

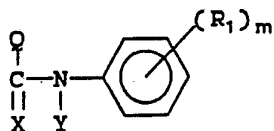


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(54) Title: SUBSTITUTED INDAZOLE ARTHROPODICIDES



(I)

(57) Abstract

Indazole arthropodicides, compositions containing them and a method for controlling arthropods employing these indazoles as the active ingredient. The indazoles have the general formula (I), wherein Q, X, Y, R₁ and m are as defined in the text.

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TitleSUBSTITUTED INDAZOLE ARTHROPODICIDES

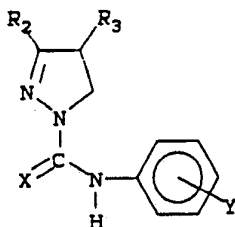
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Background of the Invention

U.S. 4,070,365 discloses insecticidal compounds
of the formula

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20 wherein

R₂ and R₃ are independently alkyl, cycloalkyl, pyridyl or thienyl optionally substituted with halogen, alkyl or nitro, or a phenyl group optionally substituted with 1 or 2 substituents selected from halogen, alkyl, haloalkyl, cycloalkyl alkylthio, alkoxy, mono or dialkylamino, nitro, phenyl optionally substituted with halogen, or cyano;

Y is halogen, NO₂, alkyl, haloalkyl, cycloalkyl, alkylthio, alkoxy, dialkylamino, alkylsulfonyl, acyl, acylamino, cyano, or a phenyl optionally substituted with halogen; and

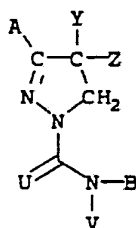
X is O or S.

35

U.S. 4,663,341 discloses insecticidal compounds
of the formula

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wherein

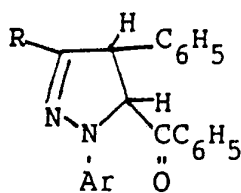
- A is unsubstituted or substituted phenyl;
- B is unsubstituted or substituted phenyl;
- U is O, S or NR;
- 20 Y is alkyl, carbonyl or phenyl each of which
may be optionally substituted; and
- Z is an organic radical other than hydrogen.

Vaughan, J. Org. Chem., 20 (1955), pages 1619
25 to 1626, discloses 1,5-diphenyl-2-pyrazoline-3-
carboxamide. No utility is given for the disclosed
compound which, in any event, does not suggest a
compound of the instant invention.

30 Harhash et al., J. Heterocyclic Chem., 21
(1984), at page 1013, discloses the preparation of
five pyrazoline compounds, none of which is disclosed
in the instant application. No utility is given for
any of said compounds:

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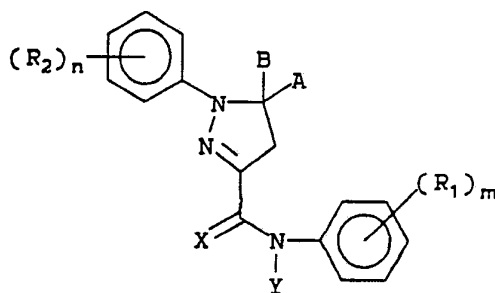
where R/Ar are

C_6H_5/C_6H_5 ;
 $CO_2C_2H_5/C_6H_5$;
 $C(O)NHC_6H_5/C_6H_5$;
 $CH=CHC_6H_5/C_6H_5$; and
 $CH_3/4-NO_2-C_6H_4$.

10

WO 88/900910 discloses insecticidal pyrazolines
such as compounds of the formula;

15

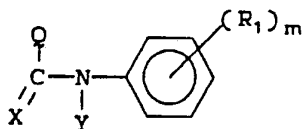


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WO 88/302995 discloses insecticidal pyrazolines
such as compounds of the formula;

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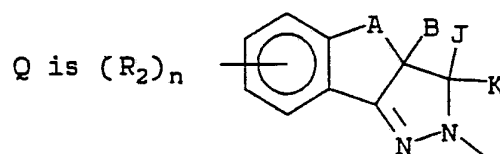
35

I

wherein,

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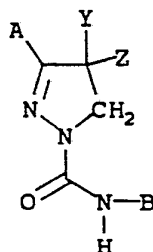
A is 1, 2 or 3-atom bridge having 0 to 3 carbon atoms and 0 to 1 oxygen atom, NR_6 group, or $S(O)_q$ group, wherein each carbon individually can be substituted with 1 to 2 substituents selected from 1 to 2 halogen, C_1 to C_6 alkyl, C_2 to C_4 alkoxy carbonyl or phenyl optionally substituted with 1 to 3 substituents selected from W and one of the carbon atoms can be C(O) or C(S).

25

EP-A-153,127 discloses insecticidal compounds of the formula

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5 wherein

A is unsubstituted or substituted phenyl;

B is unsubstituted or substituted phenyl;

U is O, S or NR;

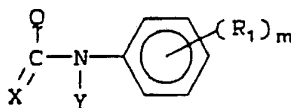
Y is alkyl, carbonyl or a phenyl group; and

10 Z is cycloalkyl, or a phenyl group.

This application is a cognate of applications bearing U.S. Serial Numbers 07/249,883 and 07/247,690.

15 Summary of the Invention

This invention pertains to the following compounds including all of their geometric and stereoisomers, agriculturally suitable salts thereof, agricultural compositions containing them and their
20 use as arthropodicides:



I

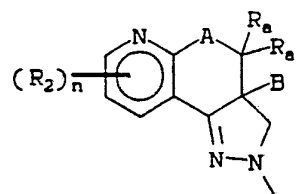
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wherein:

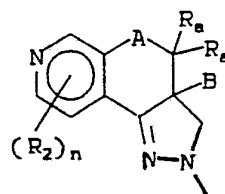
Q is

35

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;



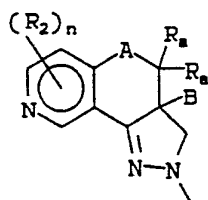
;

Q-1

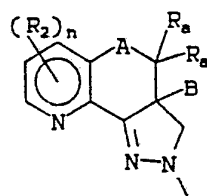
Q-2

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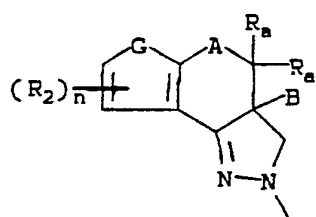
;

Q-3

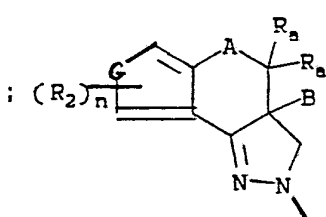
Q-4

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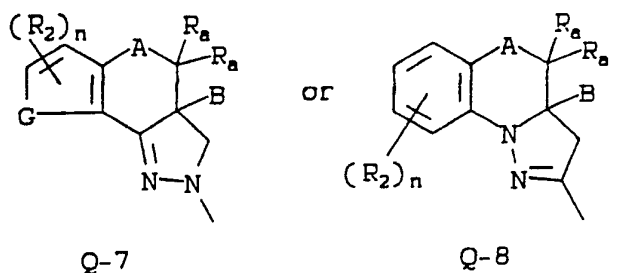
Q-5

Q-6

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15

G is O or S;

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A is a 0, 1 or 2-atom bridge comprising 0 to 2 carbon atoms, 0 to 1 oxygen atoms, 0 to 1 S(O)_q groups or 0 to 1 NR₆ groups wherein each carbon atom is optionally substituted with 1 to 2 substituents selected from R_a;

25

B is H, C₁ to C₆ alkyl, C₃ to C₆ cycloalkyl optionally substituted with 1 to 2 halogens or 1 to 2 CH₃, C₄ to C₆ cycloalkylalkyl, C₁ to C₆ haloalkyl, C₂ to C₆ alkenyl, C₂ to C₆ alkynyl, C₂ to C₆ alkoxyalkyl, C₂ to C₆ cyanoalkyl, C₃ to C₈ alkoxycarbonylalkyl, CO₂R₃, C(O)R₃, C(O)NR₃R₄, C(S)NR₃R₄, C(S)R₃, C(S)SR₃, phenyl, phenyl substituted with (R₅)_p, benzyl, benzyl substituted with 1 to 3 substituents independently selected from W, or OR₇ when Q is Q₁ to Q₇;

30

35

W is halogen, CN, NO₂, C₁ to C₂ alkyl, C₁ to C₂ haloalkyl, C₁ to C₂ alkoxy, C₁ to C₂ haloalkoxy, C₁ to C₂ alkylthio, C₁ to C₂ haloalkylthio, C₁ to C₂ alkylsulfonyl or C₁ to C₂ haloalkylsulfonyl;

- 5 R_1 , R_2 and R_5 are independently selected from
 R_3 , halogen, CN, N_3 , SCN, NO_2 , OR_3 , SR_3 ,
 SOR_3 , SO_2R_3 , $OC(O)R_3$, OSO_2R_3 , CO_2R_3 , $C(O)R_3$,
 $C(O)NR_3R_4$, $SO_2NR_3R_4$, NR_3R_4 , $NR_4C(O)R_3$,
 $OC(O)NHR_3$, $NR_4C(O)NHR_3$ and $NR_4SO_2R_3$, or when
10 m , n or p is 2, R_1 , R_2 or R_5 can be $-OCH_2O-$,
 $-OCH_2CH_2O-$, or $-CH_2CH_2O-$, each of which can
be substituted with 1 to 4 halogen atoms or 1
to 2 methyl groups;
- 15 R_3 is H, C_1 to C_6 alkyl, C_1 to C_6 haloalkyl, C_2
to C_6 alkenyl, C_2 to C_6 haloalkenyl, C_2 to C_6
alkynyl, C_2 to C_6 haloalkynyl, C_2 to C_6
alkoxyalkyl, C_2 to C_6 alkylthioalkyl, C_1 to
 C_6 nitroalkyl, C_2 to C_6 cyanoalkyl, C_3 to C_8
alkoxycarbonylalkyl, C_3 to C_6 cycloalkyl,
20 C_3 to C_6 halocycloalkyl, phenyl, benzyl, or
phenyl or benzyl substituted with 1 to 3
substituents independently selected from W;
- R_4 is H, C_1 to C_4 alkyl or R_3 and R_4 can be
taken together as $(CH_2)_4$, $(CH_2)_5$ or
 $(CH_2CH_2OCH_2CH_2)$;
- 25 R_6 is H, C_1 to C_4 alkyl, C_1 to C_4 haloalkyl, C_2
to C_4 alkenyl, C_2 to C_4 haloalkenyl, C_2 to C_4
alkynyl, phenyl optionally substituted with
W, or benzyl optionally substituted with W;
- 30 R_7 is H, C_1 to C_4 alkyl, C_2 to C_4 alkenyl, C_2
to C_4 alkynyl, C_2 to C_4 alkylcarbonyl, C_2 to
 C_4 alkoxycarbonyl;

R_a is independently selected from H, C_1 to C_6 alkyl, C_2 to C_4 alkoxy carbonyl and phenyl optionally substituted with 1 to 3 substituents independently selected from W;

X is O or S;

n is 1 to 2;

m is 1 to 3;

10 p is 1 to 3;

q is 0 to 2;

Y is H, C_1 to C_6 alkyl, C_2 to C_6 alkoxyalkyl, CHO, C_2 to C_6 alkylcarbonyl, C_2 to C_6 alkoxy carbonyl, C_2 to C_6 haloalkylcarbonyl, C_1 to C_6 alkylthio, C_1 to C_6 haloalkylthio, phenylthio, phenylthio substituted with 1 to 3 substituents independently selected from W, or S-J;

20 J is $NR_8\overset{\overset{O}{\parallel}}{C}R_9$, $NR_8S(O)_tR_9$, $NR_8\overset{\overset{Y_1Y_1R_{10}}{\parallel}}{P}Y_1R_{11}$, $NR_8\overset{\overset{Y_1Y_1R_{11}}{\parallel}}{P}R_{10}$

$\underline{J}_1$ $\underline{J}_2$ $\underline{J}_3$ $\underline{J}_4$

25 $\overset{\overset{O}{\parallel}}{C}R_9$ $\overset{\overset{O}{\parallel}}{P}\begin{matrix} OR_{10} \\ OR_{11} \end{matrix}$ NR_8R_{12} or SR_{10}

$\underline{J}_5$ $\underline{J}_6$ $\underline{J}_7$ $\underline{J}_8$

R_8 and R_{12} are independently selected from C_1 to C_6 alkyl, C_1 to C_6 haloalkyl, C_3 to C_6 cycloalkyl, C_4 to C_7 cycloalkylalkyl, phenyl optionally substituted with 1 to 2 substituents independently selected from W, benzyl optionally substituted with 1 to 2 substituents independently selected from W, phenethyl optionally substituted with 1 to 2 substituents independently selected from W, C_2 to C_6 cyanoalkyl, C_2 to C_6 alkoxyalkyl, C_3

to C₈ alkoxy-carbonylalkyl and C₄ to C₈ di-
alkylaminocarbonylalkyl, or R₈ and R₁₂ can be
taken together as (CH₂)₄, (CH₂)₅ or
(CH₂)₂O(CH₂)₂;
R₉ is F, C₁ to C₂₂ alkyl, C₁ to C₆ haloalkyl,
C₁ to C₂₂ alkoxy, C₂ to C₈ dialkylamino,
piperidinyl, pyrrolidinyl, morpholino, C₁ to
C₄ haloalkoxy, C₁ to C₄ alkoxy substituted
with cyano, nitro, C₂ to C₄ alkoxy, C₄ to C₈
alkoxyalkoxy, C₁ to C₂ alkylthio, C₂ to C₃
alkoxy-carbonyl, C₃ to C₅ dialkylaminocarbonyl
or phenyl, or R₉ is phenyl optionally substi-
tuted with 1 to 2 substituents independently
selected from W, or phenoxy optionally
substituted with 1 to 2 substituents
independently selected from W;
R₁₀ and R₁₁ are independently selected from C₁
to C₄ alkyl, C₂ to C₄ haloalkyl and phenyl
optionally substituted with 1 to 2 substi-
tuents independently selected from W, or R₁₀
and R₁₁ can be taken together as (CH₂)₂,
(CH₂)₃ or CH₂C(CH₃)₂CH₂;
t is 0 to 2; and
Y₁ is O or S.

In the above definitions, the term "alkyl", used
either alone or in compound words such as "alkylthio"
or "haloalkyl", denotes straight chain or branched
alkyl such as methyl, ethyl, n-propyl, isopropyl or
the different butyl, pentyl, hexyl isomers.

Alkoxy denotes methoxy, ethoxy, n-propyloxy, iso-
propyloxy and the different butoxy or pentoxy isomers.

Alkenyl denotes straight chain or branched
alkenes such as vinyl, 1-propenyl, 2-propenyl,
3-propenyl and the different butenyl, pentenyl and
hexenyl isomers.

Alkynyl denotes straight chain or branched
5 alkynes such as ethynyl, 1-propynyl, 2-propynyl and
the different butynyl, pentynyl and hexynyl isomers.

Alkylthio denotes methylthio, ethylthio and the
different propylthio and butylthio isomers.

Alkylsulfinyl, alkylsulfonyl, alkylamino, and
10 the like, are defined analogously to the above
examples.

Cycloalkyl denotes cyclopropyl, cyclobutyl,
cyclopentyl and cyclohexyl.

The term "halogen", either alone or in compound
15 words such as "haloalkyl", denotes fluorine, chlorine,
bromine or iodine. When used in compound words such
as "haloalkyl" said alkyl may be partially or fully
substituted with halogen atoms, which may be the same
or different. Examples of haloalkyl include $\text{CH}_2\text{CH}_2\text{F}$,
20 CF_2CF_3 and CH_2CHFCl . The terms "halocycloalkyl",
"haloalkenyl" and "haloalkynyl" are defined
analogously to the term "haloalkyl".

The total number of carbon atoms in a substituent group is indicated by the " C_i to C_j " prefix
25 where i and j are integers. For example, C_1 to C_3
alkylsulfonyl would designate methylsulfonyl through
propylsulfonyl; C_2 alkoxyalkoxy would designate
 OCH_2OCH_3 ; C_4 alkoxyalkoxy would designate the various
isomers of an alkoxy group substituted with
30 a second alkoxy group containing a total of 4 carbon
atoms, examples including $\text{OCH}_2\text{OCH}_2\text{CH}_2\text{CH}_3$ and
 $\text{OCH}_2\text{CH}_2\text{OCH}_2\text{CH}_3$; C_2 cyanoalkyl would designate CH_2CN
and C_3 cyanoalkyl would designate $\text{CH}_2\text{CH}_2\text{CN}$ and
 $\text{CH}(\text{CN})\text{CH}_3$; C_2 alkylcarbonyl would designate $\text{C}(\text{O})\text{CH}_3$
35 and C_4 alkylcarbonyl would include $\text{C}(\text{O})\text{CH}_2\text{CH}_2\text{CH}_3$
and $\text{C}(\text{O})\text{CH}(\text{CH}_3)_2$; and as a final example, C_3 alkoxy-
carbonylalkyl would designate $\text{CH}_2\text{CO}_2\text{CH}_3$ and C_4 alkoxy-
carbonylalkyl would include $\text{CH}_2\text{CH}_2\text{CO}_2\text{CH}_3$, $\text{CH}_2\text{CO}_2\text{CH}_2\text{CH}_3$
and $\text{CH}(\text{CH}_3)\text{CO}_2\text{CH}_3$.

Preferred Compounds A are those of Formula I
wherein:

- 5
A is CR_aR_a , S, O or NR_6 ;
B is H, C_1 to C_6 alkyl, C_1 to C_6 haloalkyl,
 C_2 to C_6 alkenyl, C_2 to C_6 alkynyl, C_2 to
 C_6 alkoxyalkyl, C_3 to C_8 alkoxycarbonylalkyl,
10 CO_2R_3 , $C(O)R_3$, $C(O)NR_3R_4$, $C(S)NR_3R_4$, $C(S)R_3$,
 $C(S)SR_3$, phenyl or phenyl substituted by
(R_5)_p;
W is Cl, F, Br, CN, CF_3 , C_1 to C_2 alkyl, C_1
to C_2 alkoxy, OCF_2H , OCF_3 or NO_2 ;
15 R_2 is R_3 , halogen, CN, SCN, NO_2 , OR_3 or SR_3 ;
 R_3 is H, C_1 to C_4 alkyl, C_1 to C_2 haloalkyl,
 C_3 to C_4 alkenyl, C_3 to C_4 haloalkenyl,
propargyl, phenyl, benzyl, or phenyl or
benzyl substituted with one of F, Cl, Br,
20 CF_3 , OCF_3 , OCF_2H or NO_2 ;
p is 1 or 2;
m is 1 or 2;
X is O;
Y is H, C_1 to C_4 alkyl, SCH_3 , $SCCl_3$, SO_2CH_3 ,
25 SC_6H_5 , 2- NO_2 - C_6H_4S , $C(O)CH_3$, $C(O)CH_2CH_3$,
 $C(O)CF_3$; CO_2CH_3 , $CO_2CH_2CH_3$, or S-J;
J is J_1 , J_2 , J_3 , J_4 or J_5 ;
 R_8 and R_{12} are independently selected from C_1
to C_6 alkyl, C_1 to C_6 haloalkyl, C_5 to C_6
30 cycloalkyl, C_3 to C_8 alkoxycarbonylalkyl,
phenyl, benzyl and phenethyl, each phenyl,
benzyl and phenethyl optionally substituted
with W, or, R_8 and R_{12} can be taken together
as $(CH_2)_4$, $(CH_2)_5$ or $(CH_2)_2O(CH_2)_2$;
35 R_{10} and R_{11} are independently selected from C_1
to C_3 alkyl or phenyl; and
t is 2.

5 Preferred Compounds B are Compounds A wherein:

B is H, C₁ to C₄ alkyl, C₃ to C₄ alkoxy carbonyl-alkyl, CO₂R₃, C(O)R₃, phenyl or phenyl substituted with (R₅)_p;

10 R₁ is halogen, CN, SCN, NO₂, OR₃, SR₃, SO₂R₃, CO₂R₃, C(O)R₃ or is R₃ with one substituent in the 4-position;

R₅ is H, R₃, halogen, CN, SCN, NO₂, OR₃, SR₃, SO₂R₃, C(O)R₃, OSO₂R₃, CO₂R₃, C(O)R₃,
15 C(O)NR₃R₄, SO₂NR₃R₄ or NR₃R₄; or, when m or p is 2;

R₁ and R₅ can be -CH₂C(CH₃)₂O-,
OCH₂CH₂O-, OCF₂CF₂O- or -CF₂CF₂O-;

20 R₃ is C₁ to C₄ alkyl, C₁ to C₂ haloalkyl, C₃ to C₄ alkenyl or propargyl;

R₄ is H or CH₃;

R_a is H, CH₃, CO₂CH₃ or CO₂CH₂CH₃;

m and p are independently 1 or 2 and one substituent is in the para-position;

25 Y is H, CH₃, COCH₃, CO₂CH₃ or S-J;

J is J₁ or J₂;

R₈ is C₁ to C₄ alkyl or phenyl optionally substituted with Cl or CH₃;

30 R₉ is C₁ to C₂₀ alkyl, C₁ to C₂₀ alkoxy, C₁ to C₆ haloalkyl, dimethylamino, phenyl optionally substituted with Cl or CH₃, or, R₉ is C₁ to C₄ alkoxy substituted with C₂ to C₄ alkoxy or 1 to 6 halogens; and

35 G is S.

Preferred Compounds C are Compounds B wherein:

R₁ is Cl, F, Br, CF₃, CN, OCF₃, OCF₂H, OCF₂CF₂H or SCF₂H;

R_2 and R_5 are independently H, Cl, F, Br, CN,
CF₃, CH₃, OCH(CH₃)₂, OCF₂H, OCF₃, SCH₃,
SCF₂H, NO₂ or OCH₂CF₃;

B is H, CH₃, CH₂CH₃, CH(CH₃)₂, CO₂CH₃, CO₂CH₂CH₃,
phenyl or phenyl substituted with (R₅)_p; and

R_a is H or CH₃.

Preferred Compounds D are Compounds C wherein:
A is O or CH₂;

Preferred Compounds E are Compounds D wherein:
Q is Q-1;

Preferred Compounds F are Compounds D wherein:
Q is Q-2;

Preferred Compounds G are Compounds D wherein:
Q is Q-3;

Preferred Compounds H are Compounds D wherein:
Q is Q-4;

Preferred Compounds I are Compounds D wherein:
Q is Q-5;

Preferred Compounds J are Compounds D wherein:
Q is Q-6;

Preferred Compounds K are Compounds D wherein:
Q is Q-7;

Preferred Compounds L are Compounds D wherein:
Q is Q-8;

Specifically preferred compounds are:

- 5 M) methyl 3,3a,4,5-tetrahydro-2-[[[4-trifluoro-
methyl)phenyl]-amino]carbonyl]-2H-pyrazolo[3,-
4-f]-quinoline-3a-carboxylate, a compound of
Preferred E;
- 10 N) methyl 3,3a,4,5-tetrahydro-2-[[[4-trifluoro-
methyl)phenyl]-amino]carbonyl]-2H-pyrazolo[4,-
3-h]-quinoline-3a-carboxylate, a compound of
Preferred H;
- 15 O) methyl 7-chloro-3,3a,4,5-tetrahydro-N-[[[4-
trifluoromethyl)phenyl]amino]carbonyl]-2H-
thieno [2,3-g]-indazole-3a-carboxylate, a
compound of Preferred I;
- 20 P) methyl 7-fluoro-3A,4-dihydro-2-[[[4-(tri-
fluoromethyl)-phenyl]amino]carbonyl]-3H-
pyrazolo[5,1-c]-[1,4]benzoxazine-3a-carboxyl-
ate, a compound of Preferred L; and
- 25 Q) 7-chloro-3A-(4-fluorophenyl)-3A,4-dihydro-N-
[4-(trifluoromethyl)phenyl]-3H-pyrazolo[5,1-
c][1,4]-benzoxazine-2-carboxamide, a compound
of Preferred L.

30 Hereafter, in the specification and claims, the
various geometric isomers, stereoisomers and
agriculturally suitable salts of each and every
compound of the invention depending on context, is/are
included in the term "compound(s)."

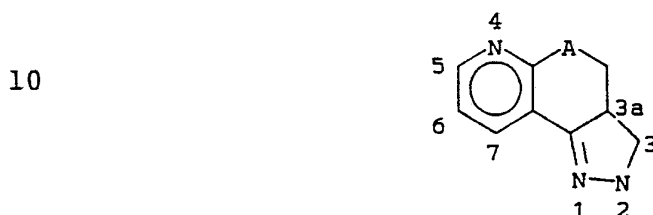
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Details of the Invention

For descriptive purposes, Q-1, where R_a is H,
will be used as a representative value of Q, when Q is

Q-1 through Q-7, in the discussssion that follows and will be referred to by the following numbering system:

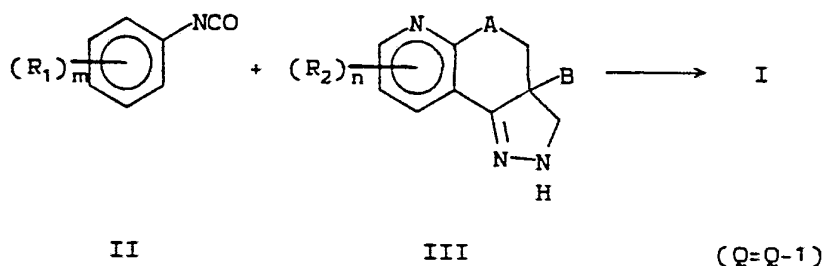
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15

Compounds of Formula I can be prepared by the reaction of aryl isocyanates of Formula II and substituted indazoles of Formula III as shown in Scheme I. Typical reactions involve the combination of equimolar amounts of II and III in conventional organic solvents including ether, tetrahydrofuran (THF), methylene chloride, chloroform and benzene. The reaction can be run at temperatures ranging from about -20°C to 100°C with temperatures in the range of about -10° to 30°C generally preferred.

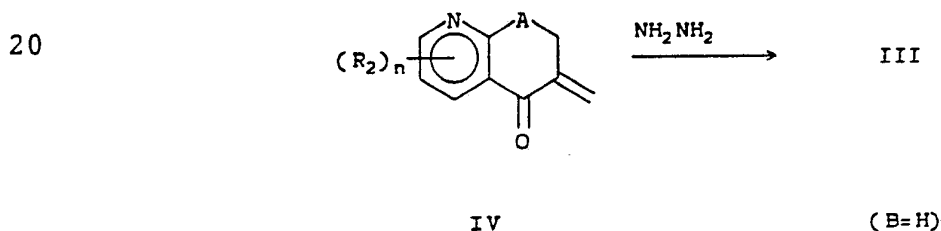
SCHEME 1



35

Substituted indazoles of Formula III, where B is equal to H, can be prepared by the reaction of hydrazine with an α , β -unsaturated ketone of Formula IV (or their precursors) by procedures well documented in the chemical literature (Scheme 2). For a review of pyrazoline synthesis, see El-Rayyes and Al-Awadi, Synthesis, 1028 (1985). For literature describing the synthesis of 3,4- and 3,5-disubstituted pyrazolines, which can be applied to the synthesis of compounds of Formula III, where B is H, see U.S. Patent 3,991,073 and U.S. Patent 4,070,365.

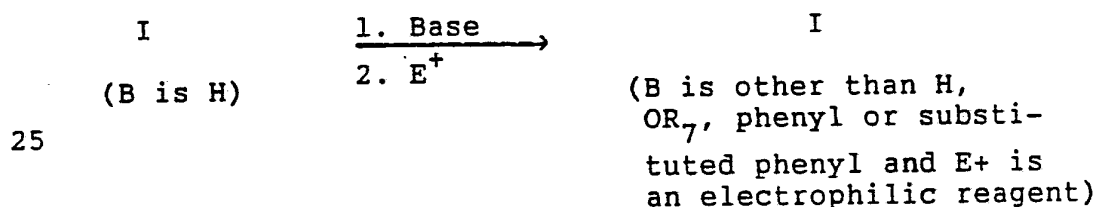
SCHEME 2



Preparation of compounds of Formula I, where B is other than H, OR₇, phenyl or substituted phenyl can be achieved by metallation of the 3a position of Formula I (where B is H) followed by reaction with a suitable electrophile as depicted in Scheme 3. Procedures for the related transformation of 4-substituted pyrazolines to 4,4-disubstituted pyrazolines are reported in U.S. Patent 4,663,341 and can be applied to substituted indazoles of Formula I. Metallation can be accomplished by deprotonation with a strong base, in a suitable solvent and at tempera-

tures ranging from -78°C to 100°C. Useful bases for this reaction include lithium dialkylamides such as lithium diisopropylamide and lithium tetramethylpiper-
5 idide and alkyl lithium reagents such as n-butyllithium and s-butyllithium. Deprotonation of compounds of Formula I, where B is equal to hydrogen, will require two equivalents of base when Y is equal to
10 hydrogen. The reaction can be conducted in many conventional organic solvents and in certain instances a cosolvent may be useful. Suitable solvents include diethylether, tetrahydrofuran, tetrahydropyran, benzene and the like. Suitable
15 electrophilic reagents for reaction with the metallated Formula I compounds include alkyl and substituted alkyl halides, alkyl chloroformates, acyl halides, isocyanates, dialkyl carbamoylhalides and related electrophiles which will be known to those
20 skilled in the art.

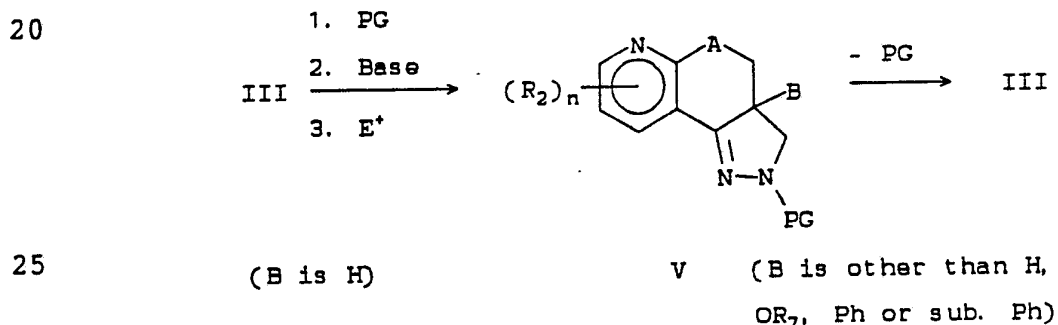
SCHEME 3



An alternative procedure for introduction of the 3a substituent, which in certain instances is preferred over that of Scheme 3 due to higher yields and/or greater ease of synthesis, proceeds via the intermediacy of Compound V, wherein the 2-nitrogen has been derivatized with a suitable protecting
30 group. Deprotonation with a strong base such as lithium diisopropylamide, typically in stoichiometric quantities, followed by reaction with any of the
35

previously described electrophiles provides compounds of Formula V where B is other than hydrogen, OR₇, phenyl or substituted phenyl. Removal of the nitrogen protecting group provides the required Formula III intermediate. Nitrogen-protecting groups are well documented in the chemical literature, as are procedures for their preparation and cleavage. Examples include acetyl, trifluoroacetyl, benzoyl, substituted benzoyl, alkoxycarbonyl, benzyl and substituted benzyl. For a review see Greene "Protective Groups in Organic Synthesis" (New York: John Wiley and Sons, 1981) pp. 218 to 287.

SCHEME 4



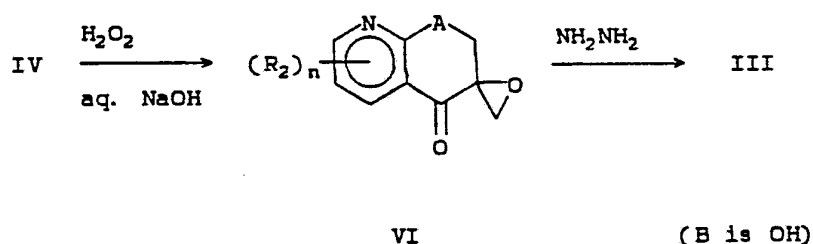
Note: E⁺ is an electrophile and PG is representative of a suitable nitrogen-protecting group.

Formula III compounds where B is equal to hydroxy are prepared by the reaction of hydrazine with a suitably substituted epoxide of Formula VI

(Scheme 5). The epoxides are available from the enones of Formula IV by procedures known in the art, the most widely employed method being epoxidation via the use of alkaline hydrogen peroxide (see, e.g., Wasson and House, Org. Syn., Coll. Vol. 4, 552 (1963)).

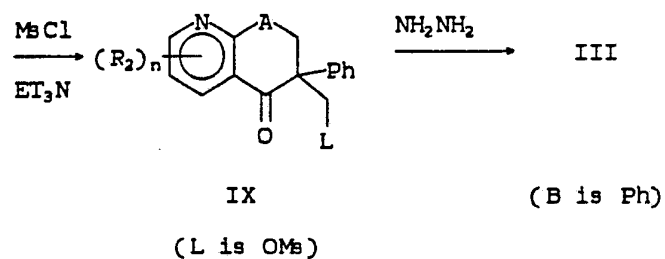
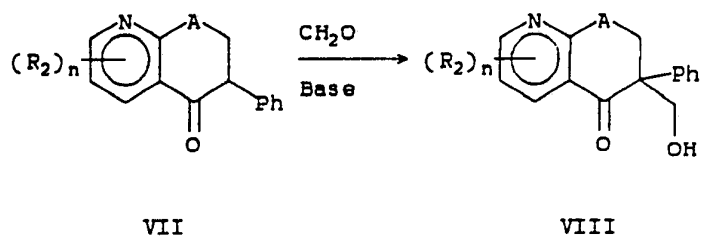
Compounds of Formula I where B is equal to OR₇ and R₇ is other than hydrogen, can be prepared from the Formula I compounds where B is equal to hydroxy via reaction with electrophilic reagents such as alkyl halides, acyl halides, alkyl chloroformates, chlorosulfonates, isocyanates and dialkyl carbamoyl-halides. Those skilled in the art will recognize that conditions necessary for this transformation including solvent, catalyst, temperature, etc., will vary with the specific electrophile chosen and the specific Formula I compound used.

SCHEME 5

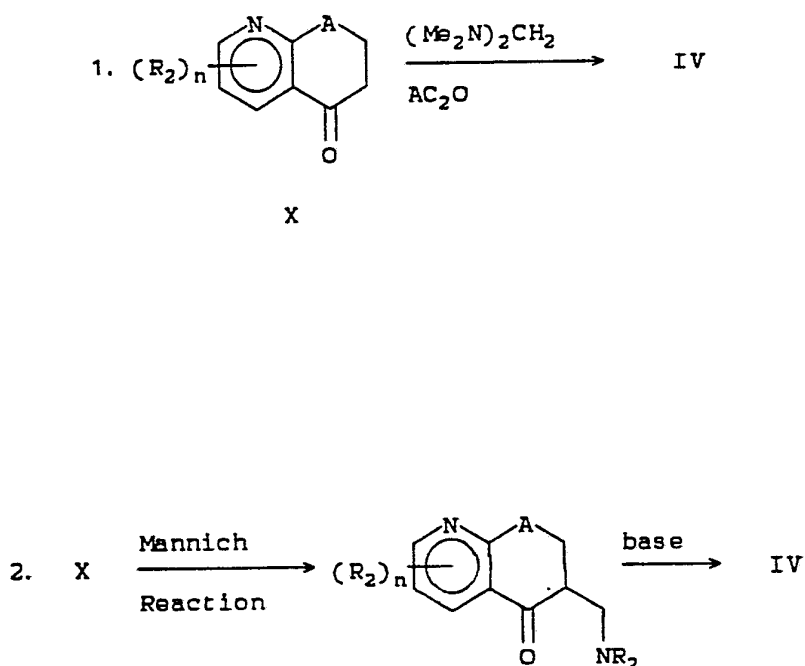


Compounds of Formula III where B is phenyl or substituted phenyl can be prepared by reaction of a ketone of Formula IX, where L is a suitable leaving group such as chloride, bromide, tosylate or mesylate, with hydrazine. The Formula IX compounds

are in turn prepared from the compounds of Formula VII in a two-step process involving first an aldol reaction of formaldehyde to produce the aldol product of Formula VIII followed by conversion of the hydroxyl group to a leaving group L. As an example, treatment of the Formula VIII compound with methanesulfonylchloride in the presence of an amine base produces the Formula IX compound where L is mesylate.

SCHEME 6

The α -methylene ketones of Formula IV can be prepared from the ketones of Formula X by a variety of procedures well documented in the literature. For example, treatment of X with tetramethyldiaminomethane and acetic anhydride produces the Formula IV compound directly. Another useful procedure is to treat the Formula X compound with formaldehyde under conditions of a Mannich reaction. The dialkylamino group can be eliminated *in situ* upon treatment with base to form the intermediate of Formula IV.

SCHEME 7

Those skilled in the art will recognize the intermediates of Formula X as substituted quinolones. Isoquinolones and the isomeric benzothiophenones used for preparation of compounds of Formula I, where Q is Q-2 through Q-7, are also known in the chemical literature as are procedures for their preparation. A few selected references include: where Q is Q-1 see J. Chem. Soc., Perkin I, 975 (1976), where Q is Q-2 see J. Amer. Chem. Soc., 107, 4998 (1985), where Q is Q-3 see J. Org. Chem. 43, 966 (1978), where Q is Q-4 see J. Het. Chem. 15, 249 (1978), when Q is Q-5 or Q-7 see Tetrahedron Letters, 2885 (1975) or J. Heterocyclic Chem., 17, 87 (1980), and where Q is Q-6 see Bull. Soc. Chim. Fr., 335 (1973).

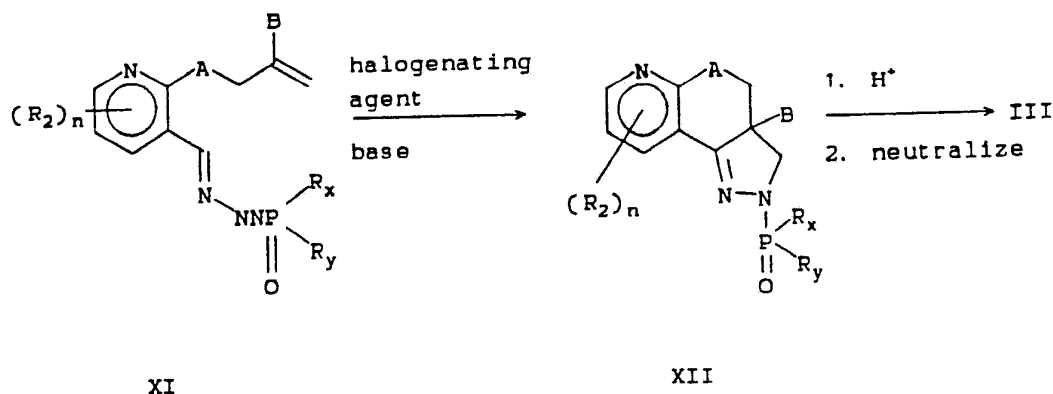
An alternative method for preparing compounds of Formula I, where Q is Q-1 through Q-7, involves intramolecular cyclization of hydrazone XI to produce the N-phosphorylated dihydropyrazole XII. The phosphorus group can then be removed under acidic conditions and neutralized with base to yield the substituted indazoles of Formula III.

SCHEME 8

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5 wherein:

R_x and R_y are independently selected from C_1 to C_4 alkyl and C_1 to C_4 alkoxy.

The intramolecular cyclization can be conducted
10 by gradual addition of a moderately reactive
halogenating agent such as N-chlorosuccinimide to a
mixture of a base, such as triethylamine, and the
compound of Formula XI in a dry inert solvent such as
ether, dichloromethane or toluene. Alternatively,
15 when Q is Q-5, Q-6 or Q-7, the base can be added
gradually to a mixture of the halogenating agent and
compound XI. It is preferable that the concentration
of reactant be kept relatively low (0.01 to 0.5 M)
and that the compound being added to the reaction
20 mixture is added gradually to avoid competing side
reactions which occur at higher concentrations. For
optimum yields, it is also important to maintain
anhydrous conditions.

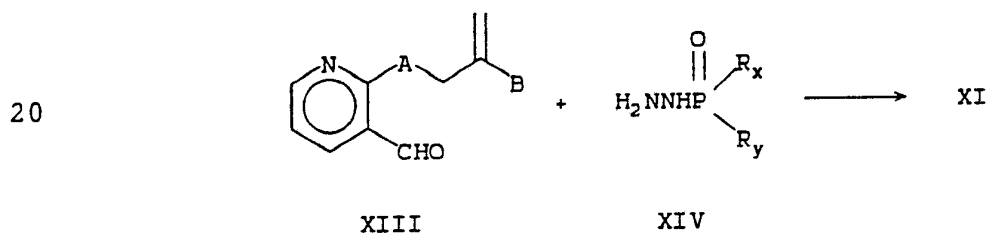
Hydrolysis of the phosphorus group is best
25 accomplished by treatment of XII with 1 to 5
equivalents of a strong acid such as hydrochloric,
sulfuric or p-toluenesulfonic in a suitable solvent
such as methanol, ethanol or tetrahydrofuran,
optionally containing about 0.1 to 10 equivalents of
30 water. The reaction can be conducted at temperatures
generally ranging from about 20 to 100°C with the
reflux temperature of the solvent being generally
preferred. Once the reaction is complete, the acid
salt can be precipitated by cooling to 0°C, or if it
35 does not precipitate, the solvent can be removed and
ether added to facilitate crystallization. The acid
salt of III can then be neutralized with an inorganic
base such as sodium carbonate or sodium bicarbonate

to give the free base III. In some instances, it is preferable to convert the acid salt of III directly to compounds of Formula I by addition of an aqueous solution of an inorganic base to a suspension of the salt III in an organic solvent such as tetrahydrofuran, followed by addition of the isocyanate II.

Compounds of Formula XI are prepared by condensation of an aldehyde of Formula XIII with a phosphorus hydrazid of Formula XIV.

SCHEME 9

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This reaction is typically run in an inert organic solvent. Alcohol solvents such as methanol and ethanol and ether solvents such as tetrahydrofuran and diethyl ether are generally preferred. The reaction can also be conducted with a catalytic amount of acid such as p-toluenesulfonic acid although typically acid catalysis is not necessary. The products of Formula XI generally precipitate from the reaction mixture as they are formed.

Starting materials of Formula XIII and XIV can be prepared by analogy with procedures known in the art.

Compounds of Formula I, where Q is Q-8, can be
5 obtained by the reaction of activated carbonyl or
thiocarbonyl compounds of Formula II with substituted
anilines in the presence or absence of an acid
acceptor or suitable condensing agent. Methods for
performing this transformation are well known in the
10 art; see, Zabicky, "The Chemistry of the Amides",
Interscience, 1970.

One particularly useful method involves the
chlorination of an acid derivative (XV, $X_1 = OH$) with
thionyl chloride or another chlorinating agent
15 followed by treatment with an aniline (XVI) in the
presence of an acid acceptor such as an amine base,
preferably triethylamine. Suitable solvents for the
chlorination reaction are inert to hydrogen chloride
and include benzene, toluene, and dichloromethane.
20 Preferred temperatures for this process are from 20°
to 100°C with temperatures between 20° and 80°C being
particularly preferred. The latter reaction can be
carried out in many different inert solvents such as
dialkylethers, chlorinated hydrocarbons, and aromatic
25 hydrocarbons. While temperatures at or below 25°C
are preferred, higher temperatures can also be
employed. These reactions are normally run at
atmospheric pressure, but can also be carried out at
elevated pressures.

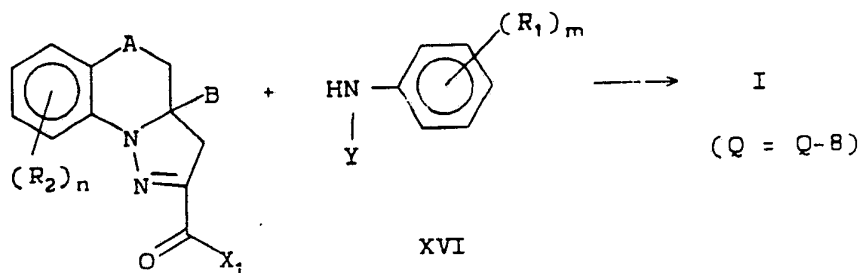
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SCHEME 10

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XV

X₁ = Cl, Br, OH, OR₃

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Esters of Formula XV ($X_1 = C_1$ to C_6 alkoxy) can be converted directly to compounds of Formula I ($Q=Q-8$) in several ways. In the presence of Lewis acids such as $AlMe_3$, anilines react readily with esters of Formula XV. The reaction is best carried out at room temperature to $120^\circ C$. Suitable solvents include dichloromethane, 1,2-dichloroethane, and toluene. The method described by Weinreb et al., Organic Synthesis, 59, 49, (1982), proceeds best with esters of lower alcohols such as methanol or ethanol.

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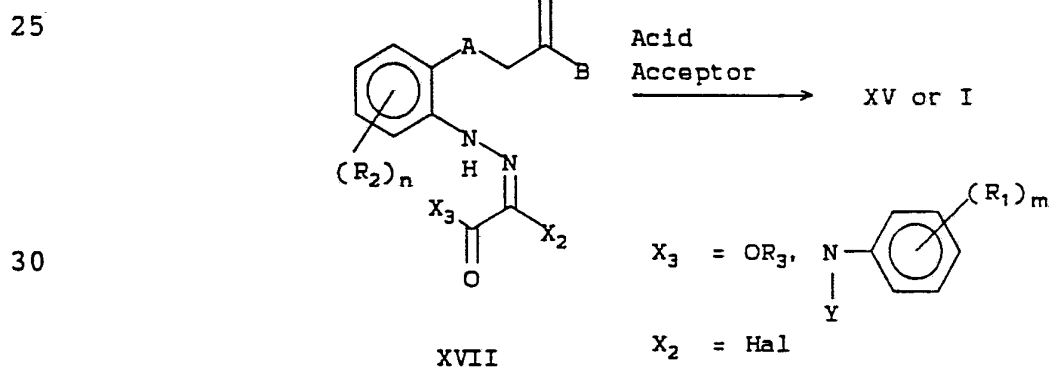
Acids of Formula XV ($X_1 = OH$) can be converted directly to compounds of Formula I by use of coupling agents known in the peptide art in conjunction with anilines. Coupling agents include dicyclohexylcarbodiimide (DCC), N-hydroxysuccinimide, 2-chloro-N-methylpyridinium iodide, carbonyl diimidazole, or other agents capable of activating an acid function

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or acting as a dehydrating agent. These and other methods are described in Gross et al., "The Peptides," 3 Vols., Academic Press, New York, 1979 to 1981.

