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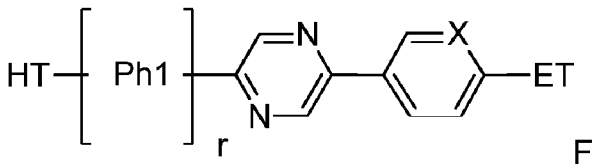
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(54) Title: ORGANIC LIGHT EMITTING POLYAROMATIC AND POLYHETEROAROMATIC HOST MATERIALS



Formula 1

(57) Abstract: Heteroaryl-aryl compounds such as compounds represented by Formula may be used in electronic devices such as organic light- emitting devices. For example, the compounds may be used as an emissive material in an emissive layer.

ORGANIC LIGHT EMITTING POLYAROMATIC AND POLYHETEROAROMATIC HOST MATERIALS

BACKGROUND

1. Field

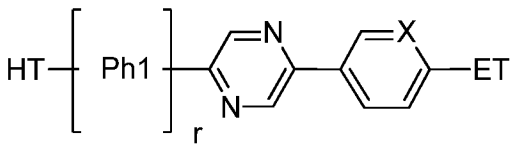
[001] The embodiments relate to emissive compounds for light-emitting layers in devices.

2. Description of the Related Art

[002] Organic light-emitting devices (OLED) are becoming increasingly important in lighting and display applications. OLEDs may include an emissive or light-emitting layer that includes a host material and an emissive component dispersed within the host material. Emissive materials of OLED devices may have problems with low stability. This potential deficiency with emissive materials may contribute to low efficiency and short lifetime of the devices comprising the emissive materials.

SUMMARY

[003] Some embodiments include an emissive compound of formula:



Formula 1

wherein, HT is optionally substituted diphenylamine or optionally substituted phenyl(naphthyl)amine, wherein Ph1 is a *p*-phenylene, wherein ET is optionally substituted benzimidazol-2-yl, optionally substituted benzoxazol-2-yl, or optionally substituted benzthiazol-2-yl, wherein X is CH or N, and wherein r is 1, 2, 3.

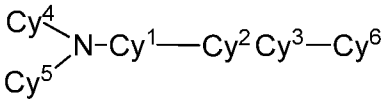
[004] With respect to Formula 1, in some embodiments, HT is unsubstituted diphenylamine, a mono-substituted diphenylamine, a di-substituted diphenylamine, an unsubstituted phenyl(naphthyl)amine, a mono-substituted phenyl(naphthyl)amine, and/or an unsubstituted carbazolyl. In some embodiments, ET is an unsubstituted benzoimidazol-2-yl.

[005] Some embodiments include a compound represented by Formula 1a:

$$HT—[Ph^1]_r—Py—Het—ET \qquad \text{Formula 1a}$$

wherein HT is optionally substituted diphenylamine or optionally substituted phenyl(naphthyl)amine; each Ph^1 is independently optionally substituted *p*-phenylene, wherein the *p*-phenylene directly bonded to HT may optionally form a bond to a phenyl of HT to form a three ring system; Py is optionally substituted pyrazin-2,5-ylene; Het is optionally substituted *p*-phenylene or optionally substituted pyridin-2,5-ylene; ET is optionally substituted benzimidazol-2-yl, optionally substituted benzoxazol-2-yl, or optionally substituted benzothiazol-2-yl; and r is 1, 2, or 3.

[006] Some embodiments include a compound represented by Formula 2:

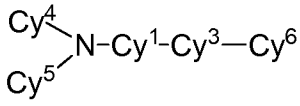


Formula 2

wherein Cy^1 is a *p*-phenylene optionally substituted with 1 or 2 substituents independently selected from C_{1-6} alkyl and F; Cy^2 is independently a 2,5-pyridyl optionally substituted with 1, 2, or 3 substituents independently selected from C_{1-6} alkyl and F, or a pyrazine optionally substituted with 1, 2, or 3 substituents independently selected from C_{1-6} alkyl and F; Cy^3 is pyridin-2,5-ylene optionally substituted with 1, 2, or 3 substituents independently selected from C_{1-6} alkyl and F, or a *p*-phenylene optionally substituted with 1 or 2 substituents independently selected from C_{1-6} alkyl and F; Cy^4 and Cy^5 are independently optionally substituted phenyl or optionally substituted naphthyl, wherein Cy^1 and Cy^5 may be joined to form, with the nitrogen atom to which they are attached, a carbazolyl ring system; and Cy^6 is 1-phenyl-1H-benzo[d]imidazol-2-yl optionally substituted with 1, 2, 3, 4, or 5 substituents independently selected from C_{1-6} alkyl and F.

[007] With respect to Formula 2, in some embodiments Cy^1, and Cy^2 are independently *p*-phenylene optionally substituted with 1 or 2 substituents independently selected from C_{1-6} alkyl and F; Cy^4 is phenyl optionally substituted with 1, 2, or 3 substituents independently selected from C_{1-6} alkyl and F; Cy^5 is phenyl optionally substituted with 1, 2, or 3 substituents independently selected from C_{1-6} alkyl and F, or a naphth-1-yl or naphth-2-yl optionally substituted with 1, 2, or 3 substituents independently selected from C_{1-6} alkyl and F; and Cy^6 is 1-phenyl-1H-benzo[d]imidazol-2-yl optionally substituted with 1, 2, 3, 4, or 5 substituents independently selected from C_{1-6} alkyl and F.

[008] Some embodiments include a compound represented by Formula 3:



Formula 3

wherein Cy^1 is an optionally substituted *p*-phenylene; Cy^3 is selected from an optionally substituted 2,5-pyrazine-3'-pyridine, and optionally substituted 2,5-pyrazine-2',5'-phenyl, an optionally substituted 2,5-bi-pyridinyl, an optionally substituted 3,3'-bi-pyridinyl, and an optionally substituted 3,2':5',3''-terpyridinyl; Cy^4 and Cy^5 are optionally substituted phenyl or optionally substituted naphthyl; and Cy^6 is optionally substituted 1-phenyl-1H-benzo[d]imidazol-2-yl.

[009] With respect to Formula 3, in some embodiments Cy^1 is an optionally substituted interphenylene, independently optionally substituted with H, F, methyl, ethyl, propyl, or isopropyl; wherein Cy^3 is independently optionally substituted with H, F, methyl, ethyl, propyl, or isopropyl; wherein wherein Cy^4 is independently optionally substituted with H, F, methyl, ethyl, propyl, or isopropyl; wherein Cy^5 is independently optionally substituted with H, F, methyl, ethyl, propyl, or isopropyl; wherein Cy^6 is independently optionally substituted with H, F, methyl, ethyl, propyl, or isopropyl.

[010] Some embodiments include optionally substituted [(para-phenylenyl-para-azolyl)]compounds, including optionally substituted N,N-diphenyl-4-(6-(1-phenyl-1H-benzo[d]imidazol-2-yl)pyridin-3-yl)aniline; N-phenyl-N-(4'-(6-(1-phenyl-1H-benzo[d]imidazol-2-yl)pyridin-3-yl)-[1,1'-biphenyl]-4-yl)naphthalen-1-amine; 4'-(6'-(1-phenyl-1H-benzo[d]imidazol-2-yl)-[3,3'-bipyridin]-6-yl)-N,N-di-*p*-tolyl-[1,1'-biphenyl]-4-amine; 9,9-dimethyl-N,N-diphenyl-7-(6'-(1-phenyl-1H-benzo[d]imidazol-2-yl)-[3,3'-bipyridin]-6-yl)-9H-fluoren-2-amine; N,N-diphenyl-4'-(6'-(1-phenyl-1H-benzo[d]imidazol-2-yl)-[3,3'-bipyridin]-6-yl)-[1,1'-biphenyl]-4-amine; 4-methyl-N-(4-(6'-(1-phenyl-1H-benzo[d]imidazol-2-yl)-[3,3'-bipyridin]-6-yl)phenyl)-N-(*p*-tolyl)aniline; N-phenyl-N-(4-(6'-(1-phenyl-1H-benzo[d]imidazol-2-yl)-[3,3'-bipyridin]-6-yl)phenyl)naphthalen-1-amine; 9,9-dimethyl-7-(6'-(1-phenyl-1H-benzo[d]imidazol-2-yl)-[3,3'-bipyridin]-6-yl)-N,N-di-*p*-tolyl-9H-fluoren-2-amine; N,N-diphenyl-4'-(6'-(1-phenyl-1H-benzo[d]imidazol-2-yl)-[2,3'-bipyridin]-5-yl)-[1,1'-biphenyl]-4-amine; 4'-(3-methyl-6'-(1-phenyl-1H-benzo[d]imidazol-2-yl)-[2,3'-bipyridin]-5-yl)-N,N-diphenyl-[1,1'-biphenyl]-4-amine, N-phenyl-N-(4'-(6'-(1-phenyl-1H-benzo[d]imidazol-2-yl)-[2,3'-

bipyridin]-5-yl)-[1,1'-biphenyl]-4-yl)naphthalen-2-amine; N-phenyl-N-(4'-(6'-(1-phenyl-1H-benzo[d]imidazol-2-yl)-[2,3'-bipyridin]-5-yl)-[1,1'-biphenyl]-4-yl)naphthalen-1-amine; 4-methyl-N-(4-(6'-(1-phenyl-1H-benzo[d]imidazol-2-yl)-[2,3'-bipyridin]-5-yl)phenyl)-N-(*p*-tolyl)aniline; N,N-diphenyl-4-(6-(1-phenyl-1H-benzo[d]imidazol-2-yl)-[3,2':5',3''-terpyridin]-6''-yl)aniline, etc.

[011] Some embodiments include a light-emitting device comprising a compound described herein.

[012] These and other embodiments are described in more detail herein. These and other embodiments are described in more detail herein.

BRIEF DESCRIPTION OF THE DRAWINGS

[013] FIG. 1 is a schematic drawing of an embodiment of an OLED device comprising a compound disclosed herein.

[014] FIG. 2 is a schematic drawing of an embodiment of an OLED device described in Example 2.

DETAILED DESCRIPTION

[015] Unless otherwise indicated, when a compound or chemical structural feature such as aryl is referred to as being "optionally substituted," it is meant that the feature may have no substituents (i.e. be unsubstituted) or may have one or more substituents. A feature that is "substituted" has one or more substituents. The term "substituent" has the ordinary meaning known to one of ordinary skill in the art. In some embodiments, the substituent may be an ordinary organic moiety known in the art, which may have a molecular weight (e.g. the sum of the atomic masses of the atoms of the substituent) of 15 g/mol to 50 g/mol, 15 g/mol to 100 g/mol, 15 g/mol to 200 g/mol, 15 g/mol to 300 g/mol, or 15 g/mol to 500 g/mol. In some embodiments, the substituent comprises: 0-30, 0-20, 0-10, or 0-5 carbon atoms; and 0-30, 0-20, 0-10, or 0-5 heteroatoms independently selected from: N, O, S, Si, F, Cl, Br, or I; provided that the substituent comprises at least one atom selected from: C, N, O, S, Si, F, Cl, Br, or I. Examples of substituents include, but are not limited to, alkyl, alkenyl, alkynyl, heteroalkyl, heteroalkenyl, heteroalkynyl, aryl, heteroaryl, hydroxy, alkoxy, aryloxy, acyl, acyloxy, alkylcarboxylate, thiol, alkylthio, cyano, halo, thiocarbonyl, O-carbamyl, N-carbamyl, O-thiocarbamyl, N-thiocarbamyl, C-amido, N-amido, S-sulfonamido, N-sulfonamido, isocyanato, thiocyanato, isothiocyanato,

nitro, silyl, sulfenyl, sulfinyl, sulfonyl, haloalkyl, haloalkoxyl, trihalomethanesulfonyl, trihalomethanesulfonamido, amino, etc. In some embodiments, two substituents may combine to form a ring.

[016] As used herein the term "alkyl" has the broadest meaning generally understood in the art, and may include a moiety composed of carbon and hydrogen containing no double or triple bonds. Alkyl may be linear alkyl, branched alkyl, cycloalkyl, or a combination thereof, and in some embodiments, may contain from one to thirty-five carbon atoms. In some embodiments, alkyl may include C_{1-10} linear alkyl, such as methyl ($-CH_3$), ethyl ($-CH_2CH_3$), n-propyl ($-CH_2CH_2CH_3$), n-butyl ($-CH_2CH_2CH_2CH_3$), n-pentyl ($-CH_2CH_2CH_2CH_2CH_3$), n-hexyl ($-CH_2CH_2CH_2CH_2CH_2CH_3$), etc.; C_{3-10} branched alkyl, such as C_3H_7 (e.g. iso-propyl), C_4H_9 (e.g. branched butyl isomers), C_5H_{11} (e.g. branched pentyl isomers), C_6H_{13} (e.g. branched hexyl isomers), C_7H_{15} (e.g. heptyl isomers), etc.; C_{3-10} cycloalkyl, such as C_3H_5 (e.g. cyclopropyl), C_4H_7 (e.g. cyclobutyl isomers such as cyclobutyl, methylcyclopropyl, etc.), C_5H_9 (e.g. cyclopentyl isomers such as cyclopentyl, methylcyclobutyl, dimethylcyclopropyl, etc.) C_6H_{11} (e.g. cyclohexyl isomers), C_7H_{13} (e.g. cycloheptyl isomers), etc.; and the like.

[017] As used herein, the term "alkoxy" includes –O-alkyl, such as $-OCH_3$, $-OC_2H_5$, $-OC_3H_7$ (e.g. propoxy isomers such as isopropoxy, n-propoxy, etc.), $-OC_4H_9$ (e.g. butyoxy isomers), $-OC_5H_{11}$ (e.g. pentoxy isomers), $-OC_6H_{13}$ (e.g. hexoxy isomers), $-OC_7H_{15}$ (e.g. heptoxy isomers), etc.

[018] With respect to an optionally substituted moiety such as optionally substituted alkyl, a phrase such as "optionally substituted C_{1-12} alkyl" refers to a C_{1-12} alkyl that may be unsubstituted, or may have 1 or more substituents, and does not limit the number of carbon atoms in any substituent. A phrase such as "C_{1-12} optionally substituted alkyl" refers to unsubstituted C_{1-12} alkyl, or substituted alkyl wherein both the alkyl parent and all substituents have from 1-12 carbon atoms. Similar conventions may be applied to other optionally substituted moieties such as aryl and heteroaryl.

[019] Substituents on alkyl may be the same as those described generally above, except that alkyl may not have an alkyl substituent. In some embodiments, substituents on alkyl are independently selected from F, Cl, Br, I, CN, CO_2H, -O-

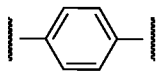
alkyl, ester groups, acyl, amine groups, and amide groups, and may have a molecular weight of about 15 to about 100 or about 500.

[020] For convenience, the term "molecular weight" is used with respect to a moiety or part of a molecule to indicate the sum of the atomic masses of the atoms in the moiety or part of a molecule, even though it may not be a complete molecule.

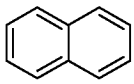
[021] The structures associated with some of the chemical names referred to herein are depicted below. These structures may be unsubstituted, as shown below, or a substituent may independently be in any position normally occupied by a hydrogen atom when the structure is unsubstituted. Unless a point of attachment is indicated by —, attachment may occur at any position normally occupied by a hydrogen atom.



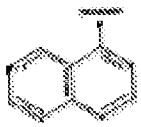
phenyl



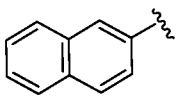
p-phenylene



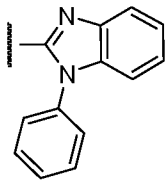
naphthyl



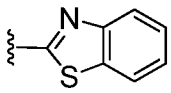
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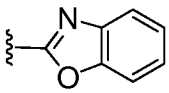
naphth-2-yl



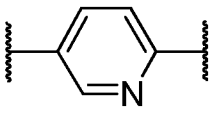
1-phenyl-1H-benzo[d]imidazol-2-yl



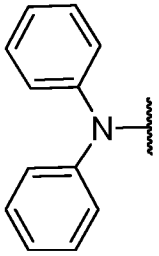
Benzothiazol-2-yl



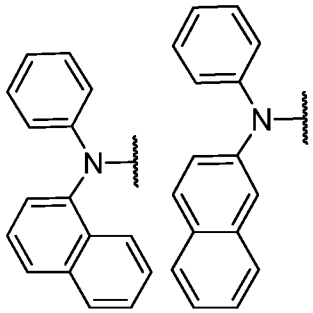
Benzoxazol-2-yl



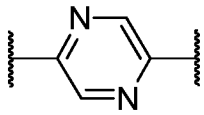
Pyridin-2,5-ylene



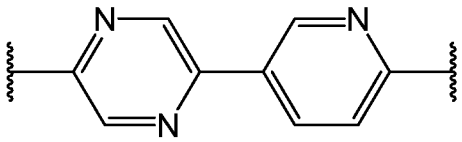
diphenylamine



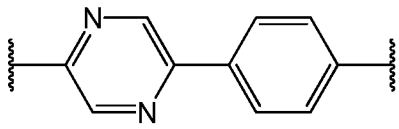
Phenyl(naphthyl)amine



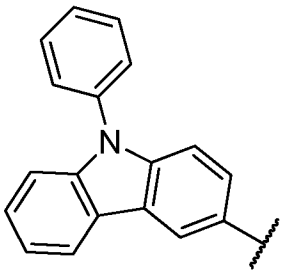
pyrazin-2,5-ylene



2,5-pyrazine-3'-pyridine

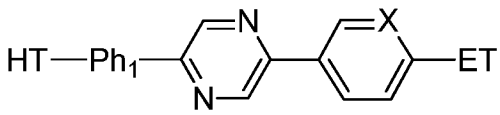


2,5-pyrazine-2',5'-phenyl

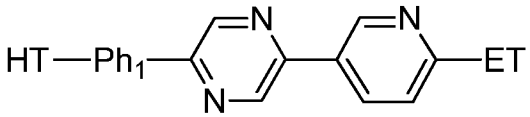


9-phenylcarbazol-3-yl

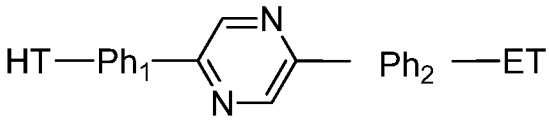
[022] In some embodiments, a compound is provided represented by the following formulae:



