(12) INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

(19) World Intellectual Property Organization
International Bureau

(43) International Publication Date
20 December 2018 (20.12.2018)

WIPO | PCT

(10) International Publication Number
WO 2018/231745 A1

(51) International Patent Classification:
A61K 31/4245 (2006.01)

(21) International Application Number:
PCT/US2018/036989

(22) International Filing Date:
12 June 2018 (12.06.2018)

(25) Filing Language: English

(26) Publication Language: English

(30) Priority Data:
62/519,575 14 June 2017 (14.06.2017) US

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(81) Designated States *(unless otherwise indicated, for every kind of national protection available)*: AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BH, BN, BR, BW, BY, BZ, CA, CH, CL, CN, CO, CR, CU, CZ, DE, DJ, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IR, IS, JO, JP, KE, KG, KH, KN, KP, KR, KW, KZ, LA, LC, LK, LR, LS, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PA, PE, PG, PH, PL, PT, QA, RO, RS, RU, RW, SA, SC, SD, SE, SG, SK, SL, SM, ST, SV, SY, TH, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW.

(84) Designated States *(unless otherwise indicated, for every kind of regional protection available)*: ARIPO (BW, GH, GM, KE, LR, LS, MW, MZ, NA, RW, SD, SL, ST, SZ, TZ, UG, ZM, ZW), Eurasian (AM, AZ, BY, KG, KZ, RU, TJ, TM), European (AL, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HR, HU, IE, IS, IT, LT, LU, LV, MC, MK, MT, NL, NO, PL, PT, RO, RS, SE, SI, SK, SM, TR), OAPI (BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, KM, ML, MR, NE, SN, TD, TG).

Published:
— *with international search report (Art. 21(3))*
— *before the expiration of the time limit for amending the claims and to be republished in the event of receipt of amendments (Rule 48.2(h))*

WO 2018/231745 A1

(54) Title: COMPOUNDS FOR MODULATING S1P1 ACTIVITY AND METHODS OF USING THE SAME

(57) Abstract: The present embodiments are directed, in part, to compounds, or pharmaceutically acceptable salts thereof, or pharmaceutical compositions thereof for modulating the activity of S_1P_1 receptor and methods of using the same.

COMPOUNDS FOR MODULATING S1P1 ACTIVITY AND METHODS OF USING THE SAME

Cross-Reference to Related Applications

This application claims priority to U.S. Provisional Application No. 62/519,575, filed June 14, 2017, which is hereby incorporated by reference in its entirety.

Field

Embodiments disclosed herein are directed, in part, to compounds, or pharmaceutically acceptable salts thereof, for modulating S1P1 receptor activity and/or methods for treating and/or preventing pain, such as neuropathic pain, chemotherapy induced neuropathic pain (CINP), chemotherapy induced peripheral neuropathy (CIPN), or treating cancer or inhibiting tumor growth, and the like as described herein.

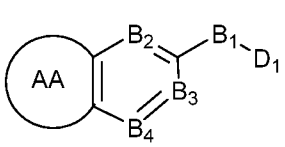
Background

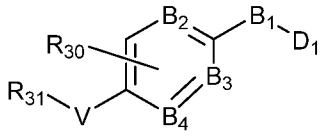
Pain is still a prevalent and pervasive problem, especially neuropathic pain, which has few good treatments or preventive therapeutics. This is especially true in conditions such chemotherapy induced neuropathic pain (CINP) and chemotherapy induced peripheral neuropathy (CIPN). Thus, there is a need for new compounds and compositions for treating and/or preventing such conditions. The compounds and compositions described herein fulfill these needs as well as others.

Summary of Embodiments

In some embodiments, compounds, or pharmaceutically acceptable salts thereof, are provided that, in part, modulate the activity of the S1P1 receptor. The compounds can have, for example, a formula as described herein. In some embodiments, the compound is selected form a compound described herein. In some embodiments, methods of treating the conditions described herein are provided. In some embodiments, the condition is CIPN, CINP, pain, neuropathy, and the like. In some embodiments, the condition is cancer and the like.

In some embodiments, the compound is a compound having a formula of Formula I or Formula II:



Formula I or 

Formula II, or a pharmaceutically acceptable salt thereof, wherein AA, B_1, B_2, B_3, B_4, D_1, V, R_{30}, and R_{31} are as provided for herein and, for example, can be selected from the respective groups of chemical moieties described herein. Also provided are processes for preparing these compounds.

In some embodiments, also provided are pharmaceutical compositions comprising one or more compounds as described herein, which can also comprise a pharmaceutically acceptable carrier. In some embodiments, the compounds described herein can be provided in any form, such as a solid or solution (e.g., aqueous solution), such as is described herein. The compounds described herein, for example, can be obtained and employed in lyophilized form alone or with suitable additives.

Also provided are methods for treating and/or preventing pain such as neuropathic pain, chemotherapy induced neuropathic pain (CINP), chemotherapy induced peripheral neuropathy (CIPN), or treating cancer or inhibiting tumor growth, and the like as described herein. In some embodiments, the methods comprise administering a one or more compounds described herein to a subject or subject.

Description Of Embodiments

Unless defined otherwise, all technical and scientific terms have the same meaning as is commonly understood by one of ordinary skill in the art to which the embodiments disclosed belongs.

As used herein, the terms "a" or "an" means that "at least one" or "one or more" unless the context clearly indicates otherwise.

As used herein, the term "about" means that the numerical value is approximate and small variations would not significantly affect the practice of the disclosed embodiments. Where a numerical limitation is used, unless indicated otherwise by the context, "about" means the numerical value can vary by ±10% and remain within the scope of the disclosed embodiments.

As used herein, the term "acylamino" means an amino group substituted by an acyl group (e.g., -O-C(=O)-H or -O-C(=O)-alkyl). An example of an acylamino is -NHC(=O)H or -NHC(=O)CH_3. The term "lower acylamino" refers to an amino group substituted by a lower acyl

group (e.g., -O-C(=O)-H or -O-C(=O)-C_{1-6}alkyl). An example of a lower acylamino is -NHC(=O)H or -NHC(=O)CH_3.

As used herein, the term "alkenyl" means a straight or branched alkyl group having one or more double carbon-carbon bonds and 2-20 carbon atoms, including, but not limited to, ethenyl, 1-propenyl, 2-propenyl, 2-methyl-1-propenyl, 1-butenyl, 2-butenyl, and the like. In some embodiments, the alkenyl chain is from 2 to 10 carbon atoms in length, from 2 to 8 carbon atoms in length, from 2 to 6 carbon atoms in length, or from 2 to 4 carbon atoms in length.

The terms "alkoxy", "phenyloxy", "benzoxy" and "pyrimidinyloxy" refer to an alkyl group, phenyl group, benzyl group, or pyrimidinyl group, respectively, each optionally substituted, that is bonded through an oxygen atom. For example, the term "alkoxy" means a straight or branched -O-alkyl group of 1 to 20 carbon atoms, including, but not limited to, methoxy, ethoxy, n-propoxy, isopropoxy, t-butoxy, and the like. In some embodiments, the alkoxy chain is from 1 to 10 carbon atoms in length, from 1 to 8 carbon atoms in length, from 1 to 6 carbon atoms in length, from 1 to 4 carbon atoms in length, from 2 to 10 carbon atoms in length, from 2 to 8 carbon atoms in length, from 2 to 6 carbon atoms in length, or from 2 to 4 carbon atoms in length.

As used herein, the term "alkyl" means a saturated hydrocarbon group which is straight-chained or branched. An alkyl group can contain from 1 to 20, from 2 to 20, from 1 to 10, from 2 to 10, from 1 to 8, from 2 to 8, from 1 to 6, from 2 to 6, from 1 to 4, from 2 to 4, from 1 to 3, or 2 or 3 carbon atoms. Examples of alkyl groups include, but are not limited to, methyl (Me), ethyl (Et), propyl (e.g., n-propyl and isopropyl), butyl (e.g., n-butyl, t-butyl, isobutyl), pentyl (e.g., n-pentyl, isopentyl, neopentyl), hexyl, isohexyl, heptyl, 4,4-dimethylpentyl, octyl, 2,2,4-trimethylpentyl, nonyl, decyl, undecyl, dodecyl,
2-methyl-1-propyl, 2-methyl-2-propyl, 2-methyl-1-butyl, 3-methyl-1-butyl, 2-methyl-3-butyl, 2-methyl-1-pentyl, 2,2-dimethyl-1-propyl, 3-methyl-1-pentyl, 4-methyl-1-pentyl,
2-methyl-2-pentyl, 3-methyl-2-pentyl, 4-methyl-2-pentyl, 2,2-dimethyl-1-butyl,
3,3-dimethyl-1-butyl, 2-ethyl-1-butyl, and the like.

As used herein, the term "allylamino" means an amino group substituted by an alkyl group having from 1 to 6 carbon atoms. An example of an alkylamino is -$NHCH_2CH_3$.

As used herein, the term "alkylene" or "alkylenyl" means a divalent alkyl linking group. An example of an alkylene (or alkylenyl) is methylene or methylenyl (-CH_2-).

As used herein, the term "alkylthio" means an -S-alkyl group having from 1 to 6 carbon atoms. An example of an alkylthio group is -SCH_2CH_3.

As used herein, the term "alkynyl" means a straight or branched alkyl group having one or more triple carbon-carbon bonds and 2-20 carbon atoms, including, but not limited to, acetylene, 1-propylene, 2-propylene, and the like. In some embodiments, the alkynyl chain is 2 to 10 carbon atoms in length, from 2 to 8 carbon atoms in length, from 2 to 6 carbon atoms in length, or from 2 to 4 carbon atoms in length.

As used herein, the term "amidino" means $-C(=NH)NH_2$.

As used herein, the term "amino" means $-NH_2$.

As used herein, the term "aminoalkoxy" means an alkoxy group substituted by an amino group. An example of an aminoalkoxy is $-OCH_2CH_2NH_2$.

As used herein, the term "aminoalkyl" means an alkyl group substituted by an amino group. An example of an aminoalkyl is $-CH_2CH_2NH_2$.

As used herein, the term "aminosulfonyl" means $-S(=O)_2NH_2$.

As used herein, the term "aminoalkylthio" means an alkylthio group substituted by an amino group. An example of an aminoalkylthio is $-SCH_2CH_2NH_2$.

As used herein, the term "amphiphilic" means a three-dimensional structure having discrete hydrophobic and hydrophilic regions. An amphiphilic compound suitably has the presence of both hydrophobic and hydrophilic elements.

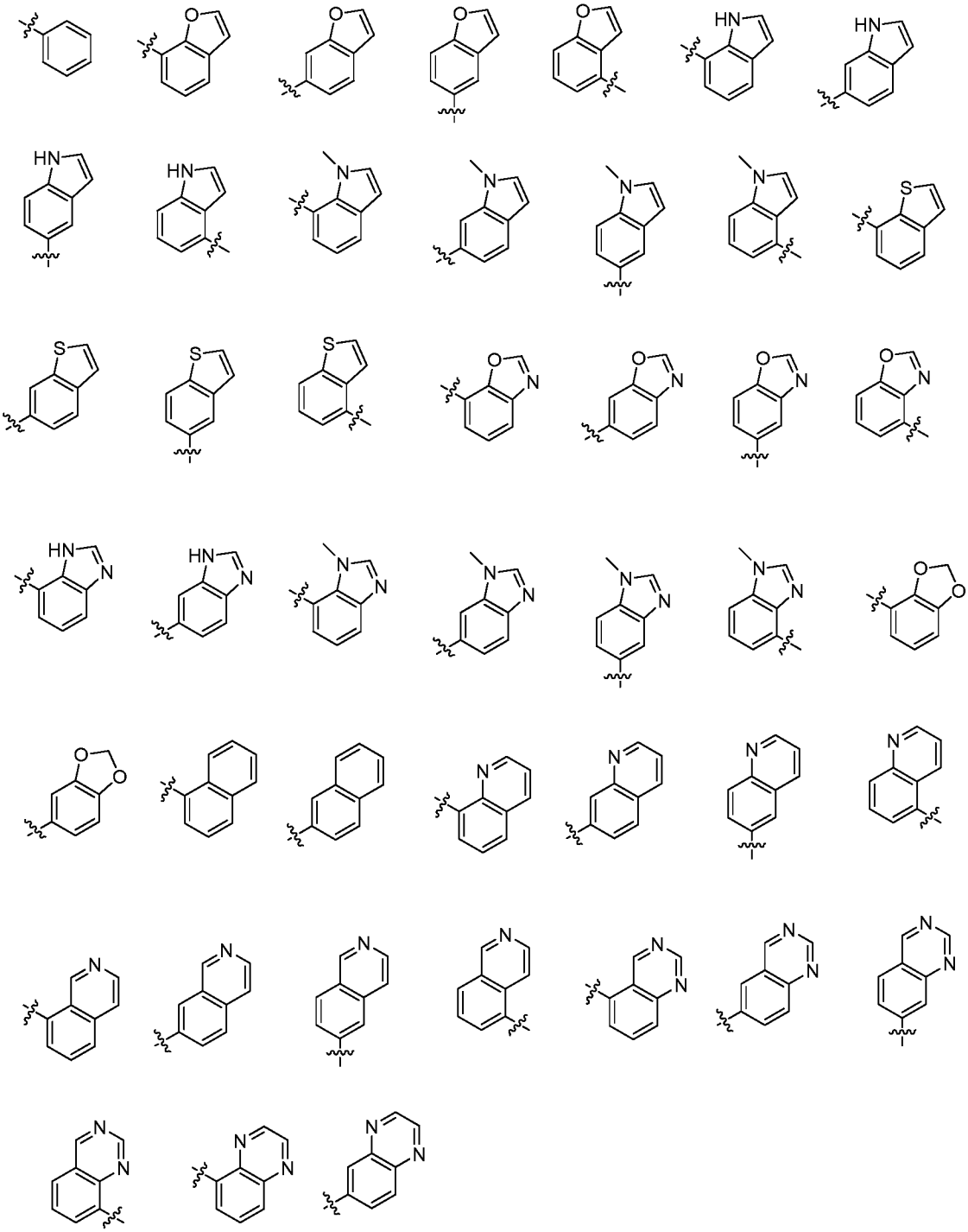
As used herein, the term "animal" includes, but is not limited to, humans and non-human vertebrates such as wild, domestic, and farm animals.

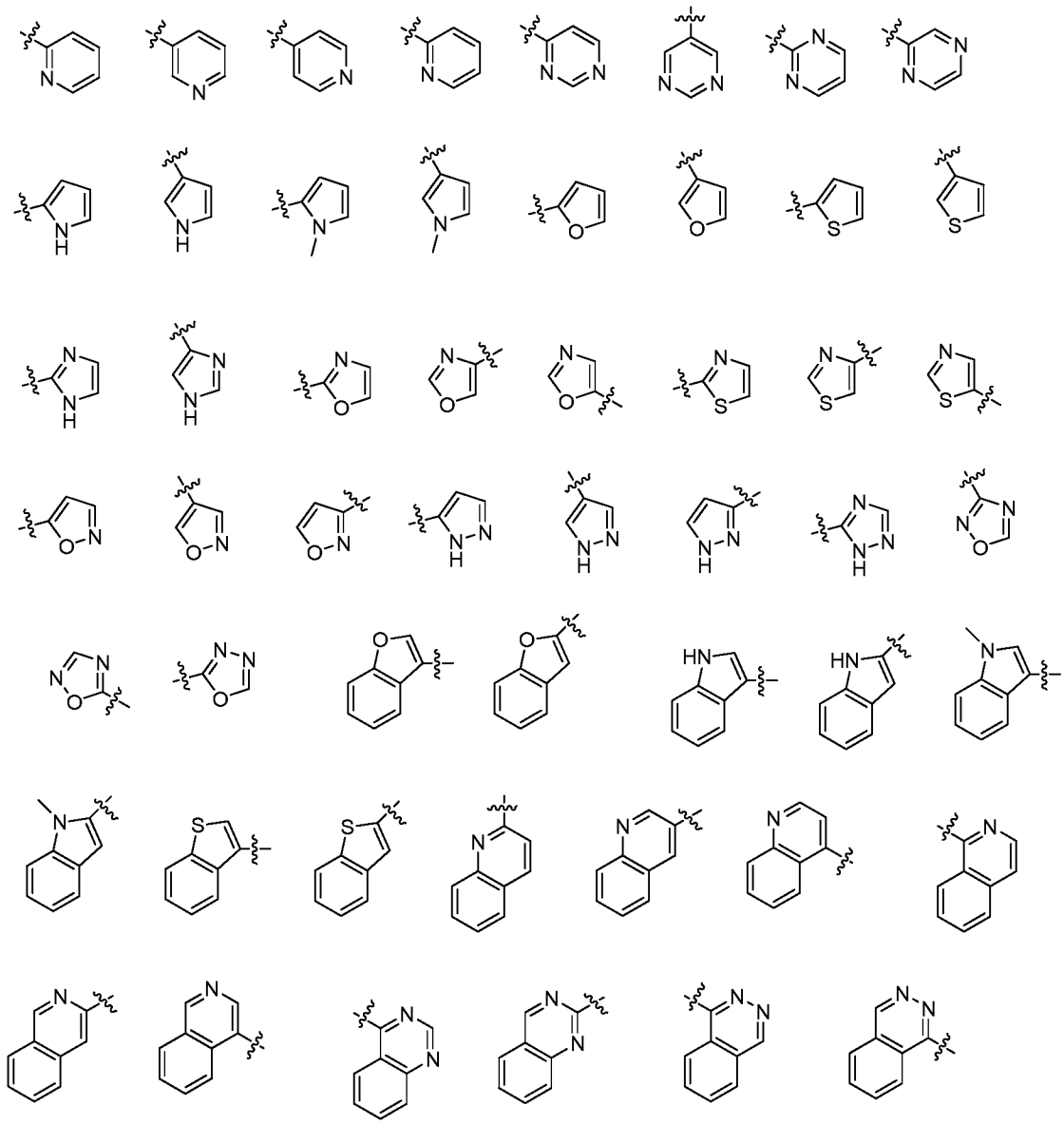
As used herein, the term "antagonize" or "antagonizing" means reducing or completely eliminating an effect, such as an activity of the S_1P_1 receptor.

As used herein, the phrase "anti-receptor effective amount" of a compound can be measured by the anti-receptor effectiveness of the compound. In some embodiments, an anti-receptor effective amount inhibits an activity of the receptor by at least 10%, by at least 20%, by at least 30%, by at least 40%, by at least 50%, by at least 60%, by at least 70%, by at least 80%, by at least 90%, or by at least 95%. In some embodiments, an "anti-receptor effective amount" is also a "therapeutically effective amount" whereby the compound reduces or eliminates at least one effect of a S_1P_1 receptor. In some embodiments, the effect is the beta-arrestin effect. In some embodiments, the effect is the G-protein mediated effect.

As used herein, the term "aryl" means a monocyclic, bicyclic, or polycyclic (e.g., having 2, 3 or 4 fused rings) aromatic hydrocarbons. In some embodiments, aryl groups have from 6 to 20 carbon atoms or from 6 to 10 carbon atoms. Examples of aryl groups include, but are not limited to,

phenyl, naphthyl, anthracenyl, phenanthrenyl, indanyl, indenyl, tetrahydronaphthyl, and the like. Examples of aryl groups include, but are not limited to:





As used herein, the term "arylalkyl" means a C_{1-6}alkyl substituted by aryl.

As used herein, the term "arylamino" means an amino group substituted by an aryl group. An example of an arylamino is -NH(phenyl).

As used herein, the term "arylene" means an aryl linking group, i.e., an aryl group that links one group to another group in a molecule.

As used herein, the term "cancer" means a spectrum of pathological symptoms associated with the initiation or progression, as well as metastasis, of malignant tumors.

As used herein, the term "carbamoyl" means -C(=O)-NH_2.

As used herein, the term "carbocycle" means a 5- or 6-membered, saturated or unsaturated cyclic ring, optionally containing O, S, or N atoms as part of the ring. Examples of carbocycles include, but are not limited to, cyclopentyl, cyclohexyl, cyclopenta-1,3-diene, phenyl, and any of the heterocycles recited above.

As used herein, the term "carrier" means a diluent, adjuvant, or excipient with which a compound is administered. Pharmaceutical carriers can be liquids, such as water and oils, including those of petroleum, animal, vegetable or synthetic origin, such as peanut oil, soybean oil, mineral oil, sesame oil and the like. The pharmaceutical carriers can also be saline, gum acacia, gelatin, starch paste, talc, keratin, colloidal silica, urea, and the like. In addition, auxiliary, stabilizing, thickening, lubricating and coloring agents can be used.

As used herein, the term, "compound" means all stereoisomers, tautomers, and isotopes of the compounds described herein.

As used herein, the terms "comprising" (and any form of comprising, such as "comprise", "comprises", and "comprised"), "having" (and any form of having, such as "have" and "has"), "including" (and any form of including, such as "includes" and "include"), or "containing" (and any form of containing, such as "contains" and "contain"), are inclusive or open-ended and do not exclude additional, unrecited elements or method steps.

As used herein, the term "contacting" means bringing together of two elements in an *in vitro* system or an *in vivo* system. For example, "contacting" a S_1P_1 receptor compound with a S_1P_1 receptor with an individual or patient or cell includes the administration of the compound to an individual or patient, such as a human, as well as, for example, introducing a compound into a sample containing a cellular or purified preparation containing the S_1P_1 receptor.

As used herein, the term "cyano" means -CN.

As used herein, the term "cycloalkyl" means non-aromatic cyclic hydrocarbons including cyclized alkyl, alkenyl, and alkynyl groups that contain up to 20 ring-forming carbon atoms. Cycloalkyl groups can include mono- or polycyclic ring systems such as fused ring systems, bridged ring systems, and spiro ring systems. In some embodiments, polycyclic ring systems include 2, 3, or 4 fused rings. A cycloalkyl group can contain from 3 to 15, from 3 to 10, from 3 to 8, from 3 to 6, from 4 to 6, from 3 to 5, or 5 or 6 ring-forming carbon atoms. Ring-forming carbon atoms of a cycloalkyl group can be optionally substituted by oxo or sulfido. Examples of cycloalkyl groups include, but are not limited to, cyclopropyl, cyclobutyl, cyclopentyl, cyclohexyl, cycloheptyl, cyclooctyl, cyclononyl, cyclopentenyl, cyclohexenyl, cyclohexadienyl, cycloheptatrienyl, norbornyl,

norpinyl, norcarnyl, adamantyl, and the like. Also included in the definition of cycloalkyl are moieties that have one or more aromatic rings fused (having a bond in common with) to the cycloalkyl ring, for example, benzo or thienyl derivatives of pentane, pentene, hexane, and the like (e.g., 2,3-dihydro-1H-indene-1-yl, or 1H-inden-2(3H)-one-1-yl).

As used herein, the term "cycloalkylalkyl" means a C_{1-6}alkyl substituted by cycloalkyl.

As used herein, the term "dialkylamino" means an amino group substituted by two alkyl groups, each having from 1 to 6 carbon atoms.

As used herein, the term "diazamino" means $-N(NH_2)_2$.

As used herein, the term "facially amphiphilic" or "facial amphiphilicity" means compounds with polar (hydrophilic) and nonpolar (hydrophobic) side chains that adopt conformation(s) leading to segregation of polar and nonpolar side chains to opposite faces or separate regions of the structure or molecule.

As used herein, the term "guanidino" means $-NH(=NH)NH_2$.

As used herein, the term "halo" means halogen groups including, but not limited to fluoro, chloro, bromo, and iodo.

As used herein, the term "haloalkoxy" means an -O-haloalkyl group. An example of an haloalkoxy group is OCF_3.

As used herein, the term "haloalkyl" means a C_{1-6}alkyl group having one or more halogen substituents. Examples of haloalkyl groups include, but are not limited to, CF_3, C_2F_5, CH_2F, CHF_2, CCl_3, $CHCl_2$, CH_2CF_3, and the like.

As used herein, the term "heteroaryl" means an aromatic heterocycle having up to 20 ring-forming atoms (e.g., C) and having at least one heteroatom ring member (ring-forming atom) such as sulfur, oxygen, or nitrogen. In some embodiments, the heteroaryl group has at least one or more heteroatom ring-forming atoms, each of which are, independently, sulfur, oxygen, or nitrogen. In some embodiments, the heteroaryl group has from 3 to 20 ring-forming atoms, from 3 to 10 ring-forming atoms, from 3 to 6 ring-forming atoms, or from 3 to 5 ring-forming atoms. In some embodiments, the heteroaryl group contains 2 to 14 carbon atoms, from 2 to 7 carbon atoms, or 5 or 6 carbon atoms. In some embodiments, the heteroaryl group has 1 to 4 heteroatoms, 1 to 3 heteroatoms, or 1 or 2 heteroatoms. Heteroaryl groups include monocyclic and polycyclic (e.g., having 2, 3 or 4 fused rings) systems. Examples of heteroaryl groups include, but are not limited to, pyridyl, pyrimidinyl, pyrazinyl, pyridazinyl, triazinyl, furyl, quinolyl, isoquinolyl, thienyl, imidazolyl, thiazolyl, indolyl (such as indol-3-yl), pyrroyl, oxazolyl, benzofuryl, benzothienyl,

benzthiazolyl, isoxazolyl, pyrazolyl, triazolyl, tetrazolyl, indazolyl, 1,2,4-thiadiazolyl, isothiazolyl, benzothienyl, purinyl, carbazolyl, benzimidazolyl, indolinyl, pyranyl, oxadiazolyl, isoxazolyl, triazolyl, thianthrenyl, pyrazolyl, indolizinyl, isoindolyl, isobenzofuranyl, benzoxazolyl, xanthenyl, 2H-pyrrolyl, pyrrolyl, 3H-indolyl,
4H-quinolizinyl, phthalazinyl, naphthyridinyl, quinazolinyl, phenanthridinyl, acridinyl, perimidinyl, phenanthrolinyl, phenazinyl, isothiazolyl, phenothiazinyl, isoxazolyl, furanyl, phenoxazinyl groups, and the like. Suitable heteroaryl groups include 1,2,3-triazole,
1,2,4-triazole, 5-amino-1,2,4-triazole, imidazole, oxazole, isoxazole, 1,2,3-oxadiazole, 1,2,4-oxadiazole, 3-amino-1,2,4-oxadiazole, 1,2,5-oxadiazole, 1,3,4-oxadiazole, pyridine, and 2-aminopyridine.

As used herein, the term "heteroarylalkyl" means a C_{1-6}alkyl group substituted by a heteroaryl group.

As used herein, the term "heteroarylamino" means an amino group substituted by a heteroaryl group. An example of a heteroarylamino is -NH-(2-pyridyl).

As used herein, the term "heteroarylene" means a heteroaryl linking group, i.e., a heteroaryl group that links one group to another group in a molecule.

As used herein, the term "heterocycle" or "heterocyclic ring" means a 5- to 7-membered mono- or bicyclic or 7- to 10-membered bicyclic heterocyclic ring system any ring of which may be saturated or unsaturated, and which consists of carbon atoms and from one to three heteroatoms chosen from N, O and S, and wherein the N and S heteroatoms may optionally be oxidized, and the N heteroatom may optionally be quaternized, and including any bicyclic group in which any of the above-defined heterocyclic rings is fused to a benzene ring. Particularly useful are rings containing one oxygen or sulfur, one to three nitrogen atoms, or one oxygen or sulfur combined with one or two nitrogen atoms. The heterocyclic ring may be attached at any heteroatom or carbon atom which results in the creation of a stable structure. Examples of heterocyclic groups include, but are not limited to, piperidinyl, piperazinyl, 2-oxopiperazinyl, 2-oxopiperidinyl, 2-oxopyrrolodinyl, 2-oxoazepinyl, azepinyl, pyrrolyl, 4-piperidonyl, pyrrolidinyl, pyrazolyl, pyrazolidinyl, imidazolyl, imidazolinyl, imidazolidinyl, pyridyl, pyrazinyl, pyrimidinyl, pyridazinyl, oxazolyl, oxazolidinyl, isoxazolyl, isoxazolidinyl, morpholinyl, thiazolyl, thiazolidinyl, isothiazolyl, quinuclidinyl, isothiazolidinyl, indolyl, quinolinyl, isoquinolinyl, benzimidazolyl, thiadiazoyl, benzopyranyl, benzothiazolyl, benzoxazolyl, furyl, tetrahydrofuryl, tetrahydropyranyl, thienyl, benzothienyl,

thiamorpholinyl, thiamorpholinyl sulfoxide, thiamorpholinyl sulfone, and oxadiazolyl. Morpholino is the same as morpholinyl.

As used herein, the term "heterocycloalkyl" means non-aromatic heterocycles having up to 20 ring-forming atoms including cyclized alkyl, alkenyl, and alkynyl groups, where one or more of the ring-forming carbon atoms is replaced by a heteroatom such as an O, N, or S atom. Hetercycloalkyl groups can be mono or polycyclic (e.g., fused, bridged, or spiro systems). In some embodiments, the heterocycloalkyl group has from 1 to 20 carbon atoms, or from 3 to 20 carbon atoms. In some embodiments, the heterocycloalkyl group contains 3 to 14 ring-forming atoms, 3 to 7 ring-forming atoms, or 5 or 6 ring-forming atoms. In some embodiments, the heterocycloalkyl group has 1 to 4 heteroatoms, 1 to 3 heteroatoms, or 1 or 2 heteroatoms. In some embodiments, the heterocycloalkyl group contains 0 to 3 double bonds. In some embodiments, the heterocycloalkyl group contains 0 to 2 triple bonds. Examples of heterocycloalkyl groups include, but are not limited to, morpholino, thiomorpholino, piperazinyl, tetrahydrofuranyl, tetrahydrothienyl, 2,3-dihydrobenzofuryl, 1,3-benzodioxole, benzo-1,4-dioxane, piperidinyl, pyrrolidinyl, isoxazolidinyl, oxazolidinyl, isothiazolidinyl, pyrazolidinyl, thiazolidinyl, imidazolidinyl, pyrrolidin-2-one-3-yl, and the like. In addition, ring-forming carbon atoms and heteroatoms of a heterocycloalkyl group can be optionally substituted by oxo or sulfido. For example, a ring-forming S atom can be substituted by 1 or 2 oxo (form a S(O) or $S(O)_2$). For another example, a ring-forming C atom can be substituted by oxo (form carbonyl). Also included in the definition of heterocycloalkyl are moieties that have one or more aromatic rings fused (having a bond in common with) to the nonaromatic heterocyclic ring including, but not limited to, pyridinyl, thiophenyl, phthalimidyl, naphthalimidyl, and benzo derivatives of heterocycles such as indolene, isoindolene, 4,5,6,7-tetrahydrothieno[2,3-c]pyridine-5-yl, 5,6-dihydrothieno[2,3-c]pyridin-7(4H)-one-5-yl, isoindolin-1-one-3-yl, and 3,4-dihydroisoquinolin-1(2H)-one-3yl groups. Ring-forming carbon atoms and heteroatoms of the heterocycloalkyl group can be optionally substituted by oxo or sulfido.

As used herein, the term "heterocycloalkylalkyl" refers to a C_{1-6}alkyl substituted by heterocycloalkyl.

As used herein, the term "hydoxy" or "hydroxyl" means an -OH group.

As used herein, the term "hydroxyalkyl" or "hydroxylalkyl" means an alkyl group substituted by a hydroxyl group. Examples of a hydroxylalkyl include, but are not limited to, $-CH_2OH$ and $-CH_2CH_2OH$.

As used herein, the term "individual" or "patient," used interchangeably, means any animal, including mammals, such as mice, rats, other rodents, rabbits, dogs, cats, swine, cattle, sheep, horses, or primates, such as humans.

As used herein, the phrase "inhibiting activity," such as enzymatic or receptor activity means reducing by any measurable amount the acitivty of an enzyme or receptor, such as the S_1P_1 receptor.

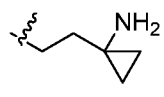
As used herein, the phrase "in need thereof" means that the animal or mammal has been identified as having a need for the particular method or treatment. In some embodiments, the identification can be by any means of diagnosis. In any of the methods and treatments described herein, the animal or mammal can be in need thereof. In some embodiments, the animal or mammal is in an environment or will be traveling to an environment in which a particular disease, disorder, or condition is prevalent.

As used herein, the phrase "*in situ* gellable" means embracing not only liquids of low viscosity that form gels upon contact with the eye or with lacrimal fluid in the exterior of the eye, but also more viscous liquids such as semi-fluid and thixotropic gels that exhibit substantially increased viscosity or gel stiffness upon administration to the eye.

As used herein, the phrase "integer from X to Y" means any integer that includes the endpoints. For example, the phrase "integer from X to Y" means 1, 2, 3, 4, or 5.

As used herein, the term "isolated" means that the compounds described herein are separated from other components of either (a) a natural source, such as a plant or cell, or (b) a synthetic organic chemical reaction mixture, such as by conventional techniques.

As used herein, the term "mammal" means a rodent (i.e., a mouse, a rat, or a guinea pig), a monkey, a cat, a dog, a cow, a horse, a pig, or a human. In some embodiments, the mammal is a human.

As used herein, the term "N-alkyl" refers to a alkyl chain that is substituted with an amine group. Non-limiting examples, include, but are not limited to 

and the like. The alkyl chain can be linear, branched, cyclic, or any combination thereof. In some embodiments, the alkyl comprises 1-10, 1-9, 1-8, 1-7, 1-6, 1-5, 1-4, 1-3, or 1-2 carbons.

As used herein, the term "nitro" means $-NO_2$.

As used herein, the term "n-membered", where n is an integer, typically describes the number of ring-forming atoms in a moiety, where the number of ring-forming atoms is n. For example,

pyridine is an example of a 6-membered heteroaryl ring and thiophene is an example of a 5-membered heteroaryl ring.

As used herein, the phrase "ophthalmically acceptable" means having no persistent detrimental effect on the treated eye or the functioning thereof, or on the general health of the subject being treated. However, it will be recognized that transient effects such as minor irritation or a "stinging" sensation are common with topical ophthalmic administration of drugs and the existence of such transient effects is not inconsistent with the composition, formulation, or ingredient (e.g., excipient) in question being "ophthalmically acceptable" as herein defined.

As used herein, the phrase "optionally substituted" means that substitution is optional and therefore includes both unsubstituted and substituted atoms and moieties. A "substituted" atom or moiety indicates that any hydrogen on the designated atom or moiety can be replaced with a selection from the indicated substituent groups, provided that the normal valency of the designated atom or moiety is not exceeded, and that the substitution results in a stable compound. For example, if a methyl group is optionally substituted, then 3 hydrogen atoms on the carbon atom can be replaced with substituent groups.

As used herein, the phrase "pharmaceutically acceptable" means those compounds, materials, compositions, and/or dosage forms which are, within the scope of sound medical judgment, suitable for use in contact with tissues of humans and animals. In some embodiments, "pharmaceutically acceptable" means approved by a regulatory agency of the Federal or a state government or listed in the U.S. Pharmacopeia or other generally recognized pharmacopeia for use in animals, and more particularly in humans.

In some embodiments, the salt of a compound described herein is a pharmaceutically acceptable salt thereof. As used herein, the phrase "pharmaceutically acceptable salt(s)," includes, but is not limited to, salts of acidic or basic groups. Compounds that are basic in nature are capable of forming a wide variety of salts with various inorganic and organic acids. Acids that may be used to prepare pharmaceutically acceptable acid addition salts of such basic compounds are those that form non-toxic acid addition salts, i.e., salts containing pharmacologically acceptable anions including, but not limited to, sulfuric, thiosulfuric, citric, maleic, acetic, oxalic, hydrochloride, hydrobromide, hydroiodide, nitrate, sulfate, bisulfate, bisulfite, phosphate, acid phosphate, isonicotinate, borate, acetate, lactate, salicylate, citrate, acid citrate, tartrate, oleate, tannate, pantothenate, bitartrate, ascorbate, succinate, maleate, gentisinate, fumarate, gluconate, glucaronate, saccharate, formate, benzoate, glutamate, methanesulfonate, ethanesulfonate, benzenesulfonate, p-

toluenesulfonate, bicarbonate, malonate, mesylate, esylate, napsydisylate, tosylate, besylate, orthophoshate, trifluoroacetate, and pamoate (i.e., 1,1′-methylene-bis-(2-hydroxy-3-naphthoate)) salts. Compounds that include an amino moiety may form pharmaceutically acceptable salts with various amino acids, in addition to the acids mentioned above. Compounds that are acidic in nature are capable of forming base salts with various pharmacologically acceptable cations. Examples of such salts include, but are not limited to, alkali metal or alkaline earth metal salts and, particularly, calcium, magnesium, ammonium, sodium, lithium, zinc, potassium, and iron salts. The present embodiments also includes quaternary ammonium salts of the compounds described herein, where the compounds have one or more tertiary amine moiety.

As used herein, the term "phenyl" means $-C_6H_5$. A phenyl group can be unsubstituted or substituted with one, two, or three suitable substituents.

As used herein, the term "prodrug" means a derivative of a known direct acting drug, which derivative has enhanced delivery characteristics and therapeutic value as compared to the drug, and is transformed into the active drug by an enzymatic or chemical process.

As used herein, the term "purified" means that when isolated, the isolate contains at least 90%, at least 95%, at least 98%, or at least 99% of a compound described herein by weight of the isolate.

As used herein, the phrase "quaternary ammonium salts" means derivatives of the disclosed compounds with one or more tertiary amine moieties wherein at least one of the tertiary amine moieties in the parent compound is modified by converting the tertiary amine moiety to a quaternary ammonium cation via alkylation (and the cations are balanced by anions such as Cl^-, CH_3COO^-, and CF_3COO^-), for example methylation or ethylation.

As used herein, the term "semicarbazone" means $=NNHC(=O)NH_2$.

As used herein, the phrase "solubilizing agent" means agents that result in formation of a micellar solution or a true solution of the drug.

As used herein, the term "solution/suspension" means a liquid composition wherein a first portion of the active agent is present in solution and a second portion of the active agent is present in particulate form, in suspension in a liquid matrix.

As used herein, the phrase "substantially isolated" means a compound that is at least partially or substantially separated from the environment in which it is formed or detected.

As used herein, the phrase "suitable substituent" or "substituent" means a group that does not nullify the synthetic or pharmaceutical utility of the compounds described herein or the intermediates

useful for preparing them. Examples of suitable substituents include, but are not limited to: C_1-C_6alkyl, C_1-C_6alkenyl, C_1-C_6alkynyl, C_5-C_6aryl, C_1-C_6alkoxy, C_3-C_5heteroaryl, C_3-C_6cycloalkyl, C_5-C_6aryloxy, -CN, -OH, oxo, halo, haloalkyl, -NO_2, -CO_2H, -NH_2, -NH(C_1-C_8alkyl), -N(C_1-C_8alkyl)$_2$, -NH(C_6aryl), -N(C_5-C_6aryl)$_2$, -CHO, -CO(C_1-C_6alkyl), -CO((C_5-C_6)aryl), -CO_2((C_1-C_6)alkyl), and -CO_2((C_5-C_6)aryl). One of skill in art can readily choose a suitable substituent based on the stability and pharmacological and synthetic activity of the compounds described herein.

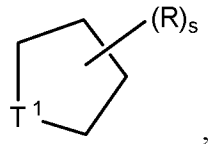
As used herein, the phrase "therapeutically effective amount" means the amount of active compound or pharmaceutical agent that elicits the biological or medicinal response that is being sought in a tissue, system, animal, individual or human by a researcher, veterinarian, medical doctor or other clinician. The therapeutic effect is dependent upon the disorder being treated or the biological effect desired. As such, the therapeutic effect can be a decrease in the severity of symptoms associated with the disorder and/or inhibition (partial or complete) of progression of the disorder, or improved treatment, healing, prevention or elimination of a disorder, or side-effects. The amount needed to elicit the therapeutic response can be determined based on the age, health, size and sex of the subject. Optimal amounts can also be determined based on monitoring of the subject's response to treatment.

As used herein, the terms "treat," "treated," or "treating" mean both therapeutic treatment and prophylactic measures wherein the object is to slow down (lessen) an undesired physiological condition, disorder or disease, or obtain beneficial or desired clinical results. Beneficial or desired clinical results include, but are not limited to, alleviation of symptoms; diminishment of extent of condition, disorder or disease; stabilized (i.e., not worsening) state of condition, disorder or disease; delay in onset or slowing of condition, disorder or disease progression; amelioration of the condition, disorder or disease state or remission (whether partial or total), whether detectable or undetectable; an amelioration of at least one measurable physical parameter, not necessarily discernible by the patient; or enhancement or improvement of condition, disorder or disease. Treatment includes eliciting a clinically significant response without excessive levels of side effects. Treatment also includes prolonging survival as compared to expected survival if not receiving treatment. Thus, "treatment of pain" or "treating pain" means an activity that alleviates or ameliorates any of the primary phenomena or secondary symptoms associated with the pain or other condition described herein.

As used herein, the term "ureido" means -NHC(=O)-NH_2.

At various places in the present specification, substituents of compounds may be disclosed in groups or in ranges. It is specifically intended that embodiments include each and every individual subcombination of the members of such groups and ranges. For example, the term "C_{1-6}alkyl" is specifically intended to individually disclose methyl, ethyl, propyl, C_4alkyl, C_5alkyl, and C_6alkyl.

For compounds in which a variable appears more than once, each variable can be a different moiety selected from the Markush group defining the variable. For example, where a structure is described having two R groups that are simultaneously present on the same compound, the two R groups can represent different moieties selected from the Markush groups defined for R. In another example, when an optionally multiple substituent is designated in the form, for example,



, then it is understood that substituent R can occur s number of times on the ring, and R can be a different moiety at each occurrence. In the above example, where the variable T^1 is defined to include hydrogens, such as when T^1 is CH_2, NH, etc., any H can be replaced with a substituent.

It is further appreciated that certain features described herein, which are, for clarity, described in the context of separate embodiments, can also be provided in combination in a single embodiment. Conversely, various features which are, for brevity, described in the context of a single embodiment, can also be provided separately or in any suitable subcombination.

It is understood that the present embodiments encompasses the use, where applicable, of stereoisomers, diastereomers and optical stereoisomers of the compounds, as well as mixtures thereof. Additionally, it is understood that stereoisomers, diastereomers, and optical stereoisomers of the compounds, and mixtures thereof, are within the scope of the embodiments. By way of non-limiting example, the mixture may be a racemate or the mixture may comprise unequal proportions of one particular stereoisomer over the other. Additionally, the compounds can be provided as a substantially pure stereoisomers, diastereomers and optical stereoisomers (such as epimers).

The compounds described herein can be asymmetric (e.g., having one or more stereocenters). All stereoisomers, such as enantiomers and diastereomers, are intended to be included within the scope of the embodiments unless otherwise indicated. Compounds that contain asymmetrically substituted carbon atoms can be isolated in optically active or racemic forms. Methods of preparation of optically active forms from optically active starting materials are known in the art, such as by resolution of racemic mixtures or by stereoselective synthesis. Many geometric isomers of olefins,

C=N double bonds, and the like can also be present in the compounds described herein, and all such stable isomers are provided herein. *Cis* and *trans* geometric isomers of the compounds are also included within the present embodiments and can be isolated as a mixture of isomers or as separated isomeric forms. Where a compound capable of stereoisomerism or geometric isomerism is designated in its structure or name without reference to specific R/S or cis/trans configurations, it is intended that all such isomers are contemplated.

In some embodiments, the composition comprises a compound, or a pharmaceutically acceptable salt thereof, that is at least 90%, at least 95%, at least 98%, or at least 99%, or 100% enantiomeric pure, which means that the ratio of one enantiomer to the other in the composition is at least 90:1 at least 95:1, at least 98:1, or at least 99:1, or is completely in the form of one enantiomer over the other.

Resolution of racemic mixtures of compounds can be carried out by any of numerous methods known in the art, including, for example, chiral HPLC, fractional recrystallization using a chiral resolving acid which is an optically active, salt-forming organic acid. Suitable resolving agents for fractional recrystallization methods include, but are not limited to, optically active acids, such as the D and L forms of tartaric acid, diacetyltartaric acid, dibenzoyltartaric acid, mandelic acid, malic acid, lactic acid, and the various optically active camphorsulfonic acids such as β-camphorsulfonic acid. Other resolving agents suitable for fractional crystallization methods include, but are not limited to, stereoisomerically pure forms of α-methylbenzylamine (e.g., *S* and *R* forms, or diastereomerically pure forms), 2-phenylglycinol, norephedrine, ephedrine, N-methylephedrine, cyclohexylethylamine, 1,2-diaminocyclohexane, and the like. Resolution of racemic mixtures can also be carried out by elution on a column packed with an optically active resolving agent (e.g., dinitrobenzoylphenylglycine). Suitable elution solvent compositions can be determined by one skilled in the art.

Compounds may also include tautomeric forms. Tautomeric forms result from the swapping of a single bond with an adjacent double bond together with the concomitant migration of a proton. Tautomeric forms include prototropic tautomers which are isomeric protonation states having the same empirical formula and total charge. Examples of prototropic tautomers include, but are not limited to, ketone-enol pairs, amide-imidic acid pairs, lactam-lactim pairs, amide-imidic acid pairs, enamine-imine pairs, and annular forms where a proton can occupy two or more positions of a heterocyclic system including, but not limited to, 1H- and 3H-imidazole, 1H-, 2H- and 4H-1,2,4-

triazole, 1H- and 2H- isoindole, and 1H- and 2H-pyrazole. Tautomeric forms can be in equilibrium or sterically locked into one form by appropriate substitution.

Compounds also include hydrates and solvates, as well as anhydrous and non-solvated forms.

Compounds can also include all isotopes of atoms occurring in the intermediates or final compounds. Isotopes include those atoms having the same atomic number but different mass numbers. For example, isotopes of hydrogen include tritium and deuterium.

In some embodiments, the compounds, or salts thereof, are substantially isolated. Partial separation can include, for example, a composition enriched in the compound. Substantial separation can include compositions containing at least about 50%, at least about 60%, at least about 70%, at least about 80%, at least about 90%, at least about 95%, at least about 97%, or at least about 99% by weight of the compound, or salt thereof. Methods for isolating compounds and their salts are routine in the art.

Although the disclosed compounds are suitable, other functional groups can be incorporated into the compound with an expectation of similar results. In particular, thioamides and thioesters are anticipated to have very similar properties. The distance between aromatic rings can impact the geometrical pattern of the compound and this distance can be altered by incorporating aliphatic chains of varying length, which can be optionally substituted or can comprise an amino acid, a dicarboxylic acid or a diamine. The distance between and the relative orientation of monomers within the compounds can also be altered by replacing the amide bond with a surrogate having additional atoms. Thus, replacing a carbonyl group with a dicarbonyl alters the distance between the monomers and the propensity of dicarbonyl unit to adopt an anti-arrangement of the two carbonyl moiety and alter the periodicity of the compound. Pyromellitic anhydride represents still another alternative to simple amide linkages which can alter the conformation and physical properties of the compound. Modern methods of solid phase organic chemistry (E. Atherton and R. C. Sheppard, Solid Phase Peptide Synthesis A Practical Approach IRL Press Oxford 1989) now allow the synthesis of homodisperse compounds with molecular weights approaching 5,000 Daltons. Other substitution patterns are equally effective.

The compounds also include derivatives referred to as prodrugs.

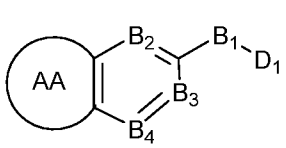
Compounds containing an amine function can also form N-oxides. A reference herein to a compound that contains an amine function also includes the N-oxide. Where a compound contains several amine functions, one or more than one nitrogen atom can be oxidized to form an N-oxide. Examples of N-oxides include N-oxides of a tertiary amine or a nitrogen atom of a nitrogen-

containing heterocycle. N-Oxides can be formed by treatment of the corresponding amine with an oxidizing agent such as hydrogen peroxide or a per-acid (e.g., a peroxycarboxylic acid) (see, Advanced Organic Chemistry, by Jerry March, 4th Edition, Wiley Interscience).

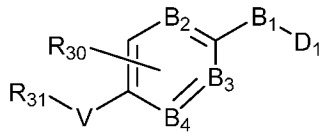
Embodiments of various compounds and salts thereof are provided. Where a variable is not specifically recited, the variable can be any option described herein, except as otherwise noted or dictated by context.

In some embodiments, the compound is as described in the appended exemplary, non-limiting claims, or a pharmaceutically acceptable salt thereof.

In some embodiments, compounds having Formula I or Formula II, or a pharmaceutically acceptable salt thereof, are provided:

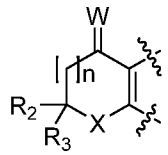


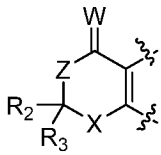
Formula I or

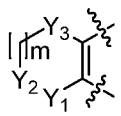


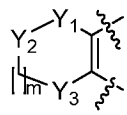
Formula II ,

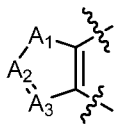
wherein:

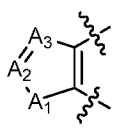
AA is 

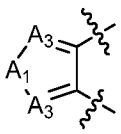
, 

, 

, 

, 

, 

, or 

;

W is O, S, or NR1;

X is O, S, or NR_4;

V is O, S, or NR_{32};

Z is CHR_{42} or NR_{43};

n is 0, 1, 2, 3, or 4;

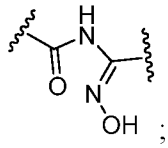
Y_1 and Y_2 are independently O, S, NR_5, C=O, C=S or $C=NR_6$;

Y_3 is O, S, CH_2, or NR_{34};

m is 0, 1, 2, or 3;

A_1 is O, S, NR_7, C=O, or C=S;

A_2 and A_3 are independently CR_{29} or N;



B_1 is an optionally substituted aryl or heteroaryl group, a carbocycle, or ;

B_2, B_3, and B_4 are independently CR_{38} or N;

D_1 is H, OH, NH_2, NO_2, cycle, optionally substituted aryl group, branched or unbranched alkyl alcohol, halo, branched or unbranched alkyl, amide, cyano, alkoxy, haloalkyl, aklylsulfonyl, nitrite, or alkylsulfanyl;

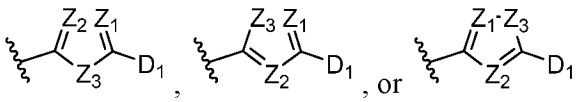
R_2 and R_3, are independently H, optionally substituted C_1-C_6 alkyl, optionally substituted C_1-C_6 hydroxyalkyl, optionally substituted C_1-C_6 alkoxy, optionally substituted cycloalkyl, or optionally substituted cycloheteroalkyl; or R_2 and R_3 are together optionally substituted cycloalkyl, or optionally substituted cycloheteroalkyl;

R_1, R_4, R_5, R_6, R_7, R_{29}, R_{31}, R_{32}, R_{33}, R_{34}, R_{38}, and R_{43} are independently H, OH, NH_2, optionally substituted C_1-C_6 alkyl, optionally substituted C_1-C_6 hydroxyalkyl, optionally substituted C_1-C_6 alkoxy, optionally substituted cycloalkyl, or optionally substituted cycloheteroalkyl.

R_{30} is independently H, CN, CF_3, optionally substituted C_1-C_6 alkyl, optionally substituted C_1-C_6 hydroxyalkyl, optionally substituted C_1-C_6 alkoxy, optionally substituted cycloalkyl, or optionally substituted cycloheteroalkyl; or optionally substituted haloalkyl;

R_{42} is independently Br, Cl, F, optionally substituted C_1-C_6 alkyl, optionally substituted C_1-C_6 hydroxyalkyl, optionally substituted C_1-C_6 alkoxy, optionally substituted cycloalkyl, or optionally substituted cycloheteroalkyl;

In some embodiments of compounds of Formula I or Formula II, D_1 and B_1 are:



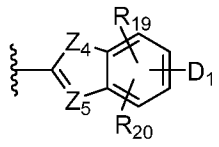
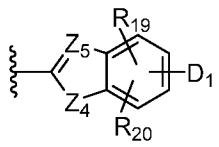
wherein:

Z_1 and Z_2 are independently N or CR_{39};

Z_3 is O, S, or NR_{27};

R_{27} and R_{39} are independently H, optionally substituted C_1-C_6 alkyl, optionally substituted C_1-C_6 hydroxyalkyl, optionally substituted C_1-C_6 alkoxy, optionally substituted cycloalkyl, or optionally substituted cycloheteroalkyl.

In some embodiments, one of Z_1 and Z_2 is N. In some embodiments, both Z_1 and Z_2 are N. In some embodiments, Z_3 is O.

In some embodiments of compounds, or a pharmaceutically acceptable salt thereof, of Formula I or Formula II, , D_1 and B_1 have a formula of:  or 

wherein:

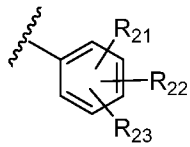
Z_4 is O, S, or NR_{28};

Z_5 is N or CH;

R_{19}, and R_{20} are each independently H, OH, NH_2, NO_2, cycle, aryl, branched or unbranched alkyl alcohol, halo, branched or unbranched alkyl, amide, cyano, alkoxy, alkylthio, haloalkyl, aklylsulfonyl, nitrite, or alkylsulfanyl; or two of R_{19}, and R_{20} together form an aryl or cycle that is attached to one or more of the atoms of B_1.

R_{28} is H, optionally substituted C_1-C_6 alkyl, optionally substituted C_1-C_6 hydroxyalkyl, optionally substituted C_1-C_6 alkoxy, optionally substituted cycloalkyl, or optionally substituted cycloheteroalkyl.

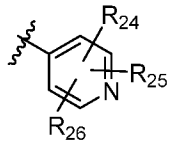
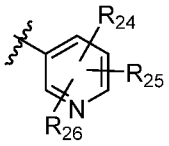
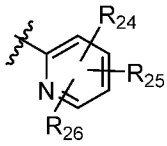
In some embodiments, Z_5 is N. In some embodiments, Z_4 is O. In some embodiments, Z_5 is N and Z_4 is O.

In some embodiments of compounds of Formula I or Formula II, D_1 is 

wherein R_{21}, R_{22}, and R_{23} are each independently H, OH, NH_2, NO_2, cycle, aryl, branched or unbranched alkyl alcohol, halo, branched or unbranched alkyl, amide, cyano, alkoxy, haloalkyl, aklylsulfonyl, nitrite, or alkylsulfanyl; or two of R_{21}, R_{22}, and R_{23} together form an aryl or cycle that is attached to one or more of the atoms of D_1.

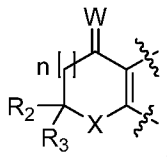
In some embodiments, one of R_{21}, R_{22}, and R_{23} is H. In some embodiments, two of R_{21}, R_{22}, and R_{23} are H. In some embodiments, R_{23} is Me, OH, NH2, Cl, $NHSO_2Me$, SO_2NH_2, NH(CO)Me, or $(CO)NH_2$. In some embodiments, R_{21} and R_{22} are H and R_{23} is Me, OH, NH2, Cl, $NHSO_2Me$, SO_2NH_2, NH(CO)Me, or $(CO)NH_2$.

In some embodiments of compounds of Formula I or Formula II, D_1 is optionally substituted aryl or optionally substituted hetero aryl.

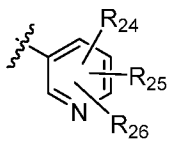
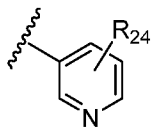
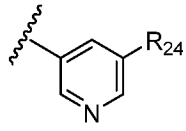
In some embodiments of compounds of Formula I or Formula II, D_1 is  ,  ,  , or

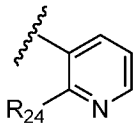
wherein R_{24}, R_{25}, and R_{26} are each independently H, OH, NH_2, NO_2, cycle (*e.g.* carbocycle or heterocyle), aryl, branched or unbranched alkyl alcohol, halo, branched or unbranched alkyl, amide, cyano, alkoxy, haloalkyl, aklylsulfonyl, nitrite, or alkylsulfanyl; or two of R_{24}, R_{25}, and R_{26} together form an aryl or cycle that is attached to one or more of the atoms of D_1.

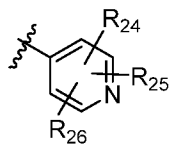
In some embodiments, one of R_{24}, R_{25}, and R_{26} is H. In some embodiments, two of R_{24}, R_{25}, and R_{26} are H. In some embodiments, R_{26} is H, Me, OH, CF_3, or OMe. In some embodiments, R_{24} and R_{25} are H and R_{26} is H, Me, OH, CF_3, or OMe.

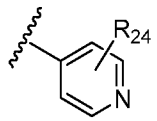
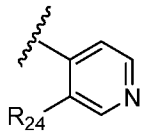
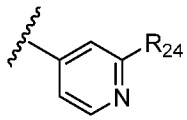
In some embodiments of compounds of Formula I or Formula II, AA is  .

In some embodiments, W is O. In some embodiments, X is O. In some embodiments, R_2 and R_3 are independently H, optionally substituted C_1-C_6 alkyl, optionally substituted C_1-C_6 hydroxyalkyl, optionally substituted C_1-C_6 alkoxy, optionally substituted cycloalkyl, or optionally substituted cycloheteroalkyl. In some embodiments, R_2 and R_3 are the same. In some embodiments, R_2 and R_3 are ethyl.

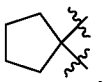
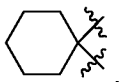
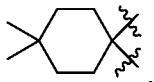
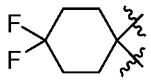
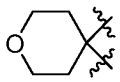
In some embodiments, D_1 is  . In some embodiments, one of R_{24}, R_{25}, and R_{26} is H. In some embodiments, two of R_{24}, R_{25}, and R_{26} are H and the other member is as defined herein. In some embodiments, D_1 is  . In some embodiments, D_1 is  .

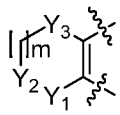
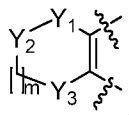
In some embodiments, R_{24} is H. In some embodiments, R_{24} is OH. In some embodiments, D_1 is  . In some embodiments, R_{24} is OMe.

In some embodiments, D_1 is  . In some embodiments, one of R_{24}, R_{25}, and R_{26} is H. In some embodiments, two of R_{24}, R_{25}, and R_{26} are H and the other member is as defined herein.

In some embodiments, D_1 is  . In some embodiments, D_1 is  . In some embodiments, D_1 is  . In some embodiments, R_{24} is halide. In some embodiments, R_{24} is F.

In some embodiments, R_{24} is Me. In some embodiments, R_{24} is OMe. In some embodiments, R_{24} is OH.

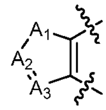
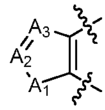
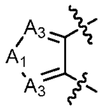
In some embodiments of compounds of Formula I or Formula II, R_2 and R_3 are together  ,  ,  ,  , or  . In some embodiments, n is 1.

In some embodiments of compounds of Formula I or Formula II, AA is  or  .

In some embodiments, Y_1 is NR_5. In some embodiments, R_5 is H.

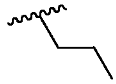
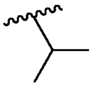
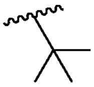
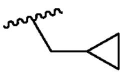
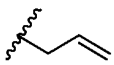
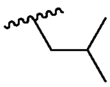
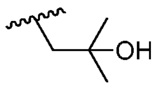
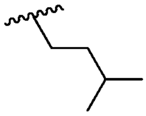
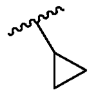
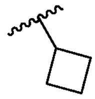
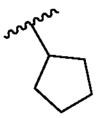
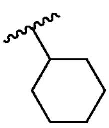
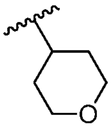
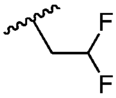
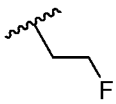
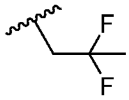
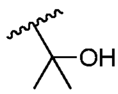
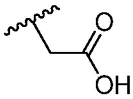
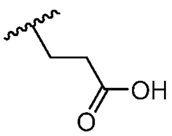
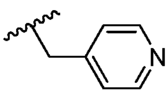
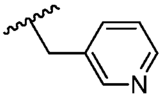
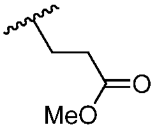
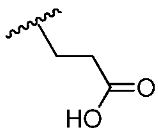
In some embodiments, Y_2 is $C{=}NR_6$. In some embodiments, R_6 is H.

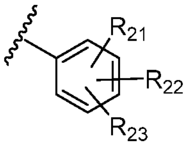
In some embodiments, Y_2 is C=O. In some embodiments, Y_3 is O. In some embodiments, Y_3 is CH_2. In some embodiments, m is 0. In some embodiments, m is 1.

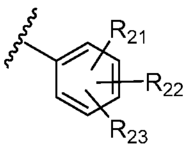
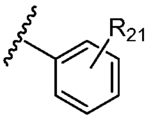
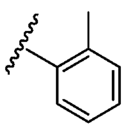
In some embodiments of compounds of Formula I or Formula II, AA is  ,  , or  .

In some embodiments, A_1 is O. In some embodiments, A_1 is S. In some embodiments, A_2 is N. In some embodiments, A_3 is N. In some embodiments, A_3 is CR_{29}. In some embodiments, R_{29} is H.

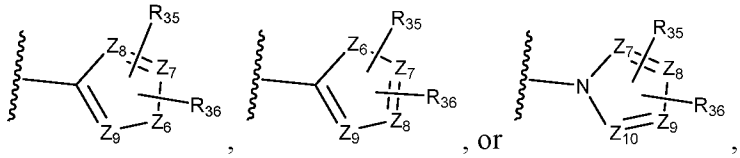
In some embodiments, A_2 is CR_{29}. In some embodiments, R_{29} is H.

In some embodiments, A_1 is NR_7. In some embodiments, R_7 is  ,  ,  ,  ,  ,  ,  ,  ,  ,  ,  ,  ,  ,  ,  ,  ,  ,  , ,  ,  ,  ,  ,  ,  , or  .

In some embodiments, D_1 is  and one of R_{21}, R_{22}, and R_{23} is H.

In some embodiments, D_1 is  and two of R_{21}, R_{22}, and R_{23} are H. In some embodiments, D_1 is  . In some embodiments, R_{21} is optionally substituted C_1-C_6 alkyl. In some embodiments, R_{21} is ethyl or methyl. In some embodiments, D_1 is  .

In some embodiments of compounds of Formula I or Formula II, D_1 is



wherein:

Z_6 is O, S, NR_{40}, or CHR_{37};

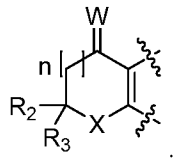
Z_7, Z_8, Z_9 and Z_{10} are independently N or CR_{41};

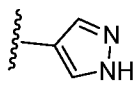
R_{35}, R_{36}, R_{37}, R_{40}, and R_{41} are each independently H, OH, NH_2, cycle, aryl, branched or unbranched alkyl alcohol, halo, branched or unbranched alkyl, amide, cyano, alkoxy, haloalkyl, aklylsulfonyl, nitrite, or alkylsulfanyl; or R_{35} and R_{36} together form an

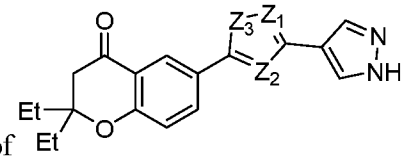
aryl or cycle that is attached to one or more of the atoms of D_1.

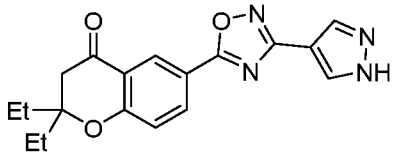
In some embodiments, one of R_{35} and R_{36} is H. In some embodiments, both R_{35} and R_{36} are H. In some embodiments, Z_6 is NH. In some embodiments, one of Z_7, Z_8 and Z_9 is N.

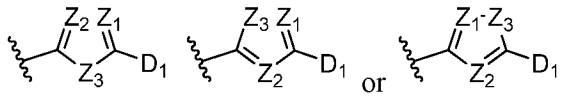
In some embodiments, Z_7 is N. In some embodiments, Z_8 is CH. In some embodiments, Z_9 is CH. In some embodiments, both Z_8 and Z_9 are CH.

In some embodiments, AA is  .

In some embodiments, W is O. In some embodiments, X is O. In some embodiments, R_2 and R_3 are independently H, optionally substituted C_1-C_6 alkyl, optionally substituted C_1-C_6 hydroxyalkyl, optionally substituted C_1-C_6 alkoxy, optionally substituted cycloalkyl, or optionally substituted cycloheteroalkyl. In some embodiments, both R_2 and R_3 are the same. In some embodiments, both R_2 and R_3 are methyl or ethyl. In some embodiments, n is 1. In some embodiments, D_1 is pyrazoly. In some embodiments, D_1 is  .

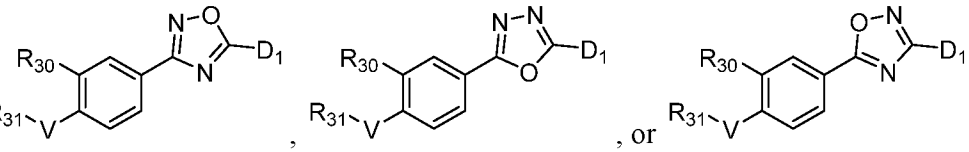
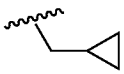
In some embodiments, the compound, or a pharmaceutically acceptable salt thereof, is a compound of Formula I having a formula of  , or a pharmaceutically acceptable salt thereof, wherein Z_1, Z_2, and Z_3 are as defined herein and above.

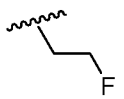
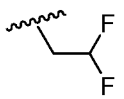
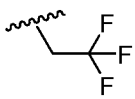
In some embodiments, Z_2 is N. In some embodiments, Z_1 is N. In some embodiments, Z_3 is O. In some embodiments, Z_2 and Z_1 are N and Z_3 is as defined herein. In some embodiments, Z_2 and Z_1 are N and Z_3 is O. In some embodiments, the compound is a compound of Formula I having a formula of  , or a pharmaceutically acceptable salt thereof.

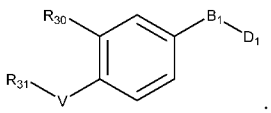
In some embodiments of compounds of Formula II, D_1 and B_1 is  .

In some embodiments, Z_3 is O and Z_1 and Z_2 are independently N or CR_{39}.

In some embodiments, Z_1 is N, Z_2 is N or CR_{39} and Z_3 is O, S, or NR_{27}. In some embodiments, Z_1 and Z_2 are N and Z_3 is O.

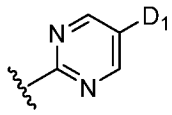
In some embodiments, the compound is a compounds of Formula II having a formula of  , or a pharmaceutically acceptable salt thereof. In some embodiments, R_{30} is CN. In some embodiments, V is NH. In some embodiments, R_{31} is C-C_5 alkyl. In some embodiments, R_{31} is  or  . In some embodiments, R_{31} is C-C_5 haloalkyl.

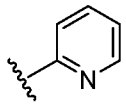
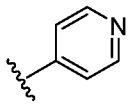
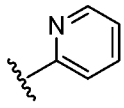
In some embodiments, R_{31} is  ,  , or  .

In some embodiments of compounds of Formula II, D_1, B_1, and AA together is  .

In some embodiments, R_{30} is CF_3. In some embodiments, V is O or NH.

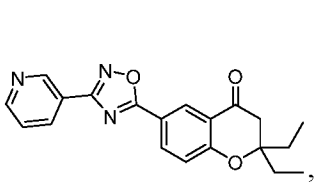
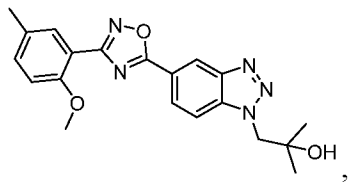
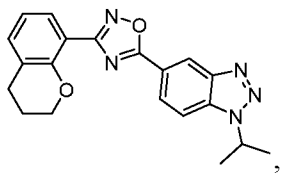
In some embodiments, R_{30} is CF_3.

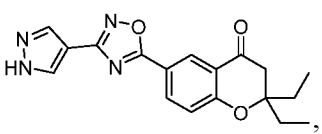
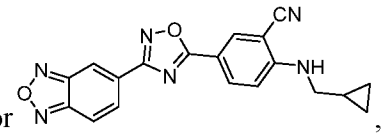
In some embodiments, B_1-D_1 is  , wherein D1 is as defined herein and above.

In some embodiments, D_1 is  ,  or  . In some embodiments, R_{31} is  .

In the preceding embodiments, or as shown below, or as illustrated in the appending claims, if a variable (substituent) is not explicitly defined then the variable is as defined above, which would be readily apparent based upon the present embodiments.

In some embodiments, the compound has a formula of:

 ,  ,  ,

 , or  , or a pharmaceutically acceptable salt thereof.

In some embodiments, the present embodiments provide a pharmaceutical composition comprising one or more compounds as provided or described herein, such as any compound of Formula I or Formula II, or a pharmaceutically acceptable salt thereof.

In some embodiments, the present embodiments provide methods of treating or preventing neuropathy, pain, inflammatory pain, cancer pain, bone cancer pain, tumor pain, pain or neuropathy resulting from disorders of the central or peripheral nervous system, neuropathic pain, pain associated with dysesthesia, allodynia or hypersensitivity, chemotherapy induced neuropathic pain, chemotherapy induced peripheral neuropathy, diabetic neuropathy or pain associated with diabetic neuropathy, post herpetic neuralgia or pain associated with post herpetic neuralgia, hiv-related neuropathy or pain associated with hiv-related neuropathy, pain or neuropathy resulting from spinal cord injury, nerve lesions, tissue injury, multiple sclerosis, stroke, nutritional deficiencies, or toxins, fibromyalgia or pain associated with fibromyalgia, phantom limb pain, complex regional pain

syndrome, carpal tunnel syndrome, sciatica, pudendal neuralgia, back or neck pain, including those resulting from degenerative disk disease, trigeminal neuralgia, headache disorders including, but not limited to migraine and cluster headache, orofacial pain, odontalgia, temporomandibular joint pain, endometrial pain, osteoarthritis, rheumatoid arthritis, atypical odontalgia, interstitial cystitis, uveitis, or any combination thereof in a subject comprising administering to the subject one or more compounds described herein, or a pharmaceutically acceptable salt thereof, or a pharmaceutical composition comprising one or more compounds described herein.

In some embodiments, the present embodiments provide methods of treating or preventing neuropathy, chemotherapy induced neuropathic pain, chemotherapy induced peripheral neuropathy, diabetic neuropathy or pain associated with diabetic neuropathy in a subject, the method comprising administering to the subject one or more compounds described herein, or a pharmaceutically acceptable salt thereof, or a pharmaceutical composition comprising one or more compounds described herein.

In some embodiments, the present embodiments provide methods of treating cancer in a subject, the method comprising administering to the subject one or more compounds described herein, or a pharmaceutically acceptable salt thereof, or a pharmaceutical composition comprising one or more compounds described herein.

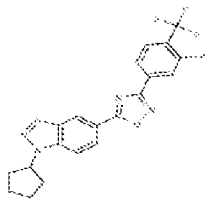
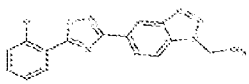
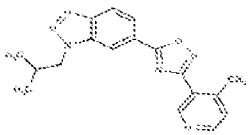
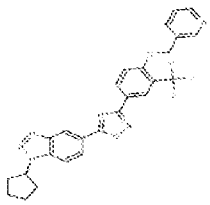
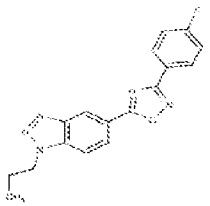
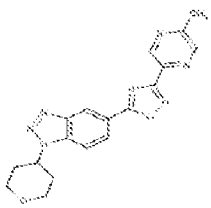
In some embodiments, the present embodiments provide methods of treating cancer in a subject, wherein the cancer is ovarian, breast, lung, brain, colon, prostate, esophageal, pancreatic, brain, glioblastoma, leukemia, multiple myeloma, lymphoma, skin cancer, acute Lymphoblastic Leukemia, acute myeloid leukemia, basal cell cancer, bile duct cancer, bladder cancer, bone cancer (Ewing sarcoma, osteosarcoma), CLL, CML, uterine cancer, cervical cancer, hairy cell leukemia, melanoma, thyroid cancer, rectal cancer, renal cell cancer, small cell lung cancer, non-small cell lung cancer, or stomach cancer.

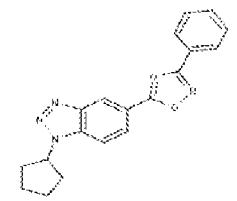
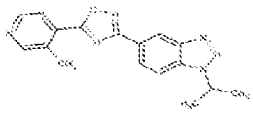
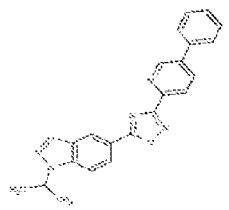
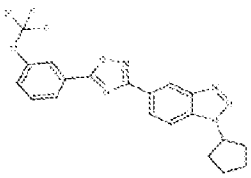
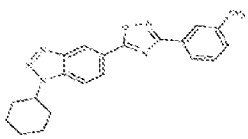
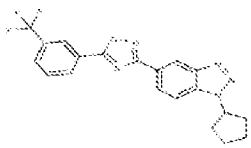
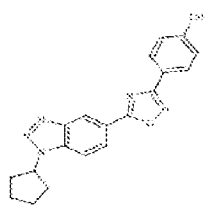
In some embodiments, wherein the subject is a subject in need thereof. In some embodiments, wherein the cancer therapeutic is selected from those described herein.

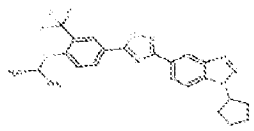
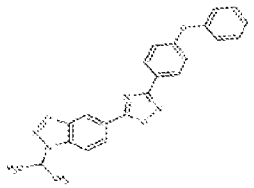
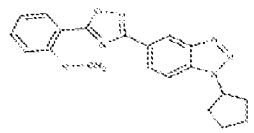
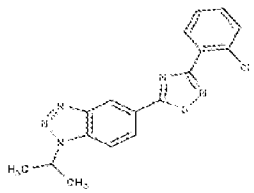
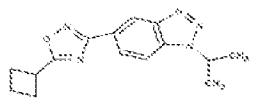
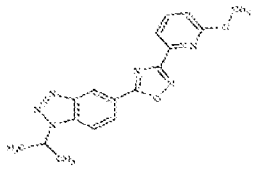
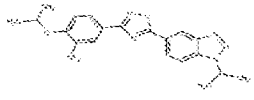
In some embodiments, the condition is prevented.

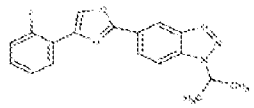
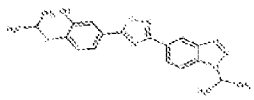
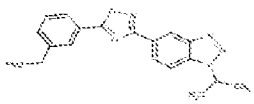
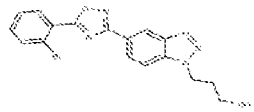
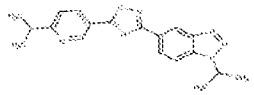
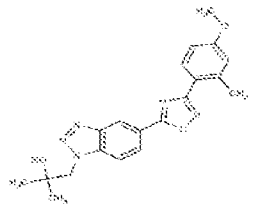
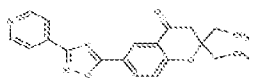
In some embodiments, a compound, or a pharmaceutically acceptable salt thereof, is chosen from a compound of as shown in the following table and/or as described herein, including in the Examples section of the present disclosure. Any of the compounds provided for herein can be prepared as pharmaceutically acceptable salts and/or as part of a pharmaceutical composition as

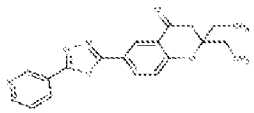
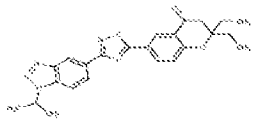
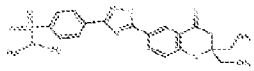
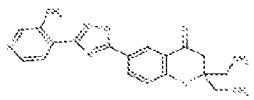
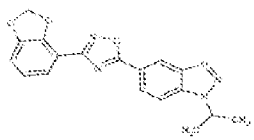
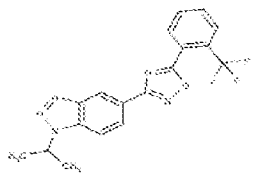
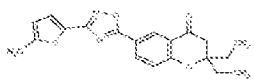
provided for herein. Examples of such salts are provided for herein. As described herein, the compounds can be prepared according to the schemes and methods described herein.

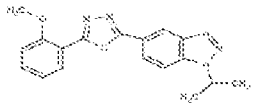
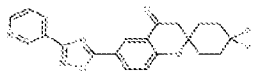
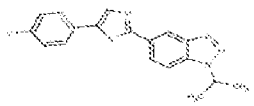
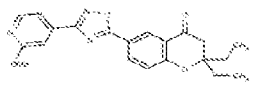
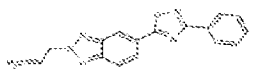
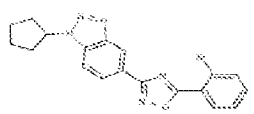
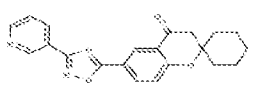
Structure	Compound Number	Chemical Name
	1	1-cyclopentyl-5-{3-[3-fluoro-4-(trifluoromethyl)phenyl]-1,2,4-oxadiazol-5-yl}-1H- 1,2,3-benzotriazole
	2	5-(2-bromophenyl)-3-(1-ethyl-1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-oxadiazole
	3	1-(2-methylpropyl)-6-[3-(4-methylpyridin-3-yl)- 1,2,4-oxadiazol-5-yl]-1H-1,2,3-benzotriazole
	4	1-cyclopentyl-5-{3-[4-(pyridin-3-ylmethoxy)-3-(trifluoromethyl)phenyl]-1,2,4-oxadiazol-5-yl}-1H- 1,2,3-benzotriazole
	5	5-[3-(4-fluorophenyl)-1,2,4-oxadiazol-5-yl]-1- propyl-1H-1,2,3-benzotriazole
	6	5-[3-(5-methylpyrazin-2-yl)-1,2,4-oxadiazol-5-yl]-1- (oxan-4-yl)-1H-1,2,3-benzotriazole

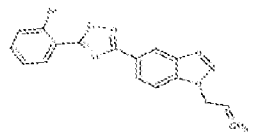
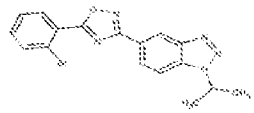
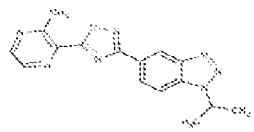
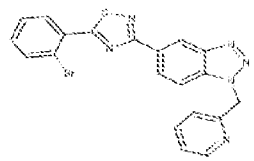
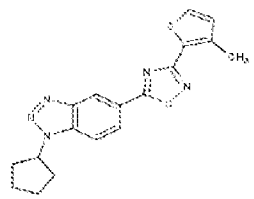
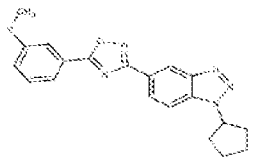
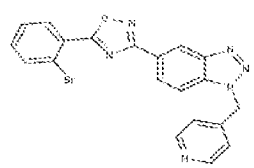
Structure	Compound Number	Chemical Name
	7	1-cyclopentyl-5-(3-phenyl-1,2,4-oxadiazol-5-yl)-1H- 1,2,3-benzotriazole
	8	3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(3-methylpyridin-4-yl)-1,2,4-oxadiazole
	9	5-[3-(5-phenylpyridin-2-yl)-1,2,4-oxadiazol-5-yl]-1- (propan-2-yl)-1H-1,2,3-benzotriazole
	10	3-(1-cyclopentyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(3-(trifluoromethoxy)phenyl)-1,2,4-oxadiazole
	11	1-cyclohexyl-5-[3-(3-methylphenyl)-1,2,4-oxadiazol-5-yl]-1H-1,2,3-benzotriazole
	12	3-(1-cyclopentyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(3-(trifluoromethyl)phenyl)-1,2,4-oxadiazole
	13	4-[5-(1-cyclopentyl-1H-1,2,3-benzotriazol-5-yl)- 1,2,4-oxadiazol-3-yl]phenol

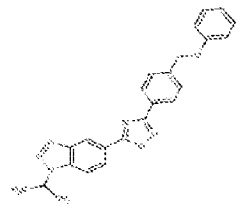
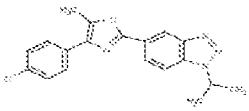
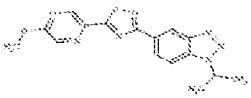
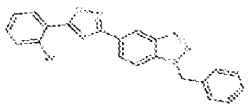
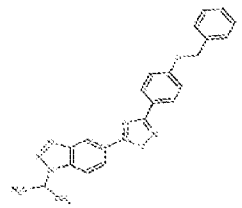
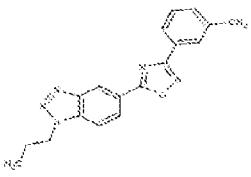
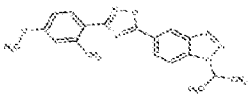
Structure	Compound Number	Chemical Name
	14	3-(1-cyclopentyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(4-isopropoxy-3-(trifluoromethyl)phenyl)-1,2,4-oxadiazole
	15	5-[3-(4-phenoxyphenyl)-1,2,4-oxadiazol-5-yl]-1- (propan-2-yl)-1H-1,2,3-benzotriazole
	16	3-(1-cyclopentyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(2-(methylthio)phenyl)-1,2,4-oxadiazole
	17	5-[3-(2-chlorophenyl)-1,2,4-oxadiazol-5-yl]-1- (propan-2-yl)-1H-1,2,3-benzotriazole
	18	5-(5-cyclobutyl-1,2,4-oxadiazol-3-yl)-1-(propan-2- yl)-1H-1,2,3-benzotriazole
	19	5-[3-(6-methoxypyridin-2-yl)-1,2,4-oxadiazol-5-yl]-1- (propan-2-yl)-1H-1,2,3-benzotriazole
	20	3-(4-isopropoxy-3-(trifluoromethyl)phenyl)-5-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-oxadiazole

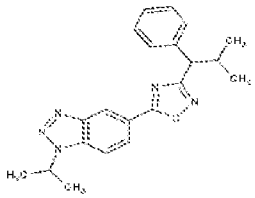
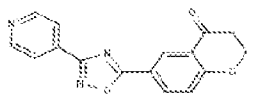
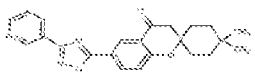
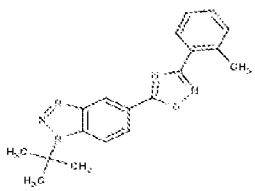
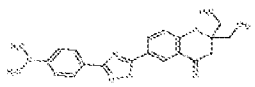
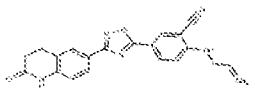
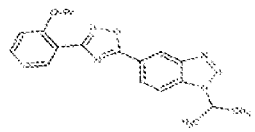
Structure	Compound Number	Chemical Name
	21	5-[4-(2-fluorophenyl)-1,3-oxazol-2-yl]-1-(propan-2- yl)-1H-1,2,3-benzotriazole
	22	2-isopropoxy-5-(3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-oxadiazol-5-yl)benzonitrile
	23	3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(3-(phenoxymethyl)phenyl)-1,2,4-oxadiazole
	24	3-(5-(5-(2-bromophenyl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)propan-1-ol
	25	3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(6-isopropylpyridin-3-yl)-1,2,4-oxadiazole
	26	1-{5-[3-(4-methoxy-2-methylphenyl)-1,2,4-oxadiazol-5-yl]-1H-1,2,3-benzotriazol-1-yl}-2-methylpropan-2- ol
	27	2,2-diethyl-6-[3-(pyridin-4-yl)-1,2,4-oxadiazol-5- yl]-3,4-dihydro-2H-1-benzopyran-4-one

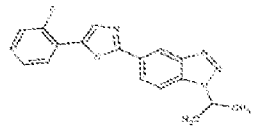
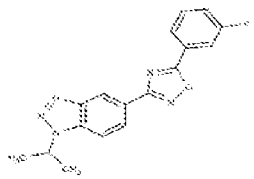
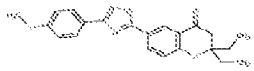
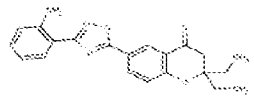
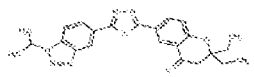
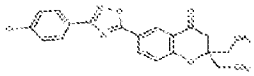
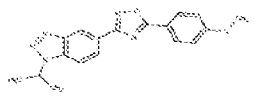
Structure	Compound Number	Chemical Name
	28	2,2-diethyl-6-(5-(pyridin-3-yl)-1,3,4-oxadiazol-2-yl)chroman-4-one
	29	2,2-diethyl-6-(3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-thiadiazol-5-yl)chroman-4-one
	30	4-(5-(2,2-diethyl-4-oxochroman-6-yl)-1,2,4-oxadiazol-3-yl)-N,N-dimethylbenzenesulfonamide
	31	2,2-diethyl-6-(3-(3-methylpyridin-4-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one
	32	3-(benzo[d][1,3]dioxol-4-yl)-5-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-oxadiazole
	33	3-(1-isopropylbenzotriazol-5-yl)-5-[2-(trifluoromethyl)phenyl]-1,2,4-oxadiazole
	34	2,2-diethyl-6-(3-(5-methylthiophen-2-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one

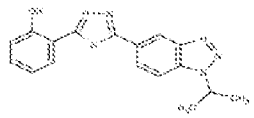
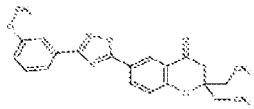
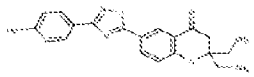
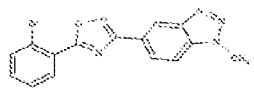
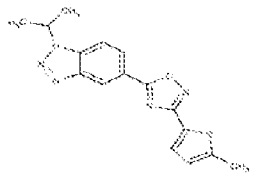
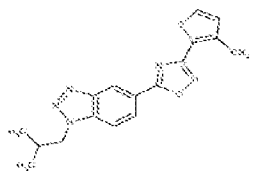
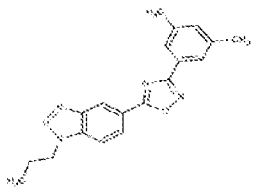
Structure	Compound Number	Chemical Name
	35	5-[5-(2-methoxyphenyl)-1,3,4-oxadiazol-2-yl]-1- (propan-2-yl)-1H-1,2,3-benzotriazole
	36	4',4'-difluoro-6-[3-(pyridin-3-yl)-1,2,4-oxadiazol-5- yl]-3,4-dihydrospiro[1-benzopyran-2,1'-cyclohexane]-4-one
	37	5-(4-fluorophenyl)-2-(1-isopropylbenzotriazol-5-yl)thiazole
	38	2,2-diethyl-6-(3-(2-methoxypyridin-4-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one
	39	5-(3-phenyl-1,2,4-oxadiazol-5-yl)-2-(prop-2-en-1- yl)-2H-1,2,3-benzotriazole
	40	5-(2-bromophenyl)-3-(1-cyclopentyl-1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-oxadiazole
	41	6-[3-(pyridin-3-yl)-1,2,4-oxadiazol-5-yl]-3,4- dihydrospiro[1-benzopyran-2,1'-cyclohexane]-4-one

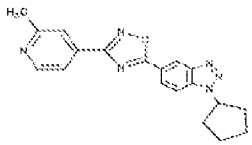
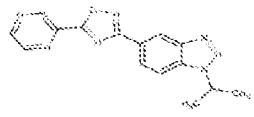
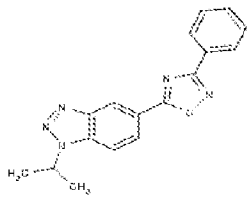
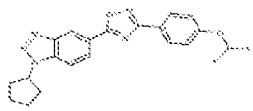
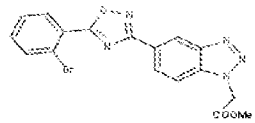
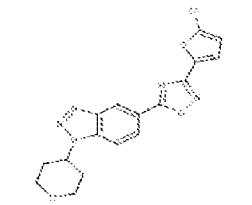
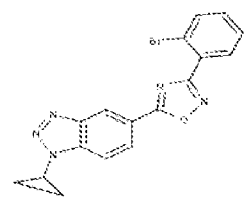
Structure	Compound Number	Chemical Name
	42	3-(1-allyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(2-bromophenyl)-1,2,4-oxadiazole
	43	5-(2-bromophenyl)-3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-oxadiazole
	44	3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(3-methylpyrazin-2-yl)-1,2,4-oxadiazole
	45	5-(2-bromophenyl)-3-(1-(pyridin-2-ylmethyl)-1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-oxadiazole
	46	1-cyclopentyl-5-[3-(3-methylthiophen-2-yl)-1,2,4-oxadiazol-5-yl]-1H-1,2,3-benzotriazole
	47	3-(1-cyclopentyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(3-(methylthio)phenyl)-1,2,4-oxadiazole
	48	5-(2-bromophenyl)-3-(1-(pyridin-4-ylmethyl)-1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-oxadiazole

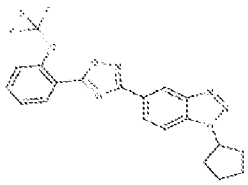
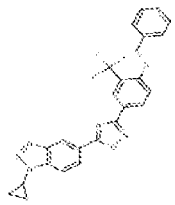
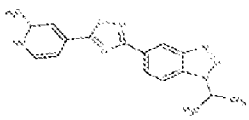
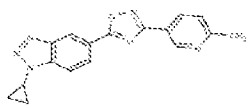
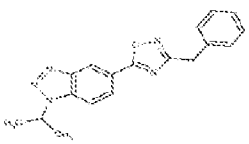
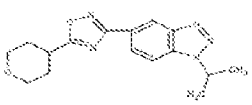
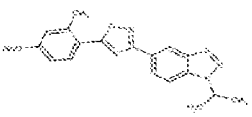
Structure	Compound Number	Chemical Name
	49	5-{3-[4-(phenoxymethyl)phenyl]-1,2,4-oxadiazol-5- yl}-1-(propan-2-yl)-1H-1,2,3-benzotriazole
	50	5-[4-(4-chlorophenyl)-5-methyl-1,3-oxazol-2-yl]-1- (propan-2-yl)-1H-1,2,3-benzotriazole
	51	3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(5-methoxypyrazin-2-yl)-1,2,4-oxadiazole
	52	3-(1-benzyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(2-bromophenyl)-1,2,4-oxadiazole
	53	5-{3-[4-(benzyloxy)phenyl]-1,2,4-oxadiazol-5-yl}-1- (propan-2-yl)-1H-1,2,3-benzotriazole
	54	5-[3-(3-methylphenyl)-1,2,4-oxadiazol-5-yl]-1- propyl-1H-1,2,3-benzotriazole
	55	5-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-3-(4-methoxy-2-methylphenyl)-1,2,4-oxadiazole

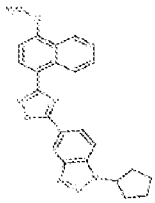
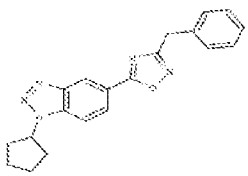
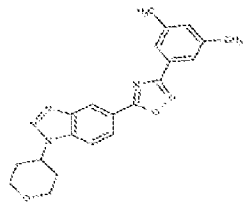
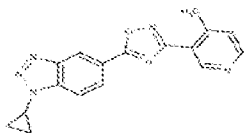
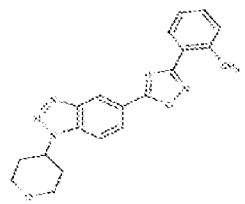
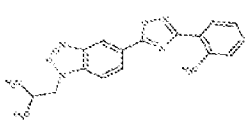
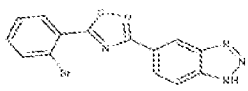
Structure	Compound Number	Chemical Name
	56	5-[3-(2-methyl-1-phenylpropyl)-1,2,4-oxadiazol-5- yl]-1-(propan-2-yl)-1H-1,2,3-benzotriazole
	57	6-[3-(pyridin-4-yl)-1,2,4-oxadiazol-5-yl]-3,4- dihydro-2H-1-benzopyran-4-one
	58	4',4'-dimethyl-6-[3-(pyridin-3-yl)-1,2,4-oxadiazol-5- yl]-3,4-dihydrospiro[1-benzopyran-2,1'-cyclohexane]-4-one
	59	1-tert-butyl-5-[3-(2-methylphenyl)-1,2,4-oxadiazol-5- yl]-1H-1,2,3-benzotriazole
	60	6-(3-(4-(dimethylamino)phenyl)-1,2,4-oxadiazol-5-yl)-2,2-diethylchroman-4-one
	61	2-(allylamino)-5-(3-(2-oxo-1,2,3,4-tetrahydroquinolin-6-yl)-1,2,4-oxadiazol-5-yl)benzonitrile
	62	3-(2-isopropoxyphenyl)-5-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-oxadiazole