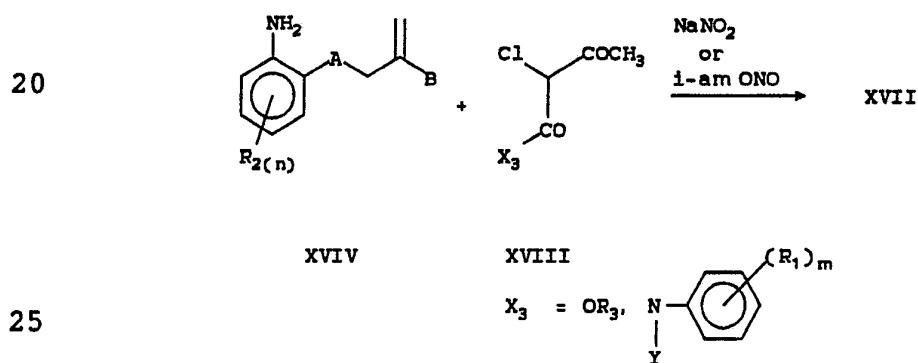
Compounds of Formula I (Q=Q-8) and intermediates of Formula XV can also be obtained by the intramolecular dipolar cycloaddition reaction of nitrile-imines, generated from substituted phenylhydrazones of Formula XVII (Scheme 11). The presence of an acid acceptor (generally an amine base, for example, triethylamine) is necessary for the formation of the nitrile-imine. Suitable solvents include but are not restricted to benzene, toluene, 1,2-dichloroethane, chloroform, and tetrahydrofuran. The reaction can be carried out at temperatures ranging from 20° to 120°C with the relative reactivity of the alkene moiety governing the required temperature for a given example.

SCHEME 11



The required hydrazones of Formula XVII can be
 5 synthesized by the Japp-Klingemann reaction (Scheme
 12). The coupling of diazonium salts with active
 methylene compounds is known. The more specific
 coupling of chloroacetoacetic acid derivatives of
 Formula XVIII with diazotized anilines of Formula XIV
 10 containing alkenyl substituents is described by Padwa
 et al. in J. Org. Chem., 43, 1664 (1978) and J. Org.
 Chem., 46, 1402 (1981). A similar process for this
 type of aniline is described by Garanti et al. in J.
 Org. Chem., 42, 1389 (1977), and J. Chem. Soc. Perkin
 15 I, 2245 (1981).

SCHEME 12



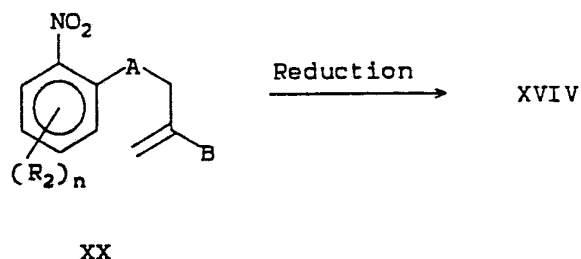
The anilines of Formula XIV can be obtained by
 35 the reduction of aromatic nitro compounds of Formula
 XX (Scheme 13). There are many methods known for this
 transformation. See, March, "Advanced Organic
 Chemistry", 1985, Wiley, page 1103-1104. A
 particularly suitable method involves the treatment of

the nitro compound with tin (II) chloride in alcoholic solvents. Refer to Bellamy et al. Tetrahedron Letters, 1984, 839.

SCHEME 13

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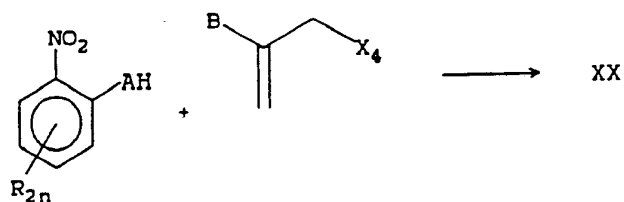
Nitro compounds of Formula XX containing a heteroatom in the alkenyl chain can be obtained by alkylation reactions (Scheme 14). Treatment of a substituted phenol, thiophenol, or aniline of Formula XXI with an acid acceptor and an allyl or homoallyl halide or sulfonate of Formula XXII gives compounds of Formula XX as products. Preferred acid acceptors for the process are inorganic bases such as potassium carbonate. Preferred solvents include dimethylformamide, dimethylsulfoxide, methylethyl ketone, and ethanol. The reaction is generally carried out at room temperature, but higher temperatures may be necessary in some cases. Alternative methods for these nitro compounds of Formula XX have been described by Oae et al. in Bull. Chem. Jap., 54, 2374 (1981).

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SCHEME 14

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XXI

XXII

 $\text{X}_4 = \text{Br}, \text{Cl}, \text{OSO}_2\text{R}_3$

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 $\text{A} = \text{S}, \text{O}, \text{NR}_6$

20

Anilines of Formula XIV containing sulfur can be obtained by alkylation on the sulfur of Formula XXIII (Scheme 15). The conditions which favor this process are alcoholic solvents and sodium hydroxide or sodium alkoxides as bases. The reaction is generally carried out using allylic halides of Formula XXII at 20° to 80° C in lower alcoholic solvents, preferably ethanol.

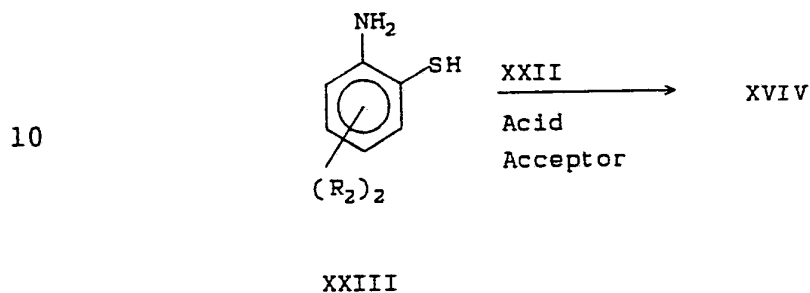
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SCHEME 15

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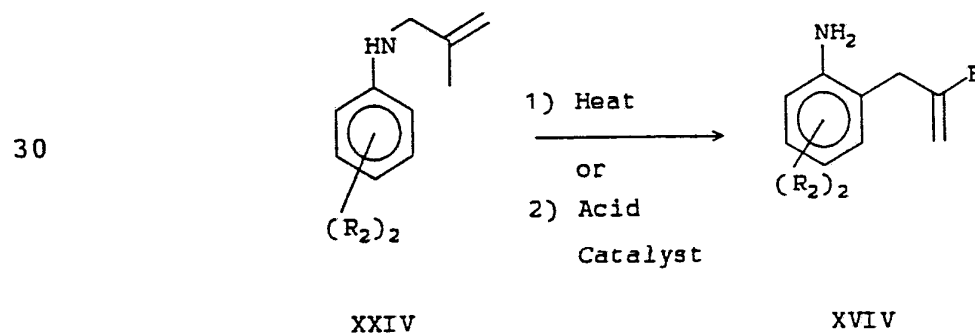


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Anilines of Formula XIV which do not contain a heteroatom in the alkenyl portion can be synthesized by the Claisen rearrangement (Scheme 16). The thermal and acid catalyzed rearrangement of N-allylanilines of Formula XXIV has been described by Hansen et al. in Helv. Chim. Acta., 60, 978 (1977).

SCHEME 16

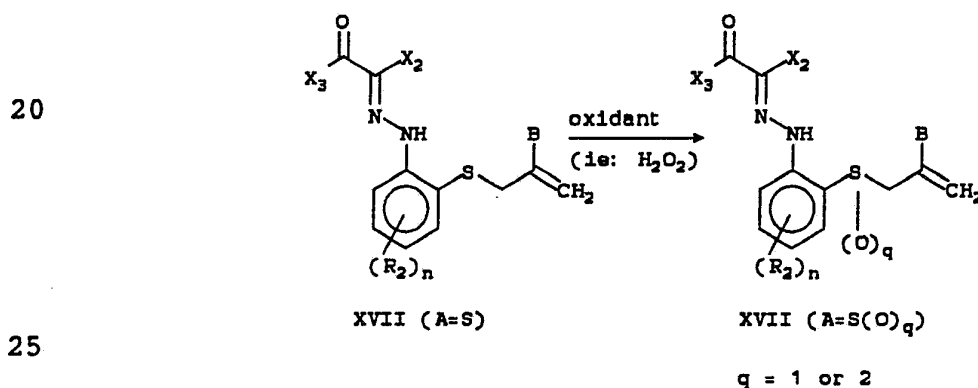
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The hydrazonyl halides of Formula XVII (A=S, q=1
 5 or 2) in which a sulfoxide or sulfone are present may
 be obtained by the oxidation of the corresponding
 sulfide of Formula XVII (A=S, q=0) (Scheme 17).
 Oxidation of hydrazones of Formula XVII (A=S, q=0) by
 hydrogen peroxide in acetic acid is known. See Zecchi
 10 et al., J. Chem. Res. 1887 (1986). By modifications
 of the amount of oxidant, reaction time and
 temperature the product obtained can be specifically
 the sulfoxide of Formula XVII (A=S, q=1) or the
 sulfone of Formula XVII (A=S, q=2).

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SCHEME 17

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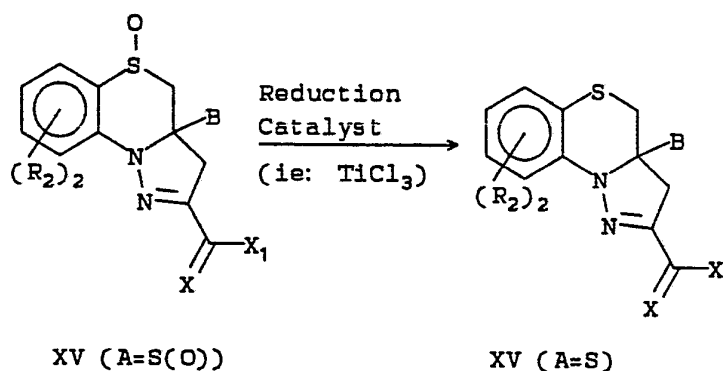
Cycloaddition of the hydrazones of Formula XVII
 (A=S, q=0) proceeds only in low yield. Synthesis of
 35 sulfur containing compounds XV (A=S, q=0) can be
 accomplished by reducing the sulfoxides of Formula XV
 (A=S, q=1) (Scheme 18). Many reagents are known in
 the art to reduce sulfoxides. See March, "Advanced
 Organic Chemistry", 1985, Wiley, page 1108. One

particularly useful method uses titanium (III) chloride at room temperature and was described by Ho
 5 in Synthetic Comm., 3, 37 (1973).

SCHEME 18

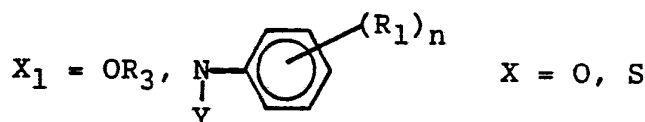
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I or XV

I or XV

30 Compounds of Formula I, where Y is H and Q is Q-1 through Q-8, can be converted to other compounds of Formula I by alkylation, acylation, and
 sulphenylation reactions to form derivatives where Y
 is other than H. Reaction of compounds of Formula I
 35 in the presence of an acid acceptor with electrophilic agents results in substitution on nitrogen. Strong bases such as sodium hydride, potassium t-butoxide, potassium hydride, and other bases known in the art to

deprotonate amides are preferred in the process. Suitable electrophiles include, but are not restricted to alkyl halides, acyl halides, acid anhydrides, carbonates, chloroformates, disulphides, and sulphenyl halides. This reaction is normally run in the the temperature range of 0-25°C, but can be run at temperature up to 120°C if unreactive electrophiles are used. Solvents not deprotonated under the reactions conditions such as tetrahydrofuran, dimethylformamide, dimethoxyethane, and diethyl ether are preferred.

Compounds of Formula I (X=O) can be converted to compounds of Formula I (X=S) by means of thiating agents. Conversion of amides to thioamides is well known in the art. Phosphorous pentasulfide either alone or in combination with organic or inorganic bases is a preferred reagent to effect this conversion. When phosphorous pentasulfide is used alone, organic bases such as pyridine are the preferred solvents. When it is used in conjunction with inorganic bases such as sodium bicarbonate, the preferred solvents are ethers such as diglyme. Temperatures between 20° to 160°C can be employed successfully with temperatures between 90° to 120°C preferred. These and other means to convert amides to thioamides are described by Lapucha, Synthesis, 256 (1987).

The following Examples further illustrate the invention.

Example 13,3a,4,5-Tetrahydro-N-[4-(trifluoromethyl)phenyl]-
5 2H-thieno[2,3-g]indazole-2-carboxamide

Step A: 6,7-Dihydro-5-methylenebenzo[b]thiophen-4(5H)-
one

10 To 20.0 mL of tetramethyldiaminomethane was
added 10.0 g of 6,7-dihydrobenzo[b]thiophen-4(5H)-one
all at once. To this mixture was added 20.0 mL of
acetic anhydride, dropwise. The reaction mixture
exothermed to 45°C and was heated to 122°C for 15
15 minutes and then cooled to 90°C where it was kept for
60 minutes. The dark solution was poured into cold
water and extracted with ether. The ether was extract-
ed with a saturated solution of NaHCO₃ and then washed
with brine. The ether layer was dried over anhydrous
20 magnesium sulfate, filtered and concentrated in vacuo
to afford a yellow oil. The yellow oil was
flash-chromatographed using 10% ethyl acetate and 90%
hexanes as eluent to afford 6.18 g of a white solid,
m.p. 47-49°C. 200 MHz¹H NMR(CDCl₃) δ 2.97 (t, 2H),
25 3.07 (t, 2H), 5.46 (s, 1H), 6.17 (s, 1H), 7.11 (d, 1H),
7.48 (d, 1H); I.R. (Nujol) 1660 cm⁻¹.

Step B: 3,3a,4,5-tetrahydro-2H-thieno[2,3-g]indazole

30 To 20 mL of anhydrous ethanol was added 1.2 g of
the product from Step A and 0.40 g of hydrazine
hydrate. The reaction mixture was heated at reflux
for 2 h, cooled, poured into cold water and extracted
with ether. The ether extracts were washed with water
35 and brine, dried over anhydrous magnesium sulfate,
filtered and utilized without concentration or
purification in Step C.

Step C:

Preparation of title compound was as follows.

- 5 To a 150 mL solution of the product from Step B in ether was added 1.50 g of α,α,α -trifluoro-p-tolyl-isocyanate. The reaction mixture was stirred at room temperature for 1 hr. where a precipitate was formed. The reaction mixture was filtered and the precipitate
10 was washed with ether to afford 0.20 g of a white solid, m.p. 219-221°C. 200 MHz ^1H NMR(CDCl_3) δ 1.98 (bm, 1H), 2.48 (bm, 1H), 3.10 (m, 2H), 3.42 (m, 2H), 4.43 (m, 1H), 7.25 (d, 1H), 7.36 (d, 1H), 7.56 (d, 2H), 7.67 (d, 2H), 8.18 (bs, 1H); I.R. (Nujol) 3370, 1668
15 cm^{-1} .

Example 2

- 7-Chloro-3a,4,-dihydro-3a-phenyl-N-[4-(trifluoromethyl)phenyl]-3H-pyrazolo[5,1-c][1,4] benzoxazine-
20 2-carboxamide

Step A: 4-chloro-1-nitro-2-(phenyl-2-propenyloxy)-benzene

- 25 A solution of 5-chloro-2-nitrophenol (7g) in dimethylformamide (40ml) was stirred at room temperature with 1-bromo-2-phenyl-2-propene (8ml) and potassium carbonate (5.5g) for 18h. The reaction mixture was diluted with water (200 ml) and extracted
30 with ether (100 ml). The ether was washed with water (3 x 100 ml). The solvent was removed under reduced pressure and the residue was crystallized from hexanes. The yellow solid (8.6 g) was the desired product. m.p. 74.5-75.5°C
35 NMR (200MHz) CDCl_3 ; δ 7.8 (d, 1H, ArH)
7.4-7.0 (m, 7H, ArH)
5.6 (s, s, 2H, CH_2)
5.0 (s, 2H, CH_2O).

Step B: 4-chloro-2-[(2-phenyl-2-propenyl)oxy]-benzenamine

The compound of Step A (7.2 g) was added to a suspension of tin (II) chloride (28 g) in ethanol (45 ml). The mixture was refluxed for 1.5 h. The reaction was diluted with ethyl acetate and neutralized by careful addition of saturated sodium bicarbonate solution. The organic solution was washed with brine and the solvent was dried over magnesium sulfate. Evaporation of the solution left a thick oil of the title compound (5.8 g).

15	NMR (200MHz) CDCl ₃	6	7.4-6.6 (m, 8H, ArH)
			5.6-5.4 (S,S, 2H, CH ₂)
			4.9 (S, 2H, CH ₂ O)
			3.2 (Br, NH ₂)

20 Step C: methyl chloro [[4-chloro-2-[(2-phenyl-
2-propenyl)oxy]phenyl]hydrazono]acetate

Using the procedure of Example 4 (Step B), the compound of Step B (5.6 g) was converted to the title compound (2.8 g). The chromatography was carried out with hexanes/ethyl acetate (8:1); m.p. 88-90°C.

30	NMR (200MHz) CDCl ₃	δ	8.6	(br. s, NH ₂)
			7.3-6.9	(m, 8H, ArH)
			5.7-5.6	(m, 2H, CH ₂)
			4.9	(s, 2H, CH ₂ O)

Step D: methyl 7-chloro-3a-4-dihydro-3a-phenyl-
3H-pyrazolo[5, 1-c][1,4]benzoxazine-
2-carboxylate

35

The compound of Step C (2.5 g) was dissolved in benzene (100 ml), treated with triethylamine (5 ml), and

heated at reflux for 24 h. The cooled mixture was diluted with ethyl acetate (100 ml) and 1N HCl (100 ml). The organic layer was dried and evaporated. The residue was chromatographed on silica gel with hexane/ethyl acetate (5:1). The title compound (1 g) was a solid. m.p. 145-146°C

NMR (200MHz) CDCl ₃	δ	7.6-6.8 (m, 8H, ArH)
10		4.65 (d, 1H, CH)
		3.9 (d, 1H, CH)
		3.8 (s, 3H, CH ₃)
		3.4 (m, 2H, CH ₂)

15 Step E:

Preparation of title compound was as follows. The compound of Step D (1.0 g) was suspended in methanol (10 ml) and treated with 50% aqueous sodium hydroxide (1 ml) and heated to reflux for 10 min. The mixture was acidified and extracted with ethyl acetate. The dried organic extract was evaporated. The residue was dissolved in benzene (15 ml) and treated with thionyl chloride (1.5 ml). The mixture was heated to reflux for 2 h and then evaporated. The residue was dissolved in tetrahydrofuran (20 ml) and one half was added to a solution of p-trifluoromethoxyaniline (0.4 g) and triethylamine (1.0 ml) in tetrahydrofuran (10 ml). After stirring for 1 h the mixture was partitioned between ethyl acetate (50 ml) and 1N HCl (50 ml). The dried organic layer was evaporated. Chromatography of the residue on silica gel in hexanes/ethyl acetate (7:1) gave the title compound (0.39 g). m.p. 140-146°C.

40

5	NMR (200MHz) CDCl ₃	δ	8.6	(br, NH)
			7.8-6.9	(m, 12H, ArH)
			4.7	(d, 1H, CH)
			3.8	(d, 1H, CH)
			3.4	(dd, 2H, CH ₂)

Example 3

10 Methyl 7-fluoro-3a,4-dihydro-2-[[[4-(trifluoromethyl)phenyl]amino]carbonyl]-3H-pyrazolo[5,1-c]-[1,4]benzoxazine-3a-carboxylate

Step A: methyl 2-[(5-fluoro-2-nitrophenoxy)methyl]-2-propenoate

The compounds 5-fluoro-2-nitrophenol (8.0 g), methyl 2-bromomethylacrylate (9.5 g) and potassium carbonate (7 g) under the conditions of Example 2, (Step A) gave the title compound (11.6 g). m.p. 89-92°C

25	NMR (200MHz) CDCl ₃	δ	8.0	(m, 1H, ArH)
			6.9	(m, 2H, ArH)
			6.4-6.2	(s, s, 2H, CH ₂)
			4.8	(s, 2H, CH ₂ O)
			3.8	(s, 3H, CH ₃ O)

Step B: methyl 2-[(2-amino-5-fluorophenoxy)methyl]-2-propenoate

30

The compound of Step A (11.0 g) was converted to the title compound (8 g) by the method of the Example 2 (Step B).

35	NMR (200MHz) CDCl ₃	δ	6.8	(m, 3H, ArH)
			6.5 & 6.0	(s, s, 2H, CH ₂)
			4.8	(s, 2H, CH ₂ O)
			4.2	(br, NH ₂)
			3.8	(s, 3H, CH ₃ O)

5 Step C: methyl 2-[[2-[2-(1-chloro-2-methoxy-2-oxo-ethylidene)hydrazino]-5-fluorophenoxy]-methyl]-2-propenoate

10 Using the procedure of Example 4 (Step C) the title compound (2.1 g) was prepared from the compound of Step B (7.5 g).

15 NMR (200MHz) CDCl₃ δ 8.7 (br. s, NH)
7.6 (m, 1H, ArH)
6.9 (m, 2H, ArH)
6.5 (s, 1H, CH₂)
6.0 (s, 1H, CH₂)
4.8 (s, 2H, CH₂)
3.8 (s, 6H, 2OCH₃)

20 Step D:

Preparation of title compound (0.13 g) was as follows. The procedure of Example 2 (Steps D and E) were used with the compound of Step C (1.8 g) and the p-trifluoromethoxyaniline was replaced with
25 p-trifluoromethyl-aniline. m.p. 177.5-181°C.

30 NMR (200MHz) CDCl₃ δ 8.6 (br, NH)
7.7-6.8 (m, 7H, ArH)
4.7 (d, 1H, CH₂O)
3.8 (s, 3H, CH₃O)
3.8-3.4 (m, 3H, CH₂, CH₂O)

35

Example 4

Methyl 3a,4-dihydro-3a-phenyl-3H-pyrazolo-
5 [5,1-cl[1,4]benzothiazine-2-carboxylate-5-oxide

Step A: 2-[(2-phenyl-2-propenyl)thio]-
benzenamine

10 The compound, 2-aminothiophenol, (12.5 g) was
added to a solution of sodium hydroxide (4.5 g) in
ethanol (100 ml) keeping the temperature less than
30°C. Then 1-bromo-2-phenyl-2-propene (21 g) was
added and the mixture was stirred at 60°C for 3h. The
15 precipitated solid was filtered and washed with
ethanol. The solvent was removed and the residue was
chromatographed on silica gel with hexanes/ethyl
acetate (7:1) to yield the title compound (14.5 g).
As an oil.

20 NMR (200MHz) CDCl₃ δ 7.3-7.0 (m, 9H, ArH)
5.3-5.0 (m, 2H, CH₂)
4.0 (Br, NH₂)
3.8 (S, 2H, CH₂S)

25 Step B: methyl chloro[[2-[(2-phenyl-2-propenyl)-
thio]-phenyl]hydrazono]acetate

The compound of Step A (14.5 g) was treated
with 6N HCl (22 ml) and water (100 ml). This mixture
30 was cooled to below 0°C and treated dropwise with an
aqueous solution of sodium nitrite (4.2 g). The
resulting mixture was decanted into an insulated
dropping funnel. The mixture was added to a cooled
(-5 to -10°C) mixture of sodium acetate (15 g) and
35 methyl 2-chloroacetoacetate (5 ml) in ethanol (100 ml)
so that the internal temperature did not exceed 5°C.

The mixture was allowed to come to room temperature over 2 h and then extracted with ether. The dried organic layer was evaporated and chromatographed on silica gel with ether/hexanes (1:2). The title compound (11.5 g) was isolated as a yellow oil.

NMR (200MHz) CDCl_3 δ 9.4 (br, NH)
7.5-7.0 (m, 9H, ArH)
5.2 (S, 1H, CH_2)
4.8 (S, 1H, CH_2)
3.9 (S, 3H, CH_3)
3.8 (S, 2H, CH_2S)

Step C: methyl chloro[[2-[(2-phenyl-2-propenyl)-sulfinyl]phenyl]-hydrazono]acetate

The compound of Step B (5 g) was stirred with occasional warming in acetic acid (45 ml) and treated with 30% aqueous hydrogen peroxide (2.0 ml). After stirring for 5 h, water (200 ml) was added and the P.h. was adjusted to 6 with sodium bicarbonate. Saturated sodium bisulfite solution (3 ml) was added and the mixture was extracted with dichloromethane (200 ml). The organic layer was dried and evaporated to give the title compound (4.9 g).

NMR (200MHz) CDCl_3 δ 7.6-7.0 (m, 9H, ArH)
5.6-4.2 (m, 4H, CH_2)
4.0 (S, 3H, CH_3O)

Step D:

Preparation of title compound (1.0 g) was as follows. The method of Example 2 (Step D) was applied to the compound of Example 12 (4.5 g).

Purification was accomplished by chromatography on silica gel with hexanes/ethyl acetate (1:1).

44

5	NRM (200MHz) CDCl ₃	δ	7.8-7.0	(m, 9H, ArH)
			4.2	(dd, 1H, CH ₂)
			3.9	(s, CH ₃ O, 3H)
			3.6	(m, 3H, CH ₂)

Example 5

3a,4-Dihydro-3a-phenyl-N-[4-(trifluoromethyl)phenyl]-
10 3H-pyrazolo[5,1-c]benzothiazine-2-carboxamide

The compound of Example 4 (Step D) (1 g) was
treated with 20% aqueous titanium (III) chloride (2
ml) in dichloromethane (20 ml) and methanol (20 ml).
15 The mixture was stirred for 20 min. at room
temperature and partitioned between ethyl acetate
(150 ml) and water (200 ml). The dried organic phase
was concentrated and the residue was subjected to the
conditions of Example 10 with p-trifluoromethyl-
20 aniline in place of p-trifluoromethoxyaniline. The
title compound (0.6 g) was isolated as a solid. m.p.
238-240°C.

25	NMR (200MHz) CDCl ₃	δ	8.6	(br, NH)
			7.8-6.9	(m, 13H, ArH)
			3.6	(s, 2H, CH ₂)
			3.4	(s, 2H, CH ₂)

By the general procedures described herein, or
obvious modifications thereof, the compounds of
30 Tables 1 through 16 can be prepared.

35

SUMMARY OF TABLES

	<u>Table</u>	<u>Q</u>	<u>Y</u>	<u>G</u>
5				
	1	Q-1	H	-
	2	Q-2	H	-
	3	Q-3	H	-
10	4	Q-4	H	-
	5	Q-5	H	S
	6	Q-6	H	S
	7	Q-7	H	S
	8	Q-5	H	O
15	9	Q-6	H	O
	10	Q-7	H	O
20	Table 11	R _a is H, X is O, G is S		
	Table 12	R _a is H, X is O, G is S, Y is S-J		
	Table 13	Q is Q-8, R _a is H, Y is H, A is CH ₂		
	Table 14	Q is Q-8, R _a is H, Y is H		
	Table 15	Q is Q-8, R _a is H		
25	Table 16	Q is Q-8, Y is H		

In the Tables that follow, the values of Q will be referred to by the following numbering system:

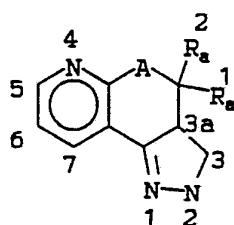
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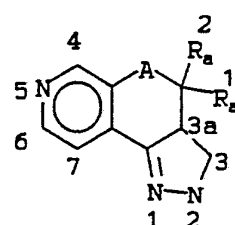
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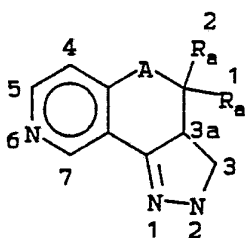


Q-1

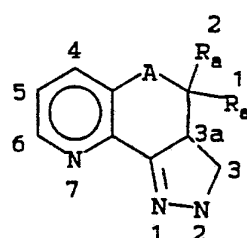


Q-2

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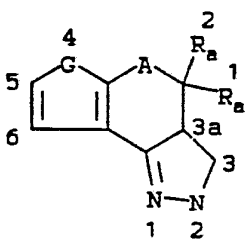


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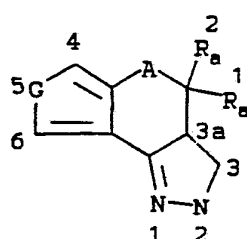


Q-4

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Q-5



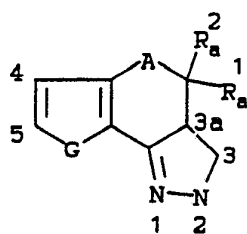
Q-6

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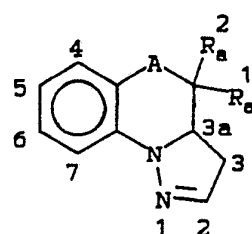
47

5

10



Q-7



Q-8

15

20

25

30

35

Table 1

5	R ₁	R ₂	A	B	X	R _a ¹ , R _a ²
10	4-CF ₃	H	CH ₂	H	O	H,H
	4-Cl	H	CH ₂	H	O	H,H
	4-Br	H	CH ₂	H	O	H,H
15	4-CF ₃	5-Cl	CH ₂	H	O	H,H
	4-Cl	5-Cl	CH ₂	H	O	H,H
	4-Br	5-Cl	CH ₂	H	O	H,H
20	4-CF ₃	5-F	CH ₂	H	O	H,H
	4-Cl	5-F	CH ₂	H	O	H,H
	4-Br	5-F	CH ₂	H	O	H,H
25	4-CF ₃	5-CN	CH ₂	H	O	H,H
	4-Cl	5-CN	CH ₂	H	O	H,H
	4-Br	5-CN	CH ₂	H	O	H,H
30	4-CF ₃	5-Br	CH ₂	H	O	H,H
	4-Cl	5-Br	CH ₂	H	O	H,H
	4-Br	5-Br	CH ₂	H	O	H,H
35	4-CF ₃	5-Me	CH ₂	H	O	H,H
	4-Cl	5-Me	CH ₂	H	O	H,H
	4-Br	5-Me	CH ₂	H	O	H,H
30	4-CF ₃	7-F	CH ₂	H	O	H,H
	4-Cl	7-F	CH ₂	H	O	H,H
	4-Br	7-F	CH ₂	H	O	H,H
30	4-CF ₃	5-NMe ₂	CH ₂	H	O	H,H
	4-Cl	5-NMe ₂	CH ₂	H	O	H,H
	4-Br	5-NMe ₂	CH ₂	H	O	H,H
35	4-CF ₃	5-CF ₃	CH ₂	H	O	H,H
	4-Cl	5-CF ₃	CH ₂	H	O	H,H
	4-Br	5-CF ₃	CH ₂	H	O	H,H
	4-CF ₃	H	CH ₂	Me	O	H,H

	R ₁	R ₂	A	B	X	R _a ¹ , R _a ²
5	4-Cl	H	CH ₂	Me	O	H,H
	4-Br	H	CH ₂	Me	O	H,H
	4-CF ₃	5-Cl	CH ₂	Me	O	H,H
	4-Cl	5-Cl	CH ₂	Me	O	H,H
10	4-Br	5-Cl	CH ₂	Me	O	H,H
	4-CF ₃	5-CF ₃	CH ₂	Me	O	H,H
	4-Cl	5-CF ₃	CH ₂	Me	O	H,H
	4-Br	5-CF ₃	CH ₂	Me	O	H,H
15	4-CF ₃	H	CH ₂	Et	O	H,H
	4-Cl	H	CH ₂	Et	O	H,H
	4-Br	H	CH ₂	Et	O	H,H
	4-CF ₃	5-F	CH ₂	Et	O	H,H
20	4-Cl	5-F	CH ₂	Et	O	H,H
	4-Br	5-F	CH ₂	Et	O	H,H
	4-CF ₃	5-CN	CH ₂	Et	O	H,H
	4-Cl	5-CN	CH ₂	Et	O	H,H
25	4-Br	5-CN	CH ₂	Et	O	H,H
	4-CF ₃	H	CH ₂	allyl	O	H,H
	4-Cl	H	CH ₂	allyl	O	H,H
	4-Br	H	CH ₂	allyl	O	H,H
30	4-CF ₃	5-Br	CH ₂	allyl	O	H,H
	4-Cl	5-Br	CH ₂	allyl	O	H,H
	4-Br	5-Br	CH ₂	allyl	O	H,H
	4-CF ₃	5-Cl	CH ₂	allyl	O	H,H
35	4-Cl	5-Cl	CH ₂	allyl	O	H,H
	4-Br	5-Cl	CH ₂	allyl	O	H,H
	4-CF ₃	H	CH ₂	CO ₂ Me	O	H,H
	4-Cl	H	CH ₂	CO ₂ Me	O	H,H
	4-Br	H	CH ₂	CO ₂ Me	O	H,H
	4-CF ₃	5-F	CH ₂	CO ₂ Me	O	H,H
	4-Cl	5-F	CH ₂	CO ₂ Me	O	H,H

	R ₁	R ₂	A	B	X	R _a ¹ , R _a ²
5	4-Br	5-F	CH ₂	CO ₂ Me	O	H,H
	4-CF ₃	5-Cl	CH ₂	CO ₂ Me	O	H,H
	4-Cl	5-Cl	CH ₂	CO ₂ Me	O	H,H
	4-Br	5-Cl	CH ₂	CO ₂ Me	O	H,H
10	4-CF ₃	5-Br	CH ₂	CO ₂ Me	O	H,H
	4-Cl	5-Br	CH ₂	CO ₂ Me	O	H,H
	4-Br	5-Br	CH ₂	CO ₂ Me	O	H,H
	4-CF ₃	5-CN	CH ₂	CO ₂ Me	O	H,H
	4-Cl	5-CN	CH ₂	CO ₂ Me	O	H,H
15	4-Br	5-CN	CH ₂	CO ₂ Me	O	H,H
	4-CF ₃	5-CF ₃	CH ₂	CO ₂ Me	O	H,H
	4-Cl	5-CF ₃	CH ₂	CO ₂ Me	O	H,H
	4-Br	5-CF ₃	CH ₂	CO ₂ Me	O	H,H
	4-CF ₃	5-Me	CH ₂	CO ₂ Me	O	H,H
20	4-Cl	5-Me	CH ₂	CO ₂ Me	O	H,H
	4-Br	5-Me	CH ₂	CO ₂ Me	O	H,H
	4-CF ₃	H	CH ₂	CO ₂ Et	O	H,H
	4-Cl	H	CH ₂	CO ₂ Et	O	H,H
	4-Br	H	CH ₂	CO ₂ Et	O	H,H
25	4-CF ₃	5-Cl	CH ₂	CO ₂ Et	O	H,H
	4-Cl	5-Cl	CH ₂	CO ₂ Et	O	H,H
	4-Br	5-Cl	CH ₂	CO ₂ Et	O	H,H
	4-CF ₃	H	CH ₂	CO ₂ -i-Pr	O	H,H
	4-Cl	H	CH ₂	CO ₂ i-Pr	O	H,H
30	4-Br	H	CH ₂	CO ₂ i-Pr	O	H,H
	4-CF ₃	H	CH ₂	CO ₂ CH ₂ CF ₃	O	H,H
	4-Cl	H	CH ₂	CO ₂ CH ₂ CF ₃	O	H,H
	4-Br	H	CH ₂	CO ₂ CH ₂ CF ₃	O	H,H
	4-CF ₃	H	CH ₂	CO ₂ allyl	O	H,H
35	4-Cl	H	CH ₂	CO ₂ allyl	O	H,H

	R ₁	R ₂	A	B	X	R _a ¹ , R _a ²
5	4-Br	H	CH ₂	CO ₂ allyl	O	H,H
	4-CF ₃	H	CH ₂	CO ₂ CH ₂ CH ₂ Cl	O	H,H
	4-Cl	H	CH ₂	CO ₂ CH ₂ CH ₂ Cl	O	H,H
	4-Br	H	CH ₂	CO ₂ CH ₂ CH ₂ Cl	O	H,H
10	4-CF ₃	H	CH ₂	Ph	O	H,H
	4-Cl	H	CH ₂	Ph	O	H,H
	4-Br	H	CH ₂	Ph	O	H,H
	4-CF ₃	5-Cl	CH ₂	Ph	O	H,H
	4-Cl	5-Cl	CH ₂	Ph	O	H,H
15	4-Br	5-Cl	CH ₂	Ph	O	H,H
	4-CF ₃	H	CH ₂	4-Cl-Ph	O	H,H
	4-Cl	H	CH ₂	4-Cl-Ph	O	H,H
	4-Br	H	CH ₂	4-Cl-Ph	O	H,H
	4-CF ₃	5-CF ₃	CH ₂	4-Cl-Ph	O	H,H
20	4-Cl	5-CF ₃	CH ₂	4-Cl-Ph	O	H,H
	4-Br	5-CF ₃	CH ₂	4-Cl-Ph	O	H,H
	4-CF ₃	H	CH ₂	4-F-Ph	O	H,H
	4-Cl	H	CH ₂	4-F-Ph	O	H,H
	4-Br	H	CH ₂	4-F-Ph	O	H,H
25	4-CF ₃	H	CH ₂	H	O	Me,H
	4-Cl	H	CH ₂	H	O	Me,H
	4-Br	H	CH ₂	H	O	Me,H
	4-CF ₃	5-Cl	CH ₂	H	O	Me,Me
	4-Cl	5-Cl	CH ₂	H	O	Me,Me
30	4-Br	5-Cl	CH ₂	H	O	Me,Me
	4-CF ₃	H	CH ₂	H	S	H,H
	4-Cl	H	CH ₂	H	S	H,H
	4-Br	H	CH ₂	H	S	H,H
	4-CF ₃	H	CH ₂	Me	S	H,H
35	4-Cl	H	CH ₂	Me	S	H,H
	4-Br	H	CH ₂	Me	S	H,H
	4-CF ₃	H	CH ₂	CO ₂ Me	S	H,H

	R ₁	R ₂	A	B	X	R _a ¹ , R _a ²
5	4-Cl	H	CH ₂	CO ₂ Me	S	H,H
	4-Br	H	CH ₂	CO ₂ Me	S	H,H
	4-CF ₃	5-Cl	CH ₂	H	S	H,H
	4-Cl	5-Cl	CH ₂	H	S	H,H
10	4-Br	5-Cl	CH ₂	H	S	H,H
	4-CF ₃	5-Cl	CH ₂	Me	S	H,H
	4-Cl	5-Cl	CH ₂	Me	S	H,H
	4-Br	5-Cl	CH ₂	Me	S	H,H
	4-CF ₃	5-Cl	CH ₂	CO ₂ Me	S	H,H
15	4-Cl	5-Cl	CH ₂	CO ₂ Me	S	H,H
	Br	5-Cl	CH ₂	CO ₂ Me	S	H,H
	4-CF ₃	5-Me	CH ₂	H	S	H,H
	4-Cl	5-Me	CH ₂	H	S	H,H
	4-Br	5-Me	CH ₂	H	S	H,H
20	4-CF ₃	H	O	H	O	H,H
	4-Cl	H	O	H	O	H,H
	4-Br	H	O	H	O	H,H
	4-CF ₃	5-Cl	O	H	O	H,H
	4-Cl	5-Cl	O	H	O	H,H
25	4-Br	5-Cl	O	H	O	H,H
	4-CF ₃	5-Br	O	H	O	H,H
	4-Cl	5-Br	O	H	O	H,H
	4-Br	5-Br	O	H	O	H,H
	4-CF ₃	5-CF ₃	O	H	O	H,H
	4-Cl	5-CF ₃	O	H	O	H,H
30	4-Br	5-CF ₃	O	H	O	H,H
	4-CF ₃	H	O	Me	O	H,H
	4-Cl	H	O	Me	O	H,H
	4-Br	H	O	Me	O	H,H
35	4-CF ₃	5-Cl	O	Me	O	H,H

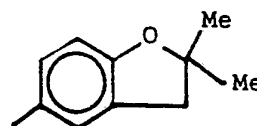
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	4-Br	5-Cl	O	Me	O	H,H
	4-CF ₃	5-Br	O	Me	O	H,H
	4-Cl	5-Br	O	Me	O	H,H
10	4-Br	5-Br	O	Me	O	H,H
	4-CF ₃	5-CF ₃	O	Me	O	H,H
	4-Cl	5-CF ₃	O	Me	O	H,H
	4-Br	5-CF ₃	O	Me	O	H,H
	4-CF ₃	5-F	O	Me	O	H,H
15	4-Cl	5-F	O	Me	O	H,H
	4-Br	5-F	O	Me	O	H,H
	4-CF ₃	H	O	CO ₂ Me	O	H,H
	4-Cl	H	O	CO ₂ Me	O	H,H
	4-Cl	H	O	CO ₂ Me	O	H,H
20	4-Br	H	O	CO ₂ Me	O	H,H
	4-CF ₃	5-Cl	O	CO ₂ Me	O	H,H
	4-Cl	5-Cl	O	CO ₂ Me	O	H,H
	4-Br	5-Cl	O	CO ₂ Me	O	H,H
	4-CF ₃	H	O	Ph	O	H,H
25	4-Cl	H	O	Ph	O	H,H
	4-Br	H	O	Ph	O	H,H
	4-CF ₃	5-Br	O	Ph	O	H,H
	4-Cl	5-Br	O	Ph	O	H,H
	4-Br	5-Br	O	Ph	O	H,H
30	4-CF ₃	H	O	H	O	Me,Me
	4-Cl	H	O	H	O	Me,Me
	4-Br	H	O	H	O	Me,Me
	4-CF ₃	H	O	H	O	H,Me
	4-Cl	H	O	H	O	H,Me
35	4-Br	H	O	H	O	H,Me

	R ₁	R ₂	A	B	X	R _a ¹ , R _a ²
5	4-CF ₃	H	O	H	O	H, Ph
	4-Cl	H	O	H	O	H, Ph
	4-Br	H	O	H	O	H, Ph
	4-CF ₃	H	O	H	O	H, CO ₂ Me
	4-Cl	H	O	H	O	H, CO ₂ Me
10	4-Br	H	O	H	O	H, CO ₂ Me
	4-CF ₃	H	O	H	S	H, H
	4-Cl	H	O	H	S	H, H
	4-Br	H	O	H	S	H, H
	4-CF ₃	H	S	H	O	H, H
15	4-Cl	H	S	H	O	H, H
	4-Br	H	S	H	O	H, H
	4-CF ₃	5-Cl	S	H	O	H, H
	4-Cl	5-Cl	S	H	O	H, H
	4-Br	5-Cl	S	H	O	H, H
20	4-CF ₃	5-Br	S	H	O	H, H
	4-Cl	5-Br	S	H	O	H, H
	4-Br	5-Br	S	H	O	H, H
	4-CF ₃	5-CF ₃	S	H	O	H, H
	4-Cl	5-CF ₃	S	H	O	H, H
25	4-Br	5-CF ₃	S	H	O	H, H
	4-CF ₃	H	S	Me	O	H, H
	4-Cl	H	S	Me	O	H, H
	4-Br	H	S	Me	O	H, H
	4-CF ₃	5-Cl	S	Me	O	H, H
30	4-Cl	5-Cl	S	Me	O	H, H
	4-Br	5-Cl	S	Me	O	H, H
	4-CF ₃	5-Br	S	Me	O	H, H
	4-Cl	5-Br	S	Me	O	H, H
	4-Br	5-Br	S	Me	O	H, H
35	4-CF ₃	5-CF ₃	S	Me	O	H, H
	4-Cl	5-CF ₃	S	Me	O	H, H
	4-Br	5-CF ₃	S	Me	O	H, H

	R ₁	R ₂	A	B	X	R _a ¹ , R _a ²
5	4-CF ₃	5-F	S	Me	O	H,H
	4-Cl	5-F	S	Me	O	H,H
	4-Br	5-F	S	Me	O	H,H
10	4-CF ₃	H	S	CO ₂ Me	O	H,H
	4-Cl	H	S	CO ₂ Me	O	H,H
	4-Br	H	S	CO ₂ Me	O	H,H
	4-CF ₃	5-Cl	S	CO ₂ Me	O	H,H
	4-Cl	5-Cl	S	CO ₂ Me	O	H,H
15	4-Br	5-Cl	S	CO ₂ Me	O	H,H
	4-CF ₃	H	S	Ph	O	H,H
	4-Cl	H	S	Ph	O	H,H
	4-Br	H	S	Ph	O	H,H
	4-CF ₃	5-Br	S	Ph	O	H,H
20	4-Cl	5-Br	S	Ph	O	H,H
	4-Br	5-Br	S	Ph	O	H,H
	4-CF ₃	H	S	H	O	Me,Me
	4-Cl	H	S	H	O	Me,Me
	4-Br	H	S	H	O	Me,Me
25	4-CF ₃	H	S	H	O	H,Me
	4-Cl	H	S	H	O	H,Me
	4-Br	H	S	H	O	H,Me
	4-CF ₃	H	S	H	O	H,Ph
	4-Cl	H	S	H	O	H,Ph
30	4-Br	H	S	H	O	H,Ph
	4-CF ₃	H	S	H	O	H,CO ₂ Me
	4-Cl	H	S	H	O	H,CO ₂ Me
	4-Br	H	S	H	O	H,CO ₂ Me
	4-CF ₃	H	S	H	S	H,H
35	4-Cl	H	S	H	S	H,H
	4-Br	H	S	H	S	H,H
	4-SMe	H	CH ₂	CO ₂ Me	O	H,H
	4-SO ₂ Me	H	CH ₂	CO ₂ Me	O	H,H
	4-OCF ₂ CF ₂ H	H	CH ₂	CO ₂ Me	O	H,H