Formula 4



Formula 5



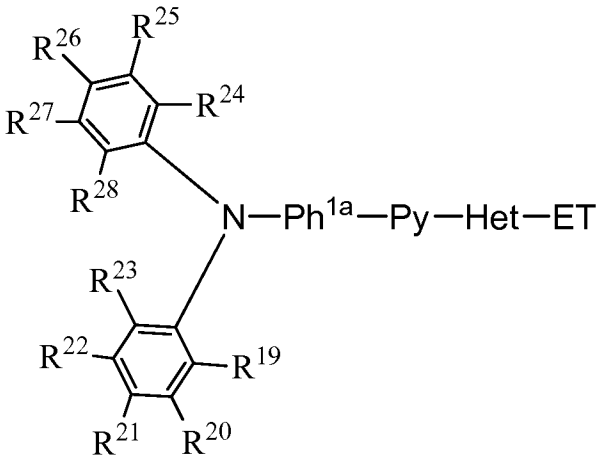
Formula 6

HT—Ph^{1a}—Ph^{1b}—Ph^{1c}—Py—Het—ET

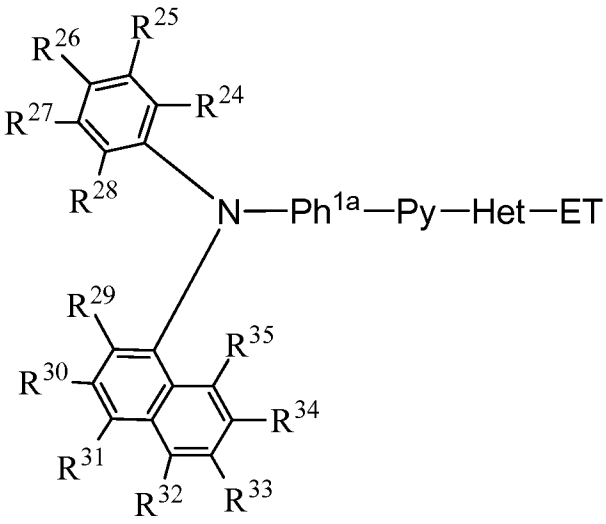
Formula 7

HT—Ph^{1a}—Py—Het—ET

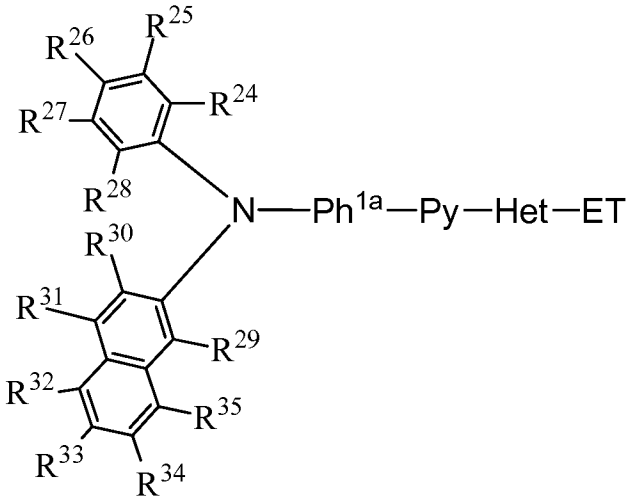
Formula 8



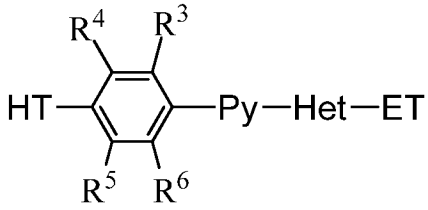
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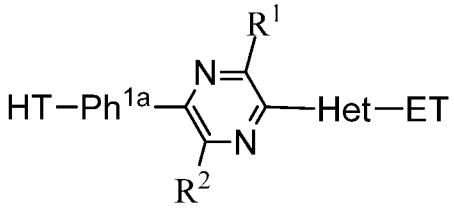
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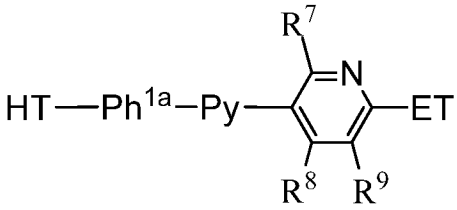
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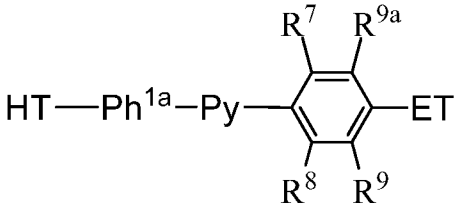
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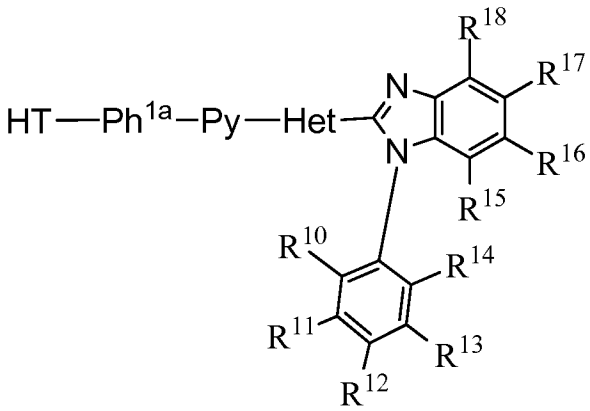
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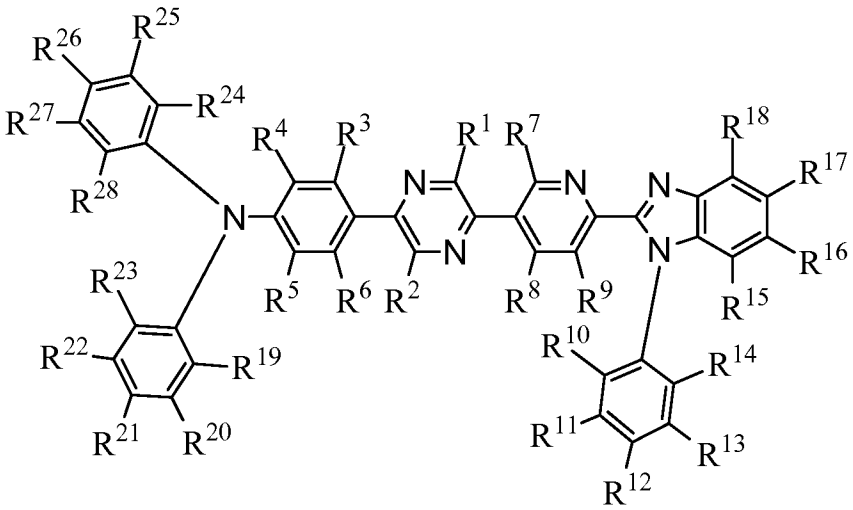
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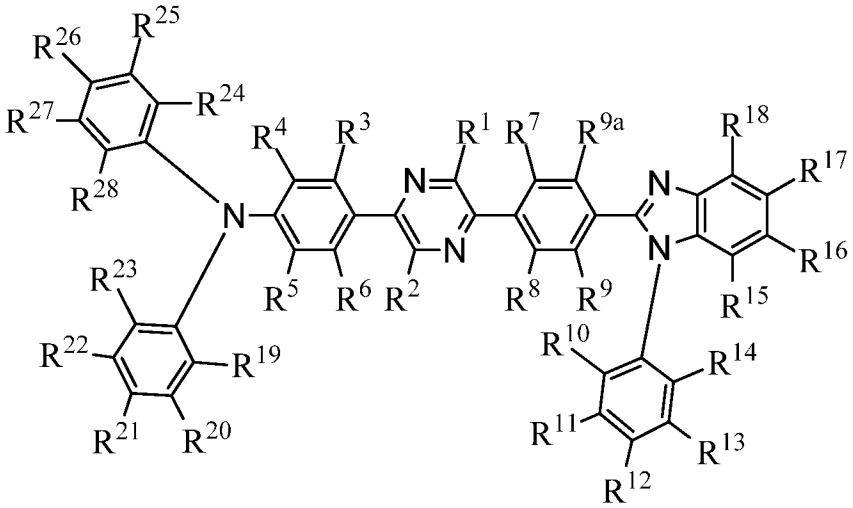
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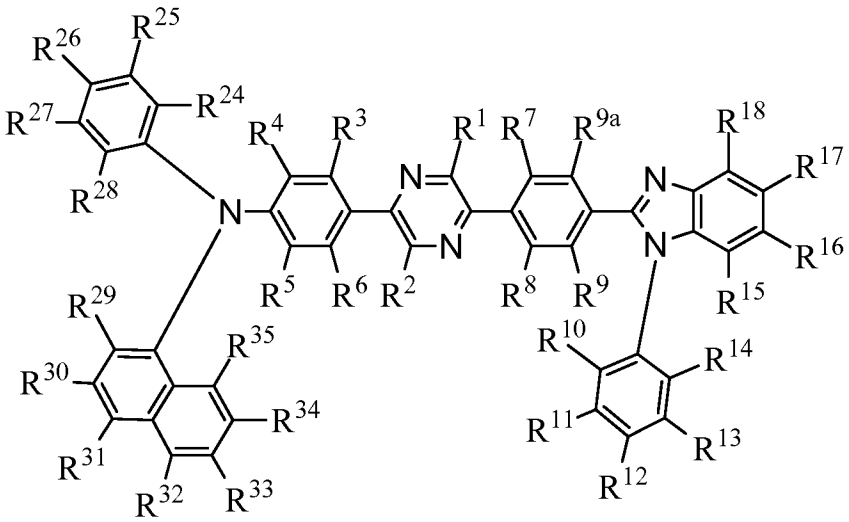
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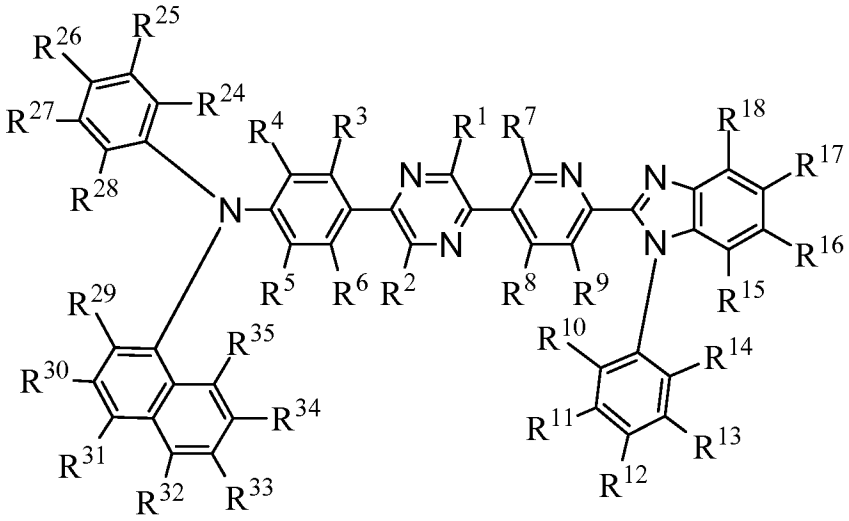
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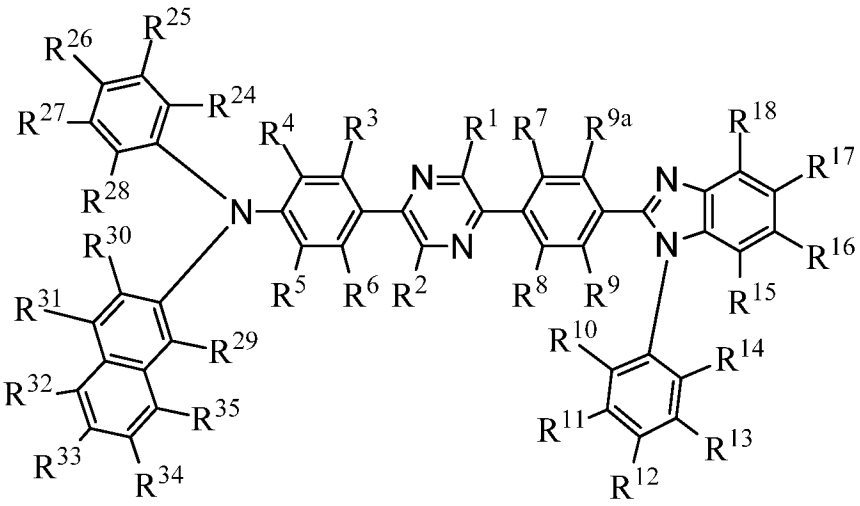
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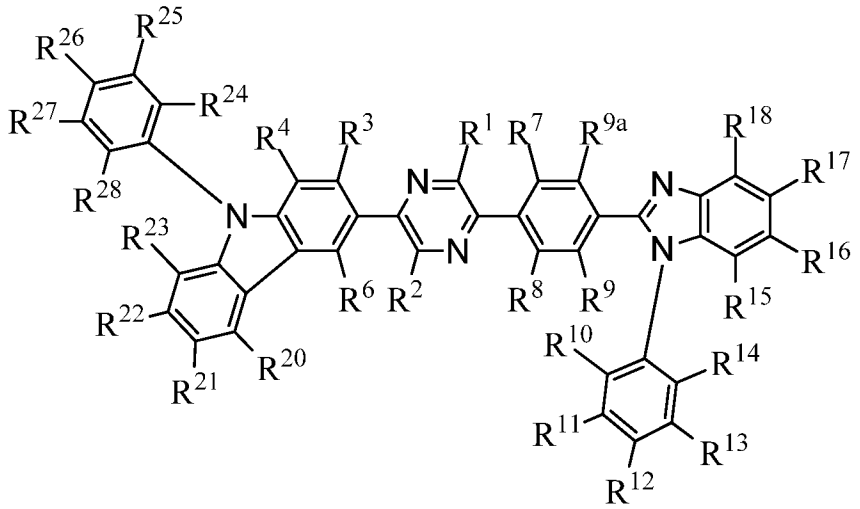
Formula 19



Formula 20



Formula 21

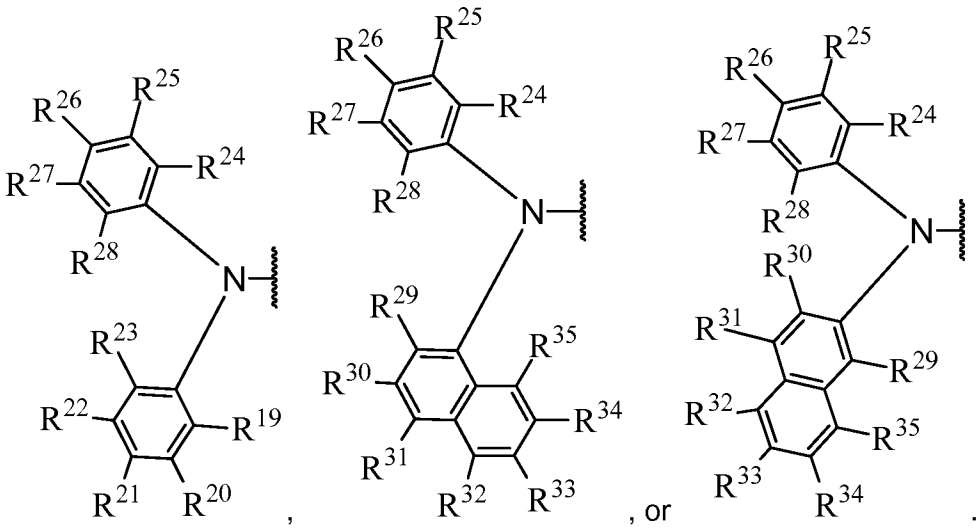


Formula 22

[023] With respect to any relevant formula or structural representation herein, HT may be optionally substituted diphenylamine or optionally substituted phenyl(naphthyl)amine. If the diphenylamine is substituted, it may have 1, 2, 3, 4, 5, 6, 7, 8, 9, or 10 substituents. In some embodiments, the diphenylamine may have 1, 2, 3, or 4 substituents, or 1 or 2 substituents. If the phenyl(naphthyl)amine is substituted, it may have 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, or 12 substituents. In some embodiments, the phenyl(naphthyl)amine may have 1, 2, 3, or 4 substituents, or 1 or 2 substituents. In some embodiments, some or all of the substituents on HT may have: from 0 to 10 carbon atoms and from 0 to 10 heteroatoms, wherein each

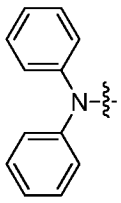
heteroatom is independently: O, N, S, F, Cl, Br, or I (provided that there is at least 1 non-hydrogen atom); and/or a molecular weight of 15 g/mol to 500 g/mol. For example, the substituents may be C_{1-10} optionally substituted alkyl, such as CH_3, C_2H_5, C_3H_7, cyclic C_3H_5, C_4H_9, cyclic C_4H_7, C_5H_{11}, cyclic C_5H_9, C_6H_{13}, cyclic C_6H_{11}, etc., which may be optionally substituted; C_{1-10} optionally substituted alkoxy; halo, such as F, Cl, Br, I; OH; CN; NO_2; C_{1-6} fluoroalkyl, such as CF_3, CF_2H, C_2F_5, etc.; a C_{1-10} ester such as $–O_2CCH_3$, $-CO_2CH_3$, $-O_2CC_2H_5$, $-CO_2C_2H_5$, $-O_2C$-phenyl, $-CO_2$-phenyl, etc.; a C_{1-10} ketone such as $–COCH_3$, $-COC_2H_5$, $-COC_3H_7$, -CO-phenyl, etc.; or C_{1-10} amino such as NH_2, $NH(CH_3)$, $N(CH_3)_2$, $N(CH_3)C_2H_5$, etc. In some embodiments, any substituents on HT can be an electron donating substituent, such as C_{1-3} alkyl, C_{1-3} -O-alkyl, NH_3, or C_{1-3} amino. In some embodiments, HT is unsubstituted.

[024] In some embodiments, HT is:

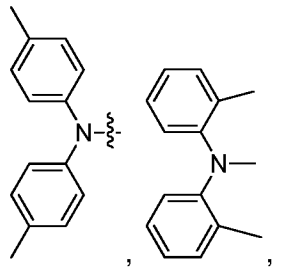


, , or .

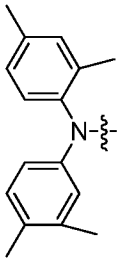
[025] In some embodiments, HT can be selected from optionally substituted carbozolyl, optionally substituted diphenylamine and/or optionally substituted phenyl(naphhyl)amine with 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11 or 12 substituents independently selected from C_{1-6} alkyl and F. In some embodiments, HT is selected from unsubstituted diphenylamine, a mono-substituted diphenylamine, a di-substituted diphenylamine, an unsubstituted phenyl(naphthyl)amine, a mono-substituted phenyl(naphthyl)amine, and/or an unsubstituted carbazolyl. Examples of the described ring systems may include any one of the following:



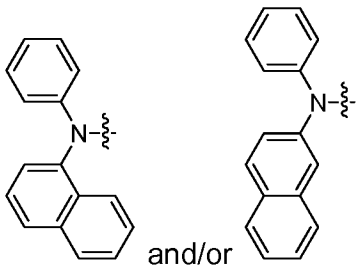
unsubstituted diphenylamine,



a mono-substituted diphenylamine,

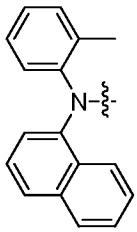


a di-substituted diphenylamine,

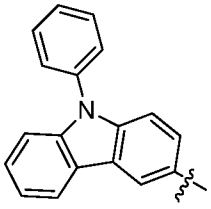


and/or

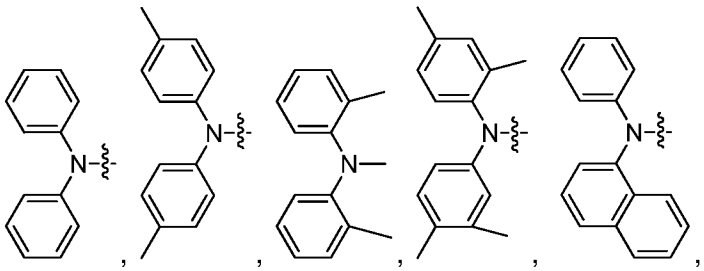
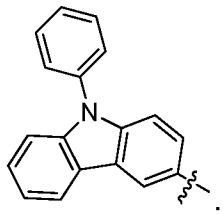
an unsubstituted phenyl(naphthyl)amine,



a mono-substituted phenyl(naphthyl)amine, and/or


an unsubstituted carbazolyl.