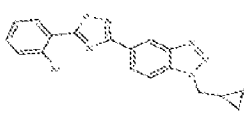
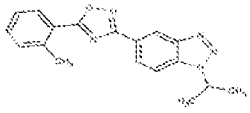
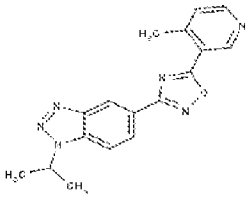
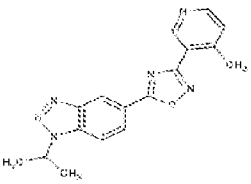
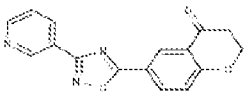
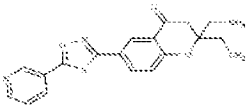
Structure	Compound Number	Chemical Name
	63	5-(2-fluorophenyl)-2-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)thiazole
	64	5-(3-fluorophenyl)-3-(1-isopropylbenzotriazol-5-yl)-1,2,4-oxadiazole
	65	2,2-diethyl-6-(3-(4-methoxyphenyl)-1,2,4-oxadiazol-5-yl)chroman-4-one
	66	2,2-diethyl-6-(3-(o-tolyl)-1,2,4-oxadiazol-5-yl)chroman-4-one
	67	2,2-diethyl-6-(5-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-1,3,4-thiadiazol-2-yl)chroman-4-one
	68	6-[3-(4-chlorophenyl)-1,2,4-oxadiazol-5-yl]-2,2-diethyl-chroman-4-one
	69	3-(1-isopropylbenzotriazol-5-yl)-5-(4-methoxyphenyl)-1,2,4-oxadiazole

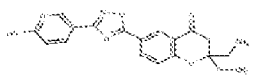
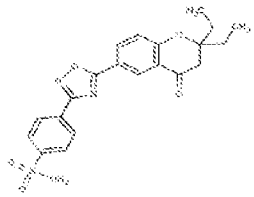
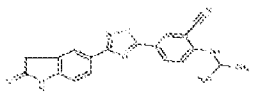
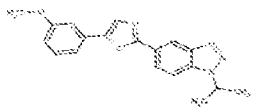
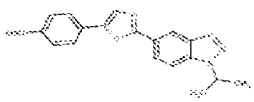
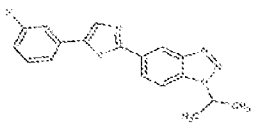
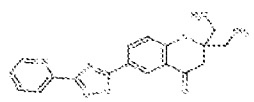
Structure	Compound Number	Chemical Name
	70	2-{5-[1-(propan-2-yl)-1H-1,2,3-benzotriazol-5-yl]- 1,3,4-thiadiazol-2-yl}phenol
	71	2,2-diethyl-6-(3-(3-methoxyphenyl)-1,2,4-oxadiazol-5-yl)chroman-4-one
	72	2,2-diethyl-6-[3-(4-hydroxyphenyl)-1,2,4-oxadiazol-5-yl]chroman-4-one
	73	5-(2-bromophenyl)-3-(1-methyl-1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-oxadiazole
	74	5-[5-(5-methylthiophen-2-yl)-1,2,4-oxadiazol-3-yl]-1- (propan-2-yl)-1H-1,2,3-benzotriazole
	75	1-(2-methylpropyl)-5-[3-(3-methylthiophen-2-yl)- 1,2,4-oxadiazol-5-yl]-1H-1,2,3-benzotriazole
	76	5-[3-(3,5-dimethylphenyl)-1,2,4-oxadiazol-5-yl]-1- propyl-1H-1,2,3-benzotriazole

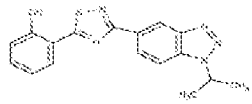
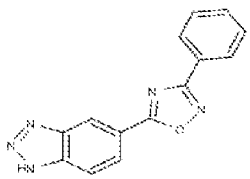
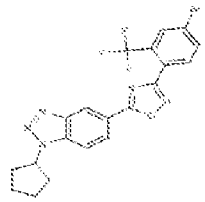
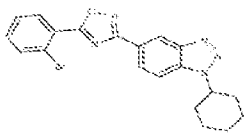
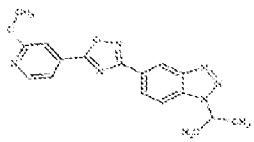
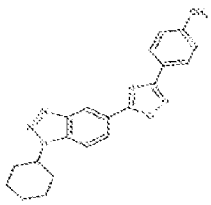
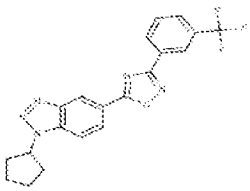
Structure	Compound Number	Chemical Name
	77	5-[3-(2-methoxypyridin-4-yl)-1,2,4-oxadiazol-5-yl]-1-methyl-2,3-dihydro-1H-1,2,3-benzotriazole; cyclopentane
	78	3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(pyrazin-2-yl)-1,2,4-oxadiazole
	79	5-(3-phenyl-1,2,4-oxadiazol-5-yl)-1-(propan-2-yl)- 1H-1,2,3-benzotriazole
	80	1-cyclopentyl-5-{3-[4-(difluoromethoxy)phenyl]- 1,2,4-oxadiazol-5-yl}-1H-1,2,3-benzotriazole
	81	methyl 2-(5-(5-(2-bromophenyl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)acetate
	82	5-[3-(5-chlorothiophen-2-yl)-1,2,4-oxadiazol-5-yl]-1- (oxan-4-yl)-1H-1,2,3-benzotriazole
	83	5-[3-(2-bromophenyl)-1,2,4-oxadiazol-5-yl]-1- cyclopropyl-1H-1,2,3-benzotriazole

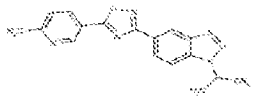
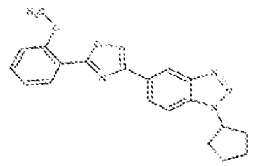
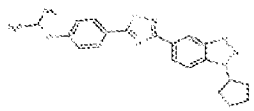
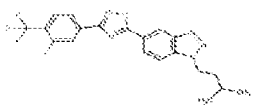
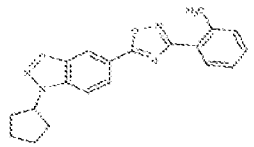
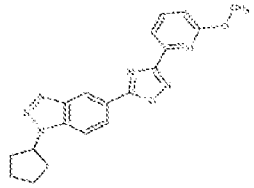
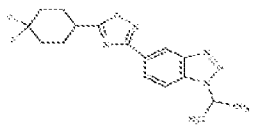
Structure	Compound Number	Chemical Name
	84	3-(1-cyclopentyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(2-(trifluoromethoxy)phenyl)-1,2,4-oxadiazole
	85	5-{3-[4-(benzyloxy)-3-(trifluoromethyl)phenyl]- 1,2,4-oxadiazol-5-yl}-1-cyclopropyl-1H-1,2,3- benzotriazole
	86	3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(2-methylpyridin-4-yl)-1,2,4-oxadiazole
	87	1-cyclopropyl-5-[3-(6-methylpyridin-3-yl)-1,2,4-oxadiazol-5-yl]-1H-1,2,3-benzotriazole
	88	5-(3-benzyl-1,2,4-oxadiazol-5-yl)-1-(propan-2-yl)- 1H-1,2,3-benzotriazole
	89	5-[5-(oxan-4-yl)-1,2,4-oxadiazol-3-yl]-1-(propan-2- yl)-1H-1,2,3-benzotriazole
	90	3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(4-methoxy-2-methylphenyl)-1,2,4-oxadiazole

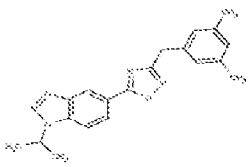
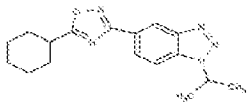
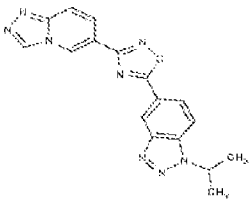
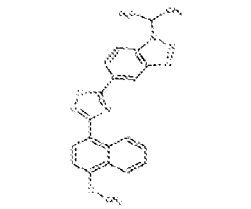
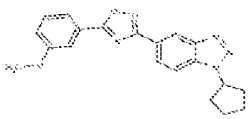
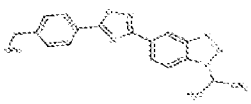
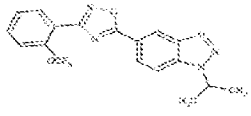
Structure	Compound Number	Chemical Name
	91	1-cyclopentyl-5-[3-(4-methoxynaphthalen-1-yl)- 1,2,4-oxadiazol-5-yl]-1H-1,2,3-benzotriazole
	92	5-(3-benzyl-1,2,4-oxadiazol-5-yl)-1-cyclopentyl-1H- 1,2,3-benzotriazole
	93	5-[3-(3,5-dimethylphenyl)-1,2,4-oxadiazol-5-yl]-1- (oxan-4-yl)-1H-1,2,3-benzotriazole
	94	1-cyclopropyl-5-[3-(4-methylpyridin-3-yl)-1,2,4-oxadiazol-5-yl]-1H-1,2,3-benzotriazole
	95	5-[3-(2-methylphenyl)-1,2,4-oxadiazol-5-yl]-1- (oxan-4-yl)-1H-1,2,3-benzotriazole
	96	5-[3-(2-methylphenyl)-1,2,4-oxadiazol-5-yl]-1-(2-methylpropyl)-1H-1,2,3-benzotriazole
	97	3-(1H-benzo[d][1,2,3]triazol-5-yl)-5-(2-bromophenyl)-1,2,4-oxadiazole

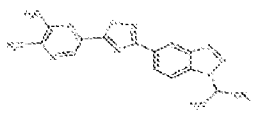
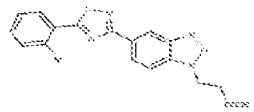
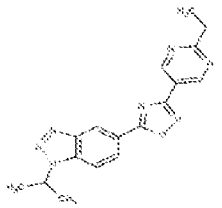
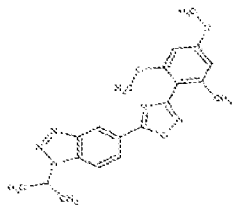
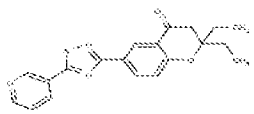
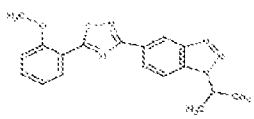
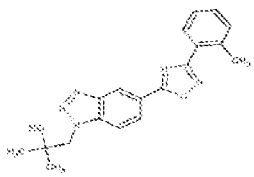
Structure	Compound Number	Chemical Name
	98	5-(2-bromophenyl)-3-(1-(cyclopropylmethyl)-1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-oxadiazole
	99	3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(o-tolyl)-1,2,4-oxadiazole
	100	3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(4-methylpyridin-3-yl)-1,2,4-oxadiazole
	101	5-[3-(4-methylpyridin-3-yl)-1,2,4-oxadiazol-5-yl]-1- (propan-2-yl)-1H-1,2,3-benzotriazole
	102	6-[3-(pyridin-3-yl)-1,2,4-oxadiazol-5-yl]-3,4- dihydro-2H-1-benzopyran-4-one
	103	2,2-diethyl-6-[3-(pyridin-3-yl)-1,2,4-oxadiazol-5- yl]-3,4-dihydro-2H-1-benzopyran-4-one
	104	2,2-diethyl-6-(5-(pyridin-3-yl)-1,3,4-thiadiazol-2-yl)chroman-4-one

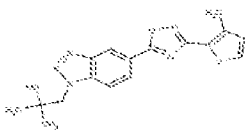
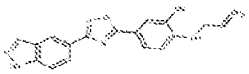
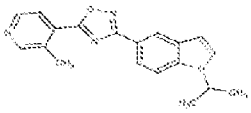
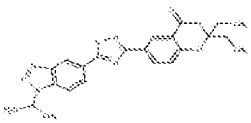
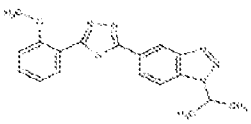
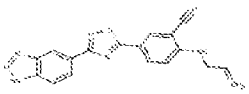
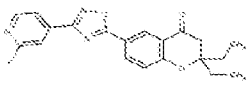
Structure	Compound Number	Chemical Name
	105	2,2-diethyl-6-[3-(6-hydroxy-3-pyridyl)-1,2,4-oxadiazol-5-yl]chroman-4-one
	106	4-(5-(2,2-diethyl-4-oxochroman-6-yl)-1,2,4-oxadiazol-3-yl)benzenesulfonamide
	107	2-(isopropylamino)-5-(3-(2-oxoindolin-5-yl)-1,2,4-oxadiazol-5-yl)benzonitrile
	108	2-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(3-methoxyphenyl)thiazole
	109	2-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(4-methoxyphenyl)thiazole
	110	5-(3-fluorophenyl)-2-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)thiazole
	111	2,2-diethyl-6-[3-(2-pyridyl)-1,2,4-oxadiazol-5-yl]chroman-4-one

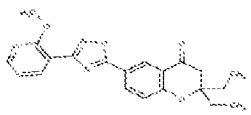
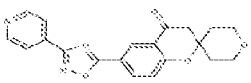
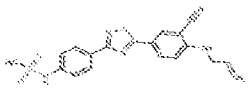
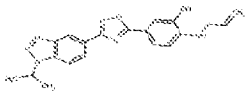
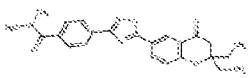
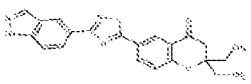
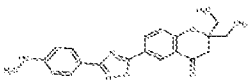
Structure	Compound Number	Chemical Name
	112	2-{3-[1-(propan-2-yl)-1H-1,2,3-benzotriazol-5-yl]- 1,2,4-thiadiazol-5-yl}phenol
	113	5-(3-phenyl-1,2,4-oxadiazol-5-yl)-1H-1,2,3- benzotriazole
	114	5-{3-[4-bromo-2-(trifluoromethyl)phenyl]-1,2,4-oxadiazol-5-yl}-1-cyclopentyl-1H-1,2,3- benzotriazole
	115	5-(2-bromophenyl)-3-(1-cyclohexyl-1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-oxadiazole
	116	3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(2-methoxypyridin-4-yl)-1,2,4-oxadiazole
	117	1-cyclohexyl-5-[3-(4-methylphenyl)-1,2,4-oxadiazol-5-yl]-1H-1,2,3-benzotriazole
	118	1-cyclopentyl-5-{3-[3-(trifluoromethyl)phenyl]- 1,2,4-oxadiazol-5-yl}-1H-1,2,3-benzotriazole

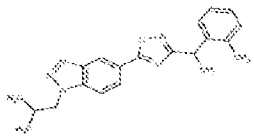
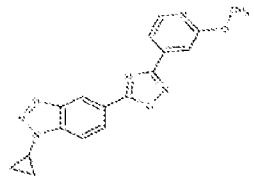
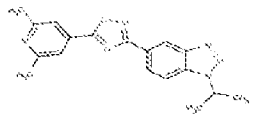
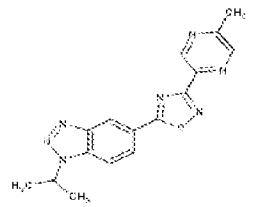
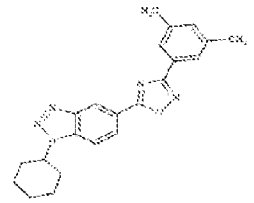
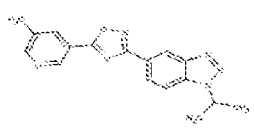
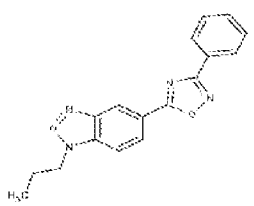
Structure	Compound Number	Chemical Name
	119	3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(6-methylpyridin-3-yl)-1,2,4-oxadiazole
	120	3-(1-cyclopentyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(2-methoxyphenyl)-1,2,4-oxadiazole
	121	3-(1-cyclopentyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(4-isopropoxyphenyl)-1,2,4-oxadiazole
	122	5-{3-[3-fluoro-4-(trifluoromethyl)phenyl]-1,2,4-oxadiazol-5-yl}-1-(3-methylbutyl)-1H-1,2,3- benzotriazole
	123	5-[3-(3,5-dimethylphenyl)-1,2,4-oxadiazol-5-yl]-1- (propan-2-yl)-1H-1,2,3-benzotriazole
	124	1-cyclopentyl-5-[3-(6-methoxypyridin-2-yl)-1,2,4-oxadiazol-5-yl]-1H-1,2,3-benzotriazole
	125	5-[5-(4,4-difluorocyclohexyl)-1,2,4-oxadiazol-3- yl]-1-(propan-2-yl)-1H-1,2,3-benzotriazole

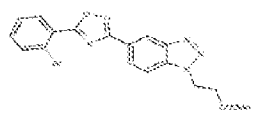
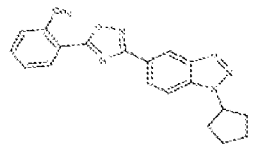
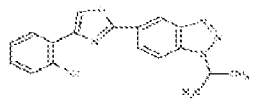
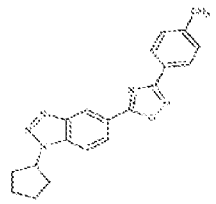
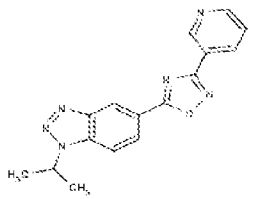
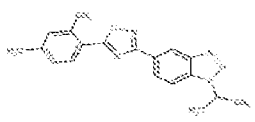
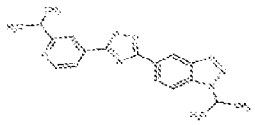
Structure	Compound Number	Chemical Name
	126	5-{3-[(3,5-dimethylphenyl)methyl]-1,2,4-oxadiazol-5- yl}-1-(propan-2-yl)-1H-1,2,3-benzotriazole
	127	5-(5-cyclohexyl-1,2,4-oxadiazol-3-yl)-1-(propan-2- yl)-1H-1,2,3-benzotriazole
	128	1-(propan-2-yl)-5-(3-{[1,2,4]triazolo[4,3- a]pyridin-6-yl}-1,2,4-oxadiazol-5-yl)-1H-1,2,3-benzotriazole
	129	5-[3-(4-methoxynaphthalen-1-yl)-1,2,4-oxadiazol-5- yl]-1-(propan-2-yl)-1H-1,2,3-benzotriazole
	130	3-(1-cyclopentyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(3-methoxyphenyl)-1,2,4-oxadiazole
	131	3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(4-(phenoxymethyl)phenyl)-1,2,4-oxadiazole
	132	5-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-3-(2-(trifluoromethoxy)phenyl)-1,2,4-oxadiazole

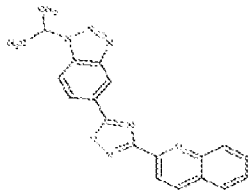
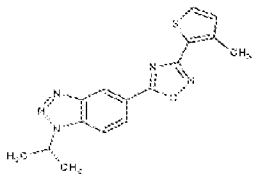
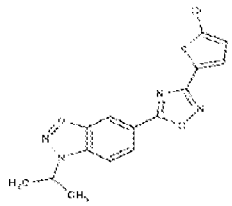
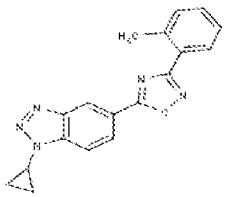
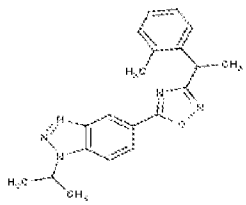
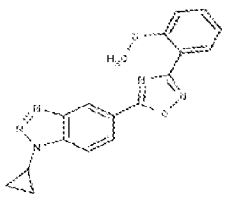
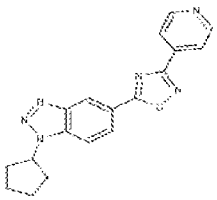
Structure	Compound Number	Chemical Name
	133	5-(5,6-dimethylpyrazin-2-yl)-3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-oxadiazole
	134	3-(5-(5-(2-bromophenyl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)propanoic acid
	135	5-[3-(2-ethylpyrimidin-5-yl)-1,2,4-oxadiazol-5-yl]-1- (propan-2-yl)-1H-1,2,3-benzotriazole
	136	5-[3-(2,4-dimethoxy-6-methylphenyl)-1,2,4- oxadiazol-5-yl]-1-(propan-2-yl)-1H-1,2,3-benzotriazole
	137	2,2-diethyl-6-(5-(pyridin-3-yl)-1,2,4-thiadiazol-3-yl)chroman-4-one
	138	5-[5-(2-methoxyphenyl)-1,2,4-thiadiazol-3-yl]-1- (propan-2-yl)-1H-1,2,3-benzotriazole
	139	2-methyl-1-{5-[3-(2-methylphenyl)-1,2,4-oxadiazol-5-yl]-1H-1,2,3-benzotriazol-1-yl}propan-2-ol

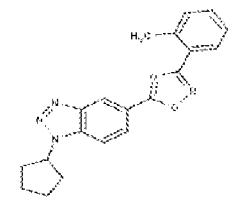
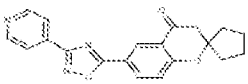
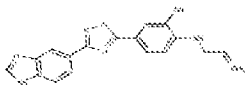
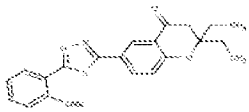
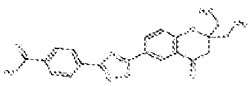
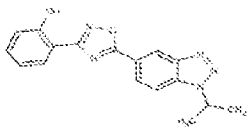
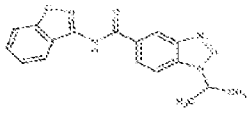
Structure	Compound Number	Chemical Name
	140	2-methyl-1-{5-[3-(3-methylthiophen-2-yl)-1,2,4-oxadiazol-5-yl]-1H-1,2,3-benzotriazol-1-yl}propan-2- ol
	141	5-(3-(1H-indazol-5-yl)-1,2,4-oxadiazol-5-yl)-2-(allylamino)benzonitrile
	142	3-(1-isopropyl-1H-indol-5-yl)-5-(3-methylpyridin-4-yl)-1,2,4-oxadiazole
	143	2,2-diethyl-6-(5-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-thiadiazol-3-yl)chroman-4-one
	144	5-[5-(2-methoxyphenyl)-1,3,4-thiadiazol-2-yl]-1- (propan-2-yl)-1H-1,2,3-benzotriazole
	145	5-(3-(1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-oxadiazol-5-yl)-2-(allylamino)benzonitrile
	146	2,2-diethyl-6-(3-(2-fluoropyridin-4-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one

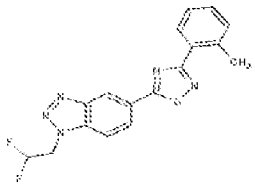
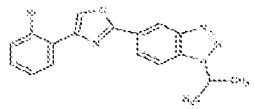
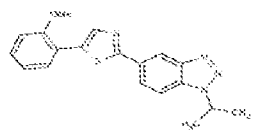
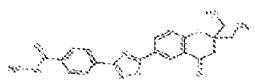
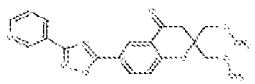
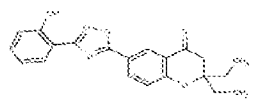
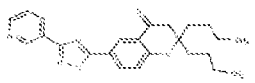
Structure	Compound Number	Chemical Name
	147	2,2-diethyl-6-(3-(2-methoxypyridin-3-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one
	148	6-[3-(pyridin-4-yl)-1,2,4-oxadiazol-5-yl]-3,4- dihydrospiro[1-benzopyran-2,4'-oxane]-4-one
	149	N-(4-(5-(4-(allylamino)-3-cyanophenyl)-1,2,4-oxadiazol-3-yl)phenyl)methanesulfonamide
	150	2-(allylamino)-5-(3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-oxadiazol-5-yl)benzonitrile
	151	4-(5-(2,2-diethyl-4-oxochroman-6-yl)-1,2,4-oxadiazol-3-yl)-N,N-dimethylbenzamide
	152	6-(3-(1H-indazol-5-yl)-1,2,4-oxadiazol-5-yl)-2,2-diethylchroman-4-one
	153	2,2-diethyl-6-(3-(4-(methylamino)phenyl)-1,2,4-oxadiazol-5-yl)chroman-4-one

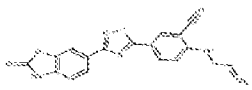
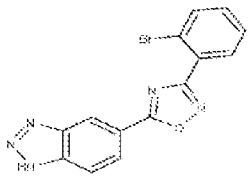
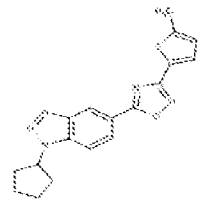
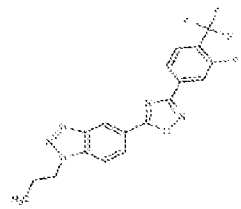
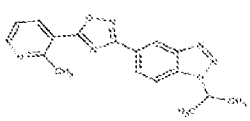
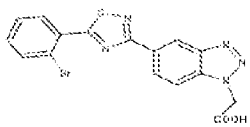
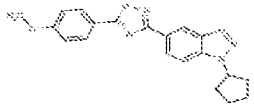
Structure	Compound Number	Chemical Name
	154	5-{3-[1-(2-methylphenyl)ethyl]-1,2,4-oxadiazol-5- yl}-1-(2-methylpropyl)-1H-1,2,3-benzotriazole
	155	1-cyclopropyl-5-[3-(2-methoxypyridin-4-yl)-1,2,4-oxadiazol-5-yl]-1H-1,2,3-benzotriazole
	156	5-(2,6-dimethylpyridin-4-yl)-3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-oxadiazole
	157	5-[3-(5-methylpyrazin-2-yl)-1,2,4-oxadiazol-5-yl]-1- (propan-2-yl)-1H-1,2,3-benzotriazole
	158	1-cyclohexyl-5-[3-(3,5-dimethylphenyl)-1,2,4- oxadiazol-5-yl]-1H-1,2,3-benzotriazole
	159	3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(5-methylpyridin-3-yl)-1,2,4-oxadiazole
	160	5-(3-phenyl-1,2,4-oxadiazol-5-yl)-1-propyl-1H- 1,2,3-benzotriazole

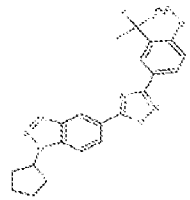
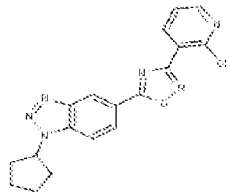
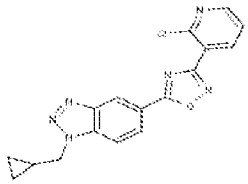
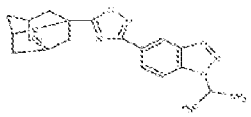
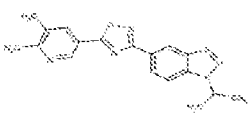
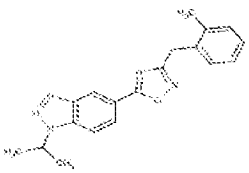
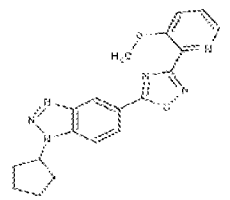
Structure	Compound Number	Chemical Name
	161	methyl 3-(5-(5-(2-bromophenyl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)propanoate
	162	3-(1-cyclopentyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(o-tolyl)-1,2,4-oxadiazole
	163	5-[4-(2-chlorophenyl)-2,3-dihydro-1,3-oxazol-2-yl]-1- (propan-2-yl)-1H-1,2,3-benzotriazole
	164	1-cyclopentyl-5-[3-(4-methylphenyl)-1,2,4- oxadiazol-5-yl]-1H-1,2,3-benzotriazole
	165	1-(propan-2-yl)-5-[3-(pyridin-3-yl)-1,2,4- oxadiazol-5-yl]-1H-1,2,3-benzotriazole
	166	5-(2,4-dimethylphenyl)-3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-oxadiazole
	167	3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(2-isopropylpyridin-4-yl)-1,2,4-oxadiazole

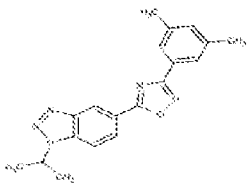
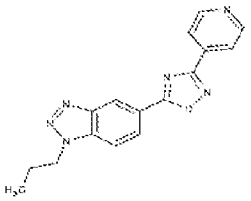
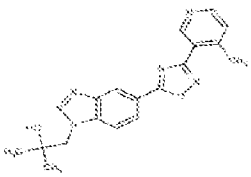
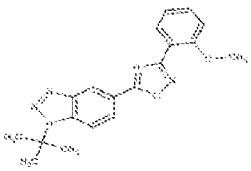
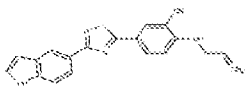
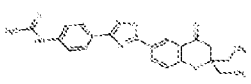
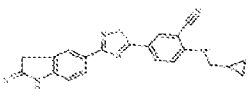
Structure	Compound Number	Chemical Name
	168	2-{5-[1-(propan-2-yl)-1H-1,2,3-benzotriazol-5-yl]- 1,2,4-oxadiazol-3-yl}quinoline
	169	5-[3-(3-methylthiophen-2-yl)-1,2,4-oxadiazol-5-yl]-1- (propan-2-yl)-1H-1,2,3-benzotriazole
	170	5-[3-(5-chlorothiophen-2-yl)-1,2,4-oxadiazol-5-yl]-1- (propan-2-yl)-1H-1,2,3-benzotriazole
	171	1-cyclopropyl-5-[3-(2-methylphenyl)-1,2,4- oxadiazol-5-yl]-1H-1,2,3-benzotriazole
	172	5-{3-[1-(2-methylphenyl)ethyl]-1,2,4-oxadiazol-5- yl}-1-(propan-2-yl)-1H-1,2,3-benzotriazole
	173	1-cyclopropyl-5-[3-(2-methoxyphenyl)-1,2,4- oxadiazol-5-yl]-1H-1,2,3-benzotriazole
	174	1-cyclopentyl-5-[3-(pyridin-4-yl)-1,2,4-oxadiazol-5- yl]-1H-1,2,3-benzotriazole

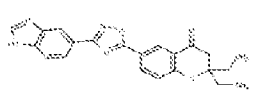
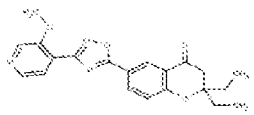
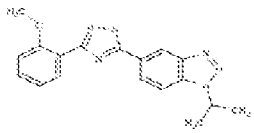
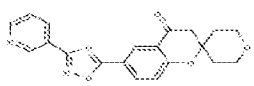
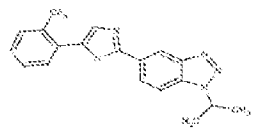
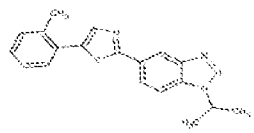
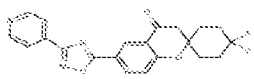
Structure	Compound Number	Chemical Name
	175	1-cyclopentyl-5-[3-(2-methylphenyl)-1,2,4- oxadiazol-5-yl]-1H-1,2,3-benzotriazole
	176	6-[3-(pyridin-4-yl)-1,2,4-oxadiazol-5-yl]-3,4- dihydrospiro[1-benzopyran-2,1'-cyclopentane]-4-one
	177	5-(3-(1H-benzo[d]imidazol-5-yl)-1,2,4-oxadiazol-5-yl)-2-(allylamino)benzonitrile
	178	2,2-diethyl-6-(5-(2-methoxyphenyl)-1,3,4-thiadiazol-2-yl)chroman-4-one
	179	4-(5-(2,2-diethyl-4-oxochroman-6-yl)-1,2,4-oxadiazol-3-yl)benzamide
	180	2-(5-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-oxadiazol-3-yl)phenol
	181	N-(benzo[d]isoxazol-3-yl)-1-isopropyl-1H-benzo[d][1,2,3]triazole-5-carboxamide

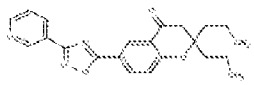
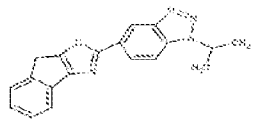
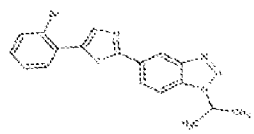
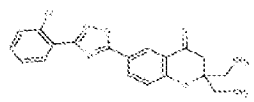
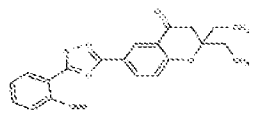
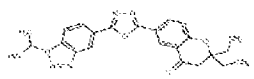
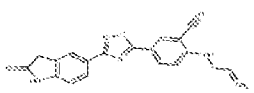
Structure	Compound Number	Chemical Name
	182	1-(2,2-difluoroethyl)-5-[3-(2-methylphenyl)-1,2,4- oxadiazol-5-yl]-1H-1,2,3-benzotriazole
	183	5-[4-(2-bromophenyl)-1,3-oxazol-2-yl]-1-(propan-2-yl)-1H-1,2,3-benzotriazole
	184	2-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(2-methoxyphenyl)thiazole
	185	4-(5-(2,2-diethyl-4-oxochroman-6-yl)-1,2,4-oxadiazol-3-yl)-N-methylbenzamide
	186	2,2-bis(methoxymethyl)-6-[3-(pyridin-3-yl)-1,2,4- oxadiazol-5-yl]-3,4-dihydro-2H-1-benzopyran-4-one
	187	2,2-diethyl-6-[3-(2-hydroxyphenyl)-1,2,4-oxadiazol-5-yl]chroman-4-one
	188	2,2-dibutyl-6-[3-(pyridin-3-yl)-1,2,4-oxadiazol-5- yl]-3,4-dihydro-2H-1-benzopyran-4-one

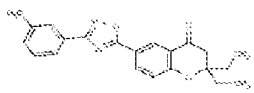
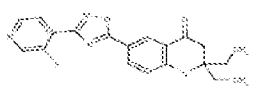
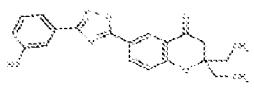
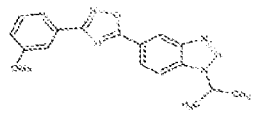
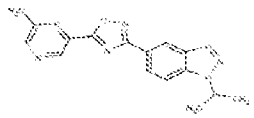
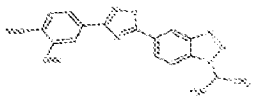
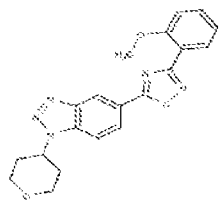
Structure	Compound Number	Chemical Name
	189	2-(allylamino)-5-(3-(2-oxo-2,3-dihydrobenzo[d]oxazol-6-yl)-1,2,4-oxadiazol-5-yl)benzonitrile
	190	5-[3-(2-bromophenyl)-1,2,4-oxadiazol-5-yl]-1H- 1,2,3-benzotriazole
	192	1-cyclopentyl-5-[3-(5-methylthiophen-2-yl)-1,2,4-oxadiazol-5-yl]-1H-1,2,3-benzotriazole
	193	5-{3-[3-fluoro-4-(trifluoromethyl)phenyl]-1,2,4-oxadiazol-5-yl}-1-propyl-1H-1,2,3-benzotriazole
	194	3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(2-methylpyridin-3-yl)-1,2,4-oxadiazole
	195	2-(5-(5-(2-bromophenyl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)acetic acid
	196	3-(1-cyclopentyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(4-methoxyphenyl)-1,2,4-oxadiazole

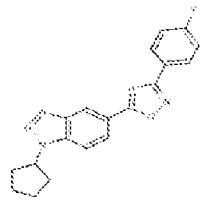
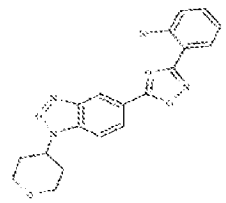
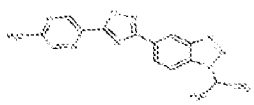
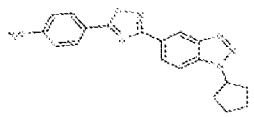
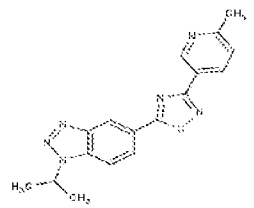
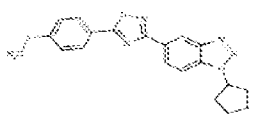
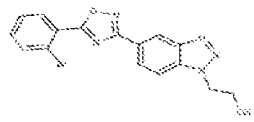
Structure	Compound Number	Chemical Name
	197	1-cyclopentyl-5-{3-[4-methoxy-3-(trifluoromethyl)phenyl]-1,2,4-oxadiazol-5-yl}-1H- 1,2,3-benzotriazole
	198	5-[3-(2-chloropyridin-3-yl)-1,2,4-oxadiazol-5-yl]-1- cyclopentyl-1H-1,2,3-benzotriazole
	199	5-[3-(2-chloropyridin-3-yl)-1,2,4-oxadiazol-5-yl]-1-(cyclopropylmethyl)-1H-1,2,3-benzotriazole
	200	5-[5-(adamantan-1-yl)-1,2,4-oxadiazol-3-yl]-1- (propan-2-yl)-1H-1,2,3-benzotriazole
	201	5-(5,6-dimethylpyridin-3-yl)-3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-oxadiazole
	202	5-{3-[(2-methylphenyl)methyl]-1,2,4-oxadiazol-5- yl}-1-(propan-2-yl)-1H-1,2,3-benzotriazole
	203	1-cyclopentyl-5-[3-(3-methoxypyridin-2-yl)-1,2,4-oxadiazol-5-yl]-1H-1,2,3-benzotriazole

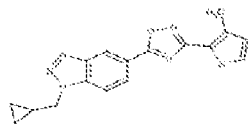
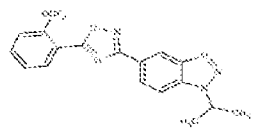
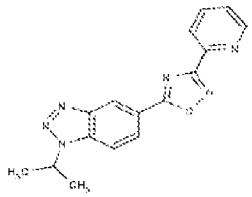
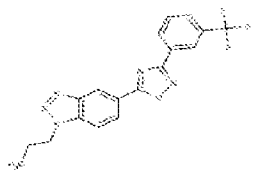
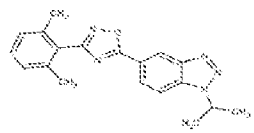
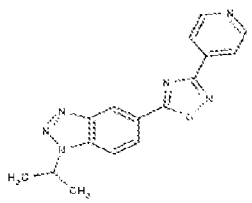
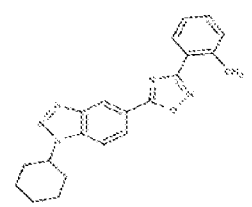
Structure	Compound Number	Chemical Name
	204	5-[3-(3,5-dimethylphenyl)-1,2,4-oxadiazol-5-yl]-1- (propan-2-yl)-1H-1,2,3-benzotriazole
	205	1-propyl-5-[3-(pyridin-4-yl)-1,2,4-oxadiazol-5-yl]- 1H-1,2,3-benzotriazole
	206	2-methyl-1-{5-[3-(4-methylpyridin-3-yl)-1,2,4- oxadiazol-5-yl]-1H-1,2,3-benzotriazol-1-yl}propan-2-ol
	207	1-tert-butyl-5-[3-(2-methoxyphenyl)-1,2,4- oxadiazol-5-yl]-1H-1,2,3-benzotriazole
	208	5-(3-(1H-indol-5-yl)-1,2,4-oxadiazol-5-yl)-2-(allylamino)benzonitrile
	209	N-(4-(5-(2,2-diethyl-4-oxochroman-6-yl)-1,2,4-oxadiazol-3-yl)phenyl)acetamide
	210	2-((cyclopropylmethyl)amino)-5-(3-(2-oxoindolin-5-yl)-1,2,4-oxadiazol-5-yl)benzonitrile

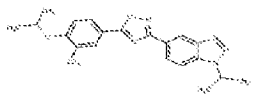
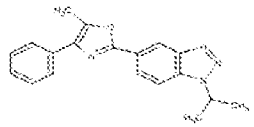
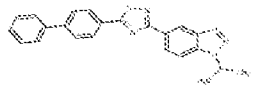
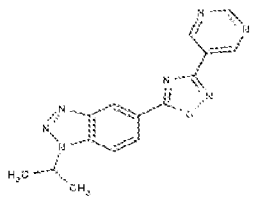
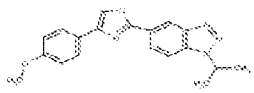
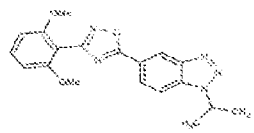
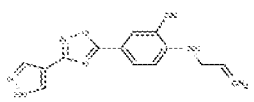
Structure	Compound Number	Chemical Name
	211	6-(3-(1H-benzo[d]imidazol-5-yl)-1,2,4-oxadiazol-5-yl)-2,2-diethylchroman-4-one
	212	2,2-diethyl-6-(3-(3-methoxypyridin-4-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one
	213	5-[3-(2-methoxyphenyl)-1,2,4-thiadiazol-5-yl]-1- (propan-2-yl)-1H-1,2,3-benzotriazole
	214	6-[3-(pyridin-3-yl)-1,2,4-oxadiazol-5-yl]-3,4- dihydrospiro[1-benzopyran-2,4'-oxane]-4-one
	215	2-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(2-(trifluoromethyl)phenyl)thiazole
	216	2-(1-isopropylbenzotriazol-5-yl)-5-(o-tolyl)thiazole
	217	4',4'-difluoro-6-[3-(pyridin-4-yl)-1,2,4-oxadiazol-5- yl]-3,4-dihydrospiro[1-benzopyran-2,1'-cyclohexane]-4-one

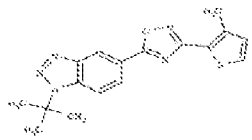
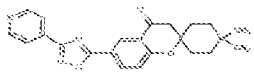
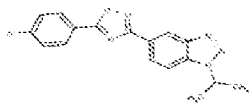
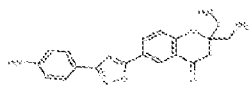
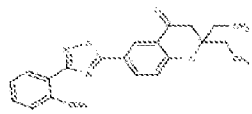
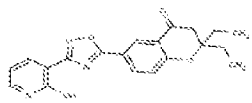
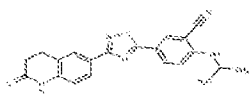
Structure	Compound Number	Chemical Name
	218	2,2-dipropyl-6-[3-(pyridin-3-yl)-1,2,4-oxadiazol-5- yl]-3,4-dihydro-2H-1-benzopyran-4-one
	219	5-{8H-indeno[1,2-d][1,3]oxazol-2-yl}-1-(propan-2- yl)-1H-1,2,3-benzotriazole
	220	5-(2-bromophenyl)-2-(1-isopropylbenzotriazol-5-yl)thiazole
	221	6-(3-(2-chlorophenyl)-1,2,4-oxadiazol-5-yl)-2,2-diethylchroman-4-one
	222	2,2-diethyl-6-(5-(2-methoxyphenyl)-1,2,4-thiadiazol-3-yl)chroman-4-one
	223	2,2-diethyl-6-(5-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-1,3,4-oxadiazol-2-yl)chroman-4-one
	224	2-(allylamino)-5-(3-(2-oxoindolin-5-yl)-1,2,4-oxadiazol-5-yl)benzonitrile

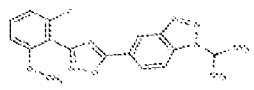
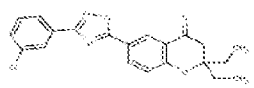
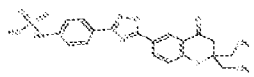
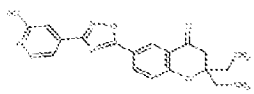
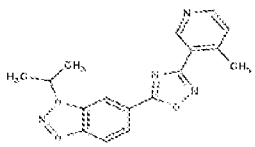
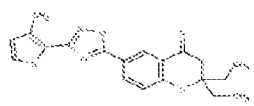
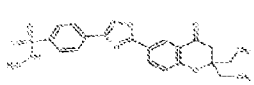
Structure	Compound Number	Chemical Name
	225	2,2-diethyl-6-(3-(m-tolyl)-1,2,4-oxadiazol-5-yl)chroman-4-one
	226	2,2-diethyl-6-(3-(3-fluoropyridin-4-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one
	227	2,2-diethyl-6-[3-(3-hydroxyphenyl)-1,2,4-oxadiazol-5-yl]chroman-4-one
	228	5-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-3-(3-methoxyphenyl)-1,2,4-oxadiazole
	229	3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(6-methylpyrazin-2-yl)-1,2,4-oxadiazole
	230	3-(3,4-dimethoxyphenyl)-5-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-oxadiazole
	231	5-[3-(2-methoxyphenyl)-1,2,4-oxadiazol-5-yl]-1- (oxan-4-yl)-1H-1,2,3-benzotriazole

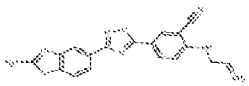
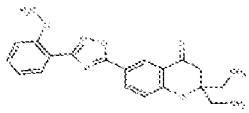
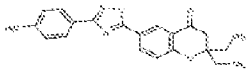
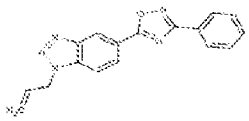
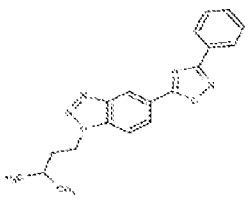
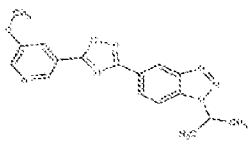
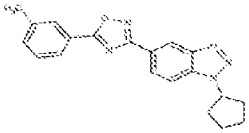
Structure	Compound Number	Chemical Name
	232	1-cyclopentyl-5-[3-(4-fluorophenyl)-1,2,4- oxadiazol-5-yl]-1H-1,2,3-benzotriazole
	233	5-[3-(2-bromophenyl)-1,2,4-oxadiazol-5-yl]-1-(oxan-4- yl)-1H-1,2,3-benzotriazole
	234	3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(5-methylpyrazin-2-yl)-1,2,4-oxadiazole
	235	3-(1-cyclopentyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(p-tolyl)-1,2,4-oxadiazole
	236	5-[3-(6-methylpyridin-3-yl)-1,2,4-oxadiazol-5-yl]-1- (propan-2-yl)-1H-1,2,3-benzotriazole
	237	3-(1-cyclopentyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(4-(methylthio)phenyl)-1,2,4-oxadiazole
	238	2-(5-(5-(2-bromophenyl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)ethanol

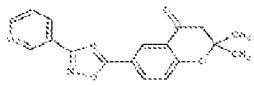
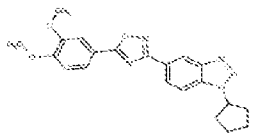
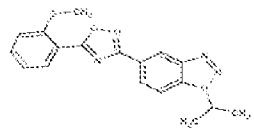
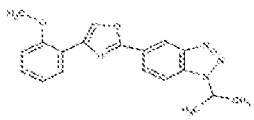
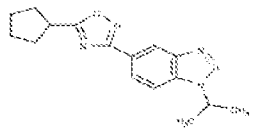
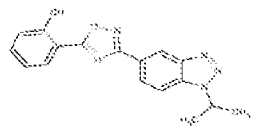
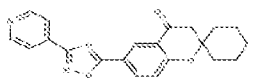
Structure	Compound Number	Chemical Name
	239	1-(cyclopropylmethyl)-5-[3-(3-methylthiophen-2-yl)- 1,2,4-oxadiazol-5-yl]-1H-1,2,3-benzotriazole
	240	3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(2-(trifluoromethoxy)phenyl)-1,2,4-oxadiazole
	241	1-(propan-2-yl)-5-[3-(pyridin-2-yl)-1,2,4- oxadiazol-5-yl]-1H-1,2,3-benzotriazole
	242	1-propyl-5-{3-[3-(trifluoromethyl)phenyl]-1,2,4-oxadiazol-5-yl}-1H-1,2,3-benzotriazole
	243	3-(2,6-dimethylphenyl)-5-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-oxadiazole
	244	1-(propan-2-yl)-5-[3-(pyridin-4-yl)-1,2,4- oxadiazol-5-yl]-1H-1,2,3-benzotriazole
	245	1-cyclohexyl-5-[3-(2-methylphenyl)-1,2,4-oxadiazol-5-yl]-1H-1,2,3-benzotriazole

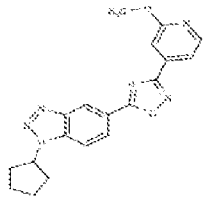
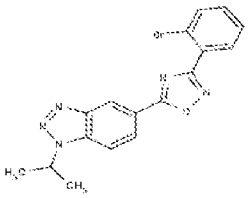
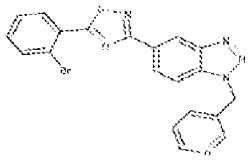
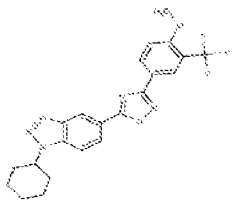
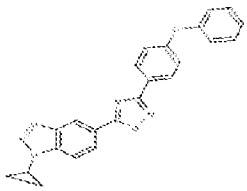
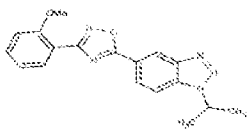
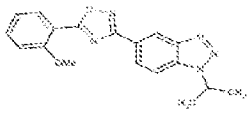
Structure	Compound Number	Chemical Name
	246	5-(4-isopropoxy-3-(trifluoromethyl)phenyl)-3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-oxadiazole
	247	5-(5-methyl-4-phenyl-1,3-oxazol-2-yl)-1-(propan-2- yl)-1H-1,2,3-benzotriazole
	248	5-([1,1'-biphenyl]-4-yl)-3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-oxadiazole
	249	1-(propan-2-yl)-5-[3-(pyrimidin-5-yl)-1,2,4- oxadiazol-5-yl]-1H-1,2,3-benzotriazole
	250	5-[4-(4-methoxyphenyl)-1,3-oxazol-2-yl]-1-(propan-2- yl)-1H-1,2,3-benzotriazole
	251	3-(2,6-dimethoxyphenyl)-5-(1-isopropylbenzotriazol-5-yl)-1,2,4-oxadiazole
	252	5-(3-(1H-pyrazol-4-yl)-1,2,4-oxadiazol-5-yl)-2-(allylamino)benzonitrile

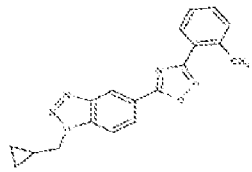
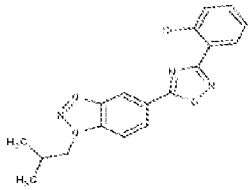
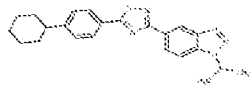
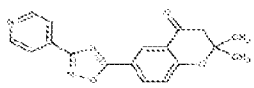
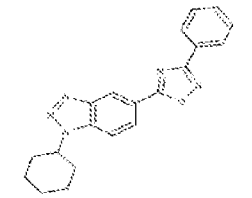
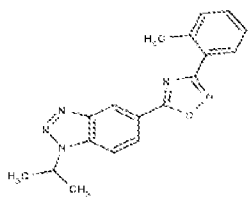
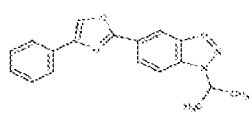
Structure	Compound Number	Chemical Name
	253	1-tert-butyl-5-[3-(3-methylthiophen-2-yl)-1,2,4-oxadiazol-5-yl]-1H-1,2,3-benzotriazole
	254	4',4'-dimethyl-6-[3-(pyridin-4-yl)-1,2,4-oxadiazol-5- yl]-3,4-dihydrospiro[1-benzopyran-2,1'-cyclohexane]-4-one
	255	5-(4-fluorophenyl)-3-(1-isopropylbenzotriazol-5-yl)-1,2,4-oxadiazole
	256	6-(3-(4-aminophenyl)-1,2,4-oxadiazol-5-yl)-2,2-diethylchroman-4-one
	257	2,2-diethyl-6-(3-(2-methoxyphenyl)-1,2,4-thiadiazol-5-yl)chroman-4-one
	258	2,2-diethyl-6-(3-(2-hydroxypyridin-3-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one
	259	2-(isopropylamino)-5-(3-(2-oxo-1,2,3,4-tetrahydroquinolin-6-yl)-1,2,4-oxadiazol-5-yl)benzonitrile

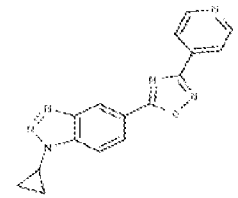
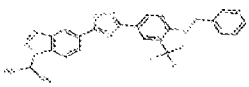
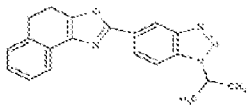
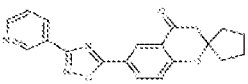
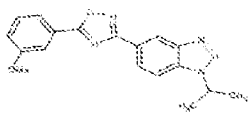
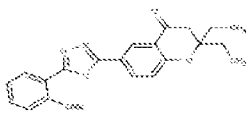
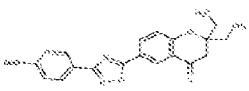
Structure	Compound Number	Chemical Name
	260	3-(2-fluoro-6-methoxy-phenyl)-5-(1-isopropylbenzotriazol-5-yl)-1,2,4-oxadiazole
	261	6-[3-(3-chlorophenyl)-1,2,4-oxadiazol-5-yl]-2,2-diethyl-chroman-4-one
	262	N-(4-(5-(2,2-diethyl-4-oxochroman-6-yl)-1,2,4-oxadiazol-3-yl)phenyl)methanesulfonamide
	263	2,2-diethyl-6-[3-(2-hydroxy-4-pyridyl)-1,2,4-oxadiazol-5-yl]chroman-4-one
	264	6-[3-(4-methylpyridin-3-yl)-1,2,4-oxadiazol-5-yl]-1- (propan-2-yl)-1H-1,2,3-benzotriazole
	265	2,2-diethyl-6-(3-(3-methylthiophen-2-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one
	266	4-(5-(2,2-diethyl-4-oxochroman-6-yl)-1,2,4-oxadiazol-3-yl)-N-methylbenzenesulfonamide

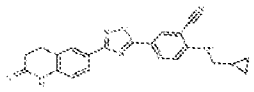
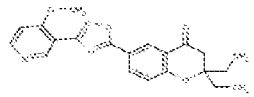
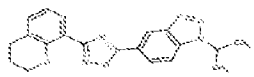
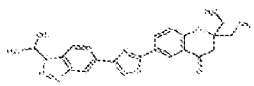
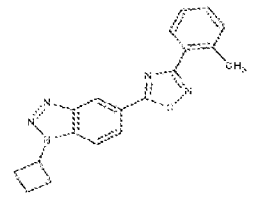
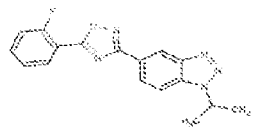
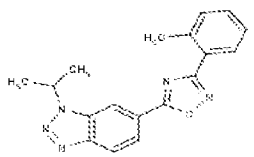
Structure	Compound Number	Chemical Name
	267	2-(allylamino)-5-(3-(2-aminobenzo[d]thiazol-5-yl)-1,2,4-oxadiazol-5-yl)benzonitrile
	268	2,2-diethyl-6-[3-(2-methoxyphenyl)-1,2,4-oxadiazol-5-yl]chroman-4-one
	269	2,2-diethyl-6-[3-(p-tolyl)-1,2,4-oxadiazol-5-yl]chroman-4-one
	270	5-(3-phenyl-1,2,4-oxadiazol-5-yl)-1-(prop-2-en-1- yl)-1H-1,2,3-benzotriazole
	271	1-(3-methylbutyl)-5-(3-phenyl-1,2,4-oxadiazol-5- yl)-1H-1,2,3-benzotriazole
	272	3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(5-methoxypyridin-3-yl)-1,2,4-oxadiazole
	273	3-(1-cyclopentyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(m-tolyl)-1,2,4-oxadiazole

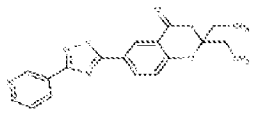
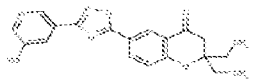
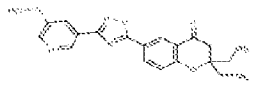
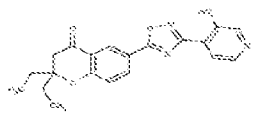
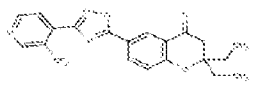
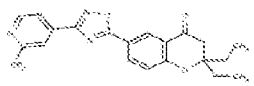
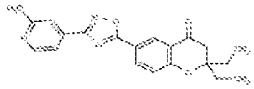
Structure	Compound Number	Chemical Name
	274	2,2-dimethyl-6-[3-(pyridin-3-yl)-1,2,4-oxadiazol-5- yl]-3,4-dihydro-2H-1-benzopyran-4-one
	275	3-(1-cyclopentyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(3,4-dimethoxyphenyl)-1,2,4-oxadiazole
	276	3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(2-(methylthio)phenyl)-1,2,4-oxadiazole
	277	5-[4-(2-methoxyphenyl)-1,3-oxazol-2-yl]-1-(propan-2- yl)-1H-1,2,3-benzotriazole
	278	5-(5-cyclopentyl-1,2,4-oxadiazol-3-yl)-1-(propan-2- yl)-1H-1,2,3-benzotriazole5-(5-cyclopentyl-1,2,4-oxadiazol-3-yl)-1-(propan-2-yl)-1H-1,2,3-benzotriazole
	279	2-(3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-oxadiazol-5-yl)benzonitrile
	280	6-[3-(pyridin-4-yl)-1,2,4-oxadiazol-5-yl]-3,4- dihydrospiro[1-benzopyran-2,1'-cyclohexane]-4-one

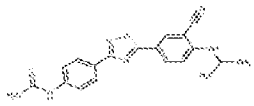
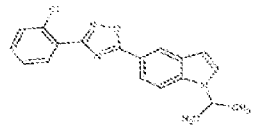
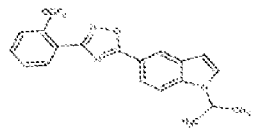
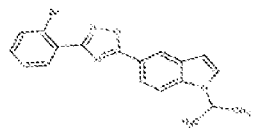
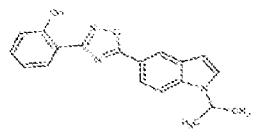
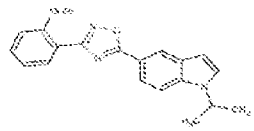
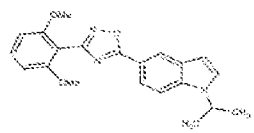
Structure	Compound Number	Chemical Name
	281	1-cyclopentyl-5-[3-(2-methoxypyridin-4-yl)-1,2,4-oxadiazol-5-yl]-1H-1,2,3-benzotriazole
	282	5-[3-(2-bromophenyl)-1,2,4-oxadiazol-5-yl]-1- (propan-2-yl)-1H-1,2,3-benzotriazole
	283	5-(2-bromophenyl)-3-(1-(pyridin-3-ylmethyl)-1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-oxadiazole
	284	1-cyclohexyl-5-{3-[4-methoxy-3-(trifluoromethyl)phenyl]-1,2,4-oxadiazol-5-yl}-1H- 1,2,3-benzotriazole
	285	1-cyclopropyl-5-[3-(4-phenoxyphenyl)-1,2,4- oxadiazol-5-yl]-1H-1,2,3-benzotriazole
	286	5-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-3-(2-methoxyphenyl)-1,2,4-oxadiazole
	287	3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(2-methoxyphenyl)-1,2,4-oxadiazole

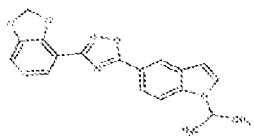
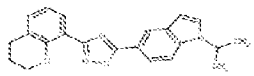
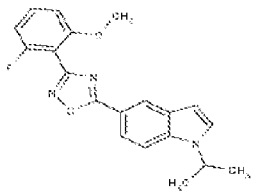
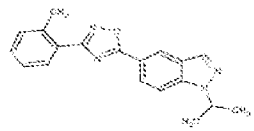
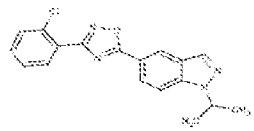
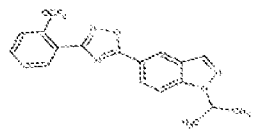
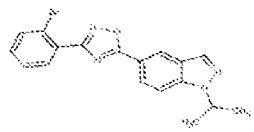
Structure	Compound Number	Chemical Name
	288	1-(cyclopropylmethyl)-5-[3-(2-methylphenyl)-1,2,4- oxadiazol-5-yl]-1H-1,2,3-benzotriazole
	289	5-[3-(2-chlorophenyl)-1,2,4-oxadiazol-5-yl]-1-(2-methylpropyl)-1H-1,2,3-benzotriazole
	290	5-(4-cyclohexylphenyl)-3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-oxadiazole
	291	2,2-dimethyl-6-[3-(pyridin-4-yl)-1,2,4-oxadiazol-5- yl]-3,4-dihydro-2H-1-benzopyran-4-one
	292	1-cyclohexyl-5-(3-phenyl-1,2,4-oxadiazol-5-yl)-1H- 1,2,3-benzotriazole
	293	5-[3-(2-methylphenyl)-1,2,4-oxadiazol-5-yl]-1- (propan-2-yl)-1H-1,2,3-benzotriazole
	294	5-(4-phenyl-1,3-oxazol-2-yl)-1-(propan-2-yl)-1H- 1,2,3-benzotriazole

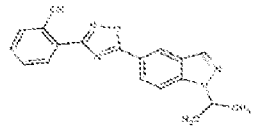
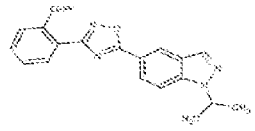
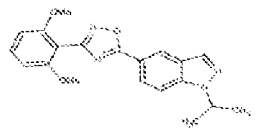
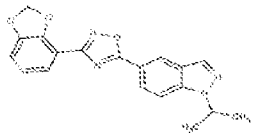
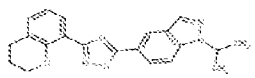
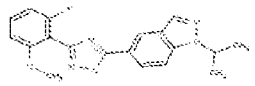
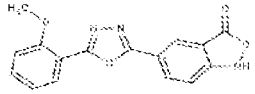
Structure	Compound Number	Chemical Name
	295	1-cyclopropyl-5-[3-(pyridin-4-yl)-1,2,4-oxadiazol-5- yl]-1H-1,2,3-benzotriazole
	296	5-{3-[4-(benzyloxy)-3-(trifluoromethyl)phenyl]- 1,2,4-oxadiazol-5-yl}-1-(propan-2-yl)-1H-1,2,3- benzotriazole
	297	5-{4H,5H-naphtho[2,1-d][1,3]oxazol-2-yl}-1-(propan-2-yl)-1H-1,2,3-benzotriazole
	298	6-[3-(pyridin-3-yl)-1,2,4-oxadiazol-5-yl]-3,4- dihydrospiro[1-benzopyran-2,1'-cyclopentane]-4-one
	299	3-(1-isopropylbenzotriazol-5-yl)-5-(3-methoxyphenyl)-1,2,4-oxadiazole
	300	2,2-diethyl-6-(5-(2-methoxyphenyl)-1,3,4-oxadiazol-2-yl)chroman-4-one
	301	2,2-diethyl-6-[3-(6-methoxy-3-pyridyl)-1,2,4-oxadiazol-5-yl]chroman-4-one

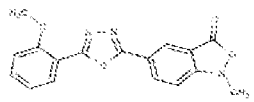
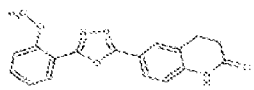
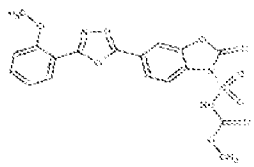
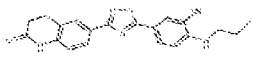
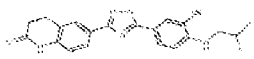
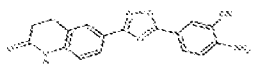
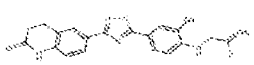
Structure	Compound Number	Chemical Name
	302	2-((cyclopropylmethyl)amino)-5-(3-(2-oxo-1,2,3,4-tetrahydroquinolin-6-yl)-1,2,4-oxadiazol-5-yl)benzonitrile
	303	2,2-diethyl-6-(3-(4-methoxypyridin-3-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one
	304	3-chroman-8-yl-5-(1-isopropylbenzotriazol-5-yl)-1,2,4-oxadiazole
	305	2,2-diethyl-6-(3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one
	306	1-cyclobutyl-5-[3-(2-methylphenyl)-1,2,4-oxadiazol-5-yl]-1H-1,2,3-benzotriazole
	307	5-(2-fluorophenyl)-3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-oxadiazole
	308	6-[3-(2-methylphenyl)-1,2,4-oxadiazol-5-yl]-1- (propan-2-yl)-1H-1,2,3-benzotriazole

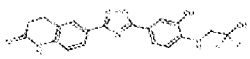
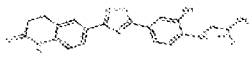
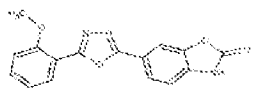
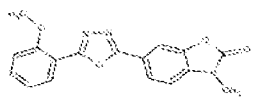
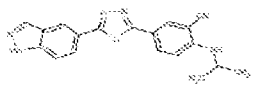
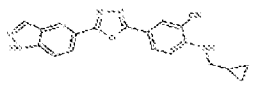
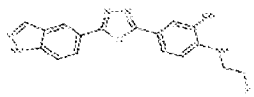
Structure	Compound Number	Chemical Name
	309	2,2-diethyl-6-(3-(pyridin-3-yl)-1,2,4-thiadiazol-5-yl)chroman-4-one
	310	2,2-diethyl-6-[3-(5-hydroxy-3-pyridyl)-1,2,4-oxadiazol-5-yl]chroman-4-one
	311	2,2-diethyl-6-(3-(5-methoxypyridin-3-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one
	312	2,2-diethyl-6-(3-(3-hydroxypyridin-4-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one
	313	2,2-diethyl-6-(3-(3-(trifluoromethyl)pyridin-4-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one
	314	2,2-diethyl-6-(3-(2-(trifluoromethyl)pyridin-4-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one
	315	2,2-diethyl-6-(3-(2-methylpyridin-4-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one

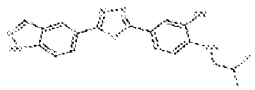
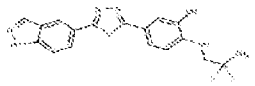
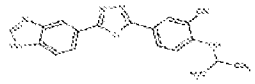
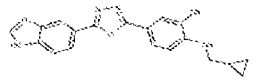
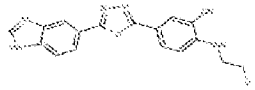
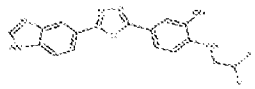
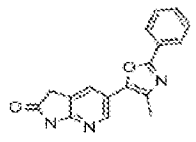
Structure	Compound Number	Chemical Name
	316	N-(4-(5-(3-cyano-4-(isopropylamino)phenyl)-1,2,4-oxadiazol-3-yl)phenyl)acetamide
	320	3-(2-chlorophenyl)-5-(1-isopropyl-1H-indol-5-yl)-1,2,4-oxadiazole
	321	5-(1-isopropyl-1H-indol-5-yl)-3-(2-(trifluoromethoxy)phenyl)-1,2,4-oxadiazole
	322	3-(2-bromophenyl)-5-(1-isopropyl-1H-indol-5-yl)-1,2,4-oxadiazole
	323	2-(5-(1-isopropyl-1H-indol-5-yl)-1,2,4-oxadiazol-3-yl)phenol
	324	3-(2-isopropoxyphenyl)-5-(1-isopropyl-1H-indol-5-yl)-1,2,4-oxadiazole
	325	3-(2,6-dimethoxyphenyl)-5-(1-isopropylindol-5-yl)-1,2,4-oxadiazole

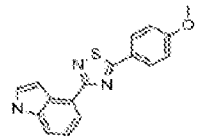
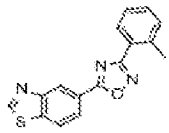
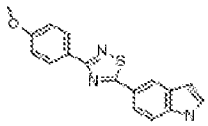
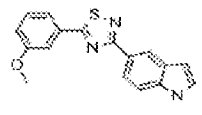
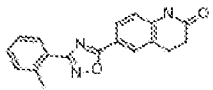
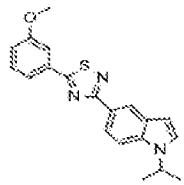
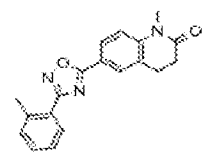
Structure	Compound Number	Chemical Name
	326	3-(benzo[d][1,3]dioxol-4-yl)-5-(1-isopropyl-1H-indol-5-yl)-1,2,4-oxadiazole
	327	3-chroman-8-yl-5-(1-isopropylindol-5-yl)-1,2,4-oxadiazole
	328	3-(2-fluoro-6-methoxy-phenyl)-5-(1-isopropylindol-5-yl)-1,2,4-oxadiazole
	329	5-(1-isopropyl-1H-indazol-5-yl)-3-(o-tolyl)-1,2,4-oxadiazole
	330	3-(2-chlorophenyl)-5-(1-isopropyl-1H-indazol-5-yl)-1,2,4-oxadiazole
	331	5-(1-isopropyl-1H-indazol-5-yl)-3-(2-(trifluoromethoxy)phenyl)-1,2,4-oxadiazole
	332	3-(2-bromophenyl)-5-(1-isopropyl-1H-indazol-5-yl)-1,2,4-oxadiazole

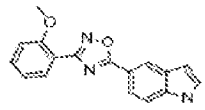
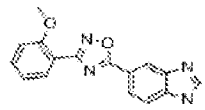
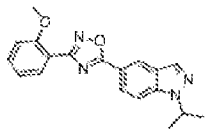
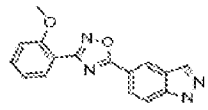
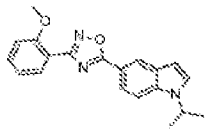
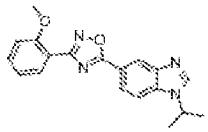
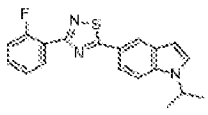
Structure	Compound Number	Chemical Name
	333	2-(5-(1-isopropyl-1H-indazol-5-yl)-1,2,4-oxadiazol-3-yl)phenol
	334	3-(2-isopropoxyphenyl)-5-(1-isopropyl-1H-indazol-5-yl)-1,2,4-oxadiazole
	335	3-(2,6-dimethoxyphenyl)-5-(1-isopropylindazol-5-yl)-1,2,4-oxadiazole
	336	3-(benzo[d][1,3]dioxol-4-yl)-5-(1-isopropyl-1H-indazol-5-yl)-1,2,4-oxadiazole
	337	3-chroman-8-yl-5-(1-isopropylindazol-5-yl)-1,2,4-oxadiazole
	338	3-(2-fluoro-6-methoxy-phenyl)-5-(1-isopropylindazol-5-yl)-1,2,4-oxadiazole
	339	5-[5-(2-methoxyphenyl)-1,3,4-oxadiazol-2-yl]-1,3- dihydro-2,1-benzoxazol-3-one

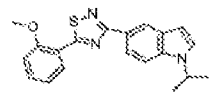
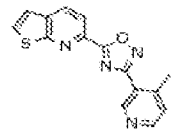
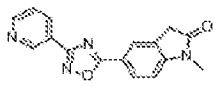
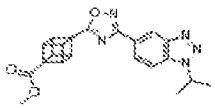
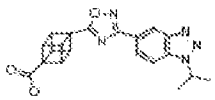
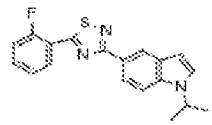
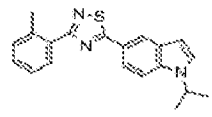
Structure	Compound Number	Chemical Name
	340	5-[5-(2-methoxyphenyl)-1,3,4-oxadiazol-2-yl]-1- methyl-1,3-dihydro-2,1-benzoxazol-3-one
	341	6-[5-(2-methoxyphenyl)-1,3,4-oxadiazol-2-yl]- 1,2,3,4-tetrahydroquinolin-2-one
	342	methyl N-({6-[5-(2-methoxyphenyl)-1,3,4-oxadiazol-2-yl]-2-oxo-2,3-dihydro-1,3-benzoxazol-3-yl}sulfonyl)carbamate
	343	2-[(2-fluoroethyl)amino]-5-[3-(2-oxo-1,2,3,4- tetrahydroquinolin-6-yl)-1,2,4-oxadiazol-5-yl]benzonitrile
	344	2-[(2,2-difluoroethyl)amino]-5-[3-(2-oxo-1,2,3,4- tetrahydroquinolin-6-yl)-1,2,4-oxadiazol-5-yl]benzonitrile
	345	2-amino-5-[3-(2-oxo-1,2,3,4-tetrahydroquinolin-6- yl)-1,2,4-oxadiazol-5-yl]benzonitrile
	346	2-[(2-fluoroprop-2-en-1-yl)amino]-5-[3-(2-oxo- 1,2,3,4-tetrahydroquinolin-6-yl)-1,2,4-oxadiazol-5- yl]benzonitrile

Structure	Compound Number	Chemical Name
	347	2-[(2,2-difluoropropyl)amino]-5-[3-(2-oxo-1,2,3,4- tetrahydroquinolin-6-yl)-1,2,4-oxadiazol-5-yl]benzonitrile
	348	2-[(2-fluoropropyl)amino]-5-[3-(2-oxo-1,2,3,4- tetrahydroquinolin-6-yl)-1,2,4-oxadiazol-5-yl]benzonitrile
	349	6-[5-(2-methoxyphenyl)-1,3,4-oxadiazol-2-yl]-2,3- dihydro-1,3-benzoxazol-2-one
	350	6-[5-(2-methoxyphenyl)-1,3,4-oxadiazol-2-yl]-3- methyl-2,3-dihydro-1,3-benzoxazol-2-one
	351	5-[5-(1H-indazol-5-yl)-1,3,4-oxadiazol-2-yl]-2- [(propan-2-yl)amino]benzonitrile
	352	2-[(cyclopropylmethyl)amino]-5-[5-(1H-indazol-5- yl)-1,3,4-oxadiazol-2-yl]benzonitrile
	353	2-[(2-fluoroethyl)amino]-5-[5-(1H-indazol-5-yl)- 1,3,4-oxadiazol-2-yl]benzonitrile

Structure	Compound Number	Chemical Name
	354	2-[(2,2-difluoroethyl)amino]-5-[5-(1H-indazol-5- yl)-1,3,4-oxadiazol-2-yl]benzonitrile
	355	2-[(2,2-difluoropropyl)amino]-5-[5-(1H-indazol-5- yl)-1,3,4-oxadiazol-2-yl]benzonitrile
	356	5-[5-(1H-1,3-benzodiazol-5-yl)-1,3,4-oxadiazol-2- yl]-2-[(propan-2-yl)amino]benzonitrile
	357	5-[5-(1H-1,3-benzodiazol-5-yl)-1,3,4-oxadiazol-2- yl]-2-[(cyclopropylmethyl)amino]benzonitrile
	358	5-[5-(1H-1,3-benzodiazol-5-yl)-1,3,4-oxadiazol-2- yl]-2-[(2-fluoroethyl)amino]benzonitrile
	359	5-[5-(1H-1,3-benzodiazol-5-yl)-1,3,4-oxadiazol-2- yl]-2-[(2,2-difluoroethyl)amino]benzonitrile
	360	5-(4-methyl-2-phenyl-1,3-oxazol-5-yl)-1H,2H,3H- pyrrolo[2,3-b]pyridin-2-one

Structure	Compound Number	Chemical Name
	361	4-[5-(4-methoxyphenyl)-1,2,4-thiadiazol-3-yl]-1H- indole
	362	5-[3-(2-methylphenyl)-1,2,4-oxadiazol-5-yl]-1,3- benzothiazole
	363	5-[3-(4-methoxyphenyl)-1,2,4-thiadiazol-5-yl]-1H- indole
	364	5-[5-(3-methoxyphenyl)-1,2,4-thiadiazol-3-yl]-1H- indole
	365	6-[3-(2-methylphenyl)-1,2,4-oxadiazol-5-yl]- 1,2,3,4-tetrahydroquinolin-2-one
	366	5-[5-(3-methoxyphenyl)-1,2,4-thiadiazol-3-yl]-1- (propan-2-yl)-1H-indole
	367	1-methyl-6-[3-(2-methylphenyl)-1,2,4-oxadiazol-5- yl]-1,2,3,4-tetrahydroquinolin-2-one

Structure	Compound Number	Chemical Name
	368	5-(1H-indol-5-yl)-3-(2-methoxyphenyl)-1,2,4-oxadiazole
	369	5-(1H-benzo[d]imidazol-5-yl)-3-(2-methoxyphenyl)-1,2,4-oxadiazole
	370	5-(1-isopropyl-1H-indazol-5-yl)-3-(2-methoxyphenyl)-1,2,4-oxadiazole
	371	5-(1H-indazol-5-yl)-3-(2-methoxyphenyl)-1,2,4-oxadiazole
	372	5-(1-isopropyl-1H-indol-5-yl)-3-(2-methoxyphenyl)-1,2,4-oxadiazole
	373	5-(1-isopropyl-1H-benzo[d]imidazol-5-yl)-3-(2-methoxyphenyl)-1,2,4-oxadiazole
	374	5-[3-(2-fluorophenyl)-1,2,4-thiadiazol-5-yl]-1- (propan-2-yl)-1H-indole

Structure	Compound Number	Chemical Name
	375	5-[5-(2-methoxyphenyl)-1,2,4-thiadiazol-3-yl]-1- (propan-2-yl)-1H-indole
	376	4-methyl-3-(5-{thieno[2,3-b]pyridin-6-yl}-1,2,4- oxadiazol-3-yl)pyridine
	377	1-methyl-5-[3-(pyridin-3-yl)-1,2,4-oxadiazol-5-yl]- 2,3-dihydro-1H-indol-2-one
	378	8-{3-[1-(propan-2-yl)-1H-1,2,3-benzotriazol-5- yl]-1,2,4-oxadiazol-5-yl}cubane-1-carboxylate
	379	8-{3-[1-(propan-2-yl)-1H-1,2,3-benzotriazol-5-yl]- 1,2,4-oxadiazol-5-yl}cubane-1-carboxylic acid
	380	5-[5-(2-fluorophenyl)-1,2,4-thiadiazol-3-yl]-1- (propan-2-yl)-1H-indole
	381	5-[3-(2-methylphenyl)-1,2,4-thiadiazol-5-yl]-1- (propan-2-yl)-1H-indole

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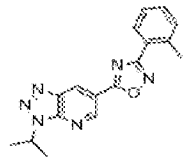
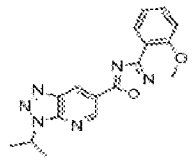
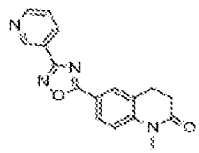
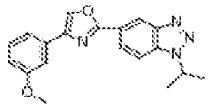
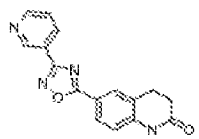
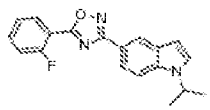
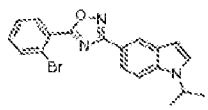
	382	3-(2-methylphenyl)-5-[3-(propan-2-yl)-3H- [1,2,3]triazolo[4,5-b]pyridin-6-yl]-1,2,4- oxadiazole
	383	3-(2-methoxyphenyl)-5-[3-(propan-2-yl)-3H- [1,2,3]triazolo[4,5-b]pyridin-6-yl]-1,2,4- oxadiazole
	384	1-methyl-6-[3-(pyridin-3-yl)-1,2,4-oxadiazol-5-yl]- 1,2,3,4-tetrahydroquinolin-2-one
	385	5-[4-(3-methoxyphenyl)-1,3-oxazol-2-yl]-1-(propan-2- yl)-1H-1,2,3-benzotriazole
	386	6-[3-(pyridin-3-yl)-1,2,4-oxadiazol-5-yl]-1,2,3,4- tetrahydroquinolin-2-one
	387	5-(2-fluorophenyl)-3-(1-isopropyl-1H-indol-5-yl)-1,2,4-oxadiazole
	388	5-(2-bromophenyl)-3-(1-isopropyl-1H-indol-5-yl)-1,2,4-oxadiazole

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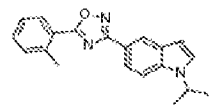
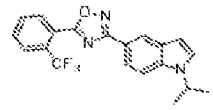
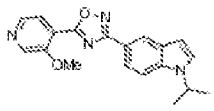
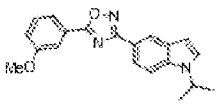
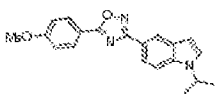
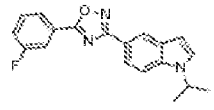
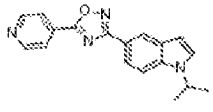
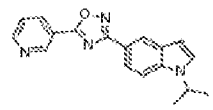
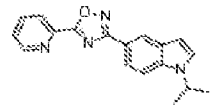
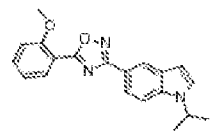
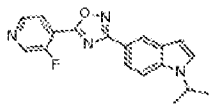
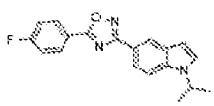
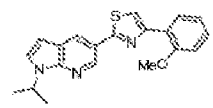
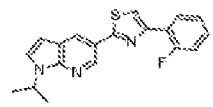
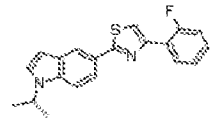
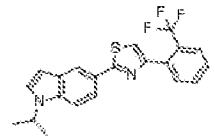
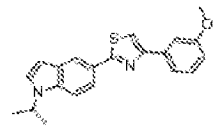
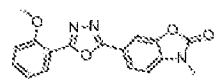
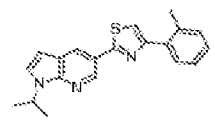
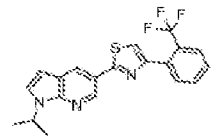
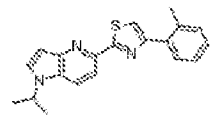
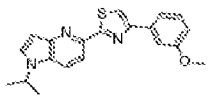
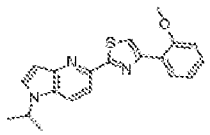
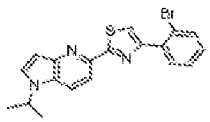
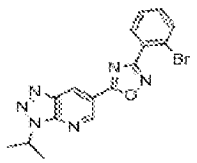
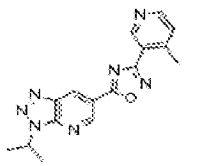
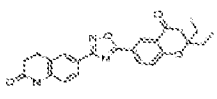
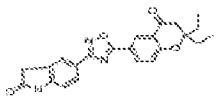
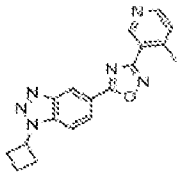
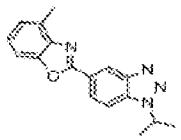
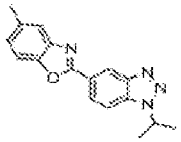
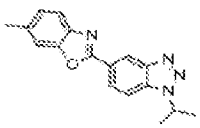
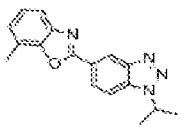
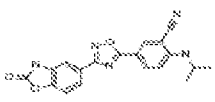
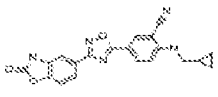
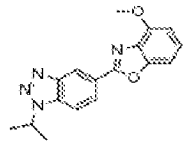
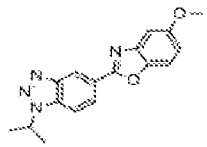
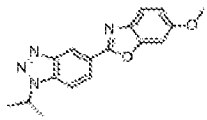
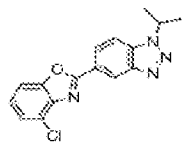
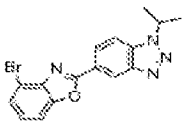
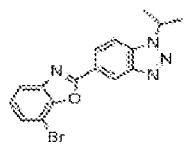
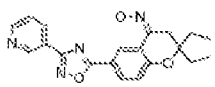
	389	3-(1-isopropyl-1H-indol-5-yl)-5-(o-tolyl)-1,2,4-oxadiazole
	390	3-(1-isopropyl-1H-indol-5-yl)-5-(2-(trifluoromethyl)phenyl)-1,2,4-oxadiazole
	391	3-(1-isopropyl-1H-indol-5-yl)-5-(3-methoxypyridin-4-yl)-1,2,4-oxadiazole
	392	3-(1-isopropyl-1H-indol-5-yl)-5-(3-methoxyphenyl)-1,2,4-oxadiazole
	393	3-(1-isopropyl-1H-indol-5-yl)-5-(4-methoxyphenyl)-1,2,4-oxadiazole
	394	5-(3-fluorophenyl)-3-(1-isopropyl-1H-indol-5-yl)-1,2,4-oxadiazole
	395	3-(1-isopropyl-1H-indol-5-yl)-5-(pyridin-4-yl)-1,2,4-oxadiazole

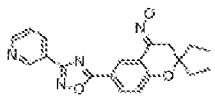
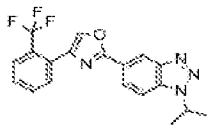
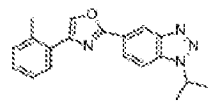
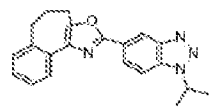
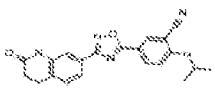
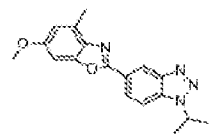
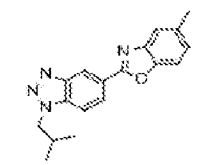
Structure	Compound Number	Chemical Name
	396	3-(1-isopropyl-1H-indol-5-yl)-5-(pyridin-3-yl)-1,2,4-oxadiazole
	397	3-(1-isopropyl-1H-indol-5-yl)-5-(pyridin-2-yl)-1,2,4-oxadiazole
	398	3-(1-isopropyl-1H-indol-5-yl)-5-(2-methoxyphenyl)-1,2,4-oxadiazole
	399	5-(3-fluoropyridin-4-yl)-3-(1-isopropyl-1H-indol-5-yl)-1,2,4-oxadiazole
	400	5-(4-fluorophenyl)-3-(1-isopropyl-1H-indol-5-yl)-1,2,4-oxadiazole
	401	2-(1-isopropyl-1H-pyrrolo[2,3-b]pyridin-5-yl)-4-(2-methoxyphenyl)thiazole
	402	4-(2-fluorophenyl)-2-(1-isopropyl-1H-pyrrolo[2,3-b]pyridin-5-yl)thiazole

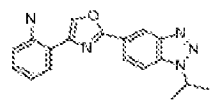
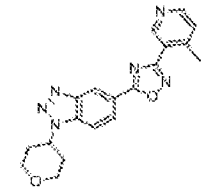
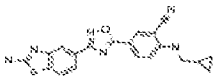
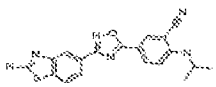
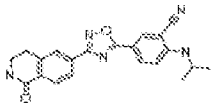
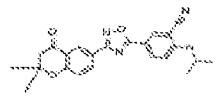
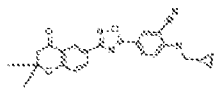
Structure	Compound Number	Chemical Name
	403	4-(2-fluorophenyl)-2-(1-isopropylindol-5-yl)thiazole
	404	2-(1-isopropylindol-5-yl)-4-[2-(trifluoromethyl)phenyl]thiazole
	405	2-(1-isopropylindol-5-yl)-4-(3-methoxyphenyl)thiazole
	406	6-[5-(2-methoxyphenyl)-1,3,4-oxadiazol-2-yl]-3- methyl-2,3-dihydro-1,3-benzoxazol-2-one
	407	2-(1-isopropylpyrrolo[2,3-b]pyridin-5-yl)-4-(o-tolyl)thiazole
	408	2-(1-isopropylpyrrolo[2,3-b]pyridin-5-yl)-4-[2-(trifluoromethyl)phenyl]thiazole
	409	2-(1-isopropylpyrrolo[3,2-b]pyridin-5-yl)-4-(o-tolyl)thiazole

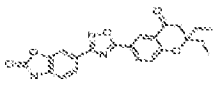
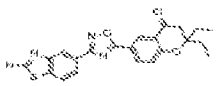
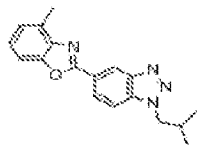
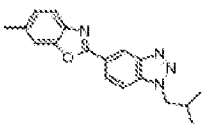
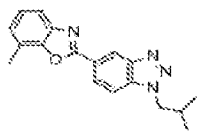
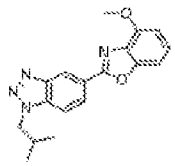
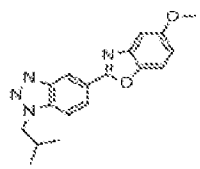
Structure	Compound Number	Chemical Name
	410	2-(1-isopropylpyrrolo[3,2-b]pyridin-5-yl)-4-(3-methoxyphenyl)thiazole
	411	2-(1-isopropyl-1H-pyrrolo[3,2-b]pyridin-5-yl)-4-(2-methoxyphenyl)thiazole
	412	4-(2-bromophenyl)-2-(1-isopropyl-1H-pyrrolo[3,2-b]pyridin-5-yl)thiazole
	413	3-(2-bromophenyl)-5-[3-(propan-2-yl)-3H- [1,2,3]triazolo[4,5-b]pyridin-6-yl]-1,2,4- oxadiazole
	414	4-methyl-3-{5-[3-(propan-2-yl)-3H- [1,2,3]triazolo[4,5-b]pyridin-6-yl]-1,2,4- oxadiazol-3-yl}pyridine
	415	6-(5-(2,2-diethyl-4-oxochroman-6-yl)-1,2,4-oxadiazol-3-yl)-3,4-dihydroquinolin-2(1H)-one
	416	5-(5-(2,2-diethyl-4-oxochroman-6-yl)-1,2,4-oxadiazol-3-yl)indolin-2-one