	R_1	R_2	A	B	X	R_a^1, R_a^2
5	4-CF ₂ Cl	H	CH ₂	CO ₂ Me	O	H,H
	4-CO ₂ Me	H	CH ₂	CO ₂ Me	O	H,H
	4-CO ₂ CF ₃	H	CH ₂	CO ₂ Me	O	H,H
	4-F	H	CH ₂	CO ₂ Me	O	H,H
10	4-CN	H	CH ₂	CO ₂ Me	O	H,H
	4-Me	H	CH ₂	CO ₂ Me	O	H,H
	3,4-CH ₂ C(Me) ₂ O ¹	H	CH ₂	CO ₂ Me	O	H,H
	3,4-CF ₂ CF ₂ O ²	H	CH ₂	CO ₂ Me	O	H,H
15	4-CF ₃ , 3-Cl	H	CH ₂	CO ₂ Me	O	H,H
	4-I	H	CH ₂	CO ₂ Me	O	H,H
	4-OMe	H	CH ₂	CO ₂ Me	O	H,H
	4-O-t-Bu	H	CH ₂	CO ₂ Me	O	H,H
20	4-t-Bu	H	CH ₂	CO ₂ Me	O	H,H
	4-CF ₃	H	CH ₂	CO ₂ H	O	H,H
	4-CF ₃	H	CH ₂	CONH ₂	O	H,H
	4-CF ₃	H	CH ₂	CONHMe	O	H,H
25	4-CF ₃	H	CH ₂	CONMe ₂	O	H,H
	4-CF ₃	H	CH ₂	CO ₂ CH ₂ Ph	O	H,H
	4-CF ₃	H	CH ₂	CH ₂ Ph	O	H,H
	4-CF ₃	H	CH ₂	OH	O	H,H
30	4-CF ₃	H	CH ₂	OAc	O	H,H
	4-CF ₃	H	CH ₂	CH ₂ CF ₃	O	H,H
	4-CF ₃	H	CH ₂	CH ₂ OCH ₃	O	H,H
	4-CF ₃	H	CH ₂	CH ₂ CO ₂ Me	O	H,H
	4-CF ₃	H	CH ₂	CH ₂ CH ₂ CN	O	H,H

1. designates Ph(R₁) as



35

2. designates Ph(R₁) as

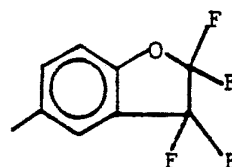


Table 2

5	R ₁	R ₂	A	B	X	R _a ¹ , R _a ²
	4-CF ₃	H	CH ₂	H	O	H,H
	4-Cl	H	CH ₂	H	O	H,H
	4-Br	H	CH ₂	H	O	H,H
10	4-CF ₃	4-F	CH ₂	H	O	H,H
	4-Cl	4-F	CH ₂	H	O	H,H
	4-Br	4-F	CH ₂	H	O	H,H
	4-CF ₃	4-Cl	CH ₂	H	O	H,H
	4-Cl	4-Cl	CH ₂	H	O	H,H
15	4-Br	4-Cl	CH ₂	H	O	H,H
	4-CF ₃	4-Me	CH ₂	H	O	H,H
	4-Cl	4-Me	CH ₂	H	O	H,H
	4-Br	4-Me	CH ₂	H	O	H,H
	4-CF ₃	4-OMe	CH ₂	H	O	H,H
20	4-Cl	4-OMe	CH ₂	H	O	H,H
	4-Br	4-OMe	CH ₂	H	O	H,H
	4-CF ₃	4-Br	CH ₂	H	O	H,H
	4-Cl	4-Br	CH ₂	H	O	H,H
	4-Br	4-Br	CH ₂	H	O	H,H
25	4-CF ₃	6-F	CH ₂	H	O	H,H
	4-Cl	6-F	CH ₂	H	O	H,H
	4-Br	6-F	CH ₂	H	O	H,H
	4-CF ₃	6-Cl	CH ₂	H	O	H,H
	4-Cl	6-Cl	CH ₂	H	O	H,H
30	4-Br	6-Cl	CH ₂	H	O	H,H
	4-CF ₃	7-F	CH ₂	H	O	H,H
	4-Cl	7-F	CH ₂	H	O	H,H
	4-Br	7-F	CH ₂	H	O	H,H
	4-CF ₃	H	CH ₂	Me	O	H,H
35	4-Cl	H	CH ₂	Me	O	H,H

	R ₁	R ₂	A	B	X	R _a ¹ , R _a ²
5	4-Br	H	CH ₂	Me	O	H,H
	4-CF ₃	4-F	CH ₂	CH ₃	O	H,H
	4-Cl	4-F	CH ₂	CH ₃	O	H,H
	4-Br	4-F	CH ₂	CH ₃	O	H,H
10	4-CF ₃	4-Cl	CH ₂	CH ₃	O	H,H
	4-Cl	4-Cl	CH ₂	CH ₃	O	H,H
	4-Br	4-Cl	CH ₂	CH ₃	O	H,H
	4-CF ₃	H	CH ₂	Et	O	H,H
15	4-Cl	H	CH ₂	Et	O	H,H
	4-Br	H	CH ₂	Et	O	H,H
	4-CF ₃	4-F	CH ₂	Et	O	H,H
	4-Cl	4-F	CH ₂	Et	O	H,H
20	4-Br	4-F	CH ₂	Et	O	H,H
	4-CF ₃	4-Cl	CH ₂	Et	O	H,H
	4-Cl	4-Cl	CH ₂	Et	O	H,H
	4-Br	4-Cl	CH ₂	CH ₂	O	H,H
25	4-CF ₃	H	CH ₂	allyl	O	H,H
	4-Cl	H	CH ₂	allyl	O	H,H
	4-Br	H	CH ₂	allyl	O	H,H
	4-CF ₃	4-F	CH ₂	allyl	O	H,H
30	4-Cl	4-F	CH ₂	allyl	O	H,H
	4-Br	4-F	CH ₂	allyl	O	H,H
	4-CF ₃	4-Cl	CH ₂	allyl	O	H,H
	4-Cl	4-Cl	CH ₂	allyl	O	H,H
35	4-Br	4-Cl	CH ₂	allyl	O	H,H
	4-CF ₃	H	CH ₂	CO ₂ Me	O	H,H
	4-Cl	H	CH ₂	CO ₂ Me	O	H,H
	4-Br	H	CH ₂	CO ₂ Me	O	H,H
	4-CF ₃	4-F	CH ₂	CO ₂ Me	O	H,H
	4-Cl	4-F	CH ₂	CO ₂ Me	O	H,H
	4-Br	4-F	CH ₂	CO ₂ Me	O	H,H

	R ₁	R ₂	A	B	X	R _a ¹ , R _a ²
5	4-CF ₃	4-Cl	CH ₂	CO ₂ Me	O	H,H
	4-Cl	4-Cl	CH ₂	CO ₂ Me	O	H,H
	4-Br	4-Cl	CH ₂	CO ₂ Me	O	H,H
	4-CF ₃	4-CN	CH ₂	CO ₂ Me	O	H,H
10	4-Cl	4-CN	CH ₂	CO ₂ Me	O	H,H
	4-Br	4-CN	CH ₂	CO ₂ Me	O	H,H
	4-CF ₃	4-Br	CH ₂	CO ₂ Me	O	H,H
	4-Cl	4-Br	CH ₂	CO ₂ Me	O	H,H
	4-Br	4-Br	CH ₂	CO ₂ Me	O	H,H
15	4-CF ₃	4-CF ₃	CH ₂	CO ₂ Me	O	H,H
	4-Cl	4-CF ₃	CH ₂	CO ₂ Me	O	H,H
	4-Br	4-CF ₃	CH ₂	CO ₂ Me	O	H,H
	4-CF ₃	4-Me	CH ₂	CO ₂ Me	O	H,H
	4-Cl	4-Me	CH ₂	CO ₂ Me	O	H,H
20	4-Br	4-Me	CH ₂	CO ₂ Me	O	H,H
	4-CF ₃	H	CH ₂	CO ₂ Et	O	H,H
	4-Cl	H	CH ₂	CO ₂ Et	O	H,H
	4-Br	H	CH ₂	CO ₂ Et	O	H,H
	4-CF ₃	4-F	CH ₂	CO ₂ Et	O	H,H
25	4-Cl	4-F	CH ₂	CO ₂ Et	O	H,H
	4-Br	4-F	CH ₂	CO ₂ Et	O	H,H
	4-CF ₃	H	CH ₂	CO ₂ -i-Pr	O	H,H
	4-Cl	H	CH ₂	CO ₂ -i-Pr	O	H,H
	4-Br	H	CH ₂	CO ₂ -i-Pr	O	H,H
30	4-CF ₃	H	CH ₂	CO ₂ CH ₂ CF ₃	O	H,H
	4-Cl	H	CH ₂	CO ₂ CH ₂ CF ₃	O	H,H
	4-Br	H	CH ₂	CO ₂ CH ₂ CF ₃	O	H,H
	4-CF ₃	H	CH ₂	CO ₂ allyl	O	H,H
	4-Cl	H	CH ₂	CO ₂ allyl	O	H,H
	4-Br	H	CH ₂	CO ₂ allyl	O	H,H
35	4-CF ₃	H	CH ₂	CO ₂ CH ₂ CH ₂ Cl	O	H,H
	4-Cl	H	CH ₂	CO ₂ CH ₂ CH ₂ Cl	O	H,H

5	R ₁	R ₂	A	B	X	R _a ¹ , R _a ²
10	4-Br	H	CH ₂	CO ₂ CH ₂ CH ₂ Cl	O	H,H
	4-CF ₃	H	CH ₂	Ph	O	H,H
	4-Cl	H	CH ₂	Ph	O	H,H
	4-Br	H	CH ₂	Ph	O	H,H
	4-CF ₃	4-F	CH ₂	Ph	O	H,H
	4-Cl	4-F	CH ₂	Ph	O	H,H
15	4-Br	4-F	CH ₂	Ph	O	H,H
	4-CF ₃	H	CH ₂	4-Cl-Ph	O	H,H
	4-Cl	H	CH ₂	4-Cl-Ph	O	H,H
	4-Br	H	CH ₂	4-Cl-Ph	O	H,H
	4-CF ₃	4-F	CH ₂	4-Cl-Ph	O	H,H
	4-Cl	4-F	CH ₂	4-Cl-Ph	O	H,H
20	4-Br	4-F	CH ₂	4-Cl-Ph	O	H,H
	4-CF ₃	H	CH ₂	4-F-Ph	O	H,H
	4-Cl	H	CH ₂	4-F-Ph	O	H,H
	4-Br	H	CH ₂	4-F-Ph	O	H,H
	4-CF ₃	H	CH ₂	H	O	H,Me
	4-Cl	H	CH ₂	H	O	H,Me
25	4-Br	H	CH ₂	H	O	H,Me
	4-CF ₃	H	CH ₂	H	O	Me,Me
	4-Cl	H	CH ₂	H	O	Me,Me
	4-Br	H	CH ₂	H	O	Me,Me
	4-CF ₃	H	CH ₂	H	S	H,H
	4-Cl	H	CH ₂	H	S	H,H
30	4-Br	H	CH ₂	H	S	H,H
	4-CF ₃	H	CH ₂	Me	S	H,H
	4-Cl	H	CH ₂	Me	S	H,H
	4-Br	H	CH ₂	Me	S	H,H
	4-CF ₃	H	CH ₂	CO ₂ Me	S	H,H
	4-Cl	H	CH ₂	CO ₂ Me	S	H,H
35	4-Br	H	CH ₂	CO ₂ Me	S	H,H

	R ₁	R ₂	A	B	X	R _a ¹ , R _a ²
5	4-CF ₃	H	CH ₂	H	S	H,H
	4-Cl	H	CH ₂	H	S	H,H
	4-Br	H	CH ₂	H	S	H,H
	4-CF ₃	4-F	CH ₂	Me	S	H,H
10	4-Cl	4-F	CH ₂	Me	S	H,H
	4-Br	4-F	CH ₂	Me	S	H,H
	4-CF ₃	4-F	CH ₂	CO ₂ Me	S	H,H
	4-Cl	4-F	CH ₂	CO ₂ Me	S	H,H
15	4-Br	4-F	CH ₂	CO ₂ Me	S	H,H
	4-CF ₃	4-F	CH ₂	H	S	H,H
	4-Cl	4-F	CH ₂	H	S	H,H
	4-Br	4-F	CH ₂	H	S	H,H
20	4-CF ₃	H	O	H	O	H,H
	4-Cl	H	O	H	O	H,H
	4-Br	H	O	H	O	H,H
	4-CF ₃	4-F	O	H	O	H,H
25	4-Cl	4-F	O	H	O	H,H
	4-Br	4-F	O	H	O	H,H
	4-CF ₃	4-Cl	O	H	O	H,H
	4-Cl	4-Cl	O	H	O	H,H
30	4-Br	4-Cl	O	H	O	H,H
	4-CF ₃	4-Me	O	H	O	H,H
	4-Cl	4-Me	O	H	O	H,H
	4-Br	4-Me	O	H	O	H,H
35	4-CF ₃	H	O	Me	O	H,H
	4-Cl	H	O	Me	O	H,H
	4-Br	H	O	Me	O	H,H
	4-CF ₃	4-F	O	Me	O	H,H
35	4-Cl	4-F	O	Me	O	H,H
	4-Br	4-F	O	Me	O	H,H
35	4-CF ₃	4-Cl	O	Me	O	H,H
	4-Cl	4-Cl	O	Me	O	H,H

	R ₁	R ₂	A	B	X	R _a ¹ , R _a ²
5	4-Cl	4-Cl	O	Me	O	H,H
	4-Br	4-Cl	O	Me	O	H,H
	4-CF ₃	4-Me	O	Me	O	H,H
	4-Cl	4-Me	O	Me	O	H,H
10	4-Br	4-Me	O	Me	O	H,H
	4-CF ₃	4-CF ₃	O	Me	O	H,H
	4-Cl	4-CF ₃	O	Me	O	H,H
	4-Br	4-CF ₃	O	Me	O	H,H
15	4-CF ₃	H	O	CO ₂ Me	O	H,H
	4-Cl	H	O	CO ₂ Me	O	H,H
	4-Br	H	O	CO ₂ Me	O	H,H
	4-CF ₃	4-F	O	CO ₂ Me	O	H,H
20	4-Cl	4-F	O	CO ₂ Me	O	H,H
	4-Br	4-F	O	CO ₂ Me	O	H,H
	4-CF ₃	H	O	Ph	O	H,H
	4-Cl	H	O	Ph	O	H,H
25	4-Br	H	O	Ph	O	H,H
	4-CF ₃	4-F	O	Ph	O	H,H
	4-Cl	4-F	O	Ph	O	H,H
	4-Br	4-F	O	Ph	O	H,H
30	4-CF ₃	H	O	H	O	Me,Me
	4-Cl	H	O	H	O	Me,Me
	4-Br	H	O	H	O	Me,Me
	4-CF ₃	H	O	H	O	H,Me
35	4-Cl	H	O	H	O	H,Me
	4-Br	H	O	H	O	H,Me
	4-CF ₃	H	O	H	O	H,Ph
	4-Cl	H	O	H	O	H,Ph
35	4-Br	H	O	H	O	H,CO ₂ Me
	4-CF ₃	H	O	H	O	H,CO ₂ Me
	4-Cl	H	O	H	O	H,CO ₂ Me
	4-Br	H	O	H	O	H,CO ₂ Me
	4-CF ₃	H	O	H	S	H,H

	R_1	R_2	A	B	X	R_a^1, R_a^2
5	4-Cl	H	O	H	S	H,H
	4-Br	H	O	H	S	H,H
	4-CF ₃	H	S	H	O	H,H
	4-Cl	H	S	H	O	H,H
10	4-Br	H	S	H	O	H,H
	4-CF ₃	4-F	S	H	O	H,H
	4-Cl	4-F	S	H	O	H,H
	4-Br	4-F	S	H	O	H,H
	4-CF ₃	4-Cl	S	H	O	H,H
15	4-Cl	4-Cl	S	H	O	H,H
	4-Br	4-Cl	S	H	O	H,H
	4-CF ₃	4-Me	S	H	O	H,H
	4-Cl	4-Me	S	H	O	H,H
	4-Br	4-Me	S	H	O	H,H
20	4-CF ₃	H	S	Me	O	H,H
	4-Cl	H	S	Me	O	H,H
	4-Br	H	S	Me	O	H,H
	4-CF ₃	4-F	S	Me	O	H,H
	4-Cl	4-F	S	Me	O	H,H
25	4-Br	4-F	S	Me	O	H,H
	4-CF ₃	4-Cl	S	Me	O	H,H
	4-Cl	4-Cl	S	Me	O	H,H
	4-Br	4-Cl	S	Me	O	H,H
	4-CF ₃	4-Me	S	Me	O	H,H
30	4-Cl	4-Me	S	Me	O	H,H
	4-Br	4-Me	S	Me	O	H,H
	4-CF ₃	6-F	S	Me	O	H,H
	4-Cl	6-F	S	Me	O	H,H
	4-Br	6-F	S	Me	O	H,H
35	4-CF ₃	H	S	CO ₂ Me	O	H,H
	4-Cl	H	S	CO ₂ Me	O	H,H
	4-Br	H	S	CO ₂ Me	O	H,H
	4-CF ₃	4-F	S	CO ₂ Me	O	H,H

	R ₁	R ₂	A	B	X	R _a ¹ , R _a ²
5	4-Cl	4-F	S	CO ₂ Me	O	H,H
	4-Br	4-F	S	CO ₂ Me	O	H,H
	4-CF ₃	4-Cl	S	Ph	O	H,H
	4-Cl	4-Cl	S	Ph	O	H,H
10	4-Br	4-Cl	S	Ph	O	H,H
	4-CF ₃	H	S	Ph	O	H,H
	4-Cl	H	S	Ph	O	H,H
	4-Br	H	S	Ph	O	H,H
15	4-CF ₃	H	S	H	O	Me,Me
	4-Cl	H	S	H	O	Me,Me
	4-Br	H	S	H	O	Me,Me
	4-CF ₃	H	S	H	O	H,Me
20	4-Cl	H	S	H	O	H,Me
	4-Br	H	S	H	O	H,Me
	4-CF ₃	H	S	H	O	H,Ph
	4-Cl	H	S	H	O	H,Ph
25	4-Br	H	S	H	O	H,CO ₂ Me
	4-CF ₃	H	S	H	O	H,CO ₂ Me
	4-Cl	H	S	H	O	H,CO ₂ Me
	4-Br	H	S	H	O	H,CO ₂ Me
30	4-CF ₃	H	S	H	S	H,H
	4-Cl	H	S	H	S	H,H
	4-Br	H	S	H	S	H,H
35						

Table 3

5

	R ₁	R ₂	A	B	X	R _a ¹ , R _a ²
10	4-CF ₃	H	CH ₂	H	O	H,H
	4-Cl	H	CH ₂	H	O	H,H
	4-Br	H	CH ₂	H	O	H,H
	4-CF ₃	5-Cl	CH ₂	H	O	H,H
	4-Cl	5-Cl	CH ₂	H	O	H,H
	4-Br	5-Cl	CH ₂	H	O	H,H
15	4-CF ₃	5-F	CH ₂	H	O	H,H
	4-Cl	5-F	CH ₂	H	O	H,H
	4-Br	5-F	CH ₂	H	O	H,H
	4-CF ₃	5-CN	CH ₂	H	O	H,H
	4-Cl	5-CN	CH ₂	H	O	H,H
	4-Br	5-CN	CH ₂	H	O	H,H
20	4-CF ₃	5-Br	CH ₂	H	O	H,H
	4-Cl	5-Br	CH ₂	H	O	H,H
	4-Br	5-Br	CH ₂	H	O	H,H
	4-CF ₃	5-Me	CH ₂	H	O	H,H
	4-Cl	5-Me	CH ₂	H	O	H,H
	4-Br	5-Me	CH ₂	H	O	H,H
25	4-CF ₃	7-F	CH ₂	H	O	H,H
	4-Cl	7-F	CH ₂	H	O	H,H
	4-Br	7-F	CH ₂	H	O	H,H
	4-CF ₃	5-NMe ₂	CH ₂	H	O	H,H
	4-Cl	5-NMe ₂	CH ₂	H	O	H,H
	4-Br	5-NMe ₂	CH ₂	H	O	H,H
30	4-CF ₃	5-CF ₃	CH ₂	H	O	H,H
	4-Cl	5-CF ₃	CH ₂	H	O	H,H

35

	R ₁	R ₂	A	B	X	R _a ¹ , R _a ²
5	4-Br	5-CF ₃	CH ₂	H	O	H,H
	4-CF ₃	H	CH ₂	Me	O	H,H
	4-Cl	H	CH ₂	Me	O	H,H
	4-Br	H	CH ₂	Me	O	H,H
10	4-CF ₃	5-Cl	CH ₂	Me	O	H,H
	4-Cl	5-Cl	CH ₂	Me	O	H,H
	4-Br	5-Cl	CH ₂	Me	O	H,H
	4-CF ₃	5-CF ₃	CH ₂	Me	O	H,H
	4-Cl	5-CF ₃	CH ₂	Me	O	H,H
15	4-Br	5-CF ₃	CH ₂	Me	O	H,H
	4-CF ₃	H	CH ₂	Et	O	H,H
	4-Cl	H	CH ₂	Et	O	H,H
	4-Br	H	CH ₂	Et	O	H,H
	4-CF ₃	5-F	CH ₂	Et	O	H,H
20	4-Cl	5-F	CH ₂	Et	O	H,H
	4-Br	5-F	CH ₂	Et	O	H,H
	4-CF ₃	5-CN	CH ₂	Et	O	H,H
	4-Cl	5-CN	CH ₂	Et	O	H,H
	4-Br	5-CN	CH ₂	Et	O	H,H
25	4-CF ₃	H	CH ₂	allyl	O	H,H
	4-Cl	H	CH ₂	allyl	O	H,H
	4-Br	H	CH ₂	allyl	O	H,H
	4-CF ₃	5-Br	CH ₂	allyl	O	H,H
	4-Cl	5-Br	CH ₂	allyl	O	H,H
30	4-Br	5-Br	CH ₂	allyl	O	H,H

	R_1	R_2	A	B	X	R_a^1, R_a^2
5	4-CF ₃	5-Cl	CH ₂	allyl	O	H,H
	4-Cl	5-Cl	CH ₂	allyl	O	H,H
	4-Br	5-Cl	CH ₂	allyl	O	H,H
10	4-CF ₃	H	CH ₂	CO ₂ Me	O	H,H
	4-Cl	H	CH ₂	CO ₂ Me	O	H,H
	4-Br	H	CH ₂	CO ₂ Me	O	H,H
	4-CF ₃	5-F	CH ₂	CO ₂ Me	O	H,H
	4-Cl	5-F	CH ₂	CO ₂ Me	O	H,H
	4-Br	5-F	CH ₂	CO ₂ Me	O	H,H
15	4-CF ₃	5-Cl	CH ₂	CO ₂ Me	O	H,H
	4-Cl	5-Cl	CH ₂	CO ₂ Me	O	H,H
	4-Br	5-Cl	CH ₂	CO ₂ Me	O	H,H
	4-CF ₃	5-Br	CH ₂	CO ₂ Me	O	H,H
	4-Cl	5-Br	CH ₂	CO ₂ Me	O	H,H
20	4-Br	5-Br	CH ₂	CO ₂ Me	O	H,H
	4-CF ₃	5-CN	CH ₂	CO ₂ Me	O	H,H
	4-Cl	5-CN	CH ₂	CO ₂ Me	O	H,H
	4-Br	5-CN	CH ₂	CO ₂ Me	O	H,H
	4-CF ₃	5-CF ₃	CH ₂	CO ₂ Me	O	H,H
25	4-Cl	5-CF ₃	CH ₂	CO ₂ Me	O	H,H
	4-Br	5-CF ₃	CH ₂	CO ₂ Me	O	H,H
	4-CF ₃	5-Me	CH ₂	CO ₂ Me	O	H,H
	4-Cl	5-Me	CH ₂	CO ₂ Me	O	H,H
	4-Br	5-Me	CH ₂	CO ₂ Me	O	H,H
30	4-CF ₃	H	CH ₂	CO ₂ Et	O	H,H

	R ₁	R ₂	A	B	X	R _a ¹ , R _a ²
5	4-Cl	H	CH ₂	CO ₂ Et	O	H,H
	4-Br	H	CH ₂	CO ₂ Et	O	H,H
	4-CF ₃	5-Cl	CH ₂	CO ₂ Et	O	H,H
	4-Cl	5-Cl	CH ₂	CO ₂ Et	O	H,H
10	4-Br	5-Cl	CH ₂	CO ₂ Et	O	H,H
	4-CF ₃	H	CH ₂	CO ₂ -i-Pr	O	H,H
	4-Cl	H	CH ₂	CO ₂ -i-Pr	O	H,H
	4-Br	H	CH ₂	CO ₂ -i-Pr	O	H,H
15	4-CF ₃	H	CH ₂	CO ₂ CH ₂ CF ₃	O	H,H
	4-Cl	H	CH ₂	CO ₂ CH ₂ CF ₃	O	H,H
	4-Br	H	CH ₂	CO ₂ CH ₂ CF ₃	O	H,H
	4-CF ₃	H	CH ₂	CO ₂ allyl	O	H,H
20	4-Cl	H	CH ₂	CO ₂ allyl	O	H,H
	4-Br	H	CH ₂	CO ₂ allyl	O	H,H
	4-CF ₃	H	CH ₂	CO ₂ CH ₂ CH ₂ Cl	O	H,H
	4-Cl	H	CH ₂	CO ₂ CH ₂ CH ₂ Cl	O	H,H
25	4-Br	H	CH ₂	CO ₂ CH ₂ CH ₂ Cl	O	H,H
	4-CF ₃	H	CH ₂	Ph	O	H,H
	4-Cl	H	CH ₂	Ph	O	H,H
	4-Br	H	CH ₂	Ph	O	H,H
30	4-CF ₃	5-Cl	CH ₂	Ph	O	H,H
	4-Cl	5-Cl	CH ₂	Ph	O	H,H
	4-Br	5-Cl	CH ₂	Ph	O	H,H
	4-CF ₃	H	CH ₂	4-Cl-Ph	O	H,H
35	4-Cl	H	CH ₂	4-Cl-Ph	O	H,H
	4-Br	H	CH ₂	4-Cl-Ph	O	H,H

	R ₁	R ₂	A	B	X	R _a ¹ , R _a ²
5	4-CF ₃	5-CF ₃	CH ₂	4-Cl-Ph	O	H,H
	4-Cl	5-CF ₃	CH ₂	4-Cl-Ph	O	H,H
	4-Br	5-CF ₃	CH ₂	4-Cl-Ph	O	H,H
	4-CF ₃	H	CH ₂	4-F-Ph	O	H,H
10	4-Cl	H	CH ₂	4-F-Ph	O	H,H
	4-Br	H	CH ₂	4-F-Ph	O	H,H
	4-CF ₃	H	CH ₂	H	O	H,Me
	4-Cl	H	CH ₂	H	O	H,Me
	4-Br	H	CH ₂	H	O	H,Me
15	4-CF ₃	5-Cl	CH ₂	H	O	Me,Me
	4-Cl	5-Cl	CH ₂	H	O	Me,Me
	4-Br	5-Cl	CH ₂	H	O	Me,Me
	4-CF ₃	H	CH ₂	H	S	H,H
	4-Cl	H	CH ₂	H	S	H,H
20	4-Br	H	CH ₂	H	S	H,H
	4-CF ₃	H	CH ₂	Me	S	H,H
	4-Cl	H	CH ₂	Me	S	H,H
	4-Br	H	CH ₂	Me	S	H,H
	4-CF ₃	H	CH ₂	CO ₂ Me	S	H,H
25	4-Cl	H	CH ₂	CO ₂ Me	S	H,H
	4-Br	H	CH ₂	CO ₂ Me	S	H,H
	4-CF ₃	5-Cl	CH ₂	H	S	H,H
	4-Cl	5-Cl	CH ₂	H	S	H,H
	4-Br	5-Cl	CH ₂	H	S	H,H
30	4-CF ₃	5-Cl	CH ₂	Me	S	H,H

	R ₁	R ₂	A	B	X	R _a ¹ , R _a ²
5	4-Cl	5-Cl	CH ₂	Me	S	H,H
	4-Br	5-Cl	CH ₂	Me	S	H,H
	4-CF ₃	5-Cl	CH ₂	CO ₂ Me	S	H,H
	4-Cl	5-Cl	CH ₂	CO ₂ Me	S	H,H
10	4-Br	5-Cl	CH ₂	CO ₂ Me	S	H,H
	4-CF ₃	5-Me	CH ₂	H	S	H,H
	4-Cl	5-Me	CH ₂	H	S	H,H
	4-Br	5-Me	CH ₂	H	S	H,H
	4-CF ₃	H	O	H	O	H,H
15	4-Cl	H	O	H	O	H,H
	4-Br	H	O	H	O	H,H
	4-CF ₃	5-Cl	O	H	O	H,H
	4-Cl	5-Cl	O	H	O	H,H
	4-Br	5-Cl	O	H	O	H,H
20	4-CF ₃	5-Br	O	H	O	H,H
	4-Cl	5-Br	O	H	O	H,H
	4-Br	5-Br	O	H	O	H,H
	4-CF ₃	5-CF ₃	O	H	O	H,H
	4-Cl	5-CF ₃	O	H	O	H,H
25	4-Br	5-CF ₃	O	H	O	H,H
	4-CF ₃	H	O	Me	O	H,H
	4-Cl	H	O	Me	O	H,H
	4-Br	H	O	Me	O	H,H
	4-CF ₃	5-Cl	O	Me	O	H,H

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	R ₁	R ₂	A	B	X	R _a ¹ , R _a ²
5	4-Cl	5-Cl	O	Me	O	H,H
	4-Br	5-Cl	O	Me	O	H,H
	4-CF ₃	5-Br	O	Me	O	H,H
	4-Cl	5-Br	O	Me	O	H,H
10	4-Br	5-Br	O	Me	O	H,H
	4-CF ₃	5-CF ₃	O	Me	O	H,H
	4-Cl	5-CF ₃	O	Me	O	H,H
	4-Br	5-CF ₃	O	Me	O	H,H
	4-CF ₃	5-F	O	Me	O	H,H
15	4-Cl	5-F	O	Me	O	H,H
	4-Br	5-F	O	Me	O	H,H
	4-CF ₃	H	O	CO ₂ Me	O	H,H
	4-Cl	H	O	CO ₂ Me	O	H,H
	4-Br	H	O	CO ₂ Me	O	H,H
20	4-CF ₃	5-Cl	O	CO ₂ Me	O	H,H
	4-Cl	5-Cl	O	CO ₂ Me	O	H,H
	4-Br	5-Cl	O	CO ₂ Me	O	H,H
	4-CF ₃	H	O	Ph	O	H,H
	4-Cl	H	O	Ph	O	H,H
25	4-Br	H	O	Ph	O	H,H
	4-CF ₃	5-Br	O	Ph	O	H,H
	4-Cl	5-Br	O	Ph	O	H,H
	4-Br	5-Br	O	Ph	O	H,H

30

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	R ₁	R ₂	A	B	X	R _a ¹ , R _a ²
5	4-CF ₃	H	O	H	O	Me, Me
	4-Cl	H	O	H	O	Me, Me
	4-Br	H	O	H	O	Me, Me
	4-CF ₃	H	O	H	O	H, Me
10	4-Cl	H	O	H	O	H, Me
	4-Br	H	O	H	O	H, Me
	4-CF ₃	H	O	H	O	H, Ph
	4-Cl	H	O	H	O	H, Ph
	4-Br	H	O	H	O	H, Ph
	4-CF ₃	H	O	H	O	H, CO ₂ Me
15	4-Cl	H	O	H	O	H, CO ₂ Me
	4-Br	H	O	H	O	H, CO ₂ Me
	4-CF ₃	H	O	H	S	H, H
	4-Cl	H	O	H	S	H, H
	4-Br	H	O	H	S	H, H
20	4-CF ₃	H	S	H	O	H, H
	4-Cl	H	S	H	O	H, H
	4-Br	H	S	H	O	H, H
	4-CF ₃	5-Cl	S	H	O	H, H
	4-Cl	5-Cl	S	H	O	H, H
25	4-Br	5-Cl	S	H	O	H, H
	4-CF ₃	5-Br	S	H	O	H, H
	4-Cl	5-Br	S	H	O	H, H
	4-Br	5-Br	S	H	O	H, H

30

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	R ₁	R ₂	A	B	X	R _a ¹ , R _a ²
5	4-CF ₃	5-CF ₃	S	H	O	H,H
	4-Cl	5-CF ₃	S	H	O	H,H
	4-Br	5-CF ₃	S	H	O	H,H
	4-CF ₃	H	S	Me	O	H,H
10	4-Cl	H	S	Me	O	H,H
	4-Br	H	S	Me	O	H,H
	4-CF ₃	5-Cl	S	Me	O	H,H
	4-Cl	5-Cl	S	Me	O	H,H
	4-Br	5-Cl	S	Me	O	H,H
15	4-CF ₃	5-Br	S	Me	O	H,H
	4-Cl	5-Br	S	Me	O	H,H
	4-Br	5-Br	S	Me	O	H,H
	4-CF ₃	5-CF ₃	S	Me	O	H,H
	4-Cl	5-CF ₃	S	Me	O	H,H
20	4-Br	5-CF ₃	S	Me	O	H,H
	4-CF ₃	5-F	S	Me	O	H,H
	4-Cl	5-F	S	Me	O	H,H
	4-Br	5-F	S	Me	O	H,H
	4-CF ₃	H	S	CO ₂ Me	O	H,H
25	4-Cl	H	S	CO ₂ Me	O	H,H
	4-Br	H	S	CO ₂ Me	O	H,H
	4-CF ₃	5-Cl	S	CO ₂ Me	O	H,H
	4-Cl	5-Cl	S	CO ₂ Me	O	H,H
	4-Br	5-Cl	S	CO ₂ Me	O	H,H
30	4-CF ₃	H	S	Ph	O	H,H

	R_1	R_2	A	B	X	R_a^1, R_a^2
5	4-Cl	H	S	Ph	O	H,H
	4-Br	H	S	Ph	O	H,H
	4-CF ₃	5-Br	S	Ph	O	H,H
10	4-Cl	5-Br	S	Ph	O	H,H
	4-Br	5-Br	S	Ph	O	H,H
	4-CF ₃	H	S	H	O	Me,Me
	4-Cl	H	S	H	O	Me,Me
	4-Br	H	S	H	O	Me,Me
15	4-CF ₃	H	S	H	O	H,Me
	4-Cl	H	S	H	O	H,Me
	4-Br	H	S	H	O	H,Me
	4-CF ₃	H	S	H	O	H,Ph
	4-Cl	H	S	H	O	H,Ph
	4-Br	H	S	H	O	H,Ph
	4-CF ₃	H	S	H	O	H,CO ₂ Me
20	4-Cl	H	S	H	O	H,CO ₂ Me
	4-Br	H	S	H	O	H,CO ₂ Me
	4-CF ₃	H	S	H	S	H,H
	4-Cl	H	S	H	S	H,H
	4-Br	H	S	H	S	H,H
25						
30						
35						

Table 4

5	R ₁	R ₂	A	B	X	R _a ¹ , R _a ²
	4-CF ₃	H	CH ₂	H	O	H,H
	4-Cl	H	CH ₂	H	O	H,H
	4-Br	H	CH ₂	H	O	H,H
10	4-CF ₃	4-Me	CH ₂	H	O	H,H
	4-Cl	4-Me	CH ₂	H	O	H,H
	4-Br	4-Me	CH ₂	H	O	H,H
	4-CF ₃	4-F	CH ₂	H	O	H,H
	4-Cl	4-F	CH ₂	H	O	H,H
	4-Br	4-F	CH ₂	H	O	H,H
15	4-CF ₃	4-Cl	CH ₂	H	O	H,H
	4-Cl	4-Cl	CH ₂	H	O	H,H
	4-Br	4-Cl	CH ₂	H	O	H,H
	4-CF ₃	5-F	CH ₂	H	O	H,H
20	4-Cl	5-F	CH ₂	H	O	H,H
	4-Br	5-F	CH ₂	H	O	H,H
	4-CF ₃	5-Cl	CH ₂	H	O	H,H
	4-Cl	5-Cl	CH ₂	H	O	H,H
	4-Br	5-Cl	CH ₂	H	O	H,H
25	4-CF ₃	5-Me	CH ₂	H	O	H,H
	4-Cl	5-Me	CH ₂	H	O	H,H
	4-Br	5-Me	CH ₂	H	O	H,H
	4-CF ₃	5-Br	CH ₂	H	O	H,H
	4-Cl	5-Br	CH ₂	H	O	H,H
	4-Br	5-Br	CH ₂	H	O	H,H
30	4-CF ₃	5-OMe	CH ₂	H	O	H,H
	4-Cl	5-OMe	CH ₂	H	O	H,H
	4-Br	5-OMe	CH ₂	H	O	H,H
	4-CF ₃	H	CH ₂	Me	O	H,H

	R ₁	R ₂	A	B	X	R _a ¹ , R _a ²
5	4-Cl	H	CH ₂	Me	O	H,H
	4-Br	H	CH ₂	Me	O	H,H
	4-CF ₃	4-F	CH ₂	Me	O	H,H
	4-Cl	4-F	CH ₂	Me	O	H,H
10	4-Br	4-F	CH ₂	Me	O	H,H
	4-CF ₃	5-F	CH ₂	Me	O	H,H
	4-Cl	5-F	CH ₂	Me	O	H,H
	4-Br	5-F	CH ₂	Me	O	H,H
	4-CF ₃	H	CH ₂	Me	O	H,H
15	4-Cl	H	CH ₂	Et	O	H,H
	4-Br	H	CH ₂	Et	O	H,H
	4-CF ₃	4-F	CH ₂	Et	O	H,H
	4-Cl	4-F	CH ₂	Et	O	H,H
	4-Br	4-F	CH ₂	Et	O	H,H
20	4-CF ₃	4-Cl	CH ₂	Et	O	H,H
	4-Cl	4-Cl	CH ₂	Et	O	H,H
	4-Br	4-Cl	CH ₂	Et	O	H,H
	4-CF ₃	H	CH ₂	allyl	O	H,H
	4-Cl	H	CH ₂	allyl	O	H,H
25	4-Br	H	CH ₂	allyl	O	H,H
	4-CF ₃	5-F	CH ₂	allyl	O	H,H
	4-Cl	5-F	CH ₂	allyl	O	H,H
	4-Br	5-F	CH ₂	allyl	O	H,H
	4-CF ₃	5-Cl	CH ₂	allyl	O	H,H
30	4-Cl	5-Cl	CH ₂	allyl	O	H,H

	R ₁	R ₂	A	B	X	R _a ¹ , R _a ²
5	4-Br	5-Cl	CH ₂	allyl	O	H,H
	4-CF ₃	H	CH ₂	CO ₂ Me	O	H,H
	4-Cl	H	CH ₂	CO ₂ Me	O	H,H
	4-Br	H	CH ₂	CO ₂ Me	O	H,H
10	4-CF ₃	4-F	CH ₂	CO ₂ Me	O	H,H
	4-Cl	4-F	CH ₂	CO ₂ Me	O	H,H
	4-Br	4-F	CH ₂	CO ₂ Me	O	H,H
	4-CF ₃	4-F	CH ₂	CO ₂ Me	O	H,H
	4-Cl	4-F	CH ₂	CO ₂ Me	O	H,H
15	4-Br	4-F	CH ₂	CO ₂ Me	O	H,H
	4-CF ₃	5-F	CH ₂	CO ₂ Me	O	H,H
	4-Cl	5-F	CH ₂	CO ₂ Me	O	H,H
	4-Br	5-F	CH ₂	CO ₂ Me	O	H,H
	4-CF ₃	4-Cl	CH ₂	CO ₂ Me	O	H,H
20	4-Cl	4-Cl	CH ₂	CO ₂ Me	O	H,H
	4-Br	4-Cl	CH ₂	CO ₂ Me	O	H,H
	4-CF ₃	5-Cl	CH ₂	CO ₂ Me	O	H,H
	4-Cl	5-Cl	CH ₂	CO ₂ Me	O	H,H
	4-Br	5-Cl	CH ₂	CO ₂ Me	O	H,H
25	4-CF ₃	5-CF ₃	CH ₂	CO ₂ Me	O	H,H
	4-Cl	5-CF ₃	CH ₂	CO ₂ Me	O	H,H
	4-Br	5-CF ₃	CH ₂	CO ₂ Me	O	H,H
	4-CF ₃	5-Me	CH ₂	CO ₂ Me	O	H,H
	4-Cl	5-Me	CH ₂	CO ₂ Me	O	H,H
30	4-Br	5-Me	CH ₂	CO ₂ Me	O	H,H

	R ₁	R ₂	A	B	X	R _a ¹ , R _a ²
5	4-CF ₃	H	CH ₂	CO ₂ Et	O	H,H
	4-Cl	H	CH ₂	CO ₂ Et	O	H,H
	4-Br	H	CH ₂	CO ₂ Et	O	H,H
	4-CF ₃	5-Me	CH ₂	CO ₂ Et	O	H,H
10	4-Cl	5-Me	CH ₂	CO ₂ Et	O	H,H
	4-Br	5-Me	CH ₂	CO ₂ Et	O	H,H
	4-CF ₃	H	CH ₂	CO ₂ i-Pr	O	H,H
	4-Cl	H	CH ₂	CO ₂ i-Pr	O	H,H
	4-Br	H	CH ₂	CO ₂ i-Pr	O	H,H
15	4-CF ₃	H	CH ₂	CO ₂ CH ₂ CF ₃	O	H,H
	4-Cl	H	CH ₂	CO ₂ CH ₂ CF ₃	O	H,H
	4-Br	H	CH ₂	CO ₂ CH ₂ CF ₃	O	H,H
	4-CF ₃	H	CH ₂	CO ₂ allyl	O	H,H
	4-Cl	H	CH ₂	CO ₂ allyl	O	H,H
20	4-Br	H	CH ₂	CO ₂ allyl	O	H,H
	4-CF ₃	H	CH ₂	CO ₂ CH ₂ CH ₂ Cl	O	H,H
	4-Cl	H	CH ₂	CO ₂ CH ₂ CH ₂ Cl	O	H,H
	4-Br	H	CH ₂	CO ₂ CH ₂ CH ₂ Cl	O	H,H
	4-CF ₃	H	CH ₂	Ph	O	H,H
25	4-Cl	H	CH ₂	Ph	O	H,H
	4-Br	H	CH ₂	Ph	O	H,H
	4-CF ₃	4-F	CH ₂	Ph	O	H,H
	4-Cl	4-F	CH ₂	Ph	O	H,H
	4-Br	4-F	CH ₂	Ph	O	H,H
30	4-CF ₃	H	CH ₂	4-Cl-Ph	O	H,H
	4-Cl	H	CH ₂	4-Cl-Ph	O	H,H

	R ₁	R ₂	A	B	X	R _a ¹ , R _a ²
5	4-Br	H	CH ₂	4-Cl-Ph	O	H,H
	4-CF ₃	5-Cl	CH ₂	4-Cl-Ph	O	H,H
	4-Cl	5-Cl	CH ₂	4-Cl-Ph	O	H,H
	4-Br	5-Cl	CH ₂	4-Cl-Ph	O	H,H
10	4-CF ₃	H	CH ₂	4-F-Ph	O	H,H
	4-Cl	H	CH ₂	4-F-Ph	O	H,H
	4-Br	H	CH ₂	4-F-Ph	O	H,H
	4-CF ₃	H	CH ₂	H	O	H,Me
	4-Cl	H	CH ₂	H	O	H,Me
15	4-Br	H	CH ₂	H	O	H,Me
	4-CF ₃	5-Cl	CH ₂	H	O	Me,Me
	4-Cl	5-Cl	CH ₂	H	O	Me,Me
	4-Br	5-Cl	CH ₂	H	O	Me,Me
	4-CF ₃	H	CH ₂	H	S	H,H
20	4-Cl	H	CH ₂	H	S	H,H
	4-Br	H	CH ₂	H	S	H,H
	4-CF ₃	H	CH ₂	Me	S	H,H
	4-Cl	H	CH ₂	Me	S	H,H
	4-Br	H	CH ₂	Me	S	H,H
25	4-CF ₃	H	CH ₂	CO ₂ Me	S	H,H
	4-Cl	H	CH ₂	CO ₂ Me	S	H,H
	4-Br	H	CH ₂	CO ₂ Me	S	H,H
	4-CF ₃	5-Cl	CH ₂	H	S	H,H
	4-Cl	5-Cl	CH ₂	H	S	H,H
30	4-Br	5-Cl	CH ₂	H	S	H,H

	R ₁	R ₂	A	B	X	R _a ¹ , R _a ²
5	4-CF ₃	5-Cl	CH ₂	Me	S	H,H
	4-Cl	5-Cl	CH ₂	Me	S	H,H
	4-Br	5-Cl	CH ₂	Me	S	H,H
	4-CF ₃	5-Cl	CH ₂	CO ₂ Me	S	H,H
10	4-Cl	5-Cl	CH ₂	CO ₂ Me	S	H,H
	4-Br	5-Cl	CH ₂	CO ₂ Me	S	H,H
	4-CF ₃	H	O	H	O	H,H
	4-Cl	H	O	H	O	H,H
	4-Br	H	O	H	O	H,H
15	4-CF ₃	5-Cl	O	H	O	H,H
	4-Cl	5-Cl	O	H	O	H,H
	4-Br	5-Cl	O	H	O	H,H
	4-CF ₃	4-F	O	H	O	H,H
	4-Cl	4-F	O	H	O	H,H
20	4-Br	4-F	O	H	O	H,H
	4-CF ₃	5-CF ₃	O	H	O	H,H
	4-Cl	5-CF ₃	O	H	O	H,H
	4-Br	5-CF ₃	O	H	O	H,H
	4-CF ₃	H	O	Me	O	H,H
25	4-Cl	H	O	Me	O	H,H
	4-Br	H	O	Me	O	H,H
	4-CF ₃	4-F	O	Me	O	H,H
	4-Cl	4-F	O	Me	O	H,H
	4-Br	4-F	O	Me	O	H,H
30						
35						