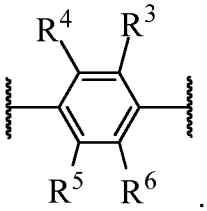
[026] In some embodiments, HT is selected any one of


, and .

[027] With respect to any relevant formula or structural representation herein, Ph^{1a} may be optionally substituted *p*-phenylene, or HT—Ph^{1a} may be 9-phenylcarbazol-3-yl. If the *p*-phenylene is substituted, it may have 1, 2, 3, or 4 substituents. In some embodiments, the *p*-phenylene is unsubstituted. In some embodiments the *p*-phenylene has 1 substituent. In some embodiments, the *p*-phenylene has 2 substituents. In some embodiments the *p*-phenylene has 3 substituents. In some embodiments the *p*-phenylene has 4 substituents. If the 9-phenylcarbazol-3-yl is substituted, it may have it may have 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, or 11, or 12 substituents. In some embodiments, the 9-phenylcarbazol-3-yl may have 1, 2, 3, or 4 substituents, or 1 or 2 substituents. In some embodiments, some or all of the substituents on Ph^{1a} or HT—Ph^{1a} may have: from 0 to 10 carbon atoms and from 0 to 10 heteroatoms, wherein each heteroatom is independently: O, N, S, F, Cl, Br, or I (provided that there is at least 1 non-hydrogen atom); and/or a molecular weight of 15 g/mol to 500 g/mol. For example, the substituents may be C_{1-10} optionally substituted alkyl, such as CH_3, C_2H_5, C_3H_7, cyclic C_3H_5, C_4H_9, cyclic C_4H_7, C_5H_{11}, cyclic C_5H_9, C_6H_{13}, cyclic C_6H_{11}, etc., which may be optionally substituted; C_{1-}

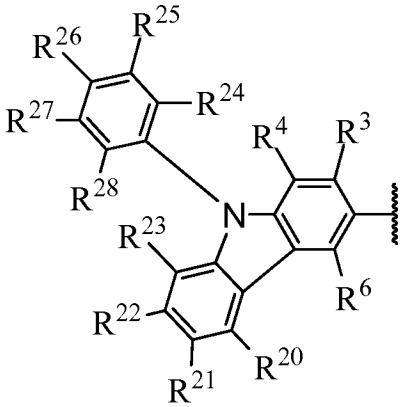
$_{10}$ optionally substituted alkoxy; halo, such as F, Cl, Br, I; OH; CN; NO_2; C_{1-6} fluoroalkyl, such as CF_3, CF_2H, C_2F_5, etc.; a C_{1-10} ester such as $–O_2CCH_3$, $-CO_2CH_3$, $-O_2CC_2H_5$, $-CO_2C_2H_5$, $-O_2C$-phenyl, $-CO_2$-phenyl, etc.; a C_{1-10} ketone such as $–COCH_3$, $-COC_2H_5$, $-COC_3H_7$, -CO-phenyl, etc.; or C_{1-10} amino such as NH_2, $NH(CH_3)$, $N(CH_3)_2$, $N(CH_3)C_2H_5$, etc. In some embodiments, any substituents on Ph^{1a} or HT—Ph^{1a} can be C_{1-3} alkyl, C_{1-3} -O-alkyl, NH_3, or C_{1-3} amino. In some embodiments, Ph^{1a} or HT—Ph^{1a} is unsubstituted.

[028] In some embodiments, Ph^{1a} is:



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[029] In some embodiments, HT—Ph^{1a} is:



[030] With respect to any relevant formula or structural representation herein, Ph^{1b} may be a bond or optionally substituted *p*-phenylene. If the *p*-phenylene is substituted, it may have 1, 2, 3, or 4 substituents. In some embodiments, the *p*-phenylene is unsubstituted. In some embodiments the *p*-phenylene has 1 substituent. In some embodiments, the *p*-phenylene has 2 substituents. In some embodiments the *p*-phenylene has 3 substituents. In some embodiments the *p*-phenylene has 4 substituents. In some embodiments, some or all of the substituents on Ph^{1b} may have: from 0 to 10 carbon atoms and from 0 to 10 heteroatoms, wherein each heteroatom is independently: O, N, S, F, Cl, Br, or I (provided that there is at least 1 non-hydrogen atom); and/or a molecular weight of 15 g/mol to 500 g/mol. For example, the substituents may be C_{1-10} optionally

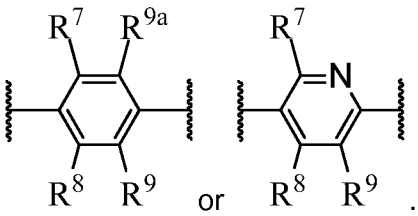
substituted alkyl, such as CH_3, C_2H_5, C_3H_7, cyclic C_3H_5, C_4H_9, cyclic C_4H_7, C_5H_{11}, cyclic C_5H_9, C_6H_{13}, cyclic C_6H_{11}, etc., which may be optionally substituted; $C_{1\text{-}10}$ optionally substituted alkoxy; halo, such as F, Cl, Br, I; OH; CN; NO_2; $C_{1\text{-}6}$ fluoroalkyl, such as CF_3, CF_2H, C_2F_5, etc.; a $C_{1\text{-}10}$ ester such as $–O_2CCH_3$, $-CO_2CH_3$, $-O_2CC_2H_5$, $-CO_2C_2H_5$, $-O_2C$-phenyl, $-CO_2$-phenyl, etc.; a $C_{1\text{-}10}$ ketone such as $–COCH_3$, $-COC_2H_5$, $-COC_3H_7$, -CO-phenyl, etc.; or $C_{1\text{-}10}$ amino such as NH_2, $NH(CH_3)$, $N(CH_3)_2$, $N(CH_3)C_2H_5$, etc. In some embodiments, any substituents on Ph^{1b} can be $C_{1\text{-}3}$ alkyl, CF_3, or F. In some embodiments, Ph^{1b} is a bond.

[031] With respect to any relevant formula or structural representation herein, Ph^{1c} may be a bond or optionally substituted *p*-phenylene. If the *p*-phenylene is substituted, it may have 1, 2, 3, or 4 substituents. In some embodiments, the *p*-phenylene is unsubstituted. In some embodiments the *p*-phenylene has 1 substituent. In some embodiments, the *p*-phenylene has 2 substituents. In some embodiments the *p*-phenylene has 3 substituents. In some embodiments the *p*-phenylene has 4 substituents. In some embodiments, some or all of the substituents on Ph^{1c} may have: from 0 to 10 carbon atoms and from 0 to 10 heteroatoms, wherein each heteroatom is independently: O, N, S, F, Cl, Br, or I (provided that there is at least 1 non-hydrogen atom); and/or a molecular weight of 15 g/mol to 500 g/mol. For example, the substituents may be $C_{1\text{-}10}$ optionally substituted alkyl, such as CH_3, C_2H_5, C_3H_7, cyclic C_3H_5, C_4H_9, cyclic C_4H_7, C_5H_{11}, cyclic C_5H_9, C_6H_{13}, cyclic C_6H_{11}, etc., which may be optionally substituted; $C_{1\text{-}10}$ optionally substituted alkoxy; halo, such as F, Cl, Br, I; OH; CN; NO_2; $C_{1\text{-}6}$ fluoroalkyl, such as CF_3, CF_2H, C_2F_5, etc.; a $C_{1\text{-}10}$ ester such as $–O_2CCH_3$, $-CO_2CH_3$, $-O_2CC_2H_5$, $-CO_2C_2H_5$, $-O_2C$-phenyl, $-CO_2$-phenyl, etc.; a $C_{1\text{-}10}$ ketone such as $–COCH_3$, $-COC_2H_5$, $-COC_3H_7$, -CO-phenyl, etc.; or $C_{1\text{-}10}$ amino such as NH_2, $NH(CH_3)$, $N(CH_3)_2$, $N(CH_3)C_2H_5$, etc. In some embodiments, any substituents on Ph^{1c} can be $C_{1\text{-}3}$ alkyl, CF_3, or F. In some embodiments, Ph^{1c} is a bond.

[032] With respect to any relevant formula or structural representation herein, Py may be optionally substituted pyrazin-2,5-ylene. If the pyrazin-2,5-ylene is substituted, it may have 1, 2, 3, or 4 substituents. In some embodiments, the pyrazin-2,5-ylene is unsubstituted. In some embodiments the pyrazin-2,5-ylene has 1 substituent. In some embodiments, the pyrazin-2,5-ylene has 2 substituents. In some embodiments, some or all of the substituents on Py may have: from 0 to 10

carbon atoms and from 0 to 10 heteroatoms, wherein each heteroatom is independently: O, N, S, F, Cl, Br, or I (provided that there is at least 1 non-hydrogen atom); and/or a molecular weight of 15 g/mol to 500 g/mol. For example, the substituents may be C_{1-10} optionally substituted alkyl, such as CH_3, C_2H_5, C_3H_7, cyclic C_3H_5, C_4H_9, cyclic C_4H_7, C_5H_{11}, cyclic C_5H_9, C_6H_{13}, cyclic C_6H_{11}, etc., which may be optionally substituted; C_{1-10} optionally substituted alkoxy; halo, such as F, Cl, Br, I; OH; CN; NO_2; C_{1-6} fluoroalkyl, such as CF_3, CF_2H, C_2F_5, etc.; a C_{1-10} ester such as $-O_2CCH_3$, $-CO_2CH_3$, $-O_2CC_2H_5$, $-CO_2C_2H_5$, $-O_2C$-phenyl, $-CO_2$-phenyl, etc.; a C_{1-10} ketone such as $-COCH_3$, $-COC_2H_5$, $-COC_3H_7$, -CO-phenyl, etc.; or C_{1-10} amino such as NH_2, $NH(CH_3)$, $N(CH_3)_2$, $N(CH_3)C_2H_5$, etc. In some embodiments, any substituents on Py can be C_{1-3} alkyl, CF_3, or F. In some embodiments, Py is unsubstituted.

[033] In some embodiments, Py is:

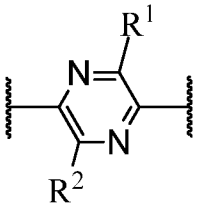


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[034] With respect to any relevant formula or structural representation herein, Het may be optionally substituted *p*-phenylene or optionally substituted pyridin-2,5-ylene. If the *p*-phenylene is substituted, it may have 1, 2, 3, or 4 substituents. In some embodiments, the *p*-phenylene is unsubstituted. In some embodiments the *p*-phenylene has 1 substituent. In some embodiments, the *p*-phenylene has 2 substituents. In some embodiments the *p*-phenylene has 3 substituents. In some embodiments the *p*-phenylene has 4 substituents. If the pyridin-2,5-ylene is substituted, it may have 1, 2, or 3 substituents. In some embodiments, the pyridin-2,5-ylene is unsubstituted. In some embodiments the pyridin-2,5-ylene has 1 substituent. In some embodiments, the pyridin-2,5-ylene has 2 substituents. In some embodiments the pyridin-2,5-ylene has 3 substituents. In some embodiments, some or all of the substituents on Het may have: from 0 to 10 carbon atoms and from 0 to 10 heteroatoms, wherein each heteroatom is independently: O, N, S, F, Cl, Br, or I (provided that there is at least 1 non-hydrogen atom); and/or a molecular weight of 15 g/mol to 500 g/mol. For example, the

substituents may be C_{1-10} optionally substituted alkyl, such as CH_3, C_2H_5, C_3H_7, cyclic C_3H_5, C_4H_9, cyclic C_4H_7, C_5H_{11}, cyclic C_5H_9, C_6H_{13}, cyclic C_6H_{11}, etc., which may be optionally substituted; C_{1-10} optionally substituted alkoxy; halo, such as F, Cl, Br, I; OH; CN; NO_2; C_{1-6} fluoroalkyl, such as CF_3, CF_2H, C_2F_5, etc.; a C_{1-10} ester such as $–O_2CCH_3$, $-CO_2CH_3$, $-O_2CC_2H_5$, $-CO_2C_2H_5$, $-O_2C$-phenyl, $-CO_2$-phenyl, etc.; a C_{1-10} ketone such as $–COCH_3$, $-COC_2H_5$, $-COC_3H_7$, -CO-phenyl, etc.; or C_{1-10} amino such as NH_2, $NH(CH_3)$, $N(CH_3)_2$, $N(CH_3)C_2H_5$, etc. In some embodiments, any substituents on Het can be C_{1-3} alkyl, CF_3, or F. In some embodiments, Het is unsubstituted.

[035] In some embodiments, Het is:



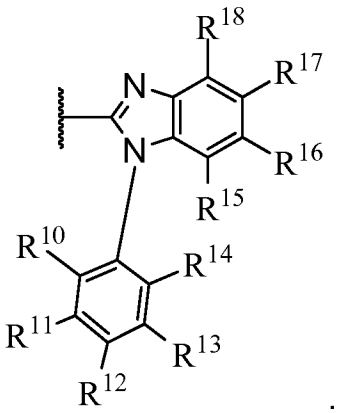
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[036] With respect to any relevant formula or structural representation herein, ET may be optionally substituted benzimidazol-2-yl, optionally substituted benzoxazol-2-yl, or optionally substituted benzothiazol-2-yl. If the benzimidazol-2-yl, benzoxazol-2-yl, or benzothiazol-2-yl is substituted, it may have 1, 2, 3, or 4 substituents. In some embodiments, the benzimidazol-2-yl, benzoxazol-2-yl, or benzothiazol-2-yl is unsubstituted. In some embodiments the benzimidazol-2-yl, benzoxazol-2-yl, or benzothiazol-2-yl has 1 substituent. In some embodiments, the benzimidazol-2-yl, benzoxazol-2-yl, or benzothiazol-2-yl has 2 substituents. In some embodiments the benzimidazol-2-yl, benzoxazol-2-yl, or benzothiazol-2-yl has 3 substituents. In some embodiments the benzimidazol-2-yl, benzoxazol-2-yl, or benzothiazol-2-yl has 4 substituents.

[037] In some embodiments, ET is optionally substituted 1-phenyl-1H-benzo[d]imidazol-2-yl. In some embodiments, the 1-phenyl-1H-benzo[d]imidazol-2-yl is unsubstituted. If the 1-phenyl-1H-benzo[d]imidazol-2-yl is substituted, it can have 1, 2, 3, 4, 5, 6, 7, 8, or 9 substituents. In some embodiments, the 1-phenyl-1H-benzo[d]imidazol-2-yl has 1, 2, 3, or 4 substituents. In some embodiments, the 1-phenyl-1H-benzo[d]imidazol-2-yl has 1 or 2 substituents. In some embodiments, some or all of the substituents on ET may have: from 0 to 10 carbon atoms and from

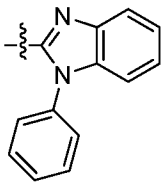
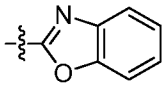
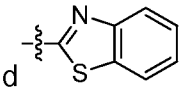
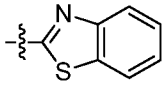
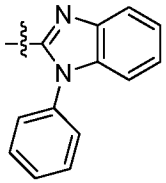
0 to 10 heteroatoms, wherein each heteroatom is independently: O, N, S, F, Cl, Br, or I (provided that there is at least 1 non-hydrogen atom); and/or a molecular weight of 15 g/mol to 500 g/mol. For example, the substituents may be C_{1-10} optionally substituted alkyl, such as CH_3, C_2H_5, C_3H_7, cyclic C_3H_5, C_4H_9, cyclic C_4H_7, C_5H_{11}, cyclic C_5H_9, C_6H_{13}, cyclic C_6H_{11}, etc., which may be optionally substituted; C_{1-10} optionally substituted alkoxy; halo, such as F, Cl, Br, I; OH; CN; NO_2; C_{1-6} fluoroalkyl, such as CF_3, CF_2H, C_2F_5, etc.; a C_{1-10} ester such as $–O_2CCH_3$, $-CO_2CH_3$, $-O_2CC_2H_5$, $-CO_2C_2H_5$, $-O_2C$-phenyl, $-CO_2$-phenyl, etc.; a C_{1-10} ketone such as $–COCH_3$, $-COC_2H_5$, $-COC_3H_7$, -CO-phenyl, etc.; or C_{1-10} amino such as NH_2, $NH(CH_3)$, $N(CH_3)_2$, $N(CH_3)C_2H_5$, etc. In some embodiments, any substituents on ET can be C_{1-3} alkyl, or an electon withdrawing substituent such as F, Cl,NO_2, CN, COH, $COCH_3$, etc. In some embodiments, ET is unsubstituted.

[038] In some embodiments, ET is:



.

[039] In some embodiments, ET can be selected from optionally substituted benzimidazol-2-yl, optionally substituted benzoxazol-2-yl, and/or optionally substituted benzthiazol-2-yl. In some embodiments, ET is an unsubstituted benzoimidazol-2-yl. In some embodiments, ET is selected from

, , and . In some embodiments, ET is an optionally substituted benzimidazol-2-yl. . In some embodiments, ET is .

[040] With respect to any relevant formula above, Ph^1 and/or Ph^2 can be an optionally substituted *p*-phenylene.

[041] With respect to any relevant formula above, X can be selected from C and N, e.g., Formula 3 and /or 2 respectively.

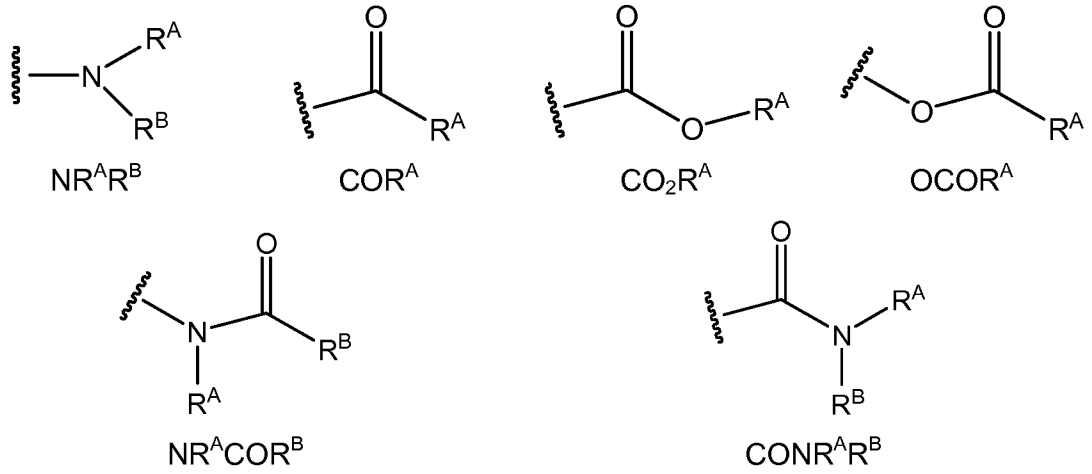
[042] In some embodiments, Ph^1 is optionally substituted *p*-phenylene with 1, 2, 3 or 4 substituents independently selected from C_{1-6} alkyl and F. In some embodiments, Ph^1 is an unsubstituted *p*-phenylene.

[043] In some embodiments, Ph^2 is optionally substituted *p*-phenylene with 1, 2, 3 or 4 substituents independently selected from C_{1-6} alkyl and F. In some embodiments, Ph^2 is an unsubstituted *p*-phenylene.