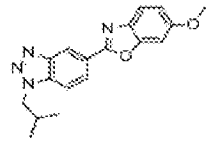
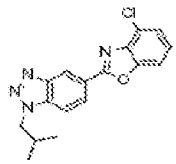
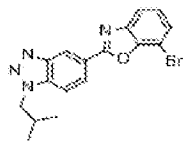
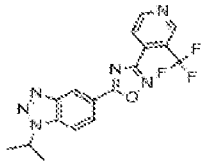
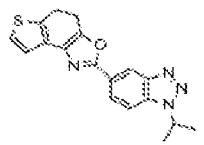
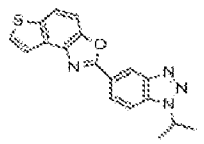
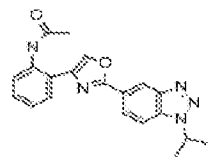
Structure	Compound Number	Chemical Name
	417	1-cyclobutyl-5-[3-(4-methylpyridin-3-yl)-1,2,4-oxadiazol-5-yl]-1H-1,2,3-benzotriazole
	418	2-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-4-methylbenzo[d]oxazole
	419	2-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-methylbenzo[d]oxazole
	420	2-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-6-methylbenzo[d]oxazole
	421	2-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-7-methylbenzo[d]oxazole
	422	2-(isopropylamino)-5-(3-(2-oxo-2,3-dihydrobenzo[d]oxazol-5-yl)-1,2,4-oxadiazol-5-yl)benzonitrile
	423	2-((cyclopropylmethyl)amino)-5-(3-(2-oxo-2,3-dihydrobenzo[d]oxazol-5-yl)-1,2,4-oxadiazol-5-yl)benzonitrile

Structure	Compound Number	Chemical Name
	424	2-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-4-methoxybenzo[d]oxazole
	425	2-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-methoxybenzo[d]oxazole
	426	2-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-6-methoxybenzo[d]oxazole
	427	4-chloro-2-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)benzo[d]oxazole
	428	4-bromo-2-(1-isopropylbenzotriazol-5-yl)-1,3-benzoxazole
	429	7-bromo-2-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)benzo[d]oxazole
	430	N-[(4Z)-2,2-diethyl-6-[3-(pyridin-3-yl)-1,2,4- oxadiazol-5-yl]-3,4-dihydro-2H-1-benzopyran-4-ylidene]hydroxylamine

Structure	Compound Number	Chemical Name
	431	N-[(4E)-2,2-diethyl-6-[3-(pyridin-3-yl)-1,2,4- oxadiazol-5-yl]-3,4-dihydro-2H-1-benzopyran-4-ylidene]hydroxylamine
	432	1-(propan-2-yl)-5-{4-[2-(trifluoromethyl)phenyl]- 1,3-oxazol-2-yl}-1H-1,2,3-benzotriazole
	433	5-[4-(2-methylphenyl)-1,3-oxazol-2-yl]-1-(propan-2- yl)-1H-1,2,3-benzotriazole
	434	4-[1-(propan-2-yl)-1H-1,2,3-benzotriazol-5-yl]-5- oxa-3-azatricyclo[8.4.0.0²,6]tetradeca-1(14),2(6),3,10,12-pentaene
	435	2-(isopropylamino)-5-(3-(2-oxo-1,2,3,4-tetrahydroquinolin-7-yl)-1,2,4-oxadiazol-5-yl)benzonitrile
	436	2-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-6-methoxy-4-methylbenzo[d]oxazole
	437	2-(1-isobutyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-methylbenzo[d]oxazole

Structure	Compound Number	Chemical Name
	438	2-{2-[1-(propan-2-yl)-1H-1,2,3-benzotriazol-5-yl]- 1,3-oxazol-4-yl}aniline
	439	5-[3-(4-methylpyridin-3-yl)-1,2,4-oxadiazol-5-yl]-1- (oxan-4-yl)-1H-1,2,3-benzotriazole
	440	5-(3-(2-aminobenzo[d]thiazol-5-yl)-1,2,4-oxadiazol-5-yl)-2-((cyclopropylmethyl)amino)benzonitrile
	441	5-(3-(2-aminobenzo[d]thiazol-5-yl)-1,2,4-oxadiazol-5-yl)-2-(isopropylamino)benzonitrile
	442	2-(isopropylamino)-5-(3-(1-oxo-1,2,3,4-tetrahydroisoquinolin-6-yl)-1,2,4-oxadiazol-5-yl)benzonitrile
	443	5-(3-(2,2-diethyl-4-oxochroman-6-yl)-1,2,4-oxadiazol-5-yl)-2-(isopropylamino)benzonitrile
	444	2-((cyclopropylmethyl)amino)-5-(3-(2,2-diethyl-4-oxochroman-6-yl)-1,2,4-oxadiazol-5-yl)benzonitrile

Structure	Compound Number	Chemical Name
	445	6-(5-(2,2-diethyl-4-oxochroman-6-yl)-1,2,4-oxadiazol-3-yl)benzo[d]oxazol-2(3H)-one
	446	6-(3-(2-aminobenzo[d]thiazol-5-yl)-1,2,4-oxadiazol-5-yl)-2,2-diethylchroman-4-one
	447	2-(1-isobutyl-1H-benzo[d][1,2,3]triazol-5-yl)-4-methylbenzo[d]oxazole
	448	2-(1-isobutyl-1H-benzo[d][1,2,3]triazol-5-yl)-6-methylbenzo[d]oxazole
	449	2-(1-isobutyl-1H-benzo[d][1,2,3]triazol-5-yl)-7-methylbenzo[d]oxazole
	450	2-(1-isobutyl-1H-benzo[d][1,2,3]triazol-5-yl)-4-methoxybenzo[d]oxazole
	451	2-(1-isobutyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-methoxybenzo[d]oxazole

Structure	Compound Number	Chemical Name
	452	2-(1-isobutyl-1H-benzo[d][1,2,3]triazol-5-yl)-6-methoxybenzo[d]oxazole
	453	4-chloro-2-(1-isobutyl-1H-benzo[d][1,2,3]triazol-5-yl)benzo[d]oxazole
	454	7-bromo-2-(1-isobutyl-1H-benzo[d][1,2,3]triazol-5-yl)benzo[d]oxazole
	455	1-(propan-2-yl)-5-{3-[3-(trifluoromethyl)pyridin-4- yl]-1,2,4-oxadiazol-5-yl}-1H-1,2,3-benzotriazole
	456	4-[1-(propan-2-yl)-1H-1,2,3-benzotriazol-5-yl]-5- oxa-10-thia-3-azatricyclo[7.3.0.0²,6]dodeca-1(9),2(6),3,11-tetraene
	457	4-[1-(propan-2-yl)-1H-1,2,3-benzotriazol-5-yl]-5- oxa-10-thia-3-azatricyclo[7.3.0.0²,6]dodeca-1(9),2(6),3,7,11-pentaene
	458	N-(2-{2-[1-(propan-2-yl)-1H-1,2,3-benzotriazol-5- yl]-1,3-oxazol-4-yl}phenyl)acetamide

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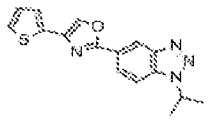
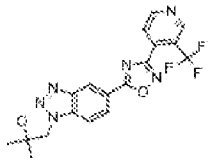
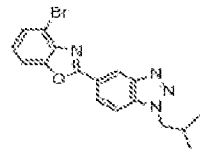
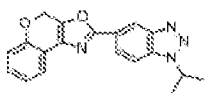
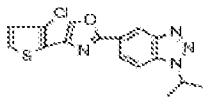
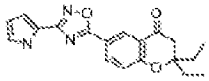
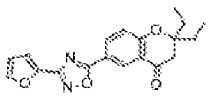
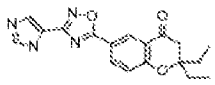
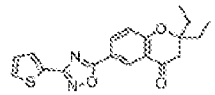
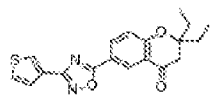
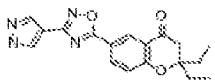
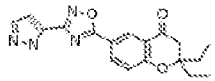
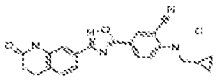
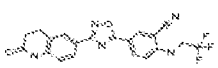
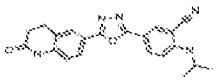
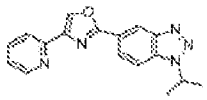
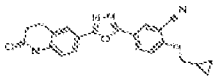
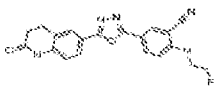
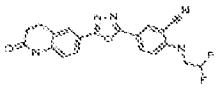
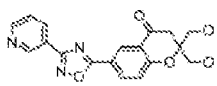
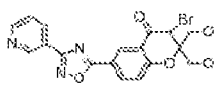
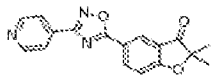
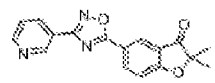
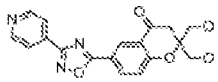
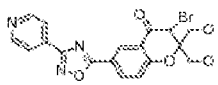
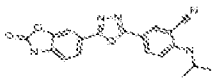
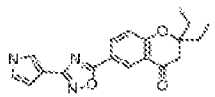
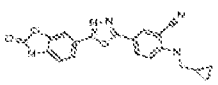
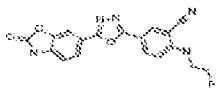
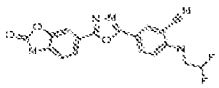
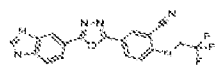
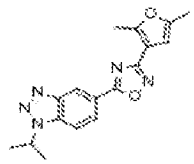
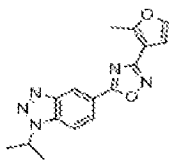
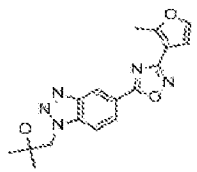
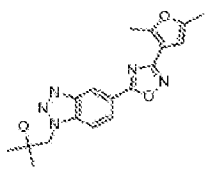
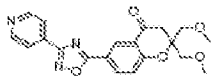
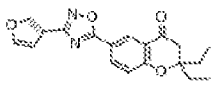
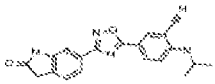
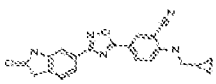
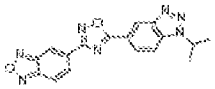
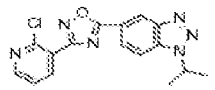
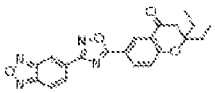
	459	1-(propan-2-yl)-5-[4-(thiophen-2-yl)-1,3-oxazol-2- yl]-1H-1,2,3-benzotriazole
	460	2-methyl-1-(5-{3-[3-(trifluoromethyl)pyridin-4-yl]-1,2,4-oxadiazol-5-yl}-1H-1,2,3-benzotriazol-1- yl)propan-2-ol
	461	4-bromo-2-(1-isobutyl-1H-benzo[d][1,2,3]triazol-5-yl)benzo[d]oxazole
	462	5-{4H-chromeno[4,3-d][1,3]oxazol-2-yl}-1-(propan-2-yl)-1H-1,2,3-benzotriazole
	463	5-[4-(3-chlorothiophen-2-yl)-1,3-oxazol-2-yl]-1- (propan-2-yl)-1H-1,2,3-benzotriazole
	464	6-(3-(1H-pyrrol-2-yl)-1,2,4-oxadiazol-5-yl)-2,2-diethylchroman-4-one
	465	2,2-diethyl-6-(3-(furan-2-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one

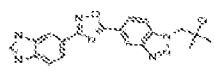
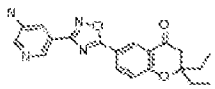
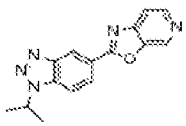
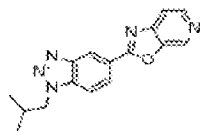
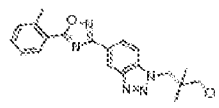
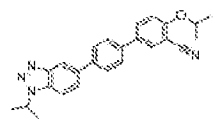
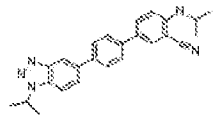
Structure	Compound Number	Chemical Name
	466	6-(3-(1H-imidazol-5-yl)-1,2,4-oxadiazol-5-yl)-2,2-diethylchroman-4-one
	467	2,2-diethyl-6-(3-(thiophen-2-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one
	468	2,2-diethyl-6-(3-(thiophen-3-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one
	469	6-(3-(1H-pyrazol-4-yl)-1,2,4-oxadiazol-5-yl)-2,2-diethylchroman-4-one
	470	6-(3-(1H-pyrazol-5-yl)-1,2,4-oxadiazol-5-yl)-2,2-diethylchroman-4-one
	471	2-((cyclopropylmethyl)amino)-5-(3-(2-oxo-1,2,3,4-tetrahydroquinolin-7-yl)-1,2,4-oxadiazol-5-yl)benzonitrile
	472	5-[3-(2-oxo-1,2,3,4-tetrahydroquinolin-6-yl)-1,2,4-oxadiazol-5-yl]-2-[(2,2,2-trifluoroethyl)amino]benzonitrile

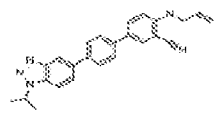
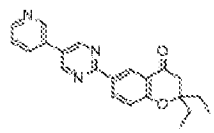
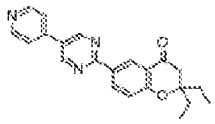
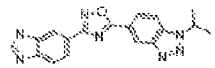
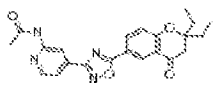
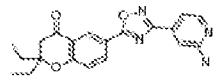
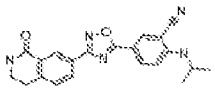
Structure	Compound Number	Chemical Name
	473	5-[5-(2-oxo-1,2,3,4-tetrahydroquinolin-6-yl)-1,3,4-oxadiazol-2-yl]-2-[(propan-2-yl)amino]benzonitrile
	474	1-(propan-2-yl)-5-[4-(pyridin-2-yl)-1,3-oxazol-2- yl]-1H-1,2,3-benzotriazole
	475	2-[(cyclopropylmethyl)amino]-5-[5-(2-oxo-1,2,3,4-tetrahydroquinolin-6-yl)-1,3,4-oxadiazol-2- yl]benzonitrile
	476	2-[(2-fluoroethyl)amino]-5-[5-(2-oxo-1,2,3,4- tetrahydroquinolin-6-yl)-1,3,4-oxadiazol-2-yl]benzonitrile
	477	2-[(2,2-difluoroethyl)amino]-5-[5-(2-oxo-1,2,3,4- tetrahydroquinolin-6-yl)-1,3,4-oxadiazol-2-yl]benzonitrile
	478	2,2-bis(hydroxymethyl)-6-[3-(pyridin-3-yl)-1,2,4- oxadiazol-5-yl]-3,4-dihydro-2H-1-benzopyran-4-one
	479	3-bromo-2,2-bis(hydroxymethyl)-6-[3-(pyridin-3-yl)- 1,2,4-oxadiazol-5-yl]-3,4-dihydro-2H-1-benzopyran-4- one

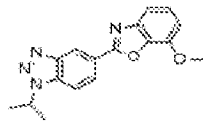
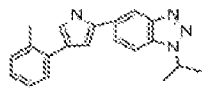
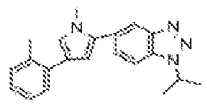
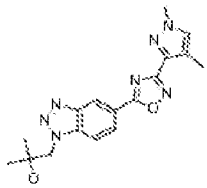
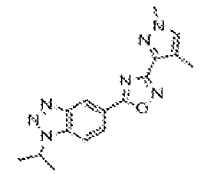
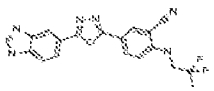
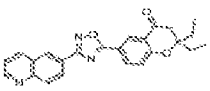
Structure	Compound Number	Chemical Name
	480	2,2-dimethyl-5-[3-(pyridin-4-yl)-1,2,4-oxadiazol-5- yl]-2,3-dihydro-1-benzofuran-3-one
	481	2,2-dimethyl-5-[3-(pyridin-3-yl)-1,2,4-oxadiazol-5- yl]-2,3-dihydro-1-benzofuran-3-one
	482	2,2-bis(hydroxymethyl)-6-[3-(pyridin-4-yl)-1,2,4- oxadiazol-5-yl]-3,4-dihydro-2H-1-benzopyran-4-one
	483	3-bromo-2,2-bis(hydroxymethyl)-6-[3-(pyridin-4-yl)- 1,2,4-oxadiazol-5-yl]-3,4-dihydro-2H-1-benzopyran-4- one
	484	5-[5-(2-oxo-2,3-dihydro-1,3-benzoxazol-6-yl)-1,3,4- oxadiazol-2-yl]-2-[(propan-2-yl)amino]benzonitrile
	485	6-(3-(1H-pyrrol-3-yl)-1,2,4-oxadiazol-5-yl)-2,2-diethylchroman-4-one
	486	2-[(cyclopropylmethyl)amino]-5-[5-(2-oxo-2,3- dihydro-1,3-benzoxazol-6-yl)-1,3,4-oxadiazol-2- yl]benzonitrile

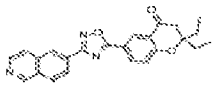
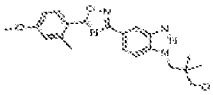
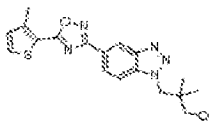
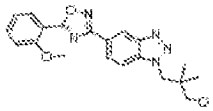
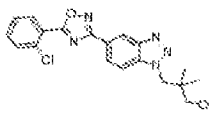
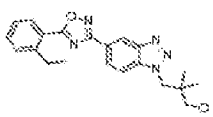
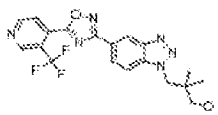
Structure	Compound Number	Chemical Name
	487	2-[(2-fluoroethyl)amino]-5-[5-(2-oxo-2,3-dihydro- 1,3-benzoxazol-6-yl)-1,3,4-oxadiazol-2-yl]benzonitrile
	488	2-[(2,2-difluoroethyl)amino]-5-[5-(2-oxo-2,3- dihydro-1,3-benzoxazol-6-yl)-1,3,4-oxadiazol-2- yl]benzonitrile
	489	5-[3-(1H-1,3-benzodiazol-5-yl)-1,2,4-oxadiazol-5- yl]-2-[(2,2,2-trifluoroethyl)amino]benzonitrile
	490	5-[3-(2,5-dimethylfuran-3-yl)-1,2,4-oxadiazol-5- yl]-1-(propan-2-yl)-1H-1,2,3-benzotriazole
	491	5-[3-(2-methylfuran-3-yl)-1,2,4-oxadiazol-5-yl]-1- (propan-2-yl)-1H-1,2,3-benzotriazole
	492	2-methyl-1-{5-[3-(2-methylfuran-3-yl)-1,2,4- oxadiazol-5-yl]-1H-1,2,3-benzotriazol-1-yl}propan-2- ol
	493	1-{5-[3-(2,5-dimethylfuran-3-yl)-1,2,4-oxadiazol-5- yl]-1H-1,2,3-benzotriazol-1-yl}-2-methylpropan-2- ol

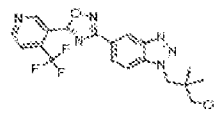
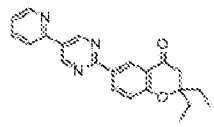
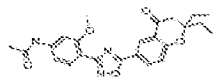
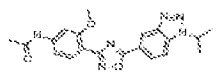
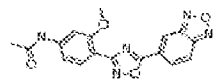
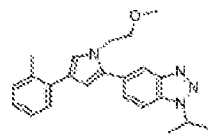
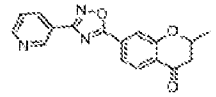
Structure	Compound Number	Chemical Name
	494	2,2-bis(methoxymethyl)-6-[3-(pyridin-4-yl)-1,2,4- oxadiazol-5-yl]-3,4-dihydro-2H-1-benzopyran-4-one
	495	2,2-diethyl-6-(3-(furan-3-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one
	496	2-(isopropylamino)-5-(3-(2-oxoindolin-6-yl)-1,2,4-oxadiazol-5-yl)benzonitrile
	497	2-((cyclopropylmethyl)amino)-5-(3-(2-oxoindolin-6-yl)-1,2,4-oxadiazol-5-yl)benzonitrile
	498	5-{5-[1-(propan-2-yl)-1H-1,2,3-benzotriazol-5-yl]-1,2,4-oxadiazol-3-yl}-2,1,3-benzoxadiazole
	499	5-[3-(2-chloropyridin-3-yl)-1,2,4-oxadiazol-5-yl]-1- (propan-2-yl)-1H-1,2,3-benzotriazole
	500	6-[3-(2,1,3-benzoxadiazol-5-yl)-1,2,4-oxadiazol-5-yl]-2,2-diethyl-3,4-dihydro-2H-1-benzopyran-4-one

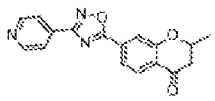
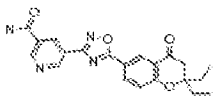
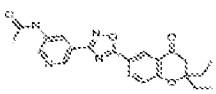
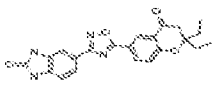
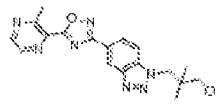
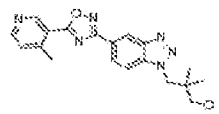
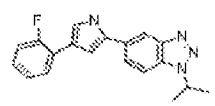
Structure	Compound Number	Chemical Name
	501	1-{5-[3-(1H-1,3-benzodiazol-6-yl)-1,2,4-oxadiazol-5- yl]-1H-1,2,3-benzotriazol-1-yl}-2-methylpropan-2- ol
	502	6-(3-(5-aminopyridin-3-yl)-1,2,4-oxadiazol-5-yl)-2,2-diethylchroman-4-one
	503	2-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)oxazolo[5,4-c]pyridine
	504	2-(1-isobutyl-1H-benzo[d][1,2,3]triazol-5-yl)oxazolo[5,4-c]pyridine
	505	2,2-dimethyl-3-(5-(5-(o-tolyl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)propan-1-ol
	506	4-isopropoxy-4'-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-[1,1'-biphenyl]-3-carbonitrile
	507	4'-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-4-(isopropylamino)-[1,1'-biphenyl]-3-carbonitrile

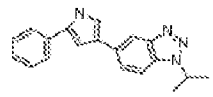
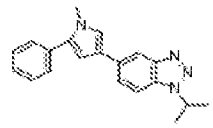
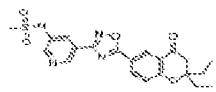
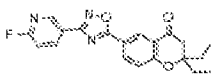
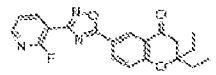
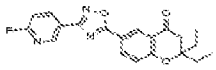
Structure	Compound Number	Chemical Name
	508	4-(allylamino)-4'-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-[1,1'-biphenyl]-3-carbonitrile
	509	2,2-diethyl-6-(5-(pyridin-3-yl)pyrimidin-2-yl)chroman-4-one
	510	2,2-diethyl-6-(5-(pyridin-4-yl)pyrimidin-2-yl)chroman-4-one
	511	5-[3-(1H-1,3-benzodiazol-6-yl)-1,2,4-oxadiazol-5- yl]-1-(propan-2-yl)-1H-1,2,3-benzotriazole
	512	N-(4-(5-(2,2-diethyl-4-oxochroman-6-yl)-1,2,4-oxadiazol-3-yl)pyridin-2-yl)acetamide
	513	6-(3-(2-aminopyridin-4-yl)-1,2,4-oxadiazol-5-yl)-2,2-diethylchroman-4-one
	514	2-(isopropylamino)-5-(3-(1-oxo-1,2,3,4-tetrahydroisoquinolin-7-yl)-1,2,4-oxadiazol-5-yl)benzonitrile

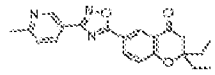
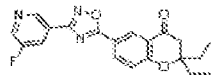
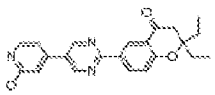
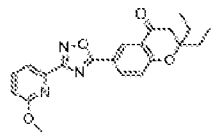
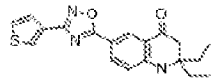
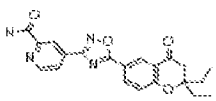
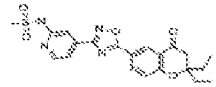
Structure	Compound Number	Chemical Name
	515	2-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-7-methoxybenzo[d]oxazole
	516	5-[4-(2-methylphenyl)-1H-pyrrol-2-yl]-1-(propan-2- yl)-1H-1,2,3-benzotriazole
	517	5-[1-methyl-4-(2-methylphenyl)-1H-pyrrol-2-yl]-1- (propan-2-yl)-1H-1,2,3-benzotriazole
	518	1-{5-[3-(1,4-dimethyl-1H-pyrazol-3-yl)-1,2,4- oxadiazol-5-yl]-1H-1,2,3-benzotriazol-1-yl}-2-methylpropan-2-ol
	519	5-[3-(1,4-dimethyl-1H-pyrazol-3-yl)-1,2,4- oxadiazol-5-yl]-1-(propan-2-yl)-1H-1,2,3-benzotriazole
	520	5-[5-(1H-1,3-benzodiazol-5-yl)-1,3,4-oxadiazol-2- yl]-2-[(2,2-difluoropropyl)amino]benzonitrile
	521	2,2-diethyl-6-(3-(quinolin-6-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one

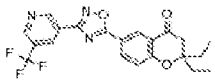
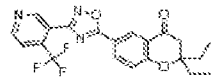
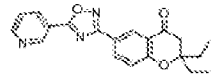
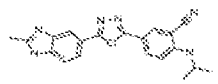
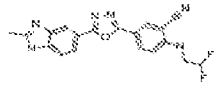
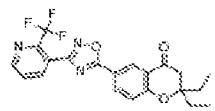
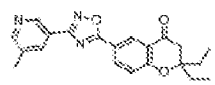
Structure	Compound Number	Chemical Name
	522	2,2-diethyl-6-(3-(isoquinolin-6-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one
	523	3-(5-(5-(4-methoxy-2-methylphenyl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)-2,2-dimethylpropan-1-ol
	524	2,2-dimethyl-3-(5-(5-(3-methylthiophen-2-yl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)propan-1-ol
	525	3-(5-(5-(2-methoxyphenyl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)-2,2-dimethylpropan-1-ol
	526	3-(5-(5-(2-chlorophenyl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)-2,2-dimethylpropan-1-ol
	527	3-(5-(5-(2-ethylphenyl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)-2,2-dimethylpropan-1-ol
	528	2,2-dimethyl-3-(5-(5-(3-(trifluoromethyl)pyridin-4-yl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)propan-1-ol

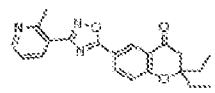
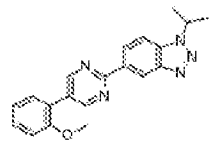
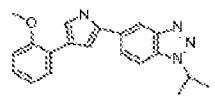
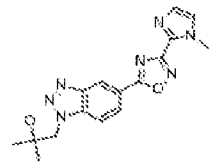
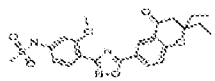
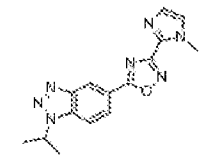
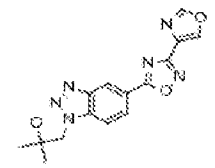
Structure	Compound Number	Chemical Name
	529	2,2-dimethyl-3-(5-(5-(4-(trifluoromethyl)pyridin-3-yl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)propan-1-ol
	530	2,2-diethyl-6-(5-(pyridin-2-yl)pyrimidin-2-yl)chroman-4-one
	531	N-{4-[5-(2,2-diethyl-4-oxo-3,4-dihydro-2H-1-benzopyran-6-yl)-1,2,4-oxadiazol-3-yl]-3-methoxyphenyl}acetamide
	532	N-(3-methoxy-4-{5-[1-(propan-2-yl)-1H-1,2,3-benzotriazol-5-yl]-1,2,4-oxadiazol-3-yl}phenyl)acetamide
	533	N-{4-[5-(2,1,3-benzoxadiazol-5-yl)-1,2,4-oxadiazol-3-yl]-3-methoxyphenyl}acetamide
	534	5-[1-(2-methoxyethyl)-4-(2-methylphenyl)-1H-pyrrol-2- yl]-1-(propan-2-yl)-1H-1,2,3-benzotriazole
	535	2-methyl-7-[3-(pyridin-3-yl)-1,2,4-oxadiazol-5-yl]- 3,4-dihydro-2H-1-benzopyran-4-one

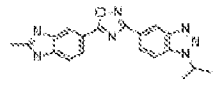
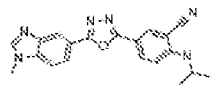
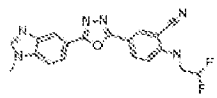
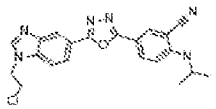
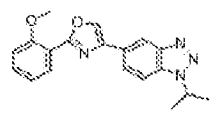
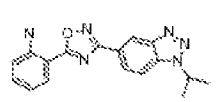
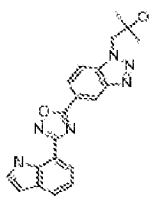
Structure	Compound Number	Chemical Name
	536	2-methyl-7-[3-(pyridin-4-yl)-1,2,4-oxadiazol-5-yl]- 3,4-dihydro-2H-1-benzopyran-4-one
	537	5-(5-(2,2-diethyl-4-oxochroman-6-yl)-1,2,4-oxadiazol-3-yl)nicotinamide
	538	N-(5-(5-(2,2-diethyl-4-oxochroman-6-yl)-1,2,4-oxadiazol-3-yl)pyridin-3-yl)acetamide
	539	5-(5-(2,2-diethyl-4-oxochroman-6-yl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d]imidazol-2(3H)-one
	540	2,2-dimethyl-3-(5-(5-(3-methylpyrazin-2-yl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)propan-1-ol
	541	2,2-dimethyl-3-(5-(5-(4-methylpyridin-3-yl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)propan-1-ol
	542	5-[4-(2-fluorophenyl)-1H-pyrrol-2-yl]-1-(propan-2- yl)-1H-1,2,3-benzotriazole

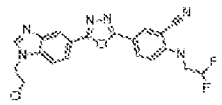
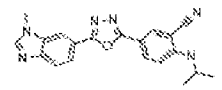
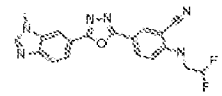
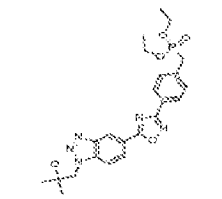
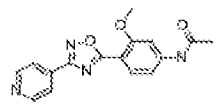
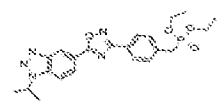
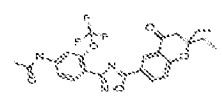
Structure	Compound Number	Chemical Name
	543	5-(5-phenyl-1H-pyrrol-3-yl)-1-(propan-2-yl)-1H- 1,2,3-benzotriazole
	544	5-(1-methyl-5-phenyl-1H-pyrrol-3-yl)-1-(propan-2- yl)-1H-1,2,3-benzotriazole
	545	N-(5-(5-(2,2-diethyl-4-oxochroman-6-yl)-1,2,4-oxadiazol-3-yl)pyridin-3-yl)methanesulfonamide
	546	2,2-diethyl-6-(3-(6-fluoropyridin-3-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one
	547	2,2-diethyl-6-(3-(2-fluoropyridin-3-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one
	548	2,2-diethyl-6-(3-(6-(trifluoromethyl)pyridin-3-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one
	549	2,2-diethyl-6-(3-(4-methylpyridin-3-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one

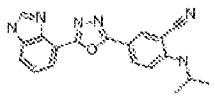
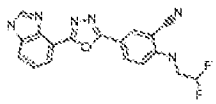
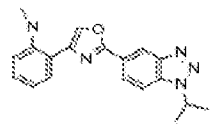
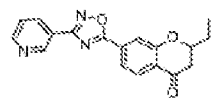
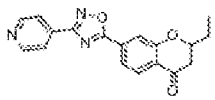
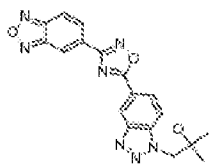
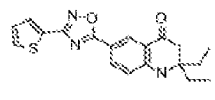
Structure	Compound Number	Chemical Name
	550	2,2-diethyl-6-(3-(6-methylpyridin-3-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one
	551	2,2-diethyl-6-(3-(5-fluoropyridin-3-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one
	552	2,2-diethyl-6-(5-(2-hydroxypyridin-4-yl)pyrimidin-2-yl)chroman-4-one
	553	2,2-diethyl-6-[3-(6-methoxypyridin-2-yl)-1,2,4-oxadiazol-5-yl]-3,4-dihydro-2H-1-benzopyran-4-one
	554	2,2-diethyl-6-(3-(thiophen-3-yl)-1,2,4-oxadiazol-5-yl)-2,3-dihydroquinolin-4(1H)-one
	555	4-(5-(2,2-diethyl-4-oxochroman-6-yl)-1,2,4-oxadiazol-3-yl)picolinamide
	556	N-(4-(5-(2,2-diethyl-4-oxochroman-6-yl)-1,2,4-oxadiazol-3-yl)pyridin-2-yl)methanesulfonamide

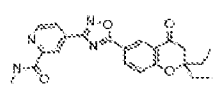
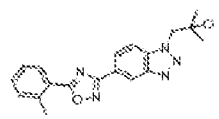
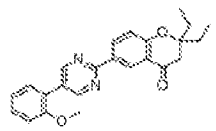
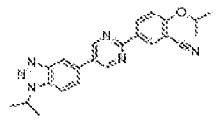
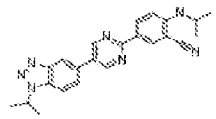
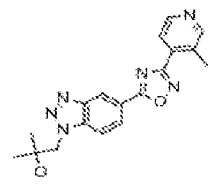
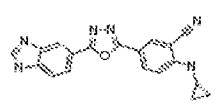
Structure	Compound Number	Chemical Name
	557	2,2-diethyl-6-(3-(5-(trifluoromethyl)pyridin-3-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one
	558	2,2-diethyl-6-(3-(4-(trifluoromethyl)pyridin-3-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one
	559	2,2-diethyl-6-(5-(pyridin-3-yl)-1,2,4-oxadiazol-3-yl)chroman-4-one
	560	5-[5-(2-methyl-1H-1,3-benzodiazol-5-yl)-1,3,4- oxadiazol-2-yl]-2-[(propan-2-yl)amino]benzonitrile
	561	2-[(2,2-difluoroethyl)amino]-5-[5-(2-methyl-1H-1,3- benzodiazol-5-yl)-1,3,4-oxadiazol-2-yl]benzonitrile
	562	2,2-diethyl-6-(3-(2-(trifluoromethyl)pyridin-3-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one
	563	2,2-diethyl-6-(3-(5-methylpyridin-3-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one

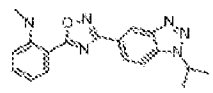
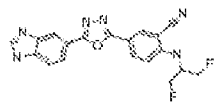
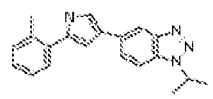
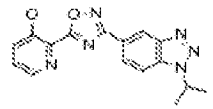
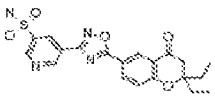
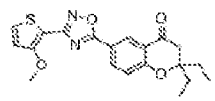
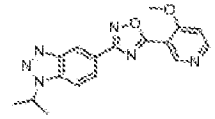
Structure	Compound Number	Chemical Name
	564	2,2-diethyl-6-(3-(2-methylpyridin-3-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one
	565	1-isopropyl-5-(5-(2-methoxyphenyl)pyrimidin-2-yl)-1H-benzo[d][1,2,3]triazole
	566	5-[4-(2-methoxyphenyl)-1H-pyrrol-2-yl]-1-(propan-2- yl)-1H-1,2,3-benzotriazole
	567	2-methyl-1-{5-[3-(1-methyl-1H-imidazol-2-yl)-1,2,4- oxadiazol-5-yl]-1H-1,2,3-benzotriazol-1-yl}propan-2- ol
	568	N-{4-[5-(2,2-diethyl-4-oxo-3,4-dihydro-2H-1-benzopyran-6-yl)-1,2,4-oxadiazol-3-yl]-3-methoxyphenyl}methanesulfonamide
	569	5-[3-(1-methyl-1H-imidazol-2-yl)-1,2,4-oxadiazol-5- yl]-1-(propan-2-yl)-1H-1,2,3-benzotriazole
	570	2-methyl-1-{5-[3-(1,3-oxazol-4-yl)-1,2,4-oxadiazol-5- yl]-1H-1,2,3-benzotriazol-1-yl}propan-2-ol

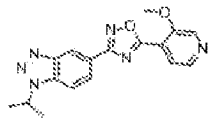
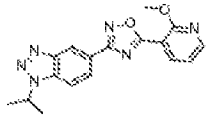
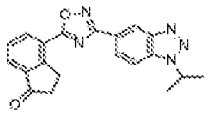
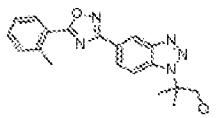
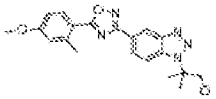
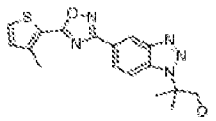
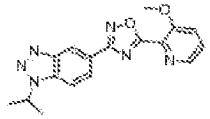
Structure	Compound Number	Chemical Name
	571	5-[5-(2-methyl-1H-1,3-benzodiazol-5-yl)-1,2,4- oxadiazol-3-yl]-1-(propan-2-yl)-1H-1,2,3-benzotriazole
	572	5-[5-(1-methyl-1H-1,3-benzodiazol-5-yl)-1,3,4- oxadiazol-2-yl]-2-[(propan-2-yl)amino]benzonitrile
	573	2-[(2,2-difluoroethyl)amino]-5-[5-(1-methyl-1H-1,3- benzodiazol-5-yl)-1,3,4-oxadiazol-2-yl]benzonitrile
	574	5-{5-[1-(2-hydroxyethyl)-1H-1,3-benzodiazol-5-yl]- 1,3,4-oxadiazol-2-yl}-2-[(propan-2-yl)amino]benzonitrile
	575	5-[2-(2-methoxyphenyl)-1,3-oxazol-4-yl]-1-(propan-2- yl)-1H-1,2,3-benzotriazole
	576	2-{3-[1-(propan-2-yl)-1H-1,2,3-benzotriazol-5-yl]- 1,2,4-oxadiazol-5-yl}aniline
	577	1-{5-[3-(1H-indol-7-yl)-1,2,4-oxadiazol-5-yl]-1H- 1,2,3-benzotriazol-1-yl}-2-methylpropan-2-ol

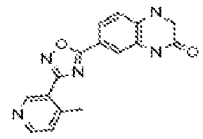
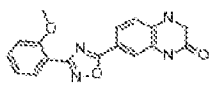
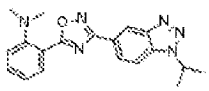
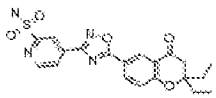
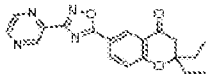
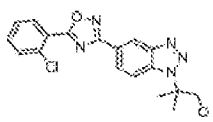
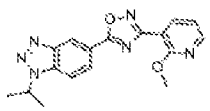
Structure	Compound Number	Chemical Name
	578	2-[(2,2-difluoroethyl)amino]-5-{5-[1-(2- hydroxyethyl)-1H-1,3-benzodiazol-5-yl]-1,3,4- oxadiazol-2-yl}benzonitrile
	579	5-[5-(1-methyl-1H-1,3-benzodiazol-6-yl)-1,3,4- oxadiazol-2-yl]-2-[(propan-2-yl)amino]benzonitrile
	580	2-[(2,2-difluoroethyl)amino]-5-[5-(1-methyl-1H-1,3- benzodiazol-6-yl)-1,3,4-oxadiazol-2-yl]benzonitrile
	581	[(4-{5-[1-(2-hydroxy-2-methylpropyl)-1H- 1,2,3-benzotriazol-5-yl]-1,2,4-oxadiazol-3- yl}phenyl)methyl]phosphonate
	582	N-{3-methoxy-4-[3-(pyridin-4-yl)-1,2,4-oxadiazol-5-yl]phenyl}acetamide
	583	diethyl [(4-{5-[1-(propan-2-yl)-1H-1,2,3- benzotriazol-5-yl]-1,2,4-oxadiazol-3-yl}phenyl)methyl]phosphonate
	584	N-{4-[5-(2,2-diethyl-4-oxo-3,4-dihydro-2H-1-benzopyran-6-yl)-1,2,4-oxadiazol-3-yl]-3-(trifluoromethoxy)phenyl}acetamide

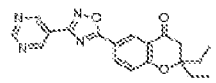
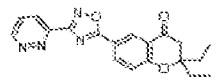
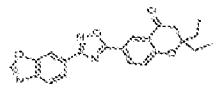
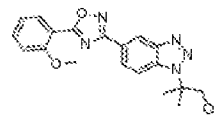
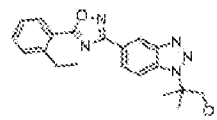
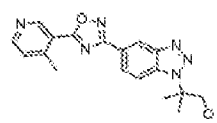
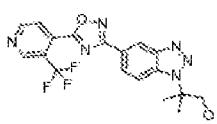
Structure	Compound Number	Chemical Name
	585	5-[5-(1H-1,3-benzodiazol-4-yl)-1,3,4-oxadiazol-2- yl]-2-[(propan-2-yl)amino]benzonitrile
	586	5-[5-(1H-1,3-benzodiazol-4-yl)-1,3,4-oxadiazol-2- yl]-2-[(2,2-difluoroethyl)amino]benzonitrile
	587	N-methyl-2-{2-[1-(propan-2-yl)-1H-1,2,3- benzotriazol-5-yl]-1,3-oxazol-4-yl}aniline
	588	2-ethyl-7-[3-(pyridin-3-yl)-1,2,4-oxadiazol-5-yl]- 3,4-dihydro-2H-1-benzopyran-4-one
	589	2-ethyl-7-[3-(pyridin-4-yl)-1,2,4-oxadiazol-5-yl]- 3,4-dihydro-2H-1-benzopyran-4-one
	590	1-{5-[3-(2,1,3-benzoxadiazol-5-yl)-1,2,4-oxadiazol-5- yl]-1H-1,2,3-benzotriazol-1-yl}-2-methylpropan-2- ol
	591	2,2-diethyl-6-(3-(thiophen-2-yl)-1,2,4-oxadiazol-5-yl)-2,3-dihydroquinolin-4(1H)-one

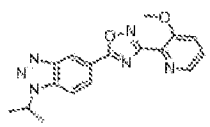
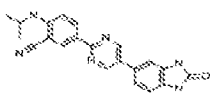
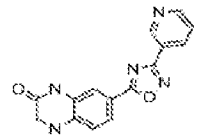
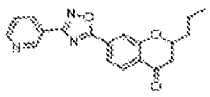
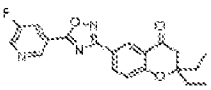
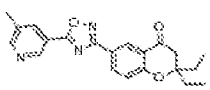
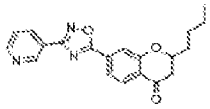
Structure	Compound Number	Chemical Name
	592	4-(5-(2,2-diethyl-4-oxochroman-6-yl)-1,2,4-oxadiazol-3-yl)-N-methylpicolinamide
	593	2-methyl-1-(5-(5-(o-tolyl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)propan-2-ol
	594	2,2-diethyl-6-(5-(2-methoxyphenyl)pyrimidin-2-yl)chroman-4-one
	595	2-isopropoxy-5-(5-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)pyrimidin-2-yl)benzonitrile
	596	5-(5-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)pyrimidin-2-yl)-2-(isopropylamino)benzonitrile
	597	2-methyl-1-{5-[3-(3-methylpyridin-4-yl)-1,2,4- oxadiazol-5-yl]-1H-1,2,3-benzotriazol-1-yl}propan-2-ol
	598	5-[5-(1H-1,3-benzodiazol-5-yl)-1,3,4-oxadiazol-2- yl]-2-(cyclopropylamino)benzonitrile

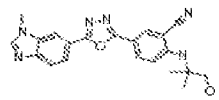
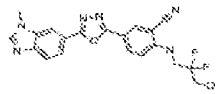
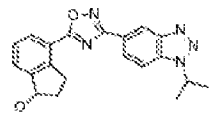
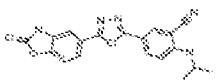
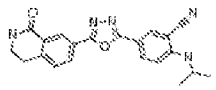
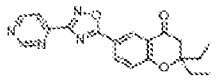
Structure	Compound Number	Chemical Name
	599	N-methyl-2-{3-[1-(propan-2-yl)-1H-1,2,3- benzotriazol-5-yl]-1,2,4-oxadiazol-5-yl}aniline
	600	5-[5-(1H-1,3-benzodiazol-5-yl)-1,3,4-oxadiazol-2- yl]-2-[(1,3-difluoropropan-2-yl)amino]benzonitrile
	601	5-[5-(2-methylphenyl)-1H-pyrrol-3-yl]-1-(propan-2- yl)-1H-1,2,3-benzotriazole
	602	2-{3-[1-(propan-2-yl)-1H-1,2,3-benzotriazol-5-yl]- 1,2,4-oxadiazol-5-yl}pyridin-3-ol
	603	5-(5-(2,2-diethyl-4-oxochroman-6-yl)-1,2,4-oxadiazol-3-yl)pyridine-3-sulfonamide
	604	2,2-diethyl-6-(3-(3-methoxythiophen-2-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one
	605	3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(4-methoxypyridin-3-yl)-1,2,4-oxadiazole

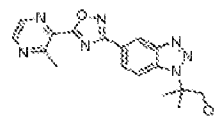
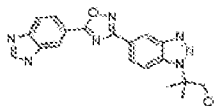
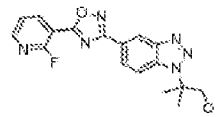
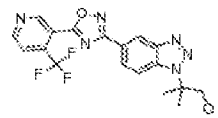
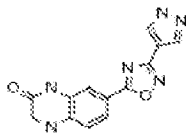
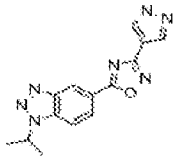
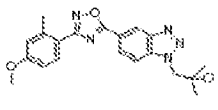
Structure	Compound Number	Chemical Name
	606	3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(3-methoxypyridin-4-yl)-1,2,4-oxadiazole
	607	3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(2-methoxypyridin-3-yl)-1,2,4-oxadiazole
	608	4-{3-[1-(propan-2-yl)-1H-1,2,3-benzotriazol-5-yl]- 1,2,4-oxadiazol-5-yl}-2,3-dihydro-1H-inden-1-one
	609	2-methyl-2-(5-(5-(o-tolyl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)propan-1-ol
	610	2-(5-(5-(4-methoxy-2-methylphenyl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)-2-methylpropan-1-ol
	611	2-methyl-2-(5-(5-(3-methylthiophen-2-yl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)propan-1-ol
	612	3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(3-methoxypyridin-2-yl)-1,2,4-oxadiazole

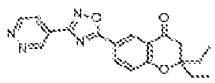
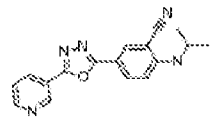
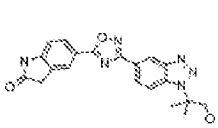
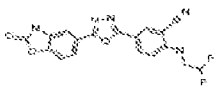
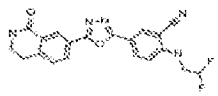
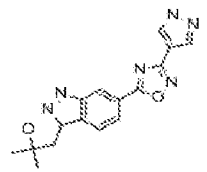
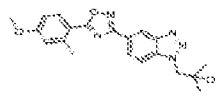
Structure	Compound Number	Chemical Name
	613	7-[3-(4-methylpyridin-3-yl)-1,2,4-oxadiazol-5-yl]- 1,2,3,4-tetrahydroquinoxalin-2-one
	614	7-[3-(2-methoxyphenyl)-1,2,4-oxadiazol-5-yl]- 1,2,3,4-tetrahydroquinoxalin-2-one
	615	N,N-dimethyl-2-{3-[1-(propan-2-yl)-1H-1,2,3- benzotriazol-5-yl]-1,2,4-oxadiazol-5-yl}aniline
	616	4-(5-(2,2-diethyl-4-oxochroman-6-yl)-1,2,4-oxadiazol-3-yl)pyridine-2-sulfonamide
	617	2,2-diethyl-6-(3-(pyrazin-2-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one
	618	2-(5-(5-(2-chlorophenyl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)-2-methylpropan-1-ol
	619	5-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-3-(2-methoxypyridin-3-yl)-1,2,4-oxadiazole

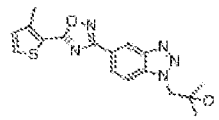
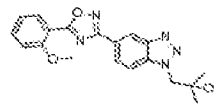
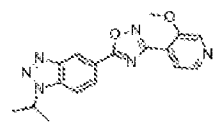
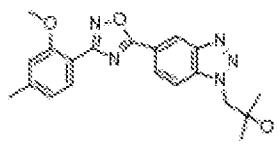
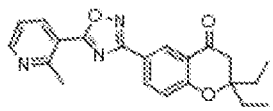
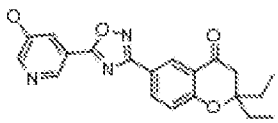
Structure	Compound Number	Chemical Name
	620	2,2-diethyl-6-(3-(pyrimidin-5-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one
	621	2,2-diethyl-6-(3-(pyridazin-3-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one
	622	6-(3-(benzo[d]oxazol-6-yl)-1,2,4-oxadiazol-5-yl)-2,2-diethylchroman-4-one
	623	2-(5-(5-(2-methoxyphenyl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)-2-methylpropan-1-ol
	624	2-(5-(5-(2-ethylphenyl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)-2-methylpropan-1-ol
	625	2-methyl-2-(5-(5-(4-methylpyridin-3-yl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)propan-1-ol
	626	2-methyl-2-(5-(5-(3-(trifluoromethyl)pyridin-4-yl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)propan-1-ol

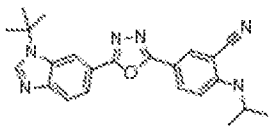
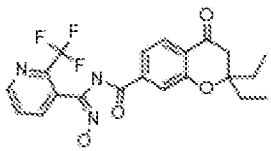
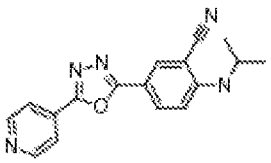
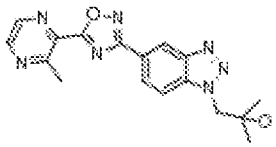
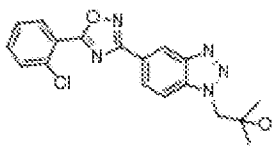
Structure	Compound Number	Chemical Name
	627	5-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-3-(3-methoxypyridin-2-yl)-1,2,4-oxadiazole
	628	2-(isopropylamino)-5-(5-(2-oxo-2,3-dihydro-1H-benzo[d]imidazol-5-yl)pyrimidin-2-yl)benzonitrile
	629	7-[3-(pyridin-3-yl)-1,2,4-oxadiazol-5-yl]-1,2,3,4- tetrahydroquinoxalin-2-one
	630	2-propyl-7-[3-(pyridin-3-yl)-1,2,4-oxadiazol-5-yl]- 3,4-dihydro-2H-1-benzopyran-4-one
	631	2,2-diethyl-6-[5-(5-fluoropyridin-3-yl)-1,2,4- oxadiazol-3-yl]-3,4-dihydro-2H-1-benzopyran-4-one
	632	2,2-diethyl-6-[5-(5-methylpyridin-3-yl)-1,2,4- oxadiazol-3-yl]-3,4-dihydro-2H-1-benzopyran-4-one
	633	2-butyl-7-[3-(pyridin-3-yl)-1,2,4-oxadiazol-5-yl]- 3,4-dihydro-2H-1-benzopyran-4-one

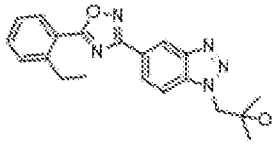
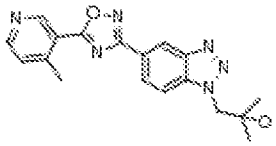
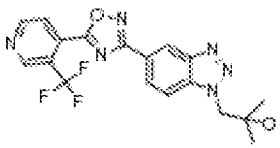
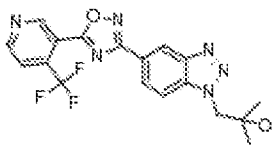
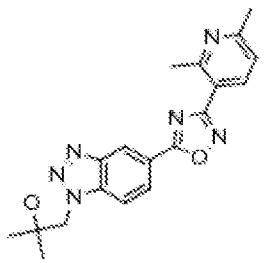
Structure	Compound Number	Chemical Name
	634	2-[(1-hydroxy-2-methylpropan-2-yl)amino]-5-[5-(1- methyl-1H-1,3-benzodiazol-6-yl)-1,3,4-oxadiazol-2- yl]benzonitrile
	635	2-[(2,2-difluoro-3-hydroxypropyl)amino]-5-[5-(1-methyl-1H-1,3-benzodiazol-6-yl)-1,3,4-oxadiazol-2- yl]benzonitrile
	636	4-{3-[1-(propan-2-yl)-1H-1,2,3-benzotriazol-5-yl]- 1,2,4-oxadiazol-5-yl}-2,3-dihydro-1H-inden-1-ol
	637	5-[5-(2-oxo-2,3-dihydro-1,3-benzoxazol-5-yl)-1,3,4- oxadiazol-2-yl]-2-[(propan-2-yl)amino]benzonitrile
	638	5-[5-(1-oxo-1,2,3,4-tetrahydroisoquinolin-7-yl)- 1,3,4-oxadiazol-2-yl]-2-[(propan-2-yl)amino]benzonitrile
	639	2,2-diethyl-6-(3-(pyrimidin-4-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one
	640	2,2-diethyl-6-(3-(pyrimidin-2-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one

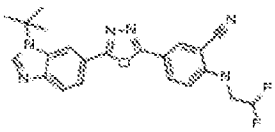
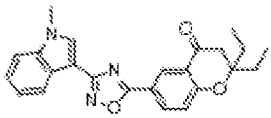
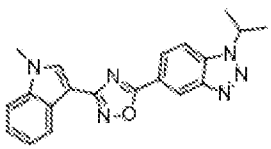
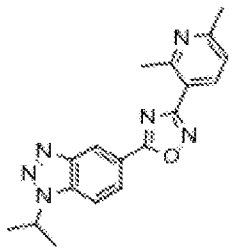
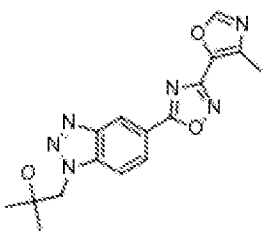
Structure	Compound Number	Chemical Name
	641	2-methyl-2-(5-(5-(3-methylpyrazin-2-yl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)propan-1-ol
	642	2-(5-(5-(1H-benzo[d]imidazol-6-yl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)-2-methylpropan-1-ol
	643	2-(5-(5-(2-fluoropyridin-3-yl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)-2-methylpropan-1-ol
	644	2-methyl-2-(5-(5-(4-(trifluoromethyl)pyridin-3-yl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)propan-1-ol
	645	7-[3-(1H-pyrazol-4-yl)-1,2,4-oxadiazol-5-yl]- 1,2,3,4-tetrahydroquinoxalin-2-one
	646	1-(propan-2-yl)-5-[3-(1H-pyrazol-4-yl)-1,2,4- oxadiazol-5-yl]-1H-1,2,3-benzotriazole
	647	1-{5-[3-(4-methoxy-2-methylphenyl)-1,2,4-oxadiazol-5-yl]-1H-1,2,3-benzotriazol-1-yl}-2-methylpropan-2- ol

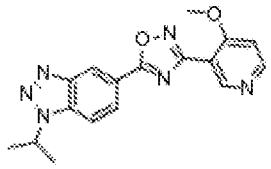
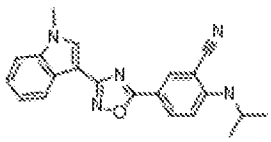
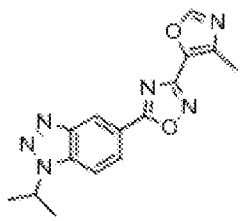
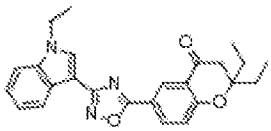
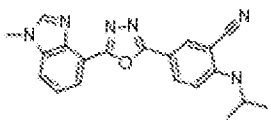
Structure	Compound Number	Chemical Name
	648	2,2-diethyl-6-(3-(pyridazin-4-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one
	649	2-(isopropylamino)-5-(5-(pyridin-3-yl)-1,3,4-oxadiazol-2-yl)benzonitrile
	650	5-(3-(1-(1-hydroxy-2-methylpropan-2-yl)-1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-oxadiazol-5-yl)indolin-2-one
	651	2-[(2,2-difluoroethyl)amino]-5-[5-(2-oxo-2,3- dihydro-1,3-benzoxazol-5-yl)-1,3,4-oxadiazol-2- yl]benzonitrile
	652	2-[(2,2-difluoroethyl)amino]-5-[5-(1-oxo-1,2,3,4-tetrahydroisoquinolin-7-yl)-1,3,4-oxadiazol-2- yl]benzonitrile
	653	2-methyl-1-{6-[3-(1H-pyrazol-4-yl)-1,2,4-oxadiazol-5- yl]-3H-indazol-3-yl}propan-2-ol
	654	1-(5-(5-(4-methoxy-2-methylphenyl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)-2-methylpropan-2-ol

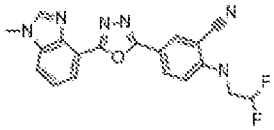
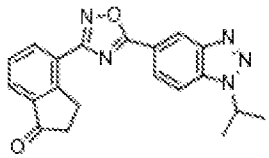
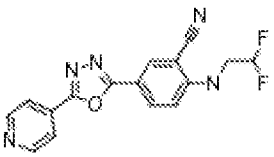
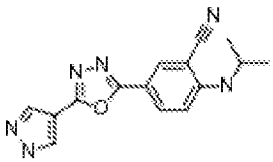
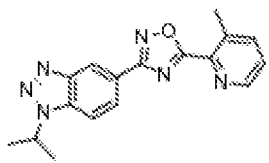
Structure	Compound Number	Chemical Name
	655	2-methyl-1-(5-(5-(3-methylthiophen-2-yl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)propan-2-ol
	656	1-(5-(5-(2-methoxyphenyl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)-2-methylpropan-2-ol
	657	5-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-3-(3-methoxypyridin-4-yl)-1,2,4-oxadiazole
	662	1-{5-[3-(2-methoxy-4-methylphenyl)-1,2,4-oxadiazol-5-yl]-1H-1,2,3-benzotriazol-1-yl}-2-methylpropan-2- ol
	663	2,2-diethyl-6-[5-(2-methylpyridin-3-yl)-1,2,4- oxadiazol-3-yl]-3,4-dihydro-2H-1-benzopyran-4-one
	664	2,2-diethyl-6-[5-(5-hydroxypyridin-3-yl)-1,2,4- oxadiazol-3-yl]-3,4-dihydro-2H-1-benzopyran-4-one

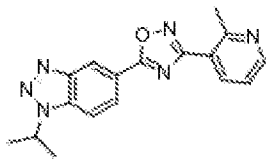
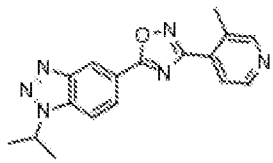
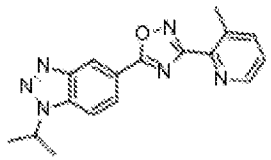
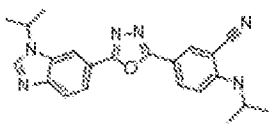
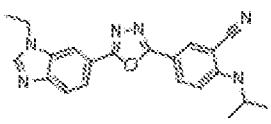
Structure	Compound Number	Chemical Name
	665	5-[5-(1-tert-butyl-1H-1,3-benzodiazol-6-yl)-1,3,4- oxadiazol-2-yl]-2-[(propan-2-yl)amino]benzonitrile
	666	2,2-diethyl-N-[(1E)-(hydroxyimino)[2-(trifluoromethyl)pyridin-3-yl]methyl]-4-oxo-3,4- dihydro-2H-1-benzopyran-7-carboxamide
	667	2-(isopropylamino)-5-(5-(pyridin-4-yl)-1,3,4-oxadiazol-2-yl)benzonitrile
	668	2-methyl-1-(5-(5-(3-methylpyrazin-2-yl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)propan-2-ol
	669	1-(5-(5-(2-chlorophenyl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)-2-methylpropan-2-ol

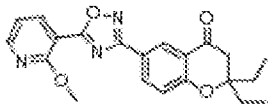
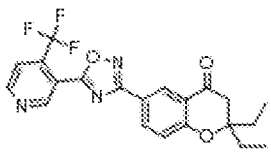
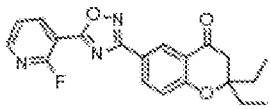
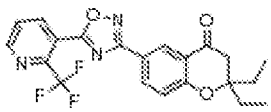
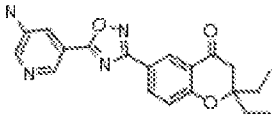
Structure	Compound Number	Chemical Name
	670	1-(5-(5-(2-ethylphenyl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)-2-methylpropan-2-ol
	671	2-methyl-1-(5-(5-(4-methylpyridin-3-yl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)propan-2-ol
	672	2-methyl-1-(5-(5-(3-(trifluoromethyl)pyridin-4-yl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)propan-2-ol
	673	2-methyl-1-(5-(5-(4-(trifluoromethyl)pyridin-3-yl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)propan-2-ol
	675	1-{5-[3-(2,6-dimethylpyridin-3-yl)-1,2,4-oxadiazol-5- yl]-1H-1,2,3-benzotriazol-1-yl}-2-methylpropan-2- ol

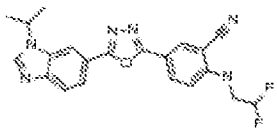
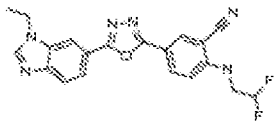
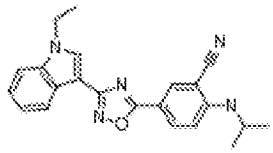
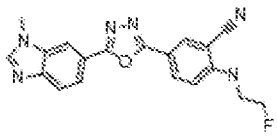
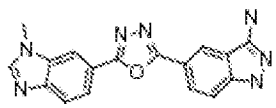
Structure	Compound Number	Chemical Name
	676	5-[5-(1-tert-butyl-1H-1,3-benzodiazol-6-yl)-1,3,4- oxadiazol-2-yl]-2-[(2,2-difluoroethyl)amino]benzonitrile
	677	2,2-diethyl-6-[3-(1-methyl-1H-indol-3-yl)-1,2,4-oxadiazol-5-yl]-3,4-dihydro-2H-1-benzopyran-4-one
	678	5-[3-(1-methyl-1H-indol-3-yl)-1,2,4-oxadiazol-5-yl]-1-(propan-2-yl)-1H-1,2,3-benzotriazole
	679	5-[3-(2,6-dimethylpyridin-3-yl)-1,2,4-oxadiazol-5- yl]-1-(propan-2-yl)-1H-1,2,3-benzotriazole
	680	2-methyl-1-{5-[3-(4-methyl-1,3-oxazol-5-yl)-1,2,4- oxadiazol-5-yl]-1H-1,2,3-benzotriazol-1-yl}propan-2- ol

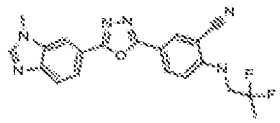
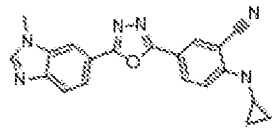
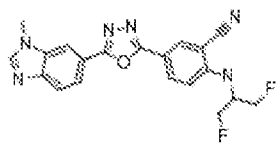
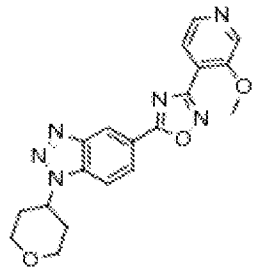
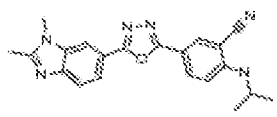
Structure	Compound Number	Chemical Name
	681	5-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-3-(4-methoxypyridin-3-yl)-1,2,4-oxadiazole
	682	5-[3-(1-methyl-1H-indol-3-yl)-1,2,4-oxadiazol-5-yl]-2-[(propan-2-yl)amino]benzonitrile
	683	5-[3-(4-methyl-1,3-oxazol-5-yl)-1,2,4-oxadiazol-5- yl]-1-(propan-2-yl)-1H-1,2,3-benzotriazole
	684	2,2-diethyl-6-[3-(1-ethyl-1H-indol-3-yl)-1,2,4-oxadiazol-5-yl]-3,4-dihydro-2H-1-benzopyran-4-one
	685	5-[5-(1-methyl-1H-1,3-benzodiazol-4-yl)-1,3,4- oxadiazol-2-yl]-2-[(propan-2-yl)amino]benzonitrile

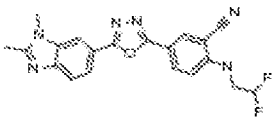
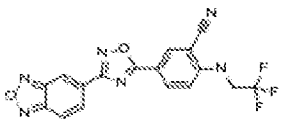
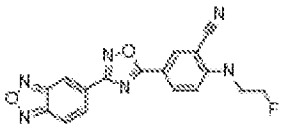
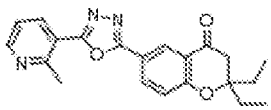
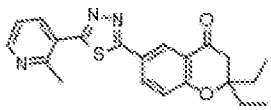
Structure	Compound Number	Chemical Name
	686	2-[(2,2-difluoroethyl)amino]-5-[5-(1-methyl-1H-1,3- benzodiazol-4-yl)-1,3,4-oxadiazol-2-yl]benzonitrile
	687	4-{5-[1-(propan-2-yl)-1H-1,2,3-benzotriazol-5-yl]- 1,2,4-oxadiazol-3-yl}-2,3-dihydro-1H-inden-1-one
	688	2-((2,2-difluoroethyl)amino)-5-(5-(pyridin-4-yl)-1,3,4-oxadiazol-2-yl)benzonitrile
	689	5-(5-(1H-pyrazol-4-yl)-1,3,4-oxadiazol-2-yl)-2-(isopropylamino)benzonitrile
	690	3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(3-methylpyridin-2-yl)-1,2,4-oxadiazole

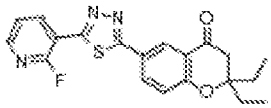
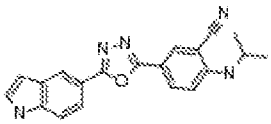
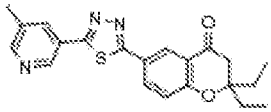
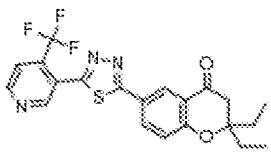
Structure	Compound Number	Chemical Name
	691	5-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-3-(2-methylpyridin-3-yl)-1,2,4-oxadiazole
	692	5-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-3-(3-methylpyridin-4-yl)-1,2,4-oxadiazole
	693	5-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-3-(3-methylpyridin-2-yl)-1,2,4-oxadiazole
	694	5-{5-[1-(propan-2-yl)-1H-1,3-benzodiazol-6-yl]- 1,3,4-oxadiazol-2-yl}-2-[(propan-2-yl)amino]benzonitrile
	695	5-[5-(1-ethyl-1H-1,3-benzodiazol-6-yl)-1,3,4- oxadiazol-2-yl]-2-[(propan-2-yl)amino]benzonitrile

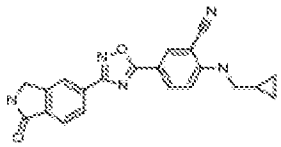
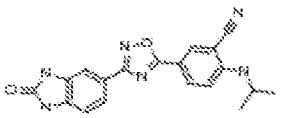
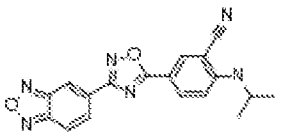
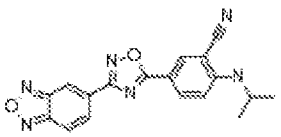
Structure	Compound Number	Chemical Name
	696	2,2-diethyl-6-[5-(2-methoxypyridin-3-yl)-1,2,4-oxadiazol-3-yl]-3,4-dihydro-2H-1-benzopyran-4-one
	697	2,2-diethyl-6-{5-[4-(trifluoromethyl)pyridin-3-yl]-1,2,4-oxadiazol-3-yl}-3,4-dihydro-2H-1-benzopyran-4- one
	698	2,2-diethyl-6-[5-(2-fluoropyridin-3-yl)-1,2,4- oxadiazol-3-yl]-3,4-dihydro-2H-1-benzopyran-4-one
	699	2,2-diethyl-6-{5-[2-(trifluoromethyl)pyridin-3-yl]-1,2,4-oxadiazol-3-yl}-3,4-dihydro-2H-1-benzopyran-4- one
	700	6-[5-(5-aminopyridin-3-yl)-1,2,4-oxadiazol-3-yl]- 2,2-diethyl-3,4-dihydro-2H-1-benzopyran-4-one

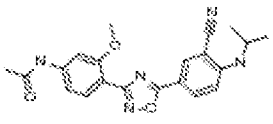
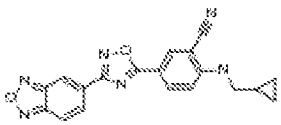
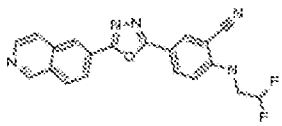
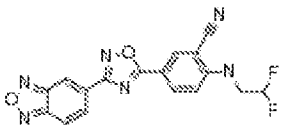
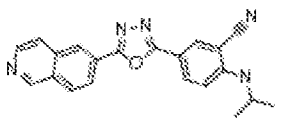
Structure	Compound Number	Chemical Name
	701	2-[(2,2-difluoroethyl)amino]-5-{5-[1-(propan-2-yl)- 1H-1,3-benzodiazol-6-yl]-1,3,4-oxadiazol-2- yl}benzonitrile
	702	2-[(2,2-difluoroethyl)amino]-5-[5-(1-ethyl-1H-1,3- benzodiazol-6-yl)-1,3,4-oxadiazol-2- yl]benzonitrile
	703	5-[3-(1-ethyl-1H-indol-3-yl)-1,2,4-oxadiazol-5-yl]-2-[(propan-2-yl)amino]benzonitrile
	704	2-[(2-fluoroethyl)amino]-5-[5-(1-methyl-1H-1,3- benzodiazol-6-yl)-1,3,4-oxadiazol-2- yl]benzonitrile
	705	5-[5-(1-methyl-1H-1,3-benzodiazol-6-yl)-1,3,4- oxadiazol-2-yl]-1H-indazol-3-amine

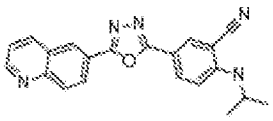
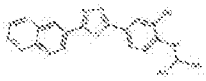
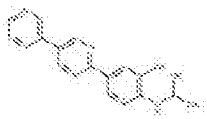
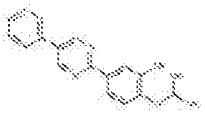
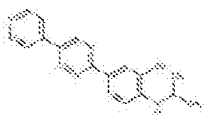
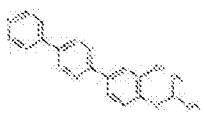
Structure	Compound Number	Chemical Name
	706	2-[(2,2-difluoropropyl)amino]-5-[5-(1-methyl-1H- 1,3-benzodiazol-6-yl)-1,3,4-oxadiazol-2-yl]benzonitrile
	707	2-(cyclopropylamino)-5-[5-(1-methyl-1H-1,3- benzodiazol-6-yl)-1,3,4-oxadiazol-2- yl]benzonitrile
	708	2-[(1,3-difluoropropan-2-yl)amino]-5-[5-(1-methyl- 1H-1,3-benzodiazol-6-yl)-1,3,4-oxadiazol-2- yl]benzonitrile
	709	5-[3-(3-methoxypyridin-4-yl)-1,2,4-oxadiazol-5-yl]-1- (oxan-4-yl)-1H-1,2,3-benzotriazole
	710	5-[5-(1,2-dimethyl-1H-1,3-benzodiazol-6-yl)-1,3,4- oxadiazol-2-yl]-2-[(propan-2-yl)amino]benzonitrile

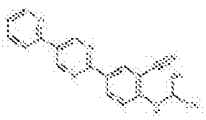
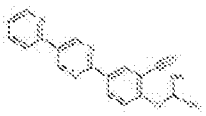
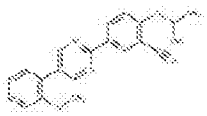
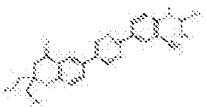
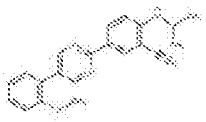
Structure	Compound Number	Chemical Name
	711	2-[(2,2-difluoroethyl)amino]-5-[5-(1,2-dimethyl-1H- 1,3-benzodiazol-6-yl)-1,3,4-oxadiazol-2-yl]benzonitrile
	712	5-[3-(2,1,3-benzoxadiazol-5-yl)-1,2,4-oxadiazol-5-yl]-2-[(2,2,2-trifluoroethyl)amino]benzonitrile
	713	5-[3-(2,1,3-benzoxadiazol-5-yl)-1,2,4-oxadiazol-5-yl]-2-[(2-fluoroethyl)amino]benzonitrile
	718	2,2-diethyl-6-(5-(2-methylpyridin-3-yl)-1,3,4-oxadiazol-2-yl)chroman-4-one
	719	2,2-diethyl-6-(5-(2-methylpyridin-3-yl)-1,3,4-thiadiazol-2-yl)chroman-4-one

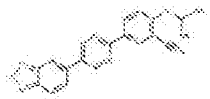
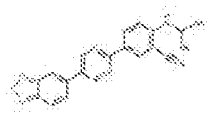
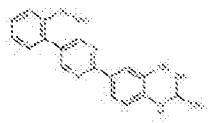
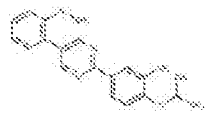
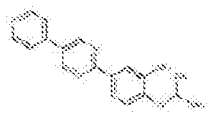
Structure	Compound Number	Chemical Name
	720	2,2-diethyl-6-(5-(2-fluoropyridin-3-yl)-1,3,4-thiadiazol-2-yl)chroman-4-one
	721	5-(5-(1H-indol-5-yl)-1,3,4-oxadiazol-2-yl)-2-(isopropylamino)benzonitrile
	724	2,2-diethyl-6-(5-(5-methylpyridin-3-yl)-1,3,4-thiadiazol-2-yl)chroman-4-one
	725	2,2-diethyl-6-(5-(4-(trifluoromethyl)pyridin-3-yl)-1,3,4-thiadiazol-2-yl)chroman-4-one
	726	2-(cyclopropylmethylamino)-5-[3-(2-oxo-3H-1,3-benzoxazol-6-yl)-1,2,4-oxadiazol-5-yl]benzonitrile

Structure	Compound Number	Chemical Name
	727	2-((cyclopropylmethyl)amino)-5-(3-(1-oxoisoindolin-5-yl)-1,2,4-oxadiazol-5-yl)benzonitrile
	728	2-(isopropylamino)-5-(3-(2-oxo-2,3-dihydro-1H-benzo[d]imidazol-5-yl)-1,2,4-oxadiazol-5-yl)benzonitrile
	729	2-((cyclopropylmethyl)amino)-5-(3-(2-oxo-2,3-dihydro-1H-benzo[d]imidazol-5-yl)-1,2,4-oxadiazol-5-yl)benzonitrile
	730	5-[3-(2,1,3-benzoxadiazol-5-yl)-1,2,4-oxadiazol-5-yl]-2-[(propan-2-yl)amino]benzonitrile
	730	5-[3-(2,1,3-benzoxadiazol-5-yl)-1,2,4-oxadiazol-5-yl]-2-[(propan-2-yl)amino]benzonitrile

Structure	Compound Number	Chemical Name
	731	N-[4-(5-{3-cyano-4-[(propan-2-yl)amino]phenyl}-1,2,4-oxadiazol-3-yl)-3-methoxyphenyl]acetamide
	732	5-[3-(2,1,3-benzoxadiazol-5-yl)-1,2,4-oxadiazol-5-yl]-2-[(2,2-difluoroethyl)amino]benzonitrile
	733	2-[(2,2-difluoroethyl)amino]-5-[5-(isoquinolin-6- yl)-1,3,4-oxadiazol-2-yl]benzonitrile
	734	5-[3-(2,1,3-benzoxadiazol-5-yl)-1,2,4-oxadiazol-5-yl]-2-[(cyclopropylmethyl)amino]benzonitrile
	735	5-[5-(isoquinolin-6-yl)-1,3,4-oxadiazol-2-yl]-2- [(propan-2-yl)amino]benzonitrile

Structure	Compound Number	Chemical Name
	736	2-[(propan-2-yl)amino]-5-[5-(quinolin-6-yl)-1,3,4- oxadiazol-2-yl]benzonitrile
	736	2-[(propan-2-yl)amino]-5-[5-(quinolin-6-yl)-1,3,4- oxadiazol-2-yl]benzonitrile
	737	2-(isopropylamino)-5-(5-(pyridin-3-yl)pyrimidin-2-yl)benzonitrile
	738	2-isopropoxy-5-(5-(pyridin-3-yl)pyrimidin-2-yl)benzonitrile
	739	2-(isopropylamino)-5-(5-(pyridin-4-yl)pyrimidin-2-yl)benzonitrile
	740	2-isopropoxy-5-(5-(pyridin-4-yl)pyrimidin-2-yl)benzonitrile

Structure	Compound Number	Chemical Name
	741	2-(isopropylamino)-5-(5-(pyridin-2-yl)pyrimidin-2-yl)benzonitrile
	742	2-isopropoxy-5-(5-(pyridin-2-yl)pyrimidin-2-yl)benzonitrile
	743	5-(5-(2-hydroxypyridin-4-yl)pyrimidin-2-yl)-2-(isopropylamino)benzonitrile
	744	5-(5-(2-hydroxypyridin-4-yl)pyrimidin-2-yl)-2-isopropoxybenzonitrile
	745	2-isopropoxy-5-(5-(2-methoxyphenyl)pyrimidin-2-yl)benzonitrile
	746	5-(5-(2,2-diethyl-4-oxochroman-6-yl)pyrimidin-2-yl)-2-(isopropylamino)benzonitrile
	747	2-(isopropylamino)-5-(5-(2-methoxyphenyl)pyrimidin-2-yl)benzonitrile

Structure	Compound Number	Chemical Name
	748	5-(5-(benzo[c][1,2,5]oxadiazol-5-yl)pyrimidin-2-yl)-2-isopropoxybenzonitrile
	749	5-(5-(benzo[c][1,2,5]oxadiazol-5-yl)pyrimidin-2-yl)-2-(isopropylamino)benzonitrile
	750	N-isopropyl-4-(5-(2-methoxyphenyl)pyrimidin-2-yl)-2-(trifluoromethyl)aniline
	751	2-(4-isopropoxy-3-(trifluoromethyl)phenyl)-5-(2-methoxyphenyl)pyrimidine
	752	2-(4-isopropoxy-3-(trifluoromethyl)phenyl)-5-(pyridin-4-yl)pyrimidine

Although the compounds described herein may be shown with specific stereochemistries around certain atoms, such as *cis* or *trans*, the compounds can also be made in the opposite orientation or in a racemic mixture. Such isomers or racemic mixtures are encompassed by the present disclosure. Additionally, although the compounds are shown collectively in a table, any

compounds, or a pharmaceutically acceptable salt thereof, can be chosen from the table and used in the embodiments provided for herein.

In some embodiments, pharmaceutical compositions comprising a compound or pharmaceutically salt thereof of any compound described herein are provided.

The compounds described herein can be made by can be made according to the methods described herein and in the examples. The methods described herein can be adapted based upon the compounds desired and described herien. In some embodiments, the method is made according to the following schemes, wherein Q and L are the substituents as shown and described herein and would be apparent to one of skill in the art based upon the present disclosure. In some embodiments, this method can be used to make one or more compounds as described herein and will be apparent to one of skill in the art which compounds can be made according to the methods described herein.

The conditions and temperatures can be varied, such as shown in the examples described herein. These schemes are non-limiting synthetic schemes and the synthetic routes can be modified as would be apparent to one of skill in the art reading the present specification. The compounds can also be prepared according to the schemes described in the Examples.

The compounds can be used to modulate the S_1P_1 receptor. Thus, in some embodiments, the compounds can be referred to as S_1P_1 receptor modulating compounds

Although the compounds in the tables above or in the examples section are shown with specific stereochemistries around certain atoms, such as *cis* or *trans*, the compounds can also be made in the opposite orientation or in a racemic mixture.

In some embodiments, the present embodiments provide pharmaceutical compositions comprising a compound or pharmaceutically salt thereof any compound described herein.

The compounds described herein can be made according to the methods described herein and in the examples. The methods described herein can be adapted based upon the compounds desired and described herien. In some embodiments, the method is made according to the following schemes, wherein Q and L are the substituents as shown and described herein and would be apparent to one of skill in the art based upon the present disclosure. In some embodiments, this method can be used to make one or more compounds as described herein and will be apparent to one of skill in the art which compounds can be made according to the methods described herein.

In some embodiments, the compounds are made according to schemes described in the examples. The schemes can be used to prepare the compounds and compositions described herein. The conditions and temperatures can be varied, or the synthesis can be performed according to the

examples described herein with modifications that are readily apparent based upon the compound being synthesized.

The conditions and temperatures can be varied, such as shown in the examples described herein. These schemes are non-limiting synthetic schemes and the synthetic routes can be modified as would be apparent to one of skill in the art reading the present specification.

The compounds described herein can be administered in any conventional manner by any route where they are active. Administration can be systemic, topical, or oral. For example, administration can be, but is not limited to, parenteral, subcutaneous, intravenous, intramuscular, intraperitoneal, transdermal, oral, buccal, sublingual, or ocular routes, or intravaginal, by inhalation, by depot injections, or by implants. The mode of administration can depend on the conditions or disease to be targeted or treated. The selection of the specific route of administration can be selected or adjusted by the clinician according to methods known to the clinician to obtain the desired clinical response.

In some embodiments, it may be desirable to administer one or more compounds, or a pharmaceutically acceptable salt thereof, locally to an area in need of treatment. This may be achieved, for example, and not by way of limitation, by local infusion during surgery, topical application, e.g., in conjunction with a wound dressing after surgery, by injection, by means of a catheter, by means of a suppository, or by means of an implant, wherein the implant is of a porous, non-porous, or gelatinous material, including membranes, such as sialastic membranes, or fibers.

The compounds described herein can be administered either alone or in combination (concurrently or serially) with other pharmaceuticals. For example, the compounds can be administered in combination with other analgesics, antidepressants, anti-anxiety compounds, anti-overactive bladder compounds, compounds for the treatment of cancer, and the like. Examples of other pharmaceuticals or medicaments are known to one of skill in the art and include, but are not limited to those described herein.

The means and methods for administration are known in the art and an artisan can refer to various pharmacologic references for guidance (see, for example, Modern Pharmaceutics, Banker & Rhodes, Marcel Dekker, Inc. (1979); and Goodman & Gilman's The Pharmaceutical Basis of Therapeutics, 6th Edition, MacMillan Publishing Co., New York (1980)).

The amount of compound to be administered is that amount which is therapeutically effective. The dosage to be administered will depend on the characteristics of the subject being treated, e.g., the particular animal treated, age, weight, health, types of concurrent treatment, if any,

and frequency of treatments, and can be easily determined by one of skill in the art (e.g., by the clinician). The standard dosing for protamine can be used and adjusted (i.e., increased or decreased) depending upon the factors described above. The selection of the specific dose regimen can be selected or adjusted or titrated by the clinician according to methods known to the clinician to obtain the desired clinical response.

The amount of a compound described herein that will be effective in the treatment and/or prevention of a particular disease, condition, or disorder will depend on the nature and extent of the disease, condition, or disorder, and can be determined by standard clinical techniques. In addition, *in vitro* or *in vivo* assays may optionally be employed to help identify optimal dosage ranges. The precise dose to be employed in the compositions will also depend on the route of administration, and the seriousness of the disorder, and should be decided according to the judgment of the practitioner and each patient's circumstances. However, a suitable dosage range for oral administration is, generally, from about 0.001 milligram to about 200 milligrams per kilogram body weight, from about 0.01 milligram to about 100 milligrams per kilogram body weight, from about 0.01 milligram to about 70 milligrams per kilogram body weight, from about 0.1 milligram to about 50 milligrams per kilogram body weight, from 0.5 milligram to about 20 milligrams per kilogram body weight, or from about 1 milligram to about 10 milligrams per kilogram body weight. In some embodiments, the oral dose is about 5 milligrams per kilogram body weight.

In some embodiments, suitable dosage ranges for intravenous (i.v.) administration are from about 0.01 mg to about 500 mg per kg body weight, from about 0.1 mg to about 100 mg per kg body weight, from about 1 mg to about 50 mg per kg body weight, or from about 10 mg to about 35 mg per kg body weight. Suitable dosage ranges for other modes of administration can be calculated based on the forgoing dosages as known by those skilled in the art. For example, recommended dosages for intranasal, transmucosal, intradermal, intramuscular, intraperitoneal, subcutaneous, epidural, sublingual, intracerebral, intravaginal, transdermal administration or administration by inhalation are in the range of from about 0.001 mg to about 200 mg per kg of body weight, from about 0.01 mg to about 100 mg per kg of body weight, from about 0.1 mg to about 50 mg per kg of body weight, or from about 1 mg to about 20 mg per kg of body weight. Effective doses may be extrapolated from dose-response curves derived from *in vitro* or animal model test systems. Such animal models and systems are well known in the art.

The compounds described herein can be formulated for parenteral administration by injection, such as by bolus injection or continuous infusion. The compounds can be administered by

continuous infusion subcutaneously over a period of about 15 minutes to about 24 hours. Formulations for injection can be presented in unit dosage form, such as in ampoules or in multi-dose containers, with an optionally added preservative. The compositions can take such forms as suspensions, solutions or emulsions in oily or aqueous vehicles, and can contain formulatory agents such as suspending, stabilizing and/or dispersing agents. In some embodiments, the injectable is in the form of short-acting, depot, or implant and pellet forms injected subcutaneously or intramuscularly. In some embodiments, the parenteral dosage form is the form of a solution, suspension, emulsion, or dry powder.

For oral administration, the compounds described herein can be formulated by combining the compounds with pharmaceutically acceptable carriers well known in the art. Such carriers enable the compounds to be formulated as tablets, pills, dragees, capsules, emulsions, liquids, gels, syrups, caches, pellets, powders, granules, slurries, lozenges, aqueous or oily suspensions, and the like, for oral ingestion by a patient to be treated. Pharmaceutical preparations for oral use can be obtained by, for example, adding a solid excipient, optionally grinding the resulting mixture, and processing the mixture of granules, after adding suitable auxiliaries, if desired, to obtain tablets or dragee cores. Suitable excipients include, but are not limited to, fillers such as sugars, including, but not limited to, lactose, sucrose, mannitol, and sorbitol; cellulose preparations such as, but not limited to, maize starch, wheat starch, rice starch, potato starch, gelatin, gum tragacanth, methyl cellulose, hydroxypropylmethyl-cellulose, sodium carboxymethylcellulose, and polyvinylpyrrolidone (PVP). If desired, disintegrating agents can be added, such as, but not limited to, the cross-linked polyvinyl pyrrolidone, agar, or alginic acid or a salt thereof such as sodium alginate.

Orally administered compositions can contain one or more optional agents, for example, sweetening agents such as fructose, aspartame or saccharin; flavoring agents such as peppermint, oil of wintergreen, or cherry; coloring agents; and preserving agents, to provide a pharmaceutically palatable preparation. Moreover, where in tablet or pill form, the compositions may be coated to delay disintegration and absorption in the gastrointestinal tract thereby providing a sustained action over an extended period of time. Selectively permeable membranes surrounding an osmotically active driving compound are also suitable for orally administered compounds. Oral compositions can include standard vehicles such as mannitol, lactose, starch, magnesium stearate, sodium saccharine, cellulose, magnesium carbonate, etc. Such vehicles are suitably of pharmaceutical grade.

Dragee cores can be provided with suitable coatings. For this purpose, concentrated sugar solutions can be used, which can optionally contain gum arabic, talc, polyvinyl pyrrolidone, carbopol

gel, polyethylene glycol, and/or titanium dioxide, lacquer solutions, and suitable organic solvents or solvent mixtures. Dyestuffs or pigments can be added to the tablets or dragee coatings for identification or to characterize different combinations of active compound doses.

Pharmaceutical preparations which can be used orally include, but are not limited to, push-fit capsules made of gelatin, as well as soft, sealed capsules made of gelatin and a plasticizer, such as glycerol or sorbitol. The push-fit capsules can contain the active ingredients in admixture with filler such as lactose, binders such as starches, and/or lubricants such as talc or magnesium stearate and, optionally, stabilizers. In soft capsules, the active compounds can be dissolved or suspended in suitable liquids, such as fatty oils, liquid paraffin, or liquid polyethylene glycols. In addition, stabilizers can be added.

For buccal administration, the compositions can take the form of, such as, tablets or lozenges formulated in a conventional manner.

For administration by inhalation, the compounds described herein can be delivered in the form of an aerosol spray presentation from pressurized packs or a nebulizer, with the use of a suitable propellant, such as dichlorodifluoromethane, trichlorofluoromethane, dichlorotetrafluoroethane, carbon dioxide or other suitable gas. In the case of a pressurized aerosol the dosage unit can be determined by providing a valve to deliver a metered amount. Capsules and cartridges of, such as gelatin for use in an inhaler or insufflator can be formulated containing a powder mix of the compound and a suitable powder base such as lactose or starch.

The compounds described herein can also be formulated in rectal compositions such as suppositories or retention enemas, such as containing conventional suppository bases such as cocoa butter or other glycerides. The compounds described herein can also be formulated in vaginal compositions such as vaginal creams, suppositories, pessaries, vaginal rings, and intrauterine devices.

In transdermal administration, the compounds can be applied to a plaster, or can be applied by transdermal, therapeutic systems that are consequently supplied to the organism. In some embodiments, the compounds are present in creams, solutions, powders, fluid emulsions, fluid suspensions, semi-solids, ointments, pastes, gels, jellies, and foams, or in patches containing any of the same.

The compounds described herein can also be formulated as a depot preparation. Such long acting formulations can be administered by implantation (for example subcutaneously or intramuscularly) or by intramuscular injection. Depot injections can be administered at about 1 to

about 6 months or longer intervals. Thus, for example, the compounds can be formulated with suitable polymeric or hydrophobic materials (for example as an emulsion in an acceptable oil) or ion exchange resins, or as sparingly soluble derivatives, for example, as a sparingly soluble salt.

In some embodiments, the compounds can be delivered in a controlled release system. In one embodiment, a pump may be used (see Langer, supra; Sefton, CRC Crit. Ref. Biomed. Eng., 1987, 14, 201; Buchwald et al., Surgery, 1980, 88, 507 Saudek et al., N. Engl. J. Med., 1989, 321, 574). In some embodiments, polymeric materials can be used (see Medical Applications of Controlled Release, Langer and Wise (eds.), CRC Pres., Boca Raton, Fla. (1974); Controlled Drug Bioavailability, Drug Product Design and Performance, Smolen and Ball (eds.), Wiley, New York (1984); Ranger et al., J. Macromol. Sci. Rev. Macromol. Chem., 1983, 23, 61; see, also Levy et al., Science, 1985, 228, 190; During et al., Ann. Neurol., 1989, 25, 351; Howard et al., J. Neurosurg., 1989, 71, 105). In yet another embodiment, a controlled-release system can be placed in proximity of the target of the compounds described herein, such as the liver, thus requiring only a fraction of the systemic dose (see, e.g., Goodson, in Medical Applications of Controlled Release, supra, vol. 2, pp. 115-138 (1984)). Other controlled-release systems discussed in the review by Langer, Science, 1990, 249, 1527-1533) may be used.

It is also known in the art that the compounds can be contained in such formulations with pharmaceutically acceptable diluents, fillers, disintegrants, binders, lubricants, surfactants, hydrophobic vehicles, water soluble vehicles, emulsifiers, buffers, humectants, moisturizers, solubilizers, preservatives and the like. The pharmaceutical compositions can also comprise suitable solid or gel phase carriers or excipients. Examples of such carriers or excipients include, but are not limited to, calcium carbonate, calcium phosphate, various sugars, starches, cellulose derivatives, gelatin, and polymers such as polyethylene glycols. In some embodiments, the compounds described herein can be used with agents including, but not limited to, topical analgesics (e.g., lidocaine), barrier devices (e.g., GelClair), or rinses (e.g., Caphosol).