	R ₁	R ₂	A	B	X	R _a ¹ , R _a ²
5	4-CF ₃	4-Cl	O	Me	O	H,H
	4-Cl	4-Cl	O	Me	O	H,H
	4-Br	4-Cl	O	Me	O	H,H
	4-CF ₃	5-F	O	Me	O	H,H
10	4-Cl	5-F	O	Me	O	H,H
	4-Br	5-F	O	Me	O	H,H
	4-CF ₃	5-Cl	O	Me	O	H,H
	4-Cl	5-Cl	O	Me	O	H,H
15	4-Br	5-Cl	O	Me	O	H,H
	4-CF ₃	H	O	CO ₂ Me	O	H,H
	4-Cl	H	O	CO ₂ Me	O	H,H
	4-Br	H	O	CO ₂ Me	O	H,H
20	4-CF ₃	5-Cl	O	CO ₂ Me	O	H,H
	4-Cl	5-Cl	O	CO ₂ Me	O	H,H
	4-Br	5-Cl	O	CO ₂ Me	O	H,H
	4-CF ₃	H	O	Ph	O	H,H
25	4-Cl	H	O	Ph	O	H,H
	4-Br	H	O	Ph	O	H,H
	4-CF ₃	5-Cl	O	Ph	O	H,H
	4-Cl	5-Cl	O	Ph	O	H,H
30	4-Br	5-Cl	O	Ph		H,H
	4-CF ₃	H	O	H	O	Me,Me
	4-Cl	H	O	H	O	Me,Me
	4-Br	H	O	H	O	Me,Me
35	4-CF ₃	H	O	H	O	H,Me
	4-Cl	H	O	H	O	H,Me
	4-Br	H	O	H	O	H,Me
	4-CF ₃	H	O	H	O	H,Ph
	4-Cl	H	O	H	O	H,Ph
	4-Br	H	O	H	O	H,Ph
	4-CF ₃	H	O	H	O	H,CO ₂ Me
	4-Cl	H	O	H	O	H,CO ₂ Me
	4-Br	H	O	H	O	H,CO ₂ Me

	R ₁	R ₂	A	B	X	R _a ¹ , R _a ²
5	4-CF ₃	H	O	H	S	H,H
	4-Cl	H	O	H	S	H,H
	4-Br	H	O	H	S	H,H
10	4-CF ₃	H	S	H	O	H,H
	4-Cl	H	S	H	O	H,H
	4-Br	H	S	H	O	H,H
	4-CF ₃	5-Cl	S	H	O	H,H
	4-Cl	5-Cl	S	H	O	H,H
	4-Br	5-Cl	S	H	O	H,H
15	4-CF ₃	4-F	S	H	O	H,H
	4-Cl	4-F	S	H	O	H,H
	4-Br	4-F	S	H	O	H,H
	4-CF ₃	5-CF ₃	S	H	O	H,H
	4-Cl	5-CF ₃	S	H	O	H,H
20	4-Br	5-CF ₃	S	H	O	H,H
	4-CF ₃	H	S	Me	O	H,H
	4-Cl	H	S	Me	O	H,H
	4-Br	H	S	Me	O	H,H
	4-CF ₃	4-F	S	Me	O	H,H
25	4-Cl	4-F	S	Me	O	H,H
	4-Br	4-F	S	Me	O	H,H
	4-CF ₃	4-Cl	S	Me	O	H,H
	4-Cl	4-Cl	S	Me	O	H,H
	4-Br	4-Cl	S	Me	O	H,H
30	4-CF ₃	5-F	S	Me	O	H,H
	4-Cl	5-F	S	Me	O	H,H
	4-Br	5-F	S	Me	O	H,H
	4-CF ₃	5-Cl	S	Me	O	H,H
	4-Cl	5-Cl	S	Me	O	H,H
35	4-Br	5-Cl	S	Me	O	H,H
	4-CF ₃	H	S	CO ₂ Me	O	H,H

	R ₁	R ₂	A	B	X	R _a ¹ , R _a ²
5	4-Cl	H	S	CO ₂ Me	O	H,H
	4-Br	H	S	CO ₂ Me	O	H,H
	4-CF ₃	5-Cl	S	CO ₂ Me	O	H,H
	4-Cl	5-Cl	S	CO ₂ Me	O	H,H
10	4-Br	5-Cl	S	CO ₂ Me	O	H,H
	4-CF ₃	H	S	Ph	O	H,H
	4-Cl	H	S	Ph	O	H,H
	4-Br	H	S	Ph	O	H,H
15	4-CF ₃	5-Cl	S	Ph	O	H,H
	4-Cl	5-Cl	S	Ph	O	H,H
	4-Br	5-Cl	S	Ph	O	H,H
	4-CF ₃	H	S	H	O	Me,Me
20	4-Cl	H	S	H	O	Me,Me
	4-Br	H	S	H	O	Me,Me
	4-CF ₃	H	S	H	O	H,Me
	4-Cl	H	S	H	O	H,Me
25	4-Br	H	S	H	O	H,Me
	4-CF ₃	H	S	H	O	H,Ph
	4-Cl	H	S	H	O	H,Ph
	4-Br	H	S	H	O	H,CO ₂ Me
30	4-CF ₃	H	S	H	O	H,CO ₂ Me
	4-Br	H	S	H	O	H,CO ₂ Me
	4-CF ₃	H	S	H	S	H,H
	4-Cl	H	S	H	S	H,H

35

Table 5

5	R ₁	R ₂	A	B	X	R _a ¹ , R _a ²
	4-CF ₃	H	CH ₂	H	O	H,H
	4-Cl	H	CH ₂	H	O	H,H
	4-Br	H	CH ₂	H	O	H,H
10	4-CF ₃	5-Cl	CH ₂	H	O	H,H
	4-Cl	5-Cl	CH ₂	H	O	H,H
	4-Br	5-Cl	CH ₂	H	O	H,H
	4-CF ₃	5-F	CH ₂	H	O	H,H
	4-Cl	5-F	CH ₂	H	O	H,H
	4-Br	5-F	CH ₂	H	O	H,H
15	4-CF ₃	5-Me	CH ₂	H	O	H,H
	4-Cl	5-Me	CH ₂	H	O	H,H
	4-Br	5-Me	CH ₂	H	O	H,H
	4-CF ₃	H	CH ₂	Me	O	H,H
	4-Cl	H	CH ₂	Me	O	H,H
	4-Br	H	CH ₂	Me	O	H,H
20	4-CF ₃	5-Cl	CH ₂	Me	O	H,H
	4-Cl	5-Cl	CH ₂	Me	O	H,H
	4-Br	5-Cl	CH ₂	Me	O	H,H
	4-CF ₃	5-F	CH ₂	Me	O	H,H
	4-Cl	5-F	CH ₂	Me	O	H,H
	4-Br	5-F	CH ₂	Me	O	H,H
25	4-CF ₃	5-Me	CH ₂	Me	O	H,H
	4-Cl	5-Me	CH ₂	Me	O	H,H
	4-Br	5-Me	CH ₂	Me	O	H,H
30	4-CF ₃	H	CH ₂	Et	O	H,H
	4-Cl	H	CH ₂	Et	O	H,H
	4-Br	H	CH ₂	Et	O	H,H
	4-CF ₃	H	CH ₂	CO ₂ Me	O	H,H
35						

	R ₁	R ₂	A	B	X	R _a ¹ , R _a ²
5	4-Cl	H	CH ₂	CO ₂ Me	O	H,H
	4-Br	H	CH ₂	CO ₂ Me	O	H,H
	4-CF ₃	5-F	CH ₂	CO ₂ Me	O	H,H
	4-Cl	5-F	CH ₂	CO ₂ Me	O	H,H
10	4-Br	5-F	CH ₂	CO ₂ Me	O	H,H
	4-CF ₃	5-Cl	CH ₂	CO ₂ Me	O	H,H
	4-Cl	5-Cl	CH ₂	CO ₂ Me	O	H,H
	4-Br	5-Cl	CH ₂	CO ₂ Me	O	H,H
15	4-CF ₃	5-Me	CH ₂	CO ₂ Me	O	H,H
	4-Cl	5-Me	CH ₂	CO ₂ Me	O	H,H
	4-Br	5-Me	CH ₂	CO ₂ Me	O	H,H
	4-CF ₃	5-Cl	CH ₂	CO ₂ Et	O	H,H
20	4-Cl	5-Cl	CH ₂	CO ₂ Et	O	H,H
	4-Br	5-Cl	CH ₂	CO ₂ Et	O	H,H
	4-CF ₃	H	CH ₂	Ph	O	H,H
	4-Cl	H	CH ₂	Ph	O	H,H
25	4-Br	H	CH ₂	Ph	O	H,H
	4-CF ₃	5-Cl	CH ₂	Ph	O	H,H
	4-Cl	5-Cl	CH ₂	Ph	O	H,H
	4-Br	5-Cl	CH ₂	Ph	O	H,H
30	4-CF ₃	H	CH ₂	4-Cl-Ph	O	H,H
	4-Cl	H	CH ₂	4-Cl-Ph	O	H,H
	4-Br	H	CH ₂	4-Cl-Ph	O	H,H
	4-CF ₃	5-Cl	CH ₂	4-Cl-Ph	O	H,H
35	4-Cl	5-Cl	CH ₂	4-Cl-Ph	O	H,H
	4-Br	5-Cl	CH ₂	4-Cl-Ph	O	H,H
	4-CF ₃	5-CO ₂ Me	CH ₂	H	O	H,H
	4-CF ₃	H	O	H	O	H,H
35	4-CF ₃	H	O	Me	O	H,H
	4-CF ₃	H	O	i-Pr	O	H,H
	4-CF ₃	H	O	CO ₂ Me	O	H,H

	R ₁	R ₂	A	B	X	R _a ¹ , R _a ²
5	4-CF ₃	H	O	Ph	O	H,H
	4-CF ₃	H	O	4-F-Ph	O	H,H
	4-CF ₃	H	O	4-Cl-Ph	O	H,H
	4-CF ₃	5-F	O	H	O	H,H
10	4-CF ₃	5-F	O	Me	O	H,H
	4-CF ₃	5-F	O	i-Pr	O	H,H
	4-CF ₃	5-F	O	CO ₂ Me	O	H,H
	4-CF ₃	5-F	O	Ph	O	H,H
	4-CF ₃	5-F	O	4-F-Ph	O	H,H
15	4-CF ₃	5-F	O	4-Cl-Ph	O	H,H
	4-CF ₃	5-Cl	O	H	O	H,H
	4-CF ₃	5-Cl	O	Me	O	H,H
	4-CF ₃	5-Cl	O	i-Pr	O	H,H
	4-CF ₃	5-Cl	O	CO ₂ Me	O	H,H
20	4-CF ₃	5-Cl	O	Ph	O	H,H
	4-CF ₃	5-Cl	O	4-F-Ph	O	H,H
	4-CF ₃	5-Cl	O	4-Cl-Ph	O	H,H
	4-OCF ₃	H	O	H	O	H,H
	4-OCF ₃	H	O	Me	O	H,H
25	4-OCF ₃	H	O	i-Pr	O	H,H
	4-OCF ₃	H	O	CO ₂ Me	O	H,H
	4-OCF ₃	H	O	Ph	O	H,H
	4-OCF ₃	H	O	4-F-Ph	O	H,H
	4-OCF ₃	H	O	4-Cl-Ph	O	H,H
30	4-OCF ₃	5-F	O	H	O	H,H
	4-OCF ₃	5-F	O	Me	O	H,H
	4-OCF ₃	5-F	O	i-Pr	O	H,H
	4-OCF ₃	5-F	O	CO ₂ Me	O	H,H
	4-OCF ₃	5-F	O	Ph	O	H,H
35	4-OCF ₃	5-F	O	4-F-Ph	O	H,H
	4-OCF ₃	5-F	O	4-Cl-Ph	O	H,H

	R ₁	R ₂	A	B	X	R _a ¹ , R _a ²
5	4-OCF ₃	5-Cl	O	H	O	H,H
	4-OCF ₃	5-Cl	O	Me	O	H,H
	4-OCF ₃	5-Cl	O	i-Pr	O	H,H
	4-OCF ₃	5-Cl	O	CO ₂ Me	O	H,H
10	4-OCF ₃	5-Cl	O	Ph	O	H,H
	4-OCF ₃	5-Cl	O	4-F-Ph	O	H,H
	4-OCF ₃	5-Cl	O	4-Cl-Ph	O	H,H
	4-Br	H	O	H	O	H,H
	4-Br	H	O	Me	O	H,H
15	4-Br	H	O	i-Pr	O	H,H
	4-Br	H	O	CO ₂ Me	O	H,H
	4-Br	H	O	Ph	O	H,H
	4-Br	H	O	4-F-Ph	O	H,H
	4-Br	H	O	4-Cl-Ph	O	H,H
20	4-Br	5-F	O	H	O	H,H
	4-Br	5-F	O	Me	O	H,H
	4-Br	5-F	O	i-Pr	O	H,H
	4-Br	5-F	O	CO ₂ Me	O	H,H
	4-Br	5-F	O	Ph	O	H,H
25	4-Br	5-F	O	4-F-Ph	O	H,H
	4-Br	5-F	O	4-Cl-Ph	O	H,H
	4-Br	5-Cl	O	H	O	H,H
	4-Br	5-Cl	O	Me	O	H,H
	4-Br	5-Cl	O	i-Pr	O	H,H
30	4-Br	5-Cl	O	CO ₂ Me	O	H,H
	4-Br	5-Cl	O	Ph	O	H,H
	4-Br	5-Cl	O	4-F-Ph	O	H,H
	4-Br	5-Cl	O	4-Cl-Ph	O	H,H
	4-Cl	H	O	H	O	H,H
35	4-Cl	H	O	Me	O	H,H
	4-Cl	H	O	i-Pr	O	H,H
	4-Cl	H	O	CO ₂ Me	O	H,H

	R_1	R_2	A	B	X	R_a^1, R_a^2
5	4-Cl	H	O	Ph	O	H,H
	4-Cl	H	O	4-F-Ph	O	H,H
	4-Cl	H	O	4-Cl-Ph	O	H,H
	4-Cl	5-F	O	H	O	H,H
10	4-Cl	5-F	O	Me	O	H,H
	4-Cl	5-F	O	i-Pr	O	H,H
	4-Cl	5-F	O	CO ₂ Me	O	H,H
	4-Cl	5-F	O	Ph	O	H,H
	4-Cl	5-F	O	4-F-Ph	O	H,H
15	4-Cl	5-F	O	4-Cl-Ph	O	H,H
	4-Cl	5-Cl	O	H	O	H,H
	4-Cl	5-Cl	O	Me	O	H,H
	4-Cl	5-Cl	O	i-Pr	O	H,H
	4-Cl	5-Cl	O	CO ₂ Me	O	H,H
20	4-Cl	5-Cl	O	Ph	O	H,H
	4-Cl	5-Cl	O	4-F-Ph	O	H,H
	4-Cl	5-Cl	O	4-Cl-Ph	O	H,H

25

30

35

Table 6

5	R ₁	R ₂	A	B	X	R _a ¹ , R _a ²
	4-CF ₃	H	CH ₂	H	O	H,H
	4-Cl	H	CH ₂	H	O	H,H
	4-Br	H	CH ₂	H	O	H,H
10	4-CF ₃	4-F	CH ₂	H	O	H,H
	4-Cl	4-F	CH ₂	H	O	H,H
	4-Br	4-F	CH ₂	H	O	H,H
	4-CF ₃	4-Cl	CH ₂	H	O	H,H
	4-Cl	4-Cl	CH ₂	H	O	H,H
15	4-Br	4-Cl	CH ₂	H	O	H,H
	4-CF ₃	4-Me	CH ₂	H	O	H,H
	4-Cl	4-Me	CH ₂	H	O	H,H
	4-Br	4-Me	CH ₂	H	O	H,H
	4-CF ₃	H	CH ₂	Me	O	H,H
20	4-Cl	H	CH ₂	Me	O	H,H
	4-Br	H	CH ₂	Me	O	H,H
	4-CF ₃	4-F	CH ₂	Me	O	H,H
	4-Cl	4-F	CH ₂	Me	O	H,H
	4-Br	4-F	CH ₂	Me	O	H,H
25	4-CF ₃	4-Cl	CH ₂	Me	O	H,H
	4-Cl	4-Cl	CH ₂	Me	O	H,H
	4-Br	4-Cl	CH ₂	Me	O	H,H
	4-CF ₃	H	CH ₂	Et	O	H,H
	4-Cl	H	CH ₂	Et	O	H,H
30	4-Br	H	CH ₂	Et	O	H,H
	4-CF ₃	4-F	CH ₂	Et	O	H,H
	4-Cl	4-F	CH ₂	Et	O	H,H
	4-Br	4-F	CH ₂	Et	O	H,H
	4-CF ₃	H	CH ₂	CO ₂ Me	O	H,H
35						

	R ₁	R ₂	A	B	X	R _a ¹ , R _a ²
5	4-Cl	H	CH ₂	CO ₂ Me	O	H,H
	4-Br	H	CH ₂	CO ₂ Me	O	H,H
	4-CF ₃	4-F	CH ₂	CO ₂ Me	O	H,H
	4-Cl	4-F	CH ₂	CO ₂ Me	O	H,H
10	4-Br	4-F	CH ₂	CO ₂ Me	O	H,H
	4-CF ₃	4-Cl	CH ₂	CO ₂ Me	O	H,H
	4-Cl	4-Cl	CH ₂	CO ₂ Me	O	H,H
	4-Br	4-Cl	CH ₂	CO ₂ Me	O	H,H
15	4-CF ₃	4-Me	CH ₂	CO ₂ Me	O	H,H
	4-Cl	4-Me	CH ₂	CO ₂ Me	O	H,H
	4-Br	4-Me	CH ₂	CO ₂ Me	O	H,H
	4-CF ₃	H	CH ₂	CO ₂ Et	O	H,H
20	4-Cl	H	CH ₂	CO ₂ Et	O	H,H
	4-Br	H	CH ₂	CO ₂ Et	O	H,H
	4-CF ₃	4-Cl	CH ₂	Ph	O	H,H
	4-Cl	4-Cl	CH ₂	Ph	O	H,H
25	4-Br	4-Cl	CH ₂	Ph	O	H,H
	4-CF ₃	H	CH ₂	Ph	O	H,H
	4-Cl	H	CH ₂	Ph	O	H,H
	4-Br	H	CH ₂	Ph	O	H,H
30	4-CF ₃	4-Cl	CH ₂	4-F-Ph	O	H,H
	4-Cl	4-Cl	CH ₂	4-F-Ph	O	H,H
	4-Br	4-Cl	CH ₂	4-F-Ph	O	H,H
	4-CF ₃	H	CH ₂	4-F-Ph	O	H,H
35	4-Cl	H	CH ₂	4-F-Ph	O	H,H
	4-Br	H	CH ₂	4-F-Ph	O	H,H

Table 7

5	R ₁	R ₂	A	B	X	R _a ¹ , R _a ²
	4-CF ₃	H	CH ₂	H	O	H,H
	4-Cl	H	CH ₂	H	O	H,H
	4-Br	H	CH ₂	H	O	H,H
10	4-CF ₃	4-F	CH ₂	H	O	H,H
	4-Cl	4-F	CH ₂	H	O	H,H
	4-Br	4-F	CH ₂	H	O	H,H
	4-CF ₃	5-Cl	CH ₂	H	O	H,H
15	4-Cl	5-Cl	CH ₂	H	O	H,H
	4-Br	5-Cl	CH ₂	H	O	H,H
	4-CF ₃	5-F	CH ₂	H	O	H,H
	4-Cl	5-F	CH ₂	H	O	H,H
20	4-Br	5-F	CH ₂	H	O	H,H
	4-CF ₃	H	CH ₂	Me	O	H,H
	4-Cl	H	CH ₂	Me	O	H,H
	4-Br	H	CH ₂	Me	O	H,H
25	4-CF ₃	4-F	CH ₂	Me	O	H,H
	4-Cl	4-F	CH ₂	Me	O	H,H
	4-Br	4-F	CH ₂	Me	O	H,H
	4-CF ₃	4-Cl	CH ₂	Me	O	H,H
30	4-Cl	4-Cl	CH ₂	Me	O	H,H
	4-Br	4-Cl	CH ₂	Me	O	H,H
	4-CF ₃	5-F	CH ₂	Me	O	H,H
	4-Cl	5-F	CH ₂	Me	O	H,H
35	4-Br	5-F	CH ₂	Me	O	H,H
	4-CF ₃	5-Cl	CH ₂	Me	O	H,H
	4-Cl	5-Cl	CH ₂	Me	O	H,H

	R ₁	R ₂	A	B	X	R _a ¹ , R _a ²
5	4-Br	5-Cl	CH ₂	Me	O	H,H
	4-CF ₃	H	CH ₂	CO ₂ Me	O	H,H
	4-Cl	H	CH ₂	CO ₂ Me	O	H,H
	4-Br	H	CH ₂	CO ₂ Me	O	H,H
10	4-CF ₃	4-F	CH ₂	CO ₂ Me	O	H,H
	4-Cl	4-F	CH ₂	CO ₂ Me	O	H,H
	4-Br	4-F	CH ₂	CO ₂ Me	O	H,H
	4-CF ₃	4-Cl	CH ₂	CO ₂ Me	O	H,H
15	4-Cl	4-Cl	CH ₂	CO ₂ Me	O	H,H
	4-Br	4-Cl	CH ₂	CO ₂ Me	O	H,H
	4-CF ₃	5-F	CH ₂	CO ₂ Me	O	H,H
	4-Cl	5-F	CH ₂	CO ₂ Me	O	H,H
20	4-Br	5-F	CH ₂	CO ₂ Me	O	H,H
	4-CF ₃	5-Cl	CH ₂	CO ₂ Me	O	H,H
	4-Cl	5-Cl	CH ₂	CO ₂ Me	O	H,H
	4-Br	5-Cl	CH ₂	CO ₂ Me	O	H,H
25	4-CF ₃	H	CH ₂	Ph	O	H,H
	4-Cl	H	CH ₂	Ph	O	H,H
	4-Br	H	CH ₂	Ph	O	H,H
	4-CF ₃	4-F	CH ₂	4-F-Ph	O	H,H
30	4-Cl	4-F	CH ₂	4-F-Ph	O	H,H
	4-Br	4-F	CH ₂	4-F-Ph	O	H,H
	4-CF ₃	5-Cl	CH ₂	4-Cl-Ph	O	H,H
	4-Cl	5-Cl	CH ₂	4-Cl-Ph	O	H,H
35	4-Br	5-Cl	CH ₂	4-Cl-Ph	O	H,H
	4-CF ₃	5-F	CH ₂	4-Cl-Ph	O	H,H
	4-Cl	5-F	CH ₂	4-Cl-Ph	O	H,H
	4-Br	5-F	CH ₂	4-Cl-Ph	O	H,H

	R ₁	R ₂	A	B	X	R _a ¹ , R _a ²
5	4-CF ₃	H	O	H	O	H,H
	4-CF ₃	H	O	Me	O	H,H
	4-CF ₃	H	O	i-Pr	O	H,H
	4-CF ₃	H	O	CO ₂ Me	O	H,H
10	4-CF ₃	H	O	Ph	O	H,H
	4-CF ₃	H	O	4-F-Ph	O	H,H
	4-CF ₃	H	O	4-Cl-Ph	O	H,H
	4-CF ₃	5-F	O	H	O	H,H
	4-CF ₃	5-F	O	Me	O	H,H
15	4-CF ₃	5-F	O	i-Pr	O	H,H
	4-CF ₃	5-F	O	CO ₂ Me	O	H,H
	4-CF ₃	5-F	O	Ph	O	H,H
	4-CF ₃	5-F	O	4-F-Ph	O	H,H
	4-CF ₃	5-F	O	4-Cl-Ph	O	H,H
20	4-CF ₃	5-Cl	O	H	O	H,H
	4-CF ₃	5-Cl	O	Me	O	H,H
	4-CF ₃	5-Cl	O	i-Pr	O	H,H
	4-CF ₃	5-Cl	O	CO ₂ Me	O	H,H
	4-CF ₃	5-Cl	O	Ph	O	H,H
25	4-CF ₃	5-Cl	O	4-F-Ph	O	H,H
	4-CF ₃	5-Cl	O	4-Cl-Ph	O	H,H
	4-OCF ₃	H	O	H	O	H,H
	4-OCF ₃	H	O	Me	O	H,H
	4-OCF ₃	H	O	i-Pr	O	H,H
30	4-OCF ₃	H	O	CO ₂ Me	O	H,H
	4-OCF ₃	H	O	Ph	O	H,H
	4-OCF ₃	H	O	4-F-Ph	O	H,H
	4-OCF ₃	H	O	4-Cl-Ph	O	H,H
	4-OCF ₃	5-F	O	H	O	H,H
35	4-OCF ₃	5-F	O	Me	O	H,H
	4-OCF ₃	5-F	O	i-Pr	O	H,H

	R ₁	R ₂	A	B	X	R _a ¹ , R _a ²
5	4-OCF ₃	5-F	O	CO ₂ Me	O	H,H
	4-OCF ₃	5-F	O	Ph	O	H,H
	4-OCF ₃	5-F	O	4-F-Ph	O	H,H
	4-OCF ₃	5-F	O	4-Cl-Ph	O	H,H
10	4-OCF ₃	5-Cl	O	H	O	H,H
	4-OCF ₃	5-Cl	O	Me	O	H,H
	4-OCF ₃	5-Cl	O	i-Pr	O	H,H
	4-OCF ₃	5-Cl	O	CO ₂ Me	O	H,H
	4-OCF ₃	5-Cl	O	Ph	O	H,H
15	4-OCF ₃	5-Cl	O	4-F-Ph	O	H,H
	4-OCF ₃	5-Cl	O	4-Cl-Ph	O	H,H
	4-Br	H	O	H	O	H,H
	4-Br	H	O	Me	O	H,H
	4-Br	H	O	i-Pr	O	H,H
20	4-Br	H	O	CO ₂ Me	O	H,H
	4-Br	H	O	Ph	O	H,H
	4-Br	H	O	4-F-Ph	O	H,H
	4-Br	H	O	4-Cl-Ph	O	H,H
	4-Br	5-F	O	H	O	H,H
25	4-Br	5-F	O	Me	O	H,H
	4-Br	5-F	O	i-Pr	O	H,H
	4-Br	5-F	O	CO ₂ Me	O	H,H
	4-Br	5-F	O	Ph	O	H,H
	4-Br	5-F	O	4-F-Ph	O	H,H
30	4-Br	5-F	O	4-Cl-Ph	O	H,H
	4-Br	5-Cl	O	H	O	H,H
	4-Br	5-Cl	O	Me	O	H,H
	4-Br	5-Cl	O	i-Pr	O	H,H
	4-Br	5-Cl	O	CO ₂ Me	O	H,H
35	4-Br	5-Cl	O	Ph	O	H,H
	4-Br	5-Cl	O	4-F-Ph	O	H,H
	4-Br	5-Cl	O	4-Cl-Ph	O	H,H

	R ₁	R ₂	A	B	X	R _a ¹ , R _a ²
5	4-Cl	H	O	H	O	H,H
	4-Cl	H	O	Me	O	H,H
	4-Cl	H	O	i-Pr	O	H,H
	4-Cl	H	O	CO ₂ Me	O	H,H
10	4-Cl	H	O	Ph	O	H,H
	4-Cl	H	O	4-F-Ph	O	H,H
	4-Cl	H	O	4-Cl-Ph	O	H,H
	4-Cl	5-F	O	H	O	H,H
	4-Cl	5-F	O	Me	O	H,H
15	4-Cl	5-F	O	i-Pr	O	H,H
	4-Cl	5-F	O	CO ₂ Me	O	H,H
	4-Cl	5-F	O	Ph	O	H,H
	4-Cl	5-F	O	4-F-Ph	O	H,H
	4-Cl	5-F	O	4-Cl-Ph	O	H,H
20	4-Cl	5-Cl	O	H	O	H,H
	4-Cl	5-Cl	O	Me	O	H,H
	4-Cl	5-Cl	O	i-Pr	O	H,H
	4-Cl	5-Cl	O	CO ₂ Me	O	H,H
	4-Cl	5-Cl	O	Ph	O	H,H
25	4-Cl	5-Cl	O	4-F-Ph	O	H,H
	4-Cl	5-Cl	O	4-Cl-Ph	O	H,H

30

35

Table 8

5	R ₁	R ₂	A	B	X	R _a ¹ , R _a ²
	4-CF ₃	H	CH ₂	H	O	H,H
	4-Cl	H	CH ₂	H	O	H,H
	4-Br	H	CH ₂	H	O	H,H
	4-CF ₃	5-Cl	CH ₂	H	O	H,H
10	4-Cl	5-Cl	CH ₂	H	O	H,H
	4-Br	5-Cl	CH ₂	H	O	H,H
	4-CF ₃	5-F	CH ₂	H	O	H,H
	4-Cl	5-F	CH ₂	H	O	H,H
15	4-Br	5-F	CH ₂	H	O	H,H
	4-CF ₃	5-Me	CH ₂	H	O	H,H
	4-Cl	5-Me	CH ₂	H	O	H,H
	4-Br	5-Me	CH ₂	H	O	H,H
20	4-CF ₃	H	CH ₂	Me	O	H,H
	4-Cl	H	CH ₂	Me	O	H,H
	4-Br	H	CH ₂	Me	O	H,H
	4-CF ₃	5-Cl	CH ₂	Me	O	H,H
25	4-Cl	5-Cl	CH ₂	Me	O	H,H
	4-Br	5-Cl	CH ₂	Me	O	H,H
	4-CF ₃	5-F	CH ₂	Me	O	H,H
	4-Cl	5-F	CH ₂	Me	O	H,H
30	4-Br	5-F	CH ₂	Me	O	H,H
	4-CF ₃	5-Me	CH ₂	Me	O	H,H
	4-Cl	5-Me	CH ₂	Me	O	H,H
	4-Br	5-Me	CH ₂	Me	O	H,H
35	4-CF ₃	H	CH ₂	Et	O	H,H
	4-Cl	H	CH ₂	Et	O	H,H
	4-Br	H	CH ₂	Et	O	H,H
	4-CF ₃	H	CH ₂	CO ₂ Me	O	H,H

	R ₁	R ₂	A	B	X	R _a ¹ , R _a ²
5	4-Cl	H	CH ₂	CO ₂ Me	O	H,H
	4-Br	H	CH ₂	CO ₂ Me	O	H,H
	4-CF ₃	5-F	CH ₂	CO ₂ Me	O	H,H
	4-Cl	5-F	CH ₂	CO ₂ Me	O	H,H
10	4-Br	5-F	CH ₂	CO ₂ Me	O	H,H
	4-CF ₃	5-Cl	CH ₂	CO ₂ Me	O	H,H
	4-Cl	5-Cl	CH ₂	CO ₂ Me	O	H,H
	4-Br	5-Cl	CH ₂	CO ₂ Me	O	H,H
	4-CF ₃	5-Me	CH ₂	CO ₂ Me	O	H,H
15	4-Cl	5-Me	CH ₂	CO ₂ Me	O	H,H
	4-Br	5-Me	CH ₂	CO ₂ Me	O	H,H
	4-CF ₃	5-Cl	CH ₂	CO ₂ Et	O	H,H
	4-Cl	5-Cl	CH ₂	CO ₂ Et	O	H,H
	4-Br	5-Cl	CH ₂	CO ₂ Et	O	H,H
20	4-CF ₃	H	CH ₂	Ph	O	H,H
	4-Cl	H	CH ₂	Ph	O	H,H
	4-Br	H	CH ₂	Ph	O	H,H
	4-CF ₃	5-Cl	CH ₂	Ph	O	H,H
	4-Cl	5-Cl	CH ₂	Ph	O	H,H
25	4-Br	5-Cl	CH ₂	Ph	O	H,H
	4-CF ₃	H	CH ₂	4-Cl-Ph	O	H,H
	4-Cl	H	CH ₂	4-Cl-Ph	O	H,H
	4-Br	H	CH ₂	4-Cl-Ph	O	H,H
	4-CF ₃	5-Cl	CH ₂	4-Cl-Ph	O	H,H
30	4-Cl	5-Cl	CH ₂	4-Cl-Ph	O	H,H
	4-Br	5-Cl	CH ₂	4-Cl-Ph	O	H,H

35

Table 9

5	R ₁	R ₂	A	B	X	R _a ¹ , R _a ²
	4-CF ₃	H	CH ₂	H	O	H,H
	4-Cl	H	CH ₂	H	O	H,H
	4-Br	H	CH ₂	H	O	H,H
10	4-CF ₃	4-F	CH ₂	H	O	H,H
	4-Cl	4-F	CH ₂	H	O	H,H
	4-Br	4-F	CH ₂	H	O	H,H
	4-CF ₃	4-Cl	CH ₂	H	O	H,H
	4-Cl	4-Cl	CH ₂	H	O	H,H
	4-Br	4-Cl	CH ₂	H	O	H,H
15	4-CF ₃	4-Me	CH ₂	H	O	H,H
	4-Cl	4-Me	CH ₂	H	O	H,H
	4-Br	4-Me	CH ₂	H	O	H,H
	4-CF ₃	H	CH ₂	Me	O	H,H
	4-Cl	H	CH ₂	Me	O	H,H
	4-Br	H	CH ₂	Me	O	H,H
20	4-CF ₃	4-F	CH ₂	Me	O	H,H
	4-Cl	4-F	CH ₂	Me	O	H,H
	4-Br	4-F	CH ₂	Me	O	H,H
	4-CF ₃	4-Cl	CH ₂	Me	O	H,H
	4-Cl	4-Cl	CH ₂	Me	O	H,H
	4-Br	4-Cl	CH ₂	Me	O	H,H
25	4-CF ₃	H	CH ₂	Et	O	H,H
	4-Cl	H	CH ₂	Et	O	H,H
	4-Br	H	CH ₂	Et	O	H,H
30	4-CF ₃	4-F	CH ₂	Et	O	H,H
	4-Cl	4-F	CH ₂	Et	O	H,H
	4-Br	4-F	CH ₂	Et	O	H,H
	4-CF ₃	H	CH ₂	CO ₂ Me	O	H,H

35

	R ₁	R ₂	A	B	X	R _a ¹ , R _a ²
5	4-Cl	H	CH ₂	CO ₂ Me	O	H,H
	4-Br	H	CH ₂	CO ₂ Me	O	H,H
	4-CF ₃	4-F	CH ₂	CO ₂ Me	O	H,H
	4-Cl	4-F	CH ₂	CO ₂ Me	O	H,H
10	4-Br	4-F	CH ₂	CO ₂ Me	O	H,H
	4-CF ₃	4-Cl	CH ₂	CO ₂ Me	O	H,H
	4-Cl	4-Cl	CH ₂	CO ₂ Me	O	H,H
	4-Br	4-Cl	CH ₂	CO ₂ Me	O	H,H
15	4-CF ₃	4-Me	CH ₂	CO ₂ Me	O	H,H
	4-Cl	4-Me	CH ₂	CO ₂ Me	O	H,H
	4-Br	4-Me	CH ₂	CO ₂ Me	O	H,H
	4-CF ₃	H	CH ₂	CO ₂ Et	O	H,H
20	4-Cl	H	CH ₂	CO ₂ Et	O	H,H
	4-Br	H	CH ₂	CO ₂ Et	O	H,H
	4-CF ₃	4-Cl	CH ₂	Ph	O	H,H
	4-Cl	4-Cl	CH ₂	Ph	O	H,H
25	4-Br	4-Cl	CH ₂	Ph	O	H,H
	4-CF ₃	H	CH ₂	Ph	O	H,H
	4-Cl	H	CH ₂	Ph	O	H,H
	4-Br	H	CH ₂	Ph	O	H,H
30	4-CF ₃	4-Cl	CH ₂	4-F-Ph	O	H,H
	4-Cl	4-Cl	CH ₂	4-F-Ph	O	H,H
	4-Br	4-Cl	CH ₂	4-F-Ph	O	H,H
	4-CF ₃	H	CH ₂	4-F-Ph	O	H,H
35	4-Cl	H	CH ₂	4-F-Ph	O	H,H
	4-Br	H	CH ₂	4-F-Ph	O	H,H

Table 10

5	R ₁	R ₂	A	B	X	R _a ¹ , R _a ²
	4-CF ₃	H	CH ₂	H	O	H,H
	4-Cl	H	CH ₂	H	O	H,H
	4-Br	H	CH ₂	H	O	H,H
10	4-CF ₃	4-F	CH ₂	H	O	H,H
	4-Cl	4-F	CH ₂	H	O	H,H
	4-Br	4-F	CH ₂	H	O	H,H
	4-CF ₃	5-Cl	CH ₂	H	O	H,H
	4-Cl	5-Cl	CH ₂	H	O	H,H
	4-Br	5-Cl	CH ₂	H	O	H,H
15	4-CF ₃	5-F	CH ₂	H	O	H,H
	4-Cl	5-F	CH ₂	H	O	H,H
	4-Br	5-F	CH ₂	H	O	H,H
	4-CF ₃	H	CH ₂	Me	O	H,H
	4-Cl	H	CH ₂	Me	O	H,H
	4-Br	H	CH ₂	Me	O	H,H
20	4-CF ₃	4-F	CH ₂	Me	O	H,H
	4-Cl	4-F	CH ₂	Me	O	H,H
	4-Br	4-F	CH ₂	Me	O	H,H
	4-CF ₃	4-Cl	CH ₂	Me	O	H,H
	4-Cl	4-Cl	CH ₂	Me	O	H,H
	4-Br	4-Cl	CH ₂	Me	O	H,H
25	4-CF ₃	5-F	CH ₂	Me	O	H,H
	4-Cl	5-F	CH ₂	Me	O	H,H
	4-Br	5-F	CH ₂	Me	O	H,H
	4-CF ₃	5-Cl	CH ₂	Me	O	H,H
	4-Cl	5-Cl	CH ₂	Me	O	H,H
	4-Br	5-Cl	CH ₂	Me	O	H,H
30	4-CF ₃	H	CH ₂	CO ₂ Me	O	H,H

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	R ₁	R ₂	A	B	X	R _a ¹ , R _a ²
5	4-Cl	H	CH ₂	CO ₂ Me	O	H,H
	4-Br	H	CH ₂	CO ₂ Me	O	H,H
	4-CF ₃	4-F	CH ₂	CO ₂ Me	O	H,H
	4-Cl	4-F	CH ₂	CO ₂ Me	O	H,H
10	4-Br	4-F	CH ₂	CO ₂ Me	O	H,H
	4-CF ₃	4-Cl	CH ₂	CO ₂ Me	O	H,H
	4-Cl	4-Cl	CH ₂	CO ₂ Me	O	H,H
	4-Br	4-Cl	CH ₂	CO ₂ Me	O	H,H
	4-CF ₃	5-F	CH ₂	CO ₂ Me	O	H,H
15	4-Cl	5-F	CH ₂	CO ₂ Me	O	H,H
	4-Br	5-F	CH ₂	CO ₂ Me	O	H,H
	4-CF ₃	5-Cl	CH ₂	CO ₂ Me	O	H,H
	4-Cl	5-Cl	CH ₂	CO ₂ Me	O	H,H
	4-Br	5-Cl	CH ₂	CO ₂ Me	O	H,H
20	4-CF ₃	H	CH ₂	Ph	O	H,H
	4-Cl	H	CH ₂	Ph	O	H,H
	4-Br	H	CH ₂	Ph	O	H,H
	4-CF ₃	4-F	CH ₂	4-F-Ph	O	H,H
	4-Cl	4-F	CH ₂	4-F-Ph	O	H,H
25	4-Br	4-F	CH ₂	4-F-Ph	O	H,H
	4-CF ₃	5-Cl	CH ₂	4-Cl-Ph	O	H,H
	4-Cl	5-Cl	CH ₂	4-Cl-Ph	O	H,H
	4-Br	5-Cl	CH ₂	4-Cl-Ph	O	H,H
	4-CF ₃	5-F	CH ₂	4-Cl-Ph	O	H,H
30	4-Cl	5-F	CH ₂	4-Cl-Ph	O	H,H
	4-Br	5-F	CH ₂	4-Cl-Ph	O	H,H

Table 11

	R ₁	R ₂	A	B	Q	Y
5	4-CF ₃	H	CH ₂	H	Q-1	Me
	4-Cl	H	CH ₂	H	Q-1	Me
	4-Br	H	CH ₂	H	Q-1	Me
	4-CF ₃	5-Cl	CH ₂	Me	Q-1	Me
10	4-Cl	5-Cl	CH ₂	Me	Q-1	Me
	4-Br	5-Cl	CH ₂	Me	Q-1	Me
	4-CF ₃	H	CH ₂	Me	Q-1	Me
	4-Cl	H	CH ₂	Me	Q-1	Me
15	4-Br	H	CH ₂	Me	Q-1	Me
	4-CF ₃	H	CH ₂	Me	Q-1	C(O)Me
	4-Cl	H	CH ₂	Me	Q-1	C(O)Me
	4-Br	H	CH ₂	Me	Q-1	C(O)Me
20	4-CF ₃	H	CH ₂	Me	Q-1	CO ₂ Me
	4-Cl	H	CH ₂	Me	Q-1	CO ₂ Me
	4-Br	H	CH ₂	Me	Q-1	CO ₂ Me
	4-CF ₃	5-Cl	CH ₂	Me	Q-1	Me
25	4-Cl	5-Cl	CH ₂	Me	Q-1	Me
	4-Br	5-Cl	CH ₂	Me	Q-1	Me
	4-CF ₃	5-Cl	CH ₂	Me	Q-1	C(O)Me
	4-Cl	5-Cl	CH ₂	Me	Q-1	C(O)Me
30	4-Br	5-Cl	CH ₂	Me	Q-1	C(O)Me
	4-CF ₃	5-Cl	CH ₂	Me	Q-1	CO ₂ Me
	4-Cl	5-Cl	CH ₂	Me	Q-1	CO ₂ Me
	4-Br	5-Cl	CH ₂	Me	Q-1	CO ₂ Me
35	4-CF ₃	5-F	CH ₂	Me	Q-1	CO ₂ Me
	4-Cl	5-F	CH ₂	Me	Q-1	CO ₂ Me
	4-Br	5-F	CH ₂	Me	Q-1	CO ₂ Me
	4-CF ₃	H	CH ₂	CO ₂ Me	Q-1	C(O)Me

	R ₁	R ₂	A	B	Q	Y
5	4-Cl	H	CH ₂	CO ₂ Me	Q-1	C(O)Me
	4-Br	H	CH ₂	CO ₂ Me	Q-1	C(O)Me
	4-CF ₃	H	CH ₂	CO ₂ Me	Q-1	Me
	4-Cl	H	CH ₂	CO ₂ Me	Q-1	Me
10	4-Br	H	CH ₂	CO ₂ Me	Q-1	Me
	4-CF ₃	H	CH ₂	CO ₂ Me	Q-1	CO ₂ Me
	4-Cl	H	CH ₂	CO ₂ Me	Q-1	CO ₂ Me
	4-Br	H	CH ₂	CO ₂ Me	Q-1	CO ₂ Me
	4-CF ₃	5-Cl	CH ₂	CO ₂ Me	Q-1	C(O)Me
15	4-Cl	5-Cl	CH ₂	CO ₂ Me	Q-1	C(O)Me
	4-Br	5-Cl	CH ₂	CO ₂ Me	Q-1	C(O)Me
	4-CF ₃	5-Cl	CH ₂	CO ₂ Me	Q-1	CO ₂ Me
	4-Cl	5-Cl	CH ₂	CO ₂ Me	Q-1	CO ₂ Me
	4-Br	5-Cl	CH ₂	CO ₂ Me	Q-1	CO ₂ Me
20	4-CF ₃	H	CH ₂	Ph	Q-1	C(O)Me
	4-Cl	H	CH ₂	Ph	Q-1	C(O)Me
	4-Br	H	CH ₂	Ph	Q-1	C(O)Me
	4-CF ₃	5-Cl	CH ₂	Ph	Q-1	C(O)Me
	4-Cl	5-Cl	CH ₂	Ph	Q-1	C(O)Me
25	4-Br	5-Cl	CH ₂	Ph	Q-1	C(O)Me
	4-CF ₃	H	CH ₂	4-Cl-Ph	Q-1	C(O)Me
	4-Cl	H	CH ₂	4-Cl-Ph	Q-1	C(O)Me
	4-Br	H	CH ₂	4-Cl-Ph	Q-1	C(O)Me
	4-CF ₃	5-Cl	CH ₂	4-Cl-Ph	Q-1	C(O)Me
30	4-Cl	5-Cl	CH ₂	4-Cl-Ph	Q-1	C(O)Me
	4-Br	5-Cl	CH ₂	4-Cl-Ph	Q-1	C(O)Me
	4-CF ₃	H	CH ₂	H	Q-2	Me
	4-Cl	H	CH ₂	H	Q-2	Me