[044] Generally R^1-R^{35}, may be H or any substituent, such as a substituent having from 0 to 6 carbon atoms and from 0 to 5 heteroatoms, wherein each heteroatom is independently: O, N, S, F, Cl, Br, or I, and/or having a molecular weight of 15 g/mol to 300 g/mol. Any of R^1-R^{35} may comprise: a) 1 or more alkyl moieties optionally substituted with, or optionally connected by or to, b) 1 or more functional groups, such as C=C, C≡C, CO, CO_2, CON, NCO_2, OH, SH, O, S, N, N=C, F, Cl, Br, I, CN, NO_2, CO_2H, NH_2, etc.; or may be a substituent having no alkyl portion, such as F, Cl, Br, I, NO_2, CN, NH_2, OH, COH, CO_2H, etc.

[045] With respect to any relevant formula or structural depiction herein, some non-limiting examples of R^1 may include R^A, F, Cl, CN, OR^A, CF_3, NO_2, NR^AR^B, COR^A, CO_2R^A, OCORA, NR^ACOR^B, $CONR^AR^B$, etc. In some embodiments, R^1 may be may be H; F; Cl; CN; CF_3; OH; NH_2; C_{1-6} alkyl, such as methyl, ethyl,

propyl isomers (e.g. n-propyl and isopropyl), cyclopropyl, butyl isomers, cyclobutyl isomers (e.g. cyclobutyl and methylcyclopropyl), pentyl isomers, cyclopentyl isomers, hexyl isomers, cyclohexyl isomers, etc.; C_{1-6} amino, such as -$NHCH_3$, -$NH(CH_3)_2$,-$NHCH_2CH_3$, etc.; C_{1-6} alkoxy, such as -O-methyl, -O-ethyl, isomers of -O-propyl, -O-cyclopropyl, isomers of -O-butyl, isomers of -O-cyclobutyl, isomers of -O-pentyl, isomers of -O-cyclopentyl, isomers of -O-hexyl, isomers of -O-cyclohexyl, etc.; CHO; C_{2-6} -CO-alkyl, such as -$COCH_3$, -COC_2H_5, -COC_3H_7, COC_4H_9, -COC_5H_{11}, etc.; CO_2H; C_{2-6} -CO_2-alkyl, -CO_2CH_3, -$CO_2C_2H_5$, -$CO_2C_3H_7$, $CO_2C_4H_9$, -COC_5H_{11}, etc. In some embodiments, R^1 may be H.



[046] Each R^A may independently be H, or C_{1-12} alkyl, including: linear or branched alkyl having a formula C_aH_{a+1}, or cycloalkyl having a formula C_aH_{a-1}, wherein a is 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, or 12, such as linear or branched alkyl of a formula: CH_3, C_2H_5, C_3H_7, C_4H_9, C_5H_{11}, C_6H_{13}, C_7H_{15}, C_8H_{17}, C_9H_{19}, $C_{10}H_{21}$, etc., or cycloalkyl of a formula: C_3H_5, C_4H_7, C_5H_9, C_6H_{11}, C_7H_{13}, C_8H_{15}, C_9H_{17}, $C_{10}H_{19}$, etc. In some embodiments, R^A may be H or C_{1-6} alkyl. In some embodiments, R^A may be H or C_{1-3} alkyl. In some embodiments, R^A may be H or CH_3. In some embodiments, R^A may be H.

[047] Each R^B may independently be H, or C_{1-12} alkyl, including: linear or branched alkyl having a formula C_aH_{a+1}, or cycloalkyl having a formula C_aH_a, wherein a is 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, or 12, such as linear or branched alkyl of a formula: CH_3, C_2H_5, C_3H_7, C_4H_9, C_5H_{11}, C_6H_{13}, C_8H_{17}, C_7H_{15}, C_9H_{19}, $C_{10}H_{21}$, etc., or cycloalkyl of a formula: C_3H_5, C_4H_7, C_5H_9, C_6H_{11}, C_7H_{13}, C_8H_{15}, C_9H_{17}, $C_{10}H_{19}$, etc. In

some embodiments, R^B may be H or C_{1-3} alkyl. In some embodiments, R^B may be H or CH_3. In some embodiments, R^B may be H.

[048] With respect to any relevant formula or structural depiction herein, some non-limiting examples of R^2 may include R^A, F, Cl, CN, OR^A, CF_3, NO_2, NR^AR^B, COR^A, CO_2R^A, OCORA, NR^ACOR^B, $CONR^AR^B$, etc. In some embodiments, R^2 may be H; F; Cl; CN; CF_3; OH; NH_2; C_{1-6} alkyl, such as methyl, ethyl, propyl isomers (e.g. n-propyl and isopropyl), cyclopropyl, butyl isomers, cyclobutyl isomers (e.g. cyclobutyl and methylcyclopropyl), pentyl isomers, cyclopentyl isomers, hexyl isomers, cyclohexyl isomers, etc.; C_{1-6} amino, such as $-NHCH_3$, $-NH(CH_3)2$,$-NHCH_2CH_3$, etc.; C_{1-6} alkoxy, such as -O-methyl, -O-ethyl, isomers of -O-propyl, -O-cyclopropyl, isomers of -O-butyl, isomers of -O-cyclobutyl, isomers of -O-pentyl, isomers of -O-cyclopentyl, isomers of -O-hexyl, isomers of -O-cyclohexyl, etc.; CHO; C_{2-6} -CO-alkyl, such as $-COCH_3$, $-COC_2H_5$, $-COC_3H_7$, COC_4H_9, $-COC_5H_{11}$, etc.; CO_2H; C_{2-6} $-CO_2$-alkyl, $-CO_2CH_3$, $-CO_2C_2H_5$, $-CO_2C_3H_7$, $CO_2C_4H_9$, $-COC_5H_{11}$, etc. In some embodiments, R^2 may be H.

[049] With respect to any relevant formula or structural depiction herein, some non-limiting examples of R^3 may include R^A, F, Cl, CN, OR^A, CF_3, NO_2, NR^AR^B, COR^A, CO_2R^A, OCORA, NR^ACOR^B, $CONR^AR^B$, etc. In some embodiments, R^3 may be H; F; Cl; CN; CF_3; OH; NH_2; C_{1-6} alkyl, such as methyl, ethyl, propyl isomers (e.g. n-propyl and isopropyl), cyclopropyl, butyl isomers, cyclobutyl isomers (e.g. cyclobutyl and methylcyclopropyl), pentyl isomers, cyclopentyl isomers, hexyl isomers, cyclohexyl isomers, etc.; C_{1-6} amino, such as $-NHCH_3$, $-NH(CH_3)2$,$-NHCH_2CH_3$, etc.; C_{1-6} alkoxy, such as -O-methyl, -O-ethyl, isomers of -O-propyl, -O-cyclopropyl, isomers of -O-butyl, isomers of -O-cyclobutyl, isomers of -O-pentyl, isomers of -O-cyclopentyl, isomers of -O-hexyl, isomers of -O-cyclohexyl, etc.; CHO; C_{2-6} -CO-alkyl, such as $-COCH_3$, $-COC_2H_5$, $-COC_3H_7$, COC_4H_9, $-COC_5H_{11}$, etc.; CO_2H; C_{2-6} $-CO_2$-alkyl, $-CO_2CH_3$, $-CO_2C_2H_5$, $-CO_2C_3H_7$, $CO_2C_4H_9$, $-COC_5H_{11}$, etc. In some embodiments, R^3 may be H.

[050] With respect to any relevant formula or structural depiction herein, some non-limiting examples of R^4 may include R^A, F, Cl, CN, OR^A, CF_3, NO_2, NR^AR^B, COR^A, CO_2R^A, OCORA, NR^ACOR^B, $CONR^AR^B$, etc. In some embodiments, R^4 may be H; F; Cl; CN; CF_3; OH; NH_2; C_{1-6} alkyl, such as methyl, ethyl, propyl isomers (e.g. n-propyl and isopropyl), cyclopropyl, butyl isomers, cyclobutyl isomers

(e.g. cyclobutyl and methylcyclopropyl), pentyl isomers, cyclopentyl isomers, hexyl isomers, cyclohexyl isomers, etc.; C_{1-6} amino, such as -$NHCH_3$, -$NH(CH_3)2$,-$NHCH_2CH_3$, etc.; C_{1-6} alkoxy, such as -O-methyl, -O-ethyl, isomers of -O-propyl, -O-cyclopropyl, isomers of -O-butyl, isomers of -O-cyclobutyl, isomers of -O-pentyl, isomers of -O-cyclopentyl, isomers of -O-hexyl, isomers of -O-cyclohexyl, etc.; CHO; C_{2-6} -CO-alkyl, such as -$COCH_3$, -COC_2H_5, -COC_3H_7, COC_4H_9, -COC_5H_{11}, etc.; CO_2H; C_{2-6} -CO_2-alkyl, -CO_2CH_3, -$CO_2C_2H_5$, -$CO_2C_3H_7$, $CO_2C_4H_9$, -COC_5H_{11}, etc. In some embodiments, R^4 may be H.

[051] With respect to any relevant formula or structural depiction herein, some non-limiting examples of R^5 may include R^A, F, Cl, CN, OR^A, CF_3, NO_2, NR^AR^B, COR^A, CO_2R^A, OCORA, NR^ACOR^B, $CONR^AR^B$, etc. In some embodiments, R^5 may be H; F; Cl; CN; CF_3; OH; NH_2; C_{1-6} alkyl, such as methyl, ethyl, propyl isomers (e.g. n-propyl and isopropyl), cyclopropyl, butyl isomers, cyclobutyl isomers (e.g. cyclobutyl and methylcyclopropyl), pentyl isomers, cyclopentyl isomers, hexyl isomers, cyclohexyl isomers, etc.; C_{1-6} amino, such as -$NHCH_3$, -$NH(CH_3)2$,-$NHCH_2CH_3$, etc.; C_{1-6} alkoxy, such as -O-methyl, -O-ethyl, isomers of -O-propyl, -O-cyclopropyl, isomers of -O-butyl, isomers of -O-cyclobutyl, isomers of -O-pentyl, isomers of -O-cyclopentyl, isomers of -O-hexyl, isomers of -O-cyclohexyl, etc.; CHO; C_{2-6} -CO-alkyl, such as -$COCH_3$, -COC_2H_5, -COC_3H_7, COC_4H_9, -COC_5H_{11}, etc.; CO_2H; C_{2-6} -CO_2-alkyl, -CO_2CH_3, -$CO_2C_2H_5$, -$CO_2C_3H_7$, $CO_2C_4H_9$, -COC_5H_{11}, etc. In some embodiments, R^5 may be H.

[052] With respect to any relevant formula or structural depiction herein, some non-limiting examples of R^6 may include R^A, F, Cl, CN, OR^A, CF_3, NO_2, NR^AR^B, COR^A, CO_2R^A, OCORA, NR^ACOR^B, $CONR^AR^B$, etc. In some embodiments, R^6 may be H; F; Cl; CN; CF_3; OH; NH_2; C_{1-6} alkyl, such as methyl, ethyl, propyl isomers (e.g. n-propyl and isopropyl), cyclopropyl, butyl isomers, cyclobutyl isomers (e.g. cyclobutyl and methylcyclopropyl), pentyl isomers, cyclopentyl isomers, hexyl isomers, cyclohexyl isomers, etc.; C_{1-6} amino, such as -$NHCH_3$, -$NH(CH_3)2$,-$NHCH_2CH_3$, etc.; C_{1-6} alkoxy, such as -O-methyl, -O-ethyl, isomers of -O-propyl, -O-cyclopropyl, isomers of -O-butyl, isomers of -O-cyclobutyl, isomers of -O-pentyl, isomers of -O-cyclopentyl, isomers of -O-hexyl, isomers of -O-cyclohexyl, etc.; CHO; C_{2-6} -CO-alkyl, such as -$COCH_3$, -COC_2H_5, -COC_3H_7, COC_4H_9, -COC_5H_{11}, etc.;

CO_2H; C_{2-6} $-CO_2$-alkyl, $-CO_2CH_3$, $-CO_2C_2H_5$, $-CO_2C_3H_7$, $CO_2C_4H_9$, $-COC_5H_{11}$, etc. In some embodiments, R^6 may be H.

[053] With respect to any relevant formula or structural depiction herein, some non-limiting examples of R^7 may include R^A, F, Cl, CN, OR^A, CF_3, NO_2, NR^AR^B, COR^A, CO_2R^A, OCORA, NR^ACOR^B, $CONR^AR^B$, etc. In some embodiments, R^7 may be H; F; Cl; CN; CF_3; OH; NH_2; C_{1-6} alkyl, such as methyl, ethyl, propyl isomers (e.g. n-propyl and isopropyl), cyclopropyl, butyl isomers, cyclobutyl isomers (e.g. cyclobutyl and methylcyclopropyl), pentyl isomers, cyclopentyl isomers, hexyl isomers, cyclohexyl isomers, etc.; C_{1-6} amino, such as $-NHCH_3$, $-NH(CH_3)2$,$-NHCH_2CH_3$, etc.; C_{1-6} alkoxy, such as -O-methyl, -O-ethyl, isomers of -O-propyl, -O-cyclopropyl, isomers of -O-butyl, isomers of -O-cyclobutyl, isomers of -O-pentyl, isomers of -O-cyclopentyl, isomers of -O-hexyl, isomers of -O-cyclohexyl, etc.; CHO; C_{2-6} -CO-alkyl, such as $-COCH_3$, $-COC_2H_5$, $-COC_3H_7$, COC_4H_9, $-COC_5H_{11}$, etc.; CO_2H; C_{2-6} $-CO_2$-alkyl, $-CO_2CH_3$, $-CO_2C_2H_5$, $-CO_2C_3H_7$, $CO_2C_4H_9$, $-COC_5H_{11}$, etc. In some embodiments, R^7 may be H.

[054] With respect to any relevant formula or structural depiction herein, some non-limiting examples of R^8 may include R^A, F, Cl, CN, OR^A, CF_3, NO_2, NR^AR^B, COR^A, CO_2R^A, OCORA, NR^ACOR^B, $CONR^AR^B$, etc. In some embodiments, R^8 may be H; F; Cl; CN; CF_3; OH; NH_2; C_{1-6} alkyl, such as methyl, ethyl, propyl isomers (e.g. n-propyl and isopropyl), cyclopropyl, butyl isomers, cyclobutyl isomers (e.g. cyclobutyl and methylcyclopropyl), pentyl isomers, cyclopentyl isomers, hexyl isomers, cyclohexyl isomers, etc.; C_{1-6} amino, such as $-NHCH_3$, $-NH(CH_3)2$,$-NHCH_2CH_3$, etc.; C_{1-6} alkoxy, such as -O-methyl, -O-ethyl, isomers of -O-propyl, -O-cyclopropyl, isomers of -O-butyl, isomers of -O-cyclobutyl, isomers of -O-pentyl, isomers of -O-cyclopentyl, isomers of -O-hexyl, isomers of -O-cyclohexyl, etc.; CHO; C_{2-6} -CO-alkyl, such as $-COCH_3$, $-COC_2H_5$, $-COC_3H_7$, COC_4H_9, $-COC_5H_{11}$, etc.; CO_2H; C_{2-6} $-CO_2$-alkyl, $-CO_2CH_3$, $-CO_2C_2H_5$, $-CO_2C_3H_7$, $CO_2C_4H_9$, $-COC_5H_{11}$, etc. In some embodiments, R^8 may be H.

[055] With respect to any relevant formula or structural depiction herein, some non-limiting examples of R^9 may include R^A, F, Cl, CN, OR^A, CF_3, NO_2, NR^AR^B, COR^A, CO_2R^A, OCORA, NR^ACOR^B, $CONR^AR^B$, etc. In some embodiments, R^9 may be H; F; Cl; CN; CF_3; OH; NH_2; C_{1-6} alkyl, such as methyl, ethyl, propyl isomers (e.g. n-propyl and isopropyl), cyclopropyl, butyl isomers, cyclobutyl isomers

(e.g. cyclobutyl and methylcyclopropyl), pentyl isomers, cyclopentyl isomers, hexyl isomers, cyclohexyl isomers, etc.; C_{1-6} amino, such as -$NHCH_3$, -$NH(CH_3)2$,-$NHCH_2CH_3$, etc.; C_{1-6} alkoxy, such as -O-methyl, -O-ethyl, isomers of -O-propyl, -O-cyclopropyl, isomers of -O-butyl, isomers of -O-cyclobutyl, isomers of -O-pentyl, isomers of -O-cyclopentyl, isomers of -O-hexyl, isomers of -O-cyclohexyl, etc.; CHO; C_{2-6} -CO-alkyl, such as -$COCH_3$, -COC_2H_5, -COC_3H_7, COC_4H_9, -COC_5H_{11}, etc.; CO_2H; C_{2-6} -CO_2-alkyl, -CO_2CH_3, -$CO_2C_2H_5$, -$CO_2C_3H_7$, $CO_2C_4H_9$, -COC_5H_{11}, etc. In some embodiments, R^9 may be H.

[056] With respect to any relevant formula or structural depiction herein, some non-limiting examples of R^{9a} may include R^A, F, Cl, CN, OR^A, CF_3, NO_2, NR^AR^B, COR^A, CO_2R^A, OCORA, NR^ACOR^B, $CONR^AR^B$, etc. In some embodiments, R^{10} may be H; F; Cl; CN; CF_3; OH; NH_2; C_{1-6} alkyl, such as methyl, ethyl, propyl isomers (e.g. n-propyl and isopropyl), cyclopropyl, butyl isomers, cyclobutyl isomers (e.g. cyclobutyl and methylcyclopropyl), pentyl isomers, cyclopentyl isomers, hexyl isomers, cyclohexyl isomers, etc.; C_{1-6} amino, such as -$NHCH_3$, -$NH(CH_3)2$,-$NHCH_2CH_3$, etc.; C_{1-6} alkoxy, such as -O-methyl, -O-ethyl, isomers of -O-propyl, -O-cyclopropyl, isomers of -O-butyl, isomers of -O-cyclobutyl, isomers of -O-pentyl, isomers of -O-cyclopentyl, isomers of -O-hexyl, isomers of -O-cyclohexyl, etc.; CHO; C_{2-6} -CO-alkyl, such as -$COCH_3$, -COC_2H_5, -COC_3H_7, COC_4H_9, -COC_5H_{11}, etc.; CO_2H; C_{2-6} -CO_2-alkyl, -CO_2CH_3, -$CO_2C_2H_5$, -$CO_2C_3H_7$, $CO_2C_4H_9$, -COC_5H_{11}, etc. In some embodiments, R^{10} may be H.

[057] With respect to any relevant formula or structural depiction herein, some non-limiting examples of R^{10} may include R^A, F, Cl, CN, OR^A, CF_3, NO_2, NR^AR^B, COR^A, CO_2R^A, OCORA, NR^ACOR^B, $CONR^AR^B$, etc. In some embodiments, R^{10} may be H; F; Cl; CN; CF_3; C_{1-6} alkyl, such as methyl, ethyl, propyl isomers (e.g. n-propyl and isopropyl), cyclopropyl, butyl isomers, cyclobutyl isomers (e.g. cyclobutyl and methylcyclopropyl), pentyl isomers, cyclopentyl isomers, hexyl isomers, cyclohexyl isomers, etc.; CHO; C_{2-6} -CO-alkyl, such as -$COCH_3$, -COC_2H_5, -COC_3H_7, COC_4H_9, -COC_5H_{11}, etc.; CO_2H; C_{2-6} -CO_2-alkyl, -CO_2CH_3, -$CO_2C_2H_5$, -$CO_2C_3H_7$, $CO_2C_4H_9$, -COC_5H_{11}, etc. In some embodiments, R^{10} may be H.