In some embodiments, the compounds described herein can be delivered in a vesicle, in particular a liposome (see, Langer, Science, 1990, 249, 1527-1533; Treat et al., in Liposomes in the Therapy of Infectious Disease and Cancer, Lopez-Berestein and Fidler (eds.), Liss, New York, pp. 353-365 (1989); Lopez-Berestein, ibid., pp. 317-327; see generally ibid.).

Suitable compositions include, but are not limited to, oral non-absorbed compositions. Suitable compositions also include, but are not limited to saline, water, cyclodextrin solutions, and buffered solutions of pH 3-9.

The compounds described herein, or pharmaceutically acceptable salts thereof, can be formulated with numerous excipients including, but not limited to, purified water, propylene glycol, PEG 400, glycerin, DMA, ethanol, benzyl alcohol, citric acid/sodium citrate (pH3), citric acid/sodium citrate (pH5), tris(hydroxymethyl)amino methane HCl (pH7.0), 0.9% saline, and 1.2% saline, and any combination thereof. In some embodiments, excipient is chosen from propylene glycol, purified water, and glycerin.

In some embodiments, the formulation can be lyophilized to a solid and reconstituted with, for example, water prior to use.

When administered to a mammal (e.g., to an animal for veterinary use or to a human for clinical use) the compounds can be administered in isolated form.

When administered to a human, the compounds can be sterile. Water is a suitable carrier when the compound of Formula I is administered intravenously. Saline solutions and aqueous dextrose and glycerol solutions can also be employed as liquid carriers, particularly for injectable solutions. Suitable pharmaceutical carriers also include excipients such as starch, glucose, lactose, sucrose, gelatin, malt, rice, flour, chalk, silica gel, sodium stearate, glycerol monostearate, talc, sodium chloride, dried skim milk, glycerol, propylene, glycol, water, ethanol and the like. The present compositions, if desired, can also contain minor amounts of wetting or emulsifying agents, or pH buffering agents.

The compositions described herein can take the form of a solution, suspension, emulsion, tablet, pill, pellet, capsule, capsule containing a liquid, powder, sustained-release formulation, suppository, aerosol, spray, or any other form suitable for use. Examples of suitable pharmaceutical carriers are described in Remington's Pharmaceutical Sciences, A.R. Gennaro (Editor) Mack Publishing Co.

In some embodiments, the compounds are formulated in accordance with routine procedures as a pharmaceutical composition adapted for administration to humans. Typically, compounds are solutions in sterile isotonic aqueous buffer. Where necessary, the compositions can also include a solubilizing agent. Compositions for intravenous administration may optionally include a local anesthetic such as lidocaine to ease pain at the site of the injection. Generally, the ingredients are supplied either separately or mixed together in unit dosage form, for example, as a dry lyophilized powder or water free concentrate in a hermetically sealed container such as an ampoule or sachette indicating the quantity of active agent. Where the compound is to be administered by infusion, it can be dispensed, for example, with an infusion bottle containing sterile pharmaceutical grade water or

saline. Where the compound is administered by injection, an ampoule of sterile water for injection or saline can be provided so that the ingredients may be mixed prior to administration.

The pharmaceutical compositions can be in unit dosage form. In such form, the composition can be divided into unit doses containing appropriate quantities of the active component. The unit dosage form can be a packaged preparation, the package containing discrete quantities of the preparations, for example, packeted tablets, capsules, and powders in vials or ampules. The unit dosage form can also be a capsule, cachet, or tablet itself, or it can be the appropriate number of any of these packaged forms.

In some embodiments, a composition is in the form of a liquid wherein the active agent (i.e., one of the facially amphiphilic polymers or oligomers disclosed herein) is present in solution, in suspension, as an emulsion, or as a solution/suspension. In some embodiments, the liquid composition is in the form of a gel. In other embodiments, the liquid composition is aqueous. In other embodiments, the composition is in the form of an ointment.

In some embodiments, the composition is in the form of a solid article. For example, in some embodiments, the ophthalmic composition is a solid article that can be inserted in a suitable location in the eye, such as between the eye and eyelid or in the conjunctival sac, where it releases the active agent as described, for example, U.S. Pat. No. 3,863,633; U.S. Pat. No. 3,867,519; U.S. Pat. No. 3,868,445; U.S. Pat. No. 3,960,150; U.S. Pat. No. 3,963,025; U.S. Pat. No. 4,186,184; U.S. Pat. No. 4,303,637; U.S. Pat. No. 5,443,505; and U.S. Pat. No. 5,869,079. Release from such an article is usually to the cornea, either via the lacrimal fluid that bathes the surface of the cornea, or directly to the cornea itself, with which the solid article is generally in intimate contact. Solid articles suitable for implantation in the eye in such fashion are generally composed primarily of polymers and can be bioerodible or non-bioerodible. Bioerodible polymers that can be used in the preparation of ocular implants carrying one or more of compounds include, but are not limited to, aliphatic polyesters such as polymers and copolymers of poly(glycolide), poly(lactide), poly(epsilon-caprolactone), poly-(hydroxybutyrate) and poly(hydroxyvalerate), polyamino acids, polyorthoesters, polyanhydrides, aliphatic polycarbonates and polyether lactones. Suitable non-bioerodible polymers include silicone elastomers.

The compositions described herein can contain preservatives. Suitable preservatives include, but are not limited to, mercury-containing substances such as phenylmercuric salts (e.g., phenylmercuric acetate, borate and nitrate) and thimerosal; stabilized chlorine dioxide; quaternary ammonium compounds such as benzalkonium chloride, cetyltrimethylammonium bromide and

cetylpyridinium chloride; imidazolidinyl urea; parabens such as methylparaben, ethylparaben, propylparaben and butylparaben, and salts thereof; phenoxyethanol; chlorophenoxyethanol; phenoxypropanol; chlorobutanol; chlorocresol; phenylethyl alcohol; disodium EDTA; and sorbic acid and salts thereof.

Optionally one or more stabilizers can be included in the compositions to enhance chemical stability where required. Suitable stabilizers include, but are not limited to, chelating agents or complexing agents, such as, for example, the calcium complexing agent ethylene diamine tetraacetic acid (EDTA). For example, an appropriate amount of EDTA or a salt thereof, e.g., the disodium salt, can be included in the composition to complex excess calcium ions and prevent gel formation during storage. EDTA or a salt thereof can suitably be included in an amount of about 0.01% to about 0.5%. In those embodiments containing a preservative other than EDTA, the EDTA or a salt thereof, more particularly disodium EDTA, can be present in an amount of about 0.025% to about 0.1% by weight.

One or more antioxidants can also be included in the compositions. Suitable antioxidants include, but are not limited to, ascorbic acid, sodium metabisulfite, sodium bisulfite, acetylcysteine, polyquaternium-1, benzalkonium chloride, thimerosal, chlorobutanol, methyl paraben, propyl paraben, phenylethyl alcohol, edetate disodium, sorbic acid, or other agents know to those of skill in the art. Such preservatives are typically employed at a level of from about 0.001% to about 1.0% by weight.

In some embodiments, the compounds are solubilized at least in part by an acceptable solubilizing agent. Certain acceptable nonionic surfactants, for example polysorbate 80, can be useful as solubilizing agents, as can ophthalmically acceptable glycols, polyglycols, e.g., polyethylene glycol 400 (PEG-400), and glycol ethers.

Suitable solubilizing agents for solution and solution/suspension compositions are cyclodextrins. Suitable cyclodextrins can be chosen from α-cyclodextrin, β-cyclodextrin, γ-cyclodextrin, alkylcyclodextrins (e.g., methyl-β-cyclodextrin, dimethyl-β-cyclodextrin, diethyl-β-cyclodextrin), hydroxyalkylcyclodextrins (e.g., hydroxyethyl-β-cyclodextrin, hydroxypropyl-β-cyclodextrin), carboxy-alkylcyclodextrins (e.g., carboxymethyl-β-cyclodextrin), sulfoalkylether cyclodextrins (e.g., sulfobutylether-β-cyclodextrin), and the like. Ophthalmic applications of cyclodextrins have been reviewed in Rajewski et al., Journal of Pharmaceutical Sciences, 1996, 85, 1155-1159.

In some embodiments, the composition optionally contains a suspending agent. For example, in those embodiments in which the composition is an aqueous suspension or

solution/suspension, the composition can contain one or more polymers as suspending agents. Useful polymers include, but are not limited to, water-soluble polymers such as cellulosic polymers, for example, hydroxypropyl methylcellulose, and water-insoluble polymers such as cross-linked carboxyl-containing polymers.

One or more acceptable pH adjusting agents and/or buffering agents can be included in the compositions, including acids such as acetic, boric, citric, lactic, phosphoric and hydrochloric acids; bases such as sodium hydroxide, sodium phosphate, sodium borate, sodium citrate, sodium acetate, sodium lactate and tris-hydroxymethylaminomethane; and buffers such as citrate/dextrose, sodium bicarbonate and ammonium chloride. Such acids, bases and buffers are included in an amount required to maintain pH of the composition in an acceptable range.

One or more acceptable salts can be included in the compositions in an amount required to bring osmolality of the composition into an acceptable range. Such salts include, but are not limited to, those having sodium, potassium or ammonium cations and chloride, citrate, ascorbate, borate, phosphate, bicarbonate, sulfate, thiosulfate or bisulfite anions. In some embodiments, salts include sodium chloride, potassium chloride, sodium thiosulfate, sodium bisulfite and ammonium sulfate. In some embodiments, the salt is sodium chloride.

Optionally one or more acceptable surfactants, preferably nonionic surfactants, or co-solvents can be included in the compositions to enhance solubility of the components of the compositions or to impart physical stability, or for other purposes. Suitable nonionic surfactants include, but are not limited to, polyoxyethylene fatty acid glycerides and vegetable oils, e.g., polyoxyethylene (60) hydrogenated castor oil; and polyoxyethylene alkylethers and alkylphenyl ethers, e.g., octoxynol 10, octoxynol 40; polysorbate 20, 60 and 80; polyoxyethylene/polyoxypropylene surfactants (e.g., Pluronic® F-68, F84 and P-103); cyclodextrin; or other agents known to those of skill in the art. Typically, such co-solvents or surfactants are employed in the compositions at a level of from about 0.01% to about 2% by weight.

In some embodiments, pharmaceutical packs or kits comprising one or more containers filled with one or more compounds described herein are provided. Optionally associated with such container(s) can be a notice in the form prescribed by a governmental agency regulating the manufacture, use or sale of pharmaceuticals or biological products, which notice reflects approval by the agency of manufacture, use or sale for human administration for treating a condition, disease, or disorder described herein. In some embodiments, the kit contains more than one compound described

herein. In some embodiments, the kit comprises a compound described herein in a single injectable dosage form, such as a single dose within an injectable device such as a syringe with a needle.

Modulation of the S_1P_1 receptor has been found to be a target for the treatment of certain disoders. The compounds described herien can be used in the preparation of a medicament or pharmaceutical composition to treat and/or prevent neuropathy, pain, inflammatory pain, cancer pain, bone cancer pain, tumor pain, pain or neuropathy resulting from disorders of the central or peripheral nervous system, neuropathic pain, pain associated with dysesthesia, allodynia or hypersensitivity, chemotherapy induced neuropathic pain, chemotherapy induced peripheral neuropathy, diabetic neuropathy or pain associated with diabetic neuropathy, post herpetic neuralgia or pain associated with post herpetic neuralgia, hiv-related neuropathy or pain associated with hiv-related neuropathy, pain or neuropathy resulting from spinal cord injury, nerve lesions, tissue injury, ms, stroke, nutritional deficiencies, or toxins, fibromyalgia or pain associated with fibromyalgia, phantom limb pain, complex regional pain syndrome, carpal tunnel syndrome, sciatica, pudendal neuralgia, back or neck pain, including those resulting from degenerative disk disease, trigeminal neuralgia, headache disorders including, but not limited to migraine and cluster headache, orofacial pain, odontalgia, temporomandibular joint pain, endometrial pain, osteoarthritis, rheumatoid arthritis, atypical odontalgia, interstitial cystitis, uveitis, or any combination thereof.

Embodiments disclosed herein also provide for the compounds for the use of treating or preventing neuropathy, pain, inflammatory pain, cancer pain, bone cancer pain, tumor pain, pain or neuropathy resulting from disorders of the central or peripheral nervous system, neuropathic pain, pain associated with dysesthesia, allodynia or hypersensitivity, chemotherapy induced neuropathic pain, chemotherapy induced peripheral neuropathy, diabetic neuropathy or pain associated with diabetic neuropathy, post herpetic neuralgia or pain associated with post herpetic neuralgia, hiv-related neuropathy or pain associated with hiv-related neuropathy, pain or neuropathy resulting from spinal cord injury, nerve lesions, tissue injury, ms, stroke, nutritional deficiencies, or toxins, fibromyalgia or pain associated with fibromyalgia, phantom limb pain, complex regional pain syndrome, carpal tunnel syndrome, sciatica, pudendal neuralgia, back or neck pain, including those resulting from degenerative disk disease, trigeminal neuralgia, headache disorders including, but not limited to migraine and cluster headache, orofacial pain, odontalgia, temporomandibular joint pain, endometrial pain, osteoarthritis, rheumatoid arthritis, atypical odontalgia, interstitial cystitis, uveitis, or any combination thereof.

In some embodiments, methods of treating and/or preventing neuropathy, pain, inflammatory pain, cancer pain, bone cancer pain, tumor pain, pain or neuropathy resulting from disorders of the central or peripheral nervous system, neuropathic pain, pain associated with dysesthesia, allodynia or hypersensitivity, chemotherapy induced neuropathic pain, chemotherapy induced peripheral neuropathy, diabetic neuropathy or pain associated with diabetic neuropathy, post herpetic neuralgia or pain associated with post herpetic neuralgia, hiv-related neuropathy or pain associated with hiv-related neuropathy, pain or neuropathy resulting from spinal cord injury, nerve lesions, tissue injury, ms, stroke, nutritional deficiencies, or toxins, fibromyalgia or pain associated with fibromyalgia, phantom limb pain, complex regional pain syndrome, carpal tunnel syndrome, sciatica, pudendal neuralgia, back or neck pain, including those resulting from degenerative disk disease, trigeminal neuralgia, headache disorders including, but not limited to migraine and cluster headache, orofacial pain, odontalgia, temporomandibular joint pain, endometrial pain, osteoarthritis, rheumatoid arthritis, atypical odontalgia, interstitial cystitis, uveitis, or any combination thereof. In some embodiments, the methods comprise administering one or more of the compounds described herein, or pharmaceutically acceptable salts thereof, to the subject to treat or prevent such conditions. In some embodiments, the condition is CINP and CIPN, or other types of neuropathic pain or neuropathy. In some embodiments, the methods are performed without causing significant lymphopenia or immunosuppression. In some embodiments, the methods are performed without causing lymphopenia or immunosuppression.

In some embodiments, the compounds, or pharmaceutically acceptable salts thereof, are administered to the subject for any condition or indication provided for herein without causing significant lymphopenia or immunosuppression. In some embodiments, the methods are performed without causing lymphopenia or immunosuppression.

In some embodiments, the methods comprise administering to the subject one or more compounds described herein or a pharmaceutically acceptable salt thereof, or a pharmaceutical composition of the same. In some embodiments, the subject is a subject in need of such treatment. As described herein, in some embodiments, the subject is a mammal, such as, but not limited to, a human.

In some embodiments, also provided are one or more compounds described above, or a pharmaceutically acceptable salt thereof, or a pharmaceutical composition comprising one or more compounds described above, for use in the manufacture of a medicament for the treatment of methods of treating and/or preventing pain, including, but not limited to the conditions described

herein, in a subject, such as those described herein. In some embodiments, the subject is a subject in need thereof.

The present embodiments also provides the use of one or more compounds described above, or a pharmaceutically acceptable salt thereof, or a pharmaceutical composition comprising one or more compounds described above, in the modulation of a S_1P_1 receptor activity, such as the presence on the surface of the cell. In some embodiments, the compounds, pharmaceutically acceptable salt thereof, or a pharmaceutical composition of the same modulate the internalization, trafficking, and/or degradation of the S_1P_1 receptor. In some embodiments, the compounds, pharmaceutically acceptable salt thereof, or a pharmaceutical composition of the same modulate the G-protein modulated pathway of the S_1P_1 receptor.

As used herein, "modulation" can refer to either inhibition or enhancement of a specific activity. For example, the modulation of the S_1P_1 receptor can refer to the inhibition and/or activation of the G-protein mediated pathway of the S_1P_1 receptor. In some embodiments, the modulation refers to the inhibition or activation of the β-arrestin mediated pathway of the S_1P_1 receptor. In some embodiments, the modulation refers to the inhibition or activation of the internalization of the S_1P_1 receptor. The activity of a S_1P_1 receptor can be measured by any method including but not limited to the methods described herein.

The compounds described herien are agonists or antagonists of the S_1P_1 receptor. The ability of the compounds to stimulate or inhibit S_1P_1 receptor signaling may be measured using any assay known in the art used to detect S_1P_1 receptor mediated signaling or S_1P_1 receptor activity, or the absence of such signaling/activity. " S_1P_1 receptor activity" refers to the ability of a S_1P_1 receptor to transduce a signal. Such activity can be measured, e.g., in a heterologous cell, by coupling an S_1P_1 receptor (or a chimeric S_1P_1 receptor) to a downstream effector such as adenylate cyclase.

A "natural ligand-induced activity" as used herein, refers to activation of the S_1P_1 receptor by a natural ligand of the S_1P_1 receptor. Activity can be assessed using any number of endpoints to measure S_1P_1 receptor activity.

Generally, assays for testing compounds that modulate S_1P_1 receptor -mediated signal transduction include the determination of any parameter that is indirectly or directly under the influence of a S_1P_1 receptor, e.g., a functional, physical, or chemical effect.

Samples or assays comprising S_1P_1 receptors that are treated with a potential activator, inhibitor, or modulator are compared to control samples without the inhibitor, activator, or modulator to examine the extent of inhibition. Control samples (untreated with inhibitors) are assigned a

relative S_1P_1 receptor activity value of 100%. Inhibition of a S_1P_1 receptor is achieved when the S_1P_1 receptor activity value relative to the control is about 80%, 50%, or 25%. Activation of a S_1P_1 receptor is achieved when the S_1P_1 receptor activity value relative to the control (untreated with activators) is 110%, 150%, or 200-500% (i.e., two to five fold higher relative to the control), or 1000-3000% or higher.

The effects of the compounds upon the function of an S_1P_1 receptor can be measured by examining any of the parameters described above. Any suitable physiological change that affects S_1P_1 receptor activity can be used to assess the influence of a compound on the S_1P_1 receptors and natural ligand-mediated S_1P_1 receptor activity. When the functional consequences are determined using intact cells or animals, one can also measure a variety of effects such as changes in intracellular second messengers such as cAMP.

Modulators of S_1P_1 receptor activity can be tested using S_1P_1 receptor polypeptides as described herein, either recombinant or naturally occurring. The protein can be isolated, expressed in a cell, expressed in a membrane derived from a cell, expressed in tissue or in an animal. For example, neuronal cells, cells of the immune system, transformed cells, or membranes can be used to test the S_1P_1 receptor polypeptides described herein. Modulation is tested using one of the in vitro or in vivo assays described herein. Signal transduction and cellular trafficking can also be examined in vitro with soluble or solid state reactions, using a chimeric molecule such as an extracellular domain of a receptor covalently linked to a heterologous signal transduction domain, or a heterologous extracellular domain covalently linked to the transmembrane and or cytoplasmic domain of a receptor. Furthermore, ligand-binding domains of the protein of interest can be used in vitro in soluble or solid state reactions to assay for ligand binding.

Ligand binding to an S_1P_1 receptor, a domain, or chimeric protein can be tested in a number of formats. Binding can be performed in solution, in a bilayer membrane, attached to a solid phase, in a lipid monolayer, or in vesicles. For example, in an assay, the binding of the natural ligand to its receptor is measured in the presence of a candidate modulator, such as the compound described herein. Alternatively, the binding of the candidate modulator may be measured in the presence of the natural ligand. Often, competitive assays that measure the ability of a compound to compete with binding of the natural ligand to the receptor are used. Binding can be tested by measuring, e.g., changes in spectroscopic characteristics (e.g., fluorescence, absorbance, refractive index), hydrodynamic (e.g., shape) changes, or changes in chromatographic or solubility properties.

Another technology that can be used to evaluate S_1P_1 receptor -protein interactions in living cells involves bioluminescence resonance energy transfer (BRET). A detailed discussion regarding BRET can be found in Kroeger *et al.*, J. Biol. Chem., 276(16):12736 43 (2001).

After the receptor is expressed in a cell the cells can be grown in appropriate media in the appropriate cell plate. The cells can be plated, for example at 5000-10000 cells per well in a 384 well plate. In some embodiments, the cells are plated at about 1000, 2000, 3000, 4000, 5000, 6000, 7000, 8000, 9000, or 10000 cells/per well. The plates can have any number of wells and the number of cells can be modified accordingly.

Any medicament having utility in an application described herein can be used in co-therapy, co-administration or co-formulation with a composition as described above. Such additional medicaments include, medicines for cancer. Many medicines that are used to treat cancer cause CIPN or CINP. Therefore, the compounds described herein can be administered either before, concurrently with, or after such therapeutics are administered to a subject. Non-limiting examples of such therapeutics include, but are not limited to: Platinum-based drugs, such as but not limited to, carboplatin (Paraplatin), cisplatin, oxaliplatin; taxanes: paclitaxel (Taxol), paclitaxel nanoparticle albumin-bound (Abraxane), docetaxel (Taxotere), and cabazitaxel (Jevtana); Epothilones, such as ixabepilone (Ixempra); Plant alkaloids: vinblastine (Velban, Alkaban-AQ), vincristine (Oncovin, Vincasar PES, Vincrex), vinorelbine (Navelbine), and etoposide (Toposar, VePesid, Etopophos); halidomide (Thalomid), lenalidomide (Revlimid), and pomalidomide (Pomalyst), Bortezomib (Velcade); carfilzomib (Kyprolis), and Eribulin (Halaven). Other examples of therapeutics that the presently described compounds can be combined with include, but are not limited to, Abitrexate (Methotrexate Injection), Abraxane (Paclitaxel Injection), Adcetris (Brentuximab Vedotin Injection), Adriamycin (Doxorubicin), Adrucil Injection (5-FU (fluorouracil)), Afinitor (Everolimus), Afinitor Disperz (Everolimus), Alimta (PEMETREXED), Alkeran Injection (Melphalan Injection), Alkeran Tablets (Melphalan), Aredia (Pamidronate), Arimidex (Anastrozole), Aromasin (Exemestane), Arranon (Nelarabine), Arzerra (Ofatumumab Injection), Avastin (Bevacizumab), Beleodaq (Belinostat Injection), Bexxar (Tositumomab), BiCNU (Carmustine), Blenoxane (Bleomycin), Blincyto (Blinatumomab Injection), Bosulif (Bosutinib), Busulfex Injection (Busulfan Injection), Campath (Alemtuzumab), Camptosar (Irinotecan), Caprelsa (Vandetanib), Casodex (Bicalutamide), CeeNU (Lomustine), CeeNU Dose Pack (Lomustine), Cerubidine (Daunorubicin), Clolar (Clofarabine Injection), Cometriq (Cabozantinib), Cosmegen (Dactinomycin), Cotellic (Cobimetinib), Cyramza (Ramucirumab Injection), CytosarU (Cytarabine),

Cytoxan (Cytoxan), Cytoxan Injection (Cyclophosphamide Injection), Dacogen (Decitabine), DaunoXome (Daunorubicin Lipid Complex Injection), Decadron (Dexamethasone), DepoCyt (Cytarabine Lipid Complex Injection), Dexamethasone Intensol (Dexamethasone), Dexpak Taperpak (Dexamethasone), Docefrez (Docetaxel), Doxil (Doxorubicin Lipid Complex Injection), Droxia (Hydroxyurea), DTIC (Decarbazine), Eligard (Leuprolide), Ellence (Ellence (epirubicin)), Eloxatin (Eloxatin (oxaliplatin)), Elspar (Asparaginase), Emcyt (Estramustine), Erbitux (Cetuximab), Erivedge (Vismodegib), Erwinaze (Asparaginase Erwinia chrysanthemi), Ethyol (Amifostine), Etopophos (Etoposide Injection), Eulexin (Flutamide), Fareston (Toremifene), Farydak (Panobinostat), Faslodex (Fulvestrant), Femara (Letrozole), Firmagon (Degarelix Injection), Fludara (Fludarabine), Folex (Methotrexate Injection), Folotyn (Pralatrexate Injection), FUDR (FUDR (floxuridine)), Gazyva (Obinutuzumab Injection), Gemzar (Gemcitabine), Gilotrif (Afatinib), Gleevec (Imatinib Mesylate), Gliadel Wafer (Carmustine wafer), Used to treat, Brain Tumors Halaven (Eribulin Injection), Herceptin (Trastuzumab), Hexalen (Altretamine), Hycamtin (Topotecan), Hycamtin (Topotecan), Hydrea (Hydroxyurea), Ibrance (Palbociclib), Iclusig (Ponatinib), Idamycin PFS (Idarubicin), Ifex (Ifosfamide), Imbruvica (Ibrutinib), Inlyta (Axitinib), Intron A alfab (Interferon alfa-2a), Iressa (Gefitinib), Istodax (Romidepsin Injection), Ixempra (Ixabepilone Injection), Jakafi (Ruxolitinib), Jevtana (Cabazitaxel Injection), Kadcyla (Ado-trastuzumab Emtansine), Keytruda (Pembrolizumab Injection), Kyprolis (Carfilzomib), Lanvima (Lenvatinib), Leukeran (Chlorambucil), Leukine (Sargramostim), Leustatin (Cladribine), Lonsurf (Trifluridine and Tipiracil), Lupron (Leuprolide), Lupron Depot (Leuprolide), Lupron DepotPED (Leuprolide), Lynparza (Olaparib), Lysodren (Mitotane), Marqibo Kit (Vincristine Lipid Complex Injection) , Matulane (Procarbazine), Megace (Megestrol), Mekinist (Trametinib), Mesnex (Mesna), Mesnex (Mesna Injection), Metastron (Strontium-89 Chloride), Mexate (Methotrexate Injection), Mustargen (Mechlorethamine), Mutamycin (Mitomycin), Myleran (Busulfan), Mylotarg (Gemtuzumab Ozogamicin), Navelbine (Vinorelbine), Neosar Injection (Cyclophosphamide Injection), Neulasta (filgrastim), Neulasta (pegfilgrastim), Neupogen (filgrastim), Nexavar (Sorafenib), Nilandron (Nilandron (nilutamide)), Nipent (Pentostatin), Nolvadex (Tamoxifen), Novantrone (Mitoxantrone), Odomzo (Sonidegib), Oncaspar (Pegaspargase), Oncovin (Vincristine), Ontak (Denileukin Diftitox), Onxol (Paclitaxel Injection), Opdivo (Nivolumab Injection), Paraplatin (Carboplatin), Perjeta (Pertuzumab Injection), Platinol (Cisplatin), Platinol (Cisplatin Injection), PlatinolAQ (Cisplatin), PlatinolAQ (Cisplatin Injection), Pomalyst (Pomalidomide), Prednisone Intensol (Prednisone), Proleukin (Aldesleukin), Purinethol (Mercaptopurine), Reclast (Zoledronic

acid), Revlimid (Lenalidomide), Rheumatrex (Methotrexate), Rituxan (Rituximab), RoferonA alfaa (Interferon alfa-2a), Rubex (Doxorubicin), Sandostatin (Octreotide), Sandostatin LAR Depot (Octreotide), Soltamox (Tamoxifen), Sprycel (Dasatinib), Sterapred (Prednisone), Sterapred DS (Prednisone), Stivarga (Regorafenib), Supprelin LA (Histrelin Implant), Sutent (Sunitinib), Sylatron (Peginterferon Alfa-2b Injection (Sylatron)), Sylvant (Siltuximab Injection), Synribo (Omacetaxine Injection), Tabloid (Thioguanine), Taflinar (Dabrafenib), Tarceva (Erlotinib), Targretin Capsules (Bexarotene), Tasigna (Decarbazine), Taxol (Paclitaxel Injection), Taxotere (Docetaxel), Temodar (Temozolomide), Temodar (Temozolomide Injection), Tepadina (Thiotepa), Thalomid (Thalidomide), TheraCys BCG (BCG), Thioplex (Thiotepa), TICE BCG (BCG), Toposar (Etoposide Injection), Torisel (Temsirolimus), Treanda (Bendamustine hydrochloride), Trelstar (Triptorelin Injection), Trexall (Methotrexate), Trisenox (Arsenic trioxide), Tykerb (lapatinib), Unituxin (Dinutuximab Injection), Valstar (Valrubicin Intravesical), Vantas (Histrelin Implant), Vectibix (Panitumumab), Velban (Vinblastine), Velcade (Bortezomib), Vepesid (Etoposide), Vepesid (Etoposide Injection), Vesanoid (Tretinoin), Vidaza (Azacitidine), Vincasar PFS (Vincristine), Vincrex (Vincristine), Votrient (Pazopanib), Vumon (Teniposide), Wellcovorin IV (Leucovorin Injection), Xalkori (Crizotinib), Xeloda (Capecitabine), Xtandi (Enzalutamide), Yervoy (Ipilimumab Injection), Yondelis (Trabectedin Injection), Zaltrap (Ziv-aflibercept Injection), Zanosar (Streptozocin), Zelboraf (Vemurafenib), Zevalin (Ibritumomab Tiuxetan), Zoladex (Goserelin), Zolinza (Vorinostat), Zometa (Zoledronic acid), Zortress (Everolimus), Zydelig (Idelalisib), Zykadia (Ceritinib), Zytiga (Abiraterone), or any combination thereof. Other examples include, but are not limited to, PD-1 antibodies, such as Nivolumab or Pembrolizumab. In some embodiments, the compounds, or pharmaceutically acceptable salts thereof, provided herein can be administered with, either concurrently or sequentially, or as part of a cancer treatment protocol, the additional therapeutics provided for herein.

In some embodiments, the compounds provided herein can also be used to treat cancer. In some embodiments, the compounds, or pharmaceutically acceptable salts thereof, can be used to inhibit tumor growth. In some embodiments, the compounds, or pharmaceutically acceptable salts thereof, are used to treat cancers, such as, but not limited to, ovarian cancer, breast cancer, lung cancer, brain cancer, colon cancer, prostate cancer, esophageal cancer, pancreatic cancer, brain cancer, glioblastoma cancer, leukemia, multiple myeloma, lymphoma, skin cancer, acute Lymphoblastic Leukemia, acute myeloid leukemia, basal cell cancer, bile duct cancer, bladder cancer, bone cancer (Ewing sarcoma, osteosarcoma), CLL, CML, uterine cancer, cervical cancer,

hairy cell leukemia, melanoma, thyroid cancer, rectal cancer, renal cell cancer, small cell lung cancer, non-small cell lung cancer, or stomach cancer. In some embodiments, the cancer is breast or ovarian cancer. In some embodiments, the compounds, or pharmaceutically acceptable salts thereof, provided herein are combined with a taxane, such as paclitaxel.

The additional medicament can be administered in co-therapy (including co-formulation) with the one or more of the compounds described herein.

In some embodiments, the response of the disease or disorder to the treatment is monitored and the treatment regimen is adjusted if necessary in light of such monitoring.

Frequency of administration is typically such that the dosing interval, for example, the period of time between one dose and the next, during waking hours is from about 2 to about 12 hours, from about 3 to about 8 hours, or from about 4 to about 6 hours. It will be understood by those of skill in the art that an appropriate dosing interval is dependent to some degree on the length of time for which the selected composition is capable of maintaining a concentration of the compound(s) in the subject and/or in the target tissue (e.g., above the EC_{50} (the minimum concentration of the compound which modulates the receptor's activity by 90%). Ideally the concentration remains above the EC_{50} for at least 100% of the dosing interval. Where this is not achievable it is desired that the concentration should remain above the EC_{50} for at least about 60% of the dosing interval, or should remain above the EC_{50} for at least about 40% of the dosing interval.

The present disclosure also provides the following non-limiting embodiments:

In order that the embodiments disclosed herein may be more efficiently understood, examples are provided below. It should be understood that these examples are for illustrative purposes only and are not to be construed as limiting the embodiments in any manner. Throughout these examples, there may be molecular cloning reactions, and other standard recombinant DNA techniques described and these were carried out according to methods described in Maniatis et al., Molecular Cloning - A Laboratory Manual, 2nd ed., Cold Spring Harbor Press (1989), using commercially available reagents, except where otherwise noted.

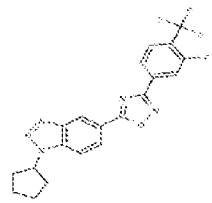
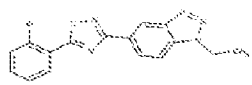
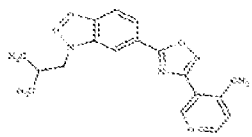
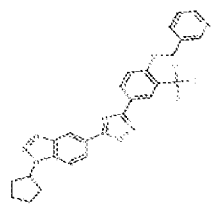
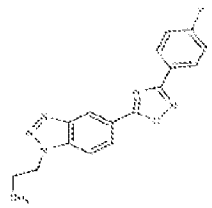
The following examples are illustrative, but not limiting, of the methods and compositions described herein. Other suitable modifications and adaptations of the variety of conditions and parameters normally encountered in therapy, synthesis, and other embodiments disclosed herein are within the spirit and scope of the embodiments.

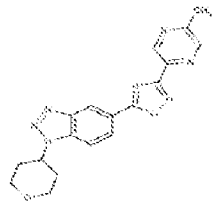
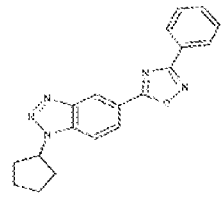
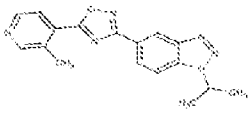
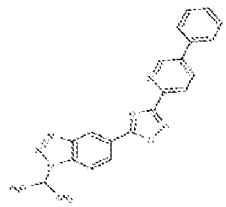
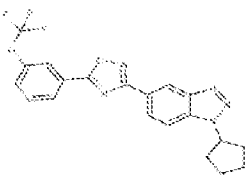
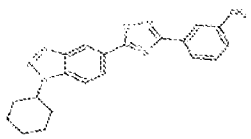
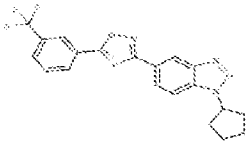
Examples

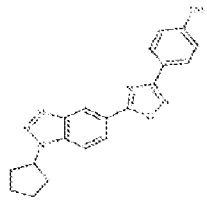
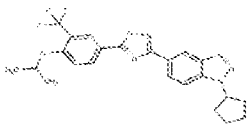
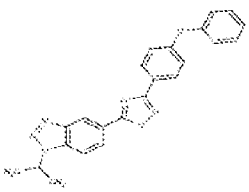
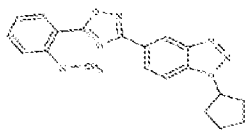
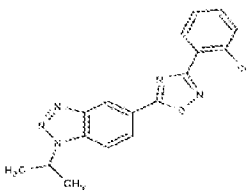
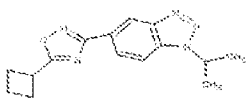
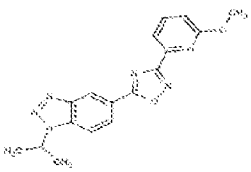
Example 1: Synthesis of Compounds

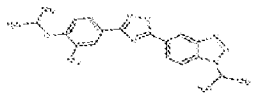
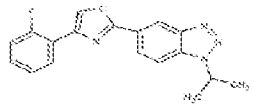
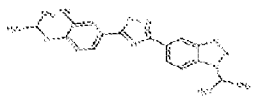
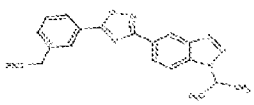
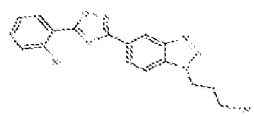
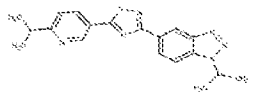
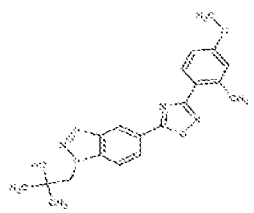
Certain synthetic schemes, both general and specific, are provided herein. The compounds disclosed herein can be made according to the methods described herein or intermediates that lead to the compounds disclosed herein can be made according to the methods described herein. The substitutions can be varied according to the compound or intermediate being made based upon the following examples and other modifications known to one of skill in the art.

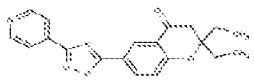
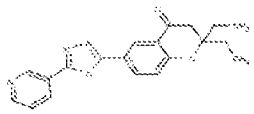
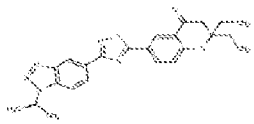
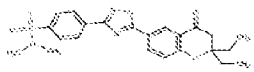
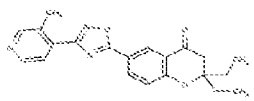
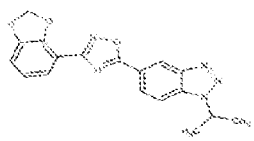
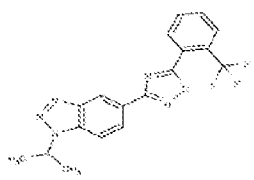
The following compounds were prepared according to the following examples or the examples were varied according to one of skill in the art to prepare the compounds.

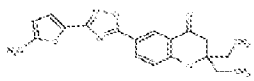
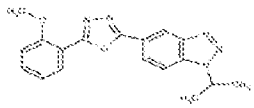
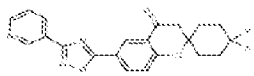
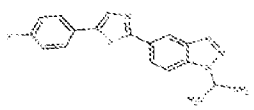
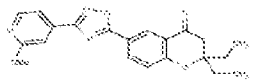
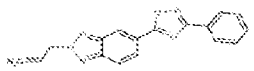
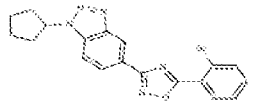
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	1	1-cyclopentyl-5-{3-[3-fluoro-4-(trifluoromethyl)phenyl]-1,2,4-oxadiazol-5-yl}-1H- 1,2,3-benzotriazole	417.37	418.1
	2	5-(2-bromophenyl)-3-(1-ethyl-1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-oxadiazole	370.21	371
	3	1-(2-methylpropyl)-6-[3-(4-methylpyridin-3-yl)- 1,2,4-oxadiazol-5-yl]-1H-1,2,3-benzotriazole	334.38	355.2
	4	1-cyclopentyl-5-{3-[4-(pyridin-3-ylmethoxy)-3-(trifluoromethyl)phenyl]-1,2,4-oxadiazol-5-yl}-1H- 1,2,3-benzotriazole	506.49	507.2
	5	5-[3-(4-fluorophenyl)-1,2,4-oxadiazol-5-yl]-1- propyl-1H-1,2,3-benzotriazole	323.33	324.2

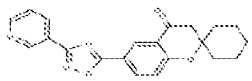
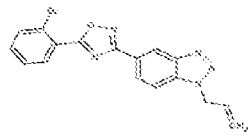
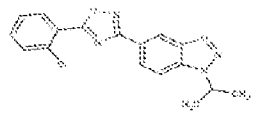
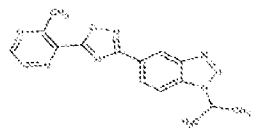
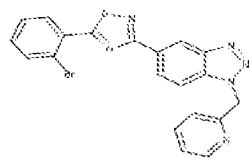
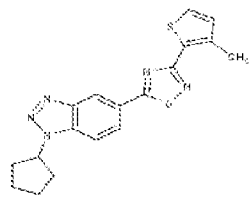
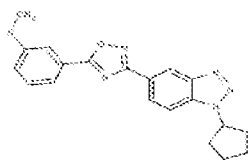
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	6	5-[3-(5-methylpyrazin-2-yl)-1,2,4-oxadiazol-5-yl]-1- (oxan-4-yl)-1H-1,2,3-benzotriazole	363.38	364.1
	7	1-cyclopentyl-5-(3-phenyl-1,2,4-oxadiazol-5-yl)-1H- 1,2,3-benzotriazole	331.38	332.1
	8	3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(3-methylpyridin-4-yl)-1,2,4-oxadiazole	320.36	321
	9	5-[3-(5-phenylpyridin-2-yl)-1,2,4-oxadiazol-5-yl]-1- (propan-2-yl)-1H-1,2,3-benzotriazole	382.43	383.1
	10	3-(1-cyclopentyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(3-(trifluoromethoxy)phenyl)-1,2,4-oxadiazole	415.38	416.1
	11	1-cyclohexyl-5-[3-(3-methylphenyl)-1,2,4-oxadiazol-5-yl]-1H-1,2,3-benzotriazole	359.43	360.2
	12	3-(1-cyclopentyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(3-(trifluoromethyl)phenyl)-1,2,4-oxadiazole	399.38	400.1

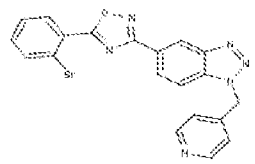
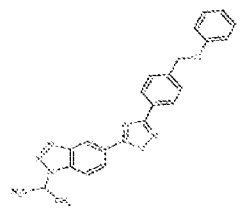
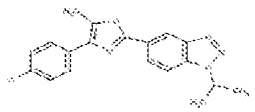
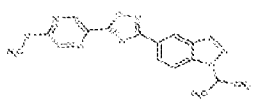
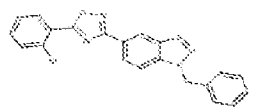
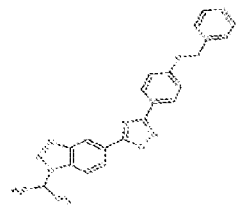
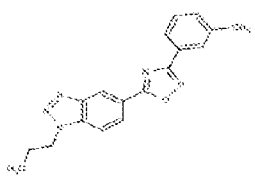
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	13	4-[5-(1-cyclopentyl-1H-1,2,3-benzotriazol-5-yl)- 1,2,4-oxadiazol-3-yl]phenol	347.38	348.1
	14	3-(1-cyclopentyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(4-isopropoxy-3-(trifluoromethyl)phenyl)-1,2,4-oxadiazole	457.46	458.1
	15	5-[3-(4-phenoxyphenyl)-1,2,4-oxadiazol-5-yl]-1- (propan-2-yl)-1H-1,2,3-benzotriazole	397.44	398.2
	16	3-(1-cyclopentyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(2-(methylthio)phenyl)-1,2,4-oxadiazole	377.47	378.1
	17	5-[3-(2-chlorophenyl)-1,2,4-oxadiazol-5-yl]-1- (propan-2-yl)-1H-1,2,3-benzotriazole	339.78	340.1
	18	5-(5-cyclobutyl-1,2,4-oxadiazol-3-yl)-1-(propan-2- yl)-1H-1,2,3-benzotriazole	283.34	284
	19	5-[3-(6-methoxypyridin-2-yl)-1,2,4-oxadiazol-5-yl]-1- (propan-2-yl)-1H-1,2,3-benzotriazole	336.36	337.1

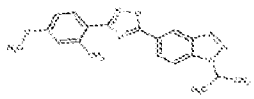
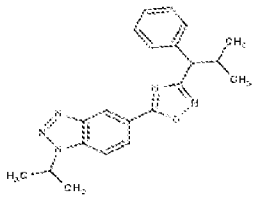
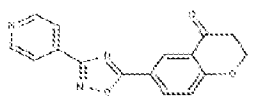
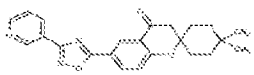
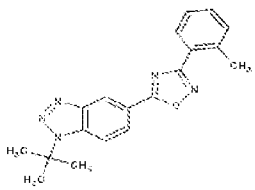
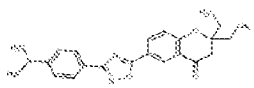
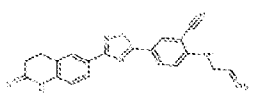
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	20	3-(4-isopropoxy-3-(trifluoromethyl)phenyl)-5-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-oxadiazole	431.42	432
	21	5-[4-(2-fluorophenyl)-1,3-oxazol-2-yl]-1-(propan-2- yl)-1H-1,2,3-benzotriazole	322.34	323
	22	2-isopropoxy-5-(3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-oxadiazol-5-yl)benzonitrile	388.43	389
	23	3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(3-(phenoxymethyl)phenyl)-1,2,4-oxadiazole	411.47	412
	24	3-(5-(5-(2-bromophenyl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)propan-1-ol	400.24	400
	25	3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(6-isopropylpyridin-3-yl)-1,2,4-oxadiazole	348.41	349.3
	26	1-{5-[3-(4-methoxy-2-methylphenyl)-1,2,4-oxadiazol-5-yl]-1H-1,2,3-benzotriazol-1-yl}-2-methylpropan-2- ol	379.42	380.1

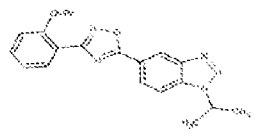
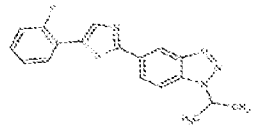
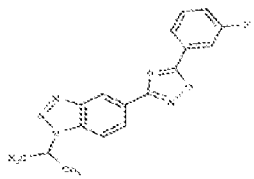
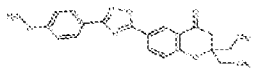
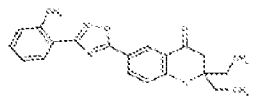
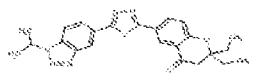
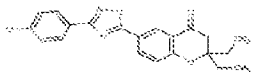
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	27	2,2-diethyl-6-[3-(pyridin-4-yl)-1,2,4-oxadiazol-5- yl]-3,4-dihydro-2H-1-benzopyran-4-one	349.39	350.1
	28	2,2-diethyl-6-(5-(pyridin-3-yl)-1,3,4-oxadiazol-2-yl)chroman-4-one	349.39	350.1
	29	2,2-diethyl-6-(3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-thiadiazol-5-yl)chroman-4-one	447.56	448.2
	30	4-(5-(2,2-diethyl-4-oxochroman-6-yl)-1,2,4-oxadiazol-3-yl)-N,N-dimethylbenzenesulfonamide	455.53	456.1
	31	2,2-diethyl-6-(3-(3-methylpyridin-4-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one	363.42	364.2
	32	3-(benzo[d][1,3]dioxol-4-yl)-5-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-oxadiazole	349.35	350.1
	33	3-(1-isopropylbenzotriazol-5-yl)-5-[2-(trifluoromethyl)phenyl]-1,2,4-oxadiazole	373.34	374.1

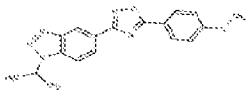
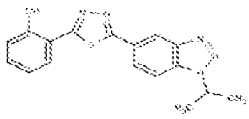
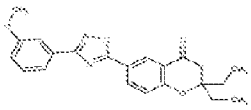
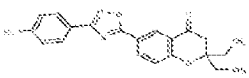
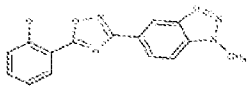
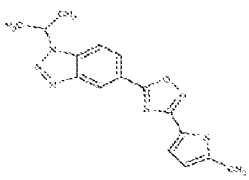
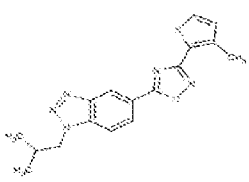
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	34	2,2-diethyl-6-(3-(5-methylthiophen-2-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one	368.45	369.3
	35	5-[5-(2-methoxyphenyl)-1,3,4-oxadiazol-2-yl]-1- (propan-2-yl)-1H-1,2,3-benzotriazole	335.37	336
	36	4',4'-difluoro-6-[3-(pyridin-3-yl)-1,2,4-oxadiazol-5- yl]-3,4-dihydrospiro[1-benzopyran-2,1'-cyclohexane]-4-one	397.38	298.1
	37	5-(4-fluorophenyl)-2-(1-isopropylbenzotriazol-5-yl)thiazole	338.40	339.2
	38	2,2-diethyl-6-(3-(2-methoxypyridin-4-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one	379.42	380.1
	39	5-(3-phenyl-1,2,4-oxadiazol-5-yl)-2-(prop-2-en-1- yl)-2H-1,2,3-benzotriazole	303.33	304.3
	40	5-(2-bromophenyl)-3-(1-cyclopentyl-1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-oxadiazole	410.28	409.9

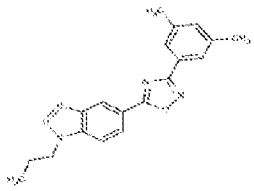
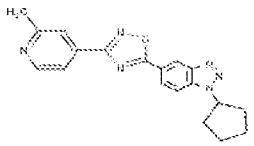
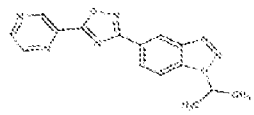
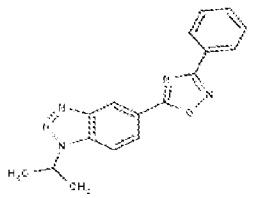
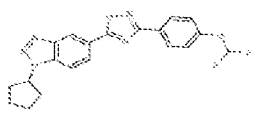
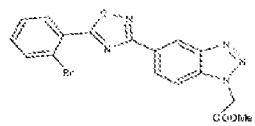
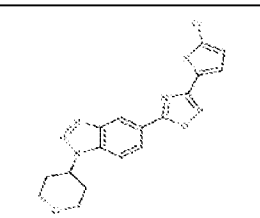
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	41	6-[3-(pyridin-3-yl)-1,2,4-oxadiazol-5-yl]-3,4- dihydrospiro[1-benzopyran-2,1'-cyclohexane]-4-one	361.40	362.1
	42	3-(1-allyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(2-bromophenyl)-1,2,4-oxadiazole	382.22	382
	43	5-(2-bromophenyl)-3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-oxadiazole	384.24	384
	44	3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(3-methylpyrazin-2-yl)-1,2,4-oxadiazole	321.34	322.1
	45	5-(2-bromophenyl)-3-(1-(pyridin-2-ylmethyl)-1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-oxadiazole	433.27	435.1
	46	1-cyclopentyl-5-[3-(3-methylthiophen-2-yl)-1,2,4-oxadiazol-5-yl]-1H-1,2,3-benzotriazole	351.43	352.1
	47	3-(1-cyclopentyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(3-(methylthio)phenyl)-1,2,4-oxadiazole	377.47	378.1

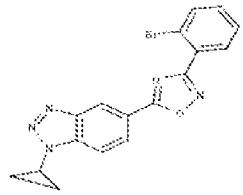
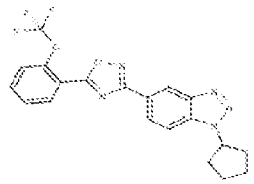
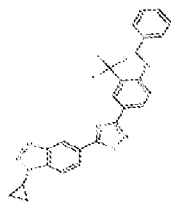
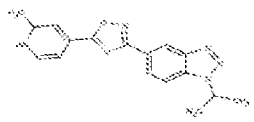
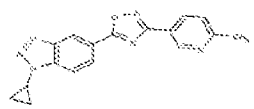
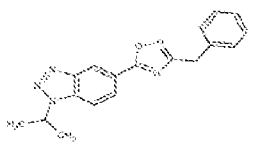
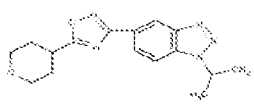
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	48	5-(2-bromophenyl)-3-(1-(pyridin-4-ylmethyl)-1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-oxadiazole	433.27	435
	49	5-{3-[4-(phenoxymethyl)phenyl]-1,2,4-oxadiazol-5- yl}-1-(propan-2-yl)-1H-1,2,3-benzotriazole	411.47	412.3
	50	5-[4-(4-chlorophenyl)-5-methyl-1,3-oxazol-2-yl]-1- (propan-2-yl)-1H-1,2,3-benzotriazole	352.82	353
	51	3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(5-methoxypyrazin-2-yl)-1,2,4-oxadiazole	337.34	338
	52	3-(1-benzyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(2-bromophenyl)-1,2,4-oxadiazole	432.28	432
	53	5-{3-[4-(benzyloxy)phenyl]-1,2,4-oxadiazol-5-yl}-1- (propan-2-yl)-1H-1,2,3-benzotriazole	411.47	412.3
	54	5-[3-(3-methylphenyl)-1,2,4-oxadiazol-5-yl]-1- propyl-1H-1,2,3-benzotriazole	319.37	320.2

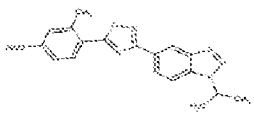
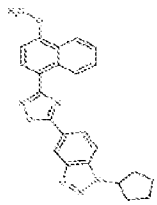
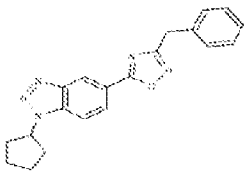
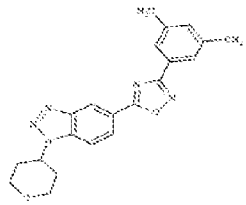
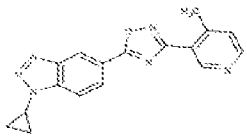
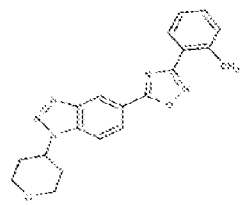
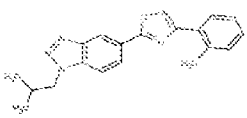
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	55	5-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-3-(4-methoxy-2-methylphenyl)-1,2,4-oxadiazole	349.39	350
	56	5-[3-(2-methyl-1-phenylpropyl)-1,2,4-oxadiazol-5- yl]-1-(propan-2-yl)-1H-1,2,3-benzotriazole	361.45	362.1
	57	6-[3-(pyridin-4-yl)-1,2,4-oxadiazol-5-yl]-3,4- dihydro-2H-1-benzopyran-4-one	293.28	294.1
	58	4',4'-dimethyl-6-[3-(pyridin-3-yl)-1,2,4-oxadiazol-5- yl]-3,4-dihydrospiro[1-benzopyran-2,1'-cyclohexane]-4-one	389.46	390.2
	59	1-tert-butyl-5-[3-(2-methylphenyl)-1,2,4-oxadiazol-5- yl]-1H-1,2,3-benzotriazole	333.40	334.1
	60	6-(3-(4-(dimethylamino)phenyl)-1,2,4-oxadiazol-5-yl)-2,2-diethylchroman-4-one	391.47	392.3
	61	2-(allylamino)-5-(3-(2-oxo-1,2,3,4-tetrahydroquinolin-6-yl)-1,2,4-oxadiazol-5-yl)benzonitrile	371.40	372.1

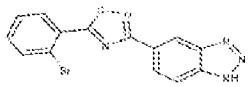
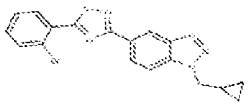
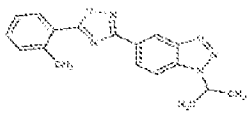
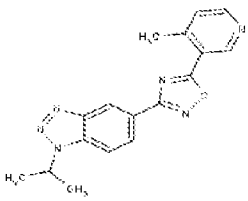
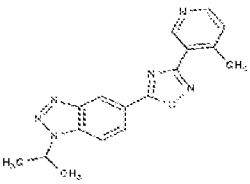
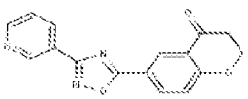
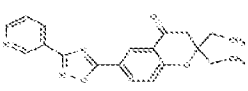
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	62	3-(2-isopropoxyphenyl)-5-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-oxadiazole	363.42	364.1
	63	5-(2-fluorophenyl)-2-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)thiazole	338.40	339.1
	64	5-(3-fluorophenyl)-3-(1-isopropylbenzotriazol-5-yl)-1,2,4-oxadiazole	323.33	324.1
	65	2,2-diethyl-6-(3-(4-methoxyphenyl)-1,2,4-oxadiazol-5-yl)chroman-4-one	378.43	379.1
	66	2,2-diethyl-6-(3-(o-tolyl)-1,2,4-oxadiazol-5-yl)chroman-4-one	362.43	363.1
	67	2,2-diethyl-6-(5-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-1,3,4-thiadiazol-2-yl)chroman-4-one	447.56	448.1
	68	6-[3-(4-chlorophenyl)-1,2,4-oxadiazol-5-yl]-2,2-diethyl-chroman-4-one	382.84	383.1

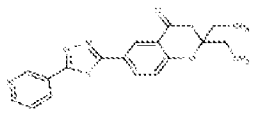
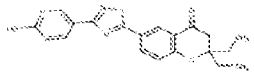
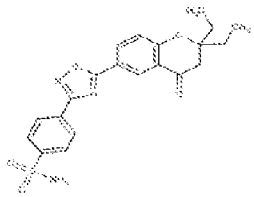
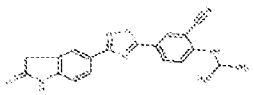
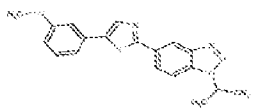
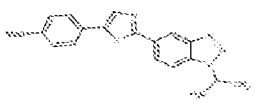
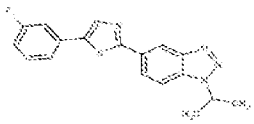
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	69	3-(1-isopropylbenzotriazol-5-yl)-5-(4-methoxyphenyl)-1,2,4-oxadiazole	335.37	336.1
	70	2-{5-[1-(propan-2-yl)-1H-1,2,3-benzotriazol-5-yl]- 1,3,4-thiadiazol-2-yl}phenol	337.40	338
	71	2,2-diethyl-6-(3-(3-methoxyphenyl)-1,2,4-oxadiazol-5-yl)chroman-4-one	378.43	379.1
	72	2,2-diethyl-6-[3-(4-hydroxyphenyl)-1,2,4-oxadiazol-5-yl]chroman-4-one	364.40	365.1
	73	5-(2-bromophenyl)-3-(1-methyl-1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-oxadiazole	356.18	356
	74	5-[5-(5-methylthiophen-2-yl)-1,2,4-oxadiazol-3-yl]-1- (propan-2-yl)-1H-1,2,3-benzotriazole	325.39	326.1
	75	1-(2-methylpropyl)-5-[3-(3-methylthiophen-2-yl)- 1,2,4-oxadiazol-5-yl]-1H-1,2,3-benzotriazole	339.42	340.1

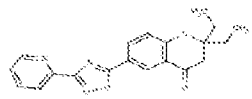
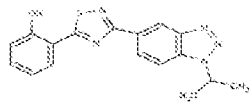
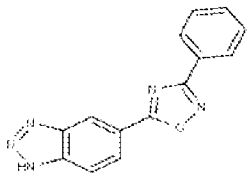
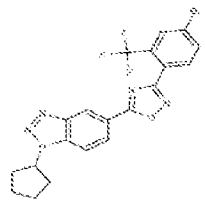
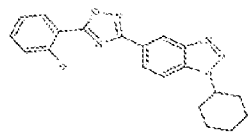
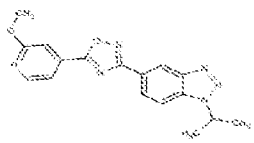
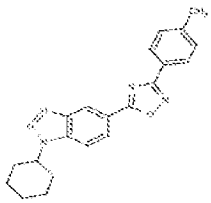
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	76	5-[3-(3,5-dimethylphenyl)-1,2,4-oxadiazol-5-yl]-1- propyl-1H-1,2,3-benzotriazole	333.40	334.3
	77	5-[3-(2-methoxypyridin-4-yl)-1,2,4-oxadiazol-5-yl]-1-methyl-2,3-dihydro-1H-1,2,3-benzotriazole; cyclopentane	346.39	347.1
	78	3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(pyrazin-2-yl)-1,2,4-oxadiazole	307.32	308
	79	5-(3-phenyl-1,2,4-oxadiazol-5-yl)-1-(propan-2-yl)- 1H-1,2,3-benzotriazole	305.34	306.3
	80	1-cyclopentyl-5-{3-[4-(difluoromethoxy)phenyl]- 1,2,4-oxadiazol-5-yl}-1H-1,2,3-benzotriazole	397.39	398.1
	81	methyl 2-(5-(5-(2-bromophenyl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)acetate	414.22	414.1
	82	5-[3-(5-chlorothiophen-2-yl)-1,2,4-oxadiazol-5-yl]-1- (oxan-4-yl)-1H-1,2,3-benzotriazole	387.84	388

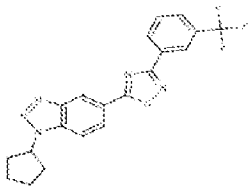
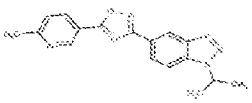
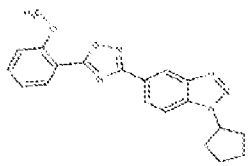
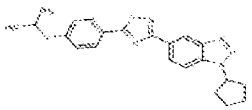
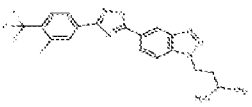
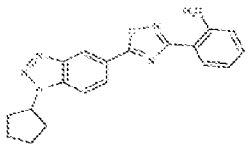
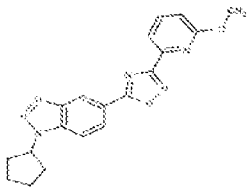
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	83	5-[3-(2-bromophenyl)-1,2,4-oxadiazol-5-yl]-1- cyclopropyl-1H-1,2,3-benzotriazole	382.22	382.2
	84	3-(1-cyclopentyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(2-(trifluoromethoxy)phenyl)-1,2,4-oxadiazole	415.38	416
	85	5-{3-[4-(benzyloxy)-3-(trifluoromethyl)phenyl]- 1,2,4-oxadiazol-5-yl}-1-cyclopropyl-1H-1,2,3- benzotriazole	477.45	478.2
	86	3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(2-methylpyridin-4-yl)-1,2,4-oxadiazole	322.37	321.1
	87	1-cyclopropyl-5-[3-(6-methylpyridin-3-yl)-1,2,4-oxadiazol-5-yl]-1H-1,2,3-benzotriazole	318.34	319.1
	88	5-(3-benzyl-1,2,4-oxadiazol-5-yl)-1-(propan-2-yl)- 1H-1,2,3-benzotriazole	319.37	320.1
	89	5-[5-(oxan-4-yl)-1,2,4-oxadiazol-3-yl]-1-(propan-2- yl)-1H-1,2,3-benzotriazole	313.36	314

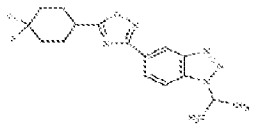
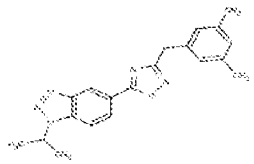
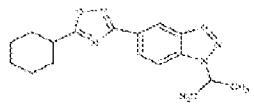
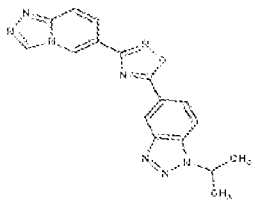
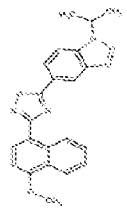
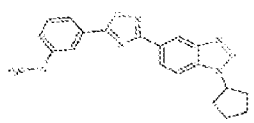
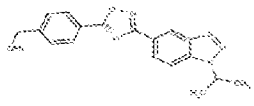
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	90	3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(4-methoxy-2-methylphenyl)-1,2,4-oxadiazole	349.39	350.1
	91	1-cyclopentyl-5-[3-(4-methoxynaphthalen-1-yl)- 1,2,4-oxadiazol-5-yl]-1H-1,2,3-benzotriazole	411.47	412.2
	92	5-(3-benzyl-1,2,4-oxadiazol-5-yl)-1-cyclopentyl-1H- 1,2,3-benzotriazole	345.41	346.1
	93	5-[3-(3,5-dimethylphenyl)-1,2,4-oxadiazol-5-yl]-1- (oxan-4-yl)-1H-1,2,3-benzotriazole	375.43	376.2
	94	1-cyclopropyl-5-[3-(4-methylpyridin-3-yl)-1,2,4-oxadiazol-5-yl]-1H-1,2,3-benzotriazole	318.34	319.3
	95	5-[3-(2-methylphenyl)-1,2,4-oxadiazol-5-yl]-1- (oxan-4-yl)-1H-1,2,3-benzotriazole	361.41	362.1
	96	5-[3-(2-methylphenyl)-1,2,4-oxadiazol-5-yl]-1-(2-methylpropyl)-1H-1,2,3-benzotriazole	333.40	334.2

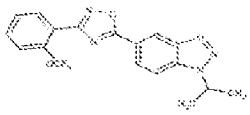
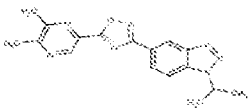
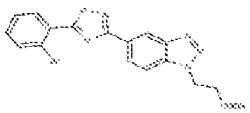
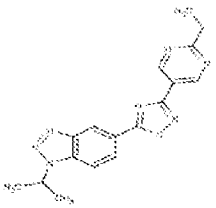
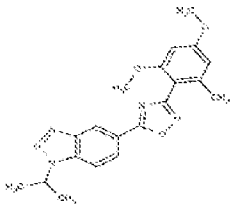
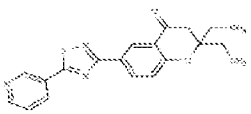
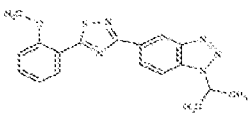
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	97	3-(1H-benzo[d][1,2,3]triazol-5-yl)-5-(2-bromophenyl)-1,2,4-oxadiazole	342.16	343.9
	98	5-(2-bromophenyl)-3-(1-(cyclopropylmethyl)-1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-oxadiazole	396.25	396
	99	3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(o-tolyl)-1,2,4-oxadiazole	319.37	320
	100	3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(4-methylpyridin-3-yl)-1,2,4-oxadiazole	320.36	321.1
	101	5-[3-(4-methylpyridin-3-yl)-1,2,4-oxadiazol-5-yl]-1- (propan-2-yl)-1H-1,2,3-benzotriazole	320.36	321.1
	102	6-[3-(pyridin-3-yl)-1,2,4-oxadiazol-5-yl]-3,4- dihydro-2H-1-benzopyran-4-one	293.28	294.1
	103	2,2-diethyl-6-[3-(pyridin-3-yl)-1,2,4-oxadiazol-5- yl]-3,4-dihydro-2H-1-benzopyran-4-one	349.39	350.2

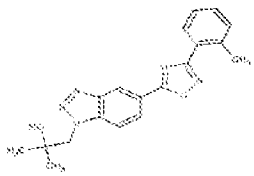
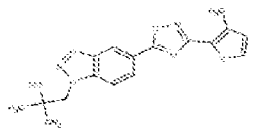
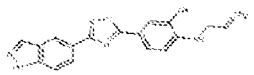
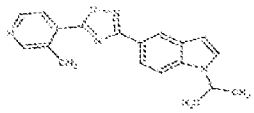
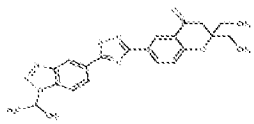
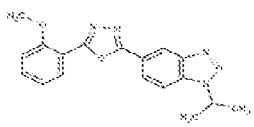
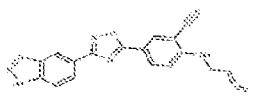
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	104	2,2-diethyl-6-(5-(pyridin-3-yl)-1,3,4-thiadiazol-2-yl)chroman-4-one	365.45	366.1
	105	2,2-diethyl-6-[3-(6-hydroxy-3-pyridyl)-1,2,4-oxadiazol-5-yl]chroman-4-one	365.39	366.1
	106	4-(5-(2,2-diethyl-4-oxochroman-6-yl)-1,2,4-oxadiazol-3-yl)benzenesulfonamide	427.48	428.1
	107	2-(isopropylamino)-5-(3-(2-oxoindolin-5-yl)-1,2,4-oxadiazol-5-yl)benzonitrile	359.39	360.1
	108	2-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(3-methoxyphenyl)thiazole	350.44	351.2
	109	2-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(4-methoxyphenyl)thiazole	350.44	351.1
	110	5-(3-fluorophenyl)-2-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)thiazole	338.40	339.1

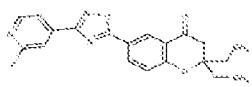
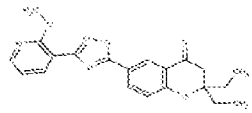
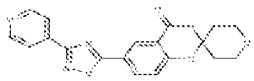
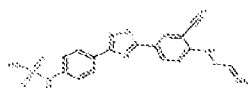
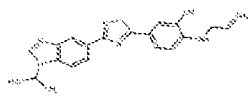
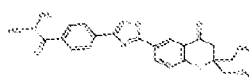
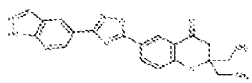
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	111	2,2-diethyl-6-[3-(2-pyridyl)-1,2,4-oxadiazol-5-yl]chroman-4-one	349.39	350.1
	112	2-{3-[1-(propan-2-yl)-1H-1,2,3-benzotriazol-5-yl]- 1,2,4-thiadiazol-5-yl}phenol	337.40	338
	113	5-(3-phenyl-1,2,4-oxadiazol-5-yl)-1H-1,2,3- benzotriazole	263.26	264.1
	114	5-{3-[4-bromo-2-(trifluoromethyl)phenyl]-1,2,4-oxadiazol-5-yl}-1-cyclopentyl-1H-1,2,3- benzotriazole	478.27	478.1
	115	5-(2-bromophenyl)-3-(1-cyclohexyl-1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-oxadiazole	424.30	426
	116	3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(2-methoxypyridin-4-yl)-1,2,4-oxadiazole	336.36	337
	117	1-cyclohexyl-5-[3-(4-methylphenyl)-1,2,4-oxadiazol-5-yl]-1H-1,2,3-benzotriazole	359.43	360.1

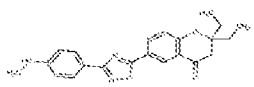
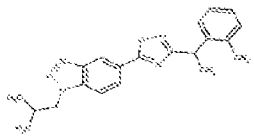
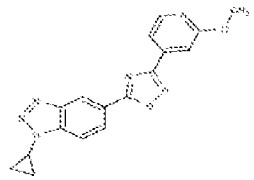
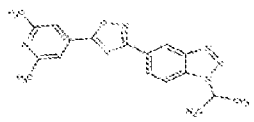
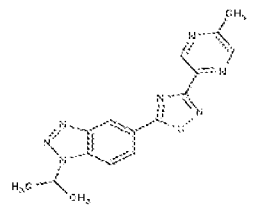
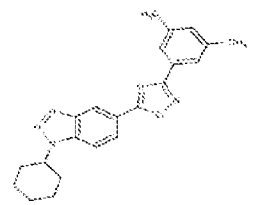
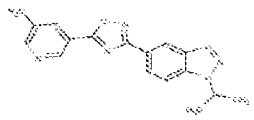
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	118	1-cyclopentyl-5-{3-[3-(trifluoromethyl)phenyl]- 1,2,4-oxadiazol-5-yl}-1H-1,2,3-benzotriazole	399.38	400.1
	119	3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(6-methylpyridin-3-yl)-1,2,4-oxadiazole	320.36	321.1
	120	3-(1-cyclopentyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(2-methoxyphenyl)-1,2,4-oxadiazole	361.41	362
	121	3-(1-cyclopentyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(4-isopropoxyphenyl)-1,2,4-oxadiazole	389.46	390.3
	122	5-{3-[3-fluoro-4-(trifluoromethyl)phenyl]-1,2,4-oxadiazol-5-yl}-1-(3-methylbutyl)-1H-1,2,3- benzotriazole	419.38	420.2
	123	5-[3-(3,5-dimethylphenyl)-1,2,4-oxadiazol-5-yl]-1- (propan-2-yl)-1H-1,2,3-benzotriazole	345.41	346.2
	124	1-cyclopentyl-5-[3-(6-methoxypyridin-2-yl)-1,2,4-oxadiazol-5-yl]-1H-1,2,3-benzotriazole	362.39	363.1

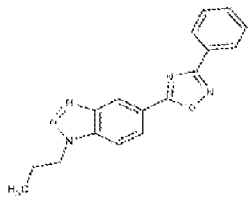
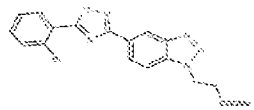
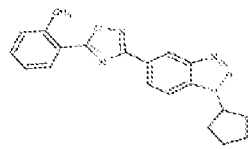
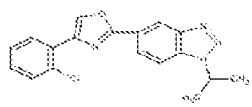
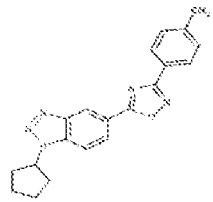
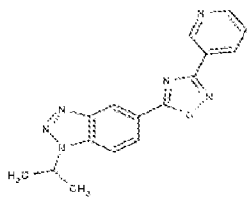
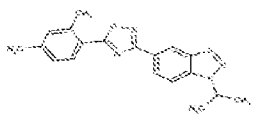
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	125	5-[5-(4,4-difluorocyclohexyl)-1,2,4-oxadiazol-3- yl]-1-(propan-2-yl)-1H-1,2,3-benzotriazole	347.37	348
	126	5-{3-[(3,5-dimethylphenyl)methyl]-1,2,4-oxadiazol-5- yl}-1-(propan-2-yl)-1H-1,2,3-benzotriazole	347.42	348.3
	127	5-(5-cyclohexyl-1,2,4-oxadiazol-3-yl)-1-(propan-2- yl)-1H-1,2,3-benzotriazole	311.39	312
	128	1-(propan-2-yl)-5-(3-{[1,2,4]triazolo[4,3- a]pyridin-6-yl}-1,2,4-oxadiazol-5-yl)-1H-1,2,3-benzotriazole	346.35	347.1
	129	5-[3-(4-methoxynaphthalen-1-yl)-1,2,4-oxadiazol-5- yl]-1-(propan-2-yl)-1H-1,2,3-benzotriazole	385.43	386.2
	130	3-(1-cyclopentyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(3-methoxyphenyl)-1,2,4-oxadiazole	361.41	362
	131	3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(4-(phenoxymethyl)phenyl)-1,2,4-oxadiazole	411.47	412

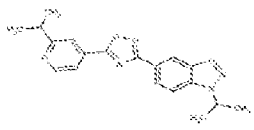
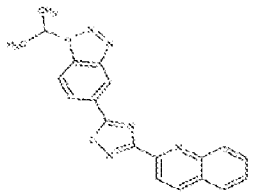
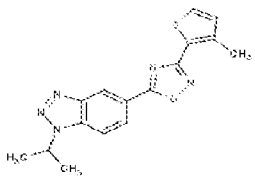
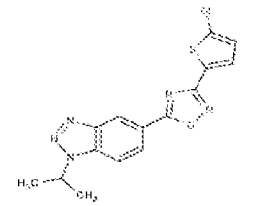
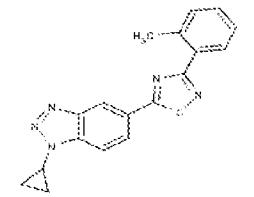
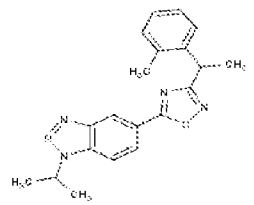
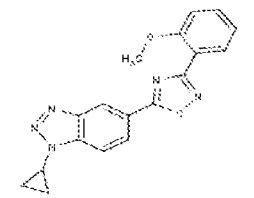
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	132	5-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-3-(2-(trifluoromethoxy)phenyl)-1,2,4-oxadiazole	389.34	390
	133	5-(5,6-dimethylpyrazin-2-yl)-3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-oxadiazole	335.37	356.1
	134	3-(5-(5-(2-bromophenyl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)propanoic acid	414.22	413.9
	135	5-[3-(2-ethylpyrimidin-5-yl)-1,2,4-oxadiazol-5-yl]-1- (propan-2-yl)-1H-1,2,3-benzotriazole	335.37	336.1
	136	5-[3-(2,4-dimethoxy-6-methylphenyl)-1,2,4- oxadiazol-5-yl]-1-(propan-2-yl)-1H-1,2,3-benzotriazole	379.42	380.3
	137	2,2-diethyl-6-(5-(pyridin-3-yl)-1,2,4-thiadiazol-3-yl)chroman-4-one	365.45	366
	138	5-[5-(2-methoxyphenyl)-1,2,4-thiadiazol-3-yl]-1- (propan-2-yl)-1H-1,2,3-benzotriazole	351.43	302

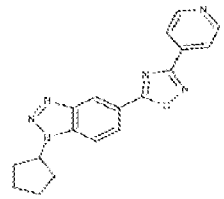
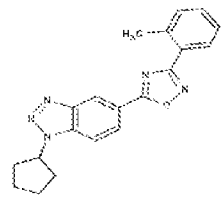
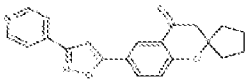
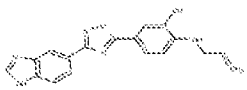
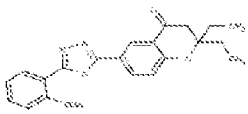
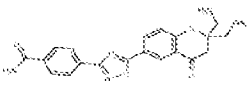
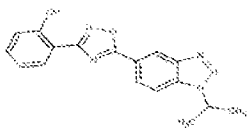
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	139	2-methyl-1-{5-[3-(2-methylphenyl)-1,2,4-oxadiazol-5-yl]-1H-1,2,3-benzotriazol-1-yl}propan-2-ol	349.39	350.1
	140	2-methyl-1-{5-[3-(3-methylthiophen-2-yl)-1,2,4-oxadiazol-5-yl]-1H-1,2,3-benzotriazol-1-yl}propan-2- ol	355.42	356.1
	141	5-(3-(1H-indazol-5-yl)-1,2,4-oxadiazol-5-yl)-2-(allylamino)benzonitrile	342.36	343.1
	142	3-(1-isopropyl-1H-indol-5-yl)-5-(3-methylpyridin-4-yl)-1,2,4-oxadiazole	318.38	318.15
	143	2,2-diethyl-6-(5-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-thiadiazol-3-yl)chroman-4-one	447.56	448.1
	144	5-[5-(2-methoxyphenyl)-1,3,4-thiadiazol-2-yl]-1- (propan-2-yl)-1H-1,2,3-benzotriazole	351.43	352
	145	5-(3-(1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-oxadiazol-5-yl)-2-(allylamino)benzonitrile	343.35	344.1

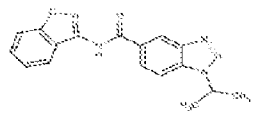
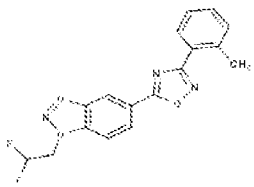
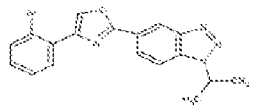
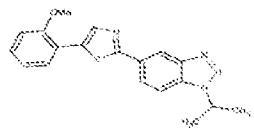
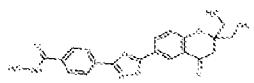
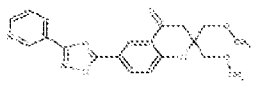
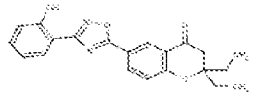
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	146	2,2-diethyl-6-(3-(2-fluoropyridin-4-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one	367.38	368.1
	147	2,2-diethyl-6-(3-(2-methoxypyridin-3-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one	379.42	380.2
	148	6-[3-(pyridin-4-yl)-1,2,4-oxadiazol-5-yl]-3,4- dihydrospiro[1-benzopyran-2,4'-oxane]-4-one	363.37	364.1
	149	N-(4-(5-(4-(allylamino)-3-cyanophenyl)-1,2,4-oxadiazol-3-yl)phenyl)methanesulfonamide	395.44	396.1
	150	2-(allylamino)-5-(3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-oxadiazol-5-yl)benzonitrile	385.43	386.3
	151	4-(5-(2,2-diethyl-4-oxochroman-6-yl)-1,2,4-oxadiazol-3-yl)-N,N-dimethylbenzamide	419.48	420.2
	152	6-(3-(1H-indazol-5-yl)-1,2,4-oxadiazol-5-yl)-2,2-diethylchroman-4-one	388.43	389.2

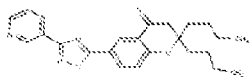
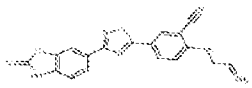
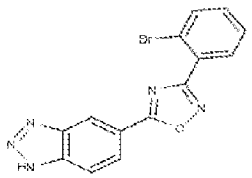
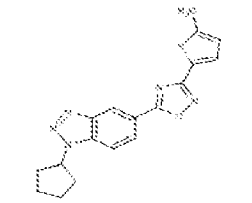
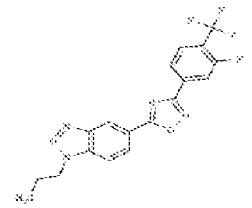
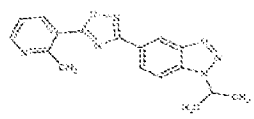
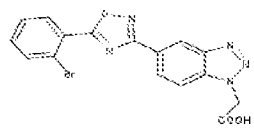
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	153	2,2-diethyl-6-(3-(4-(methylamino)phenyl)-1,2,4-oxadiazol-5-yl)chroman-4-one	377.44	378.2
	154	5-{3-[1-(2-methylphenyl)ethyl]-1,2,4-oxadiazol-5- yl}-1-(2-methylpropyl)-1H-1,2,3-benzotriazole	361.45	362.2
	155	1-cyclopropyl-5-[3-(2-methoxypyridin-4-yl)-1,2,4-oxadiazol-5-yl]-1H-1,2,3-benzotriazole	334.34	335.1
	156	5-(2,6-dimethylpyridin-4-yl)-3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-oxadiazole	334.38	335.2
	157	5-[3-(5-methylpyrazin-2-yl)-1,2,4-oxadiazol-5-yl]-1- (propan-2-yl)-1H-1,2,3-benzotriazole	321.34	322.1
	158	1-cyclohexyl-5-[3-(3,5-dimethylphenyl)-1,2,4- oxadiazol-5-yl]-1H-1,2,3-benzotriazole	373.46	374.2
	159	3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(5-methylpyridin-3-yl)-1,2,4-oxadiazole	320.36	321.1

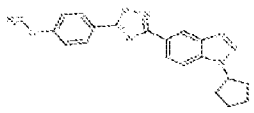
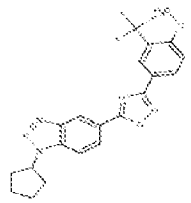
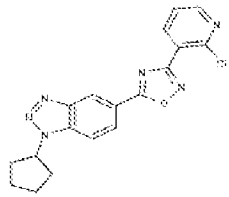
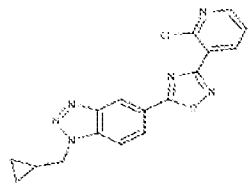
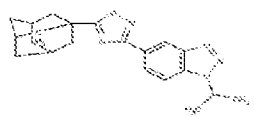
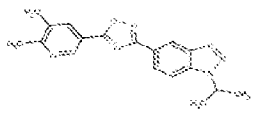
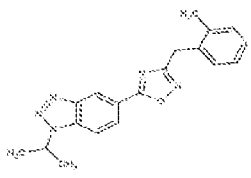
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	160	5-(3-phenyl-1,2,4-oxadiazol-5-yl)-1-propyl-1H- 1,2,3-benzotriazole	305.34	306.1
	161	methyl 3-(5-(5-(2-bromophenyl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)propanoate	428.25	429.9
	162	3-(1-cyclopentyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(o-tolyl)-1,2,4-oxadiazole	345.41	346.1
	163	5-[4-(2-chlorophenyl)-2,3-dihydro-1,3-oxazol-2-yl]-1- (propan-2-yl)-1H-1,2,3-benzotriazole	338.80	339
	164	1-cyclopentyl-5-[3-(4-methylphenyl)-1,2,4- oxadiazol-5-yl]-1H-1,2,3-benzotriazole	345.41	346.3
	165	1-(propan-2-yl)-5-[3-(pyridin-3-yl)-1,2,4- oxadiazol-5-yl]-1H-1,2,3-benzotriazole	306.33	307.3
	166	5-(2,4-dimethylphenyl)-3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-oxadiazole	333.40	334.2

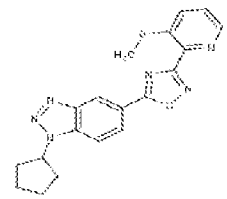
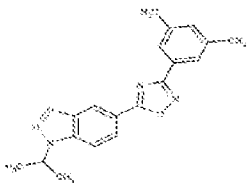
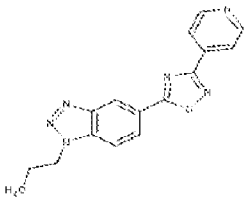
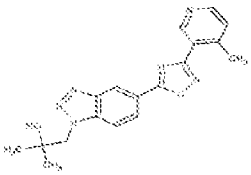
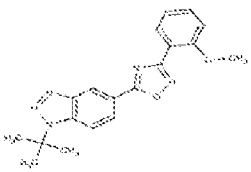
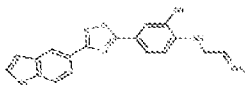
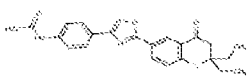
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	167	3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(2-isopropylpyridin-4-yl)-1,2,4-oxadiazole	348.41	349.1
	168	2-{5-[1-(propan-2-yl)-1H-1,2,3-benzotriazol-5-yl]- 1,2,4-oxadiazol-3-yl}quinoline	356.39	357.1
	169	5-[3-(3-methylthiophen-2-yl)-1,2,4-oxadiazol-5-yl]-1- (propan-2-yl)-1H-1,2,3-benzotriazole	325.39	326.1
	170	5-[3-(5-chlorothiophen-2-yl)-1,2,4-oxadiazol-5-yl]-1- (propan-2-yl)-1H-1,2,3-benzotriazole	345.81	346.1
	171	1-cyclopropyl-5-[3-(2-methylphenyl)-1,2,4- oxadiazol-5-yl]-1H-1,2,3-benzotriazole	317.35	318.3
	172	5-{3-[1-(2-methylphenyl)ethyl]-1,2,4-oxadiazol-5- yl}-1-(propan-2-yl)-1H-1,2,3-benzotriazole	347.42	348.1
	173	1-cyclopropyl-5-[3-(2-methoxyphenyl)-1,2,4- oxadiazol-5-yl]-1H-1,2,3-benzotriazole	333.35	334.2

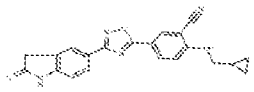
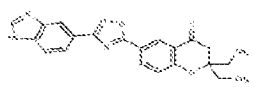
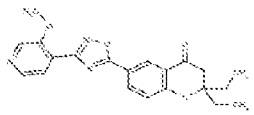
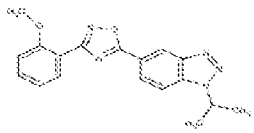
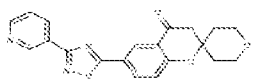
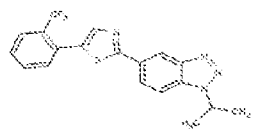
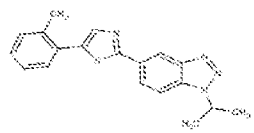
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	174	1-cyclopentyl-5-[3-(pyridin-4-yl)-1,2,4-oxadiazol-5- yl]-1H-1,2,3-benzotriazole	332.37	333.1
	175	1-cyclopentyl-5-[3-(2-methylphenyl)-1,2,4- oxadiazol-5-yl]-1H-1,2,3-benzotriazole	345.41	346.2
	176	6-[3-(pyridin-4-yl)-1,2,4-oxadiazol-5-yl]-3,4- dihydrospiro[1-benzopyran-2,1'-cyclopentane]-4-one	347.37	348.1
	177	5-(3-(1H-benzo[d]imidazol-5-yl)-1,2,4-oxadiazol-5-yl)-2-(allylamino)benzonitrile	342.36	343.1
	178	2,2-diethyl-6-(5-(2-methoxyphenyl)-1,3,4-thiadiazol-2-yl)chroman-4-one	394.49	395.2
	179	4-(5-(2,2-diethyl-4-oxochroman-6-yl)-1,2,4-oxadiazol-3-yl)benzamide	391.43	392.1
	180	2-(5-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-oxadiazol-3-yl)phenol	321.34	322.1

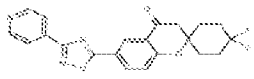
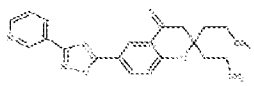
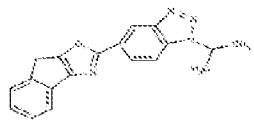
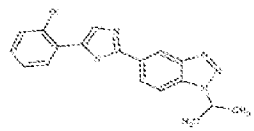
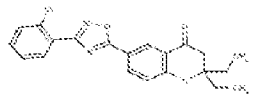
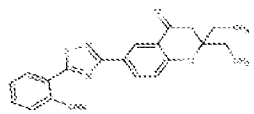
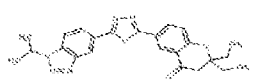
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	181	N-(benzo[d]isoxazol-3-yl)-1-isopropyl-1H-benzo[d][1,2,3]triazole-5-carboxamide	321.34	322.1
	182	1-(2,2-difluoroethyl)-5-[3-(2-methylphenyl)-1,2,4- oxadiazol-5-yl]-1H-1,2,3-benzotriazole	341.32	342.1
	183	5-[4-(2-bromophenyl)-1,3-oxazol-2-yl]-1-(propan-2-yl)-1H-1,2,3-benzotriazole	383.25	383
	184	2-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(2-methoxyphenyl)thiazole	350.44	351
	185	4-(5-(2,2-diethyl-4-oxochroman-6-yl)-1,2,4-oxadiazol-3-yl)-N-methylbenzamide	405.45	406.1
	186	2,2-bis(methoxymethyl)-6-[3-(pyridin-3-yl)-1,2,4- oxadiazol-5-yl]-3,4-dihydro-2H-1-benzopyran-4-one	381.39	282.2
	187	2,2-diethyl-6-[3-(2-hydroxyphenyl)-1,2,4-oxadiazol-5-yl]chroman-4-one	364.40	365.1

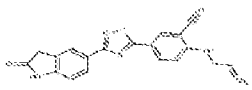
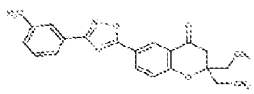
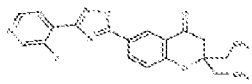
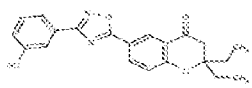
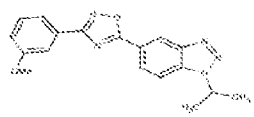
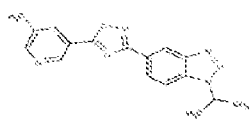
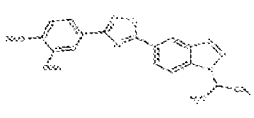
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	188	2,2-dibutyl-6-[3-(pyridin-3-yl)-1,2,4-oxadiazol-5- yl]-3,4-dihydro-2H-1-benzopyran-4-one	405.50	406.2
	189	2-(allylamino)-5-(3-(2-oxo-2,3-dihydrobenzo[d]oxazol-6-yl)-1,2,4-oxadiazol-5-yl)benzonitrile	359.35	360.1
	190	5-[3-(2-bromophenyl)-1,2,4-oxadiazol-5-yl]-1H- 1,2,3-benzotriazole	342.16	342
	192	1-cyclopentyl-5-[3-(5-methylthiophen-2-yl)-1,2,4-oxadiazol-5-yl]-1H-1,2,3-benzotriazole	351.43	352.1
	193	5-{3-[3-fluoro-4-(trifluoromethyl)phenyl]-1,2,4-oxadiazol-5-yl}-1-propyl-1H-1,2,3-benzotriazole	391.33	392.1
	194	3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(2-methylpyridin-3-yl)-1,2,4-oxadiazole	320.36	321
	195	2-(5-(5-(2-bromophenyl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)acetic acid	400.19	400