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	R ₁	R ₂	A	B	Q	Y
5	4-Br	H	CH ₂	H	Q-2	Me
	4-CF ₃	H	CH ₂	H	Q-2	C(O)Me
	4-Cl	H	CH ₂	H	Q-2	C(O)Me
	4-Br	H	CH ₂	H	Q-2	C(O)Me
10	4-CF ₃	H	CH ₂	CO ₂ Me	Q-2	Me
	4-Cl	H	CH ₂	CO ₂ Me	Q-2	Me
	4-Br	H	CH ₂	CO ₂ Me	Q-2	Me
	4-CF ₃	H	CH ₂	CO ₂ Me	Q-2	C(O)Me
	4-Cl	H	CH ₂	CO ₂ Me	Q-2	C(O)Me
15	4-Br	H	CH ₂	CO ₂ Me	Q-2	C(O)Me
	4-CF ₃	H	CH ₂	CO ₂ Me	Q-2	CO ₂ Me
	4-Cl	H	CH ₂	CO ₂ Me	Q-2	CO ₂ Me
	4-Br	H	CH ₂	CO ₂ Me	Q-2	CO ₂ Me
	4-CF ₃	4-F	CH ₂	H	Q-2	Me
20	4-Cl	4-F	CH ₂	H	Q-2	Me
	4-Br	4-F	CH ₂	H	Q-2	Me
	4-CF ₃	4-F	CH ₂	H	Q-2	C(O)Me
	4-Cl	4-F	CH ₂	H	Q-2	C(O)Me
	4-Br	4-F	CH ₂	H	Q-2	C(O)Me
25	4-CF ₃	4-F	CH ₂	CO ₂ Me	Q-2	CO ₂ Me
	4-Cl	4-F	CH ₂	CO ₂ Me	Q-2	CO ₂ Me
	4-Br	4-F	CH ₂	CO ₂ Me	Q-2	CO ₂ Me
	4-CF ₃	4-F	CH ₂	CO ₂ Me	Q-2	C(O)Me
	4-Cl	4-F	CH ₂	CO ₂ Me	Q-2	Ac
30	4-Br	4-F	CH ₂	CO ₂ Me	Q-2	Ac
	4-CF ₃	H	CH ₂	H	Q-3	Me
	4-Cl	H	CH ₂	H	Q-3	Me
	4-Br	H	CH ₂	H	Q-3	Ac

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	R ₁	R ₂	A	B	Q	Y
5	4-CF ₃	H	CH ₂	H	Q-3	C(O)Me
	4-Cl	H	CH ₂	H	Q-3	CO ₂ Me
	4-Br	H	CH ₂	H	Q-3	CO ₂ Me
	4-CF ₃	5-Cl	CH ₂	H	Q-3	Me
10	4-Cl	5-Cl	CH ₂	H	Q-3	Me
	4-Br	5-Cl	CH ₂	H	Q-3	C(O)Me
	4-CF ₃	5-Cl	CH ₂	H	Q-3	C(O)Me
	4-Cl	5-Cl	CH ₂	H	Q-3	CO ₂ Me
	4-Br	5-Cl	CH ₂	H	Q-3	CO ₂ Me
15	4-CF ₃	H	CH ₂	CO ₂ Me	Q-3	Me
	4-Cl	H	CH ₂	CO ₂ Me	Q-3	Me
	4-Br	H	CH ₂	CO ₂ Me	Q-3	C(O)Me
	4-CF ₃	H	CH ₂	CO ₂ Me	Q-3	C(O)Me
	4-Cl	H	CH ₂	CO ₂ Me	Q-3	C(O)Me
20	4-Br	H	CH ₂	CO ₂ Me	Q-3	C(O)Me
	4-CF ₃	H	CH ₂	CO ₂ Me	Q-3	CO ₂ Me
	4-Cl	H	CH ₂	CO ₂ Me	Q-3	CO ₂ Me
	4-Br	H	CH ₂	CO ₂ Me	Q-3	CO ₂ Me
	4-CF ₃	5-Cl	CH ₂	CO ₂ Me	Q-3	Me
25	4-Cl	5-Cl	CH ₂	CO ₂ Me	Q-3	Me
	4-Br	5-Cl	CH ₂	CO ₂ Me	Q-3	Me
	4-CF ₃	5-Cl	CH ₂	CO ₂ Me	Q-3	C(O)Me
	4-Cl	5-Cl	CH ₂	CO ₂ Me	Q-3	C(O)Me
	4-Br	5-Cl	CH ₂	CO ₂ Me	Q-3	C(O)Me
30	4-CF ₃	H	CH ₂	H	Q-5	C(O)Me
	4-Cl	H	CH ₂	H	Q-5	C(O)Me
	4-Br	H	CH ₂	H	Q-5	C(O)Me
	4-CF ₃	H	CH ₂	H	Q-5	CO ₂ Me

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	R ₁	R ₂	A	B	Q	Y
5	4-Cl	H	CH ₂	H	Q-5	CO ₂ Me
	4-Br	H	CH ₂	H	Q-5	CO ₂ Me
	4-CF ₃	5-Cl	CH ₂	CO ₂ Me	Q-5	C(O)Me
	4-Cl	5-Cl	CH ₂	CO ₂ Me	Q-5	C(O)Me
10	4-Br	5-Cl	CH ₂	CO ₂ Me	Q-5	C(O)Me
	4-CF ₃	5-Cl	CH ₂	CO ₂ Me	Q-5	CO ₂ Me
	4-Cl	5-Cl	CH ₂	CO ₂ Me	Q-5	CO ₂ Me
	4-Br	5-Cl	CH ₂	CO ₂ Me	Q-5	CO ₂ Me
	4-CF ₃	5-Cl	CH ₂	Me	Q-5	C(O)Me
15	4-Cl	5-Cl	CH ₂	Me	Q-5	C(O)Me
	4-Br	5-Cl	CH ₂	Me	Q-5	C(O)Me
	4-CF ₃	H	CH ₂	H	Q-7	CO ₂ Me
	4-Cl	H	CH ₂	H	Q-7	CO ₂ Me
	4-Br	H	CH ₂	H	Q-7	CO ₂ Me
20	4-CF ₃	5-Cl	CH ₂	H	Q-7	C(O)Me
	4-Cl	5-Cl	CH ₂	H	Q-7	C(O)Me
	4-Br	5-Cl	CH ₂	H	Q-7	C(O)Me
	4-CF ₃	5-Cl	CH ₂	CO ₂ Me	Q-7	CO ₂ Me
	4-Cl	5-Cl	CH ₂	CO ₂ Me	Q-7	CO ₂ Me
25	4-Br	5-Cl	CH ₂	CO ₂ Me	Q-7	CO ₂ Me
	4-CF ₃	5-Cl	CH ₂	CO ₂ Me	Q-7	C(O)Me
	4-Cl	5-Cl	CH ₂	CO ₂ Me	Q-7	C(O)Me
	4-Br	5-Cl	CH ₂	CO ₂ Me	Q-7	C(O)Me
	4-CF ₃	H	O	H	Q-1	Me
30	4-Cl	H	O	H	Q-1	C(O)Me
	4-Br	H	O	H	Q-1	CO ₂ Me
	4-CF ₃	H	O	Me	Q-1	Me
	4-Cl	H	O	Me	Q-1	C(O)Me
	4-Br	H	O	Me	Q-1	CO ₂ Me

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	R ₁	R ₂	A	B	Q	Y
5	4-CF ₃	5-Cl	O	H	Q-1	Me
	4-Cl	5-Cl	O	H	Q-1	C(O)Me
	4-Br	5-Cl	O	H	Q-1	CO ₂ Me
	4-CF ₃	H	O	H	Q-2	Me
10	4-Cl	H	O	H	Q-2	C(O)Me
	4-Br	H	O	H	Q-2	CO ₂ Me
	4-CF ₃	H	O	H	Q-2	Me
	4-Cl	H	O	H	Q-2	C(O)Me
	4-Br	H	O	H	Q-2	CO ₂ Me
	4-CF ₃	H	O	H	Q-3	Me
15	4-Cl	H	O	H	Q-3	C(O)Me
	4-Br	H	O	H	Q-3	CO ₂ Me
	4-CF ₃	H	O	H	Q-3	Me
	4-Cl	H	O	H	Q-3	C(O)Me
	4-Br	H	O	H	Q-3	CO ₂ Me
	4-CF ₃	H	O	H	Q-5	Me
20	4-Cl	H	O	H	Q-5	C(O)Me
	4-Br	H	O	H	Q-5	CO ₂ Me
	4-CF ₃	H	O	H	Q-5	Me
	4-Cl	H	O	H	Q-5	C(O)Me
	4-Br	H	O	H	Q-5	CO ₂ Me
25	4-CF ₃	H	S	H	Q-1	Me
	4-Cl	H	S	H	Q-1	C(O)Me
	4-Br	H	S	H	Q-1	CO ₂ Me
	4-CF ₃	H	S	CO ₂ Me	Q-1	Me
	4-Cl	H	S	CO ₂ Me	Q-1	C(O)Me
	4-Br	H	S	CO ₂ Me	Q-1	CO ₂ Me
30	4-CF ₃	H	S	H	Q-2	Me
	4-Cl	H	S	H	Q-2	C(O)Me
	4-Br	H	S	H	Q-2	CO ₂ Me
	4-CF ₃	H	S	CO ₂ Me	Q-2	Me
35						

5	R ₁	R ₂	A	B	Q	Y
	4-Cl	H	S	CO ₂ Me	Q-2	C(O)Me
	4-Br	H	S	CO ₂ Me	Q-2	CO ₂ Me
	4-CF ₃	H	S	H	Q-3	Me
10	4-Cl	H	S	H	Q-3	C(O)Me
	4-Br	H	S	H	Q-3	CO ₂ Me
	4-CF ₃	H	S	CO ₂ Me	Q-3	Me
	4-Cl	H	S	CO ₂ Me	Q-3	C(O)Me
	4-Br	H	S	CO ₂ Me	Q-3	CO ₂ Me
15	4-CF ₃	H	S	H	Q-5	Me
	4-Cl	H	S	H	Q-5	C(O)Me
	4-Br	H	S	H	Q-5	CO ₂ Me
	4-CF ₃	H	S	CO ₂ Me	Q-5	Me
	4-Cl	H	S	CO ₂ Me	Q-5	C(O)Me
	4-Br	H	S	CO ₂ Me	Q-5	CO ₂ Me
20	4-CF ₃	H	S	H	Q-7	Me
	4-Cl	H	S	H	Q-7	C(O)Me
	4-Br	H	S	H	Q-7	CO ₂ Me
	4-CF ₃	H	CH ₂	H	Q-1	N(Me)CO Et
	4-Cl	H	CH ₂	H	Q-1	N(Me)CO Et
25	4-Br	H	CH ₂	H	Q-1	N(Me)CO Et
	4-CF ₃	H	CH ₂	H	Q-1	N(Me)CO nBu
	4-Cl	H	CH ₂	H	Q-1	N(Me)CO nBu
30	4-Br	H	CH ₂	H	Q-1	N(Me)CO nBu

Table 12

5	R ₁	R ₂	A	B	Q	J
10	4-CF ₃	5-Cl	CH ₂	H	Q-1	N(iPr)CO ₂ Et
	4-Cl	5-Cl	CH ₂	H	Q-1	N(iPr)CO ₂ Et
	4-Br	5-Cl	CH ₂	H	Q-1	N(iPr)CO ₂ Et
	4-CF ₃	5-Cl	CH ₂	H	Q-1	N(Et)CO ₂ Et
	4-Cl	5-Cl	CH ₂	H	Q-1	N(Et)CO ₂ Et
	4-Br	5-Cl	CH ₂	H	Q-1	N(Et)CO ₂ Et
15	4-CF ₃	H	CH ₂	CO ₂ Me	Q-1	N(Et)CO ₂ Et
	4-Cl	H	CH ₂	CO ₂ Me	Q-1	N(Et)CO ₂ Et
	4-Br	H	CH ₂	CO ₂ Me	Q-1	N(Et)CO ₂ Et
	4-CF ₃	H	CH ₂	CO ₂ Me	Q-1	N(iPr)CO ₂ Et
	4-Cl	H	CH ₂	CO ₂ Me	Q-1	N(iPr)CO ₂ Et
	4-Br	H	CH ₂	CO ₂ Me	Q-1	N(iPr)CO ₂ Et
20	4-CF ₃	5-Cl	CH ₂	CO ₂ Me	Q-1	N(iPr)CO ₂ Et
	4-Cl	5-Cl	CH ₂	CO ₂ Me	Q-1	N(iPr)CO ₂ Et
	4-Br	5-Cl	CH ₂	CO ₂ Me	Q-1	N(iPr)CO ₂ Et
	4-CF ₃	5-Cl	CH ₂	CO ₂ Me	Q-1	N(Me)CO ₂ nHex
	4-Cl	5-Cl	CH ₂	CO ₂ Me	Q-1	N(Me)CO ₂ nHex
	4-Br	5-Cl	CH ₂	CO ₂ Me	Q-1	N(Me)CO ₂ nHex
25	4-CF ₃	5-Cl	CH ₂	Ph	Q-1	N(Me)CO ₂ Et
	4-Cl	5-Cl	CH ₂	Ph	Q-1	N(Me)CO ₂ Et
	4-Br	5-Cl	CH ₂	Ph	Q-1	N(Me)CO ₂ Et
	4-CF ₃	H	CH ₂	H	Q-3	N(Me)CO ₂ Et
	4-Cl	H	CH ₂	H	Q-3	N(Me)CO ₂ Et
	4-Br	H	CH ₂	H	Q-3	N(Me)CO ₂ Et
30	4-CF ₃	H	CH ₂	H	Q-3	N(Me)CO ₂ nBu
	4-Cl	H	CH ₂	H	Q-3	N(Me)CO ₂ nBu
	4-CF ₃	H	CH ₂	H	Q-3	N(Me)CO ₂ nBu
	4-Cl	H	CH ₂	H	Q-3	N(Me)CO ₂ nBu

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5	R ₁	R ₂	A	B	Q	J
10	4-Br	H	CH ₂	H	Q-3	N(Me)CO ₂ nBu
	4-CF ₃	5-Cl	CH ₂	H	Q-3	N(iPr)CO ₂ Et
	4-Cl	5-Cl	CH ₂	H	Q-3	N(iPr)CO ₂ Et
	4-Br	5-Cl	CH ₂	H	Q-3	N(iPr)CO ₂ Et
	4-CF ₃	5-Cl	CH ₂	H	Q-3	N(Et)CO ₂ Et
	4-Cl	5-Cl	CH ₂	H	Q-3	N(Et)CO ₂ Et
15	4-Br	5-Cl	CH ₂	H	Q-3	N(Et)CO ₂ Et
	4-CF ₃	H	CH ₂	CO ₂ Me	Q-3	N(Et)CO ₂ Et
	4-Cl	H	CH ₂	CO ₂ Me	Q-3	N(Et)CO ₂ Et
	4-Br	H	CH ₂	CO ₂ Me	Q-3	N(Et)CO ₂ Et
	4-CF ₃	H	CH ₂	CO ₂ Me	Q-3	N(iPr)CO ₂ Et
	4-Cl	H	CH ₂	CO ₂ Me	Q-3	N(iPr)CO ₂ Et
20	4-Br	H	CH ₂	CO ₂ Me	Q-3	N(iPr)CO ₂ Et
	4-CF ₃	5-Cl	CH ₂	CO ₂ Me	Q-3	N(iPr)CO ₂ Et
	4-Cl	5-Cl	CH ₂	CO ₂ Me	Q-3	N(iPr)CO ₂ Et
	4-Br	5-Cl	CH ₂	CO ₂ Me	Q-3	N(iPr)CO ₂ Et
	4-CF ₃	5-Cl	CH ₂	CO ₂ Me	Q-3	N(Me)CO ₂ nHex
	4-Cl	5-Cl	CH ₂	CO ₂ Me	Q-3	N(Me)CO ₂ nHex
25	4-Br	5-Cl	CH ₂	CO ₂ Me	Q-3	N(Me)CO ₂ nHex
	4-CF ₃	5-Cl	CH ₂	Ph	Q-3	N(Me)CO ₂ Et
	4-Cl	5-Cl	CH ₂	Ph	Q-3	N(Me)CO ₂ Et
	4-Br	5-Cl	CH ₂	Ph	Q-3	N(Me)CO ₂ Et
	4-CF ₃	H	CH ₂	H	Q-4	N(Me)CO ₂ Et
	4-Cl	H	CH ₂	H	Q-4	N(Me)CO ₂ Et

	R ₁	R ₂	A	B	Q	J
5	4-Br	H	CH ₂	H	Q-4	N(Me)CO ₂ Et
	4-CF ₃	H	CH ₂	H	Q-4	N(Me)CO ₂ nBu
	4-Cl	H	CH ₂	H	Q-4	N(Me)CO ₂ nBu
	4-Br	H	CH ₂	H	Q-4	N(Me)CO ₂ nBu
10	4-CF ₃	5-Cl	CH ₂	H	Q-4	N(iPr)CO ₂ Et
	4-Cl	5-Cl	CH ₂	H	Q-4	N(iPr)CO ₂ Et
	4-Br	5-Cl	CH ₂	H	Q-4	N(iPr)CO ₂ Et
	4-CF ₃	5-Cl	CH ₂	H	Q-4	N(Et)CO ₂ Et
	4-Cl	5-Cl	CH ₂	H	Q-4	N(Et)CO ₂ Et
15	4-Br	5-Cl	CH ₂	H	Q-4	N(Et)CO ₂ Et
	4-CF ₃	H	CH ₂	CO ₂ Me	Q-4	N(Et)CO ₂ Et
	4-Cl	H	CH ₂	CO ₂ Me	Q-4	N(Et)CO ₂ Et
	4-Br	H	CH ₂	CO ₂ Me	Q-4	N(Et)CO ₂ Et
	4-CF ₃	H	CH ₂	CO ₂ Me	Q-4	N(iPr)CO ₂ Et
20	4-Cl	H	CH ₂	CO ₂ Me	Q-4	N(iPr)CO ₂ Et
	4-Br	H	CH ₂	CO ₂ Me	Q-4	N(iPr)CO ₂ Et
	4-CF ₃	5-Cl	CH ₂	CO ₂ Me	Q-4	N(iPr)CO ₂ Et
	4-Cl	5-Cl	CH ₂	CO ₂ Me	Q-4	N(iPr)CO ₂ Et
	4-Br	5-Cl	CH ₂	CO ₂ Me	Q-4	N(iPr)CO ₂ Et
25	4-CF ₃	5-Cl	CH ₂	CO ₂ Me	Q-4	N(Me)CO ₂ nHex
	4-Cl	5-Cl	CH ₂	CO ₂ Me	Q-4	N(Me)CO ₂ nHex
	4-Br	5-Cl	CH ₂	CO ₂ Me	Q-4	N(Me)CO ₂ nHex
	4-CF ₃	5-Cl	CH ₂	Ph	Q-4	N(Me)CO ₂ Et
	4-Cl	5-Cl	CH ₂	Ph	Q-4	N(Me)CO ₂ Et
30	4-Br	5-Cl	CH ₂	Ph	Q-4	N(Me)CO ₂ Et
	4-CF ₃	H	CH ₂	H	Q-5	N(Me)CO ₂ Et
	4-Cl	H	CH ₂	H	Q-5	N(Me)CO ₂ Et
	4-Br	H	CH ₂	H	Q-5	N(Me)CO ₂ Et

	R ₁	R ₂	A	B	Q	J
5	4-CF ₃	H	CH ₂	H	Q-5	N(Me)CO ₂ nBu
	4-Cl	H	CH ₂	H	Q-5	N(Me)CO ₂ nBu
	4-Br	H	CH ₂	H	Q-5	N(Me)CO ₂ nBu
	4-CF ₃	5-Cl	CH ₂	H	Q-5	N(iPr)CO ₂ Et
10	4-Cl	5-Cl	CH ₂	H	Q-5	N(iPr)CO ₂ Et
	4-Br	5-Cl	CH ₂	H	Q-5	N(iPr)CO ₂ Et
	4-CF ₃	5-Cl	CH ₂	H	Q-5	N(Et)CO ₂ Et
	4-Cl	5-Cl	CH ₂	H	Q-5	N(Et)CO ₂ Et
	4-Br	5-Cl	CH ₂	H	Q-5	N(Et)CO ₂ Et
15	4-CF ₃	H	CH ₂	CO ₂ Me	Q-5	N(Et)CO ₂ Et
	4-Cl	H	CH ₂	CO ₂ Me	Q-5	N(Et)CO ₂ Et
	4-Br	H	CH ₂	CO ₂ Me	Q-5	N(Et)CO ₂ Et
	4-CF ₃	H	CH ₂	CO ₂ Me	Q-5	N(iPr)CO ₂ Et
	4-Cl	H	CH ₂	CO ₂ Me	Q-5	N(iPr)CO ₂ Et
20	4-Br	H	CH ₂	CO ₂ Me	Q-5	N(iPr)CO ₂ Et
	4-CF ₃	5-Cl	CH ₂	CO ₂ Me	Q-5	N(iPr)CO ₂ Et
	4-Cl	5-Cl	CH ₂	CO ₂ Me	Q-5	N(iPr)CO ₂ Et
	4-Br	5-Cl	CH ₂	CO ₂ Me	Q-5	N(iPr)CO ₂ Et
	4-CF ₃	5-Cl	CH ₂	CO ₂ Me	Q-5	N(Me)CO ₂ nHex
25	4-Cl	5-Cl	CH ₂	CO ₂ Me	Q-5	N(Me)CO ₂ nHex
	4-Br	5-Cl	CH ₂	CO ₂ Me	Q-5	N(Me)CO ₂ nHex
	4-CF ₃	5-Cl	CH ₂	Ph	Q-5	N(Me)CO ₂ Et
	4-Cl	5-Cl	CH ₂	Ph	Q-5	N(Me)CO ₂ Et
	4-Br	5-Cl	CH ₂	Ph	Q-5	N(Me)CO ₂ Et
30	4-CF ₃	H	CH ₂	H	Q-1	N(Me)SO ₂ Ph
	4-Cl	H	CH ₂	H	Q-1	N(Me)SO ₂ Ph
	4-Br	H	CH ₂	H	Q-1	N(Me)SO ₂ Ph
	4-CF ₃	H	CH ₂	CO ₂ Me	Q-1	N(Me)SO ₂ Ph

	R ₁	R ₂	A	B	Q	J
5	4-Cl	H	CH ₂	CO ₂ Me	Q-1	N(Me)SO ₂ Ph
	4-Br	H	CH ₂	CO ₂ Me	Q-1	N(Me)SO ₂ Ph
	4-CF ₃	H	CH ₂	Ph	Q-1	N(Me)SO ₂ Ph
	4-Cl	H	CH ₂	Ph	Q-1	N(Me)SO ₂ Ph
10	4-Br	H	CH ₂	Ph	Q-1	N(Me)SO ₂ Ph
	4-CF ₃	H	CH ₂	Me	Q-1	N(Me)SO ₂ Ph
	4-Cl	H	CH ₂	Me	Q-1	N(Me)SO ₂ Ph
	4-Br	H	CH ₂	Me	Q-1	N(Me)SO ₂ Ph
15	4-CF ₃	5-Cl	CH ₂	H	Q-1	N(Me)SO ₂ Me
	4-Cl	5-Cl	CH ₂	H	Q-1	N(Me)SO ₂ Me
	4-Br	5-Cl	CH ₂	H	Q-1	N(Me)SO ₂ Me
	4-CF ₃	5-Cl	CH ₂	CO ₂ Me	Q-1	N(Me)SO ₂ Me
20	4-Cl	5-Cl	CH ₂	CO ₂ Me	Q-1	N(Me)SO ₂ Me
	4-Br	5-Cl	CH ₂	CO ₂ Me	Q-1	N(Me)SO ₂ Me
	4-CF ₃	5-Cl	CH ₂	Ph	Q-1	N(Me)SO ₂ Me
	4-Cl	5-Cl	CH ₂	Ph	Q-1	N(Me)SO ₂ Me
25	4-Br	5-Cl	CH ₂	Ph	Q-1	N(Me)SO ₂ Me
	4-CF ₃	5-Me	CH ₂	H	Q-1	N(Me)SO ₂ Me
	4-Cl	5-Me	CH ₂	H	Q-1	N(Me)SO ₂ Me
	4-Br	5-Me	CH ₂	H	Q-1	N(Me)SO ₂ Me
30	4-CF ₃	5-Me	CH ₂	CO ₂ Me	Q-1	N(Me)SO ₂ Ph-4-Me
	4-Cl	5-Me	CH ₂	CO ₂ Me	Q-1	N(Me)SO ₂ Ph-4-Me
	4-Br	5-Me	CH ₂	CO ₂ Me	Q-1	N(Me)SO ₂ Ph-4-Me
	4-CF ₃	H	CH ₂	H	Q-2	N(Me)SO ₂ Ph
35	4-Cl	H	CH ₂	H	Q-2	N(Me)SO ₂ Ph
	4-Br	H	CH ₂	H	Q-2	N(Me)SO ₂ Ph
	4-CF ₃	H	CH ₂	CO ₂ Me	Q-2	N(Me)SO ₂ Ph
	4-Cl	H	CH ₂	CO ₂ Me	Q-2	N(Me)SO ₂ Ph

	R ₁	R ₂	A	B	Q	J
5	4-Br	H	CH ₂	CO ₂ Me	Q-2	N(Me)SO ₂ Ph
	4-CF ₃	H	CH ₂	Ph	Q-2	N(Me)SO ₂ Ph
	4-Cl	H	CH ₂	Ph	Q-2	N(Me)SO ₂ Ph
	4-Br	H	CH ₂	Ph	Q-2	N(Me)SO ₂ Ph
10	4-CF ₃	H	CH ₂	Me	Q-2	N(Me)SO ₂ Ph
	4-Cl	H	CH ₂	Me	Q-2	N(Me)SO ₂ Ph
	4-Br	H	CH ₂	Me	Q-2	N(Me)SO ₂ Ph
	4-CF ₃	H	CH ₂	H	Q-3	N(Me)SO ₂ Ph
	4-Cl	H	CH ₂	H	Q-3	N(Me)SO ₂ Ph
15	4-Br	H	CH ₂	H	Q-3	N(Me)SO ₂ Ph
	4-CF ₃	H	CH ₂	CO ₂ Me	Q-3	N(Me)SO ₂ Ph
	4-Cl	H	CH ₂	CO ₂ Me	Q-3	N(Me)SO ₂ Ph
	4-Br	H	CH ₂	CO ₂ Me	Q-3	N(Me)SO ₂ Ph
	4-CF ₃	H	CH ₂	Ph	Q-3	N(Me)SO ₂ Ph
20	4-Cl	H	CH ₂	Ph	Q-3	N(Me)SO ₂ Ph
	4-Br	H	CH ₂	Ph	Q-3	N(Me)SO ₂ Ph
	4-CF ₃	H	CH ₂	Me	Q-3	N(Me)SO ₂ Ph
	4-Cl	H	CH ₂	Me	Q-3	N(Me)SO ₂ Ph
	4-Br	H	CH ₂	Me	Q-3	N(Me)SO ₂ Ph
25	4-CF ₃	5-Cl	CH ₂	H	Q-3	N(Me)SO ₂ Me
	4-Cl	5-Cl	CH ₂	H	Q-3	N(Me)SO ₂ Me
	4-Br	5-Cl	CH ₂	H	Q-3	N(Me)SO ₂ Me
	4-CF ₃	5-Cl	CH ₂	CO ₂ Me	Q-3	N(Me)SO ₂ Me
	4-Cl	5-Cl	CH ₂	CO ₂ Me	Q-3	N(Me)SO ₂ Me
30	4-Br	5-Cl	CH ₂	CO ₂ Me	Q-3	N(Me)SO ₂ Me
	4-CF ₃	5-Cl	CH ₂	Ph	Q-3	N(Me)SO ₂ Me
	4-Cl	5-Cl	CH ₂	Ph	Q-3	N(Me)SO ₂ Me
	4-Br	5-Cl	CH ₂	Ph	Q-3	N(Me)SO ₂ Me

35

	R ₁	R ₂	A	B	Q	J
5	4-CF ₃	5-Me	CH ₂	H	Q-3	N(Me)SO ₂ Me
	4-Cl	5-Me	CH ₂	H	Q-3	N(Me)SO ₂ Me
	4-Br	5-Me	CH ₂	H	Q-3	N(Me)SO ₂ Me
	4-CF ₃	5-Me	CH ₂	CO ₂ Me	Q-3	N(Me)SO ₂ Ph-4-Me
10	4-Cl	5-Me	CH ₂	CO ₂ Me	Q-3	N(Me)SO ₂ Ph-4-Me
	4-Br	5-Me	CH ₂	CO ₂ Me	Q-3	N(Me)SO ₂ Ph-4-Me
	4-CF ₃	H	CH ₂	H	Q-4	N(Me)SO ₂ Ph
	4-Cl	H	CH ₂	H	Q-4	N(Me)SO ₂ Ph
	4-Br	H	CH ₂	H	Q-4	N(Me)SO ₂ Ph
15	4-CF ₃	H	CH ₂	CO ₂ Me	Q-4	N(Me)SO ₂ Ph
	4-Cl	H	CH ₂	CO ₂ Me	Q-4	N(Me)SO ₂ Ph
	4-Br	H	CH ₂	CO ₂ Me	Q-4	N(Me)SO ₂ Ph
	4-CF ₃	H	CH ₂	Ph	Q-4	N(Me)SO ₂ Ph
	4-Cl	H	CH ₂	Ph	Q-4	N(Me)SO ₂ Ph
20	4-Br	H	CH ₂	Ph	Q-4	N(Me)SO ₂ Ph
	4-CF ₃	H	CH ₂	Me	Q-4	N(Me)SO ₂ Ph
	4-Cl	H	CH ₂	Me	Q-4	N(Me)SO ₂ Ph
	4-Br	H	CH ₂	Me	Q-4	N(Me)SO ₂ Ph
	4-CF ₃	5-Cl	CH ₂	H	Q-4	N(Me)SO ₂ Me
25	4-Cl	5-Cl	CH ₂	H	Q-4	N(Me)SO ₂ Me
	4-Br	5-Cl	CH ₂	H	Q-4	N(Me)SO ₂ Me
	4-CF ₃	5-Cl	CH ₂	CO ₂ Me	Q-4	N(Me)SO ₂ Me
	4-Cl	5-Cl	CH ₂	CO ₂ Me	Q-4	N(Me)SO ₂ Me
	4-Br	5-Cl	CH ₂	CO ₂ Me	Q-4	N(Me)SO ₂ Me
30	4-CF ₃	5-Cl	CH ₂	Ph	Q-4	N(Me)SO ₂ Me
	4-Cl	5-Cl	CH ₂	Ph	Q-4	N(Me)SO ₂ Me
	4-Br	5-Cl	CH ₂	Ph	Q-4	N(Me)SO ₂ Me
	4-CF ₃	5-Me	CH ₂	H	Q-4	N(Me)SO ₂ Me

	R ₁	R ₂	A	B	Q	J
5	4-Cl	5-Me	CH ₂	H	Q-4	N(Me)SO ₂ Me
	4-Br	5-Me	CH ₂	H	Q-4	N(Me)SO ₂ Me
	4-CF ₃	5-Me	CH ₂	CO ₂ Me	Q-4	N(Me)SO ₂ Ph-4-Me
	4-Cl	5-Me	CH ₂	CO ₂ Me	Q-4	N(Me)SO ₂ Ph-4-Me
10	4-Br	5-Me	CH ₂	CO ₂ Me	Q-4	N(Me)SO ₂ Ph-4-Me
	4-CF ₃	H	CH ₂	H	Q-5	N(Me)SO ₂ Ph
	4-Cl	H	CH ₂	H	Q-5	N(Me)SO ₂ Ph
	4-Br	H	CH ₂	H	Q-5	N(Me)SO ₂ Ph
	4-CF ₃	H	CH ₂	CO ₂ Me	Q-5	N(Me)SO ₂ Ph
15	4-Cl	H	CH ₂	CO ₂ Me	Q-5	N(Me)SO ₂ Ph
	4-Br	H	CH ₂	CO ₂ Me	Q-5	N(Me)SO ₂ Ph
	4-CF ₃	H	CH ₂	Ph	Q-5	N(Me)SO ₂ Ph
	4-Cl	H	CH ₂	Ph	Q-5	N(Me)SO ₂ Ph
	4-Br	H	CH ₂	Ph	Q-5	N(Me)SO ₂ Ph
20	4-CF ₃	H	CH ₂	Me	Q-5	N(Me)SO ₂ Ph
	4-Cl	H	CH ₂	Me	Q-5	N(Me)SO ₂ Ph
	4-Br	H	CH ₂	Me	Q-5	N(Me)SO ₂ Ph
	4-CF ₃	5-Cl	CH ₂	H	Q-5	N(Me)SO ₂ Me
	4-Cl	5-Cl	CH ₂	H	Q-5	N(Me)SO ₂ Me
25	4-Br	5-Cl	CH ₂	H	Q-5	N(Me)SO ₂ Me
	4-CF ₃	5-Cl	CH ₂	CO ₂ Me	Q-5	N(Me)SO ₂ Me
	4-Cl	5-Cl	CH ₂	CO ₂ Me	Q-5	N(Me)SO ₂ Me
	4-Br	5-Cl	CH ₂	CO ₂ Me	Q-5	N(Me)SO ₂ Me
	4-CF ₃	5-Cl	CH ₂	Ph	Q-5	N(Me)SO ₂ Me
30	4-Cl	5-Cl	CH ₂	Ph	Q-5	N(Me)SO ₂ Me
	4-Br	5-Cl	CH ₂	Ph	Q-5	N(Me)SO ₂ Me
	4-CF ₃	5-Me	CH ₂	H	Q-5	N(Me)SO ₂ Me
	4-Cl	5-Me	CH ₂	H	Q-5	N(Me)SO ₂ Me

	R ₁	R ₂	A	B	Q	J
5	4-Br	5-Me	CH ₂	H	Q-5	N(Me)SO ₂ Me
	4-CF ₃	5-Me	CH ₂	CO ₂ Me	Q-5	N(Me)SO ₂ Ph-4-Me
	4-Cl	5-Me	CH ₂	CO ₂ Me	Q-5	N(Me)SO ₂ Ph-4-Me
	4-Br	5-Me	CH ₂	CO ₂ Me	Q-5	N(Me)SO ₂ Ph-4-Me
10	4-CF ₃	H	CH ₂	H	Q-7	N(Me)SO ₂ Ph
	4-Cl	H	CH ₂	H	Q-7	N(Me)SO ₂ Ph
	4-Br	H	CH ₂	H	Q-7	N(Me)SO ₂ Ph
	4-CF ₃	H	CH ₂	CO ₂ Me	Q-7	N(Me)SO ₂ Ph
	4-Cl	H	CH ₂	CO ₂ Me	Q-7	N(Me)SO ₂ Ph
15	4-Br	H	CH ₂	CO ₂ Me	Q-7	N(Me)SO ₂ Ph
	4-CF ₃	H	CH ₂	Ph	Q-7	N(Me)SO ₂ Ph
	4-Cl	H	CH ₂	Ph	Q-7	N(Me)SO ₂ Ph
	4-Br	H	CH ₂	Ph	Q-7	N(Me)SO ₂ Ph
	4-CF ₃	H	CH ₂	Me	Q-7	N(Me)SO ₂ Ph
20	4-Cl	H	CH ₂	Me	Q-7	N(Me)SO ₂ Ph
	4-Br	H	CH ₂	Me	Q-7	N(Me)SO ₂ Ph
	4-CF ₃	5-Cl	CH ₂	H	Q-7	N(Me)SO ₂ Me
	4-Cl	5-Cl	CH ₂	H	Q-7	N(Me)SO ₂ Me
	4-Br	5-Cl	CH ₂	H	Q-7	N(Me)SO ₂ Me
25	4-CF ₃	5-Cl	CH ₂	CO ₂ Me	Q-7	N(Me)SO ₂ Me
	4-Cl	5-Cl	CH ₂	CO ₂ Me	Q-7	N(Me)SO ₂ Me
	4-Br	5-Cl	CH ₂	CO ₂ Me	Q-7	N(Me)SO ₂ Me
	4-CF ₃	5-Cl	CH ₂	Ph	Q-7	N(Me)SO ₂ Me
	4-Cl	5-Cl	CH ₂	Ph	Q-7	N(Me)SO ₂ Me
30	4-Br	5-Cl	CH ₂	Ph	Q-7	N(Me)SO ₂ Me
	4-CF ₃	5-Me	CH ₂	H	Q-7	N(Me)SO ₂ Me
	4-Cl	5-Me	CH ₂	H	Q-7	N(Me)SO ₂ Me
	4-Br	5-Me	CH ₂	H	Q-7	N(Me)SO ₂ Me

	R ₁	R ₂	A	B	Q	J
5	4-CF ₃	5-Me	CH ₂	CO ₂ Me	Q-7	N(Me)SO ₂ Ph-4-Me
	4-Cl	5-Me	CH ₂	CO ₂ Me	Q-7	N(Me)SO ₂ Ph-4-Me
	4-Br	5-Me	CH ₂	CO ₂ Me	Q-7	N(Me)SO ₂ Ph-4-Me
	4-CF ₃	H	CH ₂	H	Q-1	CO ₂ Me
10	4-Cl	H	CH ₂	H	Q-1	CO ₂ Me
	4-Br	H	CH ₂	H	Q-1	CO ₂ Me
	4-CF ₃	H	CH ₂	CO ₂ Me	Q-1	CO ₂ Me
	4-Cl	H	CH ₂	CO ₂ Me	Q-1	CO ₂ Me
	4-Br	H	CH ₂	CO ₂ Me	Q-1	CO ₂ Me
15	4-CF ₃	H	CH ₂	Ph	Q-1	CO ₂ Me
	4-Cl	H	CH ₂	Ph	Q-1	CO ₂ Me
	4-Br	H	CH ₂	Ph	Q-1	CO ₂ Me
	4-CF ₃	H	CH ₂	Me	Q-1	CO ₂ Et
	4-Cl	H	CH ₂	Me	Q-1	CO ₂ Et
20	4-Br	H	CH ₂	Me	Q-1	CO ₂ Et
	4-CF ₃	5-Cl	CH ₂	H	Q-1	CO ₂ nPr
	4-Cl	5-Cl	CH ₂	H	Q-1	CO ₂ nPr
	4-Br	5-Cl	CH ₂	H	Q-1	CO ₂ nPr
	4-CF ₃	5-Cl	CH ₂	CO ₂ Me	Q-1	CO ₂ nPr
25	4-Cl	5-Cl	CH ₂	CO ₂ Me	Q-1	CO ₂ nPr
	4-Br	5-Cl	CH ₂	CO ₂ Me	Q-1	CO ₂ nPr
	4-CF ₃	5-Cl	CH ₂	Ph	Q-1	CO ₂ CH ₂ CH ₂ OEt
	4-Cl	5-Cl	CH ₂	Ph	Q-1	CO ₂ CH ₂ CH ₂ OEt
	4-Br	5-Cl	CH ₂	Ph	Q-1	CO ₂ CH ₂ CH ₂ OEt
30	4-CF ₃	5-Me	CH ₂	H	Q-1	CO ₂ CH ₂ Ph
	4-Cl	5-Me	CH ₂	H	Q-1	CO ₂ CH ₂ Ph
	4-Br	5-Me	CH ₂	H	Q-1	CO ₂ CH ₂ Ph
	4-CF ₃	5-Me	CH ₂	CO ₂ Me	Q-1	CO ₂ CH ₂ Ph

	R ₁	R ₂	A	B	Q	J
5	4-Cl	5-Me	CH ₂	CO ₂ Me	Q-1	CO ₂ CH ₂ Ph
	4-Br	5-Me	CH ₂	CO ₂ Me	Q-1	CO ₂ CH ₂ Ph
	4-CF ₃	H	CH ₂	H	Q-1	CO ₂ nBu
	4-Cl	H	CH ₂	H	Q-1	CO ₂ nBu
10	4-Br	H	CH ₂	H	Q-1	CO ₂ nBu
	4-CF ₃	H	CH ₂	CO ₂ Me	Q-1	CO ₂ nBu
	4-Cl	H	CH ₂	CO ₂ Me	Q-1	CO ₂ nBu
	4-Br	H	CH ₂	CO ₂ Me	Q-1	CO ₂ nBu
	4-CF ₃	H	CH ₂	Ph	Q-1	CO ₂ nBu
15	4-Cl	H	CH ₂	Ph	Q-1	CO ₂ nBu
	4-Br	H	CH ₂	Ph	Q-1	CO ₂ nBu
	4-CF ₃	H	CH ₂	Me	Q-1	CO ₂ nBu
	4-Cl	H	CH ₂	Me	Q-1	CO ₂ nBu
	4-Br	H	CH ₂	Me	Q-1	CO ₂ nBu
20	4-CF ₃	5-Cl	CH ₂	H	Q-1	CO ₂ nBu
	4-Cl	5-Cl	CH ₂	H	Q-1	CO ₂ nBu
	4-Br	5-Cl	CH ₂	H	Q-1	CO ₂ nBu
	4-CF ₃	5-Cl	CH ₂	CO ₂ Me	Q-1	CO ₂ nBu
	4-Cl	5-Cl	CH ₂	CO ₂ Me	Q-1	CO ₂ nBu
25	4-Br	5-Cl	CH ₂	CO ₂ Me	Q-1	CO ₂ nBu
	4-CF ₃	5-Cl	CH ₂	Ph	Q-1	CO ₂ nBu
	4-Cl	5-Cl	CH ₂	Ph	Q-1	CO ₂ nBu
	4-Br	5-Cl	CH ₂	Ph	Q-1	CO ₂ nBu
	4-CF ₃	5-Me	CH ₂	H	Q-1	CO ₂ nBu
30	4-Cl	5-Me	CH ₂	H	Q-1	CO ₂ nBu
	4-Br	5-Me	CH ₂	H	Q-1	CO ₂ nBu
	4-CF ₃	5-Me	CH ₂	CO ₂ Me	Q-1	CO ₂ nBu
	4-Cl	5-Me	CH ₂	CO ₂ Me	Q-1	CO ₂ nBu

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	R ₁	R ₂	A	B	Q	J
5	4-Br	5-Me	CH ₂	CO ₂ Me	Q-1	CO ₂ nBu
	4-CF ₃	H	CH ₂	H	Q-3	CO ₂ Me
	4-Cl	H	CH ₂	H	Q-3	CO ₂ Me
	4-Br	H	CH ₂	H	Q-3	CO ₂ Me
10	4-CF ₃	H	CH ₂	CO ₂ Me	Q-3	CO ₂ Me
	4-Cl	H	CH ₂	CO ₂ Me	Q-3	CO ₂ Me
	4-Br	H	CH ₂	CO ₂ Me	Q-3	CO ₂ Me
	4-CF ₃	H	CH ₂	Ph	Q-3	CO ₂ Me
	4-Cl	H	CH ₂	Ph	Q-3	CO ₂ Me
15	4-Br	H	CH ₂	Ph	Q-3	CO ₂ Me
	4-CF ₃	H	CH ₂	Me	Q-3	CO ₂ Et
	4-Cl	H	CH ₂	Me	Q-3	CO ₂ Et
	4-Br	H	CH ₂	Me	Q-3	CO ₂ Et
	4-CF ₃	5-Cl	CH ₂	H	Q-3	CO ₂ nPr
20	4-Cl	5-Cl	CH ₂	H	Q-3	CO ₂ nPr
	4-Br	5-Cl	CH ₂	H	Q-3	CO ₂ nPr
	4-CF ₃	5-Cl	CH ₂	CO ₂ Me	Q-3	CO ₂ nPr
	4-Cl	5-Cl	CH ₂	CO ₂ Me	Q-3	CO ₂ nPr
	4-Br	5-Cl	CH ₂	CO ₂ Me	Q-3	CO ₂ nPr
25	4-CF ₃	5-Cl	CH ₂	Ph	Q-3	CO ₂ CH ₂ CH ₂ OEt
	4-Cl	5-Cl	CH ₂	Ph	Q-3	CO ₂ CH ₂ CH ₂ OEt
	4-Br	5-Cl	CH ₂	Ph	Q-3	CO ₂ CH ₂ CH ₂ OEt
	4-CF ₃	5-Me	CH ₂	H	Q-3	CO ₂ CH ₂ Ph
	4-Cl	5-Me	CH ₂	H	Q-3	CO ₂ CH ₂ Ph
30	4-Br	5-Me	CH ₂	H	Q-3	CO ₂ CH ₂ Ph
	4-CF ₃	5-Me	CH ₂	CO ₂ Me	Q-3	CO ₂ CH ₂ Ph
	4-Cl	5-Me	CH ₂	CO ₂ Me	Q-3	CO ₂ CH ₂ Ph
	4-Br	5-Me	CH ₂	CO ₂ Me	Q-3	CO ₂ CH ₂ Ph

	R ₁	R ₂	A	B	Q	J
5	4-CF ₃	H	CH ₂	H	Q-3	CO ₂ nBu
	4-Cl	H	CH ₂	H	Q-3	CO ₂ nBu
	4-Br	H	CH ₂	H	Q-3	CO ₂ nBu
	4-CF ₃	H	CH ₂	CO ₂ Me	Q-3	CO ₂ nBu
10	4-Cl	H	CH ₂	CO ₂ Me	Q-3	CO ₂ nBu
	4-Br	H	CH ₂	CO ₂ Me	Q-3	CO ₂ nBu
	4-CF ₃	H	CH ₂	Ph	Q-3	CO ₂ nBu
	4-Cl	H	CH ₂	Ph	Q-3	CO ₂ nBu
15	4-Br	H	CH ₂	Ph	Q-3	CO ₂ nBu
	4-CF ₃	H	CH ₂	Me	Q-3	CO ₂ nBu
	4-Cl	H	CH ₂	Me	Q-3	CO ₂ nBu
	4-Br	H	CH ₂	Me	Q-3	CO ₂ nBu
20	4-CF ₃	5-Cl	CH ₂	H	Q-3	CO ₂ nBu
	4-Cl	5-Cl	CH ₂	H	Q-3	CO ₂ nBu
	4-Br	5-Cl	CH ₂	H	Q-3	CO ₂ nBu
	4-CF ₃	5-Cl	CH ₂	CO ₂ Me	Q-3	CO ₂ nBu
25	4-Cl	5-Cl	CH ₂	CO ₂ Me	Q-3	CO ₂ nBu
	4-Br	5-Cl	CH ₂	CO ₂ Me	Q-3	CO ₂ nBu
	4-CF ₃	5-Cl	CH ₂	Ph	Q-3	CO ₂ nBu
	4-Cl	5-Cl	CH ₂	Ph	Q-3	CO ₂ nBu
30	4-Br	5-Cl	CH ₂	Ph	Q-3	CO ₂ nBu
	4-CF ₃	5-Me	CH ₂	H	Q-3	CO ₂ nBu
	4-Cl	5-Me	CH ₂	H	Q-3	CO ₂ nBu
	4-Br	5-Me	CH ₂	H	Q-3	CO ₂ nBu
35	4-CF ₃	5-Me	CH ₂	CO ₂ Me	Q-3	CO ₂ nBu
	4-Cl	5-Me	CH ₂	CO ₂ Me	Q-3	CO ₂ nBu
	4-Br	5-Me	CH ₂	CO ₂ Me	Q-3	CO ₂ nBu
	4-CF ₃	H	CH ₂	H	Q-4	CO ₂ Me