[058] With respect to any relevant formula or structural depiction herein, some non-limiting examples of R^{11} may include R^A, F, Cl, CN, OR^A, CF_3, NO_2, NR^AR^B, COR^A, CO_2R^A, OCORA, NR^ACOR^B, $CONR^AR^B$, etc. In some embodiments,

R^{11} may be H; F; Cl; CN; CF_3; C_{1-6} alkyl, such as methyl, ethyl, propyl isomers (e.g. n-propyl and isopropyl), cyclopropyl, butyl isomers, cyclobutyl isomers (e.g. cyclobutyl and methylcyclopropyl), pentyl isomers, cyclopentyl isomers, hexyl isomers, cyclohexyl isomers, etc.; CHO; C_{2-6} -CO-alkyl, such as $-COCH_3$, $-COC_2H_5$, $-COC_3H_7$, COC_4H_9, $-COC_5H_{11}$, etc.; CO_2H; C_{2-6} $-CO_2$-alkyl, $-CO_2CH_3$, $-CO_2C_2H_5$, $-CO_2C_3H_7$, $CO_2C_4H_9$, $-COC_5H_{11}$, etc. In some embodiments, R^{11} may be H.

[059] With respect to any relevant formula or structural depiction herein, some non-limiting examples of R^{12} may include R^A, F, Cl, CN, OR^A, CF_3, NO_2, NR^AR^B, COR^A, CO_2R^A, OCORA, NR^ACOR^B, $CONR^AR^B$, etc. In some embodiments, R^{12} may be H; F; Cl; CN; CF_3; C_{1-6} alkyl, such as methyl, ethyl, propyl isomers (e.g. n-propyl and isopropyl), cyclopropyl, butyl isomers, cyclobutyl isomers (e.g. cyclobutyl and methylcyclopropyl), pentyl isomers, cyclopentyl isomers, hexyl isomers, cyclohexyl isomers, etc.; CHO; C_{2-6} -CO-alkyl, such as $-COCH_3$, $-COC_2H_5$, $-COC_3H_7$, COC_4H_9, $-COC_5H_{11}$, etc.; CO_2H; C_{2-6} $-CO_2$-alkyl, $-CO_2CH_3$, $-CO_2C_2H_5$, $-CO_2C_3H_7$, $CO_2C_4H_9$, $-COC_5H_{11}$, etc. In some embodiments, R^{12} may be H.

[060] With respect to any relevant formula or structural depiction herein, some non-limiting examples of R^{13} may include R^A, F, Cl, CN, OR^A, CF_3, NO_2, NR^AR^B, COR^A, CO_2R^A, OCORA, NR^ACOR^B, $CONR^AR^B$, etc. In some embodiments, R^{13} may be H; F; Cl; CN; CF_3; C_{1-6} alkyl, such as methyl, ethyl, propyl isomers (e.g. n-propyl and isopropyl), cyclopropyl, butyl isomers, cyclobutyl isomers (e.g. cyclobutyl and methylcyclopropyl), pentyl isomers, cyclopentyl isomers, hexyl isomers, cyclohexyl isomers, etc.; CHO; C_{2-6} -CO-alkyl, such as $-COCH_3$, $-COC_2H_5$, $-COC_3H_7$, COC_4H_9, $-COC_5H_{11}$, etc.; CO_2H; C_{2-6} $-CO_2$-alkyl, $-CO_2CH_3$, $-CO_2C_2H_5$, $-CO_2C_3H_7$, $CO_2C_4H_9$, $-COC_5H_{11}$, etc. In some embodiments, R^{13} may be H.

[061] With respect to any relevant formula or structural depiction herein, some non-limiting examples of R^{14} may include R^A, F, Cl, CN, OR^A, CF_3, NO_2, NR^AR^B, COR^A, CO_2R^A, OCORA, NR^ACOR^B, $CONR^AR^B$, etc. In some embodiments, R^{14} may be H; F; Cl; CN; CF_3; C_{1-6} alkyl, such as methyl, ethyl, propyl isomers (e.g. n-propyl and isopropyl), cyclopropyl, butyl isomers, cyclobutyl isomers (e.g. cyclobutyl and methylcyclopropyl), pentyl isomers, cyclopentyl isomers, hexyl isomers, cyclohexyl isomers, etc.; CHO; C_{2-6} -CO-alkyl, such as $-COCH_3$, $-COC_2H_5$, $-COC_3H_7$, COC_4H_9, $-COC_5H_{11}$, etc.; CO_2H; C_{2-6} $-CO_2$-alkyl, $-CO_2CH_3$, $-CO_2C_2H_5$, $-CO_2C_3H_7$, $CO_2C_4H_9$, $-COC_5H_{11}$, etc. In some embodiments, R^{14} may be H.

[062] With respect to any relevant formula or structural depiction herein, some non-limiting examples of R^{15} may include R^A, F, Cl, CN, OR^A, CF_3, NO_2, NR^AR^B, COR^A, CO_2R^A, OCORA, NR^ACOR^B, $CONR^AR^B$, etc. In some embodiments, R^{15} may be H; F; Cl; CN; CF_3; C_{1-6} alkyl, such as methyl, ethyl, propyl isomers (e.g. n-propyl and isopropyl), cyclopropyl, butyl isomers, cyclobutyl isomers (e.g. cyclobutyl and methylcyclopropyl), pentyl isomers, cyclopentyl isomers, hexyl isomers, cyclohexyl isomers, etc.; CHO; C_{2-6} -CO-alkyl, such as $-COCH_3$, $-COC_2H_5$, $-COC_3H_7$, COC_4H_9, $-COC_5H_{11}$, etc.; CO_2H; C_{2-6} $-CO_2$-alkyl, $-CO_2CH_3$, $-CO_2C_2H_5$, $-CO_2C_3H_7$, $CO_2C_4H_9$, $-COC_5H_{11}$, etc. In some embodiments, R^{15} may be H.

[063] With respect to any relevant formula or structural depiction herein, some non-limiting examples of R^{16} may include R^A, F, Cl, CN, OR^A, CF_3, NO_2, NR^AR^B, COR^A, CO_2R^A, OCORA, NR^ACOR^B, $CONR^AR^B$, etc. In some embodiments, R^{16} may be H; F; Cl; CN; CF_3; C_{1-6} alkyl, such as methyl, ethyl, propyl isomers (e.g. n-propyl and isopropyl), cyclopropyl, butyl isomers, cyclobutyl isomers (e.g. cyclobutyl and methylcyclopropyl), pentyl isomers, cyclopentyl isomers, hexyl isomers, cyclohexyl isomers, etc.; CHO; C_{2-6} -CO-alkyl, such as $-COCH_3$, $-COC_2H_5$, $-COC_3H_7$, COC_4H_9, $-COC_5H_{11}$, etc.; CO_2H; C_{2-6} $-CO_2$-alkyl, $-CO_2CH_3$, $-CO_2C_2H_5$, $-CO_2C_3H_7$, $CO_2C_4H_9$, $-COC_5H_{11}$, etc. In some embodiments, R^{16} may be H.

[064] With respect to any relevant formula or structural depiction herein, some non-limiting examples of R^{17} may include R^A, F, Cl, CN, OR^A, CF_3, NO_2, NR^AR^B, COR^A, CO_2R^A, OCORA, NR^ACOR^B, $CONR^AR^B$, etc. In some embodiments, R^{17} may be H; F; Cl; CN; CF_3; C_{1-6} alkyl, such as methyl, ethyl, propyl isomers (e.g. n-propyl and isopropyl), cyclopropyl, butyl isomers, cyclobutyl isomers (e.g. cyclobutyl and methylcyclopropyl), pentyl isomers, cyclopentyl isomers, hexyl isomers, cyclohexyl isomers, etc.; CHO; C_{2-6} -CO-alkyl, such as $-COCH_3$, $-COC_2H_5$, $-COC_3H_7$, COC_4H_9, $-COC_5H_{11}$, etc.; CO_2H; C_{2-6} $-CO_2$-alkyl, $-CO_2CH_3$, $-CO_2C_2H_5$, $-CO_2C_3H_7$, $CO_2C_4H_9$, $-COC_5H_{11}$, etc. In some embodiments, R^{17} may be H.

[065] With respect to any relevant formula or structural depiction herein, some non-limiting examples of R^{18} may include R^A, F, Cl, CN, OR^A, CF_3, NO_2, NR^AR^B, COR^A, CO_2R^A, OCORA, NR^ACOR^B, $CONR^AR^B$, etc. In some embodiments, R^{18} may be H; F; Cl; CN; CF_3; C_{1-6} alkyl, such as methyl, ethyl, propyl isomers (e.g. n-propyl and isopropyl), cyclopropyl, butyl isomers, cyclobutyl isomers (e.g. cyclobutyl and methylcyclopropyl), pentyl isomers, cyclopentyl isomers, hexyl

isomers, cyclohexyl isomers, etc.; CHO; C_{2-6} -CO-alkyl, such as $-COCH_3$, $-COC_2H_5$, $-COC_3H_7$, COC_4H_9, $-COC_5H_{11}$, etc.; CO_2H; C_{2-6} $-CO_2$-alkyl, $-CO_2CH_3$, $-CO_2C_2H_5$, $-CO_2C_3H_7$, $CO_2C_4H_9$, $-COC_5H_{11}$, etc. In some embodiments, R^{18} may be H.

[066] With respect to any relevant formula or structural depiction herein, some non-limiting examples of R^{19} may include R^A, F, Cl, CN, OR^A, CF_3, NO_2, NR^AR^B, COR^A, CO_2R^A, OCORA, NR^ACOR^B, $CONR^AR^B$, etc. In some embodiments, R^{19} may be H; F; Cl; CF_3; OH; NH_2; C_{1-6} alkyl, such as methyl, ethyl, propyl isomers (e.g. n-propyl and isopropyl), cyclopropyl, butyl isomers, cyclobutyl isomers (e.g. cyclobutyl and methylcyclopropyl), pentyl isomers, cyclopentyl isomers, hexyl isomers, cyclohexyl isomers, etc.; or C_{1-6} alkoxy, such as -O-methyl, -O-ethyl, isomers of -O-propyl, -O-cyclopropyl, isomers of -O-butyl, isomers of -O-cyclobutyl, isomers of -O-pentyl, isomers of -O-cyclopentyl, isomers of -O-hexyl, isomers of -O-cyclohexyl, etc. In some embodiments, R^{19} may be H. In some embodiments R^{19} is methyl.

[067] With respect to any relevant formula or structural depiction herein, some non-limiting examples of R^{20} may include R^A, F, Cl, CN, OR^A, CF_3, NO_2, NR^AR^B, COR^A, CO_2R^A, OCORA, NR^ACOR^B, $CONR^AR^B$, etc. In some embodiments, R^{20} may be H; F; Cl; CF_3; OH; NH_2; C_{1-6} alkyl, such as methyl, ethyl, propyl isomers (e.g. n-propyl and isopropyl), cyclopropyl, butyl isomers, cyclobutyl isomers (e.g. cyclobutyl and methylcyclopropyl), pentyl isomers, cyclopentyl isomers, hexyl isomers, cyclohexyl isomers, etc.; or C_{1-6} alkoxy, such as -O-methyl, -O-ethyl, isomers of -O-propyl, -O-cyclopropyl, isomers of -O-butyl, isomers of -O-cyclobutyl, isomers of -O-pentyl, isomers of -O-cyclopentyl, isomers of -O-hexyl, isomers of -O-cyclohexyl, etc. In some embodiments, R^{20} may be H.

[068] With respect to any relevant formula or structural depiction herein, some non-limiting examples of R^{21} may include R^A, F, Cl, CN, OR^A, CF_3, NO_2, NR^AR^B, COR^A, CO_2R^A, OCORA, NR^ACOR^B, $CONR^AR^B$, etc. In some embodiments, R^{21} may be H; F; Cl; CF_3; OH; NH_2; C_{1-6} alkyl, such as methyl, ethyl, propyl isomers (e.g. n-propyl and isopropyl), cyclopropyl, butyl isomers, cyclobutyl isomers (e.g. cyclobutyl and methylcyclopropyl), pentyl isomers, cyclopentyl isomers, hexyl isomers, cyclohexyl isomers, etc.; or C_{1-6} alkoxy, such as -O-methyl, -O-ethyl, isomers of -O-propyl, -O-cyclopropyl, isomers of -O-butyl, isomers of -O-cyclobutyl, isomers of -O-pentyl, isomers of -O-cyclopentyl, isomers of -O-hexyl, isomers of

-O-cyclohexyl, etc. In some embodiments, R^{21} may be H. In some embodiments R^{21} is methyl.

[069] With respect to any relevant formula or structural depiction herein, some non-limiting examples of R^{22} may include R^A, F, Cl, CN, OR^A, CF_3, NO_2, NR^AR^B, COR^A, CO_2R^A, OCORA, NR^ACOR^B, $CONR^AR^B$, etc. In some embodiments, R^{22} may be H; F; Cl; CF_3; OH; NH_2; C_{1-6} alkyl, such as methyl, ethyl, propyl isomers (e.g. n-propyl and isopropyl), cyclopropyl, butyl isomers, cyclobutyl isomers (e.g. cyclobutyl and methylcyclopropyl), pentyl isomers, cyclopentyl isomers, hexyl isomers, cyclohexyl isomers, etc.; or C_{1-6} alkoxy, such as -O-methyl, -O-ethyl, isomers of -O-propyl, -O-cyclopropyl, isomers of -O-butyl, isomers of -O-cyclobutyl, isomers of -O-pentyl, isomers of -O-cyclopentyl, isomers of -O-hexyl, isomers of -O-cyclohexyl, etc. In some embodiments, R^{22} may be H.

[070] With respect to any relevant formula or structural depiction herein, some non-limiting examples of R^{23} may include R^A, F, Cl, CN, OR^A, CF_3, NO_2, NR^AR^B, COR^A, CO_2R^A, OCORA, NR^ACOR^B, $CONR^AR^B$, etc. In some embodiments, R^{23} may be H; F; Cl; CF_3; OH; NH_2; C_{1-6} alkyl, such as methyl, ethyl, propyl isomers (e.g. n-propyl and isopropyl), cyclopropyl, butyl isomers, cyclobutyl isomers (e.g. cyclobutyl and methylcyclopropyl), pentyl isomers, cyclopentyl isomers, hexyl isomers, cyclohexyl isomers, etc.; or C_{1-6} alkoxy, such as -O-methyl, -O-ethyl, isomers of -O-propyl, -O-cyclopropyl, isomers of -O-butyl, isomers of -O-cyclobutyl, isomers of -O-pentyl, isomers of -O-cyclopentyl, isomers of -O-hexyl, isomers of -O-cyclohexyl, etc. In some embodiments, R^{23} may be H.

[071] With respect to any relevant formula or structural depiction herein, some non-limiting examples of R^{24} may include R^A, F, Cl, CN, OR^A, CF_3, NO_2, NR^AR^B, COR^A, CO_2R^A, OCORA, NR^ACOR^B, $CONR^AR^B$, etc. In some embodiments, R^{24} may be H; F; Cl; CF_3; OH; NH_2; C_{1-6} alkyl, such as methyl, ethyl, propyl isomers (e.g. n-propyl and isopropyl), cyclopropyl, butyl isomers, cyclobutyl isomers (e.g. cyclobutyl and methylcyclopropyl), pentyl isomers, cyclopentyl isomers, hexyl isomers, cyclohexyl isomers, etc.; or C_{1-6} alkoxy, such as -O-methyl, -O-ethyl, isomers of -O-propyl, -O-cyclopropyl, isomers of -O-butyl, isomers of -O-cyclobutyl, isomers of -O-pentyl, isomers of -O-cyclopentyl, isomers of -O-hexyl, isomers of -O-cyclohexyl, etc. In some embodiments, R^{24} may be H. In some embodiments R^{24} is methyl.

[072] In some embodiments, R_{19} and R_{24} are methyl.

[073] With respect to any relevant formula or structural depiction herein, some non-limiting examples of R^{25} may include R^A, F, Cl, CN, OR^A, CF_3, NO_2, NR^AR^B, COR^A, CO_2R^A, OCORA, NR^ACOR^B, $CONR^AR^B$, etc. In some embodiments, R^{25} may be H; F; Cl; CF_3; OH; NH_2; C_{1-6} alkyl, such as methyl, ethyl, propyl isomers (e.g. n-propyl and isopropyl), cyclopropyl, butyl isomers, cyclobutyl isomers (e.g. cyclobutyl and methylcyclopropyl), pentyl isomers, cyclopentyl isomers, hexyl isomers, cyclohexyl isomers, etc.; or C_{1-6} alkoxy, such as -O-methyl, -O-ethyl, isomers of -O-propyl, -O-cyclopropyl, isomers of -O-butyl, isomers of -O-cyclobutyl, isomers of -O-pentyl, isomers of -O-cyclopentyl, isomers of -O-hexyl, isomers of -O-cyclohexyl, etc. In some embodiments, R^{25} may be H.

[074] With respect to any relevant formula or structural depiction herein, some non-limiting examples of R^{26} may include R^A, F, Cl, CN, OR^A, CF_3, NO_2, NR^AR^B, COR^A, CO_2R^A, OCORA, NR^ACOR^B, $CONR^AR^B$, etc. In some embodiments, R^{26} may be H; F; Cl; CF_3; OH; NH_2; C_{1-6} alkyl, such as methyl, ethyl, propyl isomers (e.g. n-propyl and isopropyl), cyclopropyl, butyl isomers, cyclobutyl isomers (e.g. cyclobutyl and methylcyclopropyl), pentyl isomers, cyclopentyl isomers, hexyl isomers, cyclohexyl isomers, etc.; or C_{1-6} alkoxy, such as -O-methyl, -O-ethyl, isomers of -O-propyl, -O-cyclopropyl, isomers of -O-butyl, isomers of -O-cyclobutyl, isomers of -O-pentyl, isomers of -O-cyclopentyl, isomers of -O-hexyl, isomers of -O-cyclohexyl, etc. In some embodiments, R^{26} may be H. In some embodiments R^{26} is methyl.

[075] In some embodiments, R_{19}, R_{21}, R_{24}, and R_{26} are methyl.

[076] In some embodiments, R_{21} and R_{26} are methyl.

[077] With respect to any relevant formula or structural depiction herein, some non-limiting examples of R^{27} may include R^A, F, Cl, CN, OR^A, CF_3, NO_2, NR^AR^B, COR^A, CO_2R^A, OCORA, NR^ACOR^B, $CONR^AR^B$, etc. In some embodiments, R^{27} may be H; F; Cl; CF_3; OH; NH_2; C_{1-6} alkyl, such as methyl, ethyl, propyl isomers (e.g. n-propyl and isopropyl), cyclopropyl, butyl isomers, cyclobutyl isomers (e.g. cyclobutyl and methylcyclopropyl), pentyl isomers, cyclopentyl isomers, hexyl isomers, cyclohexyl isomers, etc.; or C_{1-6} alkoxy, such as -O-methyl, -O-ethyl, isomers of -O-propyl, -O-cyclopropyl, isomers of -O-butyl, isomers of -O-cyclobutyl,

isomers of -O-pentyl, isomers of -O-cyclopentyl, isomers of -O-hexyl, isomers of -O-cyclohexyl, etc. In some embodiments, R^{27} may be H.