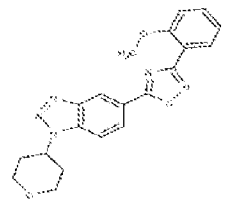
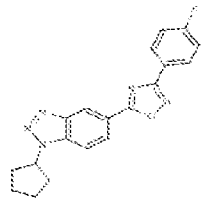
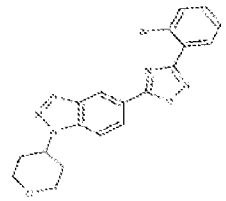
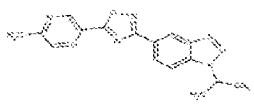
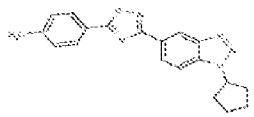
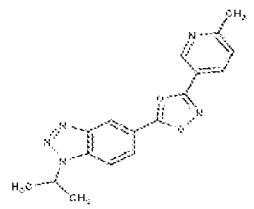
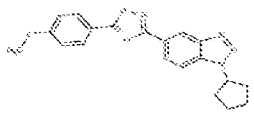
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	196	3-(1-cyclopentyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(4-methoxyphenyl)-1,2,4-oxadiazole	361.41	362
	197	1-cyclopentyl-5-{3-[4-methoxy-3-(trifluoromethyl)phenyl]-1,2,4-oxadiazol-5-yl}-1H- 1,2,3-benzotriazole	429.40	430.1
	198	5-[3-(2-chloropyridin-3-yl)-1,2,4-oxadiazol-5-yl]-1- cyclopentyl-1H-1,2,3-benzotriazole	366.81	367.1
	199	5-[3-(2-chloropyridin-3-yl)-1,2,4-oxadiazol-5-yl]-1-(cyclopropylmethyl)-1H-1,2,3-benzotriazole	352.78	353.1
	200	5-[5-(adamantan-1-yl)-1,2,4-oxadiazol-3-yl]-1- (propan-2-yl)-1H-1,2,3-benzotriazole	363.47	364
	201	5-(5,6-dimethylpyridin-3-yl)-3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-oxadiazole	334.38	335.1
	202	5-{3-[(2-methylphenyl)methyl]-1,2,4-oxadiazol-5- yl}-1-(propan-2-yl)-1H-1,2,3-benzotriazole	333.40	334.1

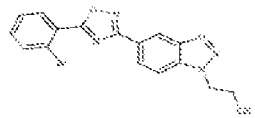
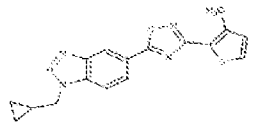
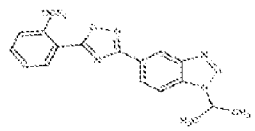
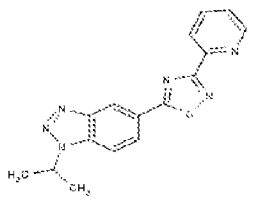
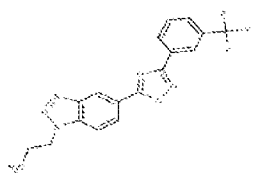
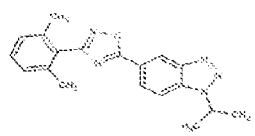
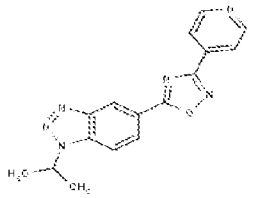
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	203	1-cyclopentyl-5-[3-(3-methoxypyridin-2-yl)-1,2,4-oxadiazol-5-yl]-1H-1,2,3-benzotriazole	362.39	363.1
	204	5-[3-(3,5-dimethylphenyl)-1,2,4-oxadiazol-5-yl]-1- (propan-2-yl)-1H-1,2,3-benzotriazole	333.40	334.1
	205	1-propyl-5-[3-(pyridin-4-yl)-1,2,4-oxadiazol-5-yl]- 1H-1,2,3-benzotriazole	306.33	307.1
	206	2-methyl-1-{5-[3-(4-methylpyridin-3-yl)-1,2,4- oxadiazol-5-yl]-1H-1,2,3-benzotriazol-1-yl}propan-2-ol	350.38	351.1
	207	1-tert-butyl-5-[3-(2-methoxyphenyl)-1,2,4- oxadiazol-5-yl]-1H-1,2,3-benzotriazole	349.39	350.2
	208	5-(3-(1H-indol-5-yl)-1,2,4-oxadiazol-5-yl)-2-(allylamino)benzonitrile	341.37	342.2
	209	N-(4-(5-(2,2-diethyl-4-oxochroman-6-yl)-1,2,4-oxadiazol-3-yl)phenyl)acetamide	405.45	406.2

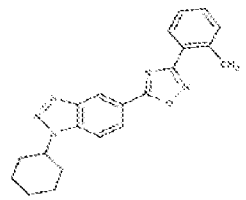
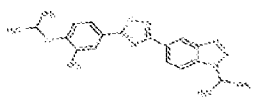
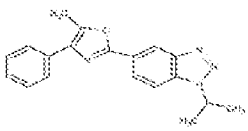
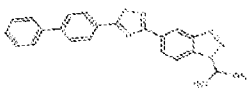
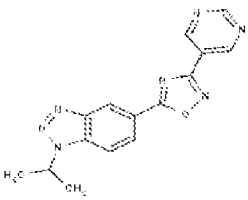
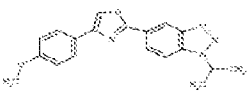
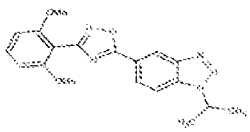
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	210	2-((cyclopropylmethyl)amino)-5-(3-(2-oxoindolin-5-yl)-1,2,4-oxadiazol-5-yl)benzonitrile	371.40	372.1
	211	6-(3-(1H-benzo[d]imidazol-5-yl)-1,2,4-oxadiazol-5-yl)-2,2-diethylchroman-4-one	388.43	389.1
	212	2,2-diethyl-6-(3-(3-methoxypyridin-4-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one	379.42	380.2
	213	5-[3-(2-methoxyphenyl)-1,2,4-thiadiazol-5-yl]-1- (propan-2-yl)-1H-1,2,3-benzotriazole	351.43	352
	214	6-[3-(pyridin-3-yl)-1,2,4-oxadiazol-5-yl]-3,4- dihydrospiro[1-benzopyran-2,4'-oxane]-4-one	363.37	364.1
	215	2-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(2-(trifluoromethyl)phenyl)thiazole	388.41	389.2
	216	2-(1-isopropylbenzotriazol-5-yl)-5-(o-tolyl)thiazole	334.44	335.1

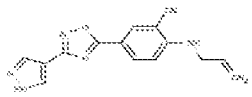
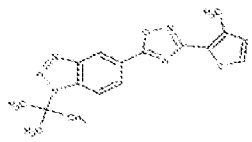
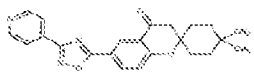
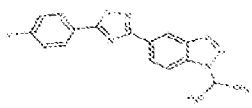
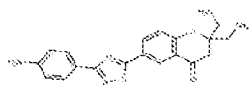
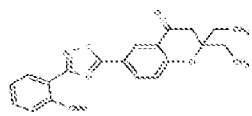
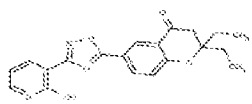
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	217	4',4'-difluoro-6-[3-(pyridin-4-yl)-1,2,4-oxadiazol-5- yl]-3,4-dihydrospiro[1-benzopyran-2,1'-cyclohexane]-4-one	397.38	398.2
	218	2,2-dipropyl-6-[3-(pyridin-3-yl)-1,2,4-oxadiazol-5- yl]-3,4-dihydro-2H-1-benzopyran-4-one	377.44	378.2
	219	5-{8H-indeno[1,2-d][1,3]oxazol-2-yl}-1-(propan-2- yl)-1H-1,2,3-benzotriazole	316.36	317
	220	5-(2-bromophenyl)-2-(1-isopropylbenzotriazol-5-yl)thiazole	399.31	401
	221	6-(3-(2-chlorophenyl)-1,2,4-oxadiazol-5-yl)-2,2-diethylchroman-4-one	382.84	383.1
	222	2,2-diethyl-6-(5-(2-methoxyphenyl)-1,2,4-thiadiazol-3-yl)chroman-4-one	394.49	395.1
	223	2,2-diethyl-6-(5-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-1,3,4-oxadiazol-2-yl)chroman-4-one	431.50	432.2

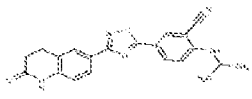
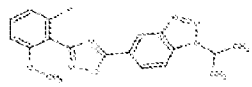
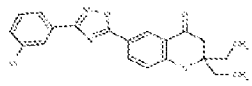
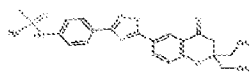
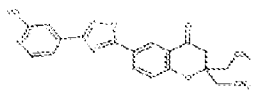
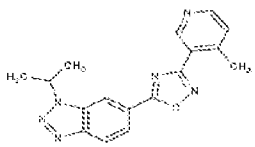
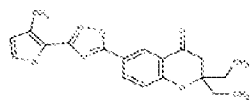
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	224	2-(allylamino)-5-(3-(2-oxoindolin-5-yl)-1,2,4-oxadiazol-5-yl)benzonitrile	357.37	358.1
	225	2,2-diethyl-6-(3-(m-tolyl)-1,2,4-oxadiazol-5-yl)chroman-4-one	362.43	363.1
	226	2,2-diethyl-6-(3-(3-fluoropyridin-4-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one	367.38	368.1
	227	2,2-diethyl-6-[3-(3-hydroxyphenyl)-1,2,4-oxadiazol-5-yl]chroman-4-one	364.40	365.1
	228	5-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-3-(3-methoxyphenyl)-1,2,4-oxadiazole	335.37	336
	229	3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(6-methylpyrazin-2-yl)-1,2,4-oxadiazole	321.34	322.1
	230	3-(3,4-dimethoxyphenyl)-5-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-oxadiazole	365.39	366

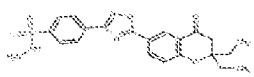
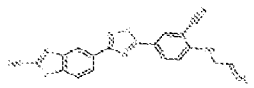
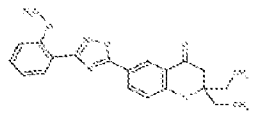
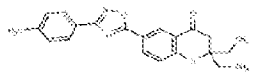
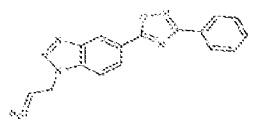
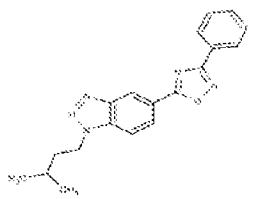
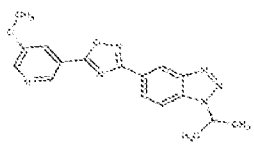
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	231	5-[3-(2-methoxyphenyl)-1,2,4-oxadiazol-5-yl]-1- (oxan-4-yl)-1H-1,2,3-benzotriazole	377.40	378.2
	232	1-cyclopentyl-5-[3-(4-fluorophenyl)-1,2,4- oxadiazol-5-yl]-1H-1,2,3-benzotriazole	349.37	350.2
	233	5-[3-(2-bromophenyl)-1,2,4-oxadiazol-5-yl]-1-(oxan-4- yl)-1H-1,2,3-benzotriazole	426.27	426.1
	234	3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(5-methylpyrazin-2-yl)-1,2,4-oxadiazole	321.34	322.1
	235	3-(1-cyclopentyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(p-tolyl)-1,2,4-oxadiazole	345.41	346
	236	5-[3-(6-methylpyridin-3-yl)-1,2,4-oxadiazol-5-yl]-1- (propan-2-yl)-1H-1,2,3-benzotriazole	320.36	321.1
	237	3-(1-cyclopentyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(4-(methylthio)phenyl)-1,2,4-oxadiazole	377.47	378.1

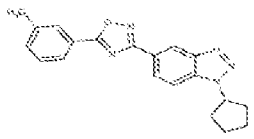
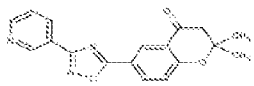
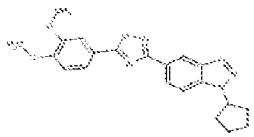
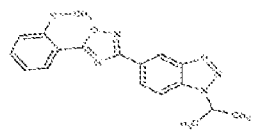
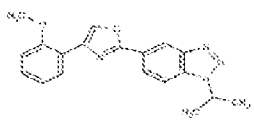
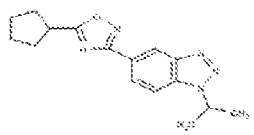
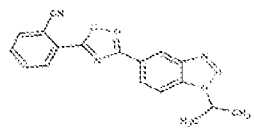
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	238	2-(5-(5-(2-bromophenyl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)ethanol	386.21	386
	239	1-(cyclopropylmethyl)-5-[3-(3-methylthiophen-2-yl)- 1,2,4-oxadiazol-5-yl]-1H-1,2,3-benzotriazole	337.40	338.2
	240	3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(2-(trifluoromethoxy)phenyl)-1,2,4-oxadiazole	389.34	390
	241	1-(propan-2-yl)-5-[3-(pyridin-2-yl)-1,2,4- oxadiazol-5-yl]-1H-1,2,3-benzotriazole	306.33	307.2
	242	1-propyl-5-{3-[3-(trifluoromethyl)phenyl]-1,2,4-oxadiazol-5-yl}-1H-1,2,3-benzotriazole	373.34	374.3
	243	3-(2,6-dimethylphenyl)-5-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-oxadiazole	333.40	334
	244	1-(propan-2-yl)-5-[3-(pyridin-4-yl)-1,2,4- oxadiazol-5-yl]-1H-1,2,3-benzotriazole	306.33	307.1

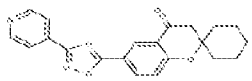
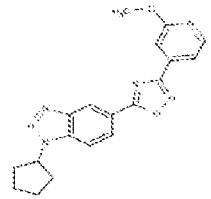
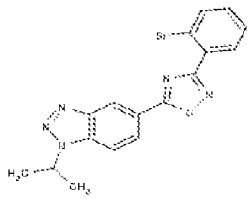
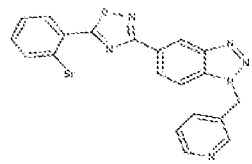
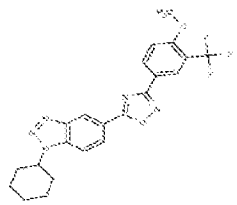
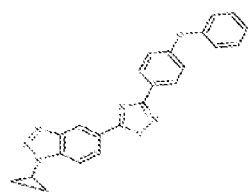
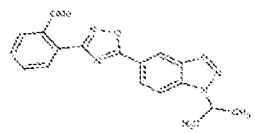
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	245	1-cyclohexyl-5-[3-(2-methylphenyl)-1,2,4-oxadiazol-5-yl]-1H-1,2,3-benzotriazole	359.43	360.2
	246	5-(4-isopropoxy-3-(trifluoromethyl)phenyl)-3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-oxadiazole	431.42	432
	247	5-(5-methyl-4-phenyl-1,3-oxazol-2-yl)-1-(propan-2- yl)-1H-1,2,3-benzotriazole	318.38	319
	248	5-([1,1'-biphenyl]-4-yl)-3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-oxadiazole	381.44	382.1
	249	1-(propan-2-yl)-5-[3-(pyrimidin-5-yl)-1,2,4- oxadiazol-5-yl]-1H-1,2,3-benzotriazole	307.32	308.1
	250	5-[4-(4-methoxyphenyl)-1,3-oxazol-2-yl]-1-(propan-2- yl)-1H-1,2,3-benzotriazole	334.38	335
	251	3-(2,6-dimethoxyphenyl)-5-(1-isopropylbenzotriazol-5-yl)-1,2,4-oxadiazole	365.39	366.1

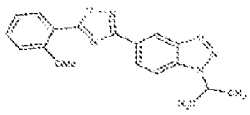
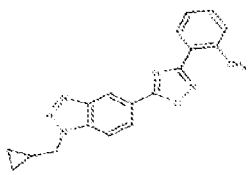
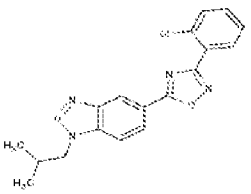
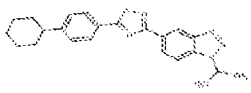
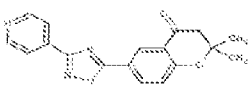
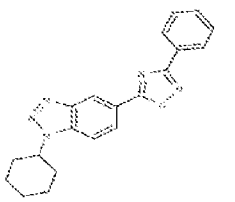
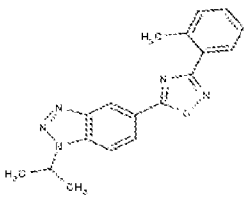
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	252	5-(3-(1H-pyrazol-4-yl)-1,2,4-oxadiazol-5-yl)-2-(allylamino)benzonitrile	292.30	293.1
	253	1-tert-butyl-5-[3-(3-methylthiophen-2-yl)-1,2,4-oxadiazol-5-yl]-1H-1,2,3-benzotriazole	339.42	340.1
	254	4',4'-dimethyl-6-[3-(pyridin-4-yl)-1,2,4-oxadiazol-5- yl]-3,4-dihydrospiro[1-benzopyran-2,1'-cyclohexane]-4-one	389.46	390.2
	255	5-(4-fluorophenyl)-3-(1-isopropylbenzotriazol-5-yl)-1,2,4-oxadiazole	323.33	324.1
	256	6-(3-(4-aminophenyl)-1,2,4-oxadiazol-5-yl)-2,2-diethylchroman-4-one	363.42	364.2
	257	2,2-diethyl-6-(3-(2-methoxyphenyl)-1,2,4-thiadiazol-5-yl)chroman-4-one	394.49	395.1
	258	2,2-diethyl-6-(3-(2-hydroxypyridin-3-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one	365.39	366.3

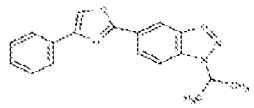
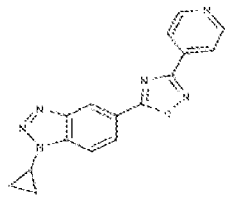
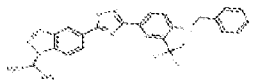
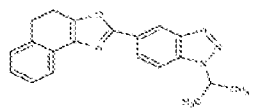
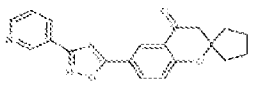
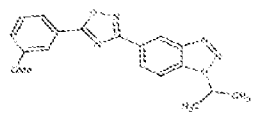
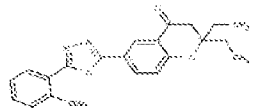
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	259	2-(isopropylamino)-5-(3-(2-oxo-1,2,3,4-tetrahydroquinolin-6-yl)-1,2,4-oxadiazol-5-yl)benzonitrile	373.42	374.1
	260	3-(2-fluoro-6-methoxy-phenyl)-5-(1-isopropylbenzotriazol-5-yl)-1,2,4-oxadiazole	353.36	354.1
	261	6-[3-(3-chlorophenyl)-1,2,4-oxadiazol-5-yl]-2,2-diethyl-chroman-4-one	382.84	383.1
	262	N-(4-(5-(2,2-diethyl-4-oxochroman-6-yl)-1,2,4-oxadiazol-3-yl)phenyl)methanesulfonamide	441.50	442
	263	2,2-diethyl-6-[3-(2-hydroxy-4-pyridyl)-1,2,4-oxadiazol-5-yl]chroman-4-one	365.39	366.1
	264	6-[3-(4-methylpyridin-3-yl)-1,2,4-oxadiazol-5-yl]-1- (propan-2-yl)-1H-1,2,3-benzotriazole	320.36	321.1
	265	2,2-diethyl-6-(3-(3-methylthiophen-2-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one	368.45	369.1

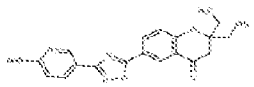
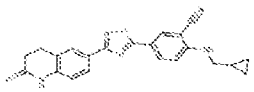
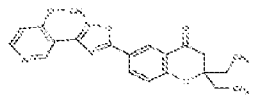
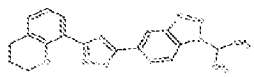
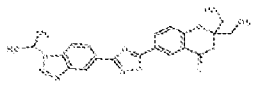
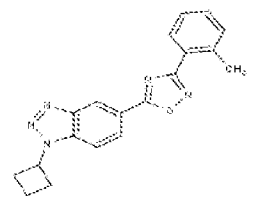
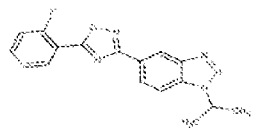
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	266	4-(5-(2,2-diethyl-4-oxochroman-6-yl)-1,2,4-oxadiazol-3-yl)-N-methylbenzenesulfonamide	441.50	442.1
	267	2-(allylamino)-5-(3-(2-aminobenzo[d]thiazol-5-yl)-1,2,4-oxadiazol-5-yl)benzonitrile	374.42	375.3
	268	2,2-diethyl-6-[3-(2-methoxyphenyl)-1,2,4-oxadiazol-5-yl]chroman-4-one	378.43	379.1
	269	2,2-diethyl-6-[3-(p-tolyl)-1,2,4-oxadiazol-5-yl]chroman-4-one	362.43	363.1
	270	5-(3-phenyl-1,2,4-oxadiazol-5-yl)-1-(prop-2-en-1- yl)-1H-1,2,3-benzotriazole	303.33	
	271	1-(3-methylbutyl)-5-(3-phenyl-1,2,4-oxadiazol-5- yl)-1H-1,2,3-benzotriazole	333.40	334.2
	272	3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(5-methoxypyridin-3-yl)-1,2,4-oxadiazole	336.36	337.1

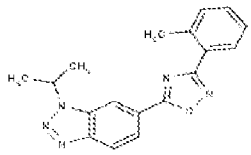
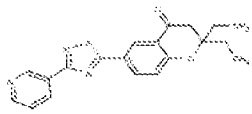
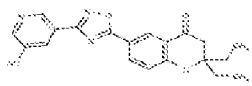
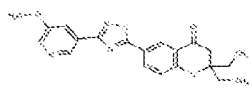
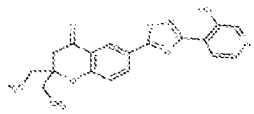
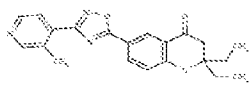
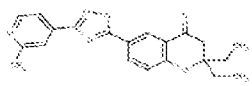
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	273	3-(1-cyclopentyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(m-tolyl)-1,2,4-oxadiazole	345.41	346
	274	2,2-dimethyl-6-[3-(pyridin-3-yl)-1,2,4-oxadiazol-5- yl]-3,4-dihydro-2H-1-benzopyran-4-one	321.34	322.1
	275	3-(1-cyclopentyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(3,4-dimethoxyphenyl)-1,2,4-oxadiazole	391.43	392.1
	276	3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(2-(methylthio)phenyl)-1,2,4-oxadiazole	351.43	352.1
	277	5-[4-(2-methoxyphenyl)-1,3-oxazol-2-yl]-1-(propan-2- yl)-1H-1,2,3-benzotriazole	334.38	335
	278	5-(5-cyclopentyl-1,2,4-oxadiazol-3-yl)-1-(propan-2- yl)-1H-1,2,3-benzotriazole5-(5-cyclopentyl-1,2,4-oxadiazol-3-yl)-1-(propan-2-yl)-1H-1,2,3-benzotriazole	297.36	298
	279	2-(3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-oxadiazol-5-yl)benzonitrile	330.35	331

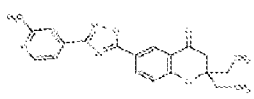
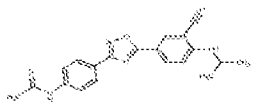
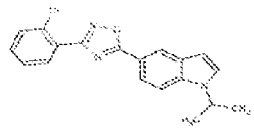
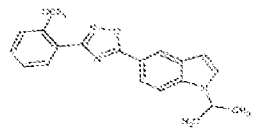
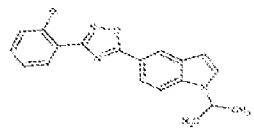
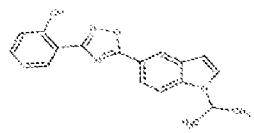
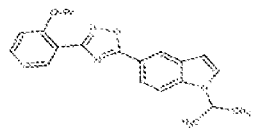
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	280	6-[3-(pyridin-4-yl)-1,2,4-oxadiazol-5-yl]-3,4- dihydrospiro[1-benzopyran-2,1'-cyclohexane]-4-one	361.40	362.1
	281	1-cyclopentyl-5-[3-(2-methoxypyridin-4-yl)-1,2,4-oxadiazol-5-yl]-1H-1,2,3-benzotriazole	362.39	363.1
	282	5-[3-(2-bromophenyl)-1,2,4-oxadiazol-5-yl]-1- (propan-2-yl)-1H-1,2,3-benzotriazole	384.24	384.2
	283	5-(2-bromophenyl)-3-(1-(pyridin-3-ylmethyl)-1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-oxadiazole	433.27	434.9
	284	1-cyclohexyl-5-{3-[4-methoxy-3-(trifluoromethyl)phenyl]-1,2,4-oxadiazol-5-yl}-1H- 1,2,3-benzotriazole	443.43	444.2
	285	1-cyclopropyl-5-[3-(4-phenoxyphenyl)-1,2,4- oxadiazol-5-yl]-1H-1,2,3-benzotriazole	395.42	396.2
	286	5-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-3-(2-methoxyphenyl)-1,2,4-oxadiazole	335.37	356

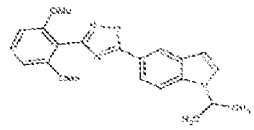
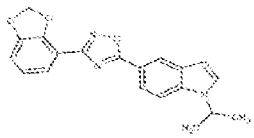
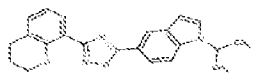
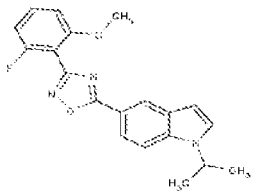
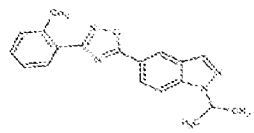
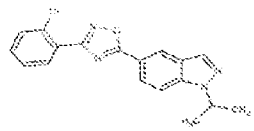
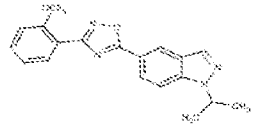
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	287	3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(2-methoxyphenyl)-1,2,4-oxadiazole	335.37	356
	288	1-(cyclopropylmethyl)-5-[3-(2-methylphenyl)-1,2,4- oxadiazol-5-yl]-1H-1,2,3-benzotriazole	331.38	332.2
	289	5-[3-(2-chlorophenyl)-1,2,4-oxadiazol-5-yl]-1-(2-methylpropyl)-1H-1,2,3-benzotriazole	353.81	354.2
	290	5-(4-cyclohexylphenyl)-3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-oxadiazole	387.49	388.1
	291	2,2-dimethyl-6-[3-(pyridin-4-yl)-1,2,4-oxadiazol-5- yl]-3,4-dihydro-2H-1-benzopyran-4-one	321.34	322.1
	292	1-cyclohexyl-5-(3-phenyl-1,2,4-oxadiazol-5-yl)-1H- 1,2,3-benzotriazole	345.41	346.3
	293	5-[3-(2-methylphenyl)-1,2,4-oxadiazol-5-yl]-1- (propan-2-yl)-1H-1,2,3-benzotriazole	319.37	320.3

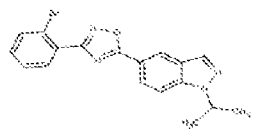
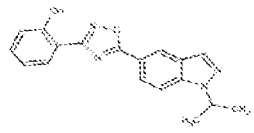
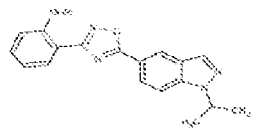
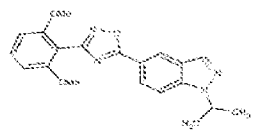
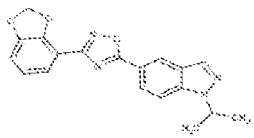
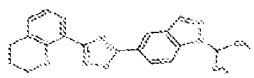
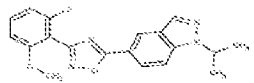
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	294	5-(4-phenyl-1,3-oxazol-2-yl)-1-(propan-2-yl)-1H- 1,2,3-benzotriazole	304.35	305
	295	1-cyclopropyl-5-[3-(pyridin-4-yl)-1,2,4-oxadiazol-5- yl]-1H-1,2,3-benzotriazole	304.31	305.2
	296	5-{3-[4-(benzyloxy)-3-(trifluoromethyl)phenyl]- 1,2,4-oxadiazol-5-yl}-1-(propan-2-yl)-1H-1,2,3- benzotriazole	479.46	480.2
	297	5-{4H,5H-naphtho[2,1-d][1,3]oxazol-2-yl}-1-(propan-2-yl)-1H-1,2,3-benzotriazole	330.39	331
	298	6-[3-(pyridin-3-yl)-1,2,4-oxadiazol-5-yl]-3,4- dihydrospiro[1-benzopyran-2,1'-cyclopentane]-4-one	347.37	348.1
	299	3-(1-isopropylbenzotriazol-5-yl)-5-(3-methoxyphenyl)-1,2,4-oxadiazole	335.37	336.1
	300	2,2-diethyl-6-(5-(2-methoxyphenyl)-1,3,4-oxadiazol-2-yl)chroman-4-one	378.43	379.3

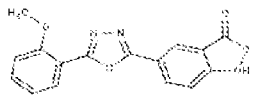
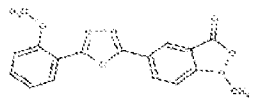
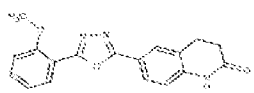
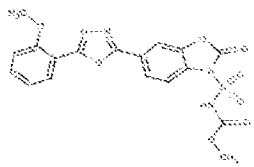
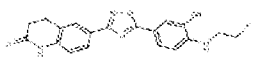
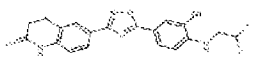
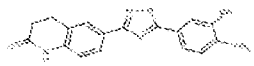
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	301	2,2-diethyl-6-[3-(6-methoxy-3-pyridyl)-1,2,4-oxadiazol-5-yl]chroman-4-one	379.42	380.3
	302	2-((cyclopropylmethyl)amino)-5-(3-(2-oxo-1,2,3,4-tetrahydroquinolin-6-yl)-1,2,4-oxadiazol-5-yl)benzonitrile	385.43	386.2
	303	2,2-diethyl-6-(3-(4-methoxypyridin-3-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one	379.42	380.3
	304	3-chroman-8-yl-5-(1-isopropylbenzotriazol-5-yl)-1,2,4-oxadiazole	361.41	362.1
	305	2,2-diethyl-6-(3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one	431.50	432.2
	306	1-cyclobutyl-5-[3-(2-methylphenyl)-1,2,4-oxadiazol-5-yl]-1H-1,2,3-benzotriazole	331.38	332.1
	307	5-(2-fluorophenyl)-3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-oxadiazole	323.33	324

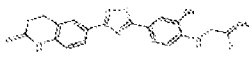
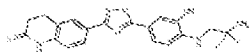
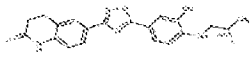
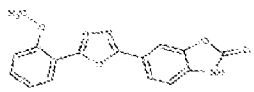
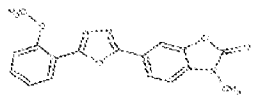
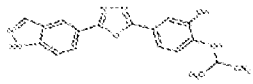
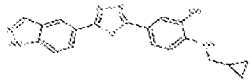
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	308	6-[3-(2-methylphenyl)-1,2,4-oxadiazol-5-yl]-1- (propan-2-yl)-1H-1,2,3-benzotriazole	319.37	320.1
	309	2,2-diethyl-6-(3-(pyridin-3-yl)-1,2,4-thiadiazol-5-yl)chroman-4-one	365.45	366
	310	2,2-diethyl-6-[3-(5-hydroxy-3-pyridyl)-1,2,4-oxadiazol-5-yl]chroman-4-one	365.39	366.1
	311	2,2-diethyl-6-(3-(5-methoxypyridin-3-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one	379.42	380.1
	312	2,2-diethyl-6-(3-(3-hydroxypyridin-4-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one	365.39	366
	313	2,2-diethyl-6-(3-(3-(trifluoromethyl)pyridin-4-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one	417.39	418
	314	2,2-diethyl-6-(3-(2-(trifluoromethyl)pyridin-4-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one	417.39	418

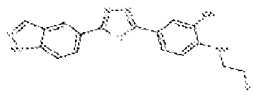
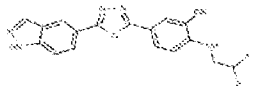
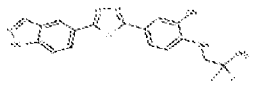
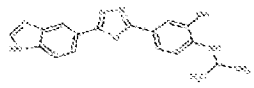
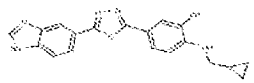
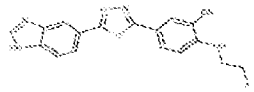
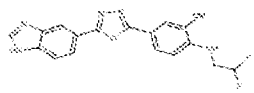
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	315	2,2-diethyl-6-(3-(2-methylpyridin-4-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one	363.42	364.1
	316	N-(4-(5-(3-cyano-4-(isopropylamino)phenyl)-1,2,4-oxadiazol-3-yl)phenyl)acetamide	361.41	362.1
	320	3-(2-chlorophenyl)-5-(1-isopropyl-1H-indol-5-yl)-1,2,4-oxadiazole	337.81	338
	321	5-(1-isopropyl-1H-indol-5-yl)-3-(2-(trifluoromethoxy)phenyl)-1,2,4-oxadiazole	387.36	388.1
	322	3-(2-bromophenyl)-5-(1-isopropyl-1H-indol-5-yl)-1,2,4-oxadiazole	382.26	384
	323	2-(5-(1-isopropyl-1H-indol-5-yl)-1,2,4-oxadiazol-3-yl)phenol	319.36	320.1
	324	3-(2-isopropoxyphenyl)-5-(1-isopropyl-1H-indol-5-yl)-1,2,4-oxadiazole	361.45	362.1

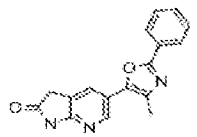
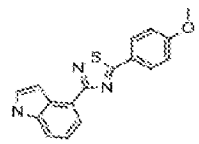
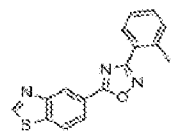
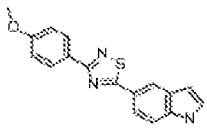
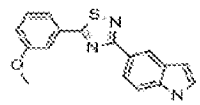
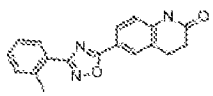
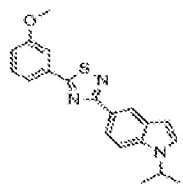
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	325	3-(2,6-dimethoxyphenyl)-5-(1-isopropylindol-5-yl)-1,2,4-oxadiazole	363.42	364.1
	326	3-(benzo[d][1,3]dioxol-4-yl)-5-(1-isopropyl-1H-indol-5-yl)-1,2,4-oxadiazole	347.37	348.1
	327	3-chroman-8-yl-5-(1-isopropylindol-5-yl)-1,2,4-oxadiazole	359.43	360.1
	328	3-(2-fluoro-6-methoxy-phenyl)-5-(1-isopropylindol-5-yl)-1,2,4-oxadiazole	351.38	352.1
	329	5-(1-isopropyl-1H-indazol-5-yl)-3-(o-tolyl)-1,2,4-oxadiazole	318.38	319.1
	330	3-(2-chlorophenyl)-5-(1-isopropyl-1H-indazol-5-yl)-1,2,4-oxadiazole	338.80	339
	331	5-(1-isopropyl-1H-indazol-5-yl)-3-(2-(trifluoromethoxy)phenyl)-1,2,4-oxadiazole	388.35	389.1

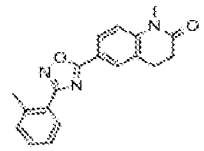
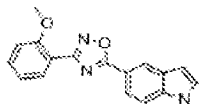
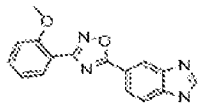
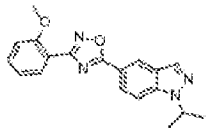
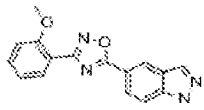
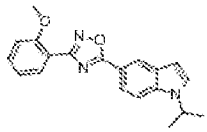
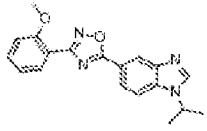
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	332	3-(2-bromophenyl)-5-(1-isopropyl-1H-indazol-5-yl)-1,2,4-oxadiazole	383.25	385.1
	333	2-(5-(1-isopropyl-1H-indazol-5-yl)-1,2,4-oxadiazol-3-yl)phenol	320.35	321.1
	334	3-(2-isopropoxyphenyl)-5-(1-isopropyl-1H-indazol-5-yl)-1,2,4-oxadiazole	362.43	363.1
	335	3-(2,6-dimethoxyphenyl)-5-(1-isopropylindazol-5-yl)-1,2,4-oxadiazole	364.41	365.1
	336	3-(benzo[d][1,3]dioxol-4-yl)-5-(1-isopropyl-1H-indazol-5-yl)-1,2,4-oxadiazole	348.36	349.1
	337	3-chroman-8-yl-5-(1-isopropylindazol-5-yl)-1,2,4-oxadiazole	360.42	361.1
	338	3-(2-fluoro-6-methoxy-phenyl)-5-(1-isopropylindazol-5-yl)-1,2,4-oxadiazole	352.37	353.1

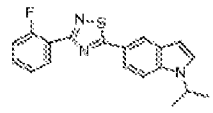
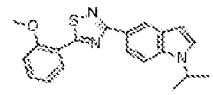
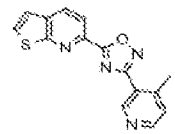
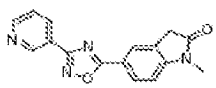
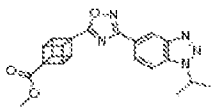
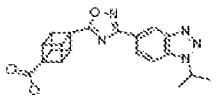
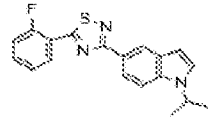
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	339	5-[5-(2-methoxyphenyl)-1,3,4-oxadiazol-2-yl]-1,3- dihydro-2,1-benzoxazol-3-one	309.28	310.2
	340	5-[5-(2-methoxyphenyl)-1,3,4-oxadiazol-2-yl]-1- methyl-1,3-dihydro-2,1-benzoxazol-3-one	323.31	324.1
	341	6-[5-(2-methoxyphenyl)-1,3,4-oxadiazol-2-yl]- 1,2,3,4-tetrahydroquinolin-2-one	321.34	322.1
	342	methyl N-({6-[5-(2-methoxyphenyl)-1,3,4-oxadiazol-2-yl]-2-oxo-2,3-dihydro-1,3-benzoxazol-3-yl}sulfonyl)carbamate	446.39	447
	343	2-[(2-fluoroethyl)amino]-5-[3-(2-oxo-1,2,3,4- tetrahydroquinolin-6-yl)-1,2,4-oxadiazol-5-yl]benzonitrile	377.38	378.1
	344	2-[(2,2-difluoroethyl)amino]-5-[3-(2-oxo-1,2,3,4- tetrahydroquinolin-6-yl)-1,2,4-oxadiazol-5-yl]benzonitrile	395.37	396.1
	345	2-amino-5-[3-(2-oxo-1,2,3,4-tetrahydroquinolin-6- yl)-1,2,4-oxadiazol-5-yl]benzonitrile	331.34	332.1

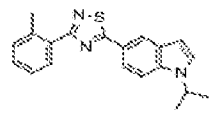
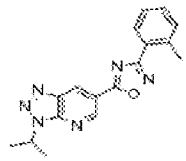
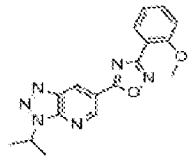
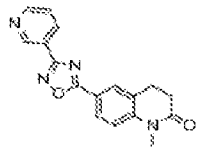
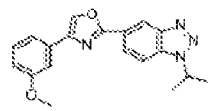
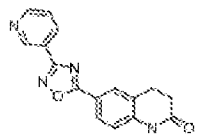
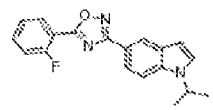
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	346	2-[(2-fluoroprop-2-en-1-yl)amino]-5-[3-(2-oxo- 1,2,3,4-tetrahydroquinolin-6-yl)-1,2,4-oxadiazol-5- yl]benzonitrile	389.39	390.1
	347	2-[(2,2-difluoropropyl)amino]-5-[3-(2-oxo-1,2,3,4- tetrahydroquinolin-6-yl)-1,2,4-oxadiazol-5-yl]benzonitrile	409.40	410.1
	348	2-[(2-fluoropropyl)amino]-5-[3-(2-oxo-1,2,3,4- tetrahydroquinolin-6-yl)-1,2,4-oxadiazol-5-yl]benzonitrile	391.41	392.1
	349	6-[5-(2-methoxyphenyl)-1,3,4-oxadiazol-2-yl]-2,3- dihydro-1,3-benzoxazol-2-one	309.28	310
	350	6-[5-(2-methoxyphenyl)-1,3,4-oxadiazol-2-yl]-3- methyl-2,3-dihydro-1,3-benzoxazol-2-one	323.31	324.1
	351	5-[5-(1H-indazol-5-yl)-1,3,4-oxadiazol-2-yl]-2- [(propan-2-yl)amino]benzonitrile	344.38	345.2
	352	2-[(cyclopropylmethyl)amino]-5-[5-(1H-indazol-5- yl)-1,3,4-oxadiazol-2-yl]benzonitrile	356.39	357.1

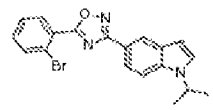
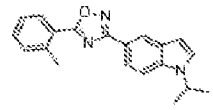
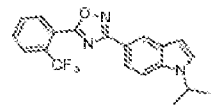
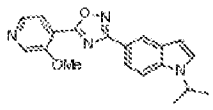
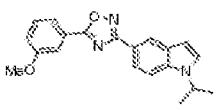
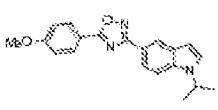
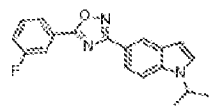
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	353	2-[(2-fluoroethyl)amino]-5-[5-(1H-indazol-5-yl)- 1,3,4-oxadiazol-2-yl]benzonitrile	348.34	349.1
	354	2-[(2,2-difluoroethyl)amino]-5-[5-(1H-indazol-5- yl)-1,3,4-oxadiazol-2-yl]benzonitrile	366.33	367.1
	355	2-[(2,2-difluoropropyl)amino]-5-[5-(1H-indazol-5- yl)-1,3,4-oxadiazol-2-yl]benzonitrile	380.36	381.1
	356	5-[5-(1H-1,3-benzodiazol-5-yl)-1,3,4-oxadiazol-2- yl]-2-[(propan-2-yl)amino]benzonitrile	344.38	345.1
	357	5-[5-(1H-1,3-benzodiazol-5-yl)-1,3,4-oxadiazol-2- yl]-2-[(cyclopropylmethyl)amino]benzonitrile	356.39	357.1
	358	5-[5-(1H-1,3-benzodiazol-5-yl)-1,3,4-oxadiazol-2- yl]-2-[(2-fluoroethyl)amino]benzonitrile	348.34	349.1
	359	5-[5-(1H-1,3-benzodiazol-5-yl)-1,3,4-oxadiazol-2- yl]-2-[(2,2-difluoroethyl)amino]benzonitrile	366.33	367.1

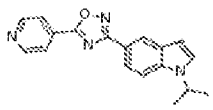
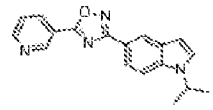
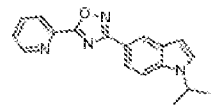
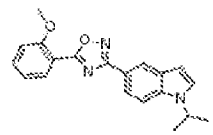
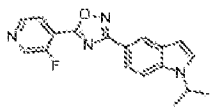
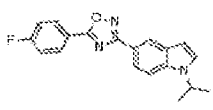
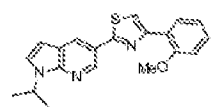
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	360	5-(4-methyl-2-phenyl-1,3-oxazol-5-yl)-1H,2H,3H- pyrrolo[2,3-b]pyridin-2-one	291.1	292.1
	361	4-[5-(4-methoxyphenyl)-1,2,4-thiadiazol-3-yl]-1H- indole	307.08	308
	362	5-[3-(2-methylphenyl)-1,2,4-oxadiazol-5-yl]-1,3- benzothiazole	293.06	294.2
	363	5-[3-(4-methoxyphenyl)-1,2,4-thiadiazol-5-yl]-1H- indole	307.08	308
	364	5-[5-(3-methoxyphenyl)-1,2,4-thiadiazol-3-yl]-1H- indole	307.08	308
	365	6-[3-(2-methylphenyl)-1,2,4-oxadiazol-5-yl]- 1,2,3,4-tetrahydroquinolin-2-one	305.12	306.1
	366	5-[5-(3-methoxyphenyl)-1,2,4-thiadiazol-3-yl]-1- (propan-2-yl)-1H-indole	349.12	350

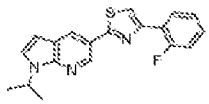
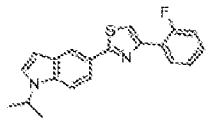
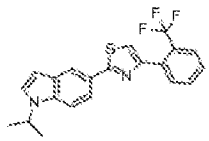
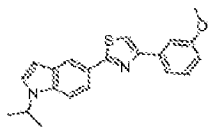
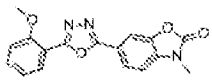
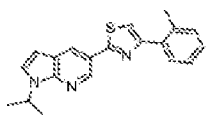
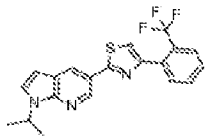
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	367	1-methyl-6-[3-(2-methylphenyl)-1,2,4-oxadiazol-5- yl]-1,2,3,4-tetrahydroquinolin-2-one	319.13	320.2
	368	5-(1H-indol-5-yl)-3-(2-methoxyphenyl)-1,2,4-oxadiazole	291.1	292
	369	5-(1H-benzo[d]imidazol-5-yl)-3-(2-methoxyphenyl)-1,2,4-oxadiazole	292.1	293.2
	370	5-(1-isopropyl-1H-indazol-5-yl)-3-(2-methoxyphenyl)-1,2,4-oxadiazole	334.14	335.3
	371	5-(1H-indazol-5-yl)-3-(2-methoxyphenyl)-1,2,4-oxadiazole	292.1	293.2
	372	5-(1-isopropyl-1H-indol-5-yl)-3-(2-methoxyphenyl)-1,2,4-oxadiazole	333.15	334.1
	373	5-(1-isopropyl-1H-benzo[d]imidazol-5-yl)-3-(2-methoxyphenyl)-1,2,4-oxadiazole	334.14	335.2

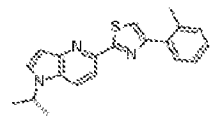
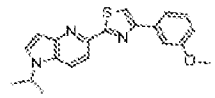
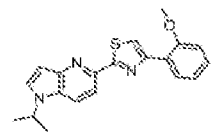
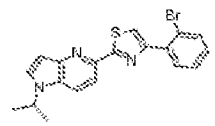
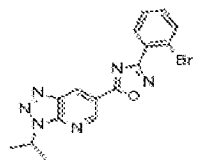
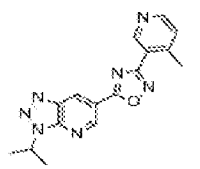
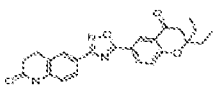
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	374	5-[3-(2-fluorophenyl)-1,2,4-thiadiazol-5-yl]-1- (propan-2-yl)-1H-indole	337.1	338
	375	5-[5-(2-methoxyphenyl)-1,2,4-thiadiazol-3-yl]-1- (propan-2-yl)-1H-indole	349.12	350
	376	4-methyl-3-(5-{thieno[2,3-b]pyridin-6-yl}-1,2,4- oxadiazol-3-yl)pyridine	294.06	295
	377	1-methyl-5-[3-(pyridin-3-yl)-1,2,4-oxadiazol-5-yl]- 2,3-dihydro-1H-indol-2-one	292.1	293.1
	378	8-{3-[1-(propan-2-yl)-1H-1,2,3-benzotriazol-5- yl]-1,2,4-oxadiazol-5-yl}cubane-1-carboxylate	389.15	390
	379	8-{3-[1-(propan-2-yl)-1H-1,2,3-benzotriazol-5-yl]- 1,2,4-oxadiazol-5-yl}cubane-1-carboxylic acid	375.13	376
	380	5-[5-(2-fluorophenyl)-1,2,4-thiadiazol-3-yl]-1- (propan-2-yl)-1H-indole	337.1	338

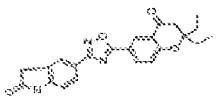
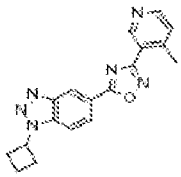
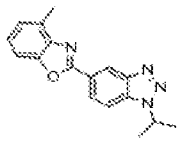
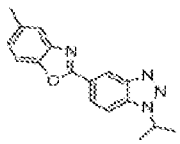
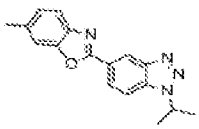
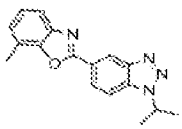
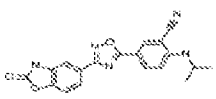
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	381	5-[3-(2-methylphenyl)-1,2,4-thiadiazol-5-yl]-1- (propan-2-yl)-1H-indole	333.13	334
	382	3-(2-methylphenyl)-5-[3-(propan-2-yl)-3H- [1,2,3]triazolo[4,5-b]pyridin-6-yl]-1,2,4- oxadiazole	320.14	321.2
	383	3-(2-methoxyphenyl)-5-[3-(propan-2-yl)-3H- [1,2,3]triazolo[4,5-b]pyridin-6-yl]-1,2,4- oxadiazole	336.13	337.1
	384	1-methyl-6-[3-(pyridin-3-yl)-1,2,4-oxadiazol-5-yl]- 1,2,3,4-tetrahydroquinolin-2-one	306.11	307.1
	385	5-[4-(3-methoxyphenyl)-1,3-oxazol-2-yl]-1-(propan-2- yl)-1H-1,2,3-benzotriazole	334.14	335
	386	6-[3-(pyridin-3-yl)-1,2,4-oxadiazol-5-yl]-1,2,3,4- tetrahydroquinolin-2-one	292.1	293.1
	387	5-(2-fluorophenyl)-3-(1-isopropyl-1H-indol-5-yl)-1,2,4-oxadiazole	321.13	322.3

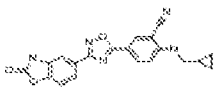
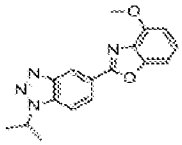
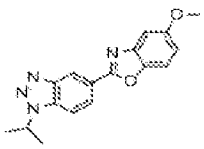
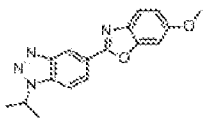
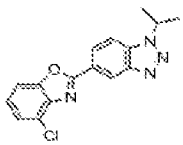
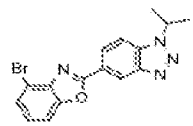
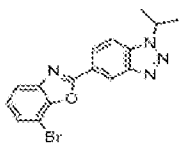
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	388	5-(2-bromophenyl)-3-(1-isopropyl-1H-indol-5-yl)-1,2,4-oxadiazole	381.05	382.2
	389	3-(1-isopropyl-1H-indol-5-yl)-5-(o-tolyl)-1,2,4-oxadiazole	317.15	318.3
	390	3-(1-isopropyl-1H-indol-5-yl)-5-(2-(trifluoromethyl)phenyl)-1,2,4-oxadiazole	371.12	372.3
	391	3-(1-isopropyl-1H-indol-5-yl)-5-(3-methoxypyridin-4-yl)-1,2,4-oxadiazole	334.14	335.3
	392	3-(1-isopropyl-1H-indol-5-yl)-5-(3-methoxyphenyl)-1,2,4-oxadiazole	333.15	334.3
	393	3-(1-isopropyl-1H-indol-5-yl)-5-(4-methoxyphenyl)-1,2,4-oxadiazole	333.15	334.2
	394	5-(3-fluorophenyl)-3-(1-isopropyl-1H-indol-5-yl)-1,2,4-oxadiazole	321.13	322.1

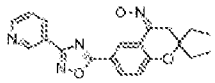
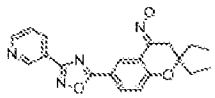
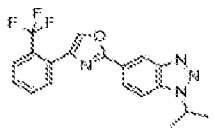
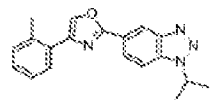
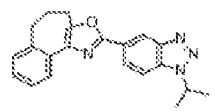
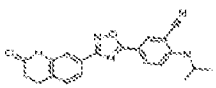
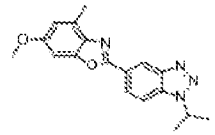
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	395	3-(1-isopropyl-1H-indol-5-yl)-5-(pyridin-4-yl)-1,2,4-oxadiazole	304.13	305.1
	396	3-(1-isopropyl-1H-indol-5-yl)-5-(pyridin-3-yl)-1,2,4-oxadiazole	304.13	305.1
	397	3-(1-isopropyl-1H-indol-5-yl)-5-(pyridin-2-yl)-1,2,4-oxadiazole	304.13	305.1
	398	3-(1-isopropyl-1H-indol-5-yl)-5-(2-methoxyphenyl)-1,2,4-oxadiazole	333.15	334.2
	399	5-(3-fluoropyridin-4-yl)-3-(1-isopropyl-1H-indol-5-yl)-1,2,4-oxadiazole	322.12	323
	400	5-(4-fluorophenyl)-3-(1-isopropyl-1H-indol-5-yl)-1,2,4-oxadiazole	321.13	322.1
	401	2-(1-isopropyl-1H-pyrrolo[2,3-b]pyridin-5-yl)-4-(2-methoxyphenyl)thiazole	349.12	350

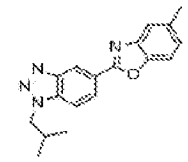
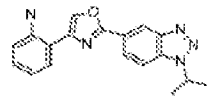
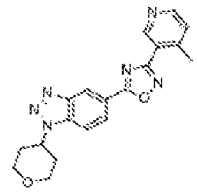
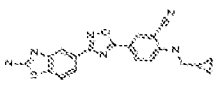
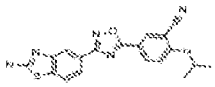
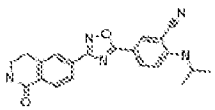
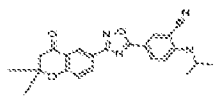
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	402	4-(2-fluorophenyl)-2-(1-isopropyl-1H-pyrrolo[2,3-b]pyridin-5-yl)thiazole	337.1	338.1
	403	4-(2-fluorophenyl)-2-(1-isopropylindol-5-yl)thiazole	336.11	337.1
	404	2-(1-isopropylindol-5-yl)-4-[2-(trifluoromethyl)phenyl]thiazole	386.11	387.1
	405	2-(1-isopropylindol-5-yl)-4-(3-methoxyphenyl)thiazole	348.13	349.1
	406	6-[5-(2-methoxyphenyl)-1,3,4-oxadiazol-2-yl]-3- methyl-2,3-dihydro-1,3-benzoxazol-2-one	323.09	324.1
	407	2-(1-isopropylpyrrolo[2,3-b]pyridin-5-yl)-4-(o-tolyl)thiazole	333.13	334.1
	408	2-(1-isopropylpyrrolo[2,3-b]pyridin-5-yl)-4-[2-(trifluoromethyl)phenyl]thiazole	387.1	388.1

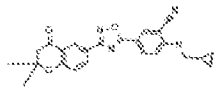
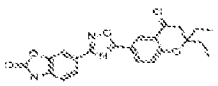
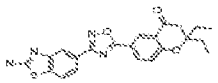
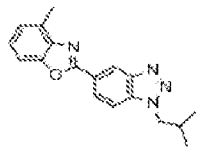
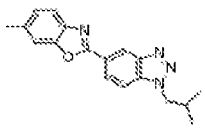
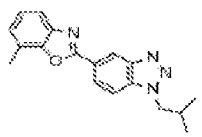
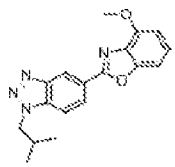
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	409	2-(1-isopropylpyrrolo[3,2-b]pyridin-5-yl)-4-(o-tolyl)thiazole	333.13	334.1
	410	2-(1-isopropylpyrrolo[3,2-b]pyridin-5-yl)-4-(3-methoxyphenyl)thiazole	349.12	350.1
	411	2-(1-isopropyl-1H-pyrrolo[3,2-b]pyridin-5-yl)-4-(2-methoxyphenyl)thiazole	349.12	350.1
	412	4-(2-bromophenyl)-2-(1-isopropyl-1H-pyrrolo[3,2-b]pyridin-5-yl)thiazole	397.02	400
	413	3-(2-bromophenyl)-5-[3-(propan-2-yl)-3H- [1,2,3]triazolo[4,5-b]pyridin-6-yl]-1,2,4- oxadiazole	384.03	385.1
	414	4-methyl-3-{5-[3-(propan-2-yl)-3H- [1,2,3]triazolo[4,5-b]pyridin-6-yl]-1,2,4- oxadiazol-3-yl}pyridine	321.13	322.1
	415	6-(5-(2,2-diethyl-4-oxochroman-6-yl)-1,2,4-oxadiazol-3-yl)-3,4-dihydroquinolin-2(1H)-one	417.17	418.2

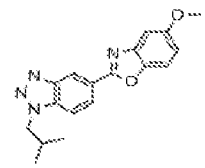
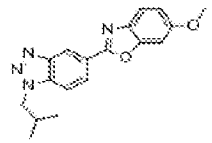
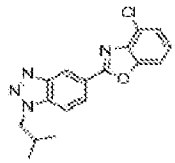
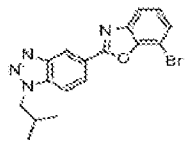
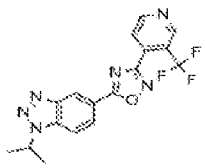
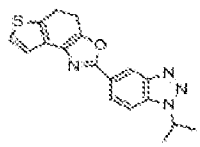
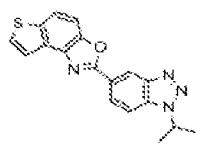
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	416	5-(5-(2,2-diethyl-4-oxochroman-6-yl)-1,2,4-oxadiazol-3-yl)indolin-2-one	403.15	404.1
	417	1-cyclobutyl-5-[3-(4-methylpyridin-3-yl)-1,2,4-oxadiazol-5-yl]-1H-1,2,3-benzotriazole	332.14	333.1
	418	2-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-4-methylbenzo[d]oxazole	292.13	293.1
	419	2-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-methylbenzo[d]oxazole	292.13	293.1
	420	2-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-6-methylbenzo[d]oxazole	292.13	293.1
	421	2-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-7-methylbenzo[d]oxazole	292.13	293.1
	422	2-(isopropylamino)-5-(3-(2-oxo-2,3-dihydrobenzo[d]oxazol-5-yl)-1,2,4-oxadiazol-5-yl)benzonitrile	361.12	362.1

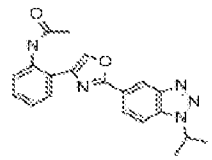
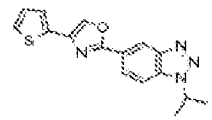
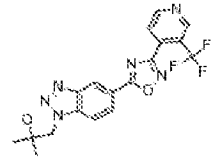
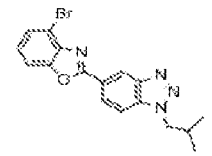
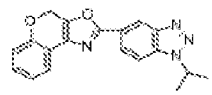
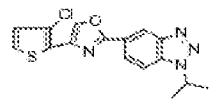
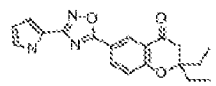
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	423	2-((cyclopropylmethyl)amino)-5-(3-(2-oxo-2,3-dihydrobenzo[d]oxazol-5-yl)-1,2,4-oxadiazol-5-yl)benzonitrile	373.12	374.2
	424	2-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-4-methoxybenzo[d]oxazole	308.13	309
	425	2-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-methoxybenzo[d]oxazole	308.13	309.1
	426	2-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-6-methoxybenzo[d]oxazole	308.13	309
	427	4-chloro-2-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)benzo[d]oxazole	312.08	313
	428	4-bromo-2-(1-isopropylbenzotriazol-5-yl)-1,3-benzoxazole	356.03	357
	429	7-bromo-2-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)benzo[d]oxazole	356.03	359

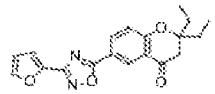
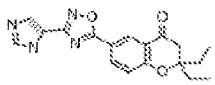
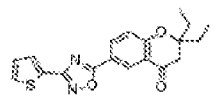
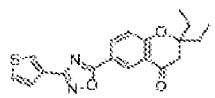
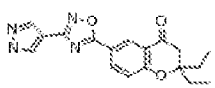
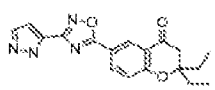
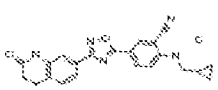
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	430	N-[(4Z)-2,2-diethyl-6-[3-(pyridin-3-yl)-1,2,4- oxadiazol-5-yl]-3,4-dihydro-2H-1-benzopyran-4-ylidene]hydroxylamine	364.15	365.1
	431	N-[(4E)-2,2-diethyl-6-[3-(pyridin-3-yl)-1,2,4- oxadiazol-5-yl]-3,4-dihydro-2H-1-benzopyran-4-ylidene]hydroxylamine	364.15	365.1
	432	1-(propan-2-yl)-5-{4-[2-(trifluoromethyl)phenyl]- 1,3-oxazol-2-yl}-1H-1,2,3-benzotriazole	372.12	373
	433	5-[4-(2-methylphenyl)-1,3-oxazol-2-yl]-1-(propan-2- yl)-1H-1,2,3-benzotriazole	318.15	319
	434	4-[1-(propan-2-yl)-1H-1,2,3-benzotriazol-5-yl]-5- oxa-3-azatricyclo[8.4.0.0²,6]tetradeca-1(14),2(6),3,10,12-pentaene	344.16	345
	435	2-(isopropylamino)-5-(3-(2-oxo-1,2,3,4-tetrahydroquinolin-7-yl)-1,2,4-oxadiazol-5-yl)benzonitrile	373.15	374
	436	2-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-6-methoxy-4-methylbenzo[d]oxazole	322.14	323

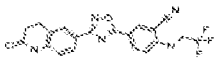
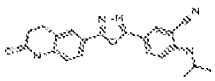
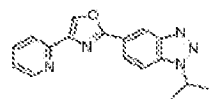
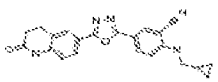
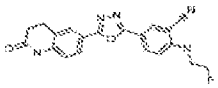
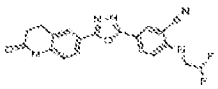
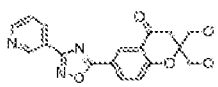
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	437	2-(1-isobutyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-methylbenzo[d]oxazole	306.15	307.2
	438	2-{2-[1-(propan-2-yl)-1H-1,2,3-benzotriazol-5-yl]- 1,3-oxazol-4-yl}aniline	319.14	320
	439	5-[3-(4-methylpyridin-3-yl)-1,2,4-oxadiazol-5-yl]-1- (oxan-4-yl)-1H-1,2,3-benzotriazole	362.15	363.1
	440	5-(3-(2-aminobenzo[d]thiazol-5-yl)-1,2,4-oxadiazol-5-yl)-2-((cyclopropylmethyl)amino)benzonitrile	388.11	389
	441	5-(3-(2-aminobenzo[d]thiazol-5-yl)-1,2,4-oxadiazol-5-yl)-2-(isopropylamino)benzonitrile	376.11	377
	442	2-(isopropylamino)-5-(3-(1-oxo-1,2,3,4-tetrahydroisoquinolin-6-yl)-1,2,4-oxadiazol-5-yl)benzonitrile	373.15	374
	443	5-(3-(2,2-diethyl-4-oxochroman-6-yl)-1,2,4-oxadiazol-5-yl)-2-(isopropylamino)benzonitrile	430.2	431

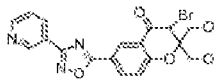
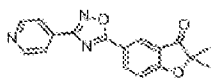
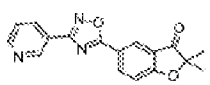
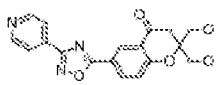
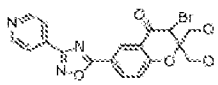
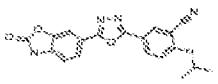
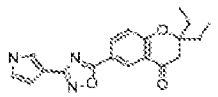
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	444	2-((cyclopropylmethyl)amino)-5-(3-(2,2-diethyl-4-oxochroman-6-yl)-1,2,4-oxadiazol-5-yl)benzonitrile	442.2	443.3
	445	6-(5-(2,2-diethyl-4-oxochroman-6-yl)-1,2,4-oxadiazol-3-yl)benzo[d]oxazol-2(3H)-one	405.13	406
	446	6-(3-(2-aminobenzo[d]thiazol-5-yl)-1,2,4-oxadiazol-5-yl)-2,2-diethylchroman-4-one	420.13	421
	447	2-(1-isobutyl-1H-benzo[d][1,2,3]triazol-5-yl)-4-methylbenzo[d]oxazole	306.15	307
	448	2-(1-isobutyl-1H-benzo[d][1,2,3]triazol-5-yl)-6-methylbenzo[d]oxazole	306.15	307
	449	2-(1-isobutyl-1H-benzo[d][1,2,3]triazol-5-yl)-7-methylbenzo[d]oxazole	306.15	307
	450	2-(1-isobutyl-1H-benzo[d][1,2,3]triazol-5-yl)-4-methoxybenzo[d]oxazole	322.14	323

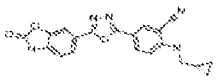
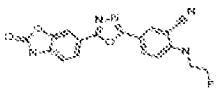
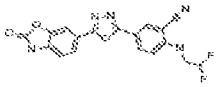
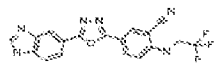
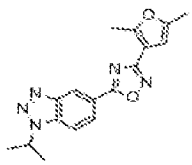
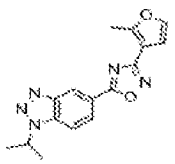
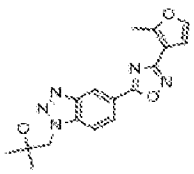
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	451	2-(1-isobutyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-methoxybenzo[d]oxazole	322.14	323
	452	2-(1-isobutyl-1H-benzo[d][1,2,3]triazol-5-yl)-6-methoxybenzo[d]oxazole	322.14	323
	453	4-chloro-2-(1-isobutyl-1H-benzo[d][1,2,3]triazol-5-yl)benzo[d]oxazole	326.09	326.9
	454	7-bromo-2-(1-isobutyl-1H-benzo[d][1,2,3]triazol-5-yl)benzo[d]oxazole	370.04	371.1
	455	1-(propan-2-yl)-5-{3-[3-(trifluoromethyl)pyridin-4- yl]-1,2,4-oxadiazol-5-yl}-1H-1,2,3-benzotriazole	374.11	375.1
	456	4-[1-(propan-2-yl)-1H-1,2,3-benzotriazol-5-yl]-5- oxa-10-thia-3-azatricyclo[7.3.0.0²,6]dodeca-1(9),2(6),3,11-tetraene	336.1	337
	457	4-[1-(propan-2-yl)-1H-1,2,3-benzotriazol-5-yl]-5- oxa-10-thia-3-azatricyclo[7.3.0.0²,6]dodeca-1(9),2(6),3,7,11-pentaene	334.09	335

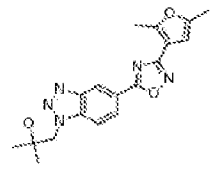
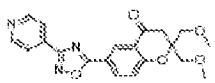
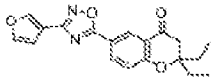
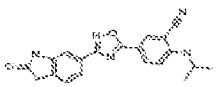
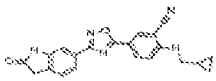
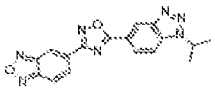
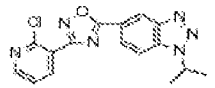
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	458	N-(2-{2-[1-(propan-2-yl)-1H-1,2,3-benzotriazol-5- yl]-1,3-oxazol-4-yl}phenyl)acetamide	361.15	362
	459	1-(propan-2-yl)-5-[4-(thiophen-2-yl)-1,3-oxazol-2- yl]-1H-1,2,3-benzotriazole	310.09	311
	460	2-methyl-1-(5-{3-[3-(trifluoromethyl)pyridin-4-yl]-1,2,4-oxadiazol-5-yl}-1H-1,2,3-benzotriazol-1- yl)propan-2-ol	404.12	405.1
	461	4-bromo-2-(1-isobutyl-1H-benzo[d][1,2,3]triazol-5-yl)benzo[d]oxazole	370.04	372.9
	462	5-{4H-chromeno[4,3-d][1,3]oxazol-2-yl}-1-(propan-2-yl)-1H-1,2,3-benzotriazole	332.13	333
	463	5-[4-(3-chlorothiophen-2-yl)-1,3-oxazol-2-yl]-1- (propan-2-yl)-1H-1,2,3-benzotriazole	344.05	345
	464	6-(3-(1H-pyrrol-2-yl)-1,2,4-oxadiazol-5-yl)-2,2-diethylchroman-4-one	337.14	338.2

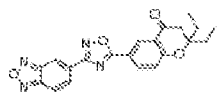
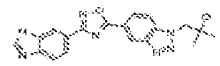
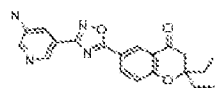
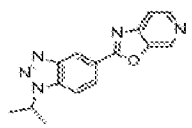
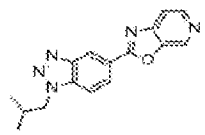
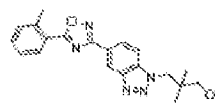
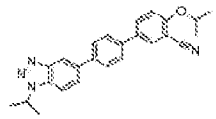
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	465	2,2-diethyl-6-(3-(furan-2-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one	338.13	339.2
	466	6-(3-(1H-imidazol-5-yl)-1,2,4-oxadiazol-5-yl)-2,2-diethylchroman-4-one	338.14	339.2
	467	2,2-diethyl-6-(3-(thiophen-2-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one	354.1	355.2
	468	2,2-diethyl-6-(3-(thiophen-3-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one	354.1	354.9
	469	6-(3-(1H-pyrazol-4-yl)-1,2,4-oxadiazol-5-yl)-2,2-diethylchroman-4-one	338.14	339.1
	470	6-(3-(1H-pyrazol-5-yl)-1,2,4-oxadiazol-5-yl)-2,2-diethylchroman-4-one	338.14	339.1
	471	2-((cyclopropylmethyl)amino)-5-(3-(2-oxo-1,2,3,4-tetrahydroquinolin-7-yl)-1,2,4-oxadiazol-5-yl)benzonitrile		385.43

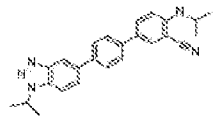
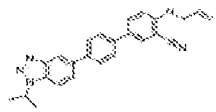
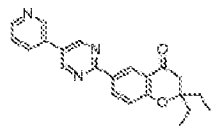
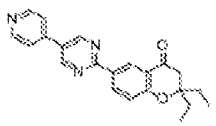
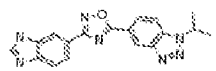
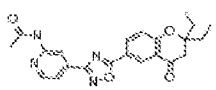
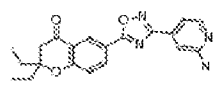
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	472	5-[3-(2-oxo-1,2,3,4-tetrahydroquinolin-6-yl)-1,2,4-oxadiazol-5-yl]-2-[(2,2,2-trifluoroethyl)amino]benzonitrile	413.11	414.1
	473	5-[5-(2-oxo-1,2,3,4-tetrahydroquinolin-6-yl)-1,3,4-oxadiazol-2-yl]-2-[(propan-2-yl)amino]benzonitrile	373.15	374.1
	474	1-(propan-2-yl)-5-[4-(pyridin-2-yl)-1,3-oxazol-2- yl]-1H-1,2,3-benzotriazole	305.13	306
	475	2-[(cyclopropylmethyl)amino]-5-[5-(2-oxo-1,2,3,4-tetrahydroquinolin-6-yl)-1,3,4-oxadiazol-2- yl]benzonitrile	385.15	386.1
	476	2-[(2-fluoroethyl)amino]-5-[5-(2-oxo-1,2,3,4- tetrahydroquinolin-6-yl)-1,3,4-oxadiazol-2-yl]benzonitrile	377.13	378.1
	477	2-[(2,2-difluoroethyl)amino]-5-[5-(2-oxo-1,2,3,4- tetrahydroquinolin-6-yl)-1,3,4-oxadiazol-2-yl]benzonitrile	395.12	396.1
	478	2,2-bis(hydroxymethyl)-6-[3-(pyridin-3-yl)-1,2,4- oxadiazol-5-yl]-3,4-dihydro-2H-1-benzopyran-4-one	353.1	354.1

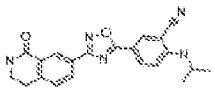
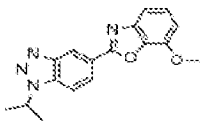
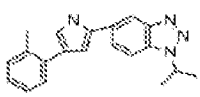
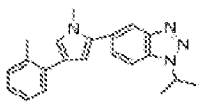
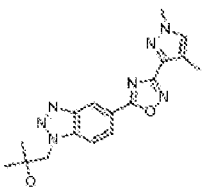
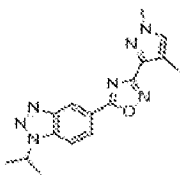
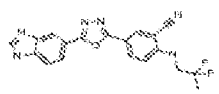
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	479	3-bromo-2,2-bis(hydroxymethyl)-6-[3-(pyridin-3-yl)- 1,2,4-oxadiazol-5-yl]-3,4-dihydro-2H-1-benzopyran-4- one	431.01	432
	480	2,2-dimethyl-5-[3-(pyridin-4-yl)-1,2,4-oxadiazol-5- yl]-2,3-dihydro-1-benzofuran-3-one	307.1	308.1
	481	2,2-dimethyl-5-[3-(pyridin-3-yl)-1,2,4-oxadiazol-5- yl]-2,3-dihydro-1-benzofuran-3-one	307.1	308.1
	482	2,2-bis(hydroxymethyl)-6-[3-(pyridin-4-yl)-1,2,4- oxadiazol-5-yl]-3,4-dihydro-2H-1-benzopyran-4-one	353.1	354.1
	483	3-bromo-2,2-bis(hydroxymethyl)-6-[3-(pyridin-4-yl)- 1,2,4-oxadiazol-5-yl]-3,4-dihydro-2H-1-benzopyran-4- one	431.01	432
	484	5-[5-(2-oxo-2,3-dihydro-1,3-benzoxazol-6-yl)-1,3,4- oxadiazol-2-yl]-2-[(propan-2-yl)amino]benzonitrile	361.12	362.1
	485	6-(3-(1H-pyrrol-3-yl)-1,2,4-oxadiazol-5-yl)-2,2-diethylchroman-4-one	337.14	338

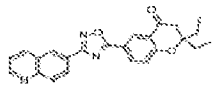
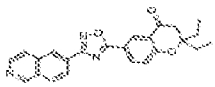
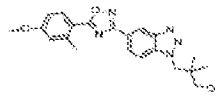
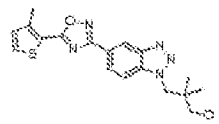
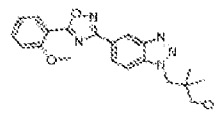
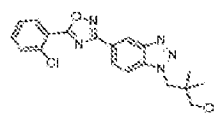
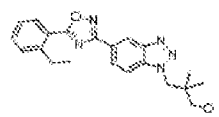
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	486	2-[(cyclopropylmethyl)amino]-5-[5-(2-oxo-2,3- dihydro-1,3-benzoxazol-6-yl)-1,3,4-oxadiazol-2- yl]benzonitrile	373.12	374.1
	487	2-[(2-fluoroethyl)amino]-5-[5-(2-oxo-2,3-dihydro- 1,3-benzoxazol-6-yl)-1,3,4-oxadiazol-2-yl]benzonitrile	365.09	366.1
	488	2-[(2,2-difluoroethyl)amino]-5-[5-(2-oxo-2,3- dihydro-1,3-benzoxazol-6-yl)-1,3,4-oxadiazol-2- yl]benzonitrile	383.08	384
	489	5-[3-(1H-1,3-benzodiazol-5-yl)-1,2,4-oxadiazol-5- yl]-2-[(2,2,2-trifluoroethyl)amino]benzonitrile	384.09	385.2
	490	5-[3-(2,5-dimethylfuran-3-yl)-1,2,4-oxadiazol-5- yl]-1-(propan-2-yl)-1H-1,2,3-benzotriazole	323.14	324.1
	491	5-[3-(2-methylfuran-3-yl)-1,2,4-oxadiazol-5-yl]-1- (propan-2-yl)-1H-1,2,3-benzotriazole	309.12	310.1
	492	2-methyl-1-{5-[3-(2-methylfuran-3-yl)-1,2,4- oxadiazol-5-yl]-1H-1,2,3-benzotriazol-1-yl}propan-2- ol	339.13	340.1

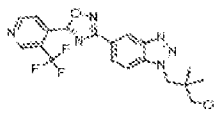
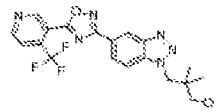
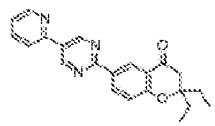
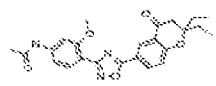
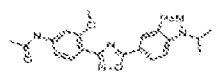
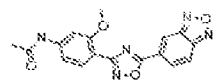
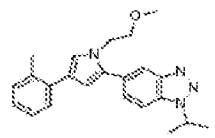
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	493	1-{5-[3-(2,5-dimethylfuran-3-yl)-1,2,4-oxadiazol-5- yl]-1H-1,2,3-benzotriazol-1-yl}-2-methylpropan-2- ol	353.15	354.1
	494	2,2-bis(methoxymethyl)-6-[3-(pyridin-4-yl)-1,2,4- oxadiazol-5-yl]-3,4-dihydro-2H-1-benzopyran-4-one	381.13	382.1
	495	2,2-diethyl-6-(3-(furan-3-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one	338.13	339
	496	2-(isopropylamino)-5-(3-(2-oxoindolin-6-yl)-1,2,4-oxadiazol-5-yl)benzonitrile	359.14	360.2
	497	2-((cyclopropylmethyl)amino)-5-(3-(2-oxoindolin-6-yl)-1,2,4-oxadiazol-5-yl)benzonitrile	371.14	372.3
	498	5-{5-[1-(propan-2-yl)-1H-1,2,3-benzotriazol-5-yl]-1,2,4-oxadiazol-3-yl}-2,1,3-benzoxadiazole	347.11	348.1
	499	5-[3-(2-chloropyridin-3-yl)-1,2,4-oxadiazol-5-yl]-1- (propan-2-yl)-1H-1,2,3-benzotriazole	340.08	341

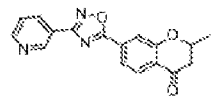
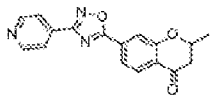
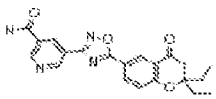
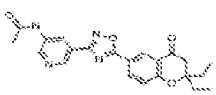
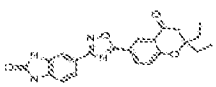
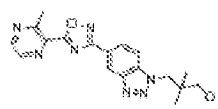
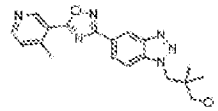
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	500	6-[3-(2,1,3-benzoxadiazol-5-yl)-1,2,4-oxadiazol-5-yl]-2,2-diethyl-3,4-dihydro-2H-1-benzopyran-4-one	390.13	391.1
	501	1-{5-[3-(1H-1,3-benzodiazol-6-yl)-1,2,4-oxadiazol-5- yl]-1H-1,2,3-benzotriazol-1-yl}-2-methylpropan-2- ol	375.14	376.1
	502	6-(3-(5-aminopyridin-3-yl)-1,2,4-oxadiazol-5-yl)-2,2-diethylchroman-4-one	364.15	365.2
	503	2-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)oxazolo[5,4-c]pyridine	279.11	280.2
	504	2-(1-isobutyl-1H-benzo[d][1,2,3]triazol-5-yl)oxazolo[5,4-c]pyridine	293.13	294.3
	505	2,2-dimethyl-3-(5-(5-(o-tolyl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)propan-1-ol	363.17	364.1
	506	4-isopropoxy-4'-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-[1,1'-biphenyl]-3-carbonitrile	396.2	397.1

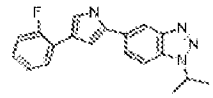
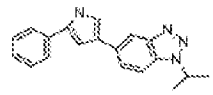
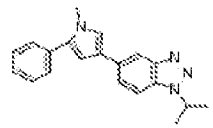
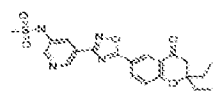
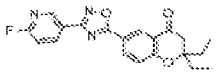
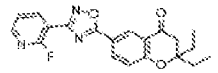
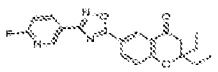
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	507	4'-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-4-(isopropylamino)-[1,1'-biphenyl]-3-carbonitrile	395.21	396.1
	508	4-(allylamino)-4'-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-[1,1'-biphenyl]-3-carbonitrile	393.2	394.1
	509	2,2-diethyl-6-(5-(pyridin-3-yl)pyrimidin-2-yl)chroman-4-one	359.16	360.3
	510	2,2-diethyl-6-(5-(pyridin-4-yl)pyrimidin-2-yl)chroman-4-one	359.16	360.3
	511	5-[3-(1H-1,3-benzodiazol-6-yl)-1,2,4-oxadiazol-5- yl]-1-(propan-2-yl)-1H-1,2,3-benzotriazole	345.13	346.1
	512	N-(4-(5-(2,2-diethyl-4-oxochroman-6-yl)-1,2,4-oxadiazol-3-yl)pyridin-2-yl)acetamide	406.16	407.3
	513	6-(3-(2-aminopyridin-4-yl)-1,2,4-oxadiazol-5-yl)-2,2-diethylchroman-4-one	364.15	365.4

Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	514	2-(isopropylamino)-5-(3-(1-oxo-1,2,3,4-tetrahydroisoquinolin-7-yl)-1,2,4-oxadiazol-5-yl)benzonitrile	373.15	374.3
	515	2-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-7-methoxybenzo[d]oxazole	308.13	309.2
	516	5-[4-(2-methylphenyl)-1H-pyrrol-2-yl]-1-(propan-2- yl)-1H-1,2,3-benzotriazole	316.17	317
	517	5-[1-methyl-4-(2-methylphenyl)-1H-pyrrol-2-yl]-1- (propan-2-yl)-1H-1,2,3-benzotriazole	330.18	331
	518	1-{5-[3-(1,4-dimethyl-1H-pyrazol-3-yl)-1,2,4- oxadiazol-5-yl]-1H-1,2,3-benzotriazol-1-yl}-2-methylpropan-2-ol	353.16	354.1
	519	5-[3-(1,4-dimethyl-1H-pyrazol-3-yl)-1,2,4- oxadiazol-5-yl]-1-(propan-2-yl)-1H-1,2,3-benzotriazole	323.15	324.1
	520	5-[5-(1H-1,3-benzodiazol-5-yl)-1,3,4-oxadiazol-2- yl]-2-[(2,2-difluoropropyl)amino]benzonitrile	380.12	381.2

Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	521	2,2-diethyl-6-(3-(quinolin-6-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one	399.16	400.4
	522	2,2-diethyl-6-(3-(isoquinolin-6-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one	399.16	400.3
	523	3-(5-(5-(4-methoxy-2-methylphenyl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)-2,2-dimethylpropan-1-ol	393.18	394.3
	524	2,2-dimethyl-3-(5-(5-(3-methylthiophen-2-yl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)propan-1-ol	369.13	370.2
	525	3-(5-(5-(2-methoxyphenyl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)-2,2-dimethylpropan-1-ol	379.16	380
	526	3-(5-(5-(2-chlorophenyl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)-2,2-dimethylpropan-1-ol	383.11	384
	527	3-(5-(5-(2-ethylphenyl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)-2,2-dimethylpropan-1-ol	377.19	378.1

Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	528	2,2-dimethyl-3-(5-(5-(3-(trifluoromethyl)pyridin-4-yl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)propan-1-ol	418.14	419
	529	2,2-dimethyl-3-(5-(5-(4-(trifluoromethyl)pyridin-3-yl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)propan-1-ol	418.14	419
	530	2,2-diethyl-6-(5-(pyridin-2-yl)pyrimidin-2-yl)chroman-4-one	359.16	360.3
	531	N-{4-[5-(2,2-diethyl-4-oxo-3,4-dihydro-2H-1-benzopyran-6-yl)-1,2,4-oxadiazol-3-yl]-3-methoxyphenyl}acetamide	435.18	436.2
	532	N-(3-methoxy-4-{5-[1-(propan-2-yl)-1H-1,2,3-benzotriazol-5-yl]-1,2,4-oxadiazol-3-yl}phenyl)acetamide	392.16	393.1
	533	N-{4-[5-(2,1,3-benzoxadiazol-5-yl)-1,2,4-oxadiazol-3-yl]-3-methoxyphenyl}acetamide	351.1	352
	534	5-[1-(2-methoxyethyl)-4-(2-methylphenyl)-1H-pyrrol-2- yl]-1-(propan-2-yl)-1H-1,2,3-benzotriazole	374.21	375

Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	535	2-methyl-7-[3-(pyridin-3-yl)-1,2,4-oxadiazol-5-yl]- 3,4-dihydro-2H-1-benzopyran-4-one	307.1	308
	536	2-methyl-7-[3-(pyridin-4-yl)-1,2,4-oxadiazol-5-yl]- 3,4-dihydro-2H-1-benzopyran-4-one	307.1	308.1
	537	5-(5-(2,2-diethyl-4-oxochroman-6-yl)-1,2,4-oxadiazol-3-yl)nicotinamide	392.15	393.2
	538	N-(5-(5-(2,2-diethyl-4-oxochroman-6-yl)-1,2,4-oxadiazol-3-yl)pyridin-3-yl)acetamide	406.16	407.3
	539	5-(5-(2,2-diethyl-4-oxochroman-6-yl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d]imidazol-2(3H)-one	404.15	405
	540	2,2-dimethyl-3-(5-(5-(3-methylpyrazin-2-yl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)propan-1-ol	365.16	366.3
	541	2,2-dimethyl-3-(5-(5-(4-methylpyridin-3-yl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)propan-1-ol	364.16	365

Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	542	5-[4-(2-fluorophenyl)-1H-pyrrol-2-yl]-1-(propan-2- yl)-1H-1,2,3-benzotriazole	320.14	321.2
	543	5-(5-phenyl-1H-pyrrol-3-yl)-1-(propan-2-yl)-1H- 1,2,3-benzotriazole	302.15	303
	544	5-(1-methyl-5-phenyl-1H-pyrrol-3-yl)-1-(propan-2- yl)-1H-1,2,3-benzotriazole	316.17	317
	545	N-(5-(5-(2,2-diethyl-4-oxochroman-6-yl)-1,2,4-oxadiazol-3-yl)pyridin-3-yl)methanesulfonamide	442.13	443.3
	546	2,2-diethyl-6-(3-(6-fluoropyridin-3-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one	367.13	368.3
	547	2,2-diethyl-6-(3-(2-fluoropyridin-3-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one	367.13	368.2
	548	2,2-diethyl-6-(3-(6-(trifluoromethyl)pyridin-3-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one	417.13	418.2

Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
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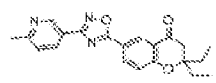
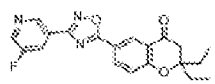
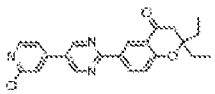
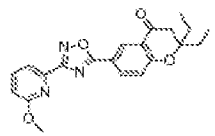
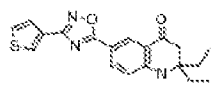
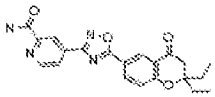
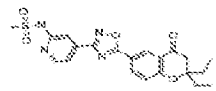
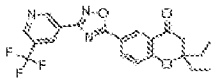
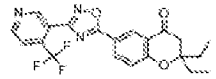
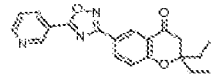
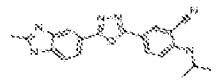
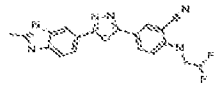
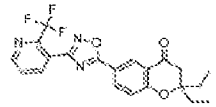
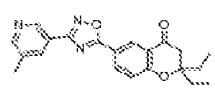
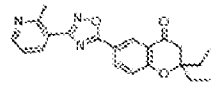
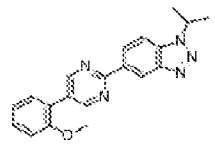
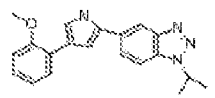
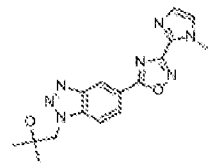
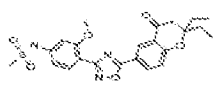
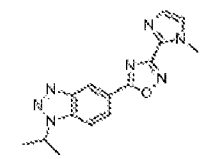
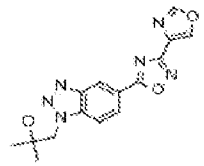
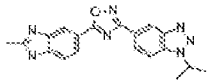
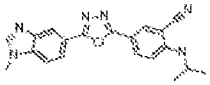
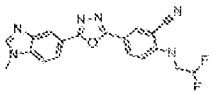
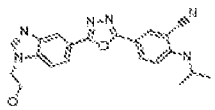
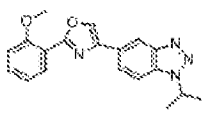
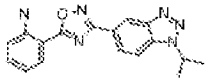
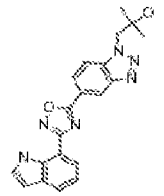
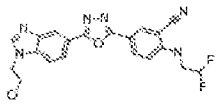
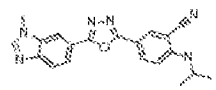
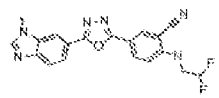
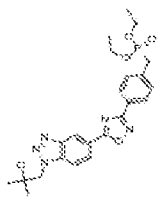
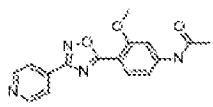
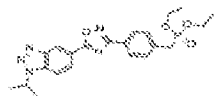
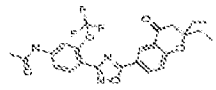
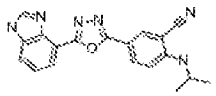
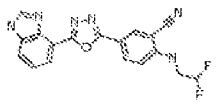
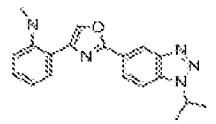
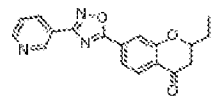
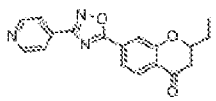
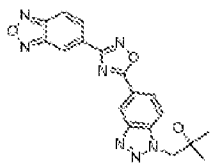
	550	2,2-diethyl-6-(3-(6-methylpyridin-3-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one	363.16	364.3
	551	2,2-diethyl-6-(3-(5-fluoropyridin-3-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one	367.13	368.2
	552	2,2-diethyl-6-(5-(2-hydroxypyridin-4-yl)pyrimidin-2-yl)chroman-4-one	375.16	376.3
	553	2,2-diethyl-6-[3-(6-methoxypyridin-2-yl)-1,2,4-oxadiazol-5-yl]-3,4-dihydro-2H-1-benzopyran-4-one	379.15	380.1
	554	2,2-diethyl-6-(3-(thiophen-3-yl)-1,2,4-oxadiazol-5-yl)-2,3-dihydroquinolin-4(1H)-one	353.12	354.2
	555	4-(5-(2,2-diethyl-4-oxochroman-6-yl)-1,2,4-oxadiazol-3-yl)picolinamide	392.15	393