	R ₁	R ₂	A	B	Q	J
5	4-Cl	H	CH ₂	H	Q-4	CO ₂ Me
	4-Br	H	CH ₂	H	Q-4	CO ₂ Me
	4-CF ₃	H	CH ₂	CO ₂ Me	Q-4	CO ₂ Me
	4-Cl	H	CH ₂	CO ₂ Me	Q-4	CO ₂ Me
10	4-Br	H	CH ₂	CO ₂ Me	Q-4	CO ₂ Me
	4-CF ₃	H	CH ₂	Ph	Q-4	CO ₂ Me
	4-Cl	H	CH ₂	Ph	Q-4	CO ₂ Me
	4-Br	H	CH ₂	Ph	Q-4	CO ₂ Me
	4-CF ₃	H	CH ₂	Me	Q-4	CO ₂ Et
15	4-Cl	H	CH ₂	Me	Q-4	CO ₂ Et
	4-Br	H	CH ₂	Me	Q-4	CO ₂ Et
	4-CF ₃	5-Cl	CH ₂	H	Q-4	CO ₂ nPr
	4-Cl	5-Cl	CH ₂	H	Q-4	CO ₂ nPr
	4-Br	5-Cl	CH ₂	H	Q-4	CO ₂ nPr
20	4-CF ₃	5-Cl	CH ₂	CO ₂ Me	Q-4	CO ₂ nPr
	4-Cl	5-Cl	CH ₂	CO ₂ Me	Q-4	CO ₂ nPr
	4-Br	5-Cl	CH ₂	CO ₂ Me	Q-4	CO ₂ nPr
	4-CF ₃	5-Cl	CH ₂	Ph	Q-4	CO ₂ CH ₂ CH ₂ OEt
	4-Cl	5-Cl	CH ₂	Ph	Q-4	CO ₂ CH ₂ CH ₂ OEt
25	4-Br	5-Cl	CH ₂	Ph	Q-4	CO ₂ CH ₂ CH ₂ OEt
	4-CF ₃	5-Me	CH ₂	H	Q-4	CO ₂ CH ₂ Ph
	4-Cl	5-Me	CH ₂	H	Q-4	CO ₂ CH ₂ Ph
	4-Br	5-Me	CH ₂	H	Q-4	CO ₂ CH ₂ Ph
	4-CF ₃	5-Me	CH ₂	CO ₂ Me	Q-4	CO ₂ CH ₂ Ph
30	4-Cl	5-Me	CH ₂	CO ₂ Me	Q-4	CO ₂ CH ₂ Ph
	4-Br	5-Me	CH ₂	CO ₂ Me	Q-4	CO ₂ CH ₂ Ph
	4-CF ₃	H	CH ₂	H	Q-4	CO ₂ nBu
	4-Cl	H	CH ₂	H	Q-4	CO ₂ nBu

35

	R ₁	R ₂	A	B	Q	J
5	4-Br	H	CH ₂	H	Q-4	CO ₂ nBu
	4-CF ₃	H	CH ₂	CO ₂ Me	Q-4	CO ₂ nBu
	4-Cl	H	CH ₂	CO ₂ Me	Q-4	CO ₂ nBu
	4-Br	H	CH ₂	CO ₂ Me	Q-4	CO ₂ nBu
10	4-CF ₃	H	CH ₂	Ph	Q-4	CO ₂ nBu
	4-Cl	H	CH ₂	Ph	Q-4	CO ₂ nBu
	4-Br	H	CH ₂	Ph	Q-4	CO ₂ nBu
	4-CF ₃	H	CH ₂	Me	Q-4	CO ₂ nBu
	4-Cl	H	CH ₂	Me	Q-4	CO ₂ nBu
15	4-Br	H	CH ₂	Me	Q-4	CO ₂ nBu
	4-CF ₃	5-Cl	CH ₂	H	Q-4	CO ₂ nBu
	4-Cl	5-Cl	CH ₂	H	Q-4	CO ₂ nBu
	4-Br	5-Cl	CH ₂	H	Q-4	CO ₂ nBu
	4-CF ₃	5-Cl	CH ₂	CO ₂ Me	Q-4	CO ₂ nBu
20	4-Cl	5-Cl	CH ₂	CO ₂ Me	Q-4	CO ₂ nBu
	4-Br	5-Cl	CH ₂	CO ₂ Me	Q-4	CO ₂ nBu
	4-CF ₃	5-Cl	CH ₂	Ph	Q-4	CO ₂ nBu
	4-Cl	5-Cl	CH ₂	Ph	Q-4	CO ₂ nBu
	4-Br	5-Cl	CH ₂	Ph	Q-4	CO ₂ nBu
25	4-CF ₃	5-Me	CH ₂	H	Q-4	CO ₂ nBu
	4-Cl	5-Me	CH ₂	H	Q-4	CO ₂ nBu
	4-Br	5-Me	CH ₂	H	Q-4	CO ₂ nBu
	4-CF ₃	5-Me	CH ₂	CO ₂ Me	Q-4	CO ₂ nBu
	4-Cl	5-Me	CH ₂	CO ₂ Me	Q-4	CO ₂ nBu
30	4-Br	5-Me	CH ₂	CO ₂ Me	Q-4	CO ₂ nBu
	4-CF ₃	H	CH ₂	H	Q-5	CO ₂ Me
	4-Cl	H	CH ₂	H	Q-5	CO ₂ Me
	4-Br	H	CH ₂	H	Q-5	CO ₂ Me

	R ₁	R ₂	A	B	Q	J
5	4-CF ₃	H	CH ₂	CO ₂ Me	Q-5	CO ₂ Me
	4-Cl	H	CH ₂	CO ₂ Me	Q-5	CO ₂ Me
	4-Br	H	CH ₂	CO ₂ Me	Q-5	CO ₂ Me
	4-CF ₃	H	CH ₂	Ph	Q-5	CO ₂ Me
10	4-Cl	H	CH ₂	Ph	Q-5	CO ₂ Me
	4-Br	H	CH ₂	Ph	Q-5	CO ₂ Me
	4-CF ₃	H	CH ₂	Me	Q-5	CO ₂ Et
	4-Cl	H	CH ₂	Me	Q-5	CO ₂ Et
	4-Br	H	CH ₂	Me	Q-5	CO ₂ Et
15	4-CF ₃	5-Cl	CH ₂	H	Q-5	CO ₂ nPr
	4-Cl	5-Cl	CH ₂	H	Q-5	CO ₂ nPr
	4-Br	5-Cl	CH ₂	H	Q-5	CO ₂ nPr
	4-CF ₃	5-Cl	CH ₂	CO ₂ Me	Q-5	CO ₂ nPr
	4-Cl	5-Cl	CH ₂	CO ₂ Me	Q-5	CO ₂ nPr
20	4-Br	5-Cl	CH ₂	CO ₂ Me	Q-5	CO ₂ nPr
	4-CF ₃	5-Cl	CH ₂	Ph	Q-5	CO ₂ CH ₂ CH ₂ OEt
	4-Cl	5-Cl	CH ₂	Ph	Q-5	CO ₂ CH ₂ CH ₂ OEt
	4-Br	5-Cl	CH ₂	Ph	Q-5	CO ₂ CH ₂ CH ₂ OEt
	4-CF ₃	5-Me	CH ₂	H	Q-5	CO ₂ CH ₂ Ph
25	4-Cl	5-Me	CH ₂	H	Q-5	CO ₂ CH ₂ Ph
	4-Br	5-Me	CH ₂	H	Q-5	CO ₂ CH ₂ Ph
	4-CF ₃	5-Me	CH ₂	CO ₂ Me	Q-5	CO ₂ CH ₂ Ph
	4-Cl	5-Me	CH ₂	CO ₂ Me	Q-5	CO ₂ CH ₂ Ph
	4-Br	5-Me	CH ₂	CO ₂ Me	Q-5	CO ₂ CH ₂ Ph
30	4-CF ₃	H	CH ₂	H	Q-5	CO ₂ nBu
	4-Cl	H	CH ₂	H	Q-5	CO ₂ nBu
	4-Br	H	CH ₂	H	Q-5	CO ₂ nBu
	4-CF ₃	H	CH ₂	CO ₂ Me	Q-5	CO ₂ nBu

	R ₁	R ₂	A	B	Q	J
5	4-Cl	H	CH ₂	CO ₂ Me	Q-5	CO ₂ nBu
	4-Br	H	CH ₂	CO ₂ Me	Q-5	CO ₂ nBu
	4-CF ₃	H	CH ₂	Ph	Q-5	CO ₂ nBu
	4-Cl	H	CH ₂	Ph	Q-5	CO ₂ nBu
10	4-Br	H	CH ₂	Ph	Q-5	CO ₂ nBu
	4-CF ₃	H	CH ₂	Me	Q-5	CO ₂ nBu
	4-Cl	H	CH ₂	Me	Q-5	CO ₂ nBu
	4-Br	H	CH ₂	Me	Q-5	CO ₂ nBu
	4-CF ₃	5-Cl	CH ₂	H	Q-5	CO ₂ nBu
15	4-Cl	5-Cl	CH ₂	H	Q-5	CO ₂ nBu
	4-Br	5-Cl	CH ₂	H	Q-5	CO ₂ nBu
	4-CF ₃	5-Cl	CH ₂	CO ₂ Me	Q-5	CO ₂ nBu
	4-Cl	5-Cl	CH ₂	CO ₂ Me	Q-5	CO ₂ nBu
	4-Br	5-Cl	CH ₂	CO ₂ Me	Q-5	CO ₂ nBu
20	4-CF ₃	5-Cl	CH ₂	Ph	Q-5	CO ₂ nBu
	4-Cl	5-Cl	CH ₂	Ph	Q-5	CO ₂ nBu
	4-Br	5-Cl	CH ₂	Ph	Q-5	CO ₂ nBu
	4-CF ₃	5-Me	CH ₂	H	Q-5	CO ₂ nBu
	4-Cl	5-Me	CH ₂	H	Q-5	CO ₂ nBu
25	4-Br	5-Me	CH ₂	H	Q-5	CO ₂ nBu
	4-CF ₃	5-Me	CH ₂	CO ₂ Me	Q-5	CO ₂ nBu
	4-Cl	5-Me	CH ₂	CO ₂ Me	Q-5	CO ₂ nBu
	4-Br	5-Me	CH ₂	CO ₂ Me	Q-5	CO ₂ nBu

30

35

TABLE 13

5	R ₁	R ₂	B	X
	H	H	H	O
	4-Cl	H	H	O
	4-F	H	H	O
	4-Br	H	H	O
	4-CF ₃	H	H	O
10	4-OCF ₂ H	H	H	O
	4-CF ₃ Cl	H	H	O
	4-CO ₂ Me	H	H	O
	4-CO ₂ -i-Pr	H	H	O
	4-NO ₂	H	H	O
15	4-SMe	H	H	O
	4-SO ₂ Me	H	H	O
	4-CF ₂ Cl	H	H	O
	4-OCF ₃	H	H	O
	4-I	H	H	O
	4-OCF ₂ CF ₂ H	H	H	O
20	4-CN	H	H	O
	4-Me	H	H	O
	3,4-CF ₂ CF ₂ O	H	H	O
	3,4-OCF ₂ CF ₂	H	H	O
	3,4-(Me) ₂ CCH ₂ O	H	O	O
25	4-Cl	H	Me	O
	4-Br	H	Me	O
	4-CF ₃	H	Me	O
	4-SMe	H	Me	O
	4-OCF ₂ H	H	Me	O
	4-CF ₃	H	Et	O
30	4-CO ₂ i-Pr	H	Me	O
	4-Cl	H	allyl	O
	4-Br	H	allyl	O
	4-CF ₃	H	allyl	O
	4-Cl	H	CH ₂ Ph	O
	4-Br	H	CH ₂ Ph	O
35	4-CF ₃	H	CH ₂ Ph	O
	4-CF ₃	H	4-F-CH ₂ Ph	O
	4-SMe	H	4-F-CH ₂ Ph	O

5	R ₁	R ₂	B	X
	4-CF ₃	H	4-F-CH ₂ Ph	O
	4-CF ₃	H	4-Cl-CH ₂ Ph	O
	4-NO ₂	H	4-Cl-CH ₂ Ph	O
	4-OCF ₂ H	H	Ph	O
10	4-OCF ₃	H	Ph	O
	4-CF ₃	H	Ph	O
	4-Cl	H	4-Cl-Ph	O
	4-Br	H	4-Cl-Ph	O
	4-OMe	H	4-Cl-Ph	O
	4-CF ₃	H	n-Bu	O
15	4-Cl	H	n-Bu	O
	4-CF ₃	H	(CH ₂) ₃ Cl	O
	4-Cl	H	(CH ₂) ₃ Cl	O
	4-Br	H	CH ₂ CF ₃	O
	4-OCF ₃	H	CH ₂ CF ₃	O
20	4-SCF ₂ H	H	CH ₂ OMe	O
	4-CF ₃	H	CH ₂ OEt	O
	4-Cl	H	CH ₂ CO ₂ Me	O
	4-Br	H	CH ₂ CO ₂ Me	O
	4-OCF ₂ H	H	CH ₂ CN	O
25	4-OCF ₂ CF ₂ H	H	(CH ₂) ₂ CN	O
	4-CF ₃	H	(CH ₂) ₂ CN	O
	4-CF ₃	H	(CH ₂) ₃ CN	O
	4-CF ₃	H	CO ₂ Me	O
	4-Cl	H	CO ₂ Me	O
30	4-Br	H	CO ₂ Me	O
	4-F	H	CO ₂ Me	O
	4-CF ₂ Cl	H	CO ₂ Me	O
	4-OCF ₃	H	CO ₂ Me	O
	3,4-CF ₂ CF ₂ O	H	CO ₂ Me	O
35	3,4-OCF ₂ CF ₂ O	H	CO ₂ Me	O
	3,4-(Me) ₂ CCH ₂ O	H	CO ₂ Me	O
	4-CF ₃	H	CO ₂ Et	O

5	R ₁	R ₂	B	X
10	4-Br	H	CO ₂ Et	O
	4-Cl	H	CO ₂ Et	O
	4-CF ₃	H	CO ₂ H	O
	4-CF ₃	H	CO ₂ Na	O
	4-CF ₃	H	CO ₂ Ph	O
	4-F	H	CO ₂ Ph	O
	4-CF ₃	H	CO ₂ CH ₂ CCl ₃	O
	4-CF ₃	H	CO ₂ CH ₂ CF ₃	O
	4-CF ₃	H	CO ₂ (CH ₂)Cl	O
	4-CF ₃	H	CO ₂ (CH ₂) ₂ Br	O
20	4-CF ₃	H	CO ₂ CH ₂ CN	O
	4-CF ₃	H	CO ₂ allyl	O
	4-CF ₃	H	CO ₂ CH ₂ Ph	O
	4-CF ₃	H	CO ₂ CH ₂ SMe	O
	4-CF ₃	H	C(O)NH ₂	O
	4-Cl	H	C(O)NH ₂	O
	4-Br	H	C(O)NHMe	O
	4-OCF ₃	H	C(O)NHMe	O
	4-CF ₃	H	C(O)NMe ₂	O
	4-Cl	H	C(O)NMe ₂	O
30	4-Br	H	C(O)NH ₂ Et	O
	4-CF ₃	H	C(O)NHMe	O
	4-CF ₃	H	C(O)NHallyl	O
	4-CF ₃	H	C(O)N(Me)allyl	O
	4-CF ₃	H	C(O)NHPh-4-Cl	O
	4-OCF ₃	H	C(S)NH ₂	O
	4-CF ₃	H	C(S)NHMe	O
	4-Cl	H	C(S)NMe ₂	O
	4-Br	H	C(S)Me	O
	4-OCF ₃	H	C(S)Et	O
35	4-CF ₃	H	C(S)NMe ₂	O
	4-Cl	H	C(S)NHMe	O

5	R ₁	R ₂	B	X
	4-Br	5-Cl	H	O
	4-CF ₃	5-Cl	Me	O
	4-OCF ₃	5-Cl	Et	O
10	4-Cl	5-Cl	H	O
	4-SMe	5-Cl	H	O
	4-CO ₂ Et	5-Cl	H	O
	4-Br	5-Cl	CO ₂ Me	O
	3-SMe	5-Cl	CO ₂ Me	O
	4-CO ₂ Et	5-Cl	CO ₂ Me	O
15	4-CF ₂	5-Cl	CO ₂ Me	O
	4-CF ₃	5-Cl	H	O
	4-CF ₃	H	CO ₂ Me	O
	4-OCF ₂ H	5-Cl	CO ₂ Me	O
	4-Cl	5-Cl	CO ₂ Me	O
	4-Br	5-Cl	C(O)Me	O
20	4-CF ₃	5-Cl	C(O)Et	O
	4-OCF ₃	5-Cl	C(O)NMe ₂	O
	4-CF ₃	5-F	H	O
	4-Cl	5-F	H	O
	4-Br	5-F	H	O
	4-OCF ₂ H	5-F	H	O
25	4-Cl	5-F	CO ₂ Me	O
	4-Br	5-F	CO ₂ Me	O
	4-CF ₃	5-F	CO ₂ Me	O
	4-OCF ₂ H	5-F	CO ₂ Me	O
	4-Cl	5-F	CO ₂ Me	O
	4-Br	5-OCF ₂ H	CO ₂ Me	O
30	4-Cl	5-OCF ₂ H	CO ₂ Me	O
	4-Br	5-OCF ₂ H	CO ₂ Me	O
	4-CF ₃	5-OCF ₂ H	CO ₂ Me	O
	4-OCF ₃	5-OCF ₂ H	CO ₂ Me	O
	4-OCF ₂ H	5-OCF ₂ H	CO ₂ Me	O
	4-Cl	5-Br	CO ₂ Me	O

5	R ₁	R ₂	B	X
10	4-Br	5-NO ₂	CO ₂ Me	O
	4-CF ₃	5-CF ₃	CO ₂ Me	O
	4-OCF ₃	5-OCH ₃	CO ₂ Me	O
	4-CF ₃	5-OCH ₂ Ph	Me	O
	4-CF ₃	5-C(O)Me	Et	O
	4-CF ₃	5-OCF ₂ CF ₂ H	CO ₂ Me	O
	4-CF ₃	5-I	Me	O
	4-CF ₃	5-OCF ₃	Et	O
	4-CF ₃	5-Et	C(O)Me	O
	4-CF ₃	5-Me	C(O)CF ₃	O
20	4-CF ₃	5-CN	Me	O
	4-CF ₃	5-OMe	CO ₂ Me	O
	4-CF ₃	5-OMe	CO ₂ Et	O
	4-CF ₃	5-OMe	H	O
	4-Cl	5-OMe	H	O
	4-CF ₃	5-CO ₂ Me	n-C ₆ H ₁₃	O
	4-CF ₃	5-SCF ₂ H	C(O)H	O
	4-CF ₃	5-SO ₂ Me	(CH ₂) ₄ Cl	O
	4-CF ₃	5,6-di-Cl	H	O
	4-CF ₃	5,6-di-Cl	CO ₂ Me	O
30	4-CF ₃	4-F	H	O
	4-Cl	4-F	CO ₂ Me	O
	4-Br	4-F	CO ₂ Me	O
	4-CF ₃	4-Cl	H	O
	4-OCF ₂ H	4-Cl	H	O
	4-OCF ₂ H	4-Cl	CO ₂ Me	O
	4-CF ₃	4-Br	H	O
	4-CF ₃	4-Br	CO ₂ Me	O
	4-CF ₃	6-Cl	CO ₂ Me	O
	4-CF ₃	6-F	CO ₂ Me	O
35	4-CF ₃	6-CF ₃	CO ₂ Me	O
	4-CF ₃	4-Cl	CO ₂ Me	O

	R ₁	R ₂	B	X
5	4-CF ₃	4-F	CO ₂ Me	O
	4-CF ₃	6-Br	CO ₂ Me	O
	4-CF ₃	6-NO ₂	CO ₂ Me	O
	4-CF ₃	6-Me	CO ₂ Me	O
10	4-CF ₃	4-Cl	CO ₂ Me	O
	4-CF ₃	4-F	CO ₂ Me	O
	4-CF ₃	4-Br	CO ₂ Me	O
	4-Cl	H	H	S
15	4-CF ₃	H	Me	S
	4-Cl	H	CO ₂ Me	S
	4-CF ₃	H	H	S
	4-Cl	H	Me	S
20	4-CF ₃	H	CO ₂ Me	S
	4-Cl	5-Cl	H	S
	4-Cl	5-F	Me	S
	4-CF ₃	5-F	CO ₂ Me	S
25	4-CF ₃	H	Ph	O
	4-OCF ₃	H	Ph	O
	4-Cl	H	Ph	O
	4-Br	H	Ph	O
30	4-CF ₃	H	4-F-Ph	O
	4-OCF ₃	H	4-F-Ph	O
	4-Cl	H	4-F-Ph	O
	4-Br	H	4-F-Ph	O
35	4-CF ₃	5-F	Ph	O
	4-OCF ₃	5-F	Ph	O
	4-Cl	5-F	Ph	O
	4-Br	5-F	Ph	O
	4-CF ₃	5-F	4-Cl-Ph	O
	4-OCF ₃	5-F	4-Cl-Ph	O
	4-Cl	5-F	4-Cl-Ph	O
	4-Br	5-F	4-Cl-Ph	O
	4-CF ₃	5-F	4-F-Ph	O
	4-OCF ₃	5-F	4-F-Ph	O
	4-Cl	5-F	4-F-Ph	O
	4-Br	5-F	4-F-Ph	O

5	R ₁	R ₂	B	X
10	4-Br	5-F	4-F-Ph	0
	4-CF ₃	5-F	Ph	0
	4-OCF ₃	5-Cl	Ph	0
	4-Cl	5-Cl	Ph	0
	4-Br	5-Cl	Ph	0
	4-CF ₃	5-Cl	4-F-Ph	0
	4-OCF ₃	5-Cl	4-F-Ph	0
	4-Cl	5-Cl	4-F-Ph	0
	4-Br	5-Cl	4-F-Ph	0
	4-CF ₃	5-Cl	4-Cl-Ph	0
15	4-OCF ₃	5-Cl	4-Cl-Ph	0
	4-Cl	5-Cl	4-Cl-Ph	0
	4-Br	5-Cl	4-Cl-Ph	0
	4-CF ₃	5-Br	4-F-Ph	0
	4-OCF ₃	5-Br	4-F-Ph	0
20	4-Cl	5-Br	4-F-Ph	0
	4-Br	5-Br	4-F-Ph	0
	4-CF ₃	5-Br	4-Cl-Ph	0
	4-OCF ₃	5-Br	4-Cl-Ph	0
	4-Cl	5-Br	4-Cl-Ph	0
25	4-Br	5-Br	4-F-Ph	0
30				
35				

TABLE 14

5	R ₁	R ₂	B	X	A
10	4-CF ₂ Cl	H	H	0	0
	4-CF ₃	H	H	0	0
	4-Br	H	H	0	0
	3-CF ₃	H	H	0	0
	4-Cl	H	H	0	0
	3-Cl	H	H	0	0
15	4-CF ₃	5-Br	H	0	0
	4-Cl	5-Br	H	0	0
	4-Br	5-Br	H	0	0
	4-Cl	7-Br	H	0	0
	4-CF ₃	7-Br	H	0	0
	4-Br	7-Br	H	0	0
20	4-Cl	5-F	H	0	0
	4-CF ₃	H	Me	0	0
	4-OCF ₂ H	5-F	Me	0	0
	4-Br	H	Me	0	0
	4-OCF ₃	H	CO ₂ Me	0	0
	4-CO ₂ Me	5-Cl	CO ₂ Me	0	0
25	4-Cl	H	CO ₂ CH ₂ CF ₃	0	0
	4-Cl	5-Cl	C(O)Me	0	0
	4-CF ₃	5-OCF ₂ H	Me	0	0
	4-CF ₃	5-F	CONHPh	0	0
	4-Cl	5-Cl	n-Pr	0	0
	4-CF ₃	5-OCF ₂ H	CO ₂ Me	0	0
30	4-Cl	H	4-Cl-Ph	0	0
	4-CF ₃	5-Cl	CO ₂ Me	S	0
	4-CF ₂ Cl	H	H	0	S
	4-Cl	5-F	H	0	S
	4-CF ₃	H	H	0	S
	4-Cl	H	H	0	S
35	4-Br	H	H	0	S
	3-CF ₃	H	H	0	S
	4-Cl	H	H	0	S

5	R ₁	R ₂	B	X	A
	3-CF ₃	5-Cl	H	0	S
	4-Cl	5-Cl	H	0	S
	3-Cl	5-Cl	H	0	S
	4-Br	5-Cl	H	0	S
10	4-Cl	5-Cl	H	0	S
	4-CF ₃	6-Cl	H	0	S
	3-CF ₃	6-Cl	H	0	S
	4-Cl	6-Cl	H	0	S
15	3-Cl	6-Cl	H	0	S
	4-Br	6-Cl	H	0	S
	4-Cl	6-Cl	H	0	S
	4-CF ₃	5-Br	H	0	S
20	3-CF ₃	5-Br	H	0	S
	4-Cl	5-Br	H	0	S
	3-Cl	5-Br	H	0	S
	4-Br	5-Br	H	0	S
25	4-Cl	5-Br	H	0	S
	4-CF ₃	4-Cl	H	0	S
	4-Cl	4-Cl	H	0	S
	4-Br	4-Cl	H	0	S
30	4-CF ₃	H	Me	0	S
	4-OCF ₂ H	5-F	Me	0	S
	4-Br	H	Me	0	S
	4-OCF ₃	H	CO ₂ Me	0	S
35	4-CO ₂ Me	5-Cl	CO ₂ Me	0	S
	4-Cl	H	CO ₂ CH ₂ CF ₃	0	S
	4-CF ₃	5-OCF ₂ H	Me	0	S
	4-CF ₃	5-F	CONHPh	0	S
35	4-Cl	5-Cl	n-Pr	0	S
	4-CF ₃	5-OCF ₂ H	CO ₂ Me	0	S
	4-Cl	H	4-Cl-Ph	0	S

	R ₁	R ₂	B	X	A
5	4-CF ₃	5-Cl	CO ₂ Me	S	S
	4-CF ₂ Cl	H	H	0	NMe
	4-Cl	5-F	H	0	NMe
	4-CF ₃	H	Me	0	NMe
10	4-OCF ₂ H	5-F	Me	0	NMe
	4-Br	H	Me	0	NMe
	4-OCF ₃	H	CO ₂ Me	0	NMe
	4-CO ₂ Me	5-Cl	CO ₂ Me	0	NMe
	4-Cl	H	CO ₂ CH ₂ CF ₃	0	NMe
15	4-CF ₃	5-OCF ₂ H	Me	0	NMe
	4-CF ₃	5-F	CONHPh	0	NMe
	4-Cl	5-Cl	n-Pr	0	NMe
	4-Cl	H	4-Cl-Ph	0	NMe
	4-CF ₃	5-Cl	CO ₂ Me	S	NMe
20	4-CF ₃	H	H	0	SO ₂
	4-Cl	H	H	0	SO ₂
	4-Br	H	H	0	SO ₂
	3-CF ₃	H	H	0	SO ₂
	4-Cl	H	H	0	SO ₂
25	3-Cl	H	H	0	SO ₂
	4-CF ₃	5-Cl	H	0	SO ₂
	3-CF ₃	5-Cl	H	0	SO ₂
	4-Cl	5-Cl	H	0	SO ₂
	3-Cl	5-Cl	H	0	SO ₂
30	4-Cl	5-Cl	H	0	SO ₂
	4-CF ₃	6-Cl	H	0	SO ₂
	3-CF ₃	6-Cl	H	0	SO ₂
	4-Cl	6-Cl	H	0	SO ₂
	3-Cl	6-Cl	H	0	SO ₂
35	4-Br	6-Cl	H	0	SO ₂
	4-Cl	6-Cl	H	0	SO ₂
	4-Cl	5-Cl	Me	0	SO ₂

	R ₁	R ₂	B	X	A
5	4-OCF ₃	H	Et	0	SO ₂
	4-Cl	H	CO ₂ Me	0	SO ₂
	4-OCF ₃	5-Cl	CO ₂ Et	0	SO ₂
	3-CF ₃	H	H	0	SO(α) ¹
10	4-CF ₃	H	H	0	SO(α)
	4-Br	H	H	0	SO(β) ¹
	4-Cl	H	H	0	SO(α)
	4-Cl	H	H	0	SO(β)
	4-Cl	H	H	0	SO(α)
15	4-Cl	H	H	0	SO(β)
	3-Cl	H	H	0	SO(α)
	3-Cl	H	H	0	SO(β)
	4-CF ₃	5-Cl	H	0	SO(α)
	4-CF ₃	5-Cl	H	0	SO(β)
	3-CF ₃	5-Cl	H	0	SO(α)
20	3-CF ₃	5-Cl	H	0	SO(β)
	4-Cl	5-Cl	H	0	SO(α)
	4-Cl	5-Cl	H	0	SO(β)
	3-Cl	5-Cl	H	0	SO(α)
	3-Cl	5-Cl	H	0	SO(β)
	4-Br	5-Cl	H	0	SO(α)
	4-Br	5-Cl	H	0	SO(β)
25	4-Cl	5-Cl	H	0	SO(α)
	4-Cl	5-Cl	H	0	SO(β)
	4-CF ₃	6-Cl	H	0	SO(α)
	4-CF ₃	6-Cl	H	0	SO(β)
	3-CF ₃	6-Cl	H	0	SO(α)
30	3-CF ₃	6-Cl	H	0	SO(β)
	4-Cl	6-Cl	H	0	SO(α)
	4-Cl	6-Cl	H	0	SO(β)
	3-Cl	6-Cl	H	0	SO(α)
	3-Cl	6-Cl	H	0	SO(β)

1. α denotes cis relationship to substituent B;

β denotes trans relationship to substituent B.

	<u>R₁</u>	<u>R₂</u>	<u>B</u>	<u>X</u>	<u>A</u>
5	3-Cl	6-Cl	H	0	SO(β)
	4-Br	6-Cl	H	0	SO(α)
	4-Br	6-Cl	H	0	SO(β)
	4-Cl	6-Cl	H	0	SO(α)
10	4-Cl	6-Cl	H	0	SO(β)
	3-CF ₃	H	H	0	SO(β)
	4-CF ₃	H	H	0	SO(β)
	4-CF ₃	5-Cl	CO ₂ Me	0	N-allyl
	4-OCF ₃	5-Cl	CO ₂ Me	0	N-CH ₂ Ph
15	4-CF ₃	H	H	0	NH
	4-CF ₃	H	CO ₂ Me	0	NH
	4-CF ₃	5-Cl	H	0	NMe
	4-CF ₃	5-Cl	CO ₂ Me	0	NMe
	4-CF ₃	5-Cl	CO ₂ Me	0	NC(O)CH ₃
20	4-CF ₃	5-Cl	CO ₂ Me	0	NCO ₂ CH ₃
	4-CF ₃	5-Cl	CO ₂ Me	0	NSO ₂ CH ₃
	4-CF ₃	5-Cl	CO ₂ Me	0	NCH ₂ Ph
	4-CF ₃	5-Cl	CO ₂ Me	0	N-allyl
	4-CF ₃	5-Cl	CO ₂ Me	0	NCO ₂ C(CH ₃) ₃
25	4-CF ₃	H	Ph	0	S
	4-OCF ₃	H	Ph	0	S
	4-Cl	H	Ph	0	S
	4-Br	H	Ph	0	S
	4-CF ₃	H	4-F-Ph	0	S
30	4-OCF ₃	H	4-F-Ph	0	S
	4-Cl	H	4-F-Ph	0	S
	4-Br	H	4-F-Ph	0	S
	4-CF ₃	5-F	Ph	0	S
	4-OCF ₃	5-F	Ph	0	S
35	4-Cl	5-F	Ph	0	S
	4-Br	5-F	Ph	0	S
	4-CF ₃	5-F	4-Cl-Ph	0	S

	R ₁	R ₂	B	X	A
5	4-Cl	5-F	4-Cl-Ph	0	S
	4-Br	5-F	4-Cl-Ph	0	S
	4-CF ₃	5-F	4-F-Ph	0	S
	4-OCF ₃	5-F	4-F-Ph	0	S
10	4-Cl	5-F	4-F-Ph	0	S
	4-Br	5-F	4-F-Ph	0	S
	4-CF ₃	5-Cl	Ph	0	S
	4-OCF ₃	5-Cl	Ph	0	S
15	4-Cl	5-Cl	Ph	0	S
	4-Br	5-Cl	Ph	0	S
	4-CF ₃	5-Cl	4-F-Ph	0	S
	4-OCF ₃	5-Cl	4-F-Ph	0	S
20	4-Cl	5-Cl	4-F-Ph	0	S
	4-Br	5-Cl	4-F-Ph	0	S
	4-CF ₃	5-Cl	4-Cl-Ph	0	S
	4-OCF ₃	5-Cl	4-Cl-Ph	0	S
25	4-Cl	5-Br	4-F-PH	0	S
	4-OCF ₃	5-Br	4-F-Ph	0	S
	4-Cl	5-Br	4-Cl-Ph	0	S
	4-Br	5-Br	4-Cl-Ph	0	S
30	4-Cl	5-Br	4-Cl-Ph	0	S
	4-CF ₃	5-Br	4-Cl-Ph	0	S
	4-CF ₃	H	Ph	0	O
	4-OCF ₃	H	Ph	0	O
35	4-Cl	H	Ph	0	O
	4-Br	H	Ph	0	O
	4-CF ₃	H	4-F-Ph	0	O
	4-OCF ₃	H	4-F-Ph	0	O
	4-Cl	H	4-F-Ph	0	O

	R ₁	R ₂	B	X	A
5	4-Br	H	4-F-Ph	0	0
	4-CF ₃	5-F	Ph	0	0
	4-OCF ₃	5-F	Ph	0	0
	4-Cl	5-F	Ph	0	0
10	4-Br	5-F	Ph	0	0
	4-CF ₃	5-F	4-Cl-Ph	0	0
	4-OCF ₃	5-F	4-Cl-Ph	0	0
	4-Cl	5-F	4-Cl-Ph	0	0
	4-Br	5-F	4-Cl-Ph	0	0
15	4-CF ₃	5-F	4-F-Ph	0	0
	4-OCF ₃	5-F	4-F-Ph	0	0
	4-Cl	5-F	4-F-Ph	0	0
	4-Br	5-F	4-F-Ph	0	0
	4-CF ₃	5-Cl	Ph	0	0
20	4-OCF ₃	5-Cl	Ph	0	0
	4-Cl	5-Cl	Ph	0	0
	4-Br	5-Cl	Ph	0	0
	4-CF ₃	5-Cl	4-F-Ph	0	0
	4-OCF ₃	5-Cl	4-F-Ph	0	0
25	4-Cl	5-Cl	4-F-Ph	0	0
	4-Br	5-Cl	4-F-Ph	0	0
	4-CF ₃	5-Cl	4-Cl-Ph	0	0
	4-OCF ₃	5-Cl	4-Cl-Ph	0	0
	4-Cl	5-Cl	4-Cl-Ph	0	0
30	4-Br	5-F	4-F-Ph	0	0
	4-CF ₃	5-Br	4-F-Ph	0	0
	4-OCF ₃	5-Br	4-F-Ph	0	0
	4-Cl	5-Br	4-F-Ph	0	0
	4-Br	5-Br	4-F-Ph	0	0
35	4-CF ₃	5-Br	4-F-Ph	0	0
	4-OCF ₃	5-Br	4-Cl-Ph	0	0
	4-Cl	5-Br	4-Cl-Ph	0	0

	R ₁	R ₂	B	X	A
5	4-Br	5-Br	4-Cl-Ph	0	O
	4-CF ₃	5-Br	4-Cl-Ph	0	O
	4-CF ₃	5-F	4-Cl-Ph	0	SO ₂
	4-Cl	5-F	4-Cl-Ph	0	SO ₂
10	4-Br	5-F	4-Cl-Ph	0	SO ₂
	4-CF ₃	5-Cl	4-Cl-Ph	0	SO ₂
	4-OCF ₃	5-Cl	4-Cl-Ph	0	SO ₂
	4-Cl	5-Cl	4-Cl-Ph	0	SO ₂
15	4-Br	5-Cl	4-Cl-Ph	0	SO ₂
	4-CF ₃	H	4-Cl-Ph	0	SO ₂
	4-OCF ₃	H	4-Cl-Ph	0	SO ₂
	4-Cl	H	4-Cl-Ph	0	SO ₂
20	4-Br	H	4-Cl-Ph	0	SO ₂
	4-CF ₃	5-F	4-Cl-Ph	0	SO
	4-OCF ₃	5-F	4-Cl-Ph	0	SO
	4-Cl	5-F	4-Cl-Ph	0	SO
25	4-Br	5-F	4-Cl-Ph	0	SO
	4-CF ₃	5-Cl	4-Cl-Ph	0	SO
	4-OCF ₃	5-Cl	4-Cl-Ph	0	SO
	4-Cl	5-Cl	4-Cl-Ph	0	SO
30	4-Br	5-Cl	4-Cl-Ph	0	SO
	4-CF ₃	H	4-Cl-Ph	0	SO
	4-OCF ₃	H	4-Cl-Ph	0	SO
	4-Cl	H	4-Cl-Ph	0	SO
35	4-Br	H	4-Cl-Ph	0	SO
	4-CF ₃	5-F	4-Cl-Ph	0	NMe
	4-OCF ₃	5-F	4-Cl-Ph	0	NMe
	4-Cl	5-F	4-Cl-Ph	0	NMe
	4-Br	5-F	4-Cl-Ph	0	NMe
	4-CF ₃	5-Cl	4-Cl-Ph	0	NMe
	4-OCF ₃	5-Cl	4-Cl-Ph	0	NMe
	4-Cl	5-Cl	4-Cl-Ph	0	NMe

	R ₁	R ₂	B	X	A
5	4-Br	5-Cl	4-Cl-Ph	0	NMe
	4-CF ₃	H	4-Cl-Ph	0	NMe
	4-OCF ₃	H	4-Cl-Ph	0	NMe
	4-Cl	H	4-Cl-Ph	0	NMe
10	4-Br	H	4-Cl-Ph	0	NMe
	4-CF ₃	5-Cl	4-Cl-Ph	0	O
	4-OCF ₃	5-Cl	4-Cl-Ph	0	O
	4-Cl	5-Cl	4-Cl-Ph	0	O
15	4-Br	5-Cl	4-Cl-Ph	0	O
	4-OCF ₂ CF ₂ H	H	Ph	0	O
	4-I	H	CH ₃	0	O
	4-COCH ₃	H	CH ₃	0	O
20	4-OCF ₂ CF ₂ H	H	CH ₃	0	O
	4-CF ₃	H	CO ₂ CH ₃	0	O
	4-Br	5-F	H	0	O
	4-OCF ₃	5-F	H	0	O
25	4-Br	5-F	H	0	O
	4-OCF ₃	5-Cl	H	0	O
	4-Br	5-Cl	H	0	O
	4-OCF ₃	5-Cl	H	0	O
30	4-Br	5-F	Me	0	O
	4-OCF ₃	5-F	Me	0	O
	4-Br	5-F	Me	0	O
	4-OCF ₃	H	CO ₂ Me	0	O
35	4-Br	H	CO ₂ Me	0	O
	4-OCF ₃	H	CO ₂ Me	0	O
	4-Cl	H	CO ₂ Me	0	O
	4-Br	H	CO ₂ Me	0	O
	4-Br	5-F	CO ₂ Me	0	O
	4-OCF ₃	5-F	CO ₂ Me	0	O
	4-Br	5-F	CO ₂ Me	0	O
	4-OCF ₃	5-Cl	CO ₂ Me	0	O

	R ₁	R ₂	B	X	A
5	4-Cl	5-Cl	CO ₂ Me	0	O
	4-Br	5-Cl	CO ₂ Me	0	O
	4-CF ₃	5-Br	CO ₂ Me	0	O
	4-OCF ₃	5-Br	CO ₂ Me	0	O
10	4-Cl	5-Br	CO ₂ Me	0	O
	4-Br	5-Br	CO ₂ Me	0	O
	4-CF ₃	5-F	CO ₂ Me	0	S
	4-OCF ₃	5-F	CO ₂ Me	0	S
	4-Cl	5-F	CO ₂ Me	0	S
15	4-Br	5-F	CO ₂ Me	0	S
	4-CF ₃	5-Cl	CO ₂ Me	0	S
	4-OCF ₃	5-Cl	CO ₂ Me	0	S
	4-Cl	5-Cl	CO ₂ Me	0	S
	4-Br	5-Cl	CO ₂ Me	0	S
20	4-CF ₃	5-F	CO ₂ Me	0	N-CH ₃
	4-OCF ₃	5-F	CO ₂ Me	0	N-CH ₃
	4-Cl	5-F	CO ₂ Me	0	N-CH ₃
	4-Br	5-F	CO ₂ Me	0	N-CH ₃
	4-CF ₃	5-Cl	CO ₂ Me	0	N-CH ₃
25	4-OCF ₃	5-Cl	CO ₂ Me	0	N-CH ₃
	4-Cl	5-Cl	CO ₂ Me	0	N-CH ₃
	4-Br	5-Cl	CO ₂ Me	0	N-CH ₃

30

35

TABLE 15

5	R ₁	R ₂	B	Y	A
	4-OCF ₃	H	H	Me	CH ₂
	4-CF ₃	H	H	C(O)Me	CH ₂
	4-F	H	CO ₂ Me	Me	CH ₂
10	4-OCF ₂ H	H	CO ₂ Me	C(O)Me	CH ₂
	4-CF ₃	H	Me	C(O)CF ₃	CH ₂
	4-Cl	H	Me	CO ₂ Et	CH ₂
	4-CF ₃	H	CO ₂ CH ₂ CF ₃	Me	CH ₂
	4-OCF ₂ H	H	CO ₂ Et	Me	CH ₂
15	4-OCF ₃	H	CO ₂ CH ₂ CH ₂ Cl	Me	CH ₂
	4-Br	H	CONHMe	Me	CH ₂
	4-CF ₃	H	CO ₂ Me	C(O)Me	CH ₂
	4-CF ₃	H	CO ₂ Me	Me	CH ₂
	4-CF ₃	H	CO ₂ Me	CO ₂ Me	CH ₂
20	4-CF ₃	5-Cl	CO ₂ Me	C(O)Me	CH ₂
	4-CF ₃	5-Cl	CO ₂ Me	Me	CH ₂
	4-CF ₃	5-Cl	CO ₂ Me	CO ₂ Me	CH ₂
	4-CF ₃	4-F	CO ₂ Me	C(O)Me	CH ₂
	4-CF ₃	5-F	CO ₂ Me	C(O)Me	CH ₂
25	4-CF ₃	4-F	CO ₂ Me	CO ₂ Me	CH ₂
	4-CF ₃	5-F	CO ₂ Me	CO ₂ Me	CH ₂
	4-CF ₃	H	H	CO ₂ -t-Bu	CH ₂
	4-CF ₃	5-Cl	CO ₂ Me	SN(iPr)P(O)(OCH ₃)(CH ₃)	CH ₂
	4-CF ₃	5-Cl	CO ₂ Me	SP(O)(OC ₂ H ₅) ₂	CH ₂
30	4-CF ₃	5-Cl	CO ₂ Me	SN(iPr) ₂	CH ₂
	4-CF ₃	H	CO ₂ Me	SN(iPr)P(O)(OC ₂ H ₅)(Ph)	CH ₂
	4-CF ₃	H	CO ₂ Me	SP(O)(OiPr) ₂	CH ₂
	4-CF ₃	H	CO ₂ Me	SN(sec Bu) ₂	CH ₂
35					

	R ₁	R ₂	B	Y	A
5					
	4-CF ₃	H	CO ₂ Me	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SNP}(\text{OEt})_2 \end{array}$	CH ₂
	4-Cl	H	CO ₂ Me	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SNP}(\text{OEt})_2 \end{array}$	CH ₂
10	4-OCF ₂ H	H	CO ₂ Me	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SNP}(\text{OEt})_2 \end{array}$	CH ₂
	4-CF ₃	5-Cl	CO ₂ Me	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SN}(\text{iPr})\text{COC}_2\text{H}_5 \end{array}$	CH ₂
	4-CF ₃	4-F	CO ₂ Me	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SN}(\text{iPr})\text{COC}_2\text{H}_5 \end{array}$	CH ₂
15	4-CF ₃	5-F	CO ₂ Me	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SN}(\text{iPr})\text{COC}_2\text{H}_5 \end{array}$	CH ₂
	4-CF ₃	5-Cl	4-Cl Phenyl	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SN}(\text{iPr})\text{COC}_2\text{H}_5 \end{array}$	CH ₂
	4-CF ₃	4-F	CO ₂ Me	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SN}(\text{iPr})\text{COC}_2\text{H}_5 \end{array}$	CH ₂
20	4-CF ₃	5-F	CO ₂ Me	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SN}(\text{iPr})\text{COC}_2\text{H}_5 \end{array}$	CH ₂
	4-CF ₃	H	CO ₂ Me	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SN}(\text{iPr})\text{COC}_2\text{H}_5 \end{array}$	CH ₂
	4-CF ₃	H	CO ₂ Me	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SN}(\text{CH}_3)\text{CO}(\text{CH}_2)_3\text{CH}_3 \end{array}$	CH ₂
25	4-Cl	H	CO ₂ Me	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SN}(\text{CH}_3)\text{CO}(\text{CH}_2)_3\text{CH}_3 \end{array}$	CH ₂
	4-CF ₃	5-Cl	CO ₂ Me	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SN}(\text{CH}_3)\text{CO}(\text{CH}_2)_3\text{CH}_3 \end{array}$	CH ₂
	4-CF ₃	4-F	CO ₂ Me	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SN}(\text{CH}_3)\text{CO}(\text{CH}_2)_3\text{CH}_3 \end{array}$	CH ₂
30	4-CF ₃	5-F	CO ₂ Me	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SN}(\text{CH}_3)\text{CO}(\text{CH}_2)_3\text{CH}_3 \end{array}$	CH ₂
	4-CF ₃	5-Cl	4-Cl-Phenyl	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SN}(\text{CH}_3)\text{CO}(\text{CH}_2)_3\text{CH}_3 \end{array}$	CH ₂
	4-CF ₃	4-F	CO ₂ Me	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SN}(\text{CH}_3)\text{CO}(\text{CH}_2)_3\text{CH}_3 \end{array}$	CH ₂
35	4-CF ₃	5-F	CO ₂ Me	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SN}(\text{CH}_3)\text{CO}(\text{CH}_2)_3\text{CH}_3 \end{array}$	CH ₂
	4-CF ₃	H	CO ₂ Me	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SN}(\text{CH}_3)\text{CO}(\text{CH}_2)_3\text{CH}_3 \end{array}$	CH ₂