[078] With respect to any relevant formula or structural depiction herein, some non-limiting examples of R^{28} may include R^A, F, Cl, CN, OR^A, CF_3, NO_2, NR^AR^B, COR^A, CO_2R^A, OCORA, NR^ACOR^B, $CONR^AR^B$, etc. In some embodiments, R^{28} may be H; F; Cl; CF_3; OH; NH_2; C_{1-6} alkyl, such as methyl, ethyl, propyl isomers (e.g. n-propyl and isopropyl), cyclopropyl, butyl isomers, cyclobutyl isomers (e.g. cyclobutyl and methylcyclopropyl), pentyl isomers, cyclopentyl isomers, hexyl isomers, cyclohexyl isomers, etc.; or C_{1-6} alkoxy, such as -O-methyl, -O-ethyl, isomers of -O-propyl, -O-cyclopropyl, isomers of -O-butyl, isomers of -O-cyclobutyl, isomers of -O-pentyl, isomers of -O-cyclopentyl, isomers of -O-hexyl, isomers of -O-cyclohexyl, etc. In some embodiments, R^{28} may be H.

[079] With respect to any relevant formula or structural depiction herein, some non-limiting examples of R^{29} may include R^A, F, Cl, CN, OR^A, CF_3, NO_2, NR^AR^B, COR^A, CO_2R^A, OCORA, NR^ACOR^B, $CONR^AR^B$, etc. In some embodiments, R^{29} may be H; F; Cl; CF_3; OH; NH_2; C_{1-6} alkyl, such as methyl, ethyl, propyl isomers (e.g. n-propyl and isopropyl), cyclopropyl, butyl isomers, cyclobutyl isomers (e.g. cyclobutyl and methylcyclopropyl), pentyl isomers, cyclopentyl isomers, hexyl isomers, cyclohexyl isomers, etc.; or C_{1-6} alkoxy, such as -O-methyl, -O-ethyl, isomers of -O-propyl, -O-cyclopropyl, isomers of -O-butyl, isomers of -O-cyclobutyl, isomers of -O-pentyl, isomers of -O-cyclopentyl, isomers of -O-hexyl, isomers of -O-cyclohexyl, etc. In some embodiments, R^{29} may be H.

[080] With respect to any relevant formula or structural depiction herein, some non-limiting examples of R^{30} may include R^A, F, Cl, CN, OR^A, CF_3, NO_2, NR^AR^B, COR^A, CO_2R^A, OCORA, NR^ACOR^B, $CONR^AR^B$, etc. In some embodiments, R^{30} may be H; F; Cl; CF_3; OH; NH_2; C_{1-6} alkyl, such as methyl, ethyl, propyl isomers (e.g. n-propyl and isopropyl), cyclopropyl, butyl isomers, cyclobutyl isomers (e.g. cyclobutyl and methylcyclopropyl), pentyl isomers, cyclopentyl isomers, hexyl isomers, cyclohexyl isomers, etc.; or C_{1-6} alkoxy, such as -O-methyl, -O-ethyl, isomers of -O-propyl, -O-cyclopropyl, isomers of -O-butyl, isomers of -O-cyclobutyl, isomers of -O-pentyl, isomers of -O-cyclopentyl, isomers of -O-hexyl, isomers of -O-cyclohexyl, etc. In some embodiments, R^{30} may be H.

[081] With respect to any relevant formula or structural depiction herein, some non-limiting examples of R^{31} may include R^A, F, Cl, CN, OR^A, CF_3, NO_2, NR^AR^B, COR^A, CO_2R^A, OCORA, NR^ACOR^B, $CONR^AR^B$, etc. In some embodiments, R^{31} may be H; F; Cl; CF_3; OH; NH_2; C_{1-6} alkyl, such as methyl, ethyl, propyl isomers (e.g. n-propyl and isopropyl), cyclopropyl, butyl isomers, cyclobutyl isomers (e.g. cyclobutyl and methylcyclopropyl), pentyl isomers, cyclopentyl isomers, hexyl isomers, cyclohexyl isomers, etc.; or C_{1-6} alkoxy, such as -O-methyl, -O-ethyl, isomers of -O-propyl, -O-cyclopropyl, isomers of -O-butyl, isomers of -O-cyclobutyl, isomers of -O-pentyl, isomers of -O-cyclopentyl, isomers of -O-hexyl, isomers of -O-cyclohexyl, etc. In some embodiments, R^{31} may be H.

[082] With respect to any relevant formula or structural depiction herein, some non-limiting examples of R^{32} may include R^A, F, Cl, CN, OR^A, CF_3, NO_2, NR^AR^B, COR^A, CO_2R^A, OCORA, NR^ACOR^B, $CONR^AR^B$, etc. In some embodiments, R^{32} may be H; F; Cl; CF_3; OH; NH_2; C_{1-6} alkyl, such as methyl, ethyl, propyl isomers (e.g. n-propyl and isopropyl), cyclopropyl, butyl isomers, cyclobutyl isomers (e.g. cyclobutyl and methylcyclopropyl), pentyl isomers, cyclopentyl isomers, hexyl isomers, cyclohexyl isomers, etc.; or C_{1-6} alkoxy, such as -O-methyl, -O-ethyl, isomers of -O-propyl, -O-cyclopropyl, isomers of -O-butyl, isomers of -O-cyclobutyl, isomers of -O-pentyl, isomers of -O-cyclopentyl, isomers of -O-hexyl, isomers of -O-cyclohexyl, etc. In some embodiments, R^{32} may be H.

[083] With respect to any relevant formula or structural depiction herein, some non-limiting examples of R^{33} may include R^A, F, Cl, CN, OR^A, CF_3, NO_2, NR^AR^B, COR^A, CO_2R^A, OCORA, NR^ACOR^B, $CONR^AR^B$, etc. In some embodiments, R^{33} may be H; F; Cl; CF_3; OH; NH_2; C_{1-6} alkyl, such as methyl, ethyl, propyl isomers (e.g. n-propyl and isopropyl), cyclopropyl, butyl isomers, cyclobutyl isomers (e.g. cyclobutyl and methylcyclopropyl), pentyl isomers, cyclopentyl isomers, hexyl isomers, cyclohexyl isomers, etc.; or C_{1-6} alkoxy, such as -O-methyl, -O-ethyl, isomers of -O-propyl, -O-cyclopropyl, isomers of -O-butyl, isomers of -O-cyclobutyl, isomers of -O-pentyl, isomers of -O-cyclopentyl, isomers of -O-hexyl, isomers of -O-cyclohexyl, etc. In some embodiments, R^{33} may be H.

[084] With respect to any relevant formula or structural depiction herein, some non-limiting examples of R^{34} may include R^A, F, Cl, CN, OR^A, CF_3, NO_2, NR^AR^B, COR^A, CO_2R^A, OCORA, NR^ACOR^B, $CONR^AR^B$, etc. In some embodiments,

R^{34} may be H; F; Cl; CF_3; OH; NH_2; C_{1-6} alkyl, such as methyl, ethyl, propyl isomers (e.g. n-propyl and isopropyl), cyclopropyl, butyl isomers, cyclobutyl isomers (e.g. cyclobutyl and methylcyclopropyl), pentyl isomers, cyclopentyl isomers, hexyl isomers, cyclohexyl isomers, etc.; or C_{1-6} alkoxy, such as -O-methyl, -O-ethyl, isomers of -O-propyl, -O-cyclopropyl, isomers of -O-butyl, isomers of -O-cyclobutyl, isomers of -O-pentyl, isomers of -O-cyclopentyl, isomers of -O-hexyl, isomers of -O-cyclohexyl, etc. In some embodiments, R^{34} may be H.

[085] With respect to any relevant formula or structural depiction herein, some non-limiting examples of R^{35} may include R^A, F, Cl, CN, OR^A, CF_3, NO_2, NR^AR^B, COR^A, CO_2R^A, OCORA, NR^ACOR^B, $CONR^AR^B$, etc. In some embodiments, R^{35} may be H; F; Cl; CF_3; OH; NH_2; C_{1-6} alkyl, such as methyl, ethyl, propyl isomers (e.g. n-propyl and isopropyl), cyclopropyl, butyl isomers, cyclobutyl isomers (e.g. cyclobutyl and methylcyclopropyl), pentyl isomers, cyclopentyl isomers, hexyl isomers, cyclohexyl isomers, etc.; or C_{1-6} alkoxy, such as -O-methyl, -O-ethyl, isomers of -O-propyl, -O-cyclopropyl, isomers of -O-butyl, isomers of -O-cyclobutyl, isomers of -O-pentyl, isomers of -O-cyclopentyl, isomers of -O-hexyl, isomers of -O-cyclohexyl, etc. In some embodiments, R^{35} may be H.

[086] Some embodiments include optionally substituted N,N-diphenyl-4-(5-(6-(1-phenyl-1H-benzo[d]imidazol-2-yl)pyridin-3-yl)pyrazin-2-yl)aniline. In some embodiments, any substituents may independently be CH_3, C_2H_5, C_3H_7, F, or CF_3. In some embodiments, the compound is unsubstituted.

[087] Some embodiments include optionally substituted 4-methyl-N-(4-(5-(4-(1-phenyl-1H-benzo[d]imidazol-2-yl)phenyl)pyrazin-2-yl)phenyl)-N-(*p*-tolyl)aniline. In some embodiments, any substituents may independently be CH_3, C_2H_5, C_3H_7, F, or CF_3. In some embodiments, the compound is unsubstituted.

[088] Some embodiments include optionally substituted N-phenyl-N-(4-(5-(6-(1-phenyl-1H-benzo[d]imidazol-2-yl)pyridin-3-yl)pyrazin-2-yl)phenyl)naphthalen-1-amine. In some embodiments, any substituents may independently be CH_3, C_2H_5, C_3H_7, F, or CF_3. In some embodiments, the compound is unsubstituted.

[089] Some embodiments include optionally substituted N-phenyl-N-(4-(5-(4-(1-phenyl-1H-benzo[d]imidazol-2-yl)phenyl)pyrazin-2-yl)phenyl)naphthalen-1-amine. In some embodiments, any substituents may independently be CH_3, C_2H_5, C_3H_7, F, or CF_3. In some embodiments, the compound is unsubstituted.

[090] Some embodiments include optionally substituted 2-methyl-N-(4-(5-(4-(1-phenyl-1H-benzo[d]imidazol-2-yl)phenyl)pyrazin-2-yl)phenyl)-N-(o-tolyl)aniline. In some embodiments, any substituents may independently be CH_3, C_2H_5, C_3H_7, F, or CF_3. In some embodiments, the compound is unsubstituted.

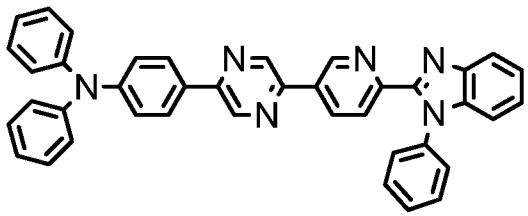
[091] Some embodiments include optionally substituted N-(2,4-dimethylphenyl)-2,4-dimethyl-N-(4-(5-(4-(1-phenyl-1H-benzo[d]imidazol-2-yl)phenyl)pyrazin-2-yl)phenyl)aniline. In some embodiments, any substituents may independently be CH_3, C_2H_5, C_3H_7, F, or CF_3. In some embodiments, the compound is unsubstituted.

[092] Some embodiments include optionally substituted N,N-diphenyl-4-(5-(4-(1-phenyl-1H-benzo[d]imidazol-2-yl)phenyl)pyrazin-2-yl)aniline. In some embodiments, any substituents may independently be CH_3, C_2H_5, C_3H_7, F, or CF_3. In some embodiments, the compound is unsubstituted.

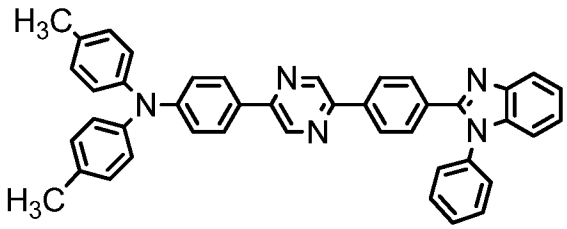
[093] Some embodiments include optionally substituted N-(4-(5-(4-(1-phenyl-1H-benzo[d]imidazol-2-yl)phenyl)pyrazin-2-yl)phenyl)-N-(o-tolyl)naphthalen-1-amine. In some embodiments, any substituents may independently be CH_3, C_2H_5, C_3H_7, F, or CF_3. In some embodiments, the compound is unsubstituted.

[094] Some embodiments include optionally substituted N-phenyl-N-(4-(5-(4-(1-phenyl-1H-benzo[d]imidazol-2-yl)phenyl)pyrazin-2-yl)phenyl)naphthalen-2-amine. In some embodiments, any substituents may independently be CH_3, C_2H_5, C_3H_7, F, or CF_3. In some embodiments, the compound is unsubstituted.

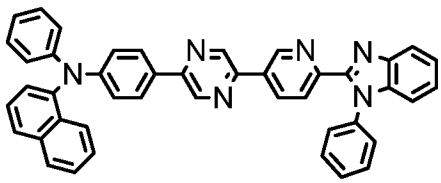
[095] Some embodiments include optionally substituted 9-phenyl-3-(5-(4-(1-phenyl-1H-benzo[d]imidazol-2-yl)phenyl)pyrazin-2-yl)-9H-carbazole. In some embodiments, any substituents may independently be CH_3, C_2H_5, C_3H_7, F, or CF_3. In some embodiments, the compound is unsubstituted.



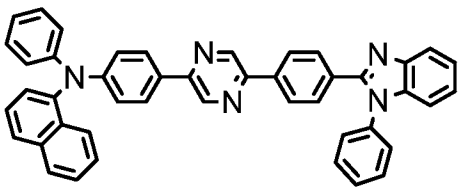
N,N-diphenyl-4-(5-(6-(1-phenyl-1H-benzo[d]imidazol-2-yl)pyridin-3-yl)pyrazin-2-yl)aniline (BE-1),



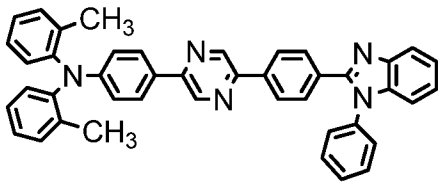
4-methyl-N-(4-(5-(4-(1-phenyl-1H-benzo[d]imidazol-2-yl)phenyl)pyrazin-2-yl)phenyl)-N-(*p*-tolyl)aniline (BE-2)



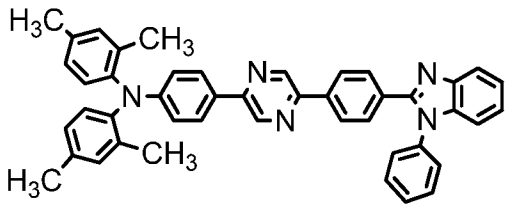
N-phenyl-N-(4-(5-(6-(1-phenyl-1H-benzo[d]imidazol-2-yl)pyridin-3-yl)pyrazin-2-yl)phenyl)naphthalen-1-amine (BE-3),



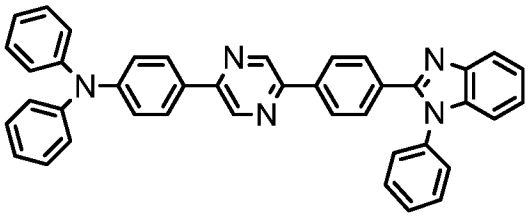
N-phenyl-N-(4-(5-(4-(1-phenyl-1H-benzo[d]imidazol-2-yl)phenyl)pyrazin-2-yl)phenyl)naphthalen-1-amine (BE-4),



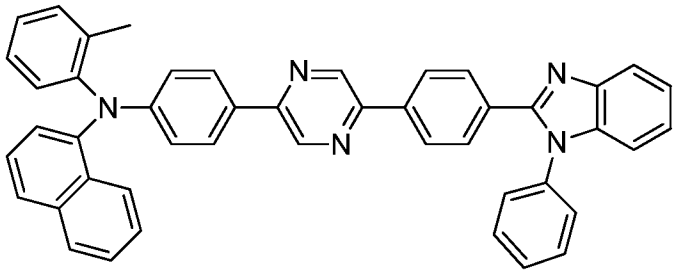
2-methyl-N-(4-(5-(4-(1-phenyl-1H-benzo[d]imidazol-2-yl)phenyl)pyrazin-2-yl)phenyl)-N-(o-tolyl)aniline (BE-5),



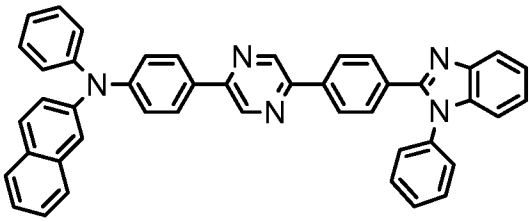
N-(2,4-dimethylphenyl)-2,4-dimethyl-N-(4-(5-(4-(1-phenyl-1H-benzo[d]imidazol-2-yl)phenyl)pyrazin-2-yl)phenyl)aniline (BE-6),



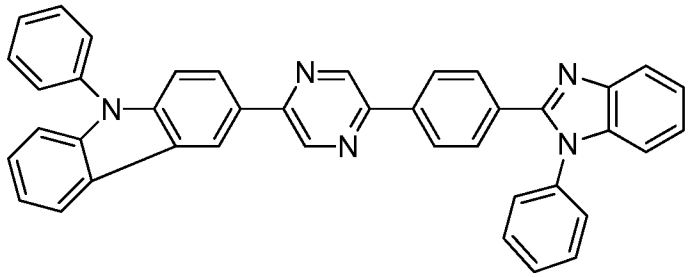
N,N-diphenyl-4-(5-(4-(1-phenyl-1H-benzo[d]imidazol-2-yl)phenyl)pyrazin-2-yl)aniline (BE-7),



N-(4-(5-(4-(1-phenyl-1H-benzo[d]imidazol-2-yl)phenyl)pyrazin-2-yl)phenyl)-N-(o-tolyl)naphthalen-1-amine (BE-8)



N-phenyl-N-(4-(5-(4-(1-phenyl-1H-benzo[d]imidazol-2-yl)phenyl)pyrazin-2-yl)phenyl)naphthalen-2-amine (BE-9)



9-phenyl-3-(5-(4-(1-phenyl-1H-benzo[d]imidazol-2-yl)phenyl)pyrazin-2-yl)-9H-carbazole (BE-10)

[096] In some embodiments, a compound of any of the formulae, structures and/or names above (hereinafter referred to as "a subject compound") may be electroluminescent, or may be fluorescent or phosphorescent. In some embodiments, the compound has fluorescence in the blue or violet visible light range or phosphorescence in the red, orange, yellow, and/or green visible light range. In some embodiments, the compound may have a lowest energy triplet state with an energy over than about 2.5 eV, such as about 2.5 eV to about 4 eV, about 2.5 eV to about 3.5 eV, or about 3 eV to about 3.5 eV.

[097] In some embodiments, a light-emitting device is provided, comprising a compound described above.

[098] In some embodiments, a light emitting device is provided, wherein the compound is an emissive material in an emissive layer.

[099] Some embodiments include a composition comprising a subject compound. A composition comprising a subject compound may further comprise a fluorescent compound or a phosphorescent compound, and may be useful for light emission in devices such as organic light-emitting devices.