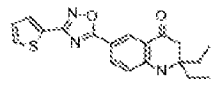
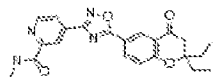
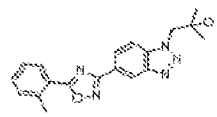
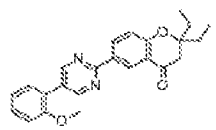
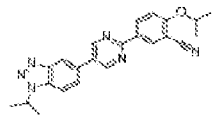
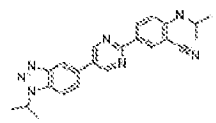
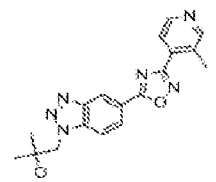
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	556	N-(4-(5-(2,2-diethyl-4-oxochroman-6-yl)-1,2,4-oxadiazol-3-yl)pyridin-2-yl)methanesulfonamide	442.13	443.3
	557	2,2-diethyl-6-(3-(5-(trifluoromethyl)pyridin-3-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one	417.13	418
	558	2,2-diethyl-6-(3-(4-(trifluoromethyl)pyridin-3-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one	417.13	418
	559	2,2-diethyl-6-(5-(pyridin-3-yl)-1,2,4-oxadiazol-3-yl)chroman-4-one	349.14	350
	560	5-[5-(2-methyl-1H-1,3-benzodiazol-5-yl)-1,3,4- oxadiazol-2-yl]-2-[(propan-2-yl)amino]benzonitrile	358.15	359.2
	561	2-[(2,2-difluoroethyl)amino]-5-[5-(2-methyl-1H-1,3- benzodiazol-5-yl)-1,3,4-oxadiazol-2-yl]benzonitrile	380.12	381.2
	562	2,2-diethyl-6-(3-(2-(trifluoromethyl)pyridin-3-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one	417.13	418

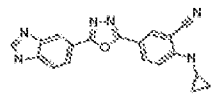
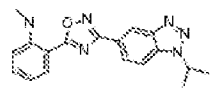
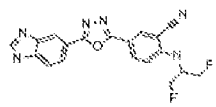
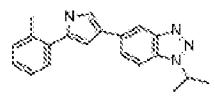
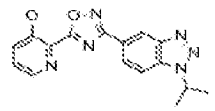
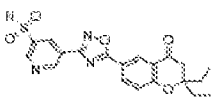
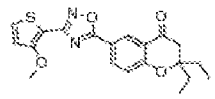
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	563	2,2-diethyl-6-(3-(5-methylpyridin-3-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one	363.16	364
	564	2,2-diethyl-6-(3-(2-methylpyridin-3-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one	363.16	364
	565	1-isopropyl-5-(5-(2-methoxyphenyl)pyrimidin-2-yl)-1H-benzo[d][1,2,3]triazole	345.16	346.1
	566	5-[4-(2-methoxyphenyl)-1H-pyrrol-2-yl]-1-(propan-2- yl)-1H-1,2,3-benzotriazole	332.16	333.2
	567	2-methyl-1-{5-[3-(1-methyl-1H-imidazol-2-yl)-1,2,4- oxadiazol-5-yl]-1H-1,2,3-benzotriazol-1-yl}propan-2- ol	339.14	340.1
	568	N-{4-[5-(2,2-diethyl-4-oxo-3,4-dihydro-2H-1-benzopyran-6-yl)-1,2,4-oxadiazol-3-yl]-3-methoxyphenyl}methanesulfonamide	471.15	472.1
	569	5-[3-(1-methyl-1H-imidazol-2-yl)-1,2,4-oxadiazol-5- yl]-1-(propan-2-yl)-1H-1,2,3-benzotriazole	309.13	310.1

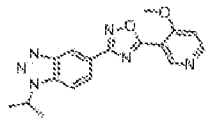
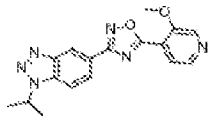
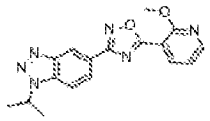
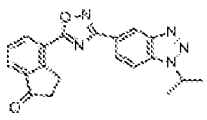
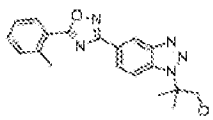
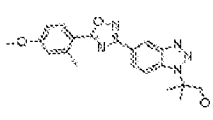
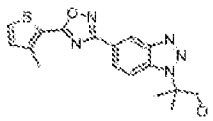
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	570	2-methyl-1-{5-[3-(1,3-oxazol-4-yl)-1,2,4-oxadiazol-5- yl]-1H-1,2,3-benzotriazol-1-yl}propan-2-ol	326.11	327
	571	5-[5-(2-methyl-1H-1,3-benzodiazol-5-yl)-1,2,4- oxadiazol-3-yl]-1-(propan-2-yl)-1H-1,2,3-benzotriazole	359.15	360
	572	5-[5-(1-methyl-1H-1,3-benzodiazol-5-yl)-1,3,4- oxadiazol-2-yl]-2-[(propan-2-yl)amino]benzonitrile	358.15	359.1
	573	2-[(2,2-difluoroethyl)amino]-5-[5-(1-methyl-1H-1,3- benzodiazol-5-yl)-1,3,4-oxadiazol-2-yl]benzonitrile	380.12	381.1
	574	5-{5-[1-(2-hydroxyethyl)-1H-1,3-benzodiazol-5-yl]- 1,3,4-oxadiazol-2-yl}-2-[(propan-2-yl)amino]benzonitrile	388.16	389.1
	575	5-[2-(2-methoxyphenyl)-1,3-oxazol-4-yl]-1-(propan-2- yl)-1H-1,2,3-benzotriazole	334.14	335
	576	2-{3-[1-(propan-2-yl)-1H-1,2,3-benzotriazol-5-yl]- 1,2,4-oxadiazol-5-yl}aniline	320.14	321.2

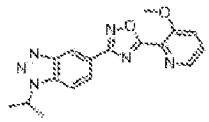
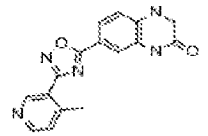
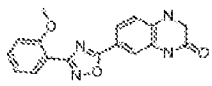
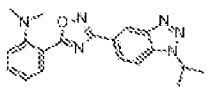
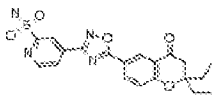
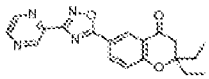
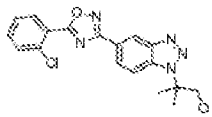
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	577	1-{5-[3-(1H-indol-7-yl)-1,2,4-oxadiazol-5-yl]-1H- 1,2,3-benzotriazol-1-yl}-2-methylpropan-2-ol	374.15	375.2
	578	2-[(2,2-difluoroethyl)amino]-5-{5-[1-(2- hydroxyethyl)-1H-1,3-benzodiazol-5-yl]-1,3,4- oxadiazol-2-yl}benzonitrile	410.13	411.1
	579	5-[5-(1-methyl-1H-1,3-benzodiazol-6-yl)-1,3,4- oxadiazol-2-yl]-2-[(propan-2-yl)amino]benzonitrile	358.15	359.2
	580	2-[(2,2-difluoroethyl)amino]-5-[5-(1-methyl-1H-1,3- benzodiazol-6-yl)-1,3,4-oxadiazol-2-yl]benzonitrile	380.12	381.1
	581	[(4-{5-[1-(2-hydroxy-2-methylpropyl)-1H- 1,2,3-benzotriazol-5-yl]-1,2,4-oxadiazol-3- yl}phenyl)methyl]phosphonate	485.18	486.2
	582	N-{3-methoxy-4-[3-(pyridin-4-yl)-1,2,4-oxadiazol-5-yl]phenyl}acetamide	310.11	311.2
	583	diethyl [(4-{5-[1-(propan-2-yl)-1H-1,2,3- benzotriazol-5-yl]-1,2,4-oxadiazol-3-yl}phenyl)methyl]phosphonate	455.17	456.1

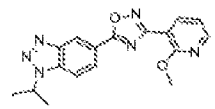
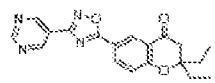
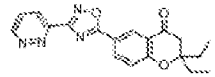
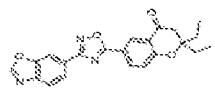
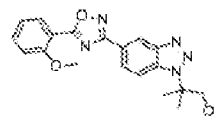
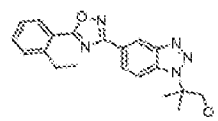
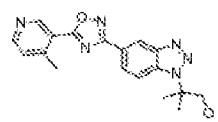
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	584	N-{4-[5-(2,2-diethyl-4-oxo-3,4-dihydro-2H-1-benzopyran-6-yl)-1,2,4-oxadiazol-3-yl]-3-(trifluoromethoxy)phenyl}acetamide	489.15	490.1
	585	5-[5-(1H-1,3-benzodiazol-4-yl)-1,3,4-oxadiazol-2- yl]-2-[(propan-2-yl)amino]benzonitrile	344.14	345.1
	586	5-[5-(1H-1,3-benzodiazol-4-yl)-1,3,4-oxadiazol-2- yl]-2-[(2,2-difluoroethyl)amino]benzonitrile	366.1	367.1
	587	N-methyl-2-{2-[1-(propan-2-yl)-1H-1,2,3- benzotriazol-5-yl]-1,3-oxazol-4-yl}aniline	333.16	334
	588	2-ethyl-7-[3-(pyridin-3-yl)-1,2,4-oxadiazol-5-yl]- 3,4-dihydro-2H-1-benzopyran-4-one	321.11	322.1
	589	2-ethyl-7-[3-(pyridin-4-yl)-1,2,4-oxadiazol-5-yl]- 3,4-dihydro-2H-1-benzopyran-4-one	321.11	322.1
	590	1-{5-[3-(2,1,3-benzoxadiazol-5-yl)-1,2,4-oxadiazol-5- yl]-1H-1,2,3-benzotriazol-1-yl}-2-methylpropan-2- ol	377.12	378.1

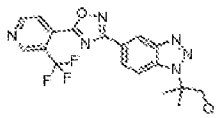
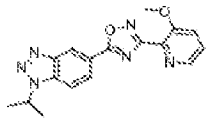
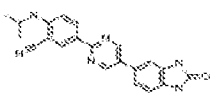
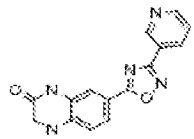
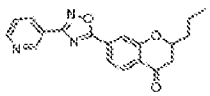
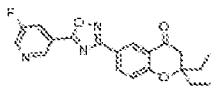
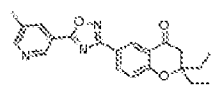
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	591	2,2-diethyl-6-(3-(thiophen-2-yl)-1,2,4-oxadiazol-5-yl)-2,3-dihydroquinolin-4(1H)-one	353.12	353.9
	592	4-(5-(2,2-diethyl-4-oxochroman-6-yl)-1,2,4-oxadiazol-3-yl)-N-methylpicolinamide	406.16	407
	593	2-methyl-1-(5-(5-(o-tolyl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)propan-2-ol	349.15	350
	594	2,2-diethyl-6-(5-(2-methoxyphenyl)pyrimidin-2-yl)chroman-4-one	388.18	389
	595	2-isopropoxy-5-(5-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)pyrimidin-2-yl)benzonitrile	398.19	399.2
	596	5-(5-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)pyrimidin-2-yl)-2-(isopropylamino)benzonitrile	397.2	398.1
	597	2-methyl-1-{5-[3-(3-methylpyridin-4-yl)-1,2,4- oxadiazol-5-yl]-1H-1,2,3-benzotriazol-1-yl}propan-2-ol	350.15	351.1

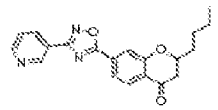
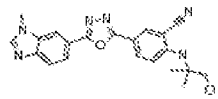
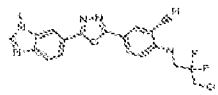
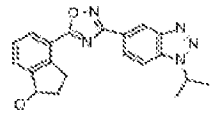
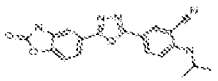
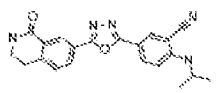
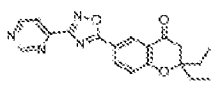
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	598	5-[5-(1H-1,3-benzodiazol-5-yl)-1,3,4-oxadiazol-2- yl]-2-(cyclopropylamino)benzonitrile	342.12	343.1
	599	N-methyl-2-{3-[1-(propan-2-yl)-1H-1,2,3- benzotriazol-5-yl]-1,2,4-oxadiazol-5-yl}aniline	334.15	335.2
	600	5-[5-(1H-1,3-benzodiazol-5-yl)-1,3,4-oxadiazol-2- yl]-2-[(1,3-difluoropropan-2-yl)amino]benzonitrile	380.12	381.1
	601	5-[5-(2-methylphenyl)-1H-pyrrol-3-yl]-1-(propan-2- yl)-1H-1,2,3-benzotriazole	316.17	317
	602	2-{3-[1-(propan-2-yl)-1H-1,2,3-benzotriazol-5-yl]- 1,2,4-oxadiazol-5-yl}pyridin-3-ol	322.12	323
	603	5-(5-(2,2-diethyl-4-oxochroman-6-yl)-1,2,4-oxadiazol-3-yl)pyridine-3-sulfonamide	428.12	428.9
	604	2,2-diethyl-6-(3-(3-methoxythiophen-2-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one	384.11	385.2

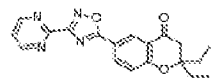
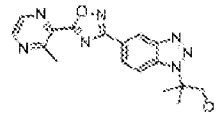
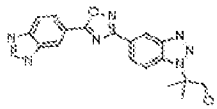
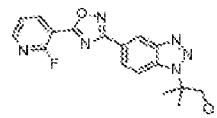
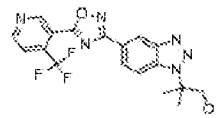
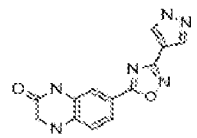
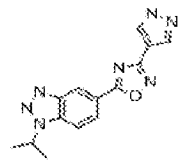
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	605	3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(4-methoxypyridin-3-yl)-1,2,4-oxadiazole	336.13	337.2
	606	3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(3-methoxypyridin-4-yl)-1,2,4-oxadiazole	336.13	337.2
	607	3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(2-methoxypyridin-3-yl)-1,2,4-oxadiazole	336.13	337.2
	608	4-{3-[1-(propan-2-yl)-1H-1,2,3-benzotriazol-5-yl]- 1,2,4-oxadiazol-5-yl}-2,3-dihydro-1H-inden-1-one	359.14	360
	609	2-methyl-2-(5-(5-(o-tolyl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)propan-1-ol	349.15	350.1
	610	2-(5-(5-(4-methoxy-2-methylphenyl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)-2-methylpropan-1-ol	379.16	380
	611	2-methyl-2-(5-(5-(3-methylthiophen-2-yl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)propan-1-ol	355.11	355.9

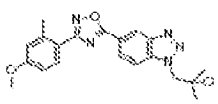
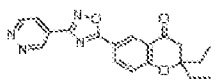
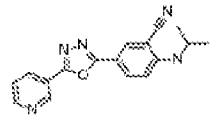
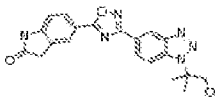
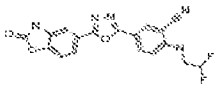
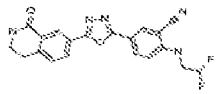
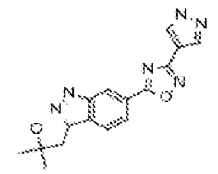
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	612	3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(3-methoxypyridin-2-yl)-1,2,4-oxadiazole	336.13	337.2
	613	7-[3-(4-methylpyridin-3-yl)-1,2,4-oxadiazol-5-yl]- 1,2,3,4-tetrahydroquinoxalin-2-one	307.11	307.1
	614	7-[3-(2-methoxyphenyl)-1,2,4-oxadiazol-5-yl]- 1,2,3,4-tetrahydroquinoxalin-2-one	322.11	322.1
	615	N,N-dimethyl-2-{3-[1-(propan-2-yl)-1H-1,2,3- benzotriazol-5-yl]-1,2,4-oxadiazol-5-yl}aniline	348.17	349.1
	616	4-(5-(2,2-diethyl-4-oxochroman-6-yl)-1,2,4-oxadiazol-3-yl)pyridine-2-sulfonamide	428.12	428.9
	617	2,2-diethyl-6-(3-(pyrazin-2-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one	350.14	351.1
	618	2-(5-(5-(2-chlorophenyl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)-2-methylpropan-1-ol	369.1	369.9

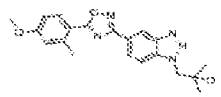
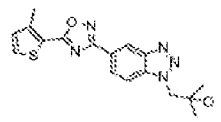
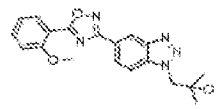
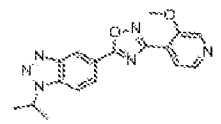
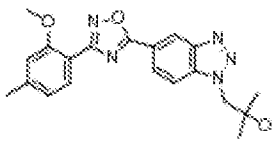
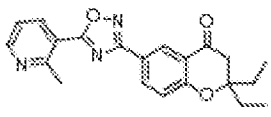
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	619	5-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-3-(2-methoxypyridin-3-yl)-1,2,4-oxadiazole	336.13	337.2
	620	2,2-diethyl-6-(3-(pyrimidin-5-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one	350.14	351.1
	621	2,2-diethyl-6-(3-(pyridazin-3-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one	350.14	351.1
	622	6-(3-(benzo[d]oxazol-6-yl)-1,2,4-oxadiazol-5-yl)-2,2-diethylchroman-4-one	389.14	390
	623	2-(5-(5-(2-methoxyphenyl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)-2-methylpropan-1-ol	365.15	365.9
	624	2-(5-(5-(2-ethylphenyl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)-2-methylpropan-1-ol	363.17	364.1
	625	2-methyl-2-(5-(5-(4-methylpyridin-3-yl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)propan-1-ol	350.15	351.1

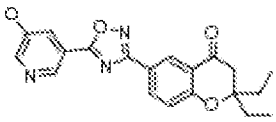
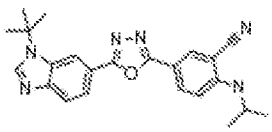
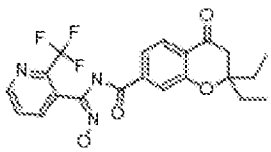
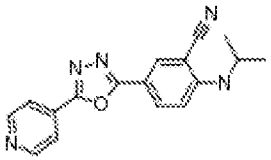
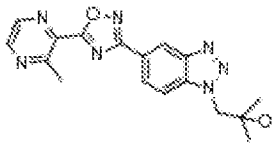
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	626	2-methyl-2-(5-(5-(3-(trifluoromethyl)pyridin-4-yl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)propan-1-ol	404.12	405.1
	627	5-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-3-(3-methoxypyridin-2-yl)-1,2,4-oxadiazole	336.13	337.1
	628	2-(isopropylamino)-5-(5-(2-oxo-2,3-dihydro-1H-benzo[d]imidazol-5-yl)pyrimidin-2-yl)benzonitrile	370.15	371.1
	629	7-[3-(pyridin-3-yl)-1,2,4-oxadiazol-5-yl]-1,2,3,4- tetrahydroquinoxalin-2-one	293.09	292.1
	630	2-propyl-7-[3-(pyridin-3-yl)-1,2,4-oxadiazol-5-yl]- 3,4-dihydro-2H-1-benzopyran-4-one	335.13	336.1
	631	2,2-diethyl-6-[5-(5-fluoropyridin-3-yl)-1,2,4- oxadiazol-3-yl]-3,4-dihydro-2H-1-benzopyran-4-one	367.13	368.1
	632	2,2-diethyl-6-[5-(5-methylpyridin-3-yl)-1,2,4- oxadiazol-3-yl]-3,4-dihydro-2H-1-benzopyran-4-one	363.16	364.1

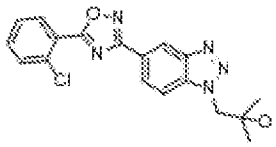
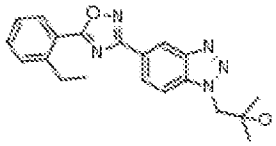
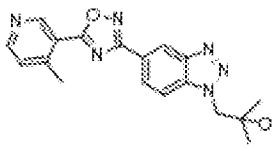
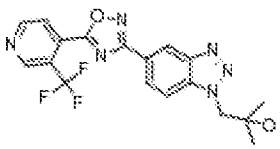
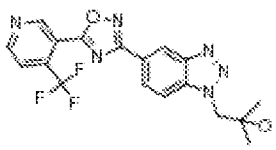
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	633	2-butyl-7-[3-(pyridin-3-yl)-1,2,4-oxadiazol-5-yl]- 3,4-dihydro-2H-1-benzopyran-4-one	349.14	350.1
	634	2-[(1-hydroxy-2-methylpropan-2-yl)amino]-5-[5-(1- methyl-1H-1,3-benzodiazol-6-yl)-1,3,4-oxadiazol-2- yl]benzonitrile	388.16	389.2
	635	2-[(2,2-difluoro-3-hydroxypropyl)amino]-5-[5-(1-methyl-1H-1,3-benzodiazol-6-yl)-1,3,4-oxadiazol-2- yl]benzonitrile	410.13	411.2
	636	4-{3-[1-(propan-2-yl)-1H-1,2,3-benzotriazol-5-yl]- 1,2,4-oxadiazol-5-yl}-2,3-dihydro-1H-inden-1-ol	361.15	362
	637	5-[5-(2-oxo-2,3-dihydro-1,3-benzoxazol-5-yl)-1,3,4- oxadiazol-2-yl]-2-[(propan-2-yl)amino]benzonitrile	361.12	362.2
	638	5-[5-(1-oxo-1,2,3,4-tetrahydroisoquinolin-7-yl)- 1,3,4-oxadiazol-2-yl]-2-[(propan-2-yl)amino]benzonitrile	373.15	374.2
	639	2,2-diethyl-6-(3-(pyrimidin-4-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one	350.14	351.1

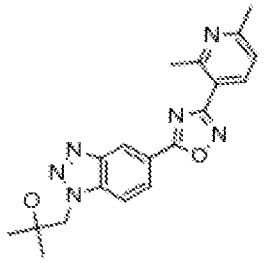
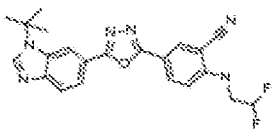
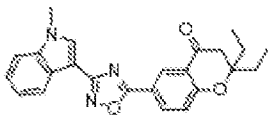
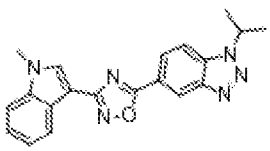
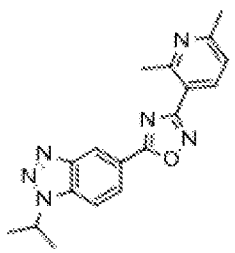
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	640	2,2-diethyl-6-(3-(pyrimidin-2-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one	350.14	351.1
	641	2-methyl-2-(5-(5-(3-methylpyrazin-2-yl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)propan-1-ol	351.14	352.2
	642	2-(5-(5-(1H-benzo[d]imidazol-6-yl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)-2-methylpropan-1-ol	375.14	376.1
	643	2-(5-(5-(2-fluoropyridin-3-yl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)-2-methylpropan-1-ol	354.12	355.1
	644	2-methyl-2-(5-(5-(4-(trifluoromethyl)pyridin-3-yl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)propan-1-ol	404.12	405.2
	645	7-[3-(1H-pyrazol-4-yl)-1,2,4-oxadiazol-5-yl]- 1,2,3,4-tetrahydroquinoxalin-2-one	282.09	281.1
	646	1-(propan-2-yl)-5-[3-(1H-pyrazol-4-yl)-1,2,4- oxadiazol-5-yl]-1H-1,2,3-benzotriazole	295.12	296.2

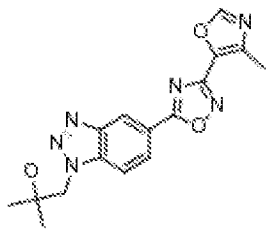
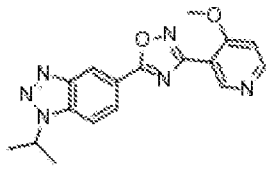
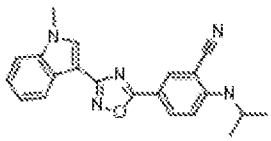
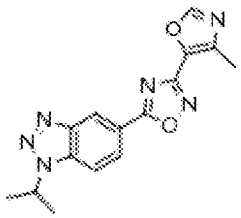
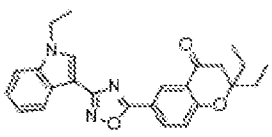
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	647	1-{5-[3-(4-methoxy-2-methylphenyl)-1,2,4-oxadiazol-5-yl]-1H-1,2,3-benzotriazol-1-yl}-2-methylpropan-2- ol	379.16	380.1
	648	2,2-diethyl-6-(3-(pyridazin-4-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one	350.14	351
	649	2-(isopropylamino)-5-(5-(pyridin-3-yl)-1,3,4-oxadiazol-2-yl)benzonitrile	305.13	306.3
	650	5-(3-(1-(1-hydroxy-2-methylpropan-2-yl)-1H-benzo[d][1,2,3]triazol-5-yl)-1,2,4-oxadiazol-5-yl)indolin-2-one	390.14	391.1
	651	2-[(2,2-difluoroethyl)amino]-5-[5-(2-oxo-2,3- dihydro-1,3-benzoxazol-5-yl)-1,3,4-oxadiazol-2- yl]benzonitrile	383.08	384
	652	2-[(2,2-difluoroethyl)amino]-5-[5-(1-oxo-1,2,3,4-tetrahydroisoquinolin-7-yl)-1,3,4-oxadiazol-2- yl]benzonitrile	395.12	396.1
	653	2-methyl-1-{6-[3-(1H-pyrazol-4-yl)-1,2,4-oxadiazol-5- yl]-3H-indazol-3-yl}propan-2-ol	324.13	326.2

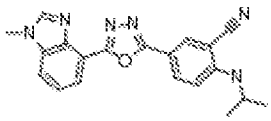
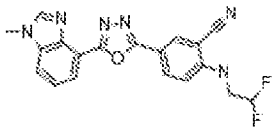
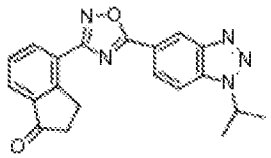
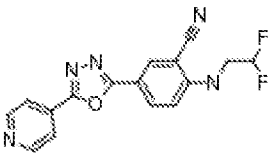
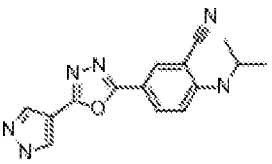
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	654	1-(5-(5-(4-methoxy-2-methylphenyl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)-2-methylpropan-2-ol	379.16	380.3
	655	2-methyl-1-(5-(5-(3-methylthiophen-2-yl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)propan-2-ol	355.11	356.2
	656	1-(5-(5-(2-methoxyphenyl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)-2-methylpropan-2-ol	365.15	366.2
	657	5-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-3-(3-methoxypyridin-4-yl)-1,2,4-oxadiazole	336.13	337.1
	662	1-{5-[3-(2-methoxy-4-methylphenyl)-1,2,4-oxadiazol-5-yl]-1H-1,2,3-benzotriazol-1-yl}-2-methylpropan-2- ol	379.16	380
	663	2,2-diethyl-6-[5-(2-methylpyridin-3-yl)-1,2,4- oxadiazol-3-yl]-3,4-dihydro-2H-1-benzopyran-4-one	363.16	364.1

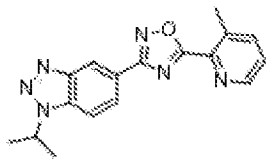
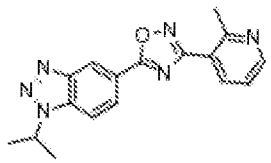
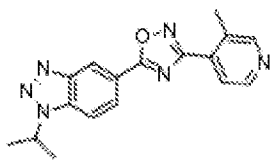
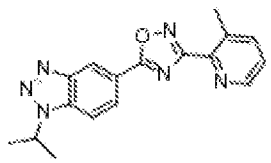
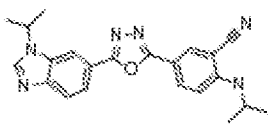
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	664	2,2-diethyl-6-[5-(5-hydroxypyridin-3-yl)-1,2,4- oxadiazol-3-yl]-3,4-dihydro-2H-1-benzopyran-4-one	365.14	366.1
	665	5-[5-(1-tert-butyl-1H-1,3-benzodiazol-6-yl)-1,3,4- oxadiazol-2-yl]-2-[(propan-2-yl)amino]benzonitrile	400.2	401.3
	666	2,2-diethyl-N-[(1E)-(hydroxyimino)[2-(trifluoromethyl)pyridin-3-yl]methyl]-4-oxo-3,4- dihydro-2H-1-benzopyran-7-carboxamide	435.14	436.2
	667	2-(isopropylamino)-5-(5-(pyridin-4-yl)-1,3,4-oxadiazol-2-yl)benzonitrile	305.13	306.3
	668	2-methyl-1-(5-(5-(3-methylpyrazin-2-yl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)propan-2-ol	351.14	352.2

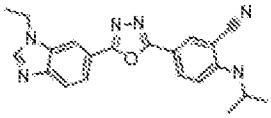
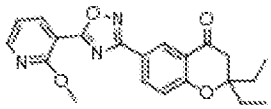
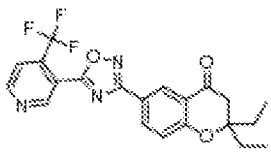
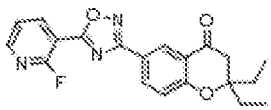
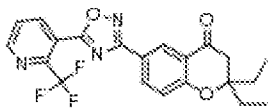
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	669	1-(5-(5-(2-chlorophenyl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)-2-methylpropan-2-ol	369.1	369.9
	670	1-(5-(5-(2-ethylphenyl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)-2-methylpropan-2-ol	363.17	364
	671	2-methyl-1-(5-(5-(4-methylpyridin-3-yl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)propan-2-ol	350.15	351.2
	672	2-methyl-1-(5-(5-(3-(trifluoromethyl)pyridin-4-yl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)propan-2-ol	404.12	405.2
	673	2-methyl-1-(5-(5-(4-(trifluoromethyl)pyridin-3-yl)-1,2,4-oxadiazol-3-yl)-1H-benzo[d][1,2,3]triazol-1-yl)propan-2-ol	404.12	405.2

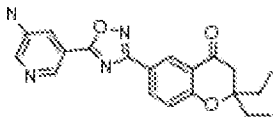
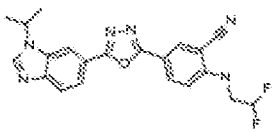
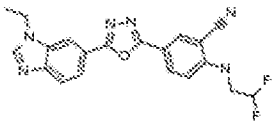
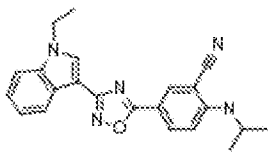
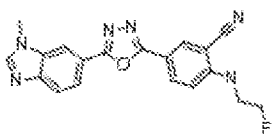
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	675	1-{5-[3-(2,6-dimethylpyridin-3-yl)-1,2,4-oxadiazol-5- yl]-1H-1,2,3-benzotriazol-1-yl}-2-methylpropan-2- ol	364.16	365.1
	676	5-[5-(1-tert-butyl-1H-1,3-benzodiazol-6-yl)-1,3,4- oxadiazol-2-yl]-2-[(2,2-difluoroethyl)amino]benzonitrile	422.17	423.1
	677	2,2-diethyl-6-[3-(1-methyl-1H-indol-3-yl)-1,2,4-oxadiazol-5-yl]-3,4-dihydro-2H-1-benzopyran-4-one	401.17	402.1
	678	5-[3-(1-methyl-1H-indol-3-yl)-1,2,4-oxadiazol-5-yl]-1-(propan-2-yl)-1H-1,2,3-benzotriazole	358.15	359.1
	679	5-[3-(2,6-dimethylpyridin-3-yl)-1,2,4-oxadiazol-5- yl]-1-(propan-2-yl)-1H-1,2,3-benzotriazole	334.15	335.1

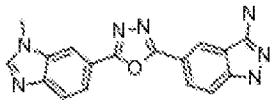
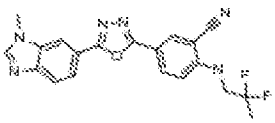
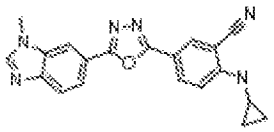
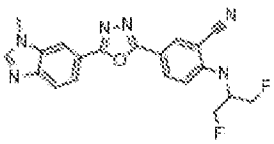
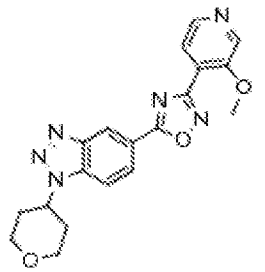
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	680	2-methyl-1-{5-[3-(4-methyl-1,3-oxazol-5-yl)-1,2,4- oxadiazol-5-yl]-1H-1,2,3-benzotriazol-1-yl}propan-2- ol	340.13	341.1
	681	5-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-3-(4-methoxypyridin-3-yl)-1,2,4-oxadiazole	336.13	337.3
	682	5-[3-(1-methyl-1H-indol-3-yl)-1,2,4-oxadiazol-5-yl]-2-[(propan-2-yl)amino]benzonitrile	357.16	358.2
	683	5-[3-(4-methyl-1,3-oxazol-5-yl)-1,2,4-oxadiazol-5- yl]-1-(propan-2-yl)-1H-1,2,3-benzotriazole	310.12	311.1
	684	2,2-diethyl-6-[3-(1-ethyl-1H-indol-3-yl)-1,2,4-oxadiazol-5-yl]-3,4-dihydro-2H-1-benzopyran-4-one	415.19	416.2

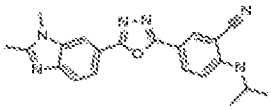
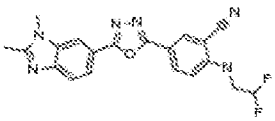
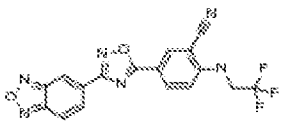
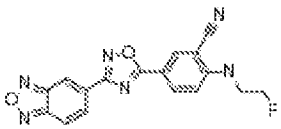
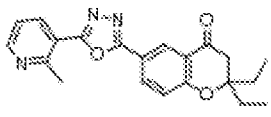
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	685	5-[5-(1-methyl-1H-1,3-benzodiazol-4-yl)-1,3,4- oxadiazol-2-yl]-2-[(propan-2-yl)amino]benzonitrile	358.15	359.2
	686	2-[(2,2-difluoroethyl)amino]-5-[5-(1-methyl-1H-1,3- benzodiazol-4-yl)-1,3,4-oxadiazol-2-yl]benzonitrile	380.12	381.2
	687	4-{5-[1-(propan-2-yl)-1H-1,2,3-benzotriazol-5-yl]- 1,2,4-oxadiazol-3-yl}-2,3-dihydro-1H-inden-1-one	359.14	360
	688	2-((2,2-difluoroethyl)amino)-5-(5-(pyridin-4-yl)-1,3,4-oxadiazol-2-yl)benzonitrile	327.09	328.3
	689	5-(5-(1H-pyrazol-4-yl)-1,3,4-oxadiazol-2-yl)-2-(isopropylamino)benzonitrile	294.12	295.3

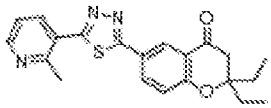
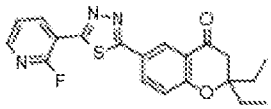
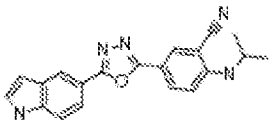
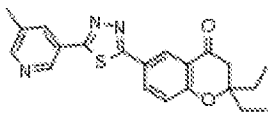
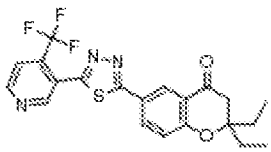
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	690	3-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-5-(3-methylpyridin-2-yl)-1,2,4-oxadiazole	320.14	321.3
	691	5-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-3-(2-methylpyridin-3-yl)-1,2,4-oxadiazole	320.14	321.2 321.2
	692	5-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-3-(3-methylpyridin-4-yl)-1,2,4-oxadiazole	320.14	321.2
	693	5-(1-isopropyl-1H-benzo[d][1,2,3]triazol-5-yl)-3-(3-methylpyridin-2-yl)-1,2,4-oxadiazole	320.14	321.1
	694	5-{5-[1-(propan-2-yl)-1H-1,3-benzodiazol-6-yl]- 1,3,4-oxadiazol-2-yl}-2-[(propan-2-yl)amino]benzonitrile	386.19	387.2

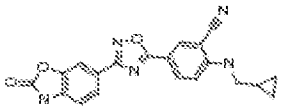
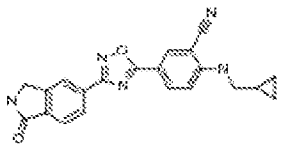
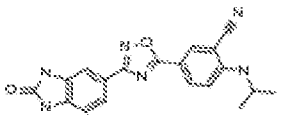
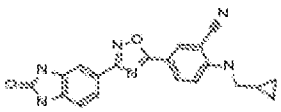
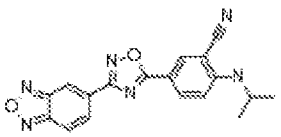
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	695	5-[5-(1-ethyl-1H-1,3-benzodiazol-6-yl)-1,3,4- oxadiazol-2-yl]-2-[(propan-2-yl)amino]benzonitrile	372.17	373.1
	696	2,2-diethyl-6-[5-(2-methoxypyridin-3-yl)-1,2,4-oxadiazol-3-yl]-3,4-dihydro-2H-1-benzopyran-4-one	379.15	380.2
	697	2,2-diethyl-6-{5-[4-(trifluoromethyl)pyridin-3-yl]-1,2,4-oxadiazol-3-yl}-3,4-dihydro-2H-1-benzopyran-4- one	417.13	418.2
	698	2,2-diethyl-6-[5-(2-fluoropyridin-3-yl)-1,2,4- oxadiazol-3-yl]-3,4-dihydro-2H-1-benzopyran-4-one	367.13	368.1
	699	2,2-diethyl-6-{5-[2-(trifluoromethyl)pyridin-3-yl]-1,2,4-oxadiazol-3-yl}-3,4-dihydro-2H-1-benzopyran-4- one	417.13	418.1

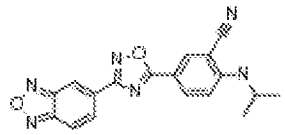
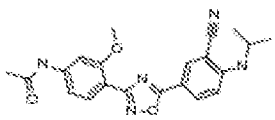
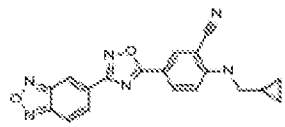
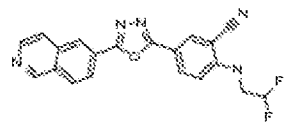
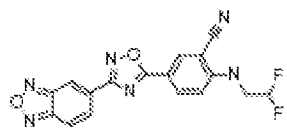
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	700	6-[5-(5-aminopyridin-3-yl)-1,2,4-oxadiazol-3-yl]- 2,2-diethyl-3,4-dihydro-2H-1-benzopyran-4-one	364.15	365.1
	701	2-[(2,2-difluoroethyl)amino]-5-{5-[1-(propan-2-yl)- 1H-1,3-benzodiazol-6-yl]-1,3,4-oxadiazol-2- yl}benzonitrile	408.15	409.1
	702	2-[(2,2-difluoroethyl)amino]-5-[5-(1-ethyl-1H-1,3- benzodiazol-6-yl)-1,3,4-oxadiazol-2- yl]benzonitrile	394.14	395.1
	703	5-[3-(1-ethyl-1H-indol-3-yl)-1,2,4-oxadiazol-5-yl]-2-[(propan-2-yl)amino]benzonitrile	371.17	372.1
	704	2-[(2-fluoroethyl)amino]-5-[5-(1-methyl-1H-1,3- benzodiazol-6-yl)-1,3,4-oxadiazol-2- yl]benzonitrile	362.13	363.1

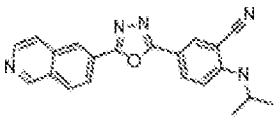
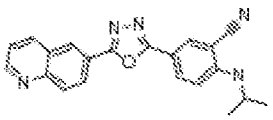
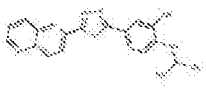
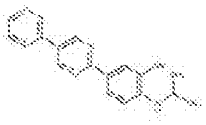
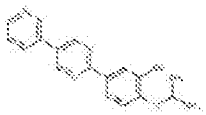
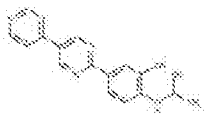
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	705	5-[5-(1-methyl-1H-1,3-benzodiazol-6-yl)-1,3,4- oxadiazol-2-yl]-1H-indazol-3-amine	331.12	332
	706	2-[(2,2-difluoropropyl)amino]-5-[5-(1-methyl-1H- 1,3-benzodiazol-6-yl)-1,3,4-oxadiazol-2-yl]benzonitrile	394.14	395.1
	707	2-(cyclopropylamino)-5-[5-(1-methyl-1H-1,3- benzodiazol-6-yl)-1,3,4-oxadiazol-2- yl]benzonitrile	356.14	357.1
	708	2-[(1,3-difluoropropan-2-yl)amino]-5-[5-(1-methyl- 1H-1,3-benzodiazol-6-yl)-1,3,4-oxadiazol-2- yl]benzonitrile	394.14	395.1
	709	5-[3-(3-methoxypyridin-4-yl)-1,2,4-oxadiazol-5-yl]-1- (oxan-4-yl)-1H-1,2,3-benzotriazole	378.14	379.1

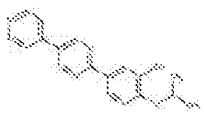
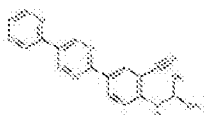
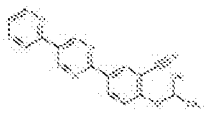
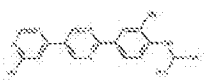
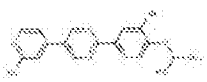
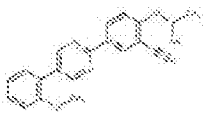
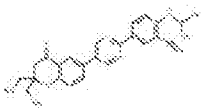
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	710	5-[5-(1,2-dimethyl-1H-1,3-benzodiazol-6-yl)-1,3,4- oxadiazol-2-yl]-2-[(propan-2-yl)amino]benzonitrile	372.17	373.1
	711	2-[(2,2-difluoroethyl)amino]-5-[5-(1,2-dimethyl-1H- 1,3-benzodiazol-6-yl)-1,3,4-oxadiazol-2-yl]benzonitrile	394.14	395.1
	712	5-[3-(2,1,3-benzoxadiazol-5-yl)-1,2,4-oxadiazol-5-yl]-2-[(2,2,2-trifluoroethyl)amino]benzonitrile	386.07	387
	713	5-[3-(2,1,3-benzoxadiazol-5-yl)-1,2,4-oxadiazol-5-yl]-2-[(2-fluoroethyl)amino]benzonitrile	350.09	351
	718	2,2-diethyl-6-(5-(2-methylpyridin-3-yl)-1,3,4-oxadiazol-2-yl)chroman-4-one	363.16	364.4

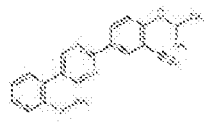
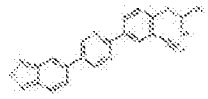
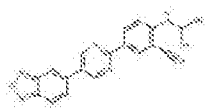
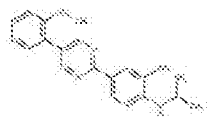
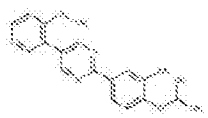
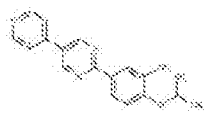
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	719	2,2-diethyl-6-(5-(2-methylpyridin-3-yl)-1,3,4-thiadiazol-2-yl)chroman-4-one	379.14	380.2
	720	2,2-diethyl-6-(5-(2-fluoropyridin-3-yl)-1,3,4-thiadiazol-2-yl)chroman-4-one	383.11	384.2
	721	5-(5-(1H-indol-5-yl)-1,3,4-oxadiazol-2-yl)-2-(isopropylamino)benzonitrile	343.14	344.4
	724	2,2-diethyl-6-(5-(5-methylpyridin-3-yl)-1,3,4-thiadiazol-2-yl)chroman-4-one	379.14	380.3
	725	2,2-diethyl-6-(5-(4-(trifluoromethyl)pyridin-3-yl)-1,3,4-thiadiazol-2-yl)chroman-4-one	433.11	434.3

Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	726	2-(cyclopropylmethylamino)-5-[3-(2-oxo-3H-1,3-benzoxazol-6-yl)-1,2,4-oxadiazol-5-yl]benzonitrile	373.12	374.1
	727	2-((cyclopropylmethyl)amino)-5-(3-(1-oxoisoindolin-5-yl)-1,2,4-oxadiazol-5-yl)benzonitrile	371.14	372.1
	728	2-(isopropylamino)-5-(3-(2-oxo-2,3-dihydro-1H-benzo[d]imidazol-5-yl)-1,2,4-oxadiazol-5-yl)benzonitrile	360.13	361.1
	729	2-((cyclopropylmethyl)amino)-5-(3-(2-oxo-2,3-dihydro-1H-benzo[d]imidazol-5-yl)-1,2,4-oxadiazol-5-yl)benzonitrile	372.13	373.1
	730	5-[3-(2,1,3-benzoxadiazol-5-yl)-1,2,4-oxadiazol-5-yl]-2-[(propan-2-yl)amino]benzonitrile	346.12	347.1

Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	730	5-[3-(2,1,3-benzoxadiazol-5-yl)-1,2,4-oxadiazol-5-yl]-2-[(propan-2-yl)amino]benzonitrile	346.12	347.1
	731	N-[4-(5-{3-cyano-4-[(propan-2-yl)amino]phenyl}-1,2,4-oxadiazol-3-yl)-3-methoxyphenyl]acetamide	391.16	392.1
	732	5-[3-(2,1,3-benzoxadiazol-5-yl)-1,2,4-oxadiazol-5-yl]-2-[(2,2-difluoroethyl)amino]benzonitrile	358.12	369
	733	2-[(2,2-difluoroethyl)amino]-5-[5-(isoquinolin-6- yl)-1,3,4-oxadiazol-2-yl]benzonitrile	377.11	378.1
	734	5-[3-(2,1,3-benzoxadiazol-5-yl)-1,2,4-oxadiazol-5-yl]-2-[(cyclopropylmethyl)amino]benzonitrile	368.08	359

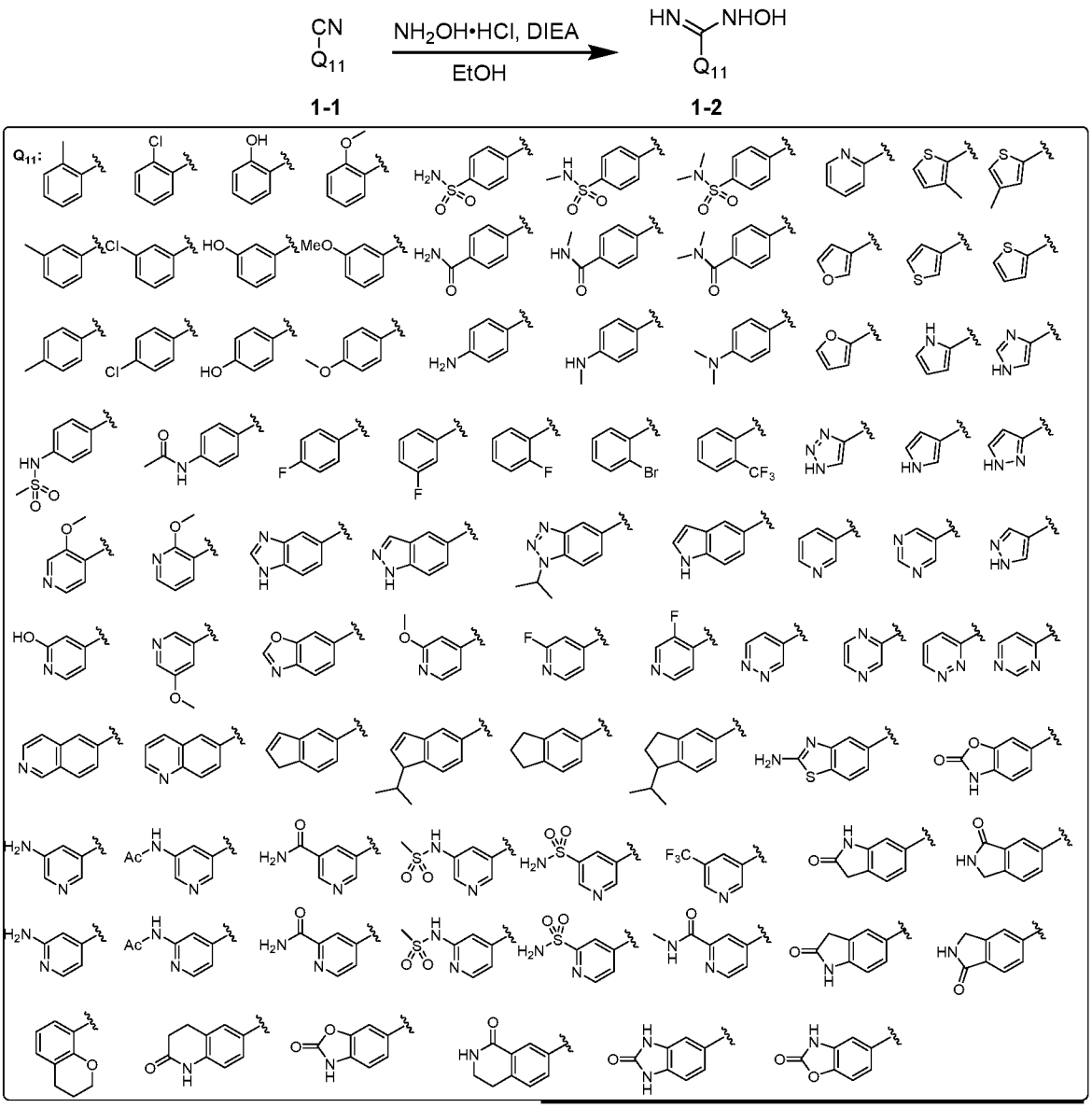
Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	735	5-[5-(isoquinolin-6-yl)-1,3,4-oxadiazol-2-yl]-2- [(propan-2-yl)amino]benzonitrile	355.14	356.1
	736	2-[(propan-2-yl)amino]-5-[5-(quinolin-6-yl)-1,3,4- oxadiazol-2-yl]benzonitrile	355.14	356.1
	736	2-[(propan-2-yl)amino]-5-[5-(quinolin-6-yl)-1,3,4- oxadiazol-2-yl]benzonitrile	355.14	356.1
	737	2-(isopropylamino)-5-(5-(pyridin-3-yl)pyrimidin-2-yl)benzonitrile	315.15	316
	738	2-isopropoxy-5-(5-(pyridin-3-yl)pyrimidin-2-yl)benzonitrile	316.13	317
	739	2-(isopropylamino)-5-(5-(pyridin-4-yl)pyrimidin-2-yl)benzonitrile	315.15	316

Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	740	2-isopropoxy-5-(5-(pyridin-4-yl)pyrimidin-2-yl)benzonitrile	316.13	317
	741	2-(isopropylamino)-5-(5-(pyridin-2-yl)pyrimidin-2-yl)benzonitrile	315.15	316
	742	2-isopropoxy-5-(5-(pyridin-2-yl)pyrimidin-2-yl)benzonitrile	316.15	317
	743	5-(5-(2-hydroxypyridin-4-yl)pyrimidin-2-yl)-2-(isopropylamino)benzonitrile	331.14	332
	744	5-(5-(2-hydroxypyridin-4-yl)pyrimidin-2-yl)-2-isopropoxybenzonitrile	332.13	333
	745	2-isopropoxy-5-(5-(2-methoxyphenyl)pyrimidin-2-yl)benzonitrile	345.15	346
	746	5-(5-(2,2-diethyl-4-oxochroman-6-yl)pyrimidin-2-yl)-2-(isopropylamino)benzonitrile	440.22	441.4

Structure	Compound Number	Chemical Name	Exact Mass	Actual Peak
	747	2-(isopropylamino)-5-(5-(2-methoxyphenyl)pyrimidin-2-yl)benzonitrile	344.16	345.3
	748	5-(5-(benzo[c][1,2,5]oxadiazol-5-yl)pyrimidin-2-yl)-2-isopropoxybenzonitrile	357.12	357.9
	749	5-(5-(benzo[c][1,2,5]oxadiazol-5-yl)pyrimidin-2-yl)-2-(isopropylamino)benzonitrile	356.14	356.9
	750	N-isopropyl-4-(5-(2-methoxyphenyl)pyrimidin-2-yl)-2-(trifluoromethyl)aniline	387.16	388
	751	2-(4-isopropoxy-3-(trifluoromethyl)phenyl)-5-(2-methoxyphenyl)pyrimidine	388.14	389
	752	2-(4-isopropoxy-3-(trifluoromethyl)phenyl)-5-(pyridin-4-yl)pyrimidine	359.13	360

General Procedure A:

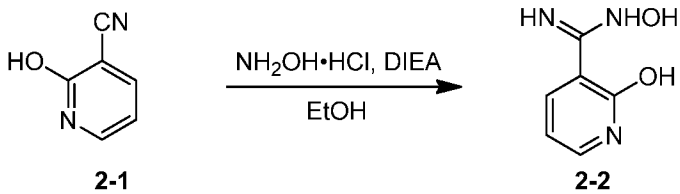
Scheme 1



Example 2

Scheme 2

Synthesis of Intermediate 2-2: N,2-dihydroxypyridine-3-carboximidamide



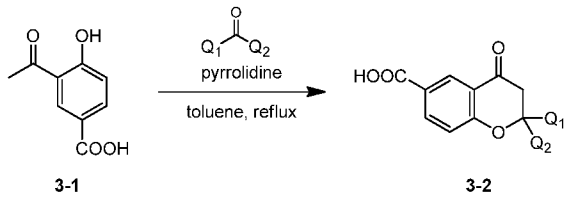
To a mixture of **2-1** (2-hydroxypyridine-3-carbonitrile)(200 mg, 1.67 mmol) in ethanol (10 mL) was added hydrochloride salt of hydroxylamine (174 mg, 2.50 mmol) , diisopropylethylamine (430 mg, 3.33 mmol) at 20 °C. The mixture was then heated to 90 °C and stirred for 16 hrs. The mixture was concentrated in vacuum to remove part of ethanol, the resulting mixture was filtered, and the solid was dried in vacuum which was used as the product in next step without further purification (185 mg, 69% yield).

^{1}H NMR (400MHz, DMSO-d_6) δ = 12.06 (br, s, 1H), 9.50 (br, s, 1H), 7.95 (dd, J = 7.2, 2.4 Hz, 1H), 7.51 (dd, J = 6.0, 2.0 Hz, 1H), 6.3 – 6.30 (m, 3H).

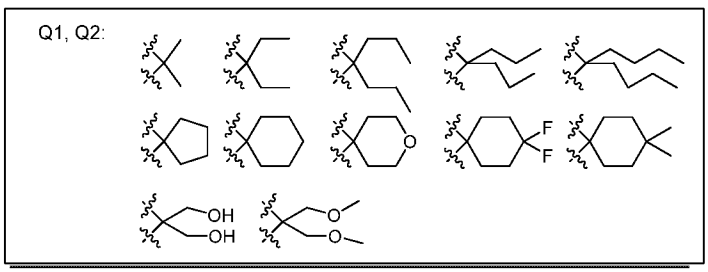
General Procedure B

Synthesis of Intermediate 3-2: 2,2-diethyl-4-oxo-3,4-dihydro-2H-1-benzopyran-6-carboxylic acid

Scheme 3

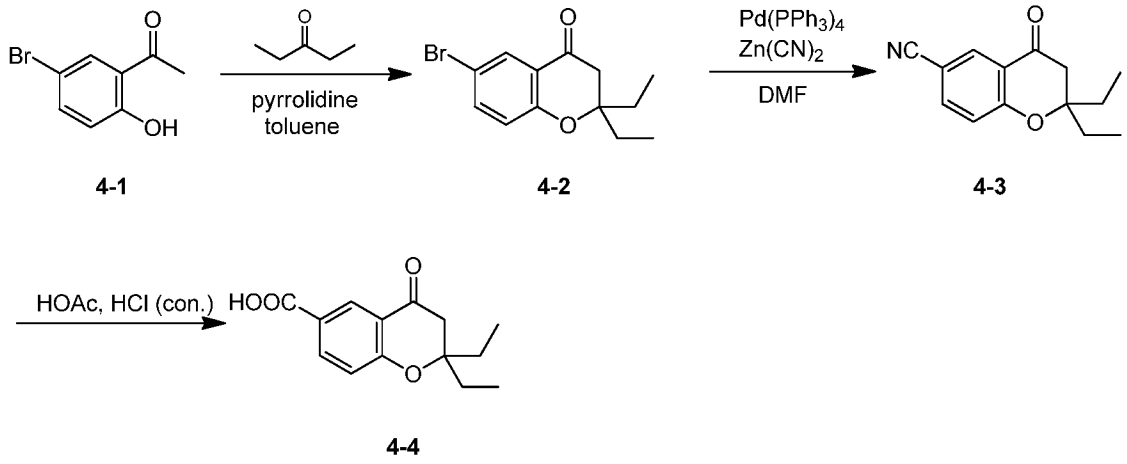


3-1 3-2



Alternative Synthesis of Intermediate 4-4: 2,2-diethyl-4-oxo-3,4-dihydro-2H-1-benzopyran-6-carboxylic acid

Scheme 4

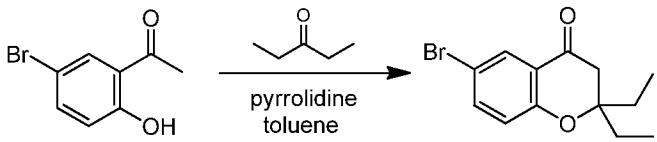


4-1 4-2 4-3

4-4

Synthesis of 4-2: 6-bromo-2,2-diethyl-3,4-dihydro-2H-1-benzopyran-4-one

Scheme 5



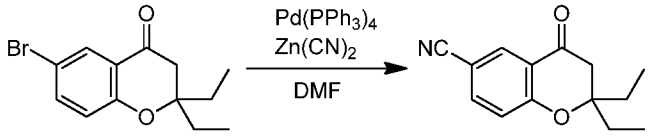
4-1 4-2

To a solution of 1-(5-bromo-2-hydroxy-phenyl)ethanone (20 g, 93.0 mmol, 1 *eq*) in methanol (400 mL) was added pyrrolidine (7.94 g, 112 mmol, 1.2 *eq*) and pentan-3-one (9.61 g, 112 mmol, 1.2 *eq*) . The mixture was stirred at 80 °C for 16 hr . The reaction mixture diluted with water (200 mL) and extracted with ethyl acetate (200 mL X 2), the combined organic layers were washed with brine (500 mL), dried over sodium sulfate, filtered and concentrated under reduced pressure to give a residue which was purified by column chromatography to give the desired product **4-2** (12 g, 46% yield) as a yellow oil.

^{1}H NMR (400MHz, $CDCl_3$) δ = 7.93 (d, *J* = 2.5 Hz, 1H), 7.52 (dd, *J* = 8.8, 2.6 Hz, 1H), 6.84 (d, *J* = 8.8 Hz, 1H), 2.70 (s, 2H), 1.86 - 1.62 (m, 4H), 0.92 (t, *J* = 7.5 Hz, 6H).

Synthesis of Intermediate 4-3: 2,2-diethyl-4-oxo-3,4-dihydro-2H-1-benzopyran-6-carbonitrile

Scheme 6



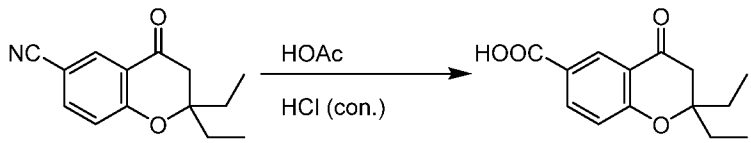
4-2 4-3

To a solution of 6-bromo-2,2-diethyl-chroman-4-one (10 g, 35.3 mmol, 1 *eq*) in DMF (100 mL) was added zinc cyanide (6.22 g, 53.0 mmol, 1.5 *eq*) and tetratriphenylphosphine palladium (4.08 g, 3.53 mmol, 0.1 *eq*). The mixture was stirred at 130 °C for 2 hr. The reaction mixture was diluted with water (100 mL) and extracted with ethyl acetate (100 mL X 3). The combined organic layers were washed with brine (200 mL), dried over sodium sulfate, filtered and concentrated under reduced pressure to give a residue which was purified by flash silica gel chromatography (petroleum ether/ethyl acetate = 100/1 to 1/1) to give the desired product **4-3** (8 g, 99% yield).

^{1}H NMR (400MHz, DMSO-d_6) δ = 8.08 (d, J = 1.9 Hz, 1H), 7.96 (dd, J = 8.7, 2.0 Hz, 1H), 7.20 (d, J = 8.7 Hz, 1H), 2.88 (s, 2H), 1.86 - 1.59 (m, 4H), 0.86 (br, t, J = 7.4 Hz, 6H).

Scheme 7

Synthesis of Intermediate 4-4: 2,2-diethyl-4-oxo-3,4-dihydro-2H-1-benzopyran-6-carboxylic acid



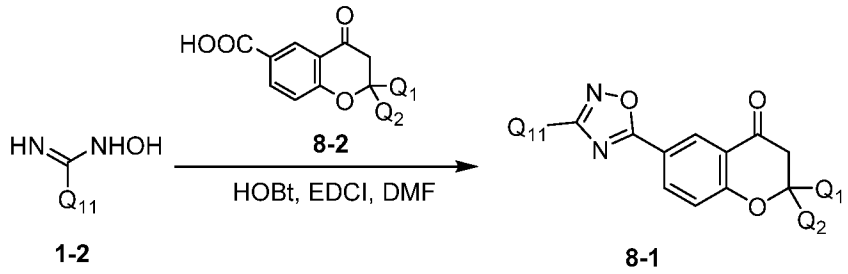
4-3 4-4

A suspension of 2,2-diethyl-4-oxo-chromane-6-carbonitrile (6.05 g, 26.4 mmol, 1 eq) in acetic acid (60 mL) and concentrated hydrochloride solution (60 mL) was stirred at 120 °C for 16 hr, The residue was triturated with water (500 mL), filtered and dried under vacuum to give the titled product **4-4** (5.8 g, 89% yield).

^{1}H NMR (400MHz, DMSO-d_6) δ = 8.27 (d, J = 1.9 Hz, 1H), 8.06 (dd, J = 8.7, 2.0 Hz, 1H), 7.11 (d, J = 8.7 Hz, 1H), 2.85 (s, 2H), 1.77 - 1.68 (m, 4H), 0.87 (t, J = 7.4 Hz, 6H).

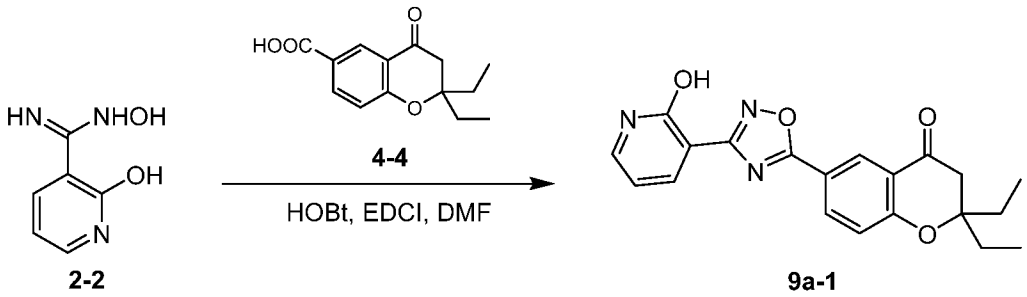
General Procedure C:

Scheme 8



Synthesis of Compound 9a-1: 2,2-diethyl-6-(3-(2-hydroxypyridin-3-yl)-1,2,4-oxadiazol-5-yl)chroman-4-one

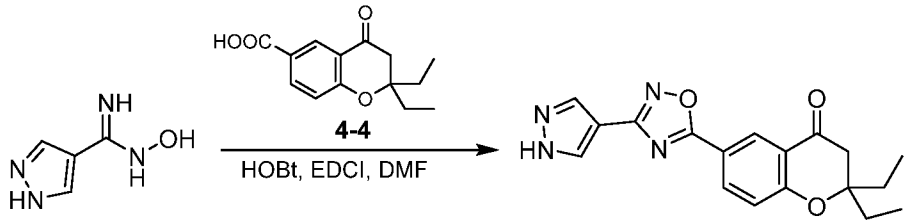
Scheme 9a



To a mixture of **4-4** (268 mg, 1.08 mmol) in *N,N*-dimethylformamide (6 mL) was added HOBt (159 mg, 1.18 mmol, 1.2 *eq*) , EDCI (225 mg, 1.18 mmol, 1.2 *eq*) at 20 °C under nitrogen atmosphere. The mixture was stirred for 30 min, then, **2-2** (150 mg, 980 umol, 1 *eq*) was added, and the resultant mixture was then heated to 120 °C and stirred for 2 hrs. The mixture was diluted with water (20 mL), extracted with ethyl acetate (20 mL X 3). The combined organic phase was washed by brine (50 mL), dried over sodium sulfate, concentrated in vacuum. The residue was purified by *prep*-HPLC (column: Phenomenex Gemini 150x25mmx10um;mobile phase: [water (0.05% ammonia hydroxide v/v)-ACN];B%: 35%-65%,12min) to give the product **9-1** as a white solid (20 mg, 6% yield). ^{1}H NMR (400MHz, DMSO-d_6) δ = 12.23 (br, s, 1H), 8.44 (d, J = 2.0 Hz, 1H), 8.33 (dd, J = 7.2, 2.0 Hz, 1H), 8.28 (dd, J = 8.8, 2.4 Hz, 1H), 7.68 (dd, J = 6.0, 2.0 Hz, 1H), 7.29 (d, J = 8.8 Hz, 1H), 6.42 (t, J = 6.8 Hz, 1H), 2.93 (s, 2H), 1.81 – 1.70 (m, 4H), 0.90 (t, J = 7.2 Hz, 6H).

Synthesis of Compound :

2,2-diethyl-6-[3-(1H-pyrazol-4-yl)-1,2,4-oxadiazol-5-yl]-3H-1-benzopyran-4-one



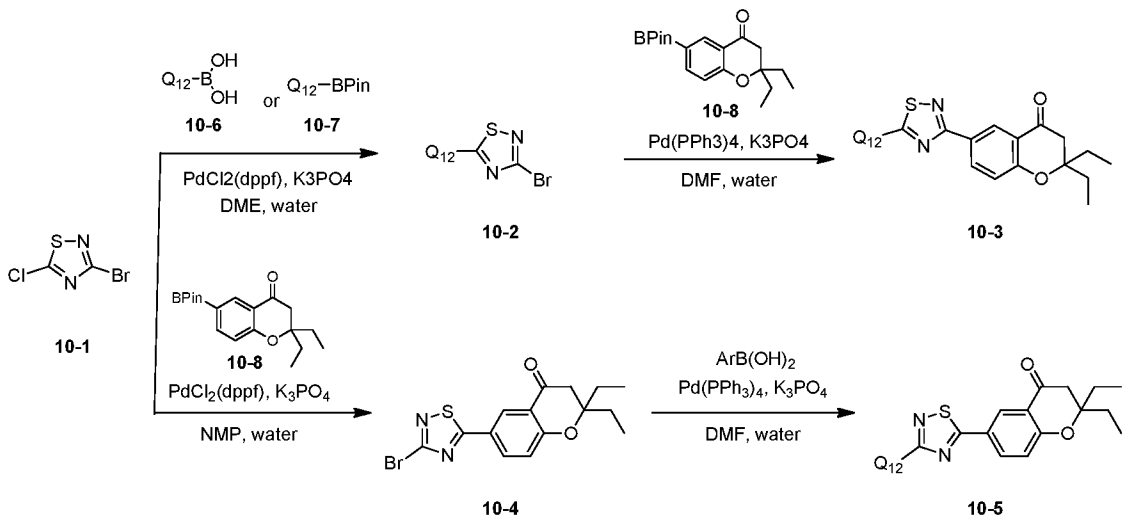
9b-1 **9b-2**

To a solution of compound **4-4** (16.41 g, 66.08 mmol, 1 *eq.*) in DMF (50 mL) was added EDCI (15.20 g, 79.29 mmol, 1.2 *eq.*) and HOBt (8.93 g, 66.08 mmol, 1.0 *eq.*), stirred at 20 °C for 0.5 hour. Then compound **9b-1** (10 g, 79.29 mmol, 1.2 *eq.*) was added. The mixture was stirred at 20 °C for 0.5 hour, then heated to 120 °C and stirred for 2 hours. The mixture was diluted with water (100 mL), extracted with EtOAc (150 mL*3), dried with sodium sulfate, filtered and concentrated. The residue was purified by silica gel column chromatography (PE:EA = 3:1) to give **9b-2** (7.2 g, yield: 30%) as white solid.

^{1}H NMR (400MHz, DMSO-d_6) δ = 13.49 (br. s, 1 H), 8.47 (s, 1 H), 8.42 (d, J = 2.3 Hz, 1 H), 8.26 (dd, J = 2.3, 8.8 Hz, 1 H), 8.06 (s, 1 H), 7.26 (d, J = 8.7 Hz, 1 H), 2.91 (s, 2 H), 1.79 - 1.69 (m, 4 H), 0.89 (t, J = 7.4 Hz, 6 H).

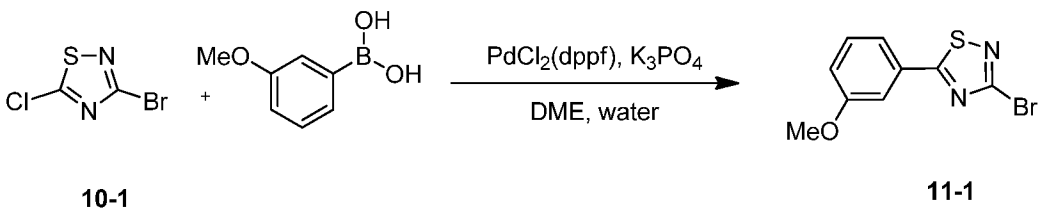
General Procedure D:

Scheme 10



Synthesis of 11-1: 3-bromo-5-(3-methoxyphenyl)-1,2,4-thiadiazole

Scheme 11



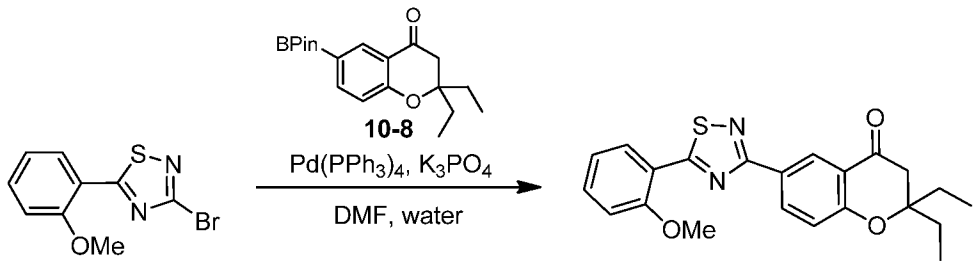
To a solution of (3-methoxyphenyl)boronic acid (247.25 mg, 1.63 mmol, 1 *eq*) in DME (5 mL) was added $Pd(dppf)Cl_2$ (119.06 mg, 162.71 umol, 0.1 *eq*), K_3PO_4 (1.04 g, 4.88 mmol, 3 *eq*) and **10-1**, 3-bromo-5-chloro-1,2,4-thiadiazole (649.07 mg, 3.25 mmol, 2 *eq*). The mixture was stirred at 80 °C for 0.5 h. The reaction mixture was diluted with water (50 mL) and extracted with EA (50 mL x *3)*. The combined organic layers were dried over Na_2SO_4, filtered and concentrated under reduced pressure to give a residue. The residue was purified by flash silica gel chromatography (*PE/EA=10/1*) to give **11-1** (3-bromo-5-(3-methoxyphenyl)-1,2,4-thiadiazole) (200 mg, 737.64 umol, 45% yield) as a white solid.

^{1}H NMR (400MHz, DMSO-d_6) δ = 8.23 (dd, *J*=1.6, 7.8 Hz, 1H), 7.78 - 7.57 (m, 1H), 7.38 (d, *J*=8.4 Hz, 1H), 7.21 (t, *J*=7.6 Hz, 1H), 4.13 (s, 3H).

Synthesis of 12-1 :

2,2-diethyl-6-[5-(2-methoxyphenyl)-1,2,4-thiadiazol-3-yl]-3,4-ihydro-2H-1-benzopyran-4-one

Scheme 12



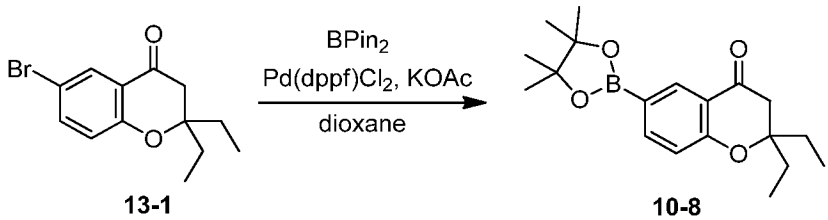
11-1 **12-1**

To a solution of 3-bromo-5-(2-methoxyphenyl)-1,2,4-thiadiazole (100 mg, 368.82 umol, 1 e*q*) and 2,2-diethyl-6-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)chroman-4-one (146.15 mg, 442.59 umol, 1.2 *eq*) in DMF (1 mL) and H_2O (0.5 mL) was added K_3PO_4 (234.87 mg, 1.11 mmol, 3 *eq*) and $Pd(PPh_3)_4$ (42.62 mg, 36.88 umol, 0.1 *eq*) and stirred at 120 °C for 0.25 h. The residue was purified by prep-HPLC (column: Phenomenex Synergi C18 150x25x10um;mobile phase: [water(0.225%FA)-ACN];B%: 70%-100%,10min) to give 2,2-diethyl-6-[5-(2-methoxyphenyl)-1,2,4-thiadiazol-3-yl]chroman-4-one (34.5 mg, 87.46 umol, 23.71% yield, 100% purity) as a yellow solid.
^{1}H NMR (400MHz, DMSO-d_6) δ = 8.66 (d, *J*=2.1 Hz, 1H), 8.52 - 8.41 (m, 2H), 7.71 - 7.62 (m, 1H), 7.39 (d, *J*=8.3 Hz, 1H), 7.26 (t, *J*=7.5 Hz, 1H), 7.19 (d, *J*=8.7 Hz, 1H), 4.14 (s, 3H), 2.88 (s, 2H), 1.76 (quint, *J*=7.2, 14.4 Hz, 4H), 0.90 (t, *J*=7.4 Hz, 6H).

Synthesis of 10-8 :

2,2-diethyl-6-(tetramethyl-1,3,2-dioxaborolan-2-yl)-3,4-dihydro-2H-1-benzopyran-4-one

Scheme 13



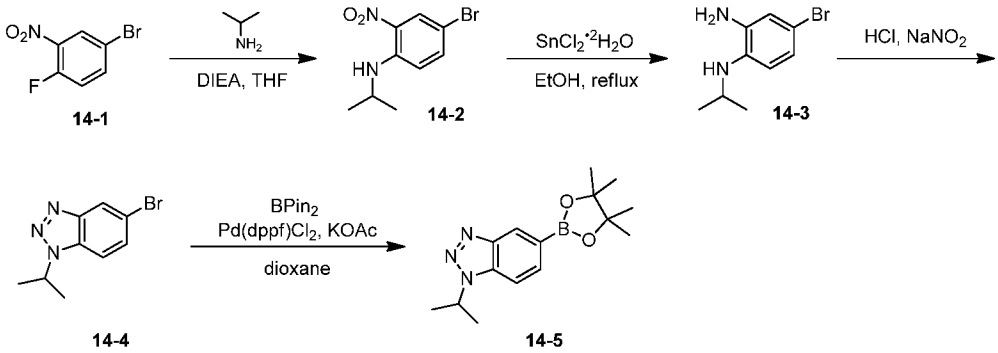
13-1 **10-8**

To a solution of 6-bromo-2,2-diethyl-chroman-4-one (1 g, 3.53 mmol, 1 *eq*) in dioxane (10 mL) was added 4,4,5,5-tetramethyl-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,3,2-dioxaborolane (986.48 mg, 3.88 mmol, 1.1 *eq*), DPPF (195.78 mg, 353.16 umol, 0.1 *eq*), $Pd(dppf)Cl_2$ (258.41 mg, 353.16 umol, 0.1 *eq*) and KOAc (415.92 mg, 4.24 mmol, 1.2 *eq*), the mixture was stirred at 100 °C for 4 h, The reaction mixture was diluted with water (100 mL) and extracted with (EA 100 mL **x** *2*). The combined organic layers were dried over Na_2SO_4, filtered and concentrated under reduced pressure to give a residue. The residue was purified by flash silica gel chromatography (*PE/EA=1/1*) to give 2,2-diethyl-6-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)chroman-4-one (1 g, 3.03 mmol, 85.75% yield) as a white solid.

^1H NMR (400MHz, CHLOROFORM-d) δ = 8.26 (d, *J*=1.6 Hz, 1H), 7.86 - 7.75 (m, 1H), 6.85 (d, *J*=8.3 Hz, 1H), 2.64 (s, 2H), 1.82 - 1.58 (m, 4H), 1.32 - 1.21 (m, 12H), 0.85 (t, *J*=7.5 Hz, 6H).

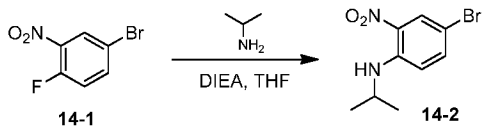
Synthesis of 14-5: 1-(propan-2-yl)-5-(tetramethyl-1,3,2-dioxaborolan-2-yl)-1H-1,2,3-benzotriazole

Scheme 14



Synthesis of 14-2 : 4-bromo-2-nitro-N-(propan-2-yl)aniline

Scheme 15



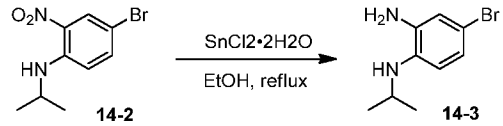
To a solution of 4-bromo-1-fluoro-2-nitro-benzene (5 g, 22.73 mmol, 2.79 mL, 1.00 *eq*) and propan-2-amine (2.02 g, 34.09 mmol, 2.92 mL, 1.50 *eq*) in THF (250.00 mL) was added DIEA (7.34 g, 56.82 mmol, 9.90 mL, 2.50 *eq*) at 10 °C and stirred for 1 h, The reaction mixture was diluted with ***water (500*** mL) and extracted with ***EA (500*** mLx*2)*. The combined organic layers were washed

with $NaHCO_3$ (500 mL), dried over ***Na_2SO_4***, filtered and concentrated under reduced pressure to give a residue. The residue was purified by flash silica gel chromatography to give 4-bromo-N-isopropyl-2-nitro-aniline (3.2 g, 12.35 mmol, 54.34% yield) as yellow oil.

^{1}H NMR (400MHz, DMSO-d_6) δ = 8.14 (d, *J*=2.4 Hz, 1H), 7.88 (br d, *J*=7.5 Hz, 1H), 7.63 (dd, *J*=2.3, 9.3 Hz, 1H), 7.07 (d, *J*=9.4 Hz, 1H), 3.92 (sxtd, *J*=6.5, 13.2 Hz, 1H), 1.25 (d, *J*=6.4 Hz, 6H).

Synthesis of 14-3 : 4-bromo-1-N-(propan-2-yl)benzene-1,2-diamine

Scheme 16



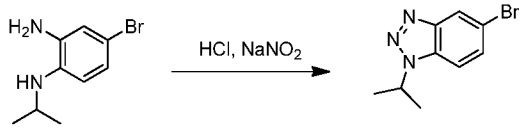
14-2 14-3

To a solution of 4-bromo-N-isopropyl-2-nitro-aniline (2 g, 7.72 mmol, 1 *eq*) in EtOH (20 mL) was added $SnCl_2.2H_2O$ (5.23 g, 23.16 mmol, 1.93 mL, 3 *eq*) and stirred at 80 °C for 16 h. The reaction mixture was quenched with aqueous NaOH (4 M, 50 mL), and then diluted with water (50 mL) and extracted with EA (100 mL **x *2)***. The combined organic layers were dried over ***Na_2SO_4***, filtered and concentrated under reduced pressure to give a residue. The residue was purified by flash silica gel chromatography (***PE/EA=100/1 to 1/1***) to give 4-bromo-N-isopropyl-benzene-1,2-diamine (850 mg, 3.71 mmol, 48.06% yield) as a black-brown solid.

^{1}H NMR (400MHz, CHLOROFORM-d) δ = 6.82 (dd, *J*=2.1, 8.4 Hz, 1H), 6.76 (d, *J*=2.2 Hz, 1H), 6.44 (d, *J*=8.3 Hz, 1H), 3.56 - 3.40 (m, 1H), 1.14 (d, *J*=6.4 Hz, 6H).

Synthesis of 14-4 : 5-bromo-1-(propan-2-yl)-1H-1,2,3-benzotriazole

Scheme 17



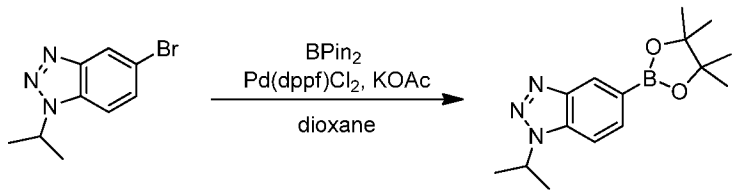
14-3 14-4

To a solution of 4-bromo-N--isopropyl-benzene-1,2-diamine (750 mg, 3.27 mmol, 1.00 *eq*) in HCl (5 mL, 6 M) was added $NaNO_2$ (271.04 mg, 3.93 mmol, 213.42 uL, 1.20 *eq*) in H_2O (2 mL) dropwise at 5 °C and stirred for 0.5 h. The reaction mixture was diluted with ***water (200*** mL) and extracted with EA (200 mLx2). The combined organic layers were dried over ***Na_2SO_4***, filtered and concentrated under reduced pressure to give a residue. The residue was purified by flash silica gel

chromatography (*1/1*) to give 5-bromo-1-isopropyl-benzotriazole (700 mg, 2.92 mmol, 89.06% yield) black-brown solid.

^{1}H NMR (400MHz, DMSO-d_6) δ = 8.32 (d, *J*=1.7 Hz, 1H), 7.94 (d, *J*=8.8 Hz, 1H), 7.60 - 7.60 (m, 1H), 7.67 (dd, *J*=1.8, 8.9 Hz, 1H), 5.32 - 5.16 (m, 1H), 1.62 (d, *J*=6.7 Hz, 6H).

Synthesis of 14-5 : 1-(propan-2-yl)-5-(tetramethyl-1,3,2-dioxaborolan-2-yl)-1H-1,2,3-benzotriazole



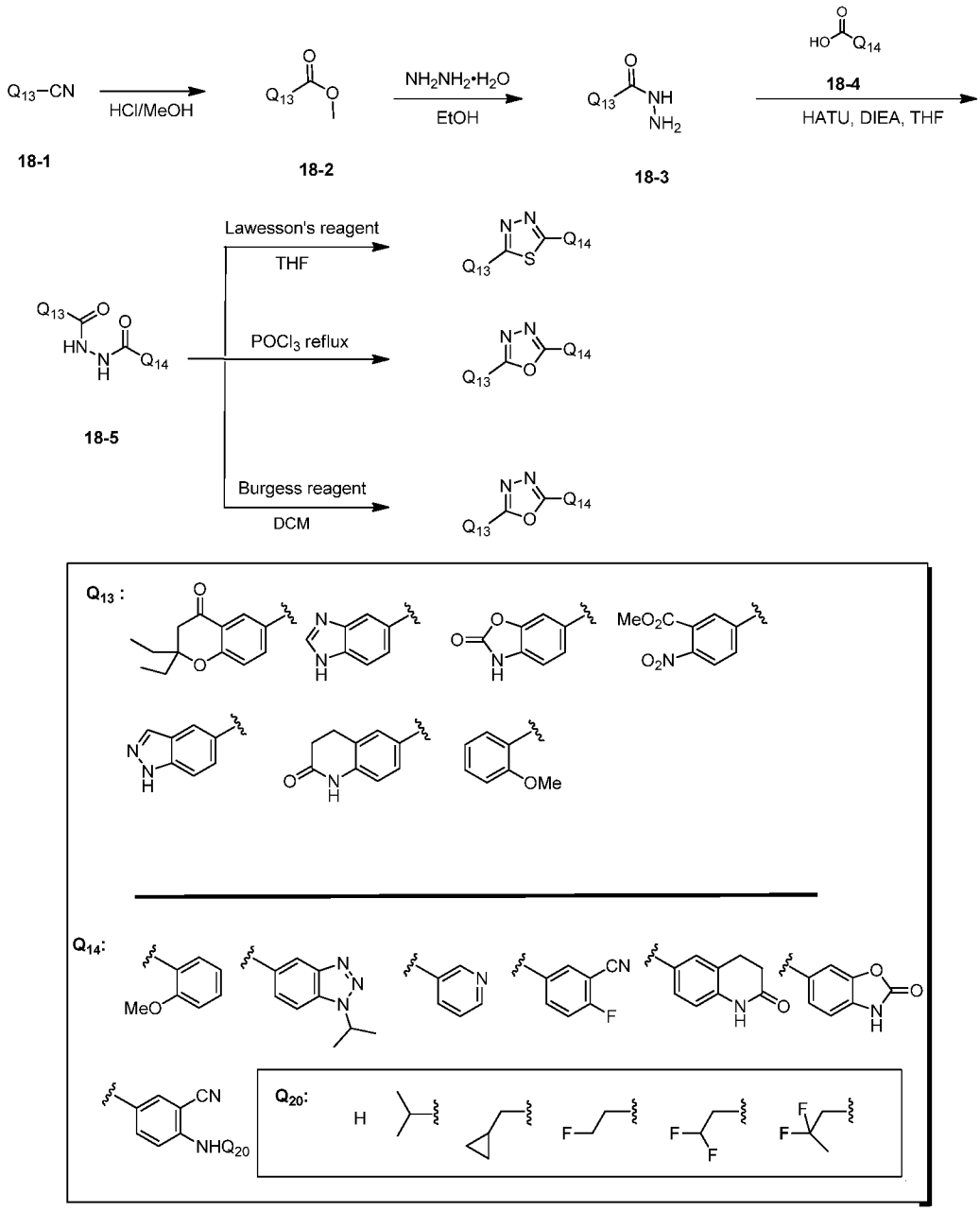
14-4 **14-5**

To a solution of 5-bromo-1-isopropyl-benzotriazole (700 mg, 2.92 mmol, 1 *eq*) in dioxane (10 mL) was added 4,4,5,5-tetramethyl-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,3,2-dioxaborolane (814.38 mg, 3.21 mmol, 1.1 *eq*), DPPF (161.63 mg, 291.55 umol, 0.1 *eq*), Pd(dppf)Cl_2 (213.33 mg, 291.55 umol, 0.1 *eq*) and KOAc (343.35 mg, 3.50 mmol, 1.2 *eq*), The mixture was stirred at 100 °C for 1 h, the mixture was diluted with water (100 mL) and extracted with (EA 100 mL x *2)*. The combined organic layers were dried over Na_2SO_4, filtered and concentrated under reduced pressure to give a residue. The residue was purified by flash silica gel chromatography (*PE/EA=100/1 to 1/1*) to give 1-isopropyl-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzotriazole (300 mg, 1.04 mmol, 35.83% yield) as a yellow solid.

^{1}H NMR (400MHz, CHLOROFORM-d) δ = 8.57 (s, 1H), 7.89 (dd, *J*=0.7, 8.3 Hz, 1H), 7.55 (dd, *J*=0.8, 8.4 Hz, 1H), 5.11 (spt, *J*=6.8 Hz, 1H), 1.75 (d, *J*=6.8 Hz, 6H), 1.47 - 1.34 (m, 12H).

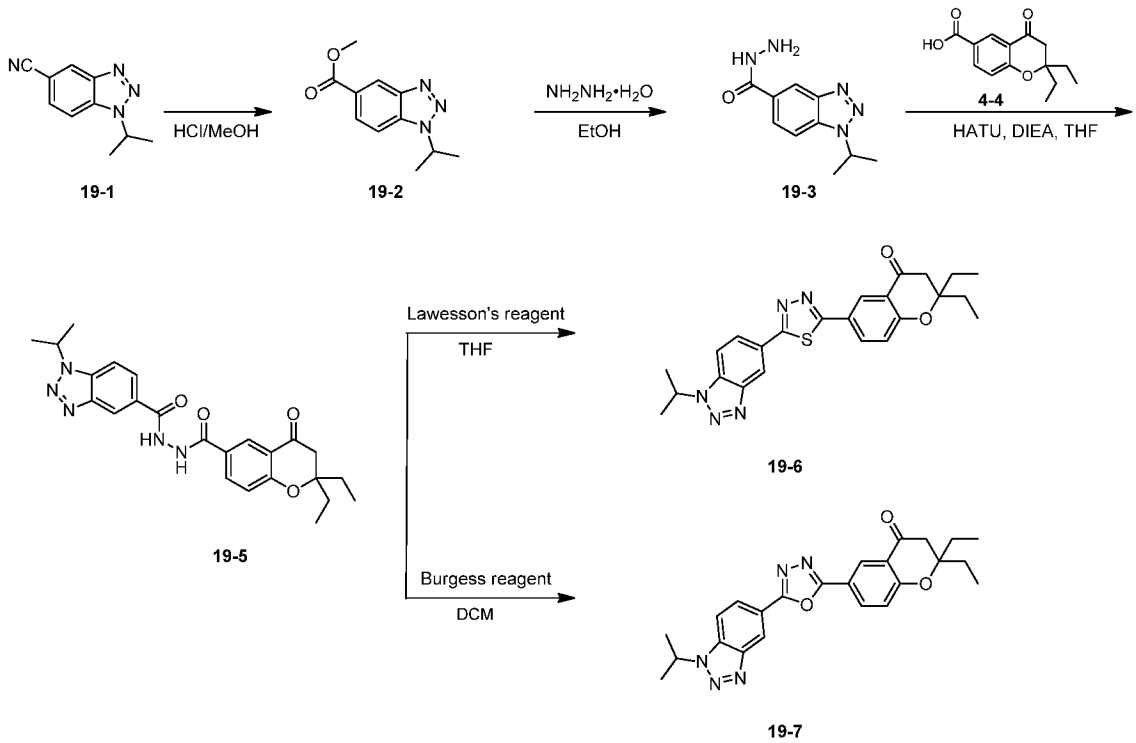
General Procedure E:

Scheme 18



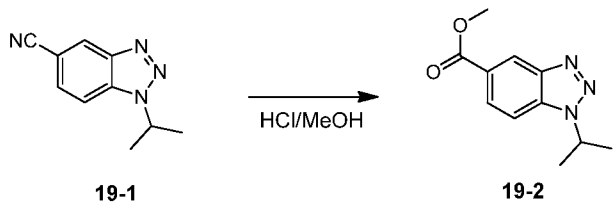
Synthesis of 19-6 and 19-7 : 2,2-diethyl-6-{5-[1-(propan-2-yl)-1H-1,2,3-benzotriazol-5-yl]-1,3,4-thiadiazol-2-yl}-3,4-dihydro-2H-1-benzopyran-4-one; 2,2-diethyl-6-{5-[1-(propan-2-yl)-1H-1,2,3-benzotriazol-5-yl]-1,3,4-oxadiazol-2-yl}-3,4-dihydro-2H-1-benzopyran-4-one

Scheme 19



Synthesis of 19-2: methyl 1-(propan-2-yl)-1H-1,2,3-benzotriazole-5-carboxylate

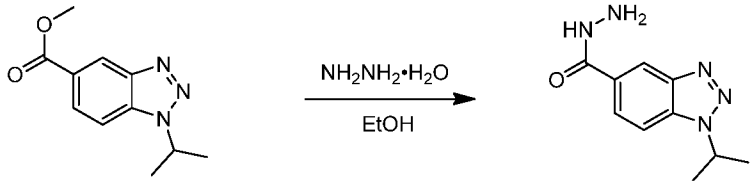
Scheme 20



A mixture of 1-isopropylbenzotriazole-5-carbonitrile (1 g, 5.37 mmol, 1 *eq.*) in HCl/MeOH (20 mL, 4 M) was stirred at 80 °C for 2 h. The mixture was concentrated, diluted with water (20 mL), extracted with EA (20 mLx2), dried over Na_2SO_4 and concentrated to dry. The crude product methyl 1-isopropylbenzotriazole-5-carboxylate (0.9 g, 4.11 mmol, 76.44% yield) was used into the next step without further purification.