	R ₁	R ₂	B	Y	A
5	4-CF ₃	H	CO ₂ Me	SN(iPr)SO ₂ CH ₃	CH ₂
	4-Cl	H	CO ₂ Me	SN(iPr)SO ₂ CH ₃	CH ₂
	4-OCF ₂ H	H	CO ₂ Me	SN(iPr)SO ₂ CH ₃	CH ₂
	4-F	H	CO ₂ Me	SN(iPr)SO ₂ CH ₃	CH ₂
10	4-CF ₃	5-Cl	CO ₂ Me	SN(iPr)SO ₂ CH ₃	CH ₂
	4-CF ₃	4-F	CO ₂ Me	SN(iPr)SO ₂ CH ₃	CH ₂
	4-CF ₃	5-F	CO ₂ Me	SN(iPr)SO ₂ CH ₃	CH ₂
	4-CF ₃	5-Cl	4-Cl-Phenyl	SN(iPr)SO ₂ CH ₃	CH ₂
	4-CF ₃	4-F	CO ₂ Me	SN(iPr)SO ₂ CH ₃	CH ₂
	4-CF ₃	5-F	CO ₂ Me	SN(iPr)SO ₂ CH ₃	CH ₂
15	4-CF ₃	H	CO ₂ Me	SN(iPr)SO ₂ CH ₃	CH ₂
	4-CF ₃	5-Cl	CO ₂ Me	SN(CH ₃)SO ₂ Ph	CH ₂
	4-CF ₃	4-F	CO ₂ Me	SN(CH ₃)SO ₂ Ph	CH ₂
	4-CF ₃	5-F	CO ₂ Me	SN(CH ₃)SO ₂ Ph	CH ₂
	4-CF ₃	5-Cl	4-Cl-Phenyl	SN(CH ₃)SO ₂ Ph	CH ₂
20	4-CF ₃	4-F	CO ₂ Me	SN(CH ₃)SO ₂ Ph	CH ₂
	4-CF ₃	5-F	CO ₂ Me	SN(CH ₃)SO ₂ Ph	CH ₂
	4-CF ₃	H	CO ₂ Me	SN(CH ₃)SO ₂ Ph	CH ₂
25	4-CF ₃	H	CO ₂ Me	$\begin{array}{c} \text{O} \\ \parallel \\ \text{S} \end{array} \text{COCH}_2\text{CH}_2\text{CH}_2\text{CH}_3$	CH ₂
	4-Cl	H	CO ₂ Me	$\begin{array}{c} \text{O} \\ \parallel \\ \text{S} \end{array} \text{COCH}_2\text{CH}_2\text{CH}_2\text{CH}_3$	CH ₂
	4-OCF ₂ H	H	CO ₂ Me	$\begin{array}{c} \text{O} \\ \parallel \\ \text{S} \end{array} \text{COCH}_2\text{CH}_2\text{CH}_2\text{CH}_3$	CH ₂
30	4-OCF ₂	H	CO ₂ Me	$\begin{array}{c} \text{O} \\ \parallel \\ \text{S} \end{array} \text{COCH}_2\text{CH}_2\text{CH}_2\text{CH}_3$	CH ₂
	4-F	H	CO ₂ Me	$\begin{array}{c} \text{O} \\ \parallel \\ \text{S} \end{array} \text{COCH}_2\text{CH}_2\text{CH}_2\text{CH}_3$	CH ₂
	4-CF ₃	5-Cl	CO ₂ Me	$\begin{array}{c} \text{O} \\ \parallel \\ \text{S} \end{array} \text{COCH}_2\text{CH}_2\text{CH}_2\text{CH}_3$	CH ₂
35	4-CF ₃	4-F	CO ₂ Me	$\begin{array}{c} \text{O} \\ \parallel \\ \text{S} \end{array} \text{COCH}_2\text{CH}_2\text{CH}_2\text{CH}_3$	CH ₂
	4-CF ₃	5-F	CO ₂ Me	$\begin{array}{c} \text{O} \\ \parallel \\ \text{S} \end{array} \text{COCH}_2\text{CH}_2\text{CH}_2\text{CH}_3$	CH ₂

	R ₁	R ₂	B	Y	A
5				O "SCOCH ₂ CH ₂ CH ₂ CH ₃	CH ₂
	4-CF ₃	5-Cl	4-Cl-Phenyl	O "SCOCH ₂ CH ₂ CH ₂ CH ₃	CH ₂
	4-CF ₃	4-F	CO ₂ Me	O "SCOCH ₂ CH ₂ CH ₂ CH ₃	CH ₂
10	4-CF ₃	5-F	CO ₂ Me	O "SCOCH ₂ CH ₂ CH ₂ CH ₃	CH ₂
	4-CF ₃	H	CO ₂ Me	O "SCOCH ₂ CH ₂ CH ₂ CH ₃	CH ₂
	4-CF ₃	5-Cl	CO ₂ Me	Me	CH ₂
	4-OCF ₃	5-Cl	CO ₂ Me	Me	CH ₂
	4-Br	5-Cl	CO ₂ Me	Me	CH ₂
15	4-CF ₃	5-F	CO ₂ Me	COCH ₃	CH ₂
	4-OCF ₃	5-F	CO ₂ Me	COCH ₃	CH ₂
	4-Br	5-F	CO ₂ Me	COCH ₃	CH ₂
	4-CF ₃	5-Cl	CO ₂ Me	CO ₂ CH ₃	CH ₂
	4-OCF ₃	5-Cl	CO ₂ Me	CO ₂ CH ₃	CH ₂
20	4-Br	5-Cl	CO ₂ Me	CO ₂ CH ₃	CH ₂
	4-CF ₃	5-F	CO ₂ Me	COCF ₃	CH ₂
	4-OCF ₃	5-F	CO ₂ Me	COCF ₃	CH ₂
	4-Br	5-F	CO ₂ Me	COCF ₃	CH ₂
	4-CF ₃	4-Cl	4-Cl-Ph	Me	CH ₂
25	4-OCF ₃	4-Cl	4-Cl-Ph	Me	CH ₂
	4-Br	4-Cl	4-Cl-Ph	Me	CH ₂
	4-CF ₃	4-Cl	4-Cl-Ph	COCH ₃	CH ₂
	4-OCF ₃	4-Cl	4-Cl-Ph	COCH ₃	CH ₂
	4-Br	4-Cl	4-Cl-Ph	COCH ₃	CH ₂
30	4-CF ₃	4-Cl	4-Cl-Ph	CO ₂ CH ₃	CH ₂
	4-OCF ₃	4-Cl	4-Cl-Ph	CO ₂ CH ₃	CH ₂
	4-Br	4-Cl	4-Cl-Ph	CO ₂ CH ₃	CH ₂
	4-CF ₃	4-Cl	4-Cl-Ph	COCF ₃	CH ₂
	4-OCF ₃	4-Cl	4-Cl-Ph	COCF ₃	CH ₂
35	4-Br	4-Cl	4-Cl-Ph	COCF ₃	CH ₂

	R ₁	R ₂	B	Y	A
5	4-CF ₃	4-Cl	4-Cl-Ph	CO ₂ CH ₂ CH ₃	CH ₂
	4-OCF ₃	4-Cl	4-Cl-Ph	CO ₂ CH ₂ CH ₃	CH ₂
	4-Br	4-Cl	4-Cl-Ph	CO ₂ CH ₂ CH ₃	CH ₂
	4-CF ₃	4-Cl	4-Cl-Ph	Me	CH ₂
	4-OCF ₃	4-Cl	4-F-Ph	Me	CH ₂
10	4-Br	4-Cl	4-F-Ph	Me	CH ₂
	4-CF ₃	4-Cl	4-F-Ph	COCH ₃	CH ₂
	4-OCF ₃	4-Cl	4-F-Ph	COCH ₃	CH ₂
	4-Br	4-Cl	4-F-Ph	COCH ₃	CH ₂
	4-CF ₃	4-Cl	4-F-Ph	CO ₂ CH ₃	CH ₂
15	4-OCF ₃	4-Cl	4-F-Ph	CO ₂ CH ₃	CH ₂
	4-Br	4-Cl	4-F-Ph	CO ₂ CH ₃	CH ₂
	4-CF ₃	4-Cl	4-F-Ph	COCH ₂ CH ₃	CH ₂
	4-OCF ₃	4-Cl	4-F-Ph	COCH ₂ CH ₃	CH ₂
	4-Br	4-Cl	4-F-Ph	COCH ₂ CH ₃	CH ₂
20	4-CF ₃	H	Me	Me	NMe
	4-CF ₃	5-Cl	CO ₂ Me	Me	S
	4-CF ₃	5-Cl	Me	Me	NMe
	4-CF ₃	5-Cl	Me	C(O)Me	S
	4-CF ₃	5-F	CO ₂ Me	C(O)Me	NMe
25	4-CF ₃	5-F	Me	C(O)Me	SO
	4-CF ₃	H	CO ₂ Me	SCCl ₃	O
	4-CF ₃	H	CO ₂ Me	SCCl ₃	NMe
	4-CF ₃	H	Me	CO ₂ Me	O
	4-CF ₃	5-OCF ₂ H	CO ₂ Me	n-Pr	NMe
30	4-CF ₃	5-CF ₃	Me	C(O)CF ₃	O
	4-CF ₃	5-CF ₃	Me	C(O)CF ₃	NMe
	4-CF ₃	5-Cl	CO ₂ Me	SMe	O
	4-CF ₃	H	H	Me	S
	4-CF ₃	H	H	CO ₂ Me	S
35	4-CF ₃	H	H	C(O)Me	S
	4-CF ₃	5-Cl	H	C(O)Me	S

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	R ₁	R ₂	B	Y	A
5	4-CF ₃	5-Cl	H	CO ₂ Me	S
	4-CF ₃	5-Cl	H	Me	S
	4-Cl	H	H	C(O)Me	S
	4-Cl	H	H	Me	S
	4-Cl	5-Cl	H	C(O)Me	S
10	4-Cl	5-Cl	H	Me	S
				O	
	4-CF ₃	5-Cl	CO ₂ Me	SN(iPr)COC ₂ H ₅	O
				O	
	4-CF ₃	4-F	CO ₂ Me	SN(iPr)COC ₂ H ₅	O
				O	
15	4-CF ₃	5-F	CO ₂ Me	SN(iPr)COC ₂ H ₅	O
				O	
	4-CF ₃	5-Cl	4-Cl-Phenyl	SN(iPr)COC ₂ H ₅	O
				O	
	4-CF ₃	4-F	4-Cl-Phenyl	SN(iPr)COC ₂ H ₅	O
				O	
20	4-CF ₃	5-F	4-Cl-Phenyl	SN(iPr)COC ₂ H ₅	O
				O	
	4-CF ₃	H	4-Cl-Phenyl	SN(iPr)COC ₂ H ₅	O
				O	
	4-CF ₃	H	CO ₂ Me	SN(CH ₃)CO(CH ₂) ₃ CH ₃	O
				O	
25	4-Cl	H	CO ₂ Me	SN(CH ₃)CO(CH ₂) ₃ CH ₃	O
				O	
	4-CF ₃	5-Cl	CO ₂ Me	SN(CH ₃)CO(CH ₂) ₃ CH ₃	O
				O	
	4-CF ₃	4-F	CO ₂ Me	SN(CH ₃)CO(CH ₂) ₃ CH ₃	O
				O	
30	4-CF ₃	5-F	CO ₂ Me	SN(CH ₃)CO(CH ₂) ₃ CH ₃	O
				O	

35

	R ₁	R ₂	B	Y	A
5				$\begin{array}{c} \text{O} \\ \parallel \\ \text{SN}(\text{CH}_3)\text{CO}(\text{CH}_2)_3\text{CH}_3 \end{array}$	
	4-CF ₃	5-Cl	4-Cl-Phenyl	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SN}(\text{CH}_3)\text{CO}(\text{CH}_2)_3\text{CH}_3 \end{array}$	O
	4-CF ₃	4-F	4-Cl-Phenyl	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SN}(\text{CH}_3)\text{CO}(\text{CH}_2)_3\text{CH}_3 \end{array}$	O
10	4-CF ₃	5-F	4-Cl-Phenyl	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SN}(\text{CH}_3)\text{CO}(\text{CH}_2)_3\text{CH}_3 \end{array}$	O
	4-CF ₃	H	4-Cl-Phenyl	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SN}(\text{CH}_3)\text{CO}(\text{CH}_2)_3\text{CH}_3 \end{array}$	O
	4-CF ₃	H	CO ₂ Me	SN(iPr)SO ₂ CH ₃	O
15	4-Cl	H	CO ₂ Me	SN(iPr)SO ₂ CH ₃	O
	4-OCF ₃	H	CO ₂ Me	SN(iPr)SO ₂ CH ₃	O
	4-CF ₃	5-Cl	CO ₂ Me	SN(iPr)SO ₂ CH ₃	O
	4-CF ₃	4-F	CO ₂ Me	SN(iPr)SO ₂ CH ₃	O
	4-CF ₃	5-F	CO ₂ Me	SN(iPr)SO ₂ CH ₃	O
20	4-CF ₃	5-Cl	4-Cl-Phenyl	SN(iPr)SO ₂ CH ₃	O
	4-CF ₃	4-F	4-Cl-Phenyl	SN(iPr)SO ₂ CH ₃	O
	4-CF ₃	5-F	4-Cl-Phenyl	SN(iPr)SO ₂ CH ₃	O
	4-CF ₃	H	4-Cl-Phenyl	SN(iPr)SO ₂ CH ₃	O
	4-CF ₃	H	CO ₂ Me	SN(CH ₃)SO ₂ Ph	O
25	4-Cl	H	CO ₂ Me	SN(CH ₃)SO ₂ Ph	O
	4-OCF ₂ H	H	CO ₂ Me	SN(CH ₃)SO ₂ Ph	O
	4-OCF ₃	H	CO ₂ Me	SN(CH ₃)SO ₂ Ph	O
	4-F	H	CO ₂ Me	SN(CH ₃)SO ₂ Ph	O
	4-CF ₃	5-Cl	CO ₂ Me	SN(CH ₃)SO ₂ Ph	O
30	4-CF ₃	4-F	CO ₂ Me	SN(CH ₃)SO ₂ Ph	O
	4-CF ₃	5-F	CO ₂ Me	SN(CH ₃)SO ₂ Ph	O
	4-CF ₃	5-Cl	4-Cl-Phenyl	SN(CH ₃)SO ₂ Ph	O
	4-CF ₃	4-F	4-Cl-Phenyl	SN(CH ₃)SO ₂ Ph	O
	4-CF ₃	5-F	4-Cl-Phenyl	SN(CH ₃)SO ₂ Ph	O
35	4-CF ₃	H	4-Cl-Phenyl	SN(CH ₃)SO ₂ Ph	O

	R ₁	R ₂	B	Y	A
5					
	4-CF ₃	H	CO ₂ Me	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SCOCH}_2\text{CH}_2\text{CH}_2\text{CH}_3 \\ \text{O} \end{array}$	O
	4-CF ₃	5-Cl	CO ₂ Me	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SCOCH}_2\text{CH}_2\text{CH}_2\text{CH}_3 \\ \text{O} \end{array}$	O
10	4-CF ₃	4-F	CO ₂ Me	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SCOCH}_2\text{CH}_2\text{CH}_2\text{CH}_3 \\ \text{O} \end{array}$	O
	4-CF ₃	5-F	CO ₂ Me	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SCOCH}_2\text{CH}_2\text{CH}_2\text{CH}_3 \\ \text{O} \end{array}$	O
	4-CF ₃	5-Cl	4-Cl-Phenyl	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SCOCH}_2\text{CH}_2\text{CH}_2\text{CH}_3 \\ \text{O} \end{array}$	O
15	4-CF ₃	4-F	4-Cl-Phenyl	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SCOCH}_2\text{CH}_2\text{CH}_2\text{CH}_3 \\ \text{O} \end{array}$	O
	4-CF ₃	5-F	4-Cl-Phenyl	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SCOCH}_2\text{CH}_2\text{CH}_2\text{CH}_3 \\ \text{O} \end{array}$	O
20	4-CF ₃	H	4-Cl-Phenyl	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SCOCH}_2\text{CH}_2\text{CH}_2\text{CH}_3 \\ \text{O} \end{array}$	O
	4-CF ₃	5-Cl	CO ₂ Me	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SN}(\text{iPr})\text{P}(\text{OCH}_3)\text{CH}_3 \\ \text{O} \end{array}$	S
	4-CF ₃	5-Cl	CO ₂ Me	$\begin{array}{c} \text{O} \\ \parallel \\ -\text{SP}(\text{OC}_2\text{H}_5)_2 \\ \text{O} \end{array}$	S
25	4-CF ₃	5-Cl	CO ₂ Me	$\begin{array}{c} \text{O} \\ \parallel \\ -\text{S}-\text{N}(\text{iPr})_2 \\ \text{O} \end{array}$	S
	4-CF ₃	H	CO ₂ Me	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SN}(\text{iPr})\text{P}(\text{OC}_2\text{H}_5)\text{Ph} \\ \text{O} \end{array}$	S
	4-CF ₃	H	CO ₂ Me	$\begin{array}{c} \text{O} \\ \parallel \\ -\text{SP}(\text{OiPr})_2 \\ \text{O} \end{array}$	S
	4-CF ₃	H	CO ₂ Me	$\begin{array}{c} \text{O} \\ \parallel \\ -\text{S}-\text{N}(\text{s-Bu})_2 \\ \text{O} \end{array}$	S
30	4-CF ₃	H	CO ₂ Me	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SNP}(\text{OEt})_2 \\ \text{O} \end{array}$	S
	4-Cl	H	CO ₂ Me	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SNP}(\text{OEt})_2 \\ \text{O} \end{array}$	S
35	4-OCF ₂ H	H	CO ₂ Me	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SNP}(\text{OEt})_2 \\ \text{O} \end{array}$	S

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	R ₁	R ₂	B	Y	A
5				O "	
	4-CF ₃	H	CO ₂ Me	SN(iPr)COC ₂ H ₅ O "	O
	4-Cl	H	CO ₂ Me	SN(iPr)COC ₂ H ₅ O "	O
10				O "	
	4-OCF ₂ H	H	CO ₂ Me	SN(iPr)COC ₂ H ₅ O "	O
	4-OCF ₃	H	CO ₂ Me	SN(iPr)COC ₂ H ₅ O "	O
15				O "	
	4-F	H	CO ₂ Me	SN(iPr)COC ₂ H ₅ O "	O
	4-CF ₃	5-Cl	CO ₂ Me	SN(iPr)COC ₂ H ₅ O "	O
	4-CF ₃	4-F	CO ₂ Me	SN(iPr)COC ₂ H ₅ O "	O
20				O "	
	4-CF ₃	5-F	CO ₂ Me	SN(iPr)COC ₂ H ₅ O "	O
	4-CF ₃	5-Cl	4-Cl-Phenyl	SN(iPr)COC ₂ H ₅ O "	O
25				O "	
	4-CF ₃	4-F	4-Cl-Phenyl	SN(iPr)COC ₂ H ₅ O "	O
	4-CF ₃	5-F	4-Cl-Phenyl	SN(iPr)COC ₂ H ₅ O "	O
	4-CF ₃	H	4-Cl-Phenyl	SN(iPr)COC ₂ H ₅ O "	O
30				O "	
	4-CF ₃	H	CO ₂ Me	SN(CH ₃)CO(CH ₂) ₃ CH ₃ O "	S
	4-Cl	H	CO ₂ Me	SN(CH ₃)CO(CH ₂) ₃ CH ₃ O "	S
35				O "	
	4-OCF ₂ H	H	CO ₂ Me	SN(CH ₃)CO(CH ₂) ₃ CH ₃ O "	S
	4-OCF ₃	H	CO ₂ Me	SN(CH ₃)CO(CH ₂) ₃ CH ₃ O "	S

	R ₁	R ₂	B	Y	A
5					
	4-F	H	CO ₂ Me	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SN}(\text{CH}_3)\text{CO}(\text{CH}_2)_3\text{CH}_3 \end{array}$	S
10	4-CF ₃	5-Cl	CO ₂ Me	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SN}(\text{CH}_3)\text{CO}(\text{CH}_2)_3\text{CH}_3 \end{array}$	S
	4-CF ₃	4-F	CO ₂ Me	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SN}(\text{CH}_3)\text{CO}(\text{CH}_2)_3\text{CH}_3 \end{array}$	S
	4-CF ₃	5-F	CO ₂ Me	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SN}(\text{CH}_3)\text{CO}(\text{CH}_2)_3\text{CH}_3 \end{array}$	S
15	4-CF ₃	5-Cl	4-Cl-Phenyl	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SN}(\text{CH}_3)\text{CO}(\text{CH}_2)_3\text{CH}_3 \end{array}$	S
	4-CF ₃	4-F	4-Cl-Phenyl	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SN}(\text{CH}_3)\text{CO}(\text{CH}_2)_3\text{CH}_3 \end{array}$	S
20	4-CF ₃	5-F	4-Cl-Phenyl	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SN}(\text{CH}_3)\text{CO}(\text{CH}_2)_3\text{CH}_3 \end{array}$	S
	4-CF ₃	5-Cl	CO ₂ Me	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SN}(\text{iPr})\text{SO}_2\text{CH}_3 \end{array}$	S
	4-CF ₃	4-F	CO ₂ Me	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SN}(\text{iPr})\text{SO}_2\text{CH}_3 \end{array}$	S
	4-CF ₃	5-F	CO ₂ Me	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SN}(\text{iPr})\text{SO}_2\text{CH}_3 \end{array}$	S
	4-CF ₃	5-Cl	4-Cl-Phenyl	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SN}(\text{iPr})\text{SO}_2\text{CH}_3 \end{array}$	S
	4-CF ₃	4-F	4-Cl-Phenyl	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SN}(\text{iPr})\text{SO}_2\text{CH}_3 \end{array}$	S
25	4-CF ₃	5-F	4-Cl-Phenyl	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SN}(\text{iPr})\text{SO}_2\text{CH}_3 \end{array}$	S
	4-CF ₃	H	4-Cl-Phenyl	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SN}(\text{iPr})\text{SO}_2\text{CH}_3 \end{array}$	S
30	4-Cl	H	CO ₂ Me	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SN}(\text{CH}_3)\text{CO}(\text{CH}_2)_3\text{CH}_3 \end{array}$	NCH ₃
	4-OCF ₂ H	H	CO ₂ Me	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SN}(\text{CH}_3)\text{CO}(\text{CH}_2)_3\text{CH}_3 \end{array}$	NCH ₃
	4-OCF ₃	H	CO ₂ Me	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SN}(\text{CH}_3)\text{CO}(\text{CH}_2)_3\text{CH}_3 \end{array}$	NCH ₃
35	4-F	H	CO ₂ Me	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SN}(\text{CH}_3)\text{CO}(\text{CH}_2)_3\text{CH}_3 \end{array}$	NCH ₃

	R ₁	R ₂	B	Y	A
5					
	4-CF ₃	5-Cl	CO ₂ Me	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SN}(\text{CH}_3)\text{CO}(\text{CH}_2)_3\text{CH}_3 \end{array}$	NCH ₃
10	4-CF ₃	4-F	CO ₂ Me	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SN}(\text{CH}_3)\text{CO}(\text{CH}_2)_3\text{CH}_3 \end{array}$	NCH ₃
	4-CF ₃	5-F	CO ₂ Me	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SN}(\text{CH}_3)\text{CO}(\text{CH}_2)_3\text{CH}_3 \end{array}$	NCH ₃
	4-CF ₃	5-Cl	4-Cl-Phenyl	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SN}(\text{CH}_3)\text{CO}(\text{CH}_2)_3\text{CH}_3 \end{array}$	NCH ₃
15	4-CF ₃	4-F	4-Cl-Phenyl	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SN}(\text{CH}_3)\text{CO}(\text{CH}_2)_3\text{CH}_3 \end{array}$	NCH ₃
	4-CF ₃	5-F	4-Cl-Phenyl	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SN}(\text{CH}_3)\text{CO}(\text{CH}_2)_3\text{CH}_3 \end{array}$	NCH ₃
20	4-CF ₃	H	4-Cl-Phenyl	$\begin{array}{c} \text{O} \\ \parallel \\ \text{SN}(\text{CH}_3)\text{CO}(\text{CH}_2)_3\text{CH}_3 \end{array}$	NCH ₃
	4-CF ₃	H	CO ₂ Me	SN(iPr)SO ₂ CH ₃	NCH ₃
	4-Cl	H	CO ₂ Me	SN(iPr)SO ₂ CH ₃	NCH ₃
	4-OCF ₂ H	H	CO ₂ Me	SN(iPr)SO ₂ CH ₃	NCH ₃
	4-OCF ₃	H	CO ₂ Me	SN(iPr)SO ₂ CH ₃	NCH ₃
25	4-F	H	CO ₂ Me	SN(iPr)SO ₂ CH ₃	NCH ₃
	4-CF ₃	5-Cl	CO ₂ Me	SN(iPr)SO ₂ CH ₃	NCH ₃
	4-CF ₃	4-F	CO ₂ Me	SN(iPr)SO ₂ CH ₃	NCH ₃
	4-CF ₃	5-F	CO ₂ Me	SN(iPr)SO ₂ CH ₃	NCH ₃
	4-CF ₃	5-Cl	4-Cl-Phenyl	SN(iPr)SO ₂ CH ₃	NCH ₃
30	4-CF ₃	4-F	4-Cl-Phenyl	SN(iPr)SO ₂ CH ₃	NCH ₃
	4-CF ₃	5-F	4-Cl-Phenyl	SN(iPr)SO ₂ CH ₃	NCH ₃
	4-CF ₃	H	4-Cl-Phenyl	SN(iPr)SO ₂ CH ₃	NCH ₃
	4-CF ₃	H	CO ₂ Me	SN(s-Bu)SO ₂ CH ₂ CH ₂ CH ₃	NCH ₃
	4-Cl	H	CO ₂ Me	SN(s-Bu)SO ₂ CH ₂ CH ₂ CH ₃	NCH ₃
35	4-OCF ₂ H	H	CO ₂ Me	SN(s-Bu)SO ₂ CH ₂ CH ₂ CH ₃	NCH ₃
	4-OCF ₃	H	CO ₂ Me	SN(s-Bu)SO ₂ CH ₂ CH ₂ CH ₃	NCH ₃
	4-F	H	CO ₂ Me	SN(s-Bu)SO ₂ CH ₂ CH ₂ CH ₃	NCH ₃

	R ₁	R ₂	B	Y	A
5	4-CF ₃	5-Cl	CO ₂ Me	SN(s-Bu)SO ₂ CH ₂ CH ₂ CH ₃	NCH ₃
	4-CF ₃	4-F	CO ₂ Me	SN(s-Bu)SO ₂ CH ₂ CH ₂ CH ₃	NCH ₃
	4-CF ₃	5-F	CO ₂ Me	SN(s-Bu)SO ₂ CH ₂ CH ₂ CH ₃	NCH ₃
	4-CF ₃	5-Cl	4-Cl-Phenyl	SN(s-Bu)SO ₂ CH ₂ CH ₂ CH ₃	NCH ₃
10	4-CF ₃	4-F	4-Cl-Phenyl	SN(s-Bu)SO ₂ CH ₂ CH ₂ CH ₃	NCH ₃
	4-CF ₃	5-F	4-Cl-Phenyl	SN(s-Bu)SO ₂ CH ₂ CH ₂ CH ₃	NCH ₃
	4-CF ₃	H	4-Cl-Phenyl	SN(s-Bu)SO ₂ CH ₂ CH ₂ CH ₃	NCH ₃
	4-CF ₃	5-Cl	CO ₂ Me	Me	S
15	4-OCF ₃	5-Cl	CO ₂ Me	Me	S
	4-Br	5-Cl	CO ₂ Me	Me	S
	4-CF ₃	5-F	CO ₂ Me	COCH ₃	S
	4-OCF ₃	5-F	CO ₂ Me	COCH ₃	S
20	4-Br	5-F	CO ₂ Me	COCH ₃	S
	4-CF ₃	5-Cl	CO ₂ Me	CO ₂ CH ₃	S
	4-OCF ₃	5-Cl	CO ₂ Me	CO ₂ CH ₃	S
	4-Br	5-Cl	CO ₂ Me	CO ₂ CH ₃	S
25	4-CF ₃	5-F	CO ₂ Me	COCF ₃	S
	4-OCF ₃	5-F	CO ₂ Me	COCF ₃	S
	4-Br	5-F	CO ₂ Me	COCF ₃	S
	4-CF ₃	4-Cl	4-Cl-Ph	Me	S
30	4-OCF ₃	4-Cl	4-Cl-Ph	Me	S
	4-Br	4-Cl	4-Cl-Ph	Me	S
	4-CF ₃	4-Cl	4-Cl-Ph	COCH ₃	S
	4-OCF ₃	4-Cl	4-Cl-Ph	COCH ₃	S
35	4-Br	4-Cl	4-Cl-Ph	COCH ₃	S
	4-CF ₃	4-Cl	4-Cl-Ph	CO ₂ CH ₃	S
	4-OCF ₃	4-Cl	4-Cl-Ph	CO ₂ CH ₃	S
	4-Br	4-Cl	4-Cl-Ph	CO ₂ CH ₃	S
	4-CF ₃	4-Cl	4-Cl-Ph	COCF ₃	S
	4-OCF ₃	4-Cl	4-Cl-Ph	COCF ₃	S
	4-Br	4-Cl	4-Cl-Ph	COCF ₃	S
	4-CF ₃	4-Cl	4-Cl-Ph	COCF ₃	S

	R ₁	R ₂	B	Y	A
5	4-CF ₃	4-Cl	4-Cl-Ph	CO ₂ CH ₂ CH ₃	S
	4-OCF ₃	4-Cl	4-Cl-Ph	CO ₂ CH ₂ CH ₃	S
	4-Br	4-Cl	4-Cl-Ph	CO ₂ CH ₂ CH ₃	S
	4-CF ₃	4-Cl	4-F-Ph	Me	S
10	4-OCF ₃	4-Cl	4-F-Ph	Me	S
	4-Br	4-Cl	4-F-Ph	Me	S
	4-CF ₃	4-Cl	4-F-Ph	COCH ₃	S
	4-OCF ₃	4-Cl	4-F-Ph	COCH ₃	S
	4-Br	4-Cl	4-F-Ph	COCH ₃	S
15	4-CF ₃	4-Cl	4-F-Ph	CO ₂ CH ₃	S
	4-OCF ₃	4-Cl	4-F-Ph	CO ₂ CH ₃	S
	4-Br	4-Cl	4-F-Ph	CO ₂ CH ₃	S
	4-CF ₃	4-Cl	4-F-Ph	COCH ₂ CH ₃	S
	4-OCF ₃	4-Cl	4-F-Ph	COCH ₂ CH ₃	S
20	4-Br	4-Cl	4-F-Ph	COCH ₂ CH ₃	S
	4-CF ₃	5-Cl	CO ₂ Me	Me	O
	4-OCF ₃	5-Cl	CO ₂ Me	Me	O
	4-Br	5-Cl	CO ₂ Me	Me	O
	4-CF ₃	5-F	CO ₂ Me	COCH ₃	O
25	4-OCF ₃	5-F	CO ₂ Me	COCH ₃	O
	4-Br	5-F	CO ₂ Me	COCH ₃	O
	4-CF ₃	5-Cl	CO ₂ Me	CO ₂ CH ₃	O
	4-OCF ₃	5-Cl	CO ₂ Me	CO ₂ CH ₃	O
	4-Br	5-Cl	CO ₂ Me	CO ₂ CH ₃	O
30	4-CF ₃	5-F	CO ₂ Me	COCF ₃	O
	4-OCF ₃	5-F	CO ₂ Me	COCF ₃	O
	4-Br	5-F	CO ₂ Me	COCF ₃	O
	4-CF ₃	4-Cl	4-Cl-Ph	Me	O
	4-OCF ₃	4-Cl	4-Cl-Ph	Me	O
35	4-Br	4-Cl	4-Cl-Ph	Me	O
	4-CF ₃	4-Cl	4-Cl-Ph	COCH ₃	O

	R ₁	R ₂	B	Y	A
5	4-OCF ₃	4-Cl	4-Cl-Ph	COCH ₃	O
	4-Br	4-Cl	4-Cl-Ph	COCH ₃	O
	4-CF ₃	4-Cl	4-Cl-Ph	CO ₂ CH ₃	O
	4-OCF ₃	4-Cl	4-Cl-Ph	CO ₂ CH ₃	O
10	4-Br	4-Cl	4-Cl-Ph	CO ₂ CH ₃	O
	4-CF ₃	4-Cl	4-Cl-Ph	COCF ₃	O
	4-OCF ₃	4-Cl	4-Cl-Ph	COCF ₃	O
	4-Br	4-Cl	4-Cl-Ph	COCF ₃	O
	4-CF ₃	4-Cl	4-Cl-Ph	CO ₂ CH ₂ CH ₃	O
15	4-OCF ₃	4-Cl	4-Cl-Ph	CO ₂ CH ₂ CH ₃	O
	4-Br	4-Cl	4-Cl-Ph	CO ₂ CH ₂ CH ₃	O
	4-CF ₃	4-Cl	4-F-Ph	Me	O
	4-OCF ₃	4-Cl	4-F-Ph	Me	O
	4-Br	4-Cl	4-F-Ph	Me	O
20	4-CF ₃	4-Cl	4-F-Ph	COCH ₃	O
	4-OCF ₃	4-Cl	4-F-Ph	COCH ₃	O
	4-Br	4-Cl	4-F-Ph	COCH ₃	O
	4-CF ₃	4-Cl	4-F-Ph	CO ₂ CH ₃	O
	4-OCF ₃	4-Cl	4-F-Ph	CO ₂ CH ₃	O
25	4-Br	4-Cl	4-F-Ph	CO ₂ CH ₃	O
	4-CF ₃	4-Cl	4-F-Ph	COCH ₂ CH ₃	O
	4-OCF ₃	4-Cl	4-F-Ph	COCH ₂ CH ₃	O
	4-Br	4-Cl	4-F-Ph	COCH ₂ CH ₃	O

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TABLE 16

	R ₁	R ₂	B	A	1 R _a	2 R _a
5	4-CF ₃	5-Cl	H	CHMe	H	H
	4-OCF ₃	5-Cl	H	CHMe	H	H
	4-Cl	5-Cl	H	CHMe	H	H
	4-Br	5-Cl	H	CHMe	H	H
10	4-OCF ₂ H	5-Cl	H	CHMe	H	H
	4-CF ₃	5-F	H	CHMe	H	H
	4-OCF ₃	5-F	H	CHMe	H	H
	4-Cl	5-F	H	CHMe	H	H
	4-Br	5-F	H	CHMe	H	H
15	4-OCF ₂ H	5-F	H	CHMe	H	H
	4-CF ₃	5-Cl	H	CH(i-Pr)	H	H
	4-Cl	5-Cl	H	CH(i-Pr)	H	H
	CF ₃	5-Cl	Me	CHMe	H	H
	OCF ₃	5-Cl	Me	CH(i-Pr)	H	H
20	OCF ₂ H	5-Cl	Me	C(Me) ₂	H	H
	Cl	5-Cl	Me	C(Me) ₂	H	H
	CF ₃	5-Cl	CO ₂ Me	C(Me) ₂	H	H
	OCF ₃	5-Cl	CO ₂ Me	C(Me) ₂	H	H
	OCF ₂ H	5-Cl	CO ₂ Me	CHEt	H	H
25	Cl	5-Cl	CO ₂ Me	CHEt	H	H
	CF ₃	5-F	Ph	CHMe	H	H
	OCF ₃	5-F	Ph	CHMe	H	H
	OCF ₂ H	5-F	Ph	CHMe	H	H
	Cl	5-F	Ph	CHMe	H	H
30	CF ₃	5-F	CO ₂ Me	CHMe	H	H
	OCF ₃	5-F	CO ₂ Me	CHMe	H	H
	CF ₃	H	H	CH ₂	Me	H
	OCF ₃	H	H	CH ₂	Me	H
	CF ₃	H	4-F-Ph	CH ₂	Me	H
35	OCF ₃	H	4-F-Ph	CH ₂	Me	H
	CF ₃	5-Cl	CO ₂ Me	CH ₂	Me	H

	R ₁	R ₂	B	A	1 R _a	2 R _a
5	OCF ₃	5-Cl	CO ₂ Me	CH ₂	Me	H
	CF ₃	5-F	CO ₂ Me	CH ₂	Me	H
	OCF ₃	5-F	CO ₂ Me	CH ₂	Me	H
	CF ₃	5-Cl	Me	CH ₂	Me	Me
10	OCF ₃	5-Cl	Me	CH ₂	Me	Me
	CF ₃	5-F	Ph	CH ₂	Me	Me
	OCF ₃	5-F	Ph	CH ₂	Me	Me
	CF ₃	5-Cl	CO ₂ Me	CH ₂	Me	Me
	OCF ₃	5-Cl	CO ₂ Me	CH ₂	Me	Me
15	CF ₃	H	H	O	Me	H
	OCF ₃	H	H	O	Me	H
	CF ₃	H	H	O	Me	Me
	OCF ₃	H	H	O	Me	Me
	CF ₃	5-Cl	CO ₂ Me	O	Me	H
20	OCF ₃	5-Cl	CO ₂ Me	O	Me	H
	CF ₃	5-Cl	CO ₂ Me	O	Me	H
	OCF ₃	5-Cl	CO ₂ Me	O	Me	H
	CF ₃	5-F	CO ₂ Me	O	Me	H
	OCF ₃	5-F	CO ₂ Me	O	Me	H
25	CF ₃	5-F	Ph	O	Me	H
	OCF ₃	5-F	Ph	O	Me	H
	CF ₃	5-F	Me	O	Me	H
	OCF ₃	5-F	Me	O	Me	H
	CF ₃	H	H	S	Me	H
30	OCF ₃	H	H	S	Me	H
	CF ₃	H	Ph	S	Me	H
	OCF ₃	5-Cl	Ph	S	Me	H
	CF ₃	5-Cl	H	S	Me	Me
	OCF ₃	5-Cl	H	S	Me	Me
35	CF ₃	5-F	Me	S	Me	H
	OCF ₃	5-F	Me	S	Me	H

	R_1	R_2	B	A	R_a^1	R_a^2
5	OCF ₃	5-Cl	H	CH ₂	Me	H
	OCF ₃	5-Cl	H	CH ₂	Me	H
	CF ₃	5-Cl	H	CH ₂	Me	Me
	OCF ₃	5-Cl	H	CH ₂	Me	Me
10	CF ₃	5-F	H	CH ₂	Me	Me
	OCF ₃	5-F	H	CH ₂	Me	Me

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Formulation and Use

The compounds of this invention will generally be used in formulation with a carrier comprising a liquid or solid diluent or an organic solvent. Useful formulations of the compounds of Formula I can be prepared in conventional ways. They include dusts, granules, pellets, solutions, suspensions, emulsions, wettable powders, emulsifiable concentrates, dry flowables and the like. Many of these can be applied directly. Sprayable formulations can be extended in suitable media and used at spray volumes of from about one to several hundred liters per hectare. High strength compositions are primarily used as intermediates for further formulation. The formulations, broadly, contain about 1% to 99% by weight of active ingredient(s) and at least one of a) about 0.1% to 20% surfactant(s) and b) about 5% to 99% solid or liquid diluent(s). More specifically, they will contain these ingredients in the following approximate proportions:

	Active Ingredient	<u>Percent by Weight</u>	
		<u>Diluent(s)</u>	<u>Surfactant(s)</u>
Wettable Powders	25-90	0-74	1-10
Oil Suspensions, Emulsions, Solutions, (including Emulsifiable Concentrates)	1-50	40-95	0-35
Dusts	1-25	70-99	0-5
Granules and Pellets	1-95	5-99	0-15
High Strength Compositions	90-99	0-10	0-2

Lower or higher levels of active ingredient can, of course, be present depending on the intended use and the physical properties of the compound. Higher ratios of surfactant to active ingredient are sometimes desirable, and are achieved by incorporation into the formulation or by tank mixing.

Typical solid diluents are described in Watkins, et al., "Handbook of Insecticide Dust Diluents and Carriers", 2nd Ed., Dorland Books, Caldwell, New Jersey. The more absorptive diluents are preferred for wettable powders and the denser ones for dusts. Typical liquid diluents and solvents are described in Marsden, "Solvents Guide," 2nd Ed., Interscience, New York, 1950. Solubility under 0.1% is preferred for suspension concentrates; solution concentrates are preferably stable against phase separation at 0°C. "McCutcheon's Detergents and Emulsifiers Annual", Allured Publ. Corp., Ridgewood, New Jersey, as well as Sisely and Wood, "Encyclopedia of Surface Active Agents", Chemical Publ. Co., Inc., New York, 1964, list surfactants and recommended uses. All formulations can contain minor amounts of additives to reduce foam, caking, corrosion, microbiological growth, etc. Preferably, ingredients should be approved by the U.S. environmental Protection Agency for the use intended.

The methods of making such compositions are well known. Solutions are prepared by simply mixing the ingredients. Fine solid compositions are made by blending and, usually, grinding as in a hammer or fluid energy mill. Suspensions are prepared by wet milling (see, for example, U.S. 3,060,084). Granules and pellets can be made by spraying the active material upon preformed granular carriers or by agglomeration techniques. See Browning,

"Agglomeration", Chemical Engineering, December 4, 1967, pages 147 and following, and "Perry's Chemical Engineer's Handbook", 4th Ed., McGraw-Hill, New York, 1963, pages 8 to 59 and following.

Many of the compounds of the invention are most efficacious when applied in the form of an emulsifiable concentrate mixed with a spray oil or spray oil concentrate. Although any oil can be used as a spray oil, spray oils usually have these characteristics: they are not phytotoxic to the crop sprayed, and they have appropriate viscosity. Petroleum based oils are commonly used for spraying. In some areas, crop oils are preferred such as the following:

Common Crop Oils Used as Spray Oils

	Corn Oil	Linseed Oil
	Cottonseed Oil	Soybean Oil
20	Coconut Oil	Sunflower Oil
	Rapeseed Oil	Olive Oil
	Peanut Oil	Palm Oil
	Safflower Oil	Sesame Oil
	Mustardseed Oil	Caster Oil

The following oils also meet the criteria for a spray oil: mineral, fish and cod liver oil.

Spray oil concentrates comprise a spray oil together with one or more additional ingredients such as emulsifiers and wetting agents. A number of useful spray oil and spray oil concentrates can be found in "A Guide to Agricultural Spray Adjuvants Used in the United States" by Thomson, Thomson Publications, California, 1986.

Examples of useful formulations of compounds of the present invention are as follows:

35

Example AEmulsifiable Concentrate

- 5 methyl 7-fluoro-3A,4-dihydro-2-[[[4-(trifluoro-
methyl)-phenyl]amino]carbonyl]-3H-pyrazolo[5,1
-c][1,4]benzoxazine-3a-carboxylate. 20%
- blend of oil soluble sulfonates
- and polyoxyethylene ethers 10%
- 10 isophorone 70%

The ingredients are combined and stirred with gentle warming to speed solution. A fine screen filter is included in packaging operation to insure the absence of any extraneous undissolved material in

15 the product.

Example BWettable Powder

- methyl 7-fluoro-3A,4-dihydro-2-[[[4-(trifluoro-
methyl)-phenyl]amino]carbonyl]-3H-pyrazolo[5,1
- 20 -c][1,4]benzoxazine-3a-carboxylate. 30%
- sodium alkyl naphthalenesulfonate 2%
- sodium ligninsulfonate 2%
- synthetic amorphous silica 3%
- kaolinite 63%

25 The active ingredient is mixed with the inert materials in a blender. After grinding in a hammer-mill, the material is re-blended and sifted through a 50 mesh screen.

Example CDust

- 30 Wettable powder of Example B 10%
- pyrophyllite (powder) 90%
- The wettable powder and the pyrophyllite diluent are thoroughly blended and then packaged. The product
- 35 is suitable for use as a dust.

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Example DGranule

- 5 methyl 7-fluoro-3A,4-dihydro-2-[[[4-(trifluoro-
methyl)-phenyl]amino]carbonyl]-3H-pyrazolo[5,1
-c][1,4]benzoxazine-3a-carboxylate. 10%
- matter, 0.71/0.30 mm; U.S.S. No.
25-50 sieves) 90%

- 10 The active ingredient is dissolved in a volatile
solvent such as acetone and sprayed upon dedusted and
pre-warmed attapulgit granules in a double cone
blender. The acetone is then driven off by heating.
The granules are then allowed to cool and are packaged.