[100] In some embodiments, an organic light-emitting device comprises a subject compound. For example, an organic component comprising a subject compound may be disposed between an anode and a cathode. The organic component may further comprise an emissive layer, wherein a subject compound is in the emissive layer. In some embodiments, the device is configured so that electrons can be transferred from the cathode to the organic component and holes can be transferred from the anode to the organic component.

[101] The subject compounds may have high photostability and thermal stability in organic light-emitting devices. The subject compounds may also have well balanced hole and electron injection rates and mobilities. This may provide OLED devices with high efficiencies and/or long lifetimes. The subject compounds may also form amorphous solids, which may make the compounds easy to form into films.

[102] Some embodiments may have a structure represented by FIG. 1. A hole-injection layer **10** is disposed on the anode **5**. A hole-transport layer **15** is disposed on the hole-injection layer **15**. The emissive layer **20** is disposed on the hole-transport layer **15**. An electron-transport layer **30** is disposed on the emissive layer **20**, and the cathode **35** is disposed on the electron-transport layer **30**.

[103] The anode may be a layer comprising a conventional material such as a metal, mixed metal, alloy, metal oxide or mixed-metal oxide, conductive polymer, and/or an inorganic material such as carbon nanotube (CNT). Examples of suitable metals include the Group 1 metals, the metals in Groups 4, 5, 6, and the Group 8-10 transition metals. If the anode layer is to be light-transmitting, metals in Group 10 and 11, such as Au, Pt, and Ag, or alloys thereof; or mixed-metal oxides of Group 12, 13, and 14 metals, such as indium-tin-oxide (ITO), indium-zinc-oxide (IZO), and the like, may be used. In some embodiments, the anode layer may be an organic material such as polyaniline. The use of polyaniline is described in "Flexible light-emitting diodes made from soluble conducting polymer," Nature, vol. 357, pp. 477-479 (11 June 1992). In some embodiments, the anode layer can have a thickness in the range of about 1 nm to about 1000 nm.

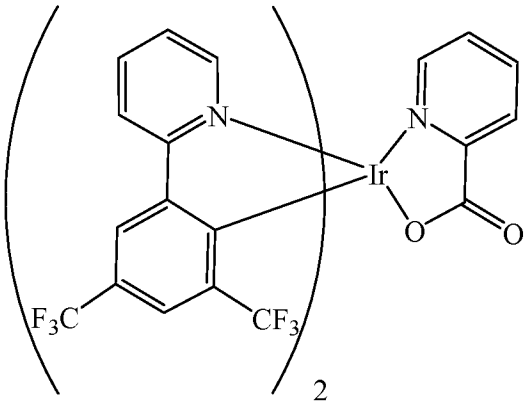
[104] A cathode may be a layer including a material having a lower work function than the anode layer. Examples of suitable materials for the cathode layer include alkali metals of Group 1, Group 2 metals, Group 12 metals including rare earth elements, lanthanides and actinides, materials such as aluminum, indium, calcium, barium, samarium and magnesium, and combinations thereof. Li-containing organometallic compounds, LiF, and Li_2O may also be deposited between the organic layer and the cathode layer to lower the operating voltage. Suitable low work function metals include but are not limited to Al, Ag, Mg, Ca, Cu, Mg/Ag, LiF/Al,

CsF, CsF/Al or alloys thereof. In some embodiments, the cathode layer can have a thickness in the range of about 1 nm to about 1000 nm.

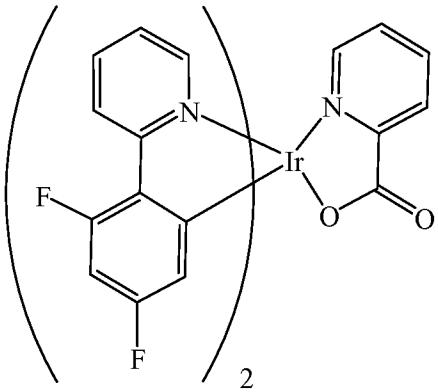
[105] In some embodiments, the organic component may comprise at least one light-emitting layer comprising a light-emitting component and a subject compound as a host. The amount of the subject compound in a light-emitting layer may vary. In one embodiment, the amount of a subject compound in a light-emitting layer is in the range of from about 1% to about 99.9% by weight of the light-emitting layer. In another embodiment, the amount of a subject compound in a light-emitting layer is in the range of from about 90% to about 99% by weight of the light-emitting layer. In another embodiment, the amount of a subject compound in a light-emitting layer is about 97% by weight of the light-emitting layer. In some embodiments, the mass of the light-emitting component is about 0.1% to about 10%, about 1% to about 5%, or about 3% of the mass of the light-emitting layer. The light-emitting component may be a fluorescent and/or a phosphorescent compound.

[106] A light-emitting component may comprise an iridium coordination compound such as: bis-{2-[3,5-bis(trifluoromethyl)phenyl]pyridinato-N,C2'}iridium(III)-picolinate; bis(2-[4,6-difluorophenyl]pyridinato-N,C2')iridium (III) picolinate; bis(2-[4,6-difluorophenyl]pyridinato-N,C2')iridium(acetylacetonate); Iridium (III) bis(4,6-difluorophenylpyridinato)-3-(trifluoromethyl)-5-(pyridin-2-yl)-1,2,4-triazolate; Iridium (III) bis(4,6-difluorophenylpyridinato)-5-(pyridin-2-yl)-1H-tetrazolate; bis[2-(4,6-difluorophenyl)pyridinato-N,$C^{2'}$]iridium(III)tetra(1-pyrazolyl)borate; Bis[2-(2'-benzothienyl)-pyridinato-N,C3'] iridium (III)(acetylacetonate); Bis[(2-phenylquinolyl)-N,C2']iridium (III) (acetylacetonate); Bis[(1-phenylisoquinolinato-N,C2')]iridium (III) (acetylacetonate); Bis[(dibenzo[f, h]quinoxalino-N,C2')iridium (III)(acetylacetonate); Tris(2,5-bis-2'-(9',9'-dihexylfluorene)pyridine)iridium (III); Tris[1-phenylisoquinolinato-N,C2']iridium (III); Tris-[2-(2'-benzothienyl)-pyridinato-N,C3'] iridium (III); Tris[1-thiophen-2-ylisoquinolinato-N,C3']iridium (III); Tris[1-(9,9-dimethyl-9H-fluoren-2-yl)isoquinolinato-(N,C3')iridium (III)); Bis(2-phenylpyridinato-N,C2')iridium(III)(acetylacetonate) [$Ir(ppy)_2(acac)$]; Bis(2-(4-tolyl)pyridinato-N,C2')iridium(III)(acetylacetonate) [$Ir(mppy)_2(acac)$]; Bis(2-(4-*tert*-butyl)pyridinato-N,C2')iridium (III)(acetylacetonate) [$Ir(t\text{-}Buppy)_2(acac)$]; Tris(2-phenylpyridinato-N,C2')iridium (III) [$Ir(ppy)_3$]; Bis(2-phenyloxazolinato-N,C2')iridium (III) (acetylacetonate) [$Ir(op)_2(acac)$]; Tris(2-(4-tolyl)pyridinato-N,C2')iridium(III)

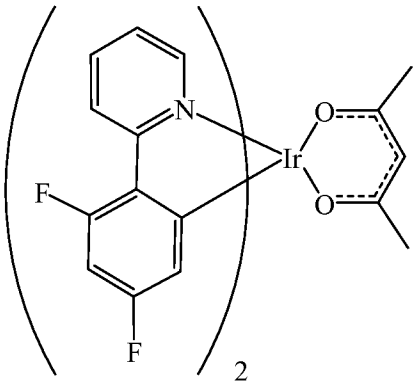
[Ir(mppy)$_3$]; Bis[2-phenylbenzothiazolato-N,C2'] iridium (III)(acetylacetonate); Bis[2-(4-tert-butylphenyl)benzothiazolato-N,C2']iridium(III)(acetylacetonate); Bis[(2-(2'-thienyl)pyridinato-N,C3')]iridium (III) (acetylacetonate); Tris[2-(9.9-dimethylfluoren-2-yl)pyridinato-(N,C3')]iridium (III); Tris[2-(9.9-dimethylfluoren-2-yl)pyridinato-(N,C3')]iridium (III); Bis[5-trifluoromethyl-2-[3-(N-phenylcarbzolyl)pyridinato-N,C2']iridium(III)(acetylacetonate); (2-PhPyCz)$_2$Ir(III)(acac); etc.



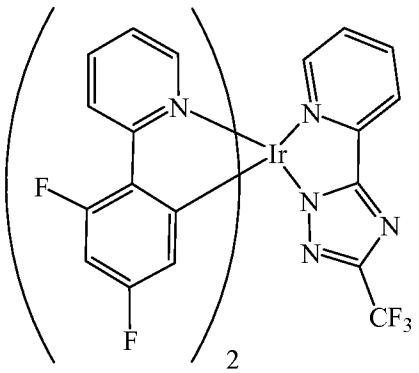
bis-{2-[3,5-bis(trifluoromethyl)phenyl]pyridinato-N,C2'}iridium(III)-picolinate (Ir(CF$_3$ppy)$_2$(Pic)



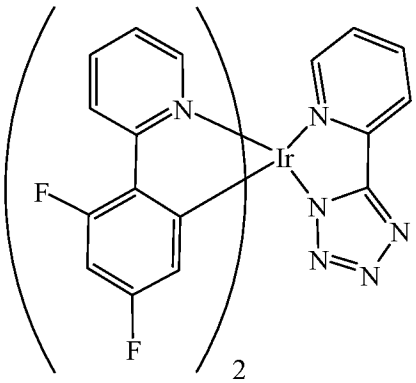
bis(2-[4,6-difluorophenyl]pyridinato-N,C2')iridium (III) picolinate [FIrPic]



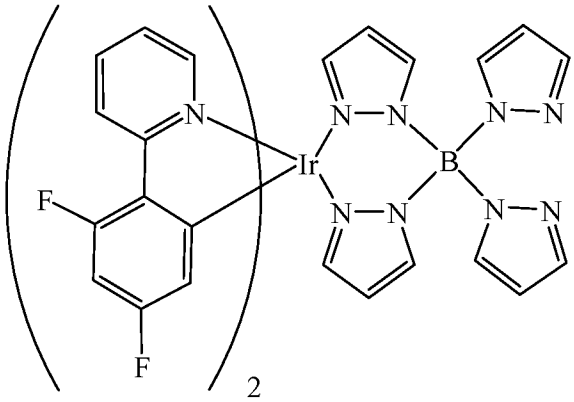
bis(2-[4,6-difluorophenyl]pyridinato-N,C2')iridium(acetylacetonate) [FIr(acac)]



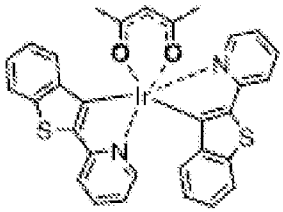
Iridium (III) bis(4,6-difluorophenylpyridinato)-3-(trifluoromethyl)-5-(pyridin-2-yl)-1,2,4-triazolate (FIrtaz)



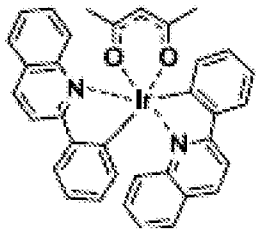
Iridium (III) bis(4,6-difluorophenylpyridinato)-5-(pyridin-2-yl)-1H-tetrazolate (FlrN4)



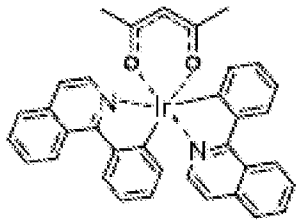
bis[2-(4,6-difluorophenyl)pyridinato-N,C$^{2'}$]iridium(III)tetra(1-pyrazolyl)borate (Fir6)



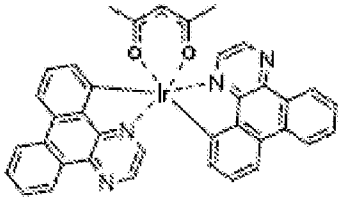
Ir(btp)$_2$(acac); (Btp)$_2$Ir(III)(acac); or Bis[2-(2'-benzothienyl)-pyridinato-N,C3'] iridium (III)(acetylacetonate)



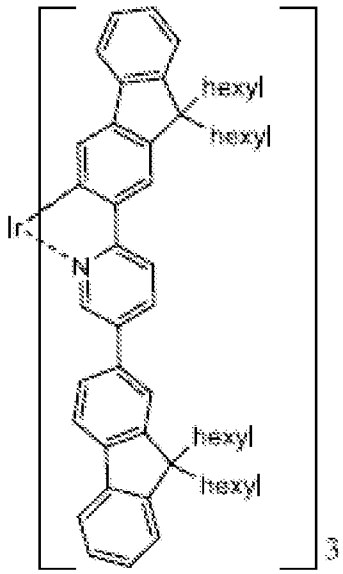
Ir(pq)2(acac); (Pq)$_2$Ir(III)(acac); or Bis[(2-phenylquinolyl)-N,C2']iridium (III) (acetylacetonate)



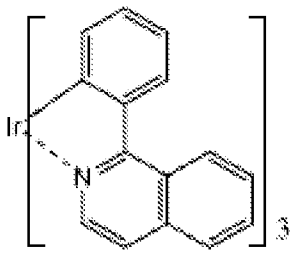
Ir(piq)2(acac); (Piq)$_2$Ir(III)(acac); or Bis[(1-phenylisoquinolinato-N,C2')]iridium (III) (acetylacetonate)



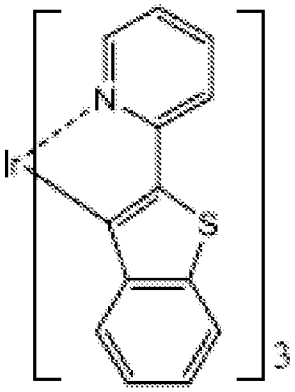
Ir(DBQ)2(acac); $(DBQ)_2Ir(acac)$; or Bis[(dibenzo[f, h]quinoxalino-N,C2')iridium (III)(acetylacetonate)



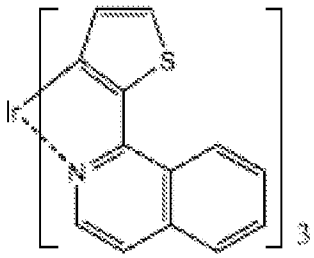
$Ir(HFP)_3$ or Tris(2,5-bis-2'-(9',9'-dihexylfluorene)pyridine)iridium (III)



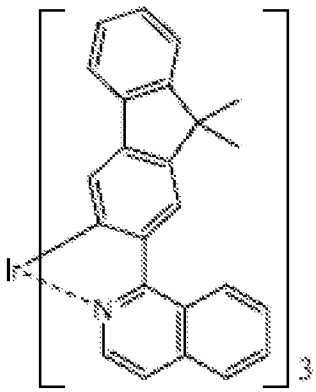
$Ir(piq)_3$; or Tris[1-phenylisoquinolinato-N,C2']iridium (III)



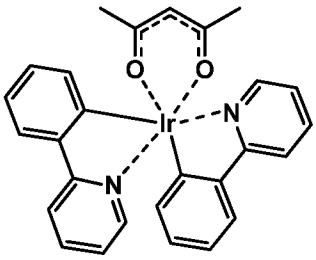
$Ir(btp)_3$ or Tris-[2-(2'-benzothienyl)-pyridinato-N,C3'] iridium (III)



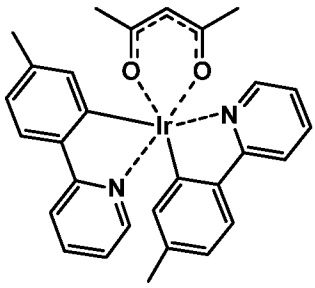
$Ir(tiq)_3$ or Tris[1-thiophen-2-ylisoquinolinato-N,C3']iridium (III)



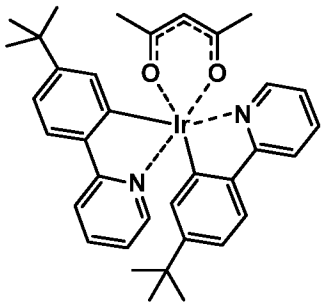
$Ir(flil)_3$; $Ir(fliq)_3$; or Tris[1-(9,9-dimethyl-9H-fluoren-2-yl)isoquinolinato-(N,C3')iridium (III))



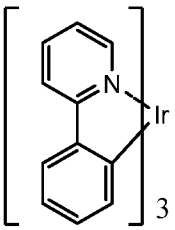
$Ir(ppy)_2(acac)$



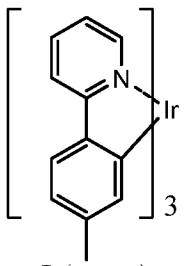
$Ir(mppy)_2(acac)$



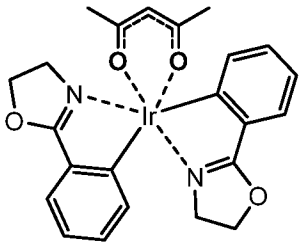
$Ir(t\text{-}Buppy)_2(acac)$



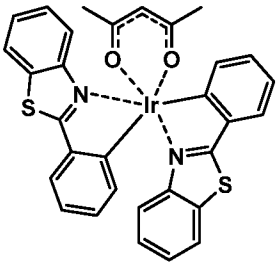
$Ir(ppy)_3$



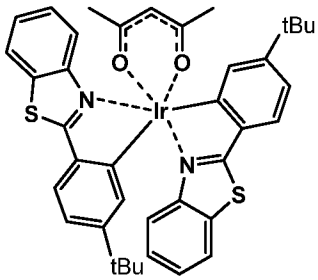
$Ir(mppy)_3$



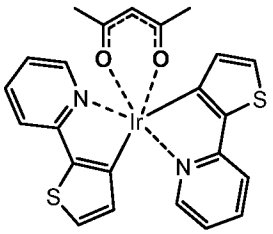
$Ir(op)_2(acac)$



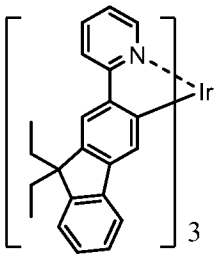
$(bt)_2Ir(III)(acac)$
Bis[2-phenylbenzothiazolato -N,C2'] iridium (III)(acetylacetonate)



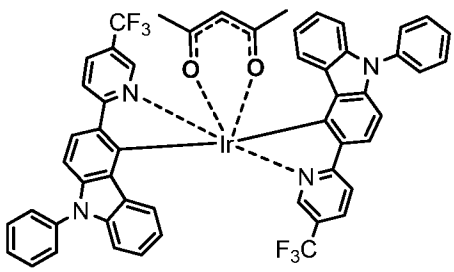
(t-$bt)_2Ir(III)(acac)$
Bis[2-(4-tert-butylphenyl)benzothiazolato-N,C2']iridium(III)(acetylacetonate)



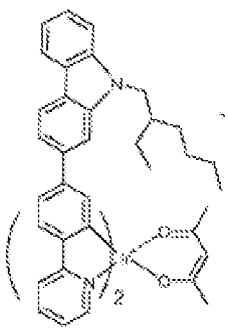
$(thp)_2Ir(III)(acac)$
Bis[(2-(2'-thienyl)pyridinato-N,C3')]iridium (III) (acetylacetonate)



$[Ir(Flpy)_3]$



$(Cz\text{-}CF_3)Ir(III)(acac)$



(2-

Tris[2-(9.9-dimethylfluoren-2-yl)pyridinato-(N,C3')]iridium (III)	Bis[5-trifluoromethyl-2-[3-(N-phenylcarbzolyl)pyridinato-N,C2']iridium(III)(acetylacetonate)	**$PhPyCz)_2Ir(III)(acac)$**

[107] The thickness of a light-emitting layer may vary. In one embodiment, a light-emitting layer has a thickness in the range of from about 1 nm to about 150 nm or about 200 nm.