Synthesis of 19-3 : 1-(propan-2-yl)-1H-1,2,3-benzotriazole-5-carbohydrazide

Scheme 21



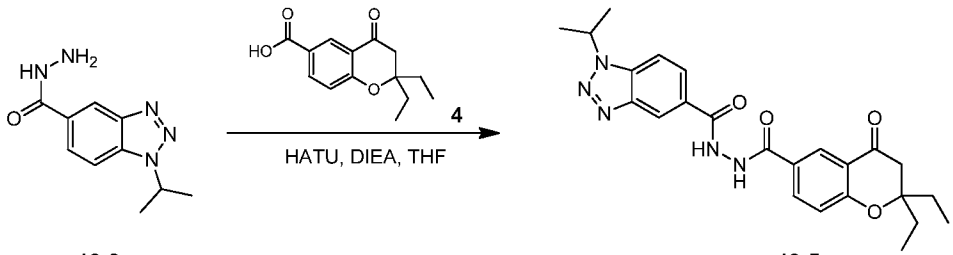
19-2 19-3

A mixture of methyl 1-isopropylbenzotriazole-5-carboxylate (0.5 g, 2.28 mmol, 1 *eq.*) and $NH_2NH_2•H_2O$ (1.14 g, 22.81 mmol, 1.11 mL, 10 *eq.*) in EtOH (10 mL) was stirred at 80 °C for 2 h. The mixture was concentrated to dry. The residue was purified by column chromatography (SiO_2, Petroleum ether/Ethyl acetate=1:1) to give 1-isopropyl Benzotriazole-5-carbohydrazide (0.38 g, 1.73 mmol, 76.00% yield) as a white solid.

Synthesis of 19-5 :

2,2-diethyl-4-oxo-N'-[1-(propan-2-yl)-1H-1,2,3-benzotriazole-5-carbonyl]-3,4-dihydro-2H-1-benzopyran-6-carbohydrazide

Scheme 22

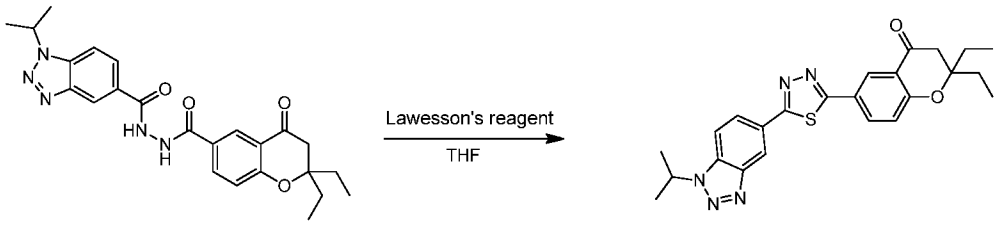


19-3 19-5

To a mixture of 2,2-diethyl-4-oxo-chromane-6-carboxylic acid (274.04 mg, 1.10 mmol, 1.1 *eq.*) and 1-isopropylbenzotriazole-5-carbohydrazide (220 mg, 1.00 mmol, 1 *eq.*) in THF (10 mL) was added HATU (419.70 mg, 1.10 mmol, 1.1 *eq.*) and DIEA (142.66 mg, 1.10 mmol, 192.26 uL, 1.1 *eq.*), the mixture was stirred at 15 °C for 2 hr. The mixture was diluted with water (50 mL), extracted with EA (50 mLx2), dried over Na_2SO_4 and concentrated in vacuum. N'-(2,2-diethyl-4-oxo-chromane-6-carbonyl)-1-isopropyl-benzotriazole-5-carbohydrazide (420 mg, 934.37 umol, 93.12% yield) was obtained as yellow solid without further purification.

Synthesis of 19-7: 2,2-diethyl-6-{5-[1-(propan-2-yl)-1H-1,2,3-benzotriazol-5-yl]-1,3,4-thiadiazol-2-yl}-3,4-dihydro-2H-1-benzopyran-4-one

Scheme 23



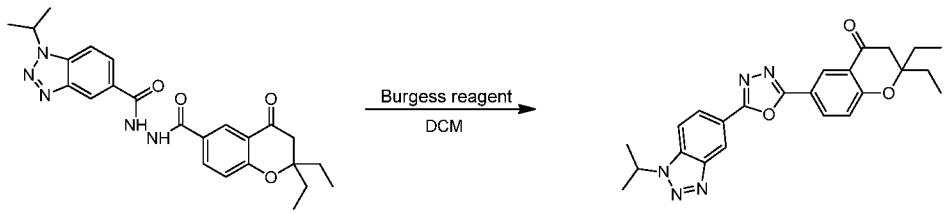
19-5 19-6

A mixture of N'-(2,2-diethyl-4-oxo-chromane-6-carbonyl)-1-isopropyl-benzotriazole-5-carbohydrazide (200 mg, 444.94 umol, 1 *eq.*) and Lawesson's reagent (359.93 mg, 889.88 umol, 2 *eq.*) in THF (2 mL) was stirred at 80 °C for 2 h. The mixture was diluted with water (20 mL), extracted with EA (20 mLx2), dried over Na_2SO_4 and concentrated to dry. The residue was purified by prep-HPLC (column: Phenomenex Synergi C18 150x25x10um; mobile phase: [water(0.1%TFA)-ACN];B%: 62%-92%,13min) to give 2,2-diethyl-6-[5-(1-isopropylbenzotriazol-5-yl)-1,3,4-thiadiazol-2-yl]chroman-4-one (61 mg, 29.99 umol, 6.74% yield, 22% purity) as a white solid. ^{1}H NMR (400MHz, CHLOROFORM-d) δ = 8.62 (d, *J*=0.6 Hz, 1H), 8.38 - 8.36 (m, 1H), 8.36 - 8.33 (m, 1H), 8.33 - 8.30 (m, 1H), 7.72 (d, *J*=8.8 Hz, 1H), 7.13 (d, *J*=8.7 Hz, 1H), 5.22 - 5.11 (m, 1H), 2.82 (s, 2H), 1.95 - 1.83 (m, 4H), 1.82 - 1.80 (m, 6H), 0.99 (t, *J*=7.5 Hz, 6H).

Synthesis of 19-7:

2,2-diethyl-6-{5-[1-(propan-2-yl)-1H-1,2,3-benzotriazol-5-yl]-1,3,4-oxadiazol-2-yl}-3,4-dihydro-2H-1-benzopyran-4-one

Scheme 24



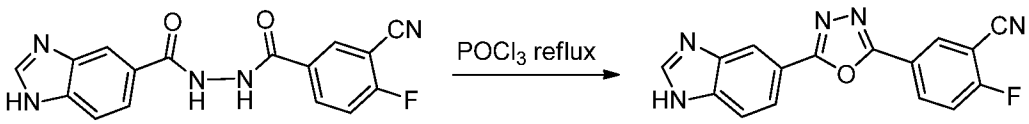
19-5 19-7

A mixture of N'-(2,2-diethyl-4-oxo-chromane-6-carbonyl)-1-isopropyl-benzotriazole-5-carbohydrazide (200 mg, 444.94 umol, 1 *eq.*) and Burgess reagent (530.17 mg, 2.22 mmol, 5 *eq.*) in DCM (2 mL) was stirred at 15 °C for 2 h. The mixture was diluted with water (20 mL), extracted with EA (20 mLx2), dried over Na_2SO_4 and concentrated to dry. The residue was purified by prep-HPLC (column: Phenomenex Synergi C18 150x25x10um; mobile phase: [water(0.1%TFA)-

ACN];B%: 55%-85%,12min) to give 2,2-diethyl-6-[5-(1-isopropylbenzotriazol-5-yl)-1,3,4-oxadiazol-2-yl]chroman-4-one (56 mg, 129.78 umol, 29.17% yield, 100% purity) as a white solid. ^{1}H NMR (400MHz, CHLOROFORM-d) δ = 8.85 (s, 1H), 8.61 (d, *J*=2.3 Hz, 1H), 8.35 (t, *J*=2.1 Hz, 1H), 8.33 (t, *J*=2.1 Hz, 1H), 7.75 (d, *J*=8.7 Hz, 1H), 7.16 (d, *J*=8.8 Hz, 1H), 5.24 - 5.11 (m, 1H), 2.84 (s, 2H), 1.94 - 1.85 (m, 2H), 1.82 (d, *J*=6.8 Hz, 5H), 1.80 - 1.75 (m, 2H), 1.00 (t, *J*=7.5 Hz, 6H)

Synthesis of 25-2: 5-[5-(1H-1,3-benzodiazol-5-yl)-1,3,4-oxadiazol-2-yl]-2-fluorobenzonitrile

Scheme 25

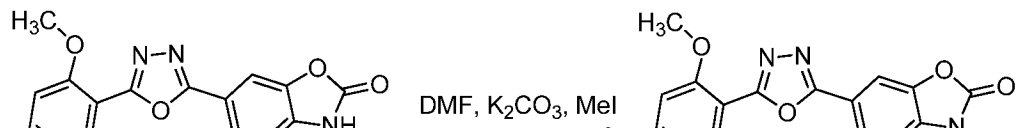


25-1 **25-2**

A suspension of **1** (N'-(1H-1,3-benzodiazole-5-carbonyl)-3-cyano-4-fluorobenzohydrazide, 541 mg, 1.67 mmol) in phosphorus oxychloride (10 mL, excess) was heated at 105°C for 3 hours. The mixture was concentrated, and the residue was suspended in water with sonication/stirring. The resulting solid was collected, washed with sat'd $NaHCO_3$ and water, then dried under N_2/vac in the filter funnel. The tan solid was suspended in MeCN and concentrated twice to remove residual water and dried under high vacuum to yield **25-2** (0.55 g, 107%). MH+ = 306.1.

Synthesis of 26-2 :
6-[5-(2-methoxyphenyl)-1,3,4-oxadiazol-2-yl]-3-methyl-2,3-dihydro-1,3-benzoxazol-2-one

Scheme 26

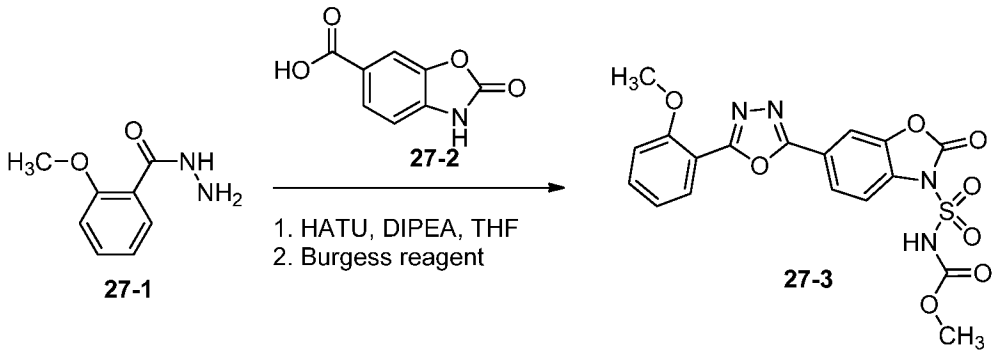


26-1 **26-2**

To a suspension of **3** (6-[5-(2-methoxyphenyl)-1,3,4-oxadiazol-2-yl]-2,3-dihydro-1,3-benzoxazol-2-one trifluoroacetate, 13 mg, 0.031 mmol) in DMF (1 mL) was added potassium carbonate (8.6 mg, 0.062 mmol) followed by methyl iodide (5.2 mg, 0.037 mmol) and the resulting white suspension heated to 100°C for 45 min. The reaction was cooled to room temperature, filtered, and purified by reverse phase chromatography, 25% - 75% MeCN/water/0.1% TFA. The product fractions lyophilized to yield **26-2** (1.6 mg, 12%). MH+ = 324.1. ^{1}H NMR (400 MHz, DMSO) 7.93 - 7.91 (3H, m), 7.59 - 7.54 (1H, m), 7.44 - 7.41 (1H, m), 7.25 - 7.22 (1H, m), 7.11 - 7.07 (1H, m), 3.88 (3H, s); 3.45 (3H, s)

Synthesis of 27-3 : methyl N-({6-[5-(2-methoxyphenyl)-1,3,4-oxadiazol-2-yl]-2-oxo-2,3-dihydro-1,3-benzoxazol-3-yl}sulfonyl)carbamate

Scheme 27



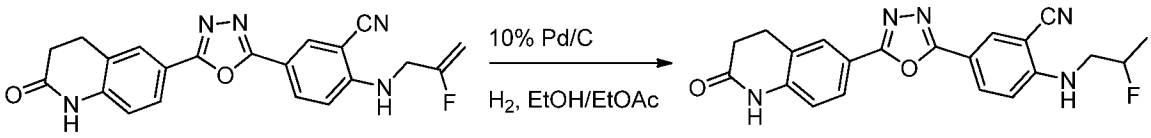
To a dry mixture of **27-1** (2-methoxyphenylhydrazide, 139 mg, 0.837 mmol), **27-2** (benzoxazol-2-one-6-carboxylic acid, 150 mg, 0.837 mmol), and HATU (318 mg, 0.837 mmol) was added THF (10 mL) to yield a hazy reddish solution. DIPEA (0.29 mL, 1.67 mmol) was added and the reaction was stirred at rt for 2 hr. Burgess reagent (499 mg, 2.09 mmol) was added one portion, and the reaction was heated to 60°C overnight. An additional 499 mg Burgess reagent was added. and continued heating. After 4 hr, 2N $KHSO_4$ (10 mL) was added and the resulting oily mixture was extracted 3X EtOAc. The combined organics were washed once with water, once with brine, filtered through cotton and concentrated to an orange solid which was purified by reverse phase chromatography, 20% - 60% MeCN/water/0.1% TFA to yield 67 mg **27-3**(18%) MH+ = 447.0. ^{1}H NMR (400 MHz,

DMSO) 8.02 - 7.97 (3H, m), 7.74 (1H, d, J=8.4 Hz), 7.64 (1H, t, J=8.2 Hz), 7.30 (1H, d, J=8.4 Hz), 7.18 (1H, t, J=7.4 Hz), 3.95 (3H, s), 3.39 (3H, s).

Synthesis of 28-2:

2-[(2-fluoropropyl)amino]-5-[5-(2-oxo-1,2,3,4-tetrahydroquinolin-6-yl)-1,3,4-oxadiazol-2-yl]benzonitrile

Scheme 28



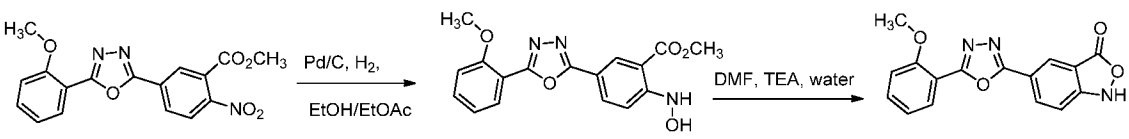
28-1 28-2

To a nitrogen purged small Parr hydrogenation bottle was added 10% Pd/C (14 mg) and moistened with a small volume of EtOH. To **28-1** (2-[(2-fluoroprop-2-en-1-yl)amino]-5-[5-(2-oxo- 1,2,3,4-tetrahydroquinolin-6-yl)-1,3,4-oxadiazol-2- yl]benzonitrile trifluoroacetate, 70 mg, 0.139 mmol) was added EtOH (10 mL) and EtOAc (90 mL) to yield a milky mixture which was added to the hydrogenation bottle. The mixture was hydrogenated under 50 psi H2 for 24 hr. MeCN was added until the milky mixture clears, then filtered through Celite and concentrated. The residue was heated in a small volume of DMF, cooled, filtered, and purified by reverse phase chromatography, 30% - 75% MeCN/water/0.1% TFA. The product fractions were lyophilized to yield **28-2** as a fluffy white solid (12.8 mg, 18%). MH+ = 392.1. ^{1}H NMR (400 MHz, DMSO) 10.40 (1H, s), 8.25 (1H, d, J=2.1 Hz), 8.11 (1H, dd, J=2.0, 9.2 Hz), 7.92 - 7.81 (2H, m), 7.22 (1H, t, J=6.3 Hz), 7.11 (1H, d, J=9.2 Hz), 7.11 (1H, d, J=9.4 Hz), 7.02 (1H, d, J=8.7 Hz), 7.04 - 7.00 (1H, m), 5.00 - 4.80 (1H, m), 3.60 - 3.51 (2H, m), 3.01 (2H, t, J=7.4 Hz), 1.35 (3H, dd, J=6.2, 24.0 Hz).

Synthesis of 29-3:

5-[5-(2-methoxyphenyl)-1,3,4-oxadiazol-2-yl]-1,3-dihydro-2,1-benzoxazol-3-one

Scheme 29



29-1 29-2 29-3

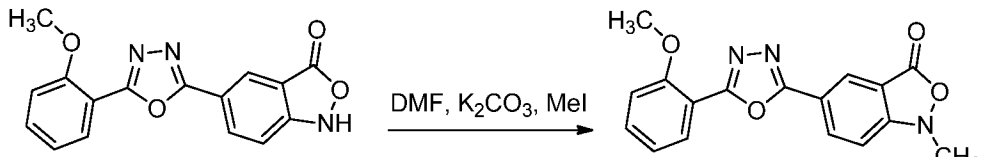
To a nitrogen purged hydrogenation bottle was added 10% Pd/C (12 mg), which was moistened with EtOH. A suspension of **29-1** (methyl 5-[5-(2-methoxyphenyl)-1,3,4-oxadiazol-2-yl]-2-nitrobenzoate, prepared according to Wuxi 1,3,4-oxadiazole experimental, 112 mg, 0.281) in EtOH (25 mL) and EtOAc (20 mL) was hydrogenated at 48 psi H_2. After 30 minutes the reaction was filtered and concentrated to solid **29-2** (113 mg, 105%), which was used without further purification. MH+ = 342.1.

To a solution of **29-2** (47 mg, 0.132 mmol) in DMF (2 mL) was added triethylamine (0.1 mL) then water (0.2 mL) and the resulting solution stirred at rt for 60 hr. The reaction mixture was purified directly by reverse phase chromatography, 20% - 65% MeCN/water/0.1% TFA to yield 8 mg **29-3** (14%). MH+ = 310.1. ^{1}H NMR (400 MHz, DMSO) 12.52 (1H, s), 8.42 - 8.38 (2H, m), 8.03 (1H, d, J=6.9 Hz), 7.65 (1H, t, J=8.3 Hz), 7.57 (1H, d, J=7.6 Hz), 7.32 (1H, d, J=8.3 Hz), 7.17 (1H, t, J=6.9 Hz), 3.96 (3H, s).

Synthesis of 30-1:

5-[5-(2-methoxyphenyl)-1,3,4-oxadiazol-2-yl]-1-methyl-1,3-dihydro-2,1-benzoxazol-3-one

Scheme 30

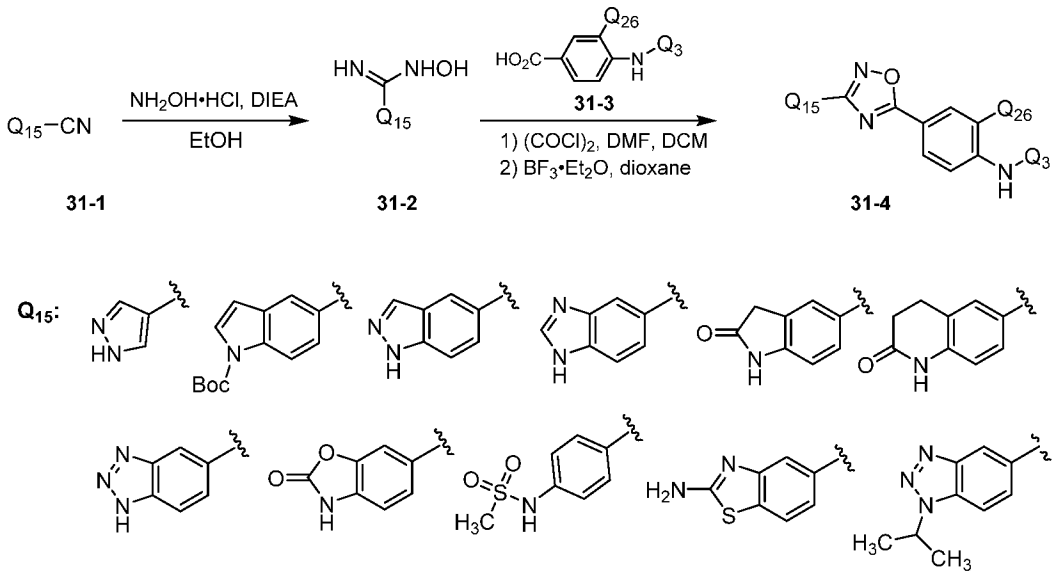


29-2 **30-1**

To a solution of **29-2** (8 mg, 0.019 mmol) in DMF (0.5 mL)was added potassium carbonate (2.6 mg, 0.019 mmol) followed by methyl iodide (4.0 mg, 0.028 mmol) and the resulting solution heated to 100°C for 15 minutes. The reaction was cooled to rt, filtered, and purified directly by reverse phase chromatography, 25% - 75% MeCN/water/0.1% TFA to yield 5.3 mg **30-1** (64%) as a white solid. MH+ = 324.1. ^{1}H NMR (400 MHz, DMSO) 8.40 (1H, d, J=8.7 Hz), 8.32 (1H, s), 7.97 (1H, d, J=8.0 Hz), 7.73 (1H, d, J=8.7 Hz), 7.58 (1H, t, J=8.3 Hz), 7.25 (1H, d, J=8.0 Hz), 7.10 (1H, t, J=7.7 Hz), 3.89 (3H, s), 3.49 (3H, s).

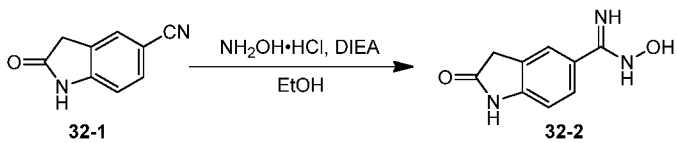
General Procedure F:

Scheme 31



Synthesis of 32-2 : N-hydroxy-2-oxo-2,3-dihydro-1H-indole-5-carboximidamide

Scheme 32



To a mixture of 2-oxoindoline-5-carbonitrile (200 mg, 1.26 mmol, 1 *eq*) in ethanol (5 mL) was added hydrochloride salt of hydroxylamine (176 mg, 2.53 mmol, 2.0 *eq*), diisopropylethylamine (327 mg, 2.53 mmol, 2.0 *eq*) at 20 °C under nitrogen atmosphere. The mixture was then heated to 90 °C and stirred for 16 hrs. The mixture was concentrated in vacuum, and a white solid was precipitated

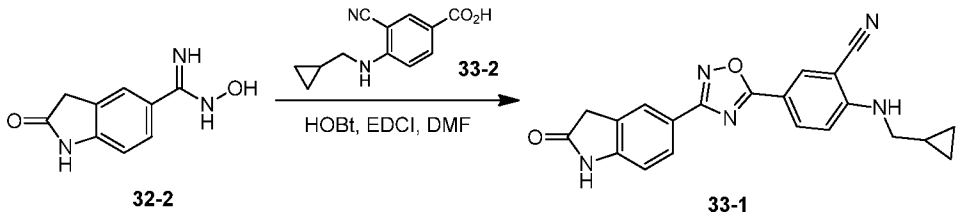
out. The suspension was filtered, and the white solid was dried in vacuum to give the product **32-2** (210 mg, 83% yield).

^{1}H NMR (400MHz, DMSO-d_6) δ = 10.46 (br, s, 1H), 9.45 (br, s, 1H), 7.51 (s, 1H), 7.50 (d, J = 10.8 Hz, 1H), 6.79 (d, J = 8.0 Hz, 1H), 5.70 (br, s, 2H), 3.49 (s, 2H).

Synthesis of 33-1:

2-[(cyclopropylmethyl)amino]-5-[3-(2-oxo-2,3-dihydro-1H-indol-5-yl)-1,2,4-oxadiazol-5-yl]benzonitrile

Scheme 33

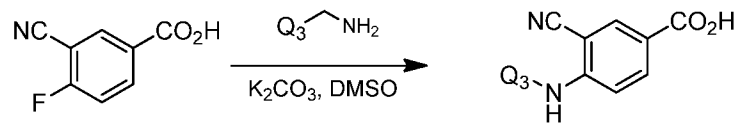


To a mixture of 3-cyano-4-(cyclopropylmethylamino)benzoic acid (107 mg, 496 umol, 1.2 eq) in *N*,*N*-dimethylformamide (1 mL) was added HOBt (67.0 mg, 496 umol, 1.2 eq), EDCI (95.1 mg, 496 umol, 1.2 eq) at 20 °C. The mixture was stirred for 30 min, then *N*-hydroxy-2-oxo-indoline-5-carboxamidine (79 mg, 413 umol, 1 eq) was added, and the resultant mixture then heated to 150 °C and stirred for 1 hour. The cooled reaction mixture was directly purified by *prep*-HPLC (column: Boston Green ODS 150x30 5u;mobile phase: [water(0.225%FA)-ACN];B%: 47%-77%,10min) to give the product **33-1** (20 mg, 12% yield).

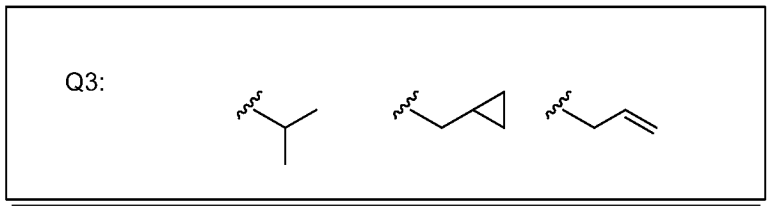
^{1}H NMR (400MHz, DMSO-d_6) δ = 10.73 (br, s, 1H), 8.23 (d, J = 2.4 Hz, 1H), 8.11 (dd, J = 9.2, 2.0 Hz, 1H), 7.93 (d, J = 8.0 Hz, 1H), 7.89 (s, 1H), 7.17 (t, J = 6.4 Hz, 1H), 7.07 (d, J = 9.2 Hz, 1H), 7.00 (d, J = 8.0 Hz, 1H), 3.61 (s, 2H), 3.20 (t, J = 6.4 Hz, 2H), 1.16 – 1.13 (m, 1H), 0.52 – 0.47 (m, 2H), 0.33 – 0.29 (m, 2H).

General Procedure G:

Scheme 34

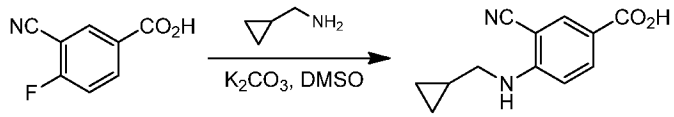


5A 5



Synthesis of 35-2 : 3-cyano-4-[(cyclopropylmethyl)amino]benzoic acid

Scheme 35



35-1 35-2

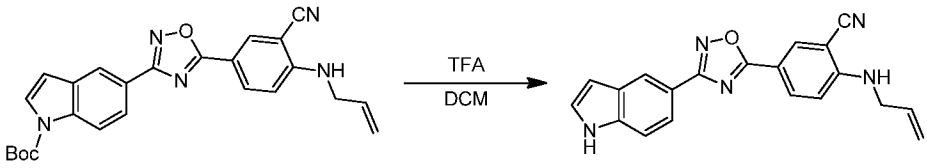
To a mixture of 3-cyano-4-fluoro-benzoic acid (5 g, 30.3 mmol, 1 eq) and cyclopropylmethanamine (5.38 g, 75.7 mmol, 2.5 eq) in dimethylsulfoxide (30 mL) was added potassium carbonate (12.6 g, 90.8 mmol, 3 eq) at 20 °C. The mixture was then heated to 100 °C and stirred for 16 hours. The mixture was filtered, and the filtrate was diluted with water (50 mL), acidified by hydrochloride solution (2N) to pH = 4~5. A yellow solid was precipitated out, the suspension was filtered, and the solid was washed by water (50 mL X 3). The solid was dried in vacuum to give the desired product **35-2** (5 g, 73% yield).

1H NMR (400MHz, DMSO-d_6) δ = 7.95 (d, J = 1.2 Hz, 1H), 7.90 (d, J = 9.2 Hz, 1H), 6.88 (d, J = 9.2 Hz, 1H), 6.85 – 6.82 (m, 1H), 3.13 (t, J = 6.0, 2H), 1.16 – 1.06 (m, 1H), 0.49 – 0.44 (m, 2H), 0.29 – 0.25 (m, 2H).

Synthesis of 36-2 :

5-[3-(1H-indol-5-yl)-1,2,4-oxadiazol-5-yl]-2-[(prop-2-en-1-yl)amino]benzonitrile

Scheme 36



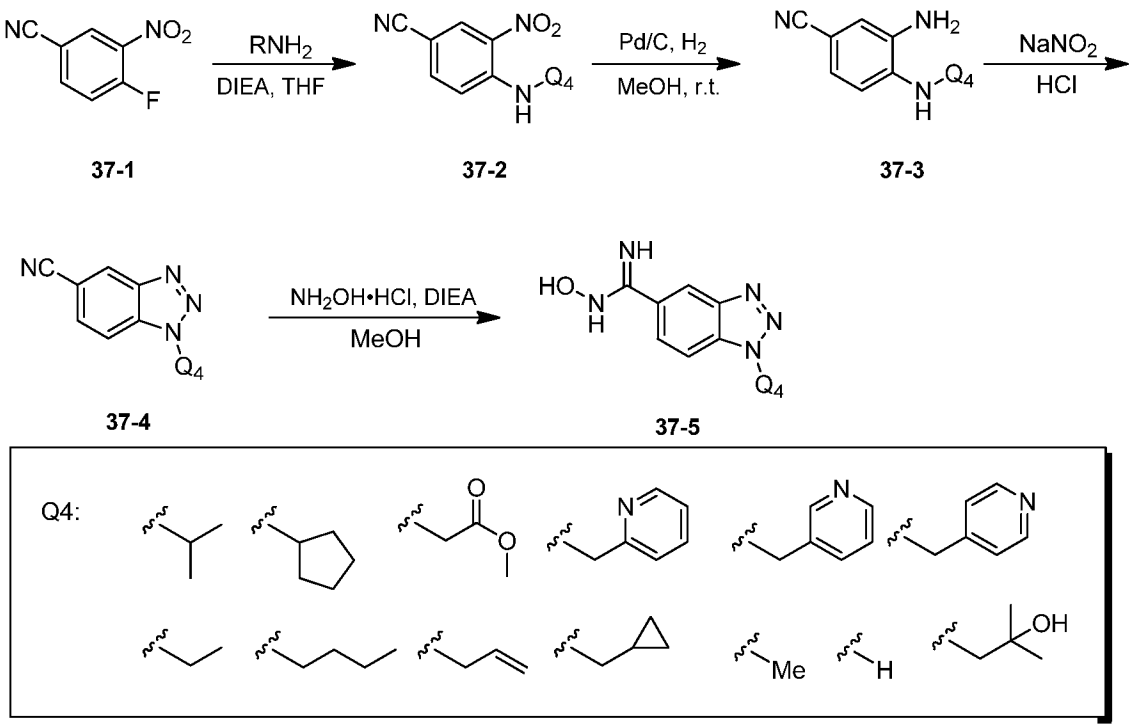
36-21 36-2

To a mixture of *tert*-butyl 5-[5-[4-(allylamino)-3-cyano-phenyl]-1,2,4-oxadiazol-3-yl]indole -1-carboxylate (60.0 mg, 136 umol, 1.00 *eq*) in dichloromethane (10.0 mL) was added trifluoroacetic acid (770 mg, 6.75 mmol, 50 *eq*) at 20 °C under nitrogen atmosphere. The mixture was stirred at 20 °C for 16 h. The mixture was concentrated in vacuum and the residue was purified by *prep*-HPLC (column: Gemini 150x25 5u;mobile phase: [water (0.05% ammonia hydroxide v/v)-ACN];B%: 47%-77%,12min) to give the product **36-2** (15 mg, 30% yield) as a white solid.

^{1}H NMR (400MHz, DMSO-d_6) δ = 8.33 (s, 1H), 8.27 (d, J = 2.0 Hz, 1H), 8.14 (dd, J = 8.8, 2.0 Hz, 1H), 7.80 (dd, J = 8.4, 1.2 Hz, 1H), 7.56 (d, J = 8.8 Hz, 1H), 7.48 (t, J = 2.4 Hz, 1H), 7.39 (t, J = 5.6 Hz, 1H), 6.91 (d, J = 8.8 Hz, 1H), 6.61 (s, 1H), 5.94 – 5.85 (m, 1H), 5.24 – 5.16 (m, 2H), 3.97 (s, 1H).

General Procedure H:

Scheme 37

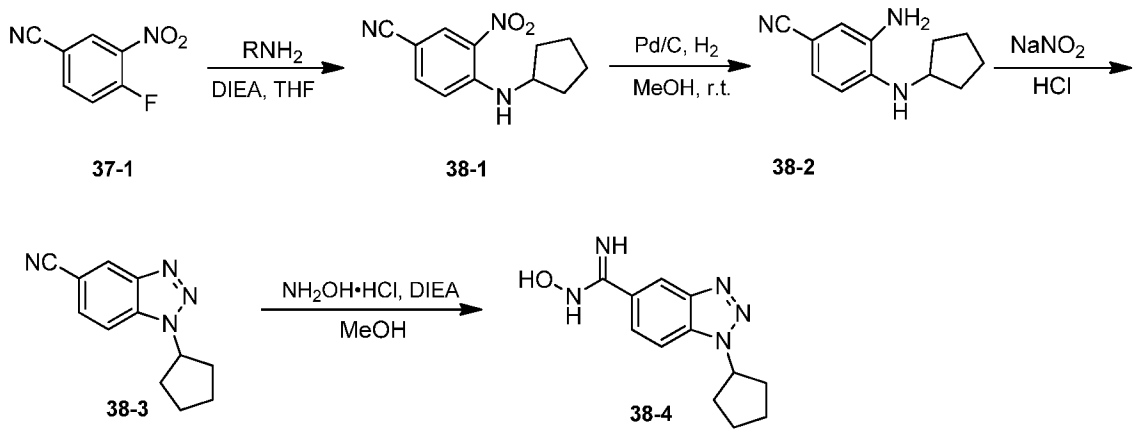


37-1 37-2 37-3

37-4 37-5

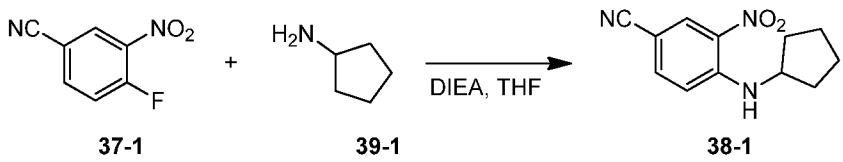
Synthesis of 38-4 : 1-cyclopentyl-N-hydroxy-1H-1,2,3-benzotriazole-5-carboximidamide

Scheme 38



Synthesis of 38-1 : 4-(cyclopentylamino)-3-nitrobenzonitrile

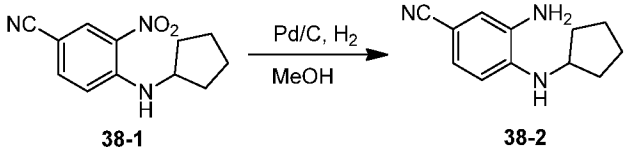
Scheme 39



Preparation of 1: To a solution of 4-fluoro-3-nitro-benzonitrile (1.00 g, 6.02 mmol, 1.00 *eq*) and cyclopentanamine (767 mg, 9.03 mmol, 1.50 *eq*) in THF (20.00 mL) was added DIEA (1.95 g, 15.05 mmol, 2.63 mL, 2.50 *eq*) and the mixture was stirred at 10 °C for 16 hour. The mixture was evaporated to dry and diluted with H_2O (50 mL), extracted with DCM (50 mLx2), dried over Na_2SO_4, filtered and concentrated to dry. Compound 4-(cyclopentylamino)-3- nitrobenzonitrile (1.36 g, 5.91 mmol, 98.10% yield) was obtained as a yellow solid which was used directly in next step.

Synthesis of 38-2 : 3-amino-4-(cyclopentylamino)benzonitrile

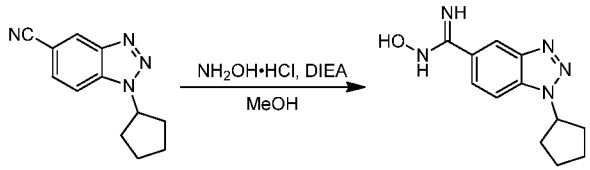
Scheme 40



Preparation of 2: To a solution of 4-(cyclopentylamino)-3-nitro-benzonitrile (5.00 g, 21.62 mmol, 1.00 *eq*) in MeOH (150.00 mL) was added Pd/C (1.00 g, 4.32 mmol, 10% purity, 0.20 *eq*). Then the mixture was stirred for 12 hours at 20°C under H_2 (50 psi). The mixture was filtered and the filtrate was concentrated to dry to get 3-amino-4-(cyclopentylamino)benzonitrile (4.20 g, 20.87 mmol, 96.52% yield) as black solid, which was used directly in the next step. ^{1}H NMR (400MHz, DMSO-d6) δ = 8.77 (s, 1H), 8.12 (d, J=8.7 Hz, 1H), 7.91 (d, J=8.7 Hz, 1H), 5.43 (m, 1H), 2.37 - 2.21 (m, 2H), 2.18 - 2.06 (m, 2H), 1.99 - 1.85 (m, 2H), 1.81 - 1.67 (m, 2H).

Synthesis of 38-4: 1-cyclopentyl-N-hydroxy-1H-1,2,3-benzotriazole-5-carboximidamide

Scheme 41



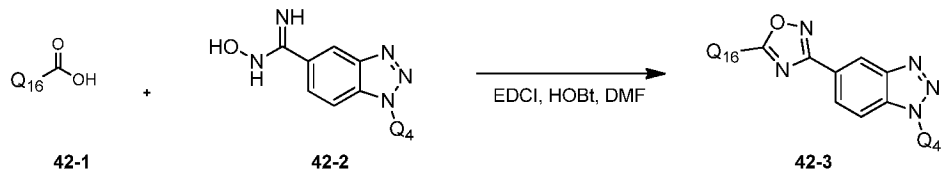
38-3 38-4

Preparation of 3: To a solution of 1-cyclopentylbenzotriazole-5-carbonitrile (1.50 g, 7.07 mmol) in ethanol (15.00 mL) was added hydroxylamine hydrochloride (736.64 mg, 10.60 mmol) and DIPEA (2.01 g, 15.55 mmol, 2.72 mL). Then the mixture was stirred at 70°C for 4 hours. The mixture was filtered to get 1-cyclopentyl-N-hydroxy-benzotriazole-5-carboxamidine (1.20 g, 4.89 mmol, 69.20% yield) as a white solid.

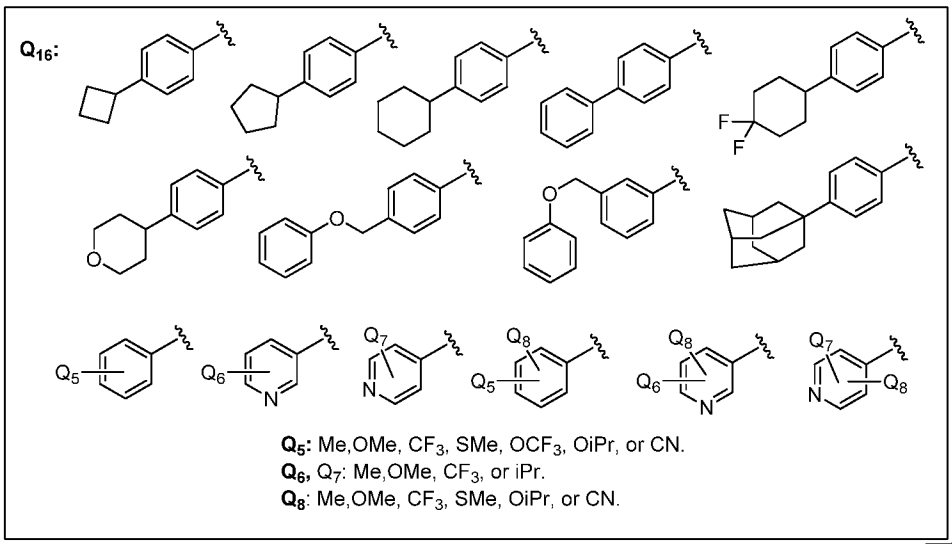
^{1}H NMR (400MHz, DMSO-d6) δ = 9.77 (s, 1H), 8.31 (s, 1H), 7.97 - 7.89 (m, 1H), 7.87 - 7.79 (m, 1H), 5.98 (s, 2H), 5.34 (q, J=7.0 Hz, 1H), 2.36 - 2.21 (m, 2H), 2.19 - 2.07 (m, 2H), 1.99 - 1.84 (m, 2H), 1.81 - 1.67 (m, 2H).

General Procedure I:

Scheme 42



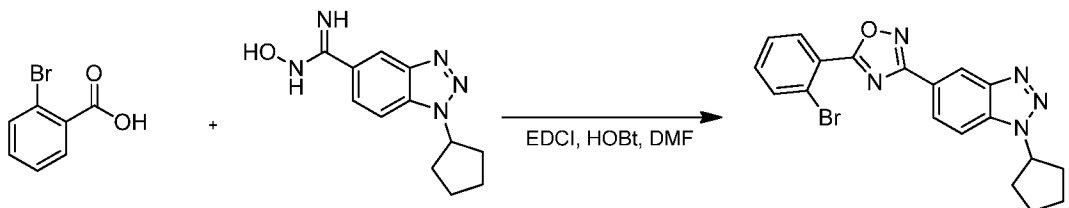
42-1 42-2 42-3



Synthesis of 42-2 :

5-[5-(2-bromophenyl)-1,2,4-oxadiazol-3-yl]-1-cyclopentyl-1H-1,2,3-benzotriazole

Scheme 43



43-1 38-4 43-2

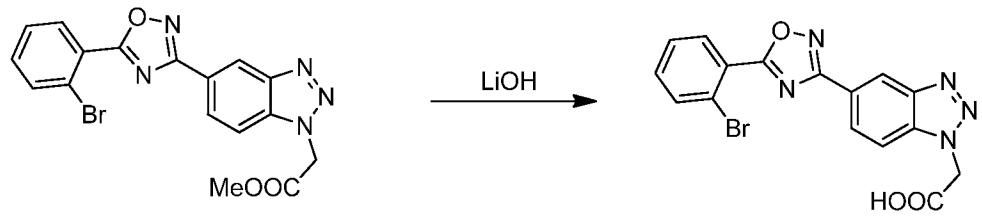
To a solution of 3-methylbenzoic acid (66.61 mg, 489.24 umol) in DMF (4.00 mL) was added EDCI (93.79 mg, 489.24 umol) and HOBt (66.11 mg, 489.24 umol). The mixture was stirred at 20°C for 1 hour and 1-cyclopentyl-N-hydroxy-benzotriazole-5-carboxamidine (100.00 mg, 407.70 umol) was added to the mixture. Then the mixture was stirred at 120°C for 12 hours under N_2. The mixture was quenched with water (30 mL) and extracted with ethyl acetate (30 mLx2). The organic layers were washed with brine (40 mL), dried over Na_2SO_4 and concentrated to dryness. The residue was purified by prep-HPLC (TFA) to get t 3-(1-cyclopentylbenzotriazol-5-yl)-5-(m-tolyl)-1,2,4-

oxadiazole (96.00 mg, 277.94 umol, 68.17% yield) as a white solid. ^{1}H NMR (400MHz, $CDCl_3$) δ = 8.93 (s, 1H), 8.30 (dd, *J*=1.3, 8.7 Hz, 1H), 8.08 (s, 1H), 8.06 (br d, *J*=6.8 Hz, 1H), 7.68 (d, *J*=8.8 Hz, 1H), 7.51 - 7.42 (m, 2H), 5.22 (quin, *J*=7.0 Hz, 1H), 2.50 (s, 3H), 2.43 - 2.32 (m, 4H), 2.15 - 2.01 (m, 2H), 1.92 - 1.81 (m, 2H).

Synthesis of 44-2 :

2-{5-[5-(2-bromophenyl)-1,2,4-oxadiazol-3-yl]-1H-1,2,3-benzotriazol-1-yl}acetic acid

Scheme 44



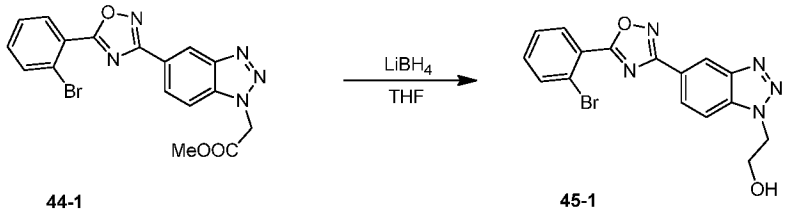
44-1 **44-2**

To a solution of methyl 2-[5-[5-(2-bromophenyl)-1,2,4-oxadiazol-3-yl]benzotriazol-1-yl] acetate (40.00 mg, 96.57 umol, 1.00 *eq*) in dioxane (2.00 mL) and H_2O (2.00 mL) was added NaOH (15.45 mg, 386.28 umol, 4.00 *eq*). Then the mixture was stirred at 20°C for 12 hours. The mixture was adjust to pH=2~3 with HCl (1N) and extracted with ethyl acetate (15 mLx2). The organic layers were dried over Na_2SO_4 and concentrated to give 2-[5-[5-(2-bromophenyl)-1,2, 4-oxadiazol-3-yl]benzotriazol-1-yl]acetic acid(17.30 mg, 43.23 umol, 44.76% yield) as a white solid. ^{1}H NMR (400MHz, DMSO-d_6) δ = 8.70 (s, 1H), 8.26 (m, 3H), 7.93 (m, 2H), 7.66 (m, 2H), 5.24 (br s, 2H)

Synthesis of 45-1 :

2-{5-[5-(2-bromophenyl)-1,2,4-oxadiazol-3-yl]-1H-1,2,3-benzotriazol-1-yl}ethan-1-ol

Scheme 45

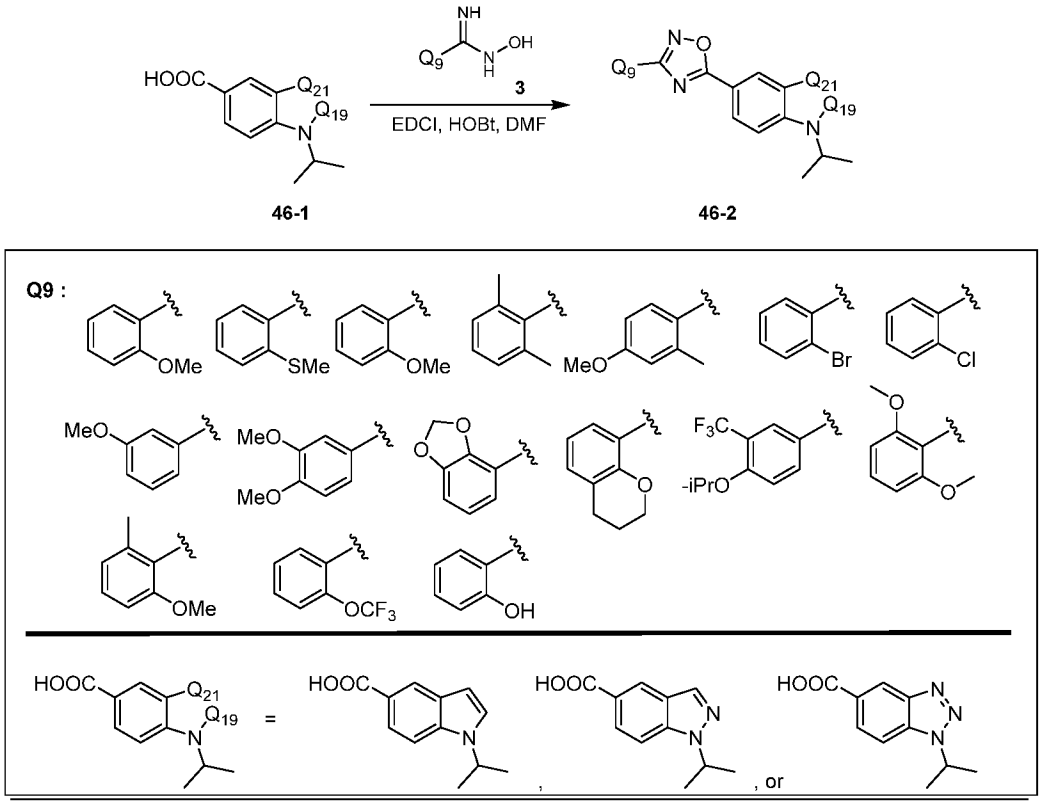


44-1 **45-1**

To a solution of methyl 2-[5-[5-(2-bromophenyl)-1,2,4-oxadiazol-3-yl]benzotriazol-1-yl] acetate (50.00 mg, 120.71 umol, 1.00 *eq*) in THF (1.00 mL) was added $LiBH_4$ (5.26 mg, 241.42 umol, 2.00 *eq*) and stirred at 10 °C for 16 h. The mixture was diluted with H_2O (20 mL) and extracted with EA (30 mLx2), the combined organic layers were dried over Na_2SO_4, filtered and concentrated to dry. The residue was purified by prep-HPLC (TFA condition) to give 2-[5-[5-(2-bromophenyl)-1,2,4-oxadiazol-3-yl]benzotriazol-1-yl]ethanol (10.00 mg, 25.89 umol, 21.45% yield) as a white solid. ^{1}H NMR (400MHz, DMSO-d_6) δ = 8.74 (s, 1H), 8.43 (br s, 1H), 8.25 (dd, *J*=1.1, 8.8 Hz, 1H), 8.17 (dd, *J*=1.9, 7.4 Hz, 1H), 8.12 (d, *J*=8.7 Hz, 1H), 8.01 - 7.92 (m, 1H), 7.74 - 7.60 (m, 2H), 4.84 (t, *J*=5.1 Hz, 2H), 3.93 (t, *J*=5.1 Hz, 2H).

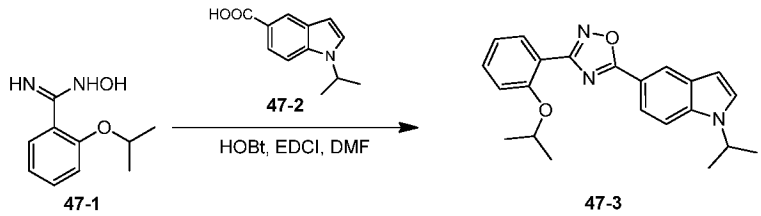
General Procedure J:

Scheme 46



Synthesis of 46-1 : 3-(2-isopropoxyphenyl)-5-(1-isopropylindol-5-yl) -1,2,4-oxadiazole

Scheme 47



47-1 47-3

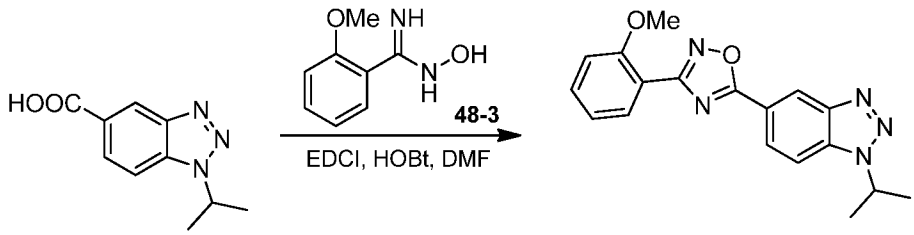
To a solution of N-hydroxy-2-isopropoxy-benzamidine (90.00 mg, 393.86 umol, 1.00 *eq*) in DMF (2.00 mL)was added 1-isopropylindole-5-carboxylic acid (80.05 mg, 393.86 umol, 1.00 *eq*), HOBt (63.86 mg, 472.63 umol, 1.20 *eq*) and EDCI (90.60 mg, 472.63 umol, 1.20 *eq*), the reaction was stirred at 120° C for 12h. The mixture was filtered and concentrated. The residue was purified by prep-HPLC to give 3-(2-isopropoxyphenyl)-5-(1-isopropylindol-5-yl) -1,2,4-oxadiazole (26.00 mg, 71.93 umol, 18.26% yield, 98.9% purity) as a yellow oil.

^{1}H NMR (400MHz, CHLOROFORM-d) δ = 8.56 (d, *J*=1.1 Hz, 1H), 8.10 (dt, *J*=1.7, 8.6 Hz, 2H), 7.53 - 7.43 (m, 2H), 7.35 (d, *J*=3.3 Hz, 1H), 7.14 - 7.07 (m, 2H), 6.69 (d, *J*=3.3 Hz, 1H), 4.81 - 4.65 (m, 2H), 1.60 (d, *J*=6.7 Hz, 7H), 1.46 (d, *J*=6.1 Hz, 6H).

Synthesis of 48-2 :

5-[3-(2-methoxyphenyl)-1,2,4-oxadiazol-5-yl]-1-(propan-2-yl)-1H-1,2,3-benzotriazole

Scheme 48



48-1 48-2

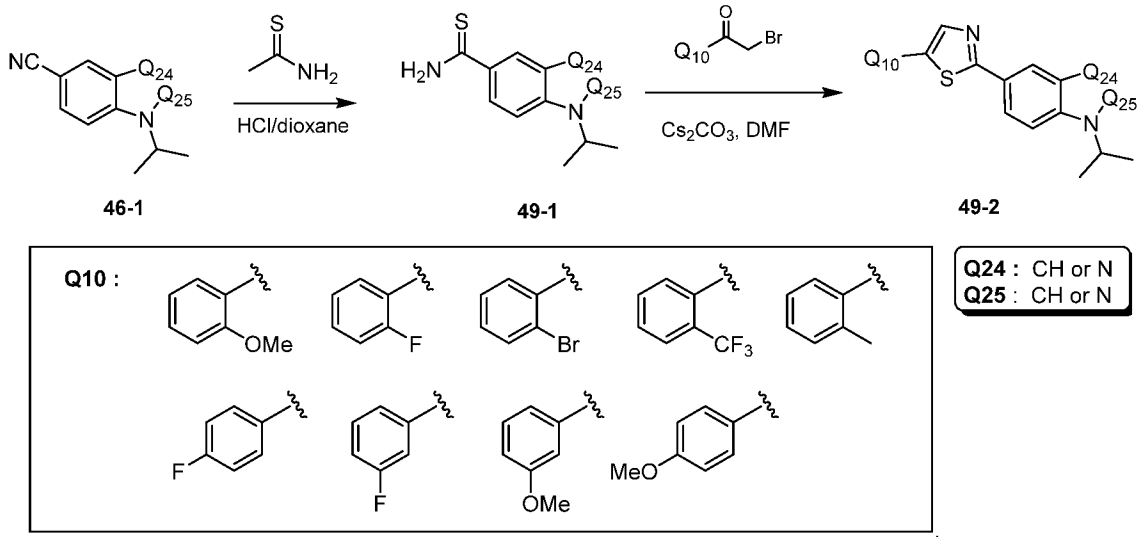
To a solution of 1-isopropylbenzotriazole-5-carboxylic acid (100.00 mg, 487.31 umol, 1.00 *eq*) in DMF (1.00 mL) was added HOBt (79.01 mg, 584.77 umol, 1.20 *eq*) and EDCI (112.10 mg, 584.77 umol, 1.20 *eq*). The mixture was stirred at 10 °C for 0.5 h, then N-hydroxy-2-methoxy-benzamidine (80.98 mg, 487.31 umol, 1.00 *eq*) was added and stirred at 120°C for 12 h. The mixture was diluted with H_2O (20 mL) and extracted with EA (30 mLx2), the combined organic layers were dried over Na_2SO_4, filtered and concentrated to dry. The residue was purified by prep-HPLC (column: Welch Ultimate AQ-C18 150x30mmx5um;mobile phase: [water(0.1%TFA)-ACN];B%:

50%-80%,13min) to give 5-(1-isopropylbenzotriazol-5-yl)-3-(2-methoxyphenyl)-1,2,4-oxadiazole (110.00 mg, 328.01 umol, 67.31% yield) as a white solid.

^{1}H NMR (400MHz, CHLOROFORM-d) δ = 8.99 (s, 1H), 8.36 (dd, *J*=1.2, 8.7 Hz, 1H), 8.17 (dd, *J*=1.6, 7.7 Hz, 1H), 7.74 (d, *J*=8.7 Hz, 1H), 7.59 - 7.48 (m, 1H), 7.20 - 7.05 (m, 2H), 5.16 (spt, *J*=6.8 Hz, 1H), 4.03 (s, 3H), 1.81 (d, *J*=6.8 Hz, 6H).

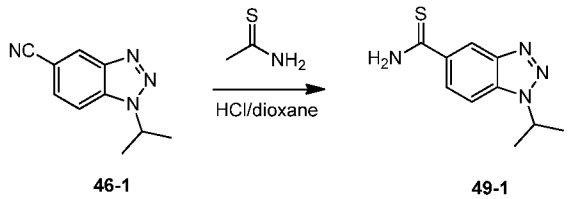
General Procedure K:

Scheme 49



Synthesis of 49-1: 1-(propan-2-yl)-1H-1,2,3-benzotriazole-5-carbothioamide

Scheme 50

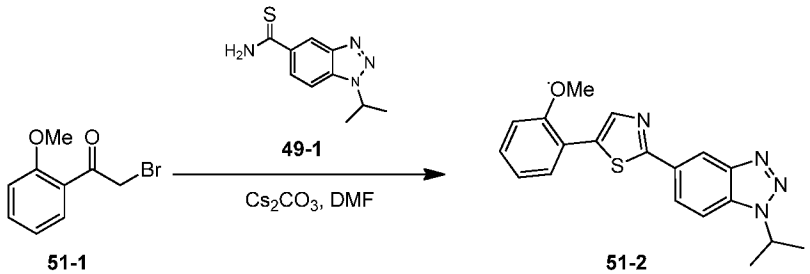


To a solution of 1-isopropylbenzotriazole-5-carbonitrile (2 g, 10.74 mmol, 1 eq) in HCl/dioxane (100 mL, 4 M) was added thioacetamide (1.61 g, 21.48 mmol, 2 eq) and stirred at 110 °C for 2 h. The reaction mixture was concentrated under reduced pressure and purified by flash silica gel chromatography (PE/EA=2/1 to 1/1) to give 1-isopropylbenzotriazole-5-carbothioamide (2.1 g, 9.53 mmol, 88.76% yield) as a yellow solid.

Synthesis of 51-2

:5-{5-[2-(methyl-λ³-oxy)phenyl]-1,3-thiazol-2-yl}-1-(propan-2-yl)-1H-1,2,3-benzotriazole

Scheme 51



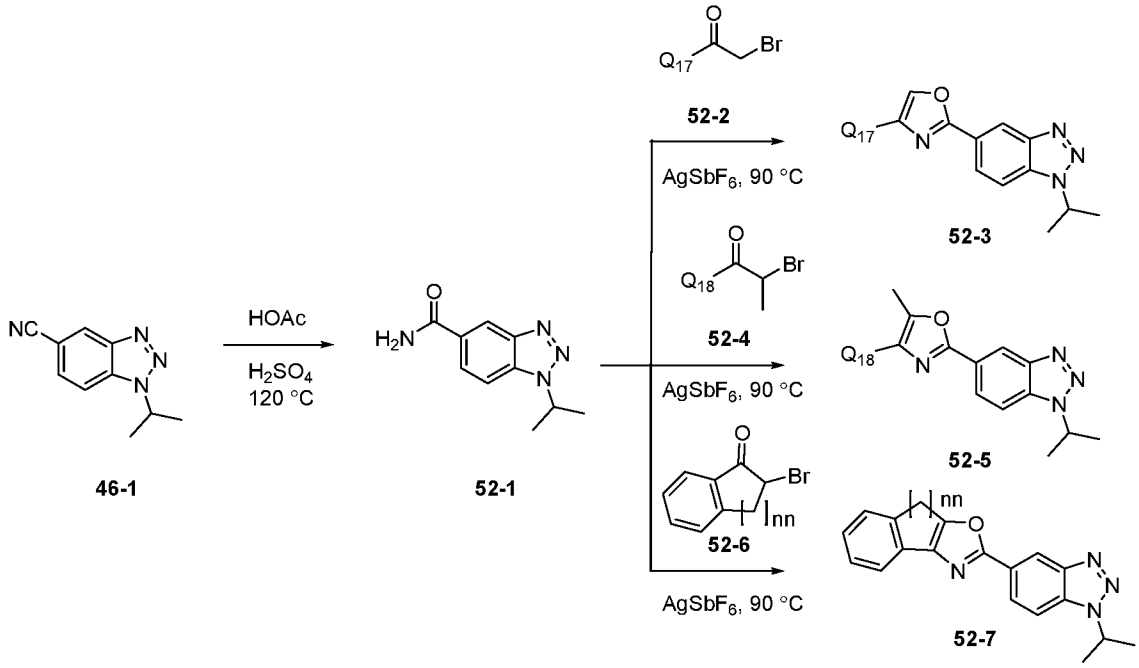
51-1 51-2

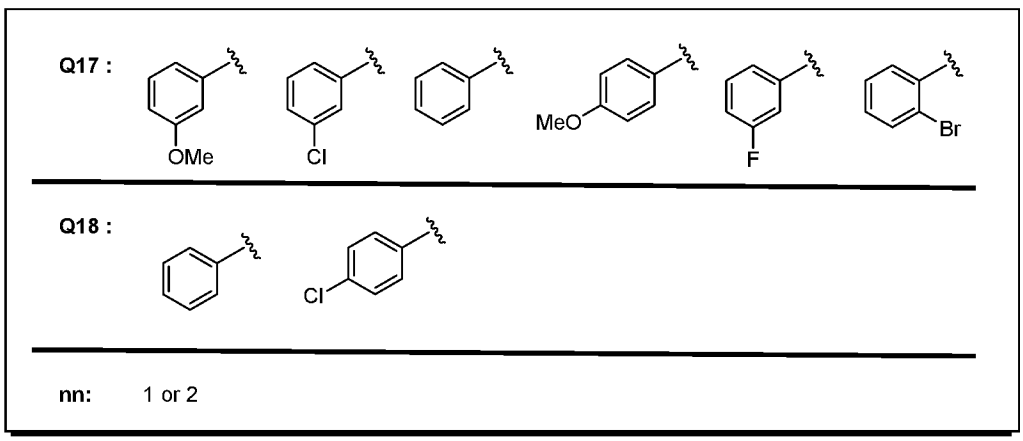
To a solution of 1-isopropylbenzotriazole-5-carbothioamide (300 mg, 1.36 mmol, 1 *eq*) in DMF (3 mL) was added Cs_2CO_3 (443.71 mg, 1.36 mmol, 1.00 *eq*) and 2-bromo-1-(2-methoxyphenyl)ethanone (311.95 mg, 1.36 mmol, 1 *eq*). The mixture was stirred at 100 °C for 12 h. The residue was purified by prep-HPLC (column: Waters Xbridge 150x25 5u;mobile phase: [water(10mM NH4HCO3)-ACN];B%: 60%-90%,10min) to give 2-(1-isopropylbenzotriazol-5-yl)-5-(2-methoxyphenyl)thiazole (190 mg, 509.65 umol, 37.42% yield, 94% purity) as a yellow solid.

^{1}H NMR (400MHz, CHLOROFORM-d) δ = 8.60 (s, 1H), 8.37 (dd, *J*=1.7, 7.8 Hz, 1H), 8.22 (dd, *J*=1.1, 8.8 Hz, 1H), 7.91 (s, 1H), 7.55 (d, *J*=8.8 Hz, 1H), 7.31 - 7.23 (m, 1H), 7.05 (t, *J*=7.5 Hz, 1H), 6.96 (d, *J*=8.3 Hz, 1H), 5.04 (spt, *J*=6.8 Hz, 1H), 3.92 (s, 3H), 1.70 (d, *J*=6.7 Hz, 6H).

General Procedure L:

Scheme 52





Synthesis of 52-1: 1-(propan-2-yl)-1H-1,2,3-benzotriazole-5-carboxamide:

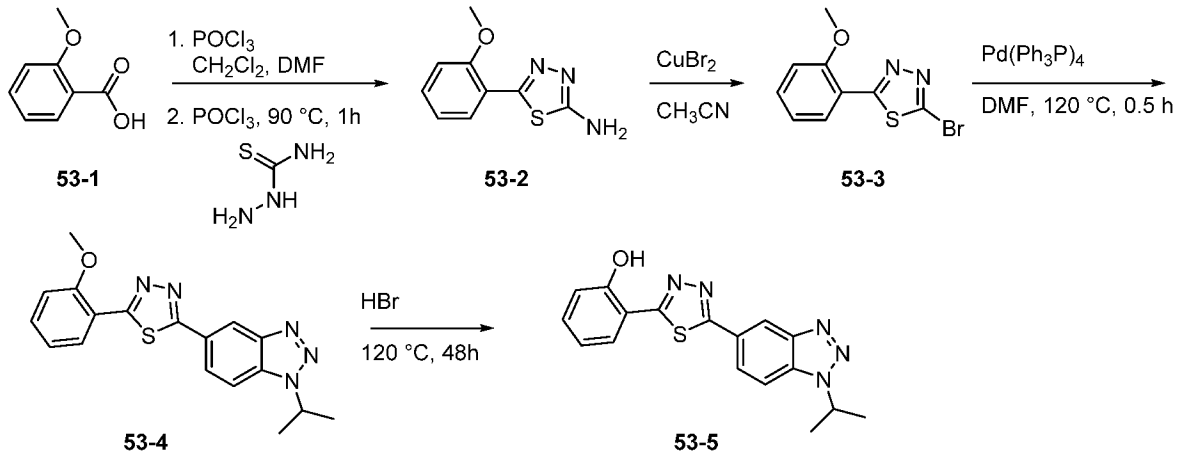
To a solution of **46-1** (1.0 g, 5.4 mmol) in HOAc (10 mL) was added H2SO4 (0.5 mL) and reaction heated in MW 90 min at 120°C. Let cool overnight. Reaction mixture poured onto ice, neutralized and extracted with EtOAc. Solvent evaporated to give a dark solid. Silica gel chromatography (10-50% acetone in hexane) gave a residue which was triturated with a small amount of acetone and an off-white solid was collected by filtration to give the title compound **(52-1)** (0.5 g, 45%).

Synthesis of 52-3: 5-(4-phenyl-1,3-oxazol-2-yl)-1-(propan-2-yl)-1H- 1,2,3-benzotriazole: To a mixture of **52-1** (50 mg, 0.25 mmol), **52-2** (51 mg, 0.25 mmol) was added AgSbF6 (86 0.25 mmol) and the mixture was heated to 90°C for about 3 hrs then cool to rt. Reaction worked up with

NaHCO3 and CH2Cl2. Organic layer separated and evaporated to give a dark oil. Residue was chromatographed (0 to 5% MeOH in CH2Cl2) to give a residue which was further purified by reverse phase HPLC. Appropriate fractions combined and lyophilized to give the title compound as an off-white solid. (7 mg, 10%).

General Procedure M

Scheme 53



Synthesis of 5-(2-methoxyphenyl)-1,3,4-thiadiazol-2-amine 53-2: To a solution of **53-1** (1.9 g, 10.0 mmol) in CH2Cl2 (50 mL) was added DMF (0.2 mL) followed by portion wise addition of oxalyl chloride (1.7 mL, 20.0 mmol) and the solution was stirred overnight at rt. Reaction mixture was evaporated in vacuum. To residue was added thiosemicarbazide (1.1 g, 15 mmol) followed by POCl3 (2.8 mL, 30 mmol) and the reaction mixture was heated to 90°C. After about 45 min to 1 hr, heat was turned off and allowed to cool overnight. Quench with ice and worked up with K2CO3 and EtOAc. Organic layer washed with sat'd NaHCO3 and dried over Na2SO4. Filtered and evaporated to give a yellow residue which was triturated with CH2Cl2 and the title compound was collected as a beige solid (0.9 g, 43%). This material was used directly in the next step.

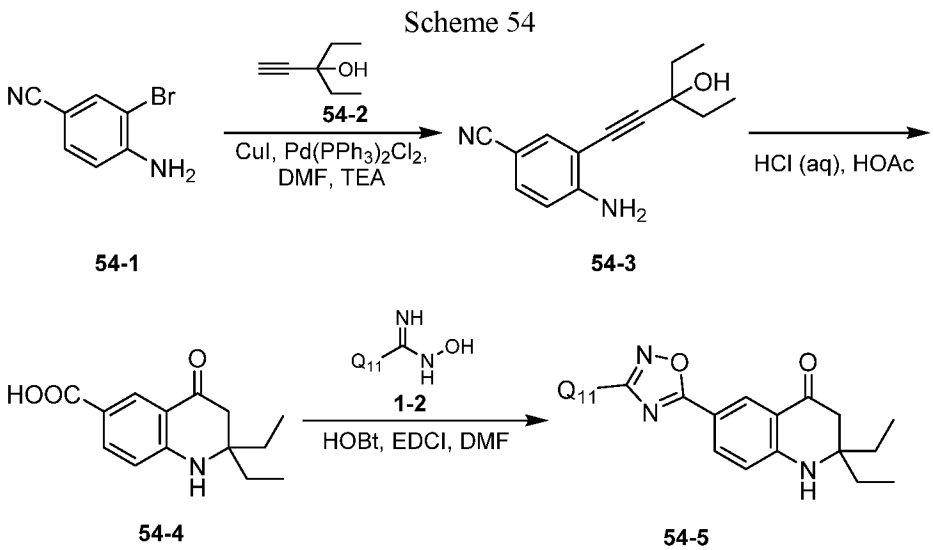
Synthesis of 2-bromo-5-(2-methoxyphenyl)-1,3,4-thiadiazole 53-3: A mixture of t-Bu-nitrite (0.9 mL, 9.6 mmol) and CuBr2 (2.2 g, 9.6 mmol) in MeCN (30 mL) was stirred for 10 min and then **53-2** (0.9 g, 1.76 mmol) was added in 2 portions. Stirred ~ 1 hr and then solvent removed in vacuum. Residue was suspended in EtOAc, washed 2x with 1 N HCl, then brine and dried over Na2SO4. Filtered and evaporated to give the title compound as a yellow-orange solid (1 g, 86%).

Synthesis of 5-[5-(2-methoxyphenyl)-1,3,4-thiadiazol-2-yl]-1- (propan-2-yl)-1H-1,2,3-benzotriazole 53-4: Combined **52-3** (95 mg, 0.25 mmol), **14-5** (45 mg, 0.3 mmol), K3PO4 (132 mg, 0.625 mmol) and Pd(Ph3P)4 (58 mg, 0.05 mmol) in a mixture of DMF (4 mL) and water (1 mL). Heated to 120°C for 30 min in MW. Evap sol to give a residue which was chromatographed on silica (0 to 30% EtOAc in hex). Appropriate fraction were combined and solvent evaporated. This residue was further purified by reverse phase HPLC to give the title compound (30 mg, 20%) as an off-white solid.

Synthesis of 2-{3-[1-(propan-2-yl)-1H-1,2,3-benzotriazol-5-yl]- 1,2,4-thiadiazol-5-yl}phenol 53-5: 53-4 (40 mg, 0.11 mmol) was dissolved in HR and heated to 120°C. After ~ 48 hrs starting material was gone. Neutralize with NaHCO3. Residue purified by reverse phase HPLC to give the title compound (10 mg, 22%). $[M+H]^+$:338.0

General Procedure N

Scheme 54



Synthesis of 54-3: 4-amino-3-(3-ethyl-3-hydroxypent-1-yn-1- yl)benzonitrile

To a solution of compound **54-1** (1 g, 5.08 mmol, 1 *eq.*) in DMF (7 mL) and TEA (2.18 g, 21.55 mmol, 3 mL, 4.25 *eq.*) was added compound 54-**2** (683.15 mg, 6.09 mmol, 783.43 uL, 1.2 *eq.*), CuI (48.33 mg, 253.77 umol, 0.05 *eq.*) and $Pd(PPh_3)_2Cl_2$ (178.12 mg, 253.77 umol, 0.05 *eq.*). The mixture was stirred at 90 °C under nitrogen atmosphere for 3 hours. TLC showed a new one spot formed. The reaction mixture was diluted with water (20 mL), extracted with EtOAc (20 mLx2),

washed with brine (20 mL), dried with sodium sulfate, filtered and concentrated. The residue was purified by flash silica gel column chromatography (PE:EA = 5:1) to give compound **3** (1 g, yield: 86%) as a yellow oil. ^{1}H NMR (400MHz, $CDCl_3$) δ = 7.52 (d, *J* = 1.6 Hz, 1 H), 7.34 (dd, *J* = 8.6, 1.8 Hz, 1 H), 6.68 (d, *J* = 8.4 Hz, 1 H), 4.76 (s, 2 H), 2.95 (s, 1 H), 2.88 (s, 1 H), 2.32 (s, 1 H), 1.85 - 1.70 (m, 4 H), 1.10 (t, *J* = 7.4 Hz, 6 H).

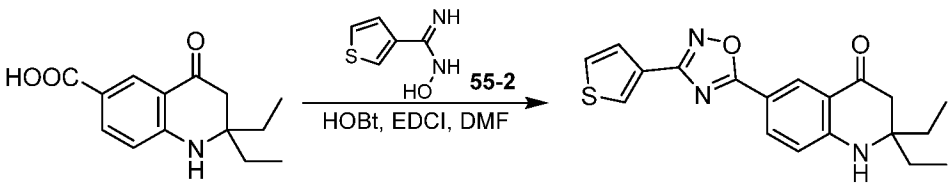
Synthesis of 54-4: 2,2-diethyl-4-oxo-1,3-dihydroquinoline-6- carboxylic acid

A mixture of compound 54-**3** (300 mg, 1.31 mmol) in concentrated hydrochloric acid solution (1 mL) and acetic acid (1 mL) was stirred at 115°C for 3 hours. The mixture was basified with 1 N sodium hydroxide solution to pH = 10, washed with EtOAc (20 mLx3), the aqueous phase was acidized with 1 N hydrochloric acid solution to pH = 3, filtered, the filtrate cake was washed with water (10 mL), dried under vacuum to give compound **54-4** (35 mg, yield: 11%) as white solid. ^{1}H NMR (400MHz, DMSO-d_6) δ = 12.08 (br. s, 1 H), 7.90 (d, *J* = 2.0 Hz, 1 H), 7.52 (dd, *J* = 2.0, 8.7 Hz, 1 H), 7.14 (s, 1 H), 6.58 (d, *J* = 8.7 Hz, 1H), 1.73 (s, 1 H), 1.36 - 1.19 (m, 4 H), 0.58 (t, *J* = 7.4 Hz, 6 H).

Synthesis of 55-1:

2,2-diethyl-6-[3-(thiophen-3-yl)-1,2,4-oxadiazol-5-yl]-1,3-dihydroquinolin-4-one

Scheme 55



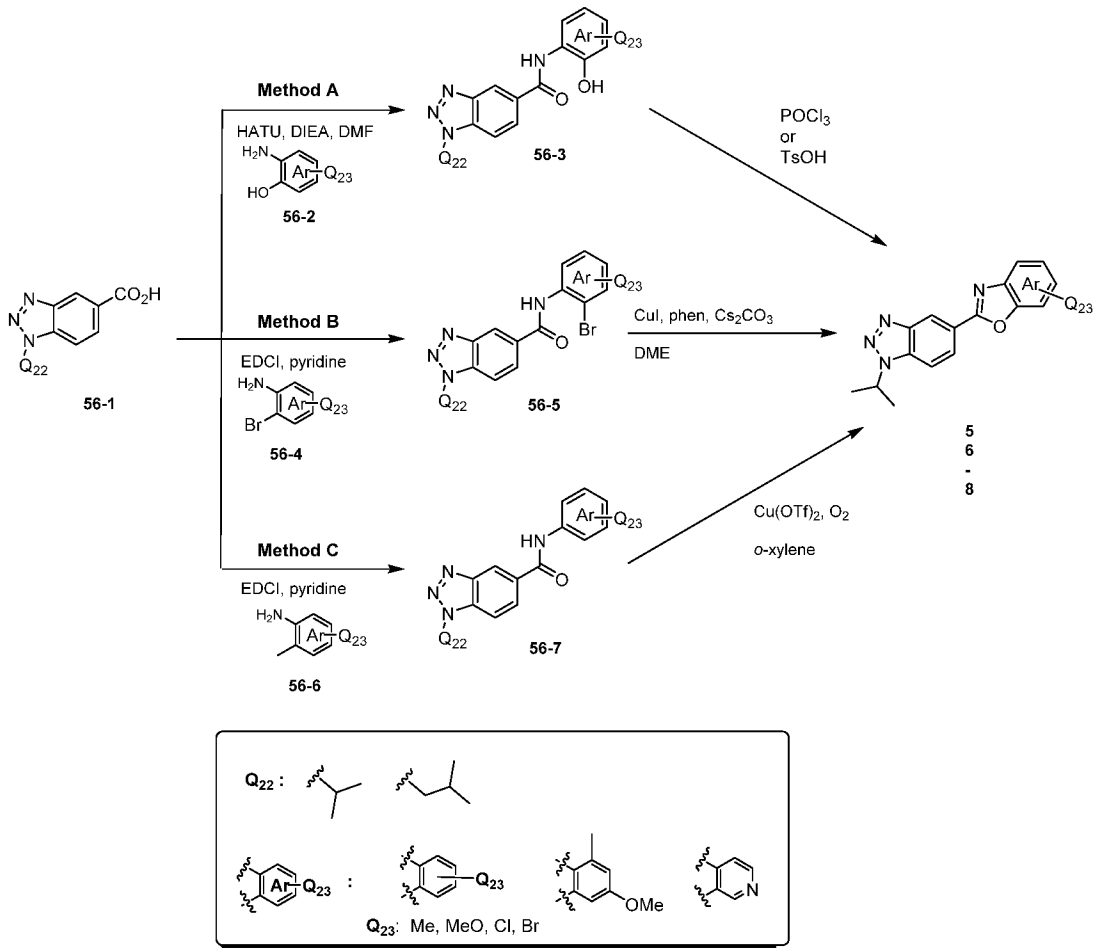
54-4 **55-1**

To a solution of compound **54-4** (100 mg, 404.39 umol, 1 *eq.*) in DMF (1 mL) was added HOBt (65.57 mg, 485.26 umol, 1.2 *eq.*) and EDCI (93.02 mg, 485.26 umol, 1.2 *eq.*). After stirring at 20 °C for 30 mins, compound **55-2** (63.24 mg, 444.82 umol, 1.1 *eq.*) was added, and stirred for another 30 mins. Then the mixture was heated to 120 °C and stirred for 2 hours. The mixture was triturated with EA (20 mL), filtered, washed with EA (10 mL), the residue was purified by *prep*-HPLC (column: Phenomenex Synergi C18 150x25x10um;mobile phase: [water(0.1%TFA)-ACN];B%: 50%-80%,13min) to give **55-1** (45 mg, yield: 29 %) as orange solid. ^{1}H NMR (400MHz, DMSO-d_6) δ = 8.36 - 8.27 (m, 2 H), 7.96 (dd, *J* = 2.0, 8.8 Hz, 1 H), 7.79 (dd, *J* = 3.0, 5.0 Hz, 1 H), 7.71 (s, 1 H),

7.62 (d, J = 5.0 Hz, 1 H), 6.99 (d, J = 8.9 Hz, 1 H), 2.59 (s, 2 H), 1.67 - 1.48 (m, 4 H), 0.86 (t, J = 7.3 Hz, 6 H).

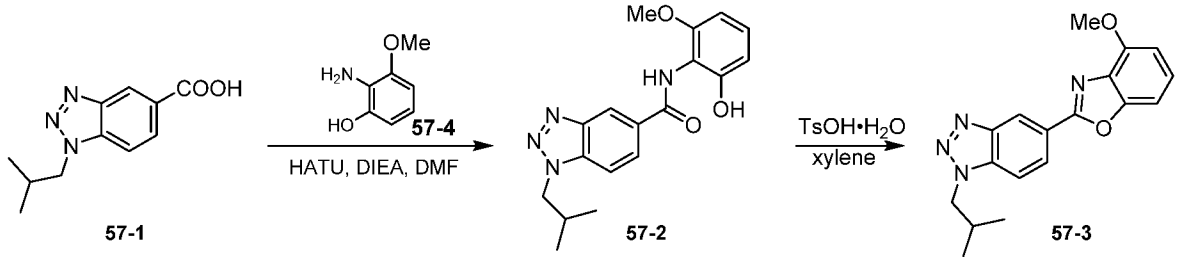
General Procedure O

Scheme 56



Synthesis of 57-3: 5-(4-methoxy-1,3-benzoxazol-2-yl)-1-(2-methylpropyl)-1,2,3-benzotriazole

Scheme 57



Synthesis of 57-2:

N-(2-hydroxy-6-methoxyphenyl)-1-(2-methylpropyl)-1,2,3-benzotriazole-5-carboxamide

To a solution of compound **57-1** (100 mg, 487.30 umol, 1 *eq.*) in DMF (3 mL) was added HOBt (65.85 mg, 487.30 umol, 1 *eq.*) and EDCI (112.10 mg, 584.76 umol, 1.2 *eq.*). After addition, the mixture was stirred at 20 °C for 0.5 hour, then compound **57-4** (81.37 mg, 584.76 umol, 1.2 *eq.*) was added, the mixture was stirred at 20 °C for further 12 hours. LCMS showed compound **57-1** consumed, and a major peak with desired MS detected. The mixture was diluted with water (20 mL), extracted with EtOAc (15 mL*2), washed with brine (20 mL), dried with sodium sulfate, filtered and concentrated, to give compound **57-2** (159 mg, crude) as brown oil, which was used in next step directly without further purification. LCMS: 327.2[M+1]

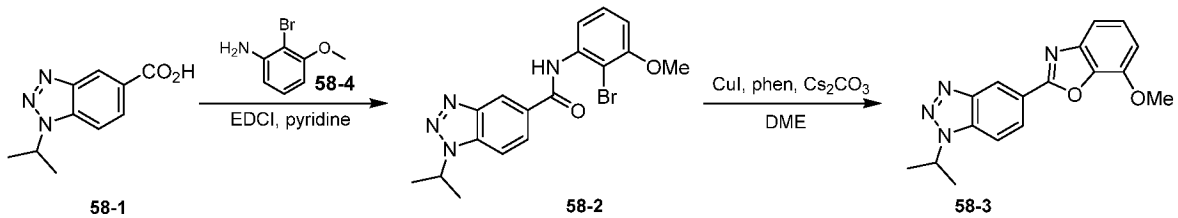
Synthesis of 57-3: 5-(4-methoxy-1,3-benzoxazol-2-yl)-1-(2-methylpropyl)-1,2,3-benzotriazole

To a solution of compound **57-2** (159 mg, crude) in xylene (10 mL) was added $TsOH{\cdot}H_2O$ (370.70 mg, 1.95 mmol, 4 *eq.*). After addition, the mixture was stirred at 120 °C for 2 hours. LCMS showed compound **57-2** consumed, and a major peak with desired Ms detected. The mixture was concentrated, diluted with saturated sodium bicarbonate solution (20 mL), extracted with EtOAc (20 mL*2), dried with sodium sulfate, filtered and concentrated. The residue was purified by *prep*-HPLC (column: Phenomenex Synergi C18 150*25*10um;mobile phase: [water(0.1%TFA)-ACN];B%: 42%-72%,10min) to give **57-3** (53 mg, yield: 35%) as grey solids.

^{1}H NMR (400MHz, $CDCl_3$) δ = 8.95 (s, 1 H), 8.51 (dd, *J* = 1.1, 8.8 Hz, 1 H), 7.69 (d, *J* = 8.8 Hz, 1 H), 7.37 - 7.31 (m, 1 H), 7.28 - 7.27 (m, 1 H), 6.85 (d, *J* = 7.9 Hz, 1 H), 5.18 - 5.08 (m, 1 H), 4.10 (s, 3 H), 1.80 (s, 3 H), 1.78 (s, 3 H)

Synthesis of 58-3: 1-isopropyl-5-(7-methoxy-1,3-benzoxazol-2-yl)-1,2,3-benzotriazole

Scheme 58



58-1 58-2 58-3

Synthesis of 58-2:

N-(2-bromo-3-methoxyphenyl)-1-isopropyl-1,2,3-benzotriazole-5-carboxamide

A mixture of compound **58-1** (200 mg, 989.86 umol, 1 *eq.*), compound **58-1** (243.76 mg, 1.19 mmol, 1.2 *eq.*) and EDCI (284.64 mg, 1.48 mmol, 1.5 *eq.*) in pyridine (3 mL) was stirred at 20 °C for 12 hours. The mixture was diluted with EtOAc (30 mL), washed with 1 N hydrochloric acid solution (20 mL*3), dried with sodium sulfate, filtered and concentrated. The residue was purified by *prep*-TLC (PE:EA = 3:1) to give compound **58-2** (150 mg,, yield: 38 %) as brown oil. LCMS: 391.1 [M+1]

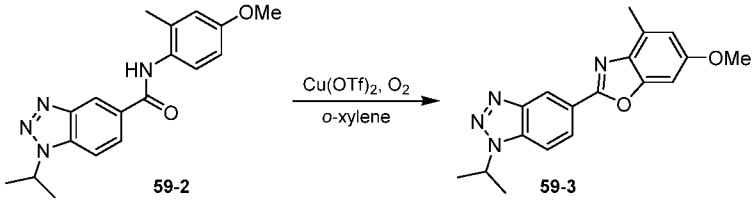
Synthesis of 58-3: 1-isopropyl-5-(7-methoxy-1,3-benzoxazol-2-yl)-1,2,3-benzotriazole

A mixture of compound **58-2** (50 mg, 128.45 umol, 1 *eq.*), 1,10-phenanthroline (2.31 mg, 12.85 umol, 0.1 *eq.*), Cs_2CO_3 (62.78 mg, 192.68 umol, 1.5 *eq.*) and CuI (1.22 mg, 6.42 umol, 0.05 *eq.*) in DME (2 mL) was heated to 85 °C and stirred for 12 hours under nitrogen atmosphere. The mixture was diluted with EtOAc (20 mL), washed with water (10 mL), dried with sodium sulfate, filtered and concentrated. The residue was purified by *prep*-HPLC (column: Phenomenex Synergi C18 150*25*10um;mobile phase: [water(0.1%TFA)-ACN];B%: 45%-75%,12min) to give **58-3** (8 mg, yield: 19%) as gray solid.

^{1}H NMR (400MHz, DMSO-d_6) δ = 8.76 (s, 1 H), 8.32 (dd, J = 1.3, 8.8 Hz, 1 H), 8.13 (d, J = 8.7 Hz, 1 H), 7.44 - 7.28 (m, 2 H), 7.07 (d, J = 7.8 Hz, 1 H), 5.29 (spt, J = 6.7 Hz, 1 H), 4.02 (s, 3 H), 1.66 (d, J = 6.6 Hz, 6 H).

Synthesis of 59-3: 1-isopropyl-5-(6-methoxy-4-methyl-1,3-benzoxazol-2-yl)-1,2,3-benzotriazole

Scheme 59



Synthesis of 59-3: 1-isopropyl-5-(6-methoxy-4-methyl-1,3-benzoxazol-2-yl)-1,2,3-benzotriazole

To a solution of compound **59-2 (1-isopropyl-N-(4-methoxy-2-methylphenyl)-1,2,3-benzotriazole-5-carboxamide) prepared according to the procedure to prepare 58-2**, (50 mg, 154.14 umol, 1 *eq.*) in o-xylene (2 mL) was added $Cu(OTf)_2$ (11.12 mg, 30.83 umol, 0.2 *eq.*). The reaction was stirred at 130 °C under oxygen atmosphere for 16 hours. The mixture was diluted with water (20 mL), extracted with EtOAc (30 mL*3), dried with sodium sulfate, filtered and concentrated. The residue was purified by *prep*-TLC (PE:EA = 4:1) to give **59-3** (1.1 mg, yield: 2%) as yellow solid.

^{1}H NMR (400MHz, $CDCl_3$) δ = 8.80 (s, 1 H), 8.33 (dd, *J* = 1.4, 8.7 Hz, 1 H), 7.59 (d, *J* = 8.8 Hz, 1 H), 6.91 (d, *J* = 2.2 Hz, 1 H), 6.72 (d, *J* = 1.5 Hz, 1 H), 5.16 - 4.93 (m, 1 H), 3.81 (s, 3 H), 2.58 (s, 3 H), 1.72 (d, *J* = 6.8 Hz, 6 H)

Example 2: In vitro activity of Compounds

Stable clonal Chinese hamster ovary K1 (CHO-K1) cells co-expressing EA-β-arrestin2 and the human sphingosine-1-phosphate receptor 1 (NM_001400, $S1P_1$) with a C-terminal Prolink™ tag were purchased from DiscoverX corporation (Cat#: 93-0207C2).

Cell culturing and assay plating

Cell lines were cultured in AssayComplete™ Media 6 (DiscoverX Corporation, Cat#: 920018GF2) at 37°C and 5% CO_2 in a humidified CO_2 and temperature-controlled incubator. To begin assay plating, cells were washed with dulbecco's phosphate buffered saline (CellGro, Cat#: 21-031-CV) and lifted from the culturing flask by incubation (37°C, 5 min) with CellStripper (Cellgro, Cat#: 25-056-CI). Lifted cells were resuspended to 250,000 cells per milliliter in AssayComplete™ Cell Plating 11 Reagent (DiscoverX Corporation, Cat#: 93-0563R11B) and plated at 5,000 cells per well in white-opaque 384 well plates (Greiner Bio-One Item #: 20-784080). Plated cells were incubated overnight at 37°C and 5% CO_2 in a humidified CO_2 and temperature-controlled incubator.

Detecting inhibition of cAMP production

Agonist-promoted G-protein responses were determined by measuring changes in intracellular cAMP using the HTRF® cAMP HiRange kit (CisBio, Cat#: 62AM6PEJ) based on time-resolved fluorescence resonance energy transfer (TR-FRET) technology. AssayComplete™ Cell Plating 11 Reagent was removed and replaced with Ham's F-12 (CellGro, Cat#: 10-080-CM) containing isobutyl-methyl-xanthine (IBMX; 500 μM; Tocris Bioscience, Cat#: 2845), and NKH-477 (1.5 μM; Tocris Bioscience, Cat#: 1603) along with test or control compounds at the desired concentrations. Following a 30-minute incubation at 37°C and 5% CO_2 in a humidified CO_2 and temperature-controlled incubator, the components of the cAMP HiRange kit were added as per the manufacturer's instructions. After an hour incubation at room temperature, plates were analyzed by a BMG PheraStar microplate reader. Responses were measured as the ratio of fluorescence emission at 665 nm to fluorescence emission at 620 nm.