15 Example E

Granule

- Wettable powder of Example B 15%
- gypsum 69%
- potassium sulfate 16%
- 20 The ingredients are blended in a rotating mixer
and water sprayed on to accomplish granulation. When
most of the material has reached the desired range of
0.1 to 0.42 mm (U.S.S. No. 18 to 40 sieves), the gran-
ules are removed, dried, and screened. Oversize
- 25 material is crushed to produce additional material in
the desired range. These granules contain 4.5% active
ingredient.

Example FSolution

- 30 methyl 7-fluoro-3A,4-dihydro-2-[[[4-
(trifluoro-methyl)-phenyl]amino]
carbonyl]-3H-pyrazolo[5,1-c][1,4]
benzoxazine-3a-carboxylate. 25%
- N-methyl-pyrrolidone 75%
- 35 The ingredients are combined and stirred to
produce a solution suitable for direct, low volume
application.

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Example GAqueous Suspension

5	Methyl 7-fluoro-3A,4-dihydro-2-[[[4-(trifluoro- methyl)-phenyl]amino]carbonyl]-3H-pyrazolo[5,1-c][1,4]benzoxazine-3a-carboxylate.	40%
	polyacrylic acid thickener	0.3%
10	dodecyclophenol polyethylene glycol ether	0.5%
	disodium phosphate	1.0%
	monosodium phosphate	0.5%
	polyvinyl alcohol	1.0%
15	water	56.7%
The ingredients are blended and ground together in a sand mill to produce particles essentially all under 5 microns in size.		

Example HOil Suspension

20	Methyl 7-fluoro-3A,4-dihydro-2-[[[4-(trifluoro- methyl)-phenyl]amino]carbonyl]-3H-pyrazolo[5,1-c][1,4]benzoxazine-3a-carboxylate.	35.0%
25	blend of polyalcohol carboxylic esters and oil soluble petroleum sulfonates	6.0%
	xylene range solvent	59.0%

30 The ingredients are combined and ground together in a sand mill to produce particles essentially all below 5 microns. The product can be used directly, extended with oils, or emulsified in water.

Example IBait Granules

35	Methyl 7-fluoro-3A,4-dihydro-2-[[[4-(trifluoro- methyl)-phenyl]amino]carbonyl]-3H-pyrazolo[5,1-c][1,4]	3.0%
----	--	------

benzoxazine-3a-carboxylate.

blend of polyethoxylated nonyl- 9.0%

5 phenols and sodium dodecyl-
benzene sulfonates

ground up corn cobs 88.0%

The active ingredient and surfactant blend are
dissolved in a suitable solvent such as acetone and
10 sprayed onto the ground corn cobs. The granules are
then dried and packaged.

Compounds of Formula I can also be mixed with one
or more other insecticides, fungicides, nematocides,
bactericides, acaricides, or other biologically active
15 compounds to form a multi-component pesticide giving
an even broader spectrum of effective agricultural
protection. Examples of other agricultural protectants
with which compounds of the present invention can be
mixed or formulated are:

20 Insecticides:

3-hydroxy-N-methylcrotonamide(dimethylphosphate)ester
(monocrotophos)

methylcarbamic acid, ester with 2,3-dihydro-2,2-
dimethyl-7-benzofuranol (carbofuran)

25 O-[2,4,5-trichloro- α -(chloromethyl)benzyl]phosphoric
acid, O',O'-dimethyl ester (tetrachlorvinphos)

2-mercaptosuccinic acid, diethyl ester, S-ester with
thionophosphoric acid, dimethyl ester (malathion)

30 phosphorothioic acid, O,O-dimethyl, O-p-nitrophenyl
ester (methyl parathion)

methylcarbamic acid, ester with α -naphthol (carbaryl)

methyl O-(methylcarbamoyl)thiolacetohydroxamate
(methomyl)

N'-(4-chloro-p-tolyl)-N,N-dimethylformamidine

35 (chlordimeform)

O,O-diethyl-O-(2-isopropyl-4-methyl-6-pyrimidylphos-
phorothioate (diazinon)

- octachlorocamphene (toxaphene)
 O-ethyl O-*p*-nitrophenyl phenylphosphonothioate (EPN)
 5 (S)- α -cyano-*m*-phenoxybenzyl(1R,3R)-3-(2,2-dibromo-
 vinyl)-2,2-dimethylcyclopropanecarboxylate (delta-
 methrin)
 Methyl N',N'-dimethyl-N-[(methylcarbamoyl)oxy]-1-thio-
 oxamimidate (oxamyl)
 10 cyano(3-phenoxyphenyl)-methyl-4-chloro- α -(1-methyl-
 ethyl)benzeneacetate (fenvalerate)
 (3-phenoxyphenyl)methyl(+)-*cis,trans*-3-(2,2-dichloro-
 ethenyl)-2,2-dimethylcyclopropanecarboxylate
 (permethrin)
 15 α -cyano-3-phenoxybenzyl 3-(2,2-dichlorovinyl)-2,2-
 dimethylcyclopropane carboxylate (cypermethrin)
 O-ethyl-S-(*p*-chlorophenyl)ethylphosphonodithioate
 (profenofos)
 phosphorothiolothionic acid, O-ethyl-O-[4-(methylthio)-
 20 phenyl]-S-*n*-propyl ester (sulprofos).

- Additional insecticides are listed hereafter by
 their common names: triflumuron, diflubenzuron,
 methoprene, buprofezin, thiodicarb, acephate,
 25 azinphos-methyl, chlorpyrifos, dimethoate, fonophos,
 isofenphos, methidathion, methamidophos,
 monocrotophos, phosmet, phosphamidon, phosalone,
 pirimicarb, phorate, profenofos, terbufos,
 trichlorfon, methoxychlor, bifenthrin, biphenate,
 30 cyfluthrin, fenpropathrin, fluvalinate, flucythrinate,
 tralomethrin, metaldehyde and rotenone.

Fungicides:

- methyl 2-benzimidazolecarbamate (carbendazim)
 tetramethylthiuram disulfide (thiuram)
 35 *n*-dodecylguanidine acetate (dodine)
 manganese ethylenebisdithiocarbamate (maneb)
 1,4-dichloro-2,5-dimethoxybenzene (chloroneb)

- methyl 1-(butylcarbamoyl)-2-benzimidazolecarbamate
(benomyl)
- 5 1-[2-(2,4-dichlorophenyl)-4-propyl-1,3-dioxolan-2-ylmethyl]-1H-1,2,4-triazole (propiconazole)
2-cyano-N-ethylcarbamoyl-2-methoxyiminoacetamide
(cymoxanil)
- 10 1-(4-chlorophenoxy)-3,3-dimethyl-1-(1H-1,2,4-triazol-1-yl)-2-butanone (triadimefon)
N-(trichloromethylthio)tetrahydrophthalimide (captan)
N-(trichloromethylthio)phthalimide (folpet)
1-[[[bis(4-fluorophenyl)][methyl]silyl]methyl]-1H-1,2,4-triazole.
- 15 Nematocides:
S-methyl 1-(dimethylcarbamoyl)-N-(methylcarbamoyloxy)-thioformimidate
S-methyl 1-carbamoyl-N-(methylcarbamoyloxy)thioformimide
- 20 N-isopropylphosphoramidic acid, O-ethyl O'-[4-(methylthio)-m-tolyl]diester (fenamiphos).
Bactericides:
tribasic copper sulfate
streptomycin sulfate.
- 25 Acaricides:
senecioic acid, ester with 2-sec-butyl-4,6-dinitrophenol (binapacryl)
6-methyl-1,3-dithiolo[4,5-c]quinoxalin-2-one
(oxythioquinox)
- 30 ethyl 4,4'-dichlorobenzilate (chlorobenzilate)
1,1-bis(p-chlorophenyl)-2,2,2-trichloroethanol
(dicofol)
bis(pentachloro-2,4-cyclopentadien-1-yl) (dienochlor)
tricyclohexyltin hydroxide (cyhexatin)
- 35 trans-5-(4-chlorophenyl)-N-cyclohexyl-4-methyl-2-oxo-thiazolidine-3-carboxamide (hexythiazox)

amitraz

propargite

5 fenbutatin-oxide

bisclofentezin.

Biological

Bacillus thuringiensis

Avermectin B.

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Utility

The compounds of this invention exhibit activity against a wide spectrum of foliar and soil inhabiting arthropods which are pests of growing and stored
15 agronomic crops, forestry, greenhouse crops, ornamentals, nursery crops, stored food and fiber products, livestock, household, and public and animal health. Those skilled in the art will recognize that not all compounds are equally effective against all
20 pests but the compounds of this invention display activity against:

larvae of the order Lepidoptera including fall and beet armyworm and other
25 Spodoptera spp., tobacco budworm, corn earworm and other Heliothis spp., European corn borer, navel orangeworm, stalk/stem borers and other pyralids, cabbage and soybean loopers and other loopers, codling
30 moth, grape berry moth and other tortricids, black cutworm, spotted cutworm, other cutworms and other

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5 noctuids, diamondback moth, green
 cloverworm, velvetbean caterpillar, green
 cloverworm, pink bollworm, gypsy moth, and
 spruce budworm;

10 foliar feeding larvae and adults of the
 order Coleoptera including Colorado potato
 beetle, Mexican bean beetle, flea beetle,
 Japanese beetles, and other leaf beetles,
 boll weevil, rice water weevil, granary
 weevil, rice weevil and other weevil
15 pests, and soil inhabiting insects such as
 Western corn rootworm and other Diabrotica
 spp., Japanese beetle, European chafer and
 other coleopteran grubs, and wireworms;

20 adults and larvae of the orders Hemiptera
 and Homoptera including tarnished plant
 bug and other plant bugs (miridae), aster
 leafhopper and other leafhoppers
 (cicadellidae), rice planthopper, brown
 planthopper, and other planthoppers
25 (fulgoroidea), psyllids, whiteflies
 (aleurodidae), aphids (aphidae), scales
 (coccidae and diaspididae), lace bugs
 (tingidae), stink bugs (pentatomidae),
 cinch bugs and other seed bugs
30 (lygaeidae), cicadas (cicadidae),
 spittlebugs (cercopids), squash bugs
 (coreidae), red bugs and cotton stainers
 (pyrrhocoridae);

35 adults, larvae and eggs of the order acari
 (mites) including European red mite, two
 spotted spider mite, rust mites, McDaniel
 mite, and foliar feed mites;

- 5 adults and immatures of the order
Orthoptera including grasshoppers;
- adults and immatures of the order Diptera
including leafminers, midges, fruit flies
(tephritidae), and soil maggots;
- 10 adults and immatures of the order
Thysanoptera including onion thrips and
other foliar feeding thrips;
- 15 insect pests of the order Hymenoptera
including carpenter ants, bees, hornets
and wasps;
- 20 insect pests of the order Diptera
including house flies, stable flies, face
flies, horn flies, blow flies, and other
muscoid fly pests, horse flies, deer flies
and other Brachycera, mosquitoes, black
flies, biting midges, sand flies,
- 25 sciarids, and other Nematocera;
- insect pests of the order Orthoptera
including cockroaches and crickets;
- 30 insect pests of the order Isoptera
including the Eastern subterranean termite
and other termites;

5 insect pests of the order Mallophaga and
Anoplura including the head louse, body
louse, chicken head louse and other
sucking and chewing parasitic lice that
attack man and animals;

10 insect pests of the order Siphonoptera
including the cat flea, dog flea and other
fleas.

The specific species for which control is
exemplified are: fall armyworm, Spodoptera
15 frugiperda; tobacco budworm, Heliothis virescens;
boll weevil, Anthonomus grandis; aster leafhopper,
Macrostelus fascifrons; southern corn rootworm,
Diabrotica undecimpunctata. The pest control
protection afforded by these compounds of the present
20 invention is not limited, however, to these species.

Application

Arthropod pests are controlled and protection of
agronomic crops, animal and human health is achieved
25 by applying one or more of the Formula I compounds of
this invention, in an effective amount, to the locus
of infestation, to the area to be protected, or
directly on the pests to be controlled. Because of
the diversity of habitat and behavior of these
30 arthropod pest species, many different methods of
application are employed. A preferred method of
application is by spraying with equipment that
distributes the compound in the environment of the
pests, on the foliage, animal, person, or premise, in
35 the soil or animal, to the plant part that is infested
or needs to be protected. Alternatively, granular

formulations of these compounds can be applied to or
5 incorporated into the soil. Other methods of
application can also be employed including direct and
residual sprays, aerial, baits, eartags, boluses,
foggers, aerosols, and many others.

The compounds of this invention can be applied
10 in their pure state, but most often application will
be of a formulation comprising one or more compounds
of this invention, with suitable carriers, diluents
and surfactants depending on the contemplated end
use. A preferred method of application involves
15 spraying a water dispersion of refined oil solution of
the compounds. Combinations with spray oils, spray
oil concentrations, and synergists such as piperonyl
butoxide often enhance the efficacy of the compounds
of Formula I.

20 The rate of application of the Formula I
compounds required for effective control will depend
on such factors as the species of arthropod to be
controlled, the pest's life cycle, life stage, its
size, location, time of year, host crop or animal,
25 feeding behavior, mating behavior, ambient moisture,
temperature, etc. In general, application rates of
about 0.01 to 2 kg of active ingredient per hectare
are sufficient to provide large-scale effective
control of pests in agronomic ecosystems under normal
30 circumstances, but as little as 0.001 kg/hectare or as
much as 8 kg/hectare may be required. For
nonagronomic applications, effective use rates will
range from about 0.1 to 5 mg/square foot but as little
as 0.01 mg/square foot or as much as 15 mg/square foot
35 may be required.

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5 The following Examples demonstrate the control
efficacy of the compounds of Formula I on specific
insect pests wherein Compounds 1 through 44 are
described in Table 17 and Compounds 45 and 46 in
Table 18; and Compound 47 in Table 19.

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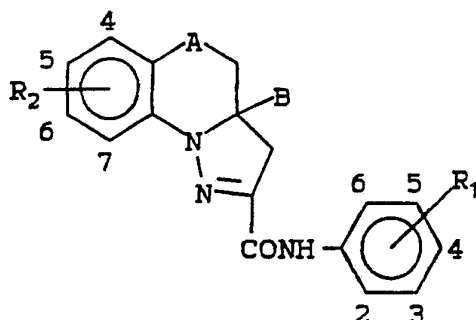
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TABLE 17

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	<u>COMPD</u>	<u>R₁</u>	<u>R₂</u>	<u>A</u>	<u>Y</u>	<u>B</u>	<u>m.p. °C</u>
20	1	4-CF ₃	H	O	H	H	157.5-158.5
	2	4-Cl	H	O	H	H	183-185
	3	4-Br	H	O	H	H	200-202
	4	4-CF ₃	H	O	H	Ph	183.5-185
25	5	4-OCF ₂ CF ₂ H	H	O	H	Ph	190-191
	6	4-Cl	H	O	H	Ph	186-188
	7	4-CF ₃	H	O	H	Me	186-187
	8	4-I	H	O	H	Me	162-163.5
	9	4-COMe	H	O	H	Me	174-177
30	10	4-OCF ₂ CF ₂ H	H	O	H	Me	oil
	11	4-CF ₃	H	O	H	Ph	106-116
	12	4-OCF ₃	5-Cl	O	H	Ph	140-146
	13	4-CF ₃	5-F	O	H	CO ₂ Me	177-181.5
	14	4-OCF ₃	5-F	O	H	4-Cl-Ph	135-139
35	15	4-Cl	5-F	O	H	4-Cl-Ph	190-191
	16	4-CF ₃	5-F	O	H	4-Cl-Ph	80-84

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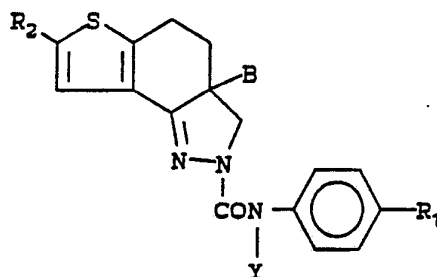
		<u>CMPD</u>	<u>R₁</u>	<u>R₂</u>	<u>A</u>	<u>Y</u>	<u>B</u>	<u>m.p. °C</u>	
5	17		4-CF ₃	6-Cl	O	H	Ph	215-215.5	
	18		4-Cl	6-Cl	O	H	Ph	180-181	7
	19		4-Br	6-Cl	O	H	Ph	173-175	
	20		4-CF ₃	H	SO ₂	H	Me	265-266	8
	21		4-Cl	H	SO ₂	H	Me	192-194	
10	22		4-CF ₃	H	S	H	Ph	238-240	
	23		4-CF ₃	H	S	H	Me	188-189	
	24		4-Cl	H	S	H	Me	169-170	
	25		4-Br	H	S	H	Me	163-165	
	26		4-CF ₃	5-Cl	O	H	4-F-Ph	178-179	
15	27		4-CF ₃	5-Cl	O	Me	4-F-Ph	155-156	
	28		4-OCF ₃	5-Cl	O	H	4-F-Ph	110-112	
	29		4-Br	5-Cl	O	H	4-F-Ph	200-201	
	30		4-CF ₃	5-F	O	H	Ph	176-178	
	31		4-Br	5-F	O	H	Ph	162-163	
20	32		4-Cl	5-F	O	H	Ph	192-193	
	33		4-OCF ₃	5-F	O	H	Ph	79-81	
	34		4-OCF ₃	5-Cl	O	H	H	157-158	
	35		4-CF ₃	5-F	O	H	Me	171-172	
	36		4-Br	5-F	O	H	Me	143-145	
25	37		4-OCF ₃	5-F	O	H	Me	124-126	
	38		4-OCF ₃	5-F	O	H	H	138-139	
	39		4-Cl	5-F	O	H	H	170-172	
	40		4-CF ₃	5-F	O	Me	H	158-160	
	41		4-CF ₃	5-Cl	O	H	H	171-172	
30	42		4-Br	5-Cl	O	H	H	177-179	
	43		4-CF ₃	5-F	O	H	H	171-173	
	44		4-Br	5-F	O	H	H	182-183	9

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TABLE 18

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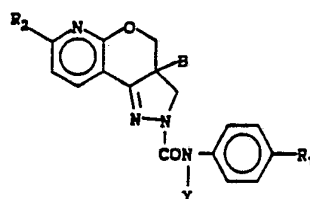
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<u>CMPD</u>	<u>R₁</u>	<u>R₂</u>	<u>B</u>	<u>Y</u>	<u>m.p. °C</u>
20					
45	CF ₃	H	H	H	219-221
46	CF ₃	Br	H	H	196-198

25

TABLE 19

30



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<u>CMPD</u>	<u>R₁</u>	<u>R₂</u>	<u>B</u>	<u>Y</u>	<u>m.p. °C</u>
47	CF ₃	H	CH ₃	H	215-217

EXAMPLE 6Fall Armyworm

5 Test units, each consisting of an 8-ounce
plastic cup containing a layer of wheat germ diet,
approximately 0.5 cm thick, were prepared. Ten
third-instar larvae of fall armyworm (Spodoptera
frugiperda) were placed into each cup. Solutions of
10 each of the test compounds (acetone/distilled water
75/25 solvent) were sprayed onto the cups, a single
solution per set of three cups. Spraying was
accomplished by passing the cups, on a conveyer belt,
directly beneath a flat fan hydraulic nozzle which
15 discharged the spray at a rate of 0.5 pounds of
active ingredient per acre (about 0.55 kg/ha) at 30
p.s.i. The cups were then covered and held at 27°C
and 50% relative humidity for 72 hours, after which
time readings were taken. The results are tabulated
20 below.

	<u>Compound</u>	<u>% Mortality</u>
	11	100
	12	100
	13	100
25	14	100
	15	100
	16	100
	26	100
	27	100
30	28	100
	29	100
	30	100
	31	100
	32	100
35	33	100

EXAMPLE 75 Tobacco Budworm

 The test procedure of Example 6 was repeated for efficacy against third-instar larvae of the tobacco budworm (Heliothis virescens) except that mortality was assessed at 48 hours. The results are tabulated
10 below.

	<u>Compound</u>	<u>% Mortality</u>
	11	100
	12	100
15	13	83
	14	100
	15	100
	16	100
	26	100
20	27	100
	28	100
	29	100
	30	100
	31	40
25	33	100

EXAMPLE 8Southern Corn Rootworm

 Test units, each consisting of an 8-ounce
30 plastic cup containing 1 sprouted corn seed, were prepared. Sets of three test units were sprayed as described in Example 6 with individual solutions of the test compounds. After the spray on the cups had dried, five third-instar larvae of the southern corn
35 rootworm (Diabrotica undecimpunctata howardi) were placed into each cup. A moistened dental wick was

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inserted into each cup to prevent drying and the cups were then covered. The cups were then held at 27°C and 50% relative humidity for 48 hours, after which time mortality readings were taken. Of the compounds tests on Southern rootworm, the following tabulation depicts the activity:

	<u>Compound</u>	<u>% Mortality</u>
10	11	100
	12	100
	13	100
	14	100
	15	100
15	16	100
	26	100
	27	100
	28	100
	29	100
20	30	100
	31	100
	32	100
	33	100

25

EXAMPLE 9Boll Weevil

Five adult boll weevils (Anthonomus grandis) were placed into each of a series of 9-ounce cups. The test procedure employed was then otherwise the same as in Example 6. Mortality readings were taken 48 hours after treatment. Of the compounds tested on boll weevil, the following tabulation depicts the activity:

35

5		
	<u>Compound</u>	<u>% Mortality</u>
	11	100
	12	100
	13	93
10	15	100
	16	93
	30	100
	31	100
	32	100

15

EXAMPLE 10Aster Leafhopper

Test units were prepared from a series of 12-ounce cups, each containing oat (Avena sativa) seedlings in a 1-inch layer of sterilized soil. The test units were sprayed as described in Example 6 with individual solutions of the below-listed compounds. After the oats had dried from the spraying, between 10 and 15 adult aster leafhoppers (Mascrosteles fascifrons) were aspirated into each of the covered cups. The cups were held at 27°C and 50% relative humidity for 48 hours, after which time mortality readings were taken. Of the compounds tested on aster leafhopper, the following tabulation depicts the activity:

35

182

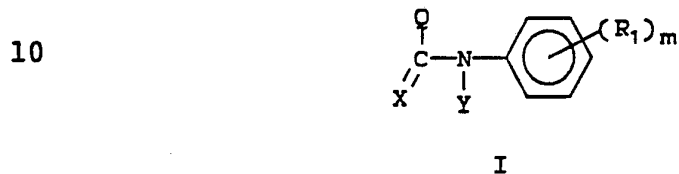
	<u>Compound</u>	<u>% Mortality</u>	
	11	88	
5	12	86	
	13	100	3
	16	100	
	26	87	4
	27	100	
10	28	95	
	29	88	
	30	100	
	33	82	
15			
20			
25			
30			
35			

183

CLAIMS

5 What is claimed is:

1. A compound of Formula I

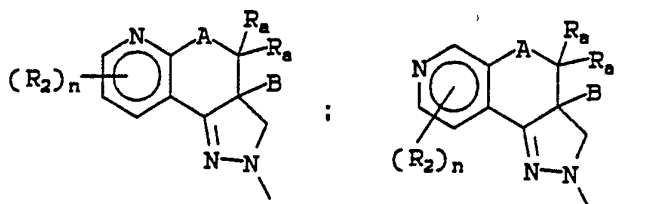


15

wherein:

Q is

20



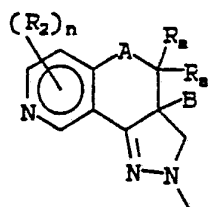
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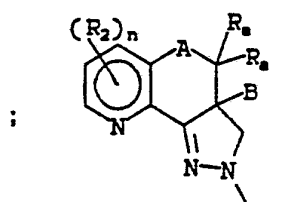
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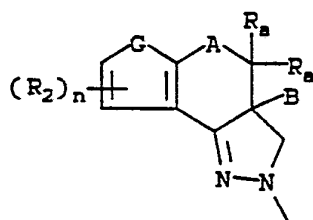


Q-3

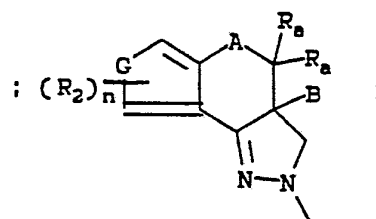


Q-4

15



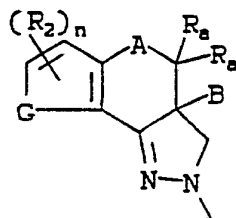
Q-5



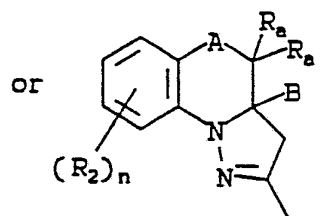
Q-6

25

30



Q-7



Q-8

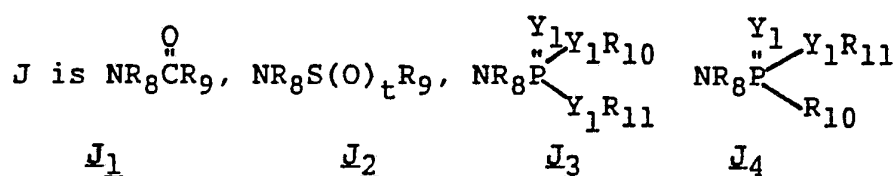
35

- 5 G is O or S;
A is a 0, 1 or 2-atom bridge comprising 0 to 2
carbon atoms, 0 to 1 oxygen atoms, 0 to 1
S(O)_q groups or 0 to 1 NR₆ groups wherein
each carbon atom is optionally substituted
10 with 1 to 2 substituents selected from R_a;
B is H, C₁ to C₆ alkyl, C₃ to C₆ cycloalkyl
optionally substituted with 1 to 2 halogens
or 1 to 2 CH₃, C₄ to C₆ cycloalkylalkyl, C₁
to C₆ haloalkyl, C₂ to C₆ alkenyl, C₂
15 to C₆ alkynyl, C₂ to C₆ alkoxyalkyl, C₂ to
C₆ cyanoalkyl, C₃ to C₈ alkoxycarbonylalkyl,
CO₂R₃, C(O)R₃, C(O)NR₃R₄, C(S)NR₃R₄, C(S)R₃,
C(S)SR₃, phenyl, phenyl substituted with
(R₅)_p, benzyl, benzyl substituted with 1 to 3
20 substituents independently selected from W,
or OR₇ when Q is Q₁ to Q₇;
W is halogen, CN, NO₂, C₁ to C₂ alkyl, C₁ to C₂
haloalkyl, C₁ to C₂ alkoxy, C₁ to C₂ halo-
alkoxy, C₁ to C₂ alkylthio, C₁ to C₂ halo-
25 alkylthio, C₁ to C₂ alkylsulfonyl or C₁ to C₂
haloalkylsulfonyl;
R₁, R₂ and R₅ are independently selected from
R₃, halogen, CN, N₃, SCN, NO₂, OR₃, SR₃,
SOR₃, SO₂R₃, OC(O)R₃, OSO₂R₃, CO₂R₃, C(O)R₃,
30 C(O)NR₃R₄, SO₂NR₃R₄, NR₃R₄, NR₄C(O)R₃,
OC(O)NHR₃, NR₄C(O)NHR₃ and NR₄SO₂R₃, or when
m, n or p is 2, R₁, R₂ or R₅ can be -OCH₂O-,
-OCH₂CH₂O-, or -CH₂CH₂O-, each of which can
be substituted with 1 to 4 halogen atoms or 1
35 to 2 methyl groups;

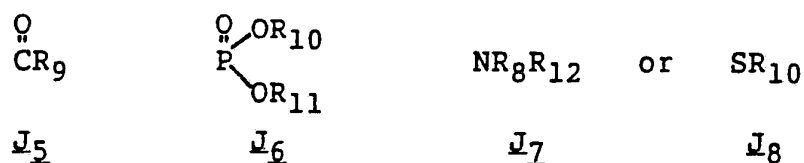
- 5 R_3 is H, C_1 to C_6 alkyl, C_1 to C_6 haloalkyl, C_2 to C_6 alkenyl, C_2 to C_6 haloalkenyl, C_2 to C_6 alkynyl, C_2 to C_6 haloalkynyl, C_2 to C_6 alkoxyalkyl, C_2 to C_6 alkylthioalkyl, C_1 to C_6 nitroalkyl, C_2 to C_6 cyanoalkyl, C_3 to C_8 alkoxycarbonylalkyl, C_3 to C_6 cycloalkyl, C_3 to C_6 halocycloalkyl, phenyl, benzyl, or phenyl or benzyl substituted with 1 to 3 substituents independently selected from W;
- 10 R_4 is H, C_1 to C_4 alkyl or R_3 and R_4 can be taken together as $(CH_2)_4$, $(CH_2)_5$ or $(CH_2CH_2OCH_2CH_2)$;
- 15 R_6 is H, C_1 to C_4 alkyl, C_1 to C_4 haloalkyl, C_2 to C_4 alkenyl, C_2 to C_4 haloalkenyl, C_2 to C_4 alkynyl, phenyl optionally substituted with W, or benzyl optionally substituted with W;
- 20 R_7 is H, C_1 to C_4 alkyl, C_2 to C_4 alkenyl, C_2 to C_4 alkynyl, C_2 to C_4 alkylcarbonyl, C_2 to C_4 alkoxycarbonyl;
- 25 R_a is independently selected from H, C_1 to C_6 alkyl, C_2 to C_4 alkoxycarbonyl and phenyl optionally substituted with 1 to 3 substituents independently selected from W;
- 30 X is O or S;
n is 1 to 2;
m is 1 to 3;
p is 1 to 3;
q is 0 to 2;
- 35

Y is H, C₁ to C₆ alkyl, C₂ to C₆ alkoxyalkyl,
 CHO, C₂ to C₆ alkylcarbonyl, C₂ to C₆
 5 alkoxycarbonyl, C₂ to C₆ haloalkylcarbonyl,
 C₁ to C₆ alkylthio, C₁ to C₆ haloalkylthio,
 phenylthio, phenylthio substituted with 1 to
 3 substituents independently selected from W,
 or S-J;

10



15



20

R₈ and R₁₂ are independently selected from C₁
 to C₆ alkyl, C₁ to C₆ haloalkyl, C₃ to C₆
 cycloalkyl, C₄ to C₇ cycloalkylalkyl, phenyl
 optionally substituted with 1 to 2 substi-
 tuents independently selected from W, benzyl
 optionally substituted with 1 to 2
 25 substituents independently selected from W,
 phenethyl optionally substituted with 1 to 2
 substituents independently selected from W,
 C₂ to C₆ cyanoalkyl, C₂ to C₆ alkoxyalkyl, C₃
 to C₈ alkoxycarbonylalkyl and C₄ to C₈ di-
 30 alkylaminocarbonylalkyl, or R₈ and R₁₂ can be
 taken together as (CH₂)₄, (CH₂)₅ or
 (CH₂)₂O(CH₂)₂;

35

R₉ is F, C₁ to C₂₂ alkyl, C₁ to C₆ haloalkyl,
 C₁ to C₂₂ alkoxy, C₂ to C₈ dialkylamino,
 piperidinyl, pyrrolidinyl, morpholino, C₁ to
 C₄ haloalkoxy, C₁ to C₄ alkoxy substituted

with cyano, nitro, C₂ to C₄ alkoxy, C₄ to C₈
alkoxyalkoxy, C₁ to C₂ alkylthio, C₂ to C₃
5 alkoxy carbonyl, C₃ to C₅ dialkylaminocarbonyl
or phenyl, or R₉ is phenyl optionally substituted
with 1 to 2 substituents independently
selected from W, or phenoxy optionally
substituted with 1 to 2 substituents
10 independently selected from W;
R₁₀ and R₁₁ are independently selected from C₁
to C₄ alkyl, C₂ to C₄ haloalkyl and phenyl
optionally substituted with 1 to 2 substituents
independently selected from W, or R₁₀
15 and R₁₁ can be taken together as (CH₂)₂,
(CH₂)₃ or CH₂C(CH₃)₂CH₂;
t is 0 to 2; and
Y₁ is O or S.

2. A compound according to Claim 1 wherein:
A is CR_aR_a, S, O or NR₆;
B is H, C₁ to C₆ alkyl, C₁ to C₆ haloalkyl,
C₂ to C₆ alkenyl, C₂ to C₆ alkynyl, C₂ to
C₆ alkoxyalkyl, C₃ to C₈ alkoxy carbonylalkyl,
25 CO₂R₃, C(O)R₃, C(O)NR₃R₄, C(S)NR₃R₄, C(S)R₃,
C(S)SR₃, phenyl or phenyl substituted by
(R₅)_p;
W is Cl, F, Br, CN, CF₃, C₁ to C₂ alkyl, C₁
to C₂ alkoxy, OCF₂H, OCF₃ or NO₂;
30 R₂ is R₃, halogen, CN, SCN, NO₂, OR₃ or SR₃;
R₃ is H, C₁ to C₄ alkyl, C₁ to C₂ haloalkyl,
C₃ to C₄ alkenyl, C₃ to C₄ haloalkenyl,
propargyl, phenyl, benzyl, or phenyl or
benzyl substituted with one of F, Cl, Br,
35 CF₃, OCF₃, OCF₂H or NO₂;
p is 1 or 2;

- m is 1 or 2;
X is O;
5 Y is H, C₁ to C₄ alkyl, SCH₃, SCCL₃, SO₂CH₃,
SC₆H₅, 2-NO₂-C₆H₄S, C(O)CH₃, C(O)CH₂CH₃,
C(O)CF₃; CO₂CH₃, CO₂CH₂CH₃, or S-J;
J is J₁, J₂, J₃, J₄ or J₅;
R₈ and R₁₂ are independently selected from C₁
10 to C₆ alkyl, C₁ to C₆ haloalkyl, C₅ to C₆
cycloalkyl, C₃ to C₈ alkoxycarbonylalkyl,
phenyl, benzyl and phenethyl, each phenyl,
benzyl and phenethyl optionally substituted
with W, or, R₈ and R₁₂ can be taken together
15 as (CH₂)₄, (CH₂)₅ or (CH₂)₂O(CH₂)₂;
R₁₀ and R₁₁ are independently selected from C₁
to C₃ alkyl or phenyl; and
t is 2.
- 20 3. A compound according to Claim 2 wherein:
B is H, C₁ to C₄ alkyl, C₃ to C₄ alkoxycarbonyl-
alkyl, CO₂R₃, C(O)R₃, phenyl or phenyl
substituted with (R₅)_p;
R₁ is halogen, CN, SCN, NO₂, OR₃, SR₃, SO₂R₃,
25 CO₂R₃, C(O)R₃ or is R₃ with one substituent
in the 4-position;
R₅ is H, R₃, halogen, CN, SCN, NO₂, OR₃, SR₃,
SO₂R₃, C(O)R₃, OSO₂R₃, CO₂R₃, C(O)R₃,
C(O)NR₃R₄, SO₂NR₃R₄ or NR₃R₄; or, when m or p
30 is 2;
R₁ and R₅ can be taken together as -CH₂C(CH₃)₂O-,
OCH₂CH₂O-, OCF₂CF₂O- or -CF₂CF₂O- to form
a 5- or 6-membered fused ring;
R₃ is C₁ to C₄ alkyl, C₁ to C₂ haloalkyl, C₃
35 to C₄ alkenyl or propargyl;
R₄ is H or CH₃;
R_a is H, CH₃, CO₂CH₃ or CO₂CH₂CH₃;

m and p are independently 1 or 2 and one substituent is in the para-position;

5 Y is H, CH₃, COCH₃, CO₂CH₃ or S-J;

J is J₁ or J₂;

R₈ is C₁ to C₄ alkyl or phenyl optionally substituted with Cl or CH₃;

10 R₉ is C₁ to C₂₀ alkyl, C₁ to C₂₀ alkoxy, C₁ to C₆ haloalkyl, dimethylamino, phenyl optionally substituted with Cl or CH₃, or, R₉ is C₁ to C₄ alkoxy substituted with C₂ to C₄ alkoxy or 1 to 6 halogens; and

G is S.

15

4. A compound according to Claim 3 wherein:

R₁ is Cl, F, Br, CF₃, CN, OCF₃, OCF₂H, OCF₂CF₂H or SCF₂H;

20 R₂ and R₅ are independently H, Cl, F, Br, CN, CF₃, CH₃, OCH(CH₃)₂, OCF₂H, OCF₃, SCH₃, SCF₂H, NO₂ or OCH₂CF₃;

B is H, CH₃, CH₂CH₃, CH(CH₃)₂, CO₂CH₃, CO₂CH₂CH₃, phenyl or phenyl substituted with (R₅)_p; and

R_a is H or CH₃.

25

5. A compound according to Claim 4 wherein:

A is O or CH₂.

6. A compound according to Claim 5 wherein:

30 Q is Q-1.

7. A compound according to Claim 5 wherein:

Q is Q-2.

35

8. A compound according to Claim 5 wherein:
Q is Q-3.

5

9. A compound according to Claim 5 wherein:
Q is Q-4.

10. A compound according to Claim 5 wherein:
Q is Q-5.

10

11. A compound according to Claim 5 wherein:
Q is Q-6.

12. A compound according to Claim 5 wherein:
Q is Q-7.

15

13. A compound according to Claim 5 wherein:
Q is Q-8.

20

14. A compound according to Claim 6 which is:
methyl 3,3a,4,5-tetrahydro-2-[[[4-trifluoro-
methyl)phenyl]-amino]carbonyl]-2H-pyrazolo[3,-
4-f]-quinoline-3a-carboxylate.

25

15. A compound according to Claim 9 which is:
methyl 3,3a,4,5-tetrahydro-2-[[[4-trifluoro-
methyl)phenyl]-amino]carbonyl]-2H-pyrazolo[4,-
3-h]-quinoline-3a-carboxylate.

30

16. A compound according to Claim 10 which is:
methyl 7-chloro-3,3a,4,5-tetrahydro-N-[[[4-
trifluoromethyl)phenyl]amino]carbonyl]-2H-
thieno [2,3-g]-indazole-3a-carboxylate.

35

- 5 17. A compound according to Claim 13 which is:
methyl 7-fluoro-3A,4-dihydro-2-[[[4-(tri-
fluoromethyl)-phenyl]amino]carbonyl]-3H-
pyrazolo[5,1-c]-[1,4]benzoxazine-3a-carboxyl-
ate.
- 10 18. A compound according to Claim 13 which is:
7-chloro-3A-(4-fluorophenyl)-3A,4-dihydro-N-
[4-(trifluoromethyl)phenyl]-3H-pyrazolo[5,1-
c][1,4]-benzoxazine-2-carboxamide.
- 15 19. An arthropodicidal composition comprising
an arthropodically effective amount of a compound
according to any one of Claims 1 to 18 and a carrier
therefor.
- 20 20. A method for controlling arthropods
comprising applying to them or their environment an
arthropodically effective amount of a compound
according to any one of Claims 1 to 18.

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INTERNATIONAL SEARCH REPORT

International Application No PCT/US 89/04013

I. CLASSIFICATION OF SUBJECT MATTER (if several classification symbols apply, indicate all) *		
According to International Patent Classification (IPC) or to both National Classification and IPC 5 C 07 D 471/04, 491/14, 495/14, 495/04, 491/04, IPC :487/04, 498/04, 513/04, A 01 N 47/38, 43/90,		
II. FIELDS SEARCHED		
Minimum Documentation Searched ⁷		
Classification System	Classification Symbols	
IPC ⁵	A 01 N 47/00, C 07 D 231/00, 471/00, 487/00, 491/00, 495/00, 498/00, 513/00	
Documentation Searched other than Minimum Documentation to the Extent that such Documents are Included in the Fields Searched *		
III. DOCUMENTS CONSIDERED TO BE RELEVANT*		
Category *	Citation of Document, ¹¹ with indication, where appropriate, of the relevant passages ¹²	Relevant to Claim No. ¹³
A,P	EP, A, 0286346 (E.I. DU PONT DE NEMOURS & CO.) 12 October 1988, see claims 1,2,12,13 --	1,5,19,20
A	WO, A, 88/06583 (E.I. DU PONT DE NEMOURS & CO.) 7 September 1988, see claims 1,11,16 --	1,19,20
A	EP, A, 0113213 (FBC LTD) 11 July 1984, see claims 1,11,12 --	1,19,20
A	GB, A, 2166137 (FMC CORP.) 30 April 1986, see claims 1,27,28 --	1,19,20
A	GB, A, 1591280 (BAYER AG) 17 June 1981, see claims 1,12,14 --	1,19,20
A	US, A, 4663341 (R.M. JACOBSON) 5 May 1987, see claims 1,20,35 (cited in the application)	1,19,20
A	& EP, A, 0153127 (cited in the application) --	
A	US, A, 4070365 (J.J. VAN DAALEN et al.) 24 January 1978, see claim 1; abstract	1,19
* Special categories of cited documents: ¹⁰ "A" document defining the general state of the art which is not considered to be of particular relevance "E" earlier document 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 "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		
IV. CERTIFICATION		
Date of the Actual Completion of the International Search	Date of Mailing of this International Search Report	
5th December 1989	06.02.90	
International Searching Authority	Signature of Authorized Officer	
EUROPEAN PATENT OFFICE	C.D. v.d. Vliet	

INTERNATIONAL SEARCH REPORT

International Application No PCT/US 89/04013 -2-

I. CLASSIFICATION OF SUBJECT MATTER (if several classification symbols apply, indicate all) *		
According to International Patent Classification (IPC) or to both National Classification and IPC ⁴ // (C 07 D 471/04, 231:00, 221:00) (C 07 D 491/14, 311:00, 231:00) IPC : 221:00) (C 07 D 495/14, 335:00, 231:00, 221:00) (C 07 D 495/04,		
II. FIELDS SEARCHED		
Minimum Documentation Searched ⁷		
Classification System	Classification Symbols	
IPC ⁴		
Documentation Searched other than Minimum Documentation to the Extent that such Documents are Included in the Fields Searched *		
III. DOCUMENTS CONSIDERED TO BE RELEVANT *		
Category *	Citation of Document, ¹¹ with indication, where appropriate, of the relevant passages ¹²	Relevant to Claim No. ¹³
	(cited in the application) --	
A	US, A, 3991073 (R. MULDER et al.) 9 November 1976, see claim 1; abstract (cited in the application) --	1,19
A	Patent Abstracts of Japan, vol. 9, no. 125 (C-283)(1848), 30 May 1985; & JP, A, 6011472 (SHOWA DENKO K.K.) 21 January 1985 --	1,19
A	Journal of Organic Chemistry, vol. 42, no. 8, 1977 L. Garanti et al.: "Intramolecular 1,3- dipolar cycloadditions of nitrile imines bearing an alkenyl substituent", pages 1389-1392, see page 1389, chart II, compound no. 11a (cited in the application) --	1
* Special categories of cited documents: ¹⁰ "A" document defining the general state of the art which is not considered to be of particular relevance "E" earlier document 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 "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		
IV. CERTIFICATION		
Date of the Actual Completion of the International Search		Date of Mailing of this International Search Report
International Searching Authority EUROPEAN PATENT OFFICE		Signature of Authorized Officer

INTERNATIONAL SEARCH REPORT

International Application No PCT/US 89/04013

-3-

I. CLASSIFICATION OF SUBJECT MATTER (if several classification symbols apply, indicate all) *		
According to International Patent Classification (IPC) or to both National Classification and IPC 333:00,231:00)(C 07 D 495/14,333:00,311:00,231:00)(C 07 D IPC ⁵ :491/04, 307:00,231:00)(C 07 D 487/04,241:00,231:00)		
II. FIELDS SEARCHED		
Minimum Documentation Searched ⁷		
Classification System ¹	Classification Symbols	
IPC ⁵		
Documentation Searched other than Minimum Documentation to the Extent that such Documents are Included in the Fields Searched *		
III. DOCUMENTS CONSIDERED TO BE RELEVANT *		
Category *	Citation of Document, ¹¹ with indication, where appropriate, of the relevant passages ¹²	Relevant to Claim No. ¹³
A	Journal of the Chemical Society, Perkin Transactions I, 1981 (London, GB) L. Bruché et al.: "Intramolecular cyclisations of nitrile imines bearing a thioether function" pages 2245-2249, see page 2245, compounds no. 6a and 6b (cited in the application)	1
A	Journal of Organic Chemistry, vol. 43, no. 9, 1978, A. Padwa et al.: "Intramolecular 1,3-dipolar cycloaddition reactions of alkenyl-substituted nitrile imines", pages 1664-1670, see page 1666, compound no. 22 (cited in the application)	1

* Special categories of cited documents: ¹⁰ "A" document defining the general state of the art which is not considered to be of particular relevance "E" earlier document 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 "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. "A" document member of the same patent family		
IV. CERTIFICATION		
Date of the Actual Completion of the International Search	Date of Mailing of this International Search Report	
International Searching Authority	Signature of Authorized Officer	
EUROPEAN PATENT OFFICE		

INTERNATIONAL SEARCH REPORT

International Application No. PCT/US 89/04013 -4-

I. CLASSIFICATION OF SUBJECT MATTER (if several classification symbols apply, indicate all) * According to International Patent Classification (IPC) or to both National Classification and IPC IPC ⁵ : (C 07 D 498/04, 265:00, 231:00) (C07 D 513/04, 279:00, 213:00)		
II. FIELDS SEARCHED		
Minimum Documentation Searched ⁷		
Classification System	Classification Symbols	
IPC ⁵		
Documentation Searched other than Minimum Documentation to the Extent that such Documents are Included in the Fields Searched *		
III. DOCUMENTS CONSIDERED TO BE RELEVANT *		
Category *	Citation of Document, ¹¹ with Indication, where appropriate, of the relevant passages ¹²	Relevant to Claim No. ¹³
* Special categories of cited documents: ¹⁰ "A" document defining the general state of the art which is not considered to be of particular relevance "E" earlier document 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 "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. "A" document member of the same patent family		
IV. CERTIFICATION		
Date of the Actual Completion of the International Search	Date of Mailing of this International Search Report	
International Searching Authority EUROPEAN PATENT OFFICE	Signature of Authorized Officer	

**ANNEX TO THE INTERNATIONAL SEARCH REPORT
ON INTERNATIONAL PATENT APPLICATION NO.**

US 8904013

SA 31170

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