[108] In some embodiments, the organic component may further comprise a hole-transport layer disposed between the anode and the light-emitting layer. The hole-transport layer may comprise at least one hole-transport material. Hole-transport materials may include, but are not limited to, an aromatic-substituted amine, a carbazole, a polyvinylcarbazole (PVK), e.g. poly(9-vinylcarbazole); polyfluorene; a polyfluorene copolymer; poly(9,9-di-n-octylfluorene-alt-benzothiadiazole); poly(paraphenylene); poly[2-(5-cyano-5-methylhexyloxy)-1,4-phenylene]; a benzidine; a phenylenediamine; a phthalocyanine metal complex; a polyacetylene; a polythiophene; a triphenylamine; an oxadiazole; copper phthalocyanine; 1,1-Bis(4-bis(4-methylphenyl) aminophenyl) cyclohexane; 2,9-Dimethyl-4,7-diphenyl-1,10-phenanthroline; 3,5-Bis(4-tert-butyl-phenyl)-4-phenyl[1,2,4]triazole; 3,4,5-Triphenyl-1,2,3-triazole; 4,4',4'-tris(3-methylphenylphenylamino)triphenylamine (MTDATA); N,N'-bis(3-methylphenyl)N,N'-diphenyl-[1,1'-biphenyl]-4,4'-diamine (TPD); 4,4'-bis[N-(naphthyl)-N-phenyl-amino]biphenyl (α-NPD); 4,4',4''-tris(carbazol-9-yl)-triphenylamine (TCTA); 4,4'-bis[N,N'-(3-tolyl)amino]-3,3'-dimethylbiphenyl (HMTPD); 4,4'-N,N'-dicarbazole-biphenyl (CBP); 1,3-N,N-dicarbazole-benzene (mCP); Bis[4-(p,p'-ditolyl-amino)phenyl]diphenylsilane (DTASi); 2,2'-bis(4-carbazolylphenyl)-1,1'-biphenyl (4CzPBP); N,N'N"-1,3,5-tricarbazoloylbenzene (tCP); N,N'-bis(4-butylphenyl)-N,N'-bis(phenyl)benzidine; or the like.

[109] In some embodiments, the organic component may further comprise an electron-transport layer disposed between the cathode and the light-emitting layer. Examples of electron-transport materials may include, but are not limited to, 2-(4-biphenylyl)-5-(4-*tert*-butylphenyl)-1,3,4-oxadiazole (PBD); 1,3-bis(N,N-t-butyl-phenyl)-1,3,4-oxadiazole (OXD-7), 1,3-bis[2-(2,2'-bipyridine-6-yl)-1,3,4-oxadiazo-5-yl]benzene; 3-phenyl-4-(1'-naphthyl)-5-phenyl-1,2,4-triazole (TAZ); 2,9-dimethyl-4,7-

diphenyl-phenanthroline (bathocuproine or BCP); aluminum tris(8-hydroxyquinolate) (Alq3); and 1,3,5-tris(2-N-phenylbenzimidazolyl)benzene; 1,3-bis[2-(2,2'-bipyridine-6-yl)-1,3,4-oxadiazo-5-yl]benzene (BPY-OXD); 3-phenyl-4-(1'-naphthyl)-5-phenyl-1,2,4-triazole (TAZ), 2,9-dimethyl-4,7-diphenyl-phenanthroline (bathocuproine or BCP); and 1,3,5-tris[2-N-phenylbenzimidazol-z-yl]benzene (TPBI). In one embodiment, the electron transport layer is aluminum quinolate (Alq_3), 2-(4-biphenylyl)-5-(4-*tert*-butylphenyl)-1,3,4-oxadiazole (PBD), phenanthroline, quinoxaline, 1,3,5-tris[N-phenylbenzimidazol-z-yl] benzene (TPBI), or a derivative or a combination thereof.

[110] If desired, additional layers may be included in the light-emitting device. These additional layers may include an electron-injecting layer (EIL), a hole-blocking layer (HBL), an exciton-blocking layer (EBL), and/or a hole-injecting layer (HIL). In addition to separate layers, some of these materials may be combined into a single layer.

[111] In some embodiments, the light-emitting device can include an electron-injecting layer between the cathode layer and the light-emitting layer. Other suitable electron-injecting materials may also be included, and are known to those skilled in the art. Examples of suitable material(s) that can be included in the electron-injecting layer include but are not limited to, an optionally substituted compound selected from the following: aluminum quinolate (Alq_3), 2-(4-biphenylyl)-5-(4-*tert*-butylphenyl)-1,3,4-oxadiazole (PBD), phenanthroline, quinoxaline, 1,3,5-tris[N-phenylbenzimidazol-z-yl] benzene (TPBI) a triazine, a metal chelate of 8-hydroxyquinoline such as tris(8-hydroxyquinoliate) aluminum, and a metal thioxinoid compound such as bis(8-quinolinethiolato) zinc. In one embodiment, the electron-injecting layer is aluminum quinolate (Alq_3), 2-(4-biphenylyl)-5-(4-*tert*-butylphenyl)-1,3,4-oxadiazole (PBD), phenanthroline, quinoxaline, 1,3,5-tris[N-phenylbenzimidazol-z-yl] benzene (TPBI), or a derivative or a combination thereof.

[112] In some embodiments, the device can include a hole-blocking layer, e.g., between the cathode and the light-emitting layer. Various suitable hole-blocking materials that can be included in the hole-blocking layer are known to those skilled in the art. Suitable hole-blocking material(s) include but are not limited to, an optionally substituted compound selected from the following: bathocuproine (BCP), 3,4,5-triphenyl-1,2,4-triazole, 3,5-bis(4-*tert*-butyl-phenyl)-4-phenyl-[1,2,4] triazole, 2,9-

dimethyl-4,7-diphenyl-1,10-phenanthroline, and 1,1-bis(4-bis(4-methylphenyl)aminophenyl)-cyclohexane.

[113] In some embodiments, the light-emitting device can include an exciton-blocking layer, e.g., between the light-emitting layer and the anode. In an embodiment, the band gap of the material(s) that comprise exciton-blocking layer is large enough to substantially prevent the diffusion of excitons. A number of suitable exciton-blocking materials that can be included in the exciton-blocking layer are known to those skilled in the art. Examples of material(s) that can compose an exciton-blocking layer include an optionally substituted compound selected from the following: aluminum quinolate (Alq_3), 4,4'-bis[N-(naphthyl)-N-phenyl-amino]biphenyl (α-NPD), 4,4'-N,N'-dicarbazole-biphenyl (CBP), and bathocuproine (BCP), and any other material(s) that have a large enough band gap to substantially prevent the diffusion of excitons.

[114] In some embodiments, the light-emitting device can include a hole-injecting layer, e.g., between the light-emitting layer and the anode. A hole-injecting layer may comprise a subject compound as a hole-injecting material. Other examples of suitable hole-injecting material(s) include, but are not limited to, an optionally substituted compound selected from the following: a polythiophene derivative such as poly(3,4-ethylenedioxythiophene (PEDOT)/polystyrene sulphonic acid (PSS), a benzidine derivative such as N, N, N', N'-tetraphenylbenzidine, poly(N,N'-bis(4-butylphenyl)-N,N'-bis(phenyl)benzidine), a triphenyl amine or phenylenediamine derivative such as N,N'-bis(4-methylphenyl)-N,N'-bis(phenyl)-1,4-phenylenediamine, 4,4',4"-tris(N-(naphthylen-2-yl)-N-phenylamino)triphenylamine, an oxadiazole derivative such as 1,3-bis(5-(4-diphenylamino)phenyl-1,3,4-oxadiazol-2-yl)benzene, a polyacetylene derivative such as poly(1,2-bis-benzylthio-acetylene), and a phthalocyanine metal complex derivative such as phthalocyanine copper.

[115] Light-emitting devices comprising a subject compound can be fabricated using techniques known in the art, as informed by the guidance provided herein. For example, a glass substrate can be coated with a high work functioning metal such as ITO which can act as an anode. After patterning the anode layer, a hole-injecting and/or hole-transport layer may be deposited on the anode in that order. A light-emitting layer that includes a light-emitting component, can be

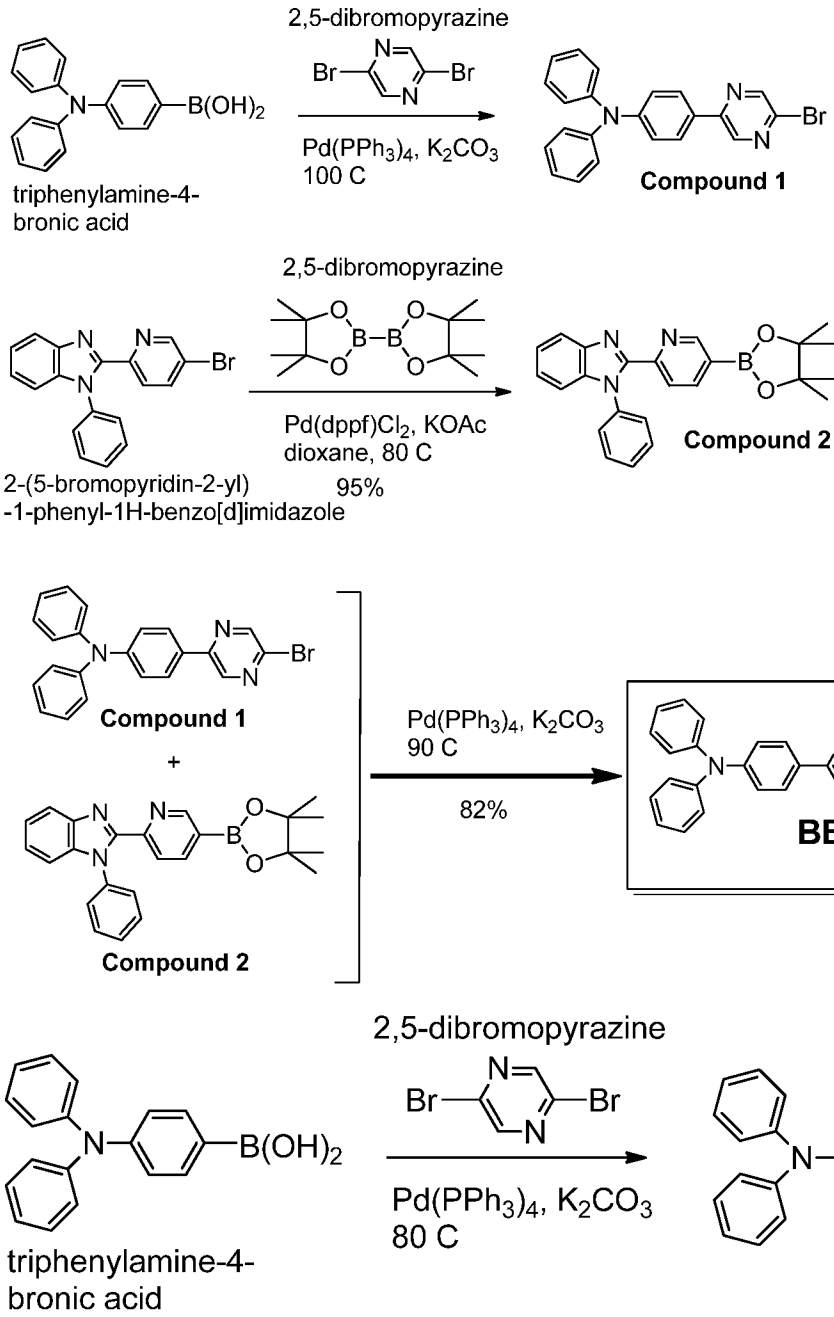
deposited on the anode, the hole-transport layer, or the hole-injecting layer. The light-emitting layer may contain a subject compound. An electron-transport layer and/or an electron-injecting layer may deposited in that order on the light-emitting component. The cathode layer, comprising a low work functioning metal (e.g., Mg:Ag), can then be deposited, e.g., by vapor deposition or sputtering. The device may also contain an exciton-blocking layer, an electron blocking layer, a hole blocking layer, a second light-emitting layer, or other layers that can be added to the device using suitable techniques.

[116] In some embodiments, a device comprising the subject compounds can provide a significantly increased device lifetime compared with commercially available compounds. In some embodiments, the devices can provide a T50(h) @ 10000 nit lifetime of at least about 125, 150, 175, 185, and/or 200 hours. In some embodiments, the desired lifetime can be determined by examining the luminescent/emissive decay of the device by measuring the luminescent, e.g., cd/m2, after applying a constant current of a 16 mA to device (corresponding to about 10000 cd/m^2) for a device having an active emissive area of about 13.2 mm^2.

3. Synthetic Examples
4. Example 1.1

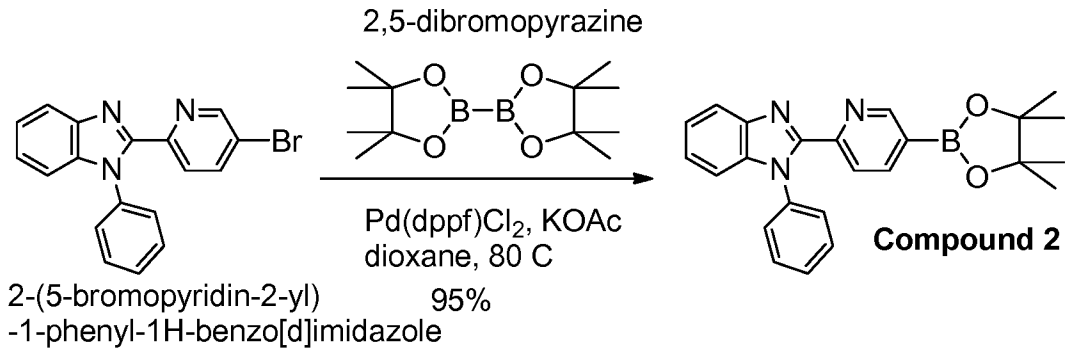
8-1. Example of synthesis

Synthesis of BE-1

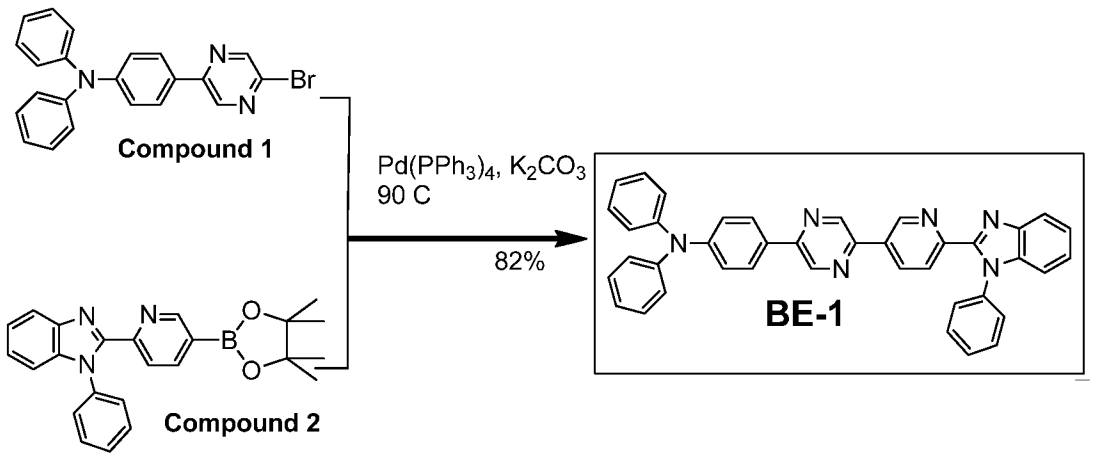


[117] 4-(5-bromopyrazin-2-yl)-N,N-diphenylaniline (**Compound 1**): A mixture of triphenylamine-4-bronic acid (1.0 g, 3.46 mmol), 2,5-dibromopyrazine (1.81 g, 7.6 mmol), $Pd(PPh_3)_4$ (0.2 g, 0.17 mmol) and K_2CO_3 (1.05g, 7.6 mmol) in dioxane/water (40 mL/8 mL) was degassed and heated at about 80ºC for about 15 hours. The whole was worked up with ethyl acetate (200 mL), washed with brine. The organic phase was dried over Na_2SO_4, loaded on silica gel, purified by flash column using the eluents of hexanes to hexanes/dichloromethane (2:1 to 1:1 to 1:2).

The desired fraction was collected, and removal of solvent gave a yellow solid (**Compound 1**) (0.99 g, in 71% yield).



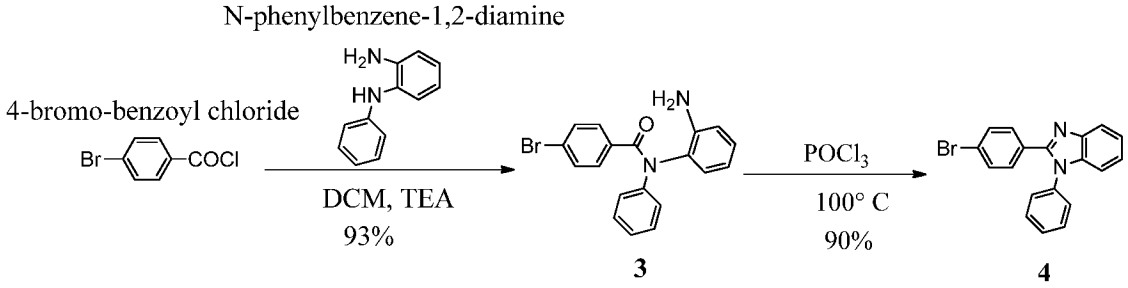
[118] 1-Phenyl-2-(5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pyridin-2-yl)-1H-benzo[d]imidazole (**Compound 2**): A mixture of 2-(5-bromopyridin-2-yl)-1-phenyl-1H-benzo[d]imidazole (1.015 g, 2.9 mmol), bis(pinacolato)diboron (0.76 g, 3 mmol), KOAc (0.49 g, 5 mmol) and Pd(dppf)Cl2 (0.11 g, 0.15 mmol) in dioxane (50 mL) was degassed and heated at about 80ºC for about 15 hours. The whole was worked up with dichloromethane/brine. The organic phase was collected and dried over Na_2SO_4. After removal of solvent, the resulting brown oil (**Compound 2**) was used for next step without further purification.

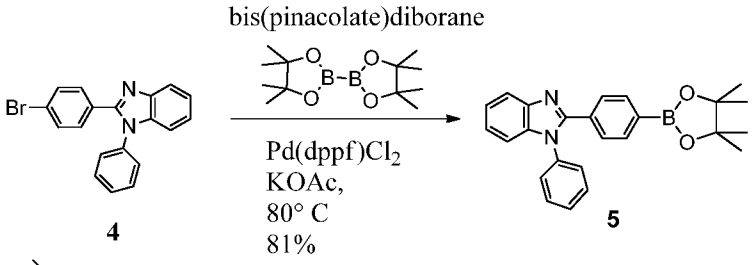