β-arrestin2 recruitment assay

Agonist-promoted β-arrestin2 recruitment to the sphingosine-1-phosphate 1 receptor was determined using the β-arrestin PathHunter® Detection kit (DiscoverX Corporation, Cat#: 93-0001). In this system, β-arrestin2 is fused to an N-terminal deletion mutant of β-galactosidase (termed the enzyme acceptor or EA) and the C-terminus of the GPCR of interest is fused to a smaller (42 amino acids), weakly-complementing fragment 15 termed ProLink™. In cells that stably express these fusion proteins, stimulation with a cognate agonist results in the interaction of β-arrestin2 and the Prolink™-tagged GPCR. This allows the complementation of the two β-galactosidase fragments and results in the formation of a functional enzyme with β-galactosidase activity. AssayComplete™ Cell Plating 11 Reagent was removed and replaced with Ham's F-12 containing IBMX (500 μM), and NKH-477 (1.5 μM) along with test or control compounds at the desired concentrations. Following a 60 minute incubation at 37°C and 5% CO_2 in a humidified CO_2 and temperature-controlled incubator, the components of the β-arrestin PathHunter® Detection kit were added as per the manufacturer's instructions. After an hour incubation at room temperature, plates were analyzed by a BMG PheraStar microplate reader.

Activity Table

The compounds as indicated herein were able to modulate the activities (inhibition of cAMP production and β-arrestin2 recruitment) of the sphingosine-1-phosphate 1 receptor as indicated herein. The tables below include the efficacy of the compound as compared to a positive control,

referred to as "SPAN". These values are normalized to fingolimod, a known agonist of the sphingosine-1-phosphate 1 receptor. The tables also include potency values (pEC50) for modulating discrete receptor-mediated activities (inhibition of cAMP production and β-arrestin2 recruitment). This value represents the estimated concentration to promote half of the maximal efficacy (or SPAN) observed for each compound.

Compound Number	hS1P1 cAMP pEC_{50}	hS1P1 cAMP SPAN	hS1P1 B-arrestin2 pEC_{50}	hS1P1 B-arrestin2 SPAN
1	<6.5	<75	<5	<75
2	<6.5	>75	>5	<75
3	>6.5	>75	>5	>75
4	<6.5	<75	<5	<75
5	<6.5	<75	<5	<75
6	<6.5	<75	<5	<75
7	<6.5	>75	<5	>75
8	<6.5	<75	<5	<75
9	<6.5	<75	<5	<75
10	<6.5	<75	<5	<75
11	<6.5	<75	<5	<75
12	<6.5	<75	<5	<75
13	>6.5	<75	>5	<75
14	>6.5	<75	>5	<75
15	<6.5	>75	<5	<75
16	<6.5	<75	>5	>75
17	>6.5	>75	>5	>75
18	<6.5	<75	<5	<75
19	<6.5	<75	>5	<75
20	>6.5	>75	>5	>75
21	<6.5	>75	<5	>75
22	>6.5	>75	>5	>75
23	<6.5	<75	<5	<75
24	<6.5	>75	<5	<75
25	<6.5	<75	<5	<75
26	>6.5	>75	>5	>75
26	>6.5	>75	>5	<75
27	<6.5	>75	>5	<75
28	<6.5	>75	<5	>75
29	<6.5	<75	<5	<75
30	<6.5	<75	<5	<75
31	>6.5	>75	>5	>75
32	>6.5	>75	>5	<75
33	>6.5	>75	>5	>75
34	<6.5	>75	>5	<75
35	<6.5	>75	<5	>75
36	<6.5	<75	<5	<75
37	<6.5	<75	<5	<75

Compound Number	hS1P1 cAMP pEC_{50}	hS1P1 cAMP SPAN	hS1P1 B-arrestin2 pEC_{50}	hS1P1 B-arrestin2 SPAN
38	<6.5	<75	<5	>75
39	<6.5	<75	<5	<75
40	>6.5	>75	>5	>75
41	<6.5	<75	<5	<75
41	<6.5	<75	<5	<75
42	<6.5	>75	<5	>75
43	>6.5	>75	>5	>75
44	<6.5	<75	<5	<75
45	<6.5	<75	<5	<75
46	>6.5	>75	>5	>75
47	<6.5	<75	<5	<75
48	<6.5	<75	<5	<75
49	<6.5	<75	<5	<75
50	<6.5	<75	<5	<75
51	<6.5	<75	<5	<75
52	<6.5	<75	<5	<75
53	<6.5	<75	<5	<75
54	<6.5	<75	<5	>75
55	>6.5	>75	>5	>75
56	<6.5	<75	<5	<75
57	<6.5	<75	<5	<75
58	<6.5	<75	<5	<75
59	>6.5	>75	>5	>75
60	<6.5	<75	<5	<75
61	>6.5	>75	>5	>75
62	<6.5	>75	<5	>75
63	>6.5	<75	<5	<75
64	>6.5	>75	<5	>75
65	<6.5	<75	<5	<75
66	>6.5	>75	>5	>75
67	<6.5	>75	>5	<75
68	<6.5	<75	<5	<75
69	<6.5	<75	>5	<75
70	>6.5	<75	>5	<75
71	<6.5	>75	<5	<75
72	>6.5	>75	>5	>75
73	<6.5	<75	>5	<75
74	<6.5	<75	<5	<75
75	>6.5	<75	>5	>75
76	<6.5	<75	<5	<75
77	<6.5	<75	<5	<75
78	<6.5	<75	<5	<75
79	>6.5	>75	>5	>75
80	>6.5	<75	<5	<75
81	<6.5	>75	<5	<75

Compound Number	hS1P1 cAMP pEC_{50}	hS1P1 cAMP SPAN	hS1P1 B-arrestin2 pEC_{50}	hS1P1 B-arrestin2 SPAN
82	<6.5	<75	<5	<75
83	>6.5	>75	>5	>75
84	<6.5	<75	>5	>75
85	<6.5	<75	<5	<75
86	<6.5	<75	<5	>75
87	<6.5	<75	<5	<75
88	<6.5	<75	<5	<75
89	<6.5	<75	<5	<75
90	<6.5	>75	>5	>75
91	<6.5	<75	<5	<75
92	<6.5	<75	<5	<75
93	<6.5	<75	<5	>75
94	<6.5	>75	<5	>75
95	<6.5	<75	<5	<75
96	>6.5	>75	>5	>75
97	<6.5	<75	<5	<75
98	<6.5	>75	>5	>75
99	>6.5	>75	>5	>75
100	<6.5	<75	<5	<75
101	>6.5	>75	>5	>75
102	<6.5	<75	<5	<75
103	>6.5	>75	>5	>75
103	>6.5	>75	>5	>75
103	>6.5	>75	>5	>75
104	>6.5	>75	<5	>75
105	<6.5	<75	<5	<75
106	>6.5	>75	>5	>75
107	>6.5	>75	>5	>75
108	>6.5	<75	<5	<75
109	<6.5	<75	>5	<75
110	<6.5	<75	<5	<75
111	<6.5	>75	<5	>75
112	>6.5	>75	>5	>75
113	<6.5	<75	<5	<75
114	<6.5	<75	<5	<75
115	>6.5	>75	>5	>75
116	<6.5	<75	<5	<75
117	<6.5	<75	<5	<75
118	<6.5	<75	<5	<75
119	<6.5	<75	<5	<75
120	>6.5	>75	>5	>75
121	<6.5	<75	<5	<75
122	<6.5	<75	<5	<75
123	>6.5	>75	>5	>75
124	<6.5	<75	<5	<75

Compound Number	hS1P1 cAMP pEC_{50}	hS1P1 cAMP SPAN	hS1P1 B-arrestin2 pEC_{50}	hS1P1 B-arrestin2 SPAN
125	<6.5	<75	<5	<75
126	<6.5	<75	<5	<75
127	<6.5	<75	<5	<75
128	<6.5	<75	<5	<75
129	<6.5	<75	<5	<75
130	<6.5	<75	<5	<75
131	<6.5	<75	<5	<75
132	>6.5	>75	>5	>75
133	<6.5	<75	<5	<75
134	<6.5	<75	<5	<75
135	<6.5	<75	<5	<75
136	<6.5	<75	<5	<75
137	>6.5	>75	<5	>75
138	>6.5	>75	>5	>75
139	>6.5	>75	>5	>75
140	>6.5	>75	>5	>75
141	>6.5	>75	>5	>75
142	>6.5	>75	>5	>75
143	<6.5	<75	<5	<75
144	<6.5	>75	>5	<75
145	>6.5	>75	>5	<75
146	>6.5	>75	>5	<75
147	>6.5	>75	>5	>75
148	<6.5	<75	<5	<75
149	>6.5	>75	>5	>75
150	>6.5	>75	>5	>75
151	<6.5	>75	<5	>75
152	<6.5	>75	>5	>75
153	<6.5	>75	>5	<75
154	<6.5	<75	<5	<75
155	<6.5	<75	<5	<75
156	>6.5	>75	>5	>75
157	<6.5	<75	<5	<75
158	<6.5	<75	<5	<75
159	<6.5	<75	<5	<75
160	<6.5	<75	<5	<75
161	<6.5	<75	<5	>75
162	<6.5	>75	>5	>75
163	>6.5	>75	>5	>75
164	<6.5	<75	<5	<75
165	<6.5	>75	<5	>75
166	<6.5	<75	<5	>75
167	<6.5	<75	<5	<75
168	<6.5	<75	<5	<75
169	>6.5	>75	>5	>75

Compound Number	hS1P1 cAMP pEC_{50}	hS1P1 cAMP SPAN	hS1P1 B-arrestin2 pEC_{50}	hS1P1 B-arrestin2 SPAN
170	<6.5	<75	<5	<75
171	>6.5	>75	>5	>75
172	<6.5	<75	<5	<75
173	>6.5	>75	>5	>75
174	>6.5	>75	<5	>75
175	>6.5	>75	>5	>75
176	<6.5	>75	<5	<75
177	>6.5	>75	>5	>75
178	<6.5	>75	>5	<75
179	>6.5	>75	>5	>75
180	<6.5	>75	<5	>75
181	<6.5	>75	<5	>75
182	>6.5	>75	>5	<75
183	>6.5	>75	>5	>75
184	<6.5	>75	<5	<75
185	>6.5	>75	>5	>75
186	<6.5	<75	<5	<75
187	<6.5	<75	<5	>75
188	<6.5	<75	<5	<75
189	>6.5	>75	>5	>75
190	<6.5	<75	<5	<75
192	<6.5	<75	<5	<75
193	<6.5	<75	<5	<75
194	<6.5	<75	<5	<75
195	<6.5	<75	<5	<75
196	<6.5	<75	<5	<75
197	<6.5	<75	<5	<75
198	>6.5	>75	>5	<75
199	<6.5	<75	<5	<75
200	<6.5	<75	<5	<75
201	<6.5	<75	<5	>75
202	<6.5	<75	<5	<75
203	<6.5	<75	<5	>75
204	<6.5	>75	>5	>75
205	<6.5	>75	<5	<75
206	<6.5	>75	<5	<75
207	>6.5	>75	>5	>75
208	>6.5	>75	>5	>75
209	>6.5	>75	>5	>75
210	>6.5	>75	>5	>75
211	<6.5	<75	>5	>75
212	>6.5	>75	>5	<75
213	<6.5	>75	<5	>75
214	<6.5	<75	<5	<75
215	<6.5	<75	<5	<75

Compound Number	hS1P1 cAMP pEC_{50}	hS1P1 cAMP SPAN	hS1P1 B-arrestin2 pEC_{50}	hS1P1 B-arrestin2 SPAN
216	<6.5	<75	<5	<75
217	<6.5	<75	<5	<75
218	<6.5	>75	<5	>75
219	>6.5	<75	>5	>75
220	<6.5	<75	<5	<75
221	>6.5	>75	>5	>75
222	<6.5	>75	>5	<75
223	<6.5	<75	<5	<75
224	>6.5	>75	>5	>75
225	<6.5	>75	>5	<75
226	<6.5	>75	<5	>75
227	>6.5	<75	<5	>75
228	<6.5	<75	<5	<75
229	<6.5	<75	>5	<75
230	<6.5	<75	<5	<75
231	<6.5	<75	<5	<75
232	<6.5	<75	<5	<75
233	<6.5	<75	<5	<75
234	<6.5	<75	<5	<75
235	<6.5	<75	<5	<75
236	<6.5	<75	<5	>75
237	<6.5	<75	<5	<75
238	<6.5	<75	<5	<75
239	<6.5	<75	<5	<75
240	<6.5	>75	<5	>75
241	<6.5	>75	<5	>75
242	<6.5	<75	<5	<75
243	<6.5	>75	<5	>75
244	>6.5	>75	>5	>75
245	<6.5	>75	>5	>75
246	>6.5	>75	>5	>75
247	<6.5	<75	<5	<75
248	<6.5	<75	<5	<75
249	<6.5	>75	<5	<75
250	<6.5	<75	<5	<75
251	<6.5	<75	<5	<75
252	>6.5	>75	>5	>75
253	>6.5	>75	>5	>75
254	>6.5	<75	<5	<75
255	<6.5	<75	<5	<75
256	>6.5	>75	>5	>75
257	<6.5	>75	<5	<75
258	<6.5	<75	<5	<75
259	>6.5	>75	>5	<75
260	<6.5	>75	<5	>75

Compound Number	hS1P1 cAMP pEC_{50}	hS1P1 cAMP SPAN	hS1P1 B-arrestin2 pEC_{50}	hS1P1 B-arrestin2 SPAN
261	<6.5	>75	>5	<75
262	>6.5	>75	>5	>75
263	>6.5	>75	>5	>75
264	<6.5	<75	<5	<75
265	>6.5	>75	>5	<75
266	<6.5	>75	>5	>75
267	>6.5	<75	>5	<75
268	>6.5	>75	>5	>75
269	<6.5	<75	<5	<75
270	<6.5	<75	<5	<75
271	<6.5	<75	<5	<75
272	<6.5	<75	<5	<75
273	<6.5	<75	<5	<75
274	<6.5	>75	>5	<75
275	<6.5	<75	<5	<75
276	>6.5	>75	>5	>75
277	>6.5	>75	>5	>75
278	<6.5	<75	<5	<75
279	<6.5	>75	<5	>75
280	<6.5	<75	<5	<75
281	<6.5	<75	<5	<75
282	>6.5	>75	>5	>75
283	<6.5	<75	<5	<75
284	<6.5	<75	<5	<75
285	<6.5	<75	<5	<75
286	>6.5	>75	>5	>75
287	>6.5	>75	>5	>75
288	<6.5	<75	<5	<75
289	<6.5	<75	<5	<75
290	<6.5	<75	<5	<75
291	<6.5	<75	<5	<75
292	<6.5	<75	<5	<75
293	>6.5	>75	>5	>75
294	<6.5	<75	<5	>75
295	<6.5	>75	<5	<75
296	<6.5	<75	<5	<75
297	<6.5	>75	<5	>75
298	<6.5	>75	>5	<75
299	<6.5	<75	<5	>75
300	<6.5	>75	<5	>75
301	<6.5	<75	<5	<75
302	>6.5	>75	>5	>75
303	<6.5	>75	<5	>75
304	>6.5	<75	>5	>75
305	<6.5	>75	<5	<75

Compound Number	hS1P1 cAMP pEC_{50}	hS1P1 cAMP SPAN	hS1P1 B-arrestin2 pEC_{50}	hS1P1 B-arrestin2 SPAN
306	>6.5	>75	>5	<75
307	>6.5	>75	>5	>75
308	<6.5	<75	<5	<75
309	<6.5	>75	<5	>75
310	>6.5	>75	>5	>75
311	<6.5	>75	<5	>75
312	<6.5	>75	<5	>75
313	>6.5	>75	<5	>75
314	<6.5	<75	<5	<75
315	>6.5	>75	>5	<75
316	>6.5	>75	<5	<75
320	>6.5	>75	>5	>75
321	<6.5	>75	>5	<75
322	>6.5	>75	>5	>75
323	<6.5	>75	<5	>75
324	<6.5	<75	<5	<75
325	<6.5	<75	<5	<75
326	<6.5	>75	>5	>75
327	<6.5	<75	>5	>75
328	<6.5	>75	>5	>75
329	>6.5	>75	>5	>75
330	>6.5	>75	>5	>75
331	>6.5	>75	>5	>75
332	>6.5	>75	>5	>75
333	>6.5	>75	<5	>75
334	<6.5	>75	<5	>75
335	<6.5	<75	<5	<75
336	>6.5	>75	>5	<75
337	>6.5	>75	>5	>75
338	<6.5	>75	<5	>75
339	<6.5	<75	<5	<75
340	<6.5	<75	<5	<75
341	<6.5	<75	<5	<75
342	<6.5	<75	<5	<75
343	>6.5	>75	>5	>75
344	>6.5	>75	>5	>75
345	<6.5	<75	<5	<75
346	>6.5	>75	>5	>75
347	>6.5	>75	>5	>75
348	>6.5	>75	>5	>75
349	>6.5	<75	<5	<75
350	<6.5	<75	<5	<75
351	>6.5	>75	>5	>75
352	>6.5	>75	>5	>75
353	>6.5	>75	>5	>75

Compound Number	hS1P1 cAMP pEC_{50}	hS1P1 cAMP SPAN	hS1P1 B-arrestin2 pEC_{50}	hS1P1 B-arrestin2 SPAN
354	>6.5	>75	>5	>75
355	>6.5	>75	>5	>75
356	>6.5	>75	>5	>75
357	>6.5	>75	>5	>75
358	>6.5	>75	>5	>75
359	>6.5	>75	>5	>75
360	<6.5	<75	<5	<75
361	<6.5	<75	<5	<75
362	<6.5	<75	<5	<75
363	<6.5	<75	<5	<75
364	<6.5	>75	<5	<75
365	<6.5	>75	>5	<75
366	<6.5	<75	<5	<75
367	<6.5	<75	<5	<75
368	<6.5	<75	<5	<75
369	<6.5	<75	<5	<75
370	>6.5	>75	>5	>75
371	<6.5	<75	<5	<75
372	>6.5	>75	>5	>75
373	<6.5	>75	<5	>75
374	<6.5	<75	<5	<75
375	>6.5	>75	>5	<75
376	<6.5	<75	<5	<75
377	<6.5	<75	<5	<75
378	<6.5	<75	<5	<75
379	<6.5	<75	<5	<75
380	<6.5	<75	<5	<75
381	<6.5	<75	>5	<75
382	>6.5	>75	>5	>75
383	>6.5	>75	>5	>75
384	<6.5	>75	<5	<75
385	<6.5	<75	<5	>75
386	<6.5	>75	<5	<75
387	<6.5	>75	>5	>75
388	>6.5	>75	>5	>75
389	>6.5	>75	>5	>75
390	>6.5	>75	>5	<75
391	>6.5	>75	>5	>75
392	<6.5	<75	<5	<75
393	<6.5	<75	<5	<75
394	<6.5	<75	>5	<75
395	>6.5	<75	>5	>75
396	<6.5	<75	<5	>75
397	<6.5	<75	<5	>75
398	>6.5	>75	>5	>75

Compound Number	hS1P1 cAMP pEC_{50}	hS1P1 cAMP SPAN	hS1P1 B-arrestin2 pEC_{50}	hS1P1 B-arrestin2 SPAN
399	>6.5	>75	>5	<75
400	<6.5	<75	<5	<75
401	<6.5	<75	<5	<75
402	>6.5	<75	<5	<75
403	<6.5	<75	<5	<75
404	<6.5	>75	<5	<75
405	<6.5	<75	<5	<75
406	>6.5	>75	>5	>75
407	<6.5	>75	<5	<75
408	<6.5	>75	<5	<75
409	<6.5	>75	<5	<75
410	<6.5	<75	<5	<75
411	<6.5	<75	<5	<75
412	<6.5	>75	<5	<75
413	>6.5	<75	>5	>75
414	>6.5	<75	<5	>75
415	>6.5	<75	<5	>75
416	>6.5	>75	>5	>75
417	>6.5	>75	>5	>75
418	>6.5	>75	>5	>75
419	>6.5	>75	>5	<75
420	>6.5	>75	<5	>75
421	<6.5	>75	<5	<75
422	>6.5	>75	>5	>75
423	>6.5	>75	>5	>75
424	>6.5	>75	<5	>75
425	>6.5	>75	>5	>75
426	>6.5	>75	<5	>75
427	<6.5	>75	<5	>75
428	<6.5	>75	<5	>75
429	<6.5	>75	<5	>75
430	<6.5	>75	<5	>75
431	<6.5	>75	<5	>75
432	>6.5	>75	>5	>75
433	>6.5	>75	>5	>75
434	<6.5	<75	<5	>75
435	>6.5	>75	>5	>75
436	>6.5	>75	<5	>75
437	>6.5	>75	>5	<75
438	>6.5	>75	>5	>75
439	<6.5	>75	<5	>75
440	>6.5	>75	>5	>75
441	>6.5	>75	>5	>75
442	>6.5	>75	>5	>75
443	>6.5	>75	>5	<75

Compound Number	hS1P1 cAMP pEC_{50}	hS1P1 cAMP SPAN	hS1P1 B-arrestin2 pEC_{50}	hS1P1 B-arrestin2 SPAN
444	<6.5	<75	>5	<75
445	>6.5	>75	>5	>75
446	<6.5	<75	<5	<75
447	>6.5	>75	>5	<75
448	<6.5	>75	<5	<75
449	<6.5	>75	<5	>75
450	>6.5	>75	>5	>75
451	>6.5	<75	>5	<75
452	<6.5	>75	>5	<75
453	>6.5	>75	>5	<75
454	>6.5	>75	>5	>75
455	>6.5	>75	>5	>75
456	>6.5	>75	<5	>75
457	>6.5	>75	<5	>75
458	<6.5	<75	<5	<75
459	<6.5	>75	<5	>75
460	<6.5	>75	<5	>75
461	<6.5	>75	<5	>75
462	>6.5	>75	<5	>75
463	>6.5	>75	>5	>75
464	>6.5	<75	<5	<75
465	>6.5	>75	>5	>75
466	<6.5	>75	<5	>75
467	>6.5	>75	>5	>75
468	>6.5	>75	>5	>75
469	>6.5	>75	>5	>75
470	<6.5	>75	<5	>75
471	>6.5	>75	>5	>75
472	>6.5	>75	>5	>75
473	>6.5	>75	>5	>75
474	<6.5	>75	<5	>75
475	>6.5	>75	>5	<75
476	>6.5	>75	>5	<75
477	>6.5	>75	>5	<75
478	<6.5	<75	<5	<75
479	<6.5	<75	<5	<75
480	<6.5	>75	<5	<75
481	<6.5	>75	>5	<75
482	<6.5	<75	<5	>75
483	<6.5	>75	<5	<75
484	>6.5	>75	>5	>75
485	>6.5	>75	<5	>75
486	>6.5	<75	<5	>75
487	<6.5	>75	>5	>75
488	>6.5	<75	>5	>75

Compound Number	hS1P1 cAMP pEC_{50}	hS1P1 cAMP SPAN	hS1P1 B-arrestin2 pEC_{50}	hS1P1 B-arrestin2 SPAN
489	>6.5	>75	>5	>75
490	>6.5	>75	>5	>75
491	>6.5	>75	>5	>75
492	<6.5	>75	<5	>75
493	<6.5	>75	<5	>75
494	<6.5	<75	>5	<75
495	>6.5	>75	>5	>75
496	>6.5	>75	>5	>75
497	>6.5	>75	>5	>75
498	>6.5	>75	<5	<75
499	>6.5	>75	>5	>75
500	<6.5	<75	<5	<75
501	<6.5	<75	<5	>75
502	>6.5	>75	>5	>75
503	<6.5	>75	<5	>75
504	<6.5	>75	<5	<75
505	<6.5	<75	<5	>75
506	>6.5	<75	>5	<75
507	>6.5	<75	<5	<75
508	<6.5	>75	<5	<75
509	<6.5	<75	<5	>75
510	>6.5	<75	>5	>75
511	>6.5	<75	>5	>75
512	>6.5	>75	>5	<75
513	>6.5	>75	>5	>75
514	>6.5	>75	>5	<75
515	>6.5	>75	>5	>75
516	<6.5	<75	>5	<75
517	<6.5	<75	>5	<75
518	<6.5	>75	<5	<75
519	>6.5	>75	>5	>75
520	>6.5	>75	>5	>75
521	<6.5	<75	<5	<75
522	<6.5	>75	<5	>75
523	<6.5	>75	<5	>75
524	>6.5	>75	>5	<75
525	<6.5	>75	<5	>75
526	<6.5	>75	<5	>75
527	<6.5	>75	<5	>75
528	<6.5	>75	<5	<75
529	<6.5	>75	>5	<75
530	<6.5	>75	<5	>75
531	>6.5	>75	>5	>75
532	>6.5	>75	>5	<75
533	<6.5	<75	<5	<75

Compound Number	hS1P1 cAMP pEC_{50}	hS1P1 cAMP SPAN	hS1P1 B-arrestin2 pEC_{50}	hS1P1 B-arrestin2 SPAN
534	<6.5	<75	<5	<75
535	<6.5	<75	>5	<75
536	<6.5	<75	>5	<75
537	>6.5	>75	>5	<75
538	>6.5	<75	>5	<75
539	>6.5	<75	>5	<75
540	<6.5	<75	<5	<75
541	<6.5	<75	<5	<75
542	<6.5	<75	>5	<75
543	>6.5	<75	<5	<75
544	<6.5	<75	>5	<75
545	>6.5	>75	>5	>75
546	<6.5	<75	<5	<75
547	>6.5	>75	>5	>75
548	<6.5	<75	<5	<75
549	>6.5	>75	>5	>75
550	<6.5	>75	>5	<75
551	>6.5	>75	>5	<75
552	<6.5	<75	<5	<75
553	<6.5	>75	>5	<75
554	>6.5	>75	>5	>75
555	>6.5	<75	>5	<75
556	>6.5	>75	>5	<75
557	<6.5	>75	>5	<75
558	>6.5	>75	>5	>75
559	>6.5	>75	>5	>75
560	>6.5	>75	>5	>75
561	>6.5	>75	>5	<75
562	>6.5	>75	>5	>75
563	>6.5	>75	>5	<75
564	>6.5	>75	>5	>75
565	>6.5	>75	>5	>75
566	<6.5	<75	<5	<75
567	<6.5	>75	<5	<75
568	>6.5	>75	>5	>75
569	<6.5	>75	<5	<75
570	<6.5	<75	<5	<75
571	>6.5	>75	>5	<75
572	<6.5	<75	<5	>75
573	<6.5	<75	<5	<75
574	<6.5	>75	<5	>75
575	>6.5	>75	>5	>75
576	>6.5	>75	>5	<75
577	<6.5	<75	>5	<75
578	<6.5	>75	<5	<75

Compound Number	hS1P1 cAMP pEC_{50}	hS1P1 cAMP SPAN	hS1P1 B-arrestin2 pEC_{50}	hS1P1 B-arrestin2 SPAN
579	>6.5	>75	>5	>75
580	>6.5	>75	>5	>75
581	<6.5	>75	<5	<75
582	<6.5	>75	<5	<75
583	<6.5	<75	<5	<75
584	>6.5	>75	>5	>75
585	>6.5	>75	>5	>75
586	>6.5	>75	>5	>75
587	<6.5	<75	<5	<75
588	<6.5	<75	<5	<75
589	<6.5	<75	<5	>75
590	<6.5	<75	<5	<75
591	>6.5	<75	>5	>75
592	<6.5	<75	<5	>75
593	>6.5	>75	>5	>75
594	>6.5	>75	>5	>75
595	>6.5	>75	>5	>75
596	>6.5	<75	>5	>75
597	>6.5	>75	>5	>75
598	>6.5	>75	>5	>75
599	>6.5	<75	>5	>75
600	>6.5	>75	>5	>75
601	<6.5	>75	>5	<75
602	<6.5	<75	<5	>75
603	>6.5	>75	>5	>75
604	>6.5	>75	>5	>75
605	>6.5	>75	>5	>75
606	>6.5	>75	>5	>75
607	>6.5	>75	>5	>75
608	>6.5	>75	>5	>75
609	>6.5	<75	<5	<75
610	<6.5	<75	<5	>75
611	>6.5	<75	>5	<75
612	>6.5	<75	>5	>75
613	<6.5	<75	<5	<75
614	<6.5	>75	<5	<75
615	>6.5	>75	>5	>75
616	>6.5	>75	>5	>75
617	<6.5	<75	<5	>75
618	<6.5	<75	>5	<75
619	>6.5	>75	>5	>75
620	>6.5	<75	>5	>75
621	<6.5	>75	<5	>75
622	>6.5	>75	<5	<75
623	<6.5	>75	<5	>75

Compound Number	hS1P1 cAMP pEC_{50}	hS1P1 cAMP SPAN	hS1P1 B-arrestin2 pEC_{50}	hS1P1 B-arrestin2 SPAN
624	<6.5	<75	<5	>75
625	<6.5	<75	<5	<75
626	<6.5	<75	<5	<75
627	<6.5	>75	<5	>75
628	>6.5	>75	>5	<75
629	<6.5	>75	<5	<75
630	<6.5	<75	<5	<75
633	<6.5	<75	<5	<75
634	<6.5	<75	<5	<75
635	>6.5	<75	>5	<75
636	>6.5	>75	>5	>75
637	>6.5	>75	>5	>75
638	>6.5	<75	<5	<75
639	<6.5	<75	<5	>75
640	<6.5	>75	<5	<75
641	<6.5	<75	<5	<75
642	<6.5	<75	<5	<75
643	<6.5	>75	<5	<75
644	<6.5	>75	<5	>75
645	<6.5	>75	<5	<75
646	<6.5	<75	<5	>75
647	>6.5	>75	>5	>75

Example 3: S_1P_1 receptor Are Effective to Treat chemotherapeutic induced peripheral neuropathy

Compounds were tested for efficacy in mouse models of chemotherapy induced peripheral neuropathy. The intraperitoneal (i.p.) injection of chemotherapeutics in rodents has been shown to induce sensory impairment and pain, similar to what is seen in humans where these sensations begin within days and last for several weeks. For these studies c57bl/6 mice are habituated to the test environment and baseline measurements of pain sensitivity are assessed. To determine mechanical responses, the threshold for responses to punctate mechanical stimuli (mechanical hyperalgesia) was tested according to the frequency method. In brief, the plantar surface of the animal hindpaw was stimulated with a single von Frey monofilament (0.4 g) for approximately 1-2 seconds. If there was a withdrawal response, it was recorded as a positive response. A response was defined as a lifting or shaking of the paw upon stimulation. This was repeated ten times for each

mouse. The final measurement for each mouse is the % non-response to stimulation for the ten trials. The %non-response to stimulation is converted to a %MPE. For paclitaxel induced peripheral neuropathy, a series of injections of PAC (6 mg/kg, i.p.) on days 1, 3, 5 and 7 is used to induce peripheral neuropathy. After approximately 14 days from the initiation of PAC injections, animals are re-assessed for mechanical sensitivity. Animals that exhibit a 50% response rate and lower can be included in studies with test compounds. On test day animals are dosed with compounds either subcutaneously or orally and tested for mechanical response by the frequency method either 30 min (s.c.) or 60 min (p.o.) after drug administration. Data is presented as a %MPE. For oxaliplatin induced peripheral neuropathy, a series of injections of OXA (4 mg/kg, i.p.) on days 1-5 is used to induce peripheral neuropathy. After approximately 14 days from the initiation of PAC injections, animals are re-assessed for mechanical sensitivity. Animals that exhibit a 50% response rate and lower can be included in studies with test compounds. On test day animals are dosed with compounds subcutaneously and tested for mechanical response by the frequency method 30 min after drug administration. Data is presented as a %MPE. One or more of the compounds show reversal of chemotherapeutic induced peripheral neuropathy.

A compound was tested for the ability to prevent the development of OXA induced peripheral neuropathy. A concurrent with the OXA injections on Day 1-5, a compound was dosed (3 mg/kg, sc) every day for 15 days. On Day 16 animals were tested for mechanical allodynia. Animals treated with a test compound did not exhibit peripheral neuropathy. The data for exemplary compounds is provided below.

Reversal of allodynia induced by Oxaliplatin in mice

Compound Number	**Screen @ 3 mg/kg sc (% MPE)**
142	>50
287	>50
55	>50

169	>50

Reversal of allodynia induced by paclitaxel in mice (s.c.)

Compound Number	**Screen @ 1 mg/kg sc (% MPE)**
293	>50
287	<50
99	>50
55	<50
142	>50
8	<50
169	>50
96	>50
277	>50
142	>50
103	>50
177	>50
26	<50
252	<50
304	>50
221	<50
33	<50
149	<50
263	>50
147	>50
212	>50
267	>50
262	>50
305	>50
224	>50
179	>50
185	>50
106	<50
306	<50
259	<50
107	<50
210	<50

Reversal of allodynia induced by paclitaxel in mice (p.o.)

Compound Number	Screen @ 3 mg/kg po (% MPE)
26	<50
99	>50
103	>50
142	>50
179	>50
262	>50
263	>50
348	>50
354	>50
355	>50
356	>50
358	>50
359	>50
415	<50
423	>50
435	>50
442	>50
455	>50
469	>50
471	<50
472	>50
489	>50
497	<50
502	>50
513	<50
514	>50
519	<50
520	>50
531	>50
547	>50
558	>50
560	>50
562	>50
563	<50
564	>50
568	<50
579	>50
580	>50

584	>50
585	<50
586	<50
598	<50
600	<50
606	>50
607	>50
608	<50
615	>50
636	<50
637	>50
726	>50
727	>50
728	>50
729	>50
730	>50
731	>50
732	>50
733	>50
734	>50
735	<50
736	>50

Example 4: The S_1P_1 Receptor Compounds Can Be Used To Treat Inflammation And Pain

Assessment of Tactile Allodynia Produced by Intraplantar Freund's Complete Adjuvant in rats:

Animals were acclimated to the vivarium for at least 48 hr prior to behavioral testing. Inflammation was induced with the administration of an intraplantar (subcutaneous injection into the plantar surface of the hind paw, i.pl.) injection of 0.10 ml Freund's Complete Adjuvant (FCA).

The experiments were conducted 24 hours after CFA administration. Rats are tested for mechanical allodynia in a Randall-Selitto apparatus. The inflamed paw is put on a pedestal and a pointed force of increasing intensity (0 to 250 grams) is applied to the paw. When the animal struggles to withdraw from the force the test is stopped and the force to induce that struggle is recorded. Data is presented as mean grams of force to withdrawal or a percentage of the maximum possible effect.

Exemplary compounds in the CFA model are shown below.

Compound Number	Active Doses, mg/kg sc (>50% MPE)
103	≥0.03
293	≥0.1
142	≥0.1
26	≥0.1
212	≥0.1
469	≥0.01

Example 5: Compounds selective for S1P1 Receptor

In vitro selectivity assays

Stable clonal Chinese hamster ovary K1 (CHO-K1) cells co-expressing EA-β-arrestin2 and the human sphingosine-1-phosphate receptor 2 (NM_004230.3, $S1P_2$), human sphingosine-1-phosphate receptor 3 (NM_005226, $S1P_3$) and sphingosine-1-phosphate receptor 5 (NM_001166215.1, $S1P_5$) with a C-terminal Prolink™ tag were purchased from DiscoverX corporation (S1P2: Cat# 93-0256C2, S1P3: Cat# 93-0217C2, S1P5: Cat# 93-0583C2).

Cell culturing and assay plating

Cell lines were cultured in AssayComplete™ Media 6 (DiscoverX Corporation, Cat#: 920018GF2) at 37°C and 5% CO_2 in a humidified CO_2 and temperature-controlled incubator. To begin assay plating, cells were washed with dulbecco's phosphate buffered saline (CellGro, Cat#: 21-031-CV) and lifted from the culturing flask by incubation (37°C, 5 min) with CellStripper (Cellgro, Cat#: 25-056-CI). Lifted cells were resuspended to 250,000 cells per milliliter in either AssayComplete™ Cell Plating 11 Reagent (S1P5 cell line) (DiscoverX Corporation, Cat#: 93-0563R11B) or AssayComplete™ Cell Plating 2 Reagent (S1P2 and S1P3 cell line) (DiscoverX Corporation, Cat#: 93-0563R2B) and plated at 5000 cells per well (S1P3 cell line) or 7500 cells per well (S1P2 and S1P5 cell line) in white-opaque 384 well plates (Greiner Bio-One Item #: 20-784080). Plated cells were incubated overnight at 37°C and 5% CO_2 in a humidified CO_2 and temperature-controlled incubator.

Detecting inhibition of cAMP production

S1P3 and S1P5 Agonist-promoted G-protein responses were determined by measuring changes in intracellular cAMP using the HTRF® cAMP HiRange kit (CisBio, Cat#: 62AM6PEJ) based on time-resolved fluorescence resonance energy transfer (TR-FRET) technology. AssayComplete™ Cell Plating 11 Reagent was removed and replaced with Ham's F-12 (CellGro, Cat#: 10-080-CM) containing isobutyl-methyl-xanthine (IBMX; 500 μM; Tocris Bioscience, Cat#: 2845), and NKH-477 (1.5 μM; Tocris Bioscience, Cat#: 1603) along with test or control compounds at the desired concentrations. Following a 30-minute room temperature incubation the components of the cAMP HiRange kit were added as per the manufacturer's instructions. After an hour incubation at room temperature, plates were analyzed by a BMG PheraStar microplate reader. Responses were measured as the ratio of signal over background, fluorescence emission at 665 nm to fluorescence emission at 620 nm.

Detecting inositol monophosphate production

S1P2 Agonist-promoted G-protein responses were determined by measuring changes in intracellular inositol monophosphate using the IP-one TB kit (CisBio, Cat#: 62IPAPEJ) based on time-resolved fluorescence resonance energy transfer (TR-FRET) technology. AssayComplete™ Cell Plating 2 Reagent was removed and replaced with 1x IP-one stimulation buffer (as per manufacturer's instructions) along with test or control compounds at the desired concentrations. Following a 60-minute incubation at 37°C and 5% CO_2 in a humidified CO_2 and temperature-controlled incubator, the components of the IP-one TB kit were added as per the manufacturer's instructions. After an hour incubation at room temperature, plates were analyzed by a BMG PheraStar microplate reader. Responses were measured as the ratio of signal over background, fluorescence emission at 665 nm to fluorescence emission at 620 nm.

Activity Table

The compounds were able to modulate the activities (inhibition of cAMP production or accumulation of inositol monophosphate) of the sphingosine-1-phosphate 2, sphingosine-1-phosphate 3, sphingosine-1-phosphate 5 receptor as indicated herein. The tables below include the efficacy of the compound as compared to a positive control, referred to as "SPAN". These values are normalized to fingolimod, a known agonist of the sphingosine-1-phosphate 3 and 5 receptor or CYM5520, a known agonist of the sphingosine-1-phosphate 2 receptor. The tables also include potency values (pEC50) for modulating discrete receptor-mediated activities (inhibition of cAMP production or inositol monophosphate accumulation). This value represents the estimated

concentration to promote half of the maximal efficacy (or SPAN) observed for each compound. Exemplary compounds that were found to be selective are shown below.

Compound number	hS1P2 IP-one pEC_{50}	hS1P2 IP-one SPAN	hS1P3 cAMP pEC_{50}	hS1P3 cAMP SPAN	hS1P5 cAMP pEC_{50}	hS1P5 cAMP SPAN
22	>5.0	<50	<5.0	<50	>5.0	<50
26	<5.0	<50	<5.0	<50	<5.0	<50
32	<5.0	<50	<5.0	<50	<5.0	<50
99	<5.0	<50	<5.0	<50	<5.0	>50
103	<5.0	<50	<5.0	<50	<5.0	<50
141	<5.0	<50	>5.0	>50	>5.0	>50
147	<5.0	<50	<5.0	<50	>5.0	<50
149	<5.0	<50	>5.0	>50	>5.0	>50
152	<5.0	<50	<5.0	<50	<5.0	<50
177	<5.0	<50	>5.0	>50	>5.0	>50
185	<5.0	<50	<5.0	<50	<5.0	>50
212	<5.0	<50	<5.0	<50	<5.0	<50
219	>5.0	<50	<5.0	<50	<5.0	<50
221	<5.0	<50	>5.0	<50	>5.0	<50
252	>5.0	<50	>5.0	<50	>5.0	>50
259	<5.0	<50	<5.0	<50	<5.0	<50
262	<5.0	>50	<5.0	<50	<5.0	<50
263	<5.0	<50	<5.0	<50	<5.0	<50
267	<5.0	<50	<5.0	<50	<5.0	<50
277	<5.0	>50	<5.0	<50	<5.0	<50
287	<5.0	<50	<5.0	<50	<5.0	<50
293	<5.0	<50	<5.0	<50	<5.0	>50
304	<5.0	<50	>5.0	<50	<5.0	<50
391	>5.0	<50	>5.0	>50	>5.0	<50
398	<5.0	<50	<5.0	<50	<5.0	<50
406	<5.0	<50	<5.0	<50	<5.0	<50
417	>5.0	<50	<5.0	<50	<5.0	<50
422	>5.0	<50	>5.0	<50		
423	>5.0	<50	>5.0	<50		
445	>5.0	<50	<5.0	<50		
455	<5.0	<50	<5.0	<50		
496	<5.0	<50	<5.0	<50		

Thus, the compounds were found to be sufficiently selective for S1P1.

Example 6: The S_1P_1 Receptor Compounds Can Be Used To Treat Diabetic Neuropathy

Assessment of Tactile Allodynia and Thermal Hyperalgesia in a Rodent Model of Diabetic Neuropathy – Streptozotocin-Induced (STZ)

A cohort of 48 male Sprague Dawley rats, weighing 225 – 250 g at arrival, was group housed under constant temperature, humidity and a 12-hour light-dark cycle. Following acclimation to the animal colony, the animals were tested for baseline withdrawal responses to mechanical allodynia and thermal hyperalgesia using the methods described below in Chaplan, S. R., Bach, F. W., Pogrel, J. W., Chung, J. M. and Yaksh, T. L. Quantitative assessment of tactile allodynia in the rat paw. J. Neurosci. Methods 53: 55-63, 1994; Joris, J.L., Dubner, R. and Hargreaves, K.M. Opioid analgesia at Peripheral Sites: a Target for Opioids Released during Stress and Inflammation? Anesthesia and Analgesia 66(12), 1277-81, 1987; and Morrow, T.J. Animal Models of Painful Diabetic Neuropathy: The STZ rat model. Current Protocols in Neuroscience, Nov; Chapter 9, Unit 9.18, 2004..

A diabetic-like state was induced with a single intraperitoneal (IP) injection of streptozotocin STZ (50 mg/kg) freshly dissolved in 10 mM citric acid buffer was injected intraperitoneally (IP) on Day 1. Two days later (on Day 3), hyperglycermia was confirmed by existence of blood glucose >350 mg/dL as measured by glucometer, and the animal health was monitored biweekly for 12 days.

For measures of mechanical allodynia, rats were preselected for experimentation only if the pain threshold 7-14 days after STZ injection (pre-treatment) was reduced by 10 grams of force relative to the response of the individual paw before STZ challenge (pre-induction), namely, with clear presence of allodynia. The rats were randomized based on pre-dose mechanical allodynia scores to balanced treatment groups. The animals were tested prior to study inclusion for mechanical allodynia by the manual von Frey test on Day 20 (Chaplan up/down method using von Frey filaments on the plantar surface of the paw). The manual von Frey test was repeated at 0.5 or 1 hr following administrations of test articles, vehicle, and reference compound via the specified route(s) and on Day 21 post-surgery.

For measures of thermal hyperalgesia, rats were pre-selected for experimentation only if the pain threshold 7-14 days after STZ injection (pre-treatment) was reduced by 75% relative to the response of the individual paw before STZ challenge (pre-induction), namely, with clear presence of hyperalgesia. The rats were randomized based on pre-dose thermal hyperalgesia scores to balanced treatment groups. Rats were preselected (with clear presence of thermal hyperalgesia) on Day 20. Thermal hyperalgesia was measured at 1 or 1.5 hr after dosing of test articles, vehicle, and reference compound via the specified route(s) on Day 21. Each rat was placed within a plastic box atop a glass floor for 20 to 30 minutes. A light beam under the floor was aimed at the plantar surface of the left

hind paw. The time was measured automatically when the paw was withdrawn away from the thermal stimulus. A cut-off latency of 23 sec was imposed. The latency to withdrawal was obtained for each rat and defined as the heat pain threshold.

Mean thresholds and withdrawal latencies were analyzed via Two Way ANOVA followed by Dunnett's Multiple Comparison tests to STZ + VEH group with differences considered significant at $p < 0.05$.

Exemplary compounds, but not limited to these, that were effective in this animal model are described below. For example, compounds 103 and 293 were tested and found to have active doses between 50 and 100 mg/kg in both mechanical allodynia and thermal hyperalgesia.

Compound #	**Active Doses in STZ Diabetic Neuropathy Model (mg/kg, po)** ($p < 0.05$ compared to STZ + VEH treated mice) **MECHANICAL**	**Active Doses in STZ Diabetic Neuropathy Model (mg/kg, po)** ($p < 0.05$ compared to STZ + VEH treated mice) **THERMAL**
103	<100	<100
293	<100	<100
469	<100	<100

Example 7: The S_1P_1 Receptor Compounds Can Be Used To Treat Peripheral Neuropathy

Assessment of Tactile Allodynia and Thermal Hyperalgesia in a Rodent Model of Peripheral Neuropathy – Spinal Nerve Ligation (SNL)

A cohort of 48 male Sprague Dawley rats, weighing 225 – 250 g at arrival, was group housed under constant temperature, humidity and a 12-hour light-dark cycle. Following acclimation to the animal colony, the animals were tested for baseline withdrawal responses to mechanical allodynia and thermal hyperalgesia using the methods described in . Chaplan, S. R., Bach, F. W., Pogrel, J. W., Chung, J. M. and Yaksh, T. L. Quantitative assessment of tactile allodynia in the rat paw. J.

Neurosci. Methods 53: 55-63, 1994; Joris, J.L., Dubner, R. and Hargreaves, K.M. Opioid analgesia at Peripheral Sites: a Target for Opioids Released during Stress and Inflammation? Anesthesia and Analgesia 66(12), 1277-81, 1987; and Kim, S. H. and Chung, J. M. An experimental model of peripheral neuropathy produced by segmental spinal nerve ligation in the rat. Pain 50: 335-63, 1992.

Animals (n = 40) were anesthetized with an intraperitoneal (IP) injection of Pentobarbital (50 mg/kg). Spinal nerve ligation (SNL) was performed by first separating the left paraspinal muscles from the spinous processes (L4 – S2). The L6-S1 facet joint was nipped. The transverse process of L6 was removed to identify the locations of the L5 and L6 spinal nerve. The left L5 and L6 spinal nerves were isolated and tightly ligated with 6.0 silk sutures. Another 8 animals were underwent sham surgery only (anesthesia, surgical opening and skin suture).

For measures of mechanical allodynia, rats were preselected for experimentation only if the pain threshold 7-14 days after SNL surgery (pre-treatment) was reduced by 10 grams of force relative to the response of the individual paw before surgery (pre-induction), namely, with clear presence of allodynia. The rats were randomized based on pre-dose mechanical allodynia scores to balanced treatment groups. The animals were tested prior to study inclusion for mechanical allodynia by the manual von Frey test on Day 20 (Chaplan up/down method using von Frey filaments on the plantar surface of the paw). The manual von Frey test was repeated at 0.5 or 1 hr following administrations of test articles, vehicle, and reference compound via the specified route(s) and on Day 21 post-surgery.

For measures of thermal hyperalgesia, rats were pre-selected for experimentation only if the pain threshold 7-14 days after spinal surgery (pre-treatment) was reduced by 75% relative to the response of the individual paw before surgery (pre-induction), namely, with clear presence of hyperalgesia. The rats were randomized based on pre-dose thermal hyperalgesia scores to balanced treatment groups. Rats were preselected (with clear presence of thermal hyperalgesia) on Day 20. Thermal hyperalgesia was measured at 1 or 1.5 hr after dosing of test articles, vehicle, and reference compound via the specified route(s) on Day 21. Each rat was placed within a plastic box atop a glass floor for 20 to 30 minutes. A light beam under the floor was aimed at the plantar surface of the left hind paw. The time was measured automatically when the paw was withdrawn away from the thermal stimulus. A cut-off latency of 23 sec was imposed. The latency to withdrawal was obtained for each rat and defined as the heat pain threshold.

Mean thresholds and withdrawal latencies were analyzed via Two Way ANOVA followed by Dunnett's Multiple Comparison tests to SNL + VEH group with differences considered significant at $p < 0.05$.

Exemplary compounds, but not limited to these, that were effective in this animal model are described below. For example, compound 103 was tested and found to have active doses between 50 and 100 mg/kg.

Compound #	**Active Doses in SNL Neuropathy Model (mg/kg)** ($p < 0.05$ compared to SNL + VEH treated mice) **MECHANICAL**	**Active Doses in SNL Neuropathy Model (mg/kg)** ($p < 0.05$ compared to SNL + VEH treated mice) **THERMAL**
103	<100	<100

Example 8: Compounds do not inhibit hERG channel activity

The standard Automated Qpatch patch-clamp assay have been used and the selective hERG inhibitor E4031, serves as a positive control.

Compound number	**IC_{50} (μM)**
E4031	0.013
26	>10
304	>10
469	>10
497	>10
520	>10
730	>10
738	>10
742	>10
743	>10
744	>10

Example 9: Compounds Do Not Cause Lymphopenia

Compounds were tested for changes in peripheral blood lymphocytes in c57bl/6 mice. In acute studies, animals (n=5/group) were dosed subcutaneously with test compound at a dose of 3 mg/kg. Animals were sacrificed at specific time points and 500 µl of whole blood was collected in EDTA (K2) Eppendorf tubes. Blood was stored on ice and shipped immediately overnight delivery to Charles River Laboratories for analysis. CRL ran samples through their WBC/differential panel on an Advia 120 instrument. We received peripheral lymphocyte counts (10^3 cells/µl) for each blood sample. Treatment group means were compared to a vehicle treatment group for statistical significance. In chronic studies, animals (n=6-8/group) were dosed subcutaneously with test compound either in a dose response paradigm (highest dose of 3 mg/kg) or in a screening paradigm at 6 mg/kg for seven days. On the seventh day, animals were sacrificed 45 minutes after the final dose. Whole blood was collected and analyzed as described for acute studies. None of the compounds showed statistically significant decreases in peripheral blood lymphocytes in acute or chronic studies. Non-limiting exemplary data is provided below.

Lymphopenia – c57bl/6 mice

Compound Number	Effect and Doses, mg/kg, sc
8	no change: 6 mg/kg, 7 days
19	no change: 6 mg/kg, 7 days
22	no change: 3 mg/kg, 7 days
32	no change: 6 mg/kg, 7 days
55	no change: 6 mg/kg, 7 days
59	no change: 6 mg/kg, 7 days
96	no change: 6 mg/kg, 7 days
99	no change: 6 mg/kg, 7 days
103	no change: 6 mg/kg, 7 days
142	no change: 6 mg/kg, 7 days
147	no change: 6 mg/kg, 7 days

169	no change: 6 mg/kg, 7 days
234	no change: 6 mg/kg, 7 days
287	no change: 6 mg/kg, 7 days
293	no change: 6 mg/kg, 7 days
304	no change: 6 mg/kg, 7 days
355	no change: 6 mg/kg, 7 days
356	no change: 6 mg/kg, 7 days
384	no change: 3 mg/kg; 45 min and 2 hr
423	no change: 6 mg/kg, 7 days
455	no change: 6 mg/kg, 7 days
469	-28% not stat sig: 6 mg/kg, 7 days
520	no change: 6 mg/kg, 7 days
531	no change: 6 mg/kg, 7 days
730	no change: 6 mg/kg, 7 days
731	-78% stat sig: 6 mg/kg, 7 days
737	-40% not stat sig: 6 mg/kg, 7 days

Example 10: **Compounds Inhibit Tumor Growth And Prolong Survivial In Tumor Model.**

Female athymic nude mice (Crl:NU(NCr)-Foxn1nu, Charles River Laboratories) were implanted with A2780 human ovarian carcinoma cells to initiate tumor growth.

Each mouse received 1 x 10^7 cells (0.1 mL cell suspension) subcutaneously in the right flank, and tumors were monitored as their volumes approached the target range of 100 to 150 mm^3. Fourteen days later, designated as Day 1 of the study, mice were sorted into six groups of ten each. The individual tumor volumes ranged from 108 to 196 mm^3 and group mean tumor volumes were 148 mm^3. Tumors were measured twice weekly for the study duration.

Paclitaxel dosing solutions were prepared in 5% ethanol, 5% Cremophor EL in D5W (Vehicle 1). Ozanimod and Compound 103 dosing solutions were prepared in 10% dimethylacetamide, 10% Cremophor EL, 80% sterile water with 10% β-cyclodextrin (Vehicle 2). Starting on Day 1 of the study, six groups (n = 10) of female athymic nude mice with established A2780 tumors were treated according to the following plan. Treatments were administered either by intravenous injection (i.v.) or oral gavage (p.o.) and were adjusted to the body weight of the individual animal. Group 1 received Vehicle 1, i.v., once every other day for five doses (qod x 5) and Vehicle 2, p.o., once daily to the end of the study (qd to end), and served as the control group for efficacy analysis. Group 2, the paclitaxel monotherapy group, received paclitaxel i.v., qod x 5 plus Vehicle 2, p.o., qd to end. Group 3, the ozanimod monotherapy group, received ozanimod p.o., qd to

end plus Vehicle 1, i.v., qod x 5. Combination Group 4 received ozanimod p.o., qd to end plus paclitaxel i.v., qod x 5. Group 5, the Compound 103 monotherapy group, received Compound 103 p.o., qd to end plus Vehicle 1, i.v., qod x 5. Combination Group 6 received Compound 103 p.o., qd to end plus paclitaxel i.v., qod x 5.

Animals were monitored individually, and each mouse was euthanized when its tumor reached the endpoint volume of 2000 mm3 or on the final day, whichever came first. The time to endpoint (TTE) was calculated for each mouse. Treatment outcome was determined from percent tumor growth delay (%TGD), defined as the percent increase in median TTE for treated versus control mice, with differences in TTE values between groups deemed statistically significant at $P < 0.05$ using logrank survival analysis. Mice were also monitored for complete regression (CR) and partial regression (PR) responses. An animal with a CR at the end of the study was additionally classified as a tumor-free survivor (TFS). Treatment tolerability was assessed by body weight measurements and frequent observation for clinical signs of treatment-related side effects.

All regimens were acceptably-tolerated based. Control tumors exhibited progressive growth, attaining the 2000 mm3 endpoint in a median 9.8 days, establishing a maximum possible TGD of 50.2 days (512%) for the 60-day study. Paclitaxel as monotherapy provided significant ($P \leq 0.001$) survival benefit (128% TGD) compared to controls, whereas the ozanimod and Compound 103 monotherapy regimens were associated with non-significant ($P > 0.05$) TGD of 31% and 15%, respectively, compared with the control. One animal receiving Compound 103 monotherapy survived the study with a sub-endpoint tumor. The combination of paclitaxel and ozanimod was associated with 185% TGD, providing statistically significant survival benefit over either of the corresponding monotherapies, and one study survivor with a CR/TFS tumor regression response. The combination of paclitaxel and Compound 103 provided 193% TGD, a significant result compared with paclitaxel monotherapy, but not statistically different ($P > 0.05$) from the result for ozanimod monotherapy.

Summary

The present example evaluated test agents ozanimod and Compound 103 each in combination with paclitaxel for efficacy in the A2780 human ovarian carcinoma model in female athymic mice. All regimens were acceptably-tolerated. Control tumors exhibited progressive growth, attaining the 2000 mm^3 endpoint in a median 9.8 days, establishing a maximum possible TGD of 50.2 days (512%) for the 60-day study. Paclitaxel as monotherapy provided significant ($P \leq 0.05$) survival

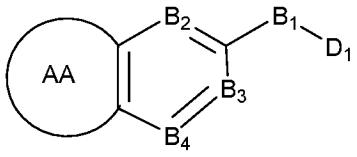
benefit (128% TGD) compared to controls, whereas the ozanimod and Compound 103 monotherapy regimens were associated with non-significant ($P > 0.05$) TGD of 31% and 15%, respectively, compared with the control. One animal receiving Compound 103 monotherapy survived the study with a sub-endpoint tumor. The combination of paclitaxel and ozanimod was associated with 185% TGD, providing statistically significant survival benefit over either of the corresponding monotherapies, and one study survivor with a CR/TFS tumor regression response. The combination of paclitaxel and Compound 103 provided 193% TGD, a significant result compared with paclitaxel monotherapy and more than additive as compared with the corresponding monotherapies..

Thus, these results demonstrate that the compounds provided herein can be used to treat cancers, such as breast or ovarian cancer.

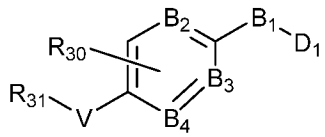
The examples and data provided herein demonstrate the unexpected properties and advantages of the compounds and pharmaceutical compositions provided herein. These properties could not have been predicted.

What Is Claimed Is:

1. A compound having Formula I or Formula II, or a pharmaceutically acceptable salt thereof:

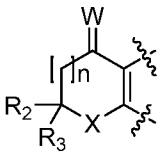
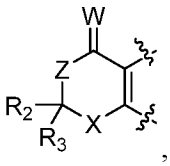
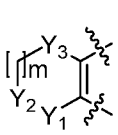
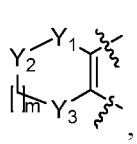
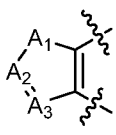
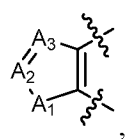
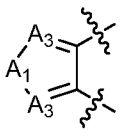


Formula I or



Formula II ,

wherein:

AA is  ,  ,  ,  ,  ,  , or  ;

W is O, S, or NR_1;

X is O, S, or NR_4;

V is O, S, or NR_{32};

Z is CHR_{42} or NR_{43};

n is 0, 1, 2, 3, or 4;

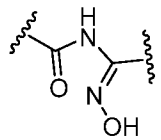
Y_1 and Y_2 are independently O, S, NR_5, C=O, C=S or $C=NR_6$;

Y_3 is O, S, CH_2, or NR_{34};

m is 0, 1, 2, or 3;

A_1 is O, S, NR_7, C=O, or C=S;

A_2 and A_3 are independently CR_{29} or N;

B_1 is an optionally substituted aryl or heteroaryl group, a carbocycle, or  ;

B_2, B_3, and B_4 are independently CR_{38} or N;

D_1 is H, OH, NH_2, NO_2, cycle, optionally substituted aryl group, branched or unbranched alkyl alcohol, halo, branched or unbranched alkyl, amide, cyano, alkoxy, haloalkyl, aklylsulfonyl, nitrite, or alkylsulfanyl;

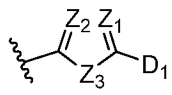
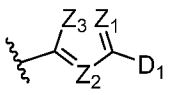
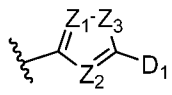
R_2 and R_3, are independently H, optionally substituted C_1-C_6 alkyl, optionally substituted C_1-C_6 hydroxyalkyl, optionally substituted C_1-C_6 alkoxy, optionally substituted cycloalkyl, or optionally substituted cycloheteroalkyl; or R_2 and R_3 are together optionally substituted cycloalkyl, or optionally substituted cycloheteroalkyl;

R_1, R_4, R_5, R_6, R_7, R_{29}, R_{31}, R_{32}, R_{33}, R_{34}, R_{38}, and R_{43} are independently H, OH, NH_2, optionally substituted C_1-C_6 alkyl, optionally substituted C_1-C_6 hydroxyalkyl, optionally substituted C_1-C_6 alkoxy, optionally substituted cycloalkyl, or optionally substituted cycloheteroalkyl.

R_{30} is independently H, CN, CF_3, optionally substituted C_1-C_6 alkyl, optionally substituted C_1-C_6 hydroxyalkyl, optionally substituted C_1-C_6 alkoxy, optionally substituted cycloalkyl, or optionally substituted cycloheteroalkyl; or optionally substituted haloalkyl;

R_{42} is independently Br, Cl, F, optionally substituted C_1-C_6 alkyl, optionally substituted C_1-C_6 hydroxyalkyl, optionally substituted C_1-C_6 alkoxy, optionally substituted cycloalkyl, or optionally substituted cycloheteroalkyl.

2. The compound of claim 1 having Formula I, or a pharmaceutically acceptable salt thereof,

wherein D_1 and B_1 have a formula of:  ,  , or 

wherein:

Z_1 and Z_2 are independently N or CR_{39};

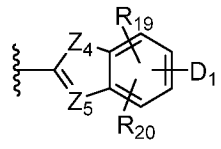
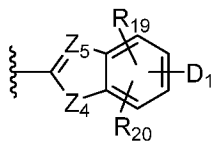
Z_3 is O, S, or NR_{27};

R_{27} and R_{39} are independently H, optionally substituted C_1-C_6 alkyl, optionally substituted C_1-C_6 hydroxyalkyl, optionally substituted C_1-C_6 alkoxy, optionally substituted cycloalkyl, or optionally substituted cycloheteroalkyl.

3. The compound of claim 2, or a pharmaceutically acceptable salt thereof, wherein one of Z_1 and Z_2 is N.

4. The compound of claim 2, or a pharmaceutically acceptable salt thereof, both Z_1 and Z_2 are N.

5. The compound of claim 2, or a pharmaceutically acceptable salt thereof, wherein Z_3 is O.

6. The compound of claim 1, or a pharmaceutically acceptable salt thereof, wherein D_1 and B_1 have a formula of:  or 

wherein:

Z_4 is O, S, or NR_{28};

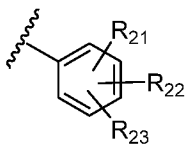
Z_5 is N or CH;

R_{19}, and R_{20} are each independently H, OH, NH_2, NO_2, cycle, aryl, branched or unbranched alkyl alcohol, halo, branched or unbranched alkyl, amide, cyano, alkoxy, alkylthio, haloalkyl, aklylsulfonyl, nitrite, or alkylsulfanyl; or two of R_{19}, and R_{20} together form an aryl or cycle that is attached to one or more of the atoms of B_1.

R_{28} is H, optionally substituted C_1-C_6 alkyl, optionally substituted C_1-C_6 hydroxyalkyl, optionally substituted C_1-C_6 alkoxy, optionally substituted cycloalkyl, or optionally substituted cycloheteroalkyl.

7. The compound of claim 6, or a pharmaceutically acceptable salt thereof, wherein Z_5 is N.

8. The compound of claim 6, or a pharmaceutically acceptable salt thereof, wherein Z_4 is O.

9. The compound of claim 1, or a pharmaceutically acceptable salt thereof, wherein D_1 is 

wherein R_{21}, R_{22}, and R_{23} are each independently H, OH, NH_2, NO_2, cycle, aryl, branched or unbranched alkyl alcohol, halo, branched or unbranched alkyl, amide, cyano, alkoxy, haloalkyl, aklylsulfonyl, nitrite, or alkylsulfanyl; or two of R_{21}, R_{22}, and R_{23} together form an aryl or cycle that is attached to one or more of the atoms of D_1.

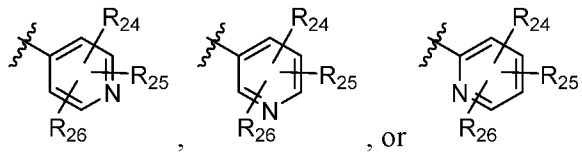
10. The compound of claim 9, or a pharmaceutically acceptable salt thereof, wherein one of R_{21}, R_{22}, and R_{23} is H.

11. The compound of claim 9, or a pharmaceutically acceptable salt thereof, wherein two of R_{21}, R_{22}, and R_{23} are H.

12. The compound of claims 11, or a pharmaceutically acceptable salt thereof, wherein R_{23} is Me, OH, NH2, Cl, $NHSO_2Me$, SO_2NH_2, NH(CO)Me, or $(CO)NH_2$.

13. The compound of claims 1, or a pharmaceutically acceptable salt thereof, wherein D_1 is optionally substituted aryl or optionally substituted hetero aryl.

14. The compound of claim 1, or a pharmaceutically acceptable salt thereof, wherein D_1 is



, , or

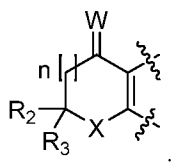
wherein R_{24}, R_{25}, and R_{26} are each independently H, OH, NH_2, NO_2, cycle, aryl, branched or unbranched alkyl alcohol, halo, branched or unbranched alkyl, amide, cyano, alkoxy, haloalkyl, aklylsulfonyl, nitrite, or alkylsulfanyl; or two of R_{24}, R_{25}, and R_{26} together form an aryl or cycle that is attached to one or more of the atoms of D_1.

15. The compound of claims 14, or a pharmaceutically acceptable salt thereof, wherein one of R_{24}, R_{25}, and R_{26} is H.

16. The compound of claims 14, or a pharmaceutically acceptable salt thereof, wherein two of R_{24}, R_{25}, and R_{26} are H.

17. The compound of claims 16, or a pharmaceutically acceptable salt thereof, wherein R_{26} is H, Me, OH, CF_3, or OMe.

18. The compound of claims 1, or a pharmaceutically acceptable salt thereof, wherein AA is



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19. The compound of claims 18, or a pharmaceutically acceptable salt thereof, wherein W is O.

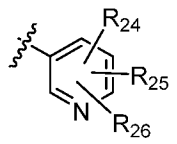
20. The compound of claims 19, or a pharmaceutically acceptable salt thereof, wherein X is O.

21. The compound of claims 20, or a pharmaceutically acceptable salt thereof, wherein R_2 and R_3 are independently H, optionally substituted C_1-C_6 alkyl, optionally substituted C_1-C_6 hydroxyalkyl, optionally substituted C_1-C_6 alkoxy, optionally substituted cycloalkyl, or optionally substituted cycloheteroalkyl.

22. The compound of claims 21, or a pharmaceutically acceptable salt thereof, wherein both R_2 and R_3 are the same.

23. The compound of claims 22, or a pharmaceutically acceptable salt thereof, wherein both R_2 and R_3 are Et.

24. The compound of claim 19, or a pharmaceutically acceptable salt thereof, wherein D_1 is



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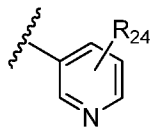
25. The compound of claims 24, or a pharmaceutically acceptable salt thereof, wherein one of R_{24}, R_{25}, and R_{26} is H.

26. The compound of claims 24, or a pharmaceutically acceptable salt thereof, wherein two of R_{24}, R_{25}, and R_{26} are H.

27. The compound of claim 26, or a pharmaceutically acceptable salt thereof, wherein D_1 is



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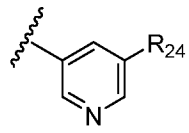
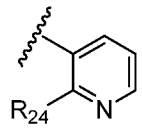
28. The compound of claim 27, or a pharmaceutically acceptable salt thereof, wherein D_1 is



29. The compound of claim 27, or a pharmaceutically acceptable salt thereof, wherein R_{24} is H.

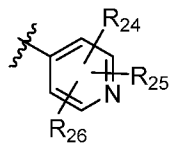
30. The compound of claim 27, or a pharmaceutically acceptable salt thereof, wherein R_{24} is OH.

31. The compound of claim 27, or a pharmaceutically acceptable salt thereof, wherein D_1 is



32. The compound of claims 31, or a pharmaceutically acceptable salt thereof, wherein R_{24} is OMe.

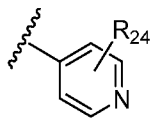
33. The compound of claim 19, or a pharmaceutically acceptable salt thereof, wherein D_1 is



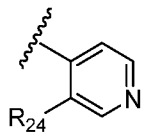
34. The compound of claims 33, or a pharmaceutically acceptable salt thereof, wherein one of R_{24}, R_{25}, and R_{26} is H.

35. The compound of claims 33, or a pharmaceutically acceptable salt thereof, wherein two of R_{24}, R_{25}, and R_{26} are H.

36. The compound of claim 35, or a pharmaceutically acceptable salt thereof, wherein D_1 is



37. The compound of claim 36, or a pharmaceutically acceptable salt thereof, wherein D_1 is



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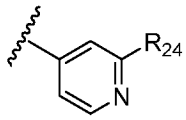
38. The compound of claim 36, or a pharmaceutically acceptable salt thereof, wherein D_1 is



.

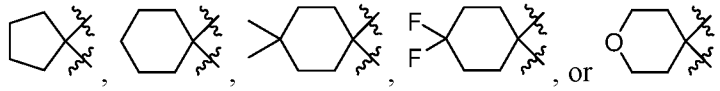
39. The compound of claim 36, or a pharmaceutically acceptable salt thereof, wherein R_{24} is halide.

40. The compound of claim 39, or a pharmaceutically acceptable salt thereof, wherein R_{24} is F.

41. The compound of claim 36, or a pharmaceutically acceptable salt thereof, wherein R_{24} is Me.

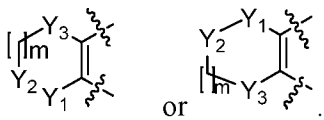
42. The compound of claim 36, or a pharmaceutically acceptable salt thereof, wherein R_{24} is OMe.

43. The compound of claim 36, or a pharmaceutically acceptable salt thereof, wherein R_{24} is OH.

44. The compound of claim 1, or a pharmaceutically acceptable salt thereof, wherein R_2 and R_3 are together  .

45. The compound of claim 44, or a pharmaceutically acceptable salt thereof, wherein n is 1.

46. The compound of claims 1, or a pharmaceutically acceptable salt thereof, wherein AA is



.

47. The compound of claim 46, or a pharmaceutically acceptable salt thereof, wherein Y_1 is NR_5.

48. The compound of claim 47, or a pharmaceutically acceptable salt thereof, wherein R_5 is H.

49. The compound of claim 46, or a pharmaceutically acceptable salt thereof, wherein Y_2 is $C{=}NR_6$.

50. The compound of claim 49, or a pharmaceutically acceptable salt thereof, wherein R_6 is H.

51. The compound of claim 46, or a pharmaceutically acceptable salt thereof, wherein Y_2 is C=O.

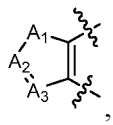
52. The compound of claim 46, or a pharmaceutically acceptable salt thereof, wherein Y_3 is O.

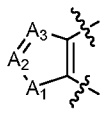
53. The compound of claim 46, or a pharmaceutically acceptable salt thereof, wherein Y_3 is CH_2.

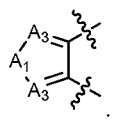
54. The compound of claim 46, or a pharmaceutically acceptable salt thereof, wherein m is 0.

55. The compound of claim 46, or a pharmaceutically acceptable salt thereof, wherein m is 1.

56. The compound of claims 1, or a pharmaceutically acceptable salt thereof, wherein AA is



,


, or


.

57. The compound of claim 56, or a pharmaceutically acceptable salt thereof, wherein A_1 is O.

58. The compound of claim 56, or a pharmaceutically acceptable salt thereof, wherein A_1 is S.

59. The compound of claim 56, or a pharmaceutically acceptable salt thereof, wherein A_2 is N.

60. The compound of claim 56, or a pharmaceutically acceptable salt thereof, wherein A_3 is N.

61. The compound of claim 56, or a pharmaceutically acceptable salt thereof, wherein A_3 is CR_{29}.

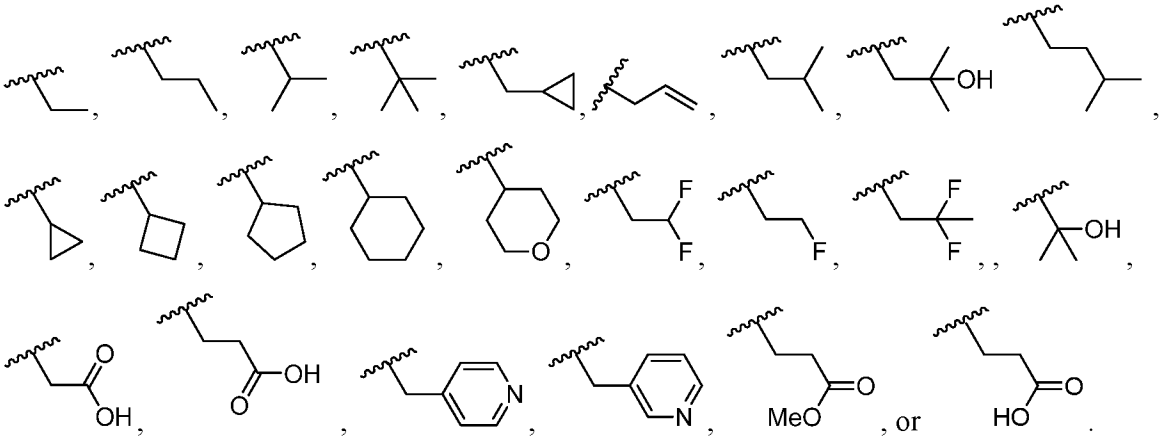
62. The compound of claim 61, or a pharmaceutically acceptable salt thereof, wherein R_{29} is H.

63. The compound of claim 56, or a pharmaceutically acceptable salt thereof, wherein A_2 is CR_{29}.

64. The compound of claim 63, or a pharmaceutically acceptable salt thereof, wherein R_{29} is H.

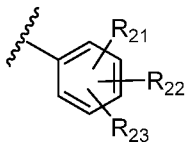
65. The compound of claim 56, or a pharmaceutically acceptable salt thereof, wherein A_1 is NR_7.

66. The compound of claim 65, or a pharmaceutically acceptable salt thereof, wherein R_7 is 

, 

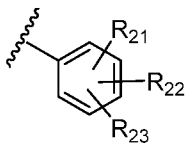
, or .

67. The compound of claim 56, or a pharmaceutically acceptable salt thereof, wherein D_1 is



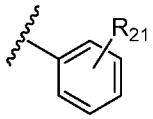
and one of R_{21}, R_{22}, and R_{23} is H.

68. The compound of claim 56, or a pharmaceutically acceptable salt thereof, wherein D_1 is



and two of R_{21}, R_{22}, and R_{23} are H.

69. The compound of claim 68, or a pharmaceutically acceptable salt thereof, wherein D_1 is

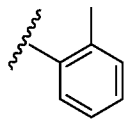


.

70. The compound of claim 69, or a pharmaceutically acceptable salt thereof, wherein R_{21} is optionally substituted C_1-C_6 alkyl.

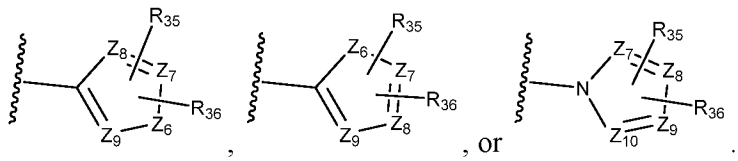
71. The compound of claim 70, or a pharmaceutically acceptable salt thereof, wherein R_{21} is Me.

72. The compound of claim 71, or a pharmaceutically acceptable salt thereof, wherein D_1 is



.

73. The compound of claim 1, or a pharmaceutically acceptable salt thereof, wherein D_1 is



, , or .

Wherein:

Z_6 is O, S, NR_{40}, or CHR_{37};

Z_7, Z_8, Z_9 and Z_{10} are independently N or CR_{41};

R_{35}, R_{36}, R_{37}, R_{40}, and R_{41} are each independently H, OH, NH_2, cycle, aryl, branched or unbranched alkyl alcohol, halo, branched or unbranched alkyl, amide, cyano, alkoxy, haloalkyl, aklylsulfonyl, nitrite, or alkylsulfanyl; or R_{35} and R_{36} together form an aryl or cycle that is attached to one or more of the atoms of D_1.

74. The compound of claim 73, or a pharmaceutically acceptable salt thereof, wherein one of R_{35} and R_{36} is H.

75. The compound of claim 73, or a pharmaceutically acceptable salt thereof, wherein both R_{35} and R_{36} are H.

76. The compound of claim 75, or a pharmaceutically acceptable salt thereof, wherein Z_6 is NH.

77. The compound of claim 76, or a pharmaceutically acceptable salt thereof, wherein one of Z_7, Z_8 and Z_9 is N.

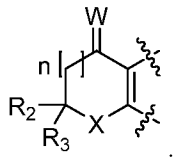
78. The compound of claim 76, or a pharmaceutically acceptable salt thereof, wherein Z_7 is N.

79. The compound of claim 78, or a pharmaceutically acceptable salt thereof, wherein Z_8 is CH.

80. The compound of claim 78, or a pharmaceutically acceptable salt thereof, wherein Z_9 is CH.

81. The compound of claim 78, or a pharmaceutically acceptable salt thereof, wherein both Z_8 and Z_9 are CH.

82. The compound of claim 73, or a pharmaceutically acceptable salt thereof, wherein AA is



83. The compound of claim 82, or a pharmaceutically acceptable salt thereof, wherein W is O.

84. The compound of claim 83, or a pharmaceutically acceptable salt thereof, wherein X is O.

85. The compound of claim 84, or a pharmaceutically acceptable salt thereof, wherein R_2 and R_3 are independently H, optionally substituted C_1-C_6 alkyl, optionally substituted C_1-C_6 hydroxyalkyl, optionally substituted C_1-C_6 alkoxy, optionally substituted cycloalkyl, or optionally substituted cycloheteroalkyl.

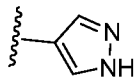
86. The compound of claim 85, or a pharmaceutically acceptable salt thereof, wherein both R_2 and R_3 are the same.

87. The compound of claim 86, or a pharmaceutically acceptable salt thereof, wherein both R_2 and R_3 are Et.

88. The compound of claim 87, or a pharmaceutically acceptable salt thereof, wherein n is 1.

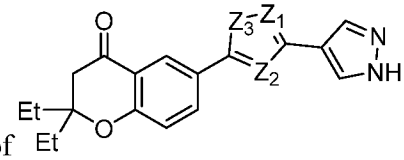
89. The compound of claim 88, or a pharmaceutically acceptable salt thereof, wherein D_1 is pyrazoly.

90. The compound of claim 89, or a pharmaceutically acceptable salt thereof, wherein D_1 is



.

91. The compound of claim 90, or a pharmaceutically acceptable salt thereof, wherein formula I has a structure of



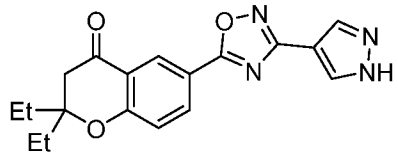
.

92. The compound of claim 91, or a pharmaceutically acceptable salt thereof, wherein Z_2 is N.

93. The compound of claim 91, or a pharmaceutically acceptable salt thereof, wherein Z_1 is N.

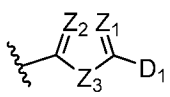
94. The compound of claim 91, or a pharmaceutically acceptable salt thereof, wherein Z_3 is O.

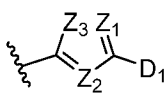
95. The compound of claim 91, or a pharmaceutically acceptable salt thereof, wherein the formula I has a formula of



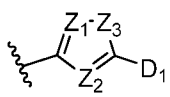
.

96. The compound of claim 1 having Formula II, or a pharmaceutically acceptable salt thereof, wherein D_1 and B_1 is





or

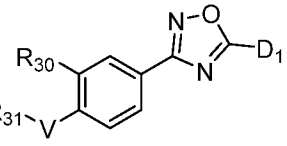
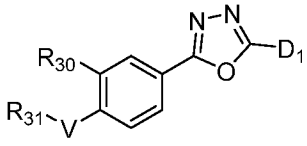
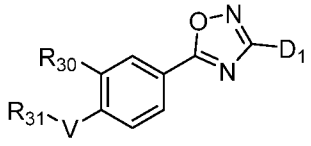


.

97. The compound of claim 96, or a pharmaceutically acceptable salt thereof, wherein Z_3 is O.

98. The compound of claim 96, or a pharmaceutically acceptable salt thereof, wherein Z_1 is N.

99. The compound of claim 96, or a pharmaceutically acceptable salt thereof, wherein Z_2 is N.

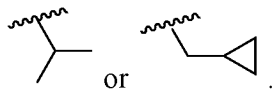
100. The compound of claim 99, or a pharmaceutically acceptable salt thereof, wherein Formula II is  ,  , or  .

101. The compound of claim 100, or a pharmaceutically acceptable salt thereof, wherein R_{30} is CN.

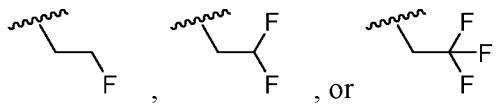
102. The compound of claim 100, or a pharmaceutically acceptable salt thereof, wherein V is NH.

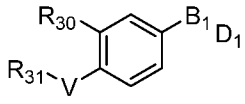
103. The compound of claim 102, or a pharmaceutically acceptable salt thereof, wherein R_{30} is CN.

104. The compound of claim 103, or a pharmaceutically acceptable salt thereof, wherein R_{31} is C-C_5 alkyl.

105. The compound of claim 104, or a pharmaceutically acceptable salt thereof, wherein R_{31} is  .

106. The compound of claim 103, or a pharmaceutically acceptable salt thereof, wherein R_{31} is C-C_5 haloalkyl.

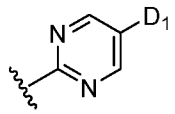
107. The compound of claim 106, or a pharmaceutically acceptable salt thereof, wherein R_{31} is  .

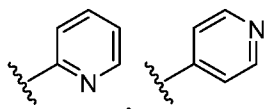
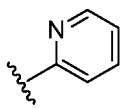
108. The compound of claim 1 having Formula II, or a pharmaceutically acceptable salt thereof, wherein D_1, B_1, and AA together is 

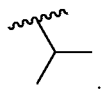
109. The compound of claim 108, or a pharmaceutically acceptable salt thereof, wherein R_{30} is CF_3.

110. The compound of claim 108, or a pharmaceutically acceptable salt thereof, wherein V is O or NH.

111. The compound of claim 110, or a pharmaceutically acceptable salt thereof, wherein R_{30} is CF_3.

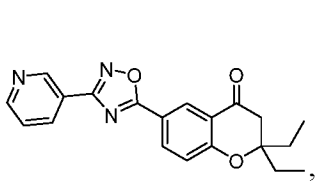
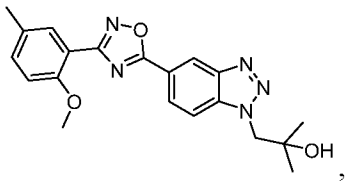
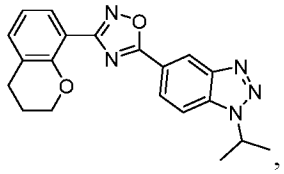
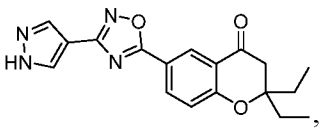
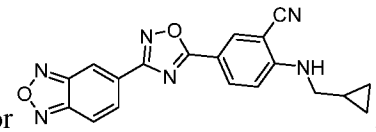
112. The compound of claim 108, or a pharmaceutically acceptable salt thereof, wherein B_1-D_1 is  .

113. The compound of claim 112, or a pharmaceutically acceptable salt thereof, wherein D_1 is  or  .

114. The compound of claim 113, or a pharmaceutically acceptable salt thereof, wherein R_{31} is  .

115. A compound or a pharmaceutically acceptable salt thereof, wherein the compound is a compound as described herein.

116. A compound having the formula of:

 ,
 ,
 ,
 , or
 , or a pharmaceutically acceptable salt thereof.

117. A pharmaceutical composition comprising a compound of any one of claims 1-116, or a pharmaceutically acceptable salt thereof.

118. A method of treating or preventing neuropathy, pain, inflammatory pain, cancer pain, bone cancer pain, tumor pain, pain or neuropathy resulting from disorders of the central or peripheral nervous system, neuropathic pain, pain associated with dysesthesia, allodynia or hypersensitivity, chemotherapy induced neuropathic pain, chemotherapy induced peripheral neuropathy, diabetic neuropathy or pain associated with diabetic neuropathy, post herpetic neuralgia or pain associated with post herpetic neuralgia, hiv-related neuropathy or pain associated with hiv-related neuropathy, pain or neuropathy resulting from spinal cord injury, nerve lesions, tissue injury, ms, stroke, nutritional deficiencies, or toxins, fibromyalgia or pain associated with fibromyalgia, phantom limb pain, complex regional pain syndrome, carpal tunnel syndrome, sciatica, pudendal neuralgia, back or neck pain, including those resulting from degenerative disk disease, trigeminal neuralgia, headache disorders including, but not limited to migraine and cluster headache, orofacial pain, odontalgia, temporomandibular joint pain, endometrial pain, osteoarthritis, rheumatoid arthritis, atypical odontalgia, interstitial cystitis, uveitis, or any combination thereof in a subject comprising administering to the subject a compound of any one of claims 1-116, or a pharmaceutically acceptable salt thereof, or a pharmaceutical composition of claim 117.

119. A method of treating or preventing neuropathy, chemotherapy induced neuropathic pain, chemotherapy induced peripheral neuropathy, diabetic neuropathy or pain associated with diabetic neuropathy in a subject, the method comprising administering to the subject a compound

of any one of claims 1-116, or a pharmaceutically acceptable salt thereof, or a pharmaceutical composition of claim 117.

120. A method of treating cancer in a subject, the method comprising administering to the subject a compound of any one of claims 1-116, or a pharmaceutically acceptable salt thereof, or a pharmaceutical composition of claim 117.

121. The method of claim 120, wherein the cancer is ovarian, breast, lung, brain, colon, prostate, esophageal, pancreatic, brain, glioblastoma, leukemia, multiple myeloma, lymphoma, skin cancer, acute Lymphoblastic Leukemia, acute myeloid leukemia, basal cell cancer, bile duct cancer, bladder cancer, bone cancer (Ewing sarcoma, osteosarcoma), CLL, CML, uterine cancer, cervical cancer, hairy cell leukemia, melanoma, thyroid cancer, rectal cancer, renal cell cancer, small cell lung cancer, non-small cell lung cancer, or stomach cancer.

122. The method of any one of claims 118-121, wherein the subject is a subject in need thereof.

123. The method of any of claim 118-121, wherein the condition is prevented.

124. The method of claim 122, wherein the cancer therapeutic is selected from those described herein.

INTERNATIONAL SEARCH REPORT

International application No.
PCT/US 18/36989

A. CLASSIFICATION OF SUBJECT MATTER
IPC(8) - A61K 31/4245 (2018.01)
CPC - A61K 31/4245, C07D 471/04, C07D 487/04

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)
See Search History Document

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched
See Search History Document

Electronic data base consulted during the international search (name of data base and, where practicable, search terms used)
See Search History Document

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	"Pubchem CID 43591546" Create Date: 21 July 2009 (21.07.2009) Date Accessed: 02 October 2018 (02.10.2018); pg. 3, compound listed	1, 18-22
A	US 2011/0212940 A1 (Burli et al.) 01 September 2011 (01.09.2011); entire document	1, 18-22
A	US 2012/0129828 A1 (Cee et al.) 24 May 2012 (24.05.2012); entire document	1, 18-22

☐ Further documents are listed in the continuation of Box C. ☐ See patent family annex.

* Special categories of cited documents:
"A" document defining the general state of the art which is not considered to be of particular relevance
"E" earlier application or patent but published on or after the international filing date
"L" document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified)
"O" document referring to an oral disclosure, use, exhibition or other means
"P" document published prior to the international filing date but later than the priority date claimed
"T" later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention
"X" document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone
"Y" document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art
"&" document member of the same patent family

Date of the actual completion of the international search	Date of mailing of the international search report
02 October 2018	25 OCT 2018

Name and mailing address of the ISA/US	Authorized officer:
Mail Stop PCT, Attn: ISA/US, Commissioner for Patents P.O. Box 1450, Alexandria, Virginia 22313-1450 Facsimile No. 571-273-8300	Lee W. Young PCT Helpdesk: 571-272-4300 PCT OSP: 571-272-7774

INTERNATIONAL SEARCH REPORT

International application No.
PCT/US 18/36989

Box No. II Observations where certain claims were found unsearchable (Continuation of item 2 of first sheet)

This international search report has not been established in respect of certain claims under Article 17(2)(a) for the following reasons:

1. ☐ Claims Nos.:
because they relate to subject matter not required to be searched by this Authority, namely:

2. ☒ Claims Nos.: 115
because they relate to parts of the international application that do not comply with the prescribed requirements to such an extent that no meaningful international search can be carried out, specifically:
claim 115 is an omnibus claim

3. ☒ Claims Nos.: 117-124
because they are dependent claims and are not drafted in accordance with the second and third sentences of Rule 6.4(a).

Box No. III Observations where unity of invention is lacking (Continuation of item 3 of first sheet)

This International Searching Authority found multiple inventions in this international application, as follows:
--continued on supplemental page--

1. ☐ As all required additional search fees were timely paid by the applicant, this international search report covers all searchable claims.

2. ☐ As all searchable claims could be searched without effort justifying additional fees, this Authority did not invite payment of additional fees.

3. ☐ As only some of the required additional search fees were timely paid by the applicant, this international search report covers only those claims for which fees were paid, specifically claims Nos.:

4. ☒ No required additional search fees were timely paid by the applicant. Consequently, this international search report is restricted to the invention first mentioned in the claims; it is covered by claims Nos.:
1 and 18-22

Remark on Protest

☐ The additional search fees were accompanied by the applicant's protest and, where applicable, the payment of a protest fee.

☐ The additional search fees were accompanied by the applicant's protest but the applicable protest fee was not paid within the time limit specified in the invitation.

☐ No protest accompanied the payment of additional search fees.

INTERNATIONAL SEARCH REPORT

International application No.

PCT/US 18/36989

--continued from Box No. III--

This application contains the following inventions or groups of inventions which are not so linked as to form a single general inventive concept under PCT Rule 13.1.

Group I+: Claims 1-114 and 116, directed to a compound of claim 1, a compound of formula I. The compound of claim 1 will be searched to the extent that it encompasses the first species of claim 1, represented by a compound of Formula I wherein AA is the first structure listed; W is O; X is O; n is 0; B1 is aryl; B2, B3, and B4 are CR38; D1 is H; R2 and R3 are H and R38 is H. It is believed that claims 1 and 18-22 reads on this first named invention, and thus these claims will be searched without fee. Applicant is invited to elect additional compounds of claim 1, wherein each additional compound elected will require one additional invention fee. Applicants must specify the claims that encompass any additionally elected compound. Applicants must further indicate, if applicable, the claims which encompass the first named invention, if different than what was indicated above for this group. Failure to clearly identify how any paid additional invention fees are to be applied to the '+' group(s) will result in only the first claimed invention to be searched. Additionally, an exemplary election wherein different actual variables are selected is suggested. An exemplary election would be a compound of Formula I wherein AA is the first structure listed; W is O; X is O; n is 0; B1 is aryl; B2, B3, and B4 are CR38; D1 is H; R2 and R3 are C2 alkyl and R38 is H (i.e., claims 1 and 18-23).

The group of inventions listed above do not relate to a single general inventive concept under PCT Rule 13.1 because, under PCT Rule 13.2, they lack the same or corresponding special technical features for the following reasons:

Special Technical Features:

Group I+ includes the technical feature of a unique compound of claim 1, formula I, which is not required by any other invention of Group I+.

Common technical features:

The inventions of Groups I+ share the technical feature of a compound of claim 1, formula I.

These shared technical features, however, do not provide a contribution over the prior art, as being anticipated by a document entitled "Pubchem CID 43591546" (hereinafter Pubchem-546). Pubchem-546 discloses a compound of formula I wherein AA is the first structure listed; W is O; X is O; n is 0; B1 is aryl; B2, B3, and B4 are CR38; D1 is H; R2 and R3 are H and R38 is H (pg. 3, compound listed).

As said compound was known in the art at the time of the invention, these cannot be considered special technical features that would otherwise unify the inventions of Groups I+. The inventions of Group I+ thus lack unity under PCT Rule 13.

Note:

Claim 115 is an omnibus claim and noted as unsearchable

claims 117-124 have been found to be unsearchable because they are not drafted in accordance with the second and third sentences of Rule 6.4(a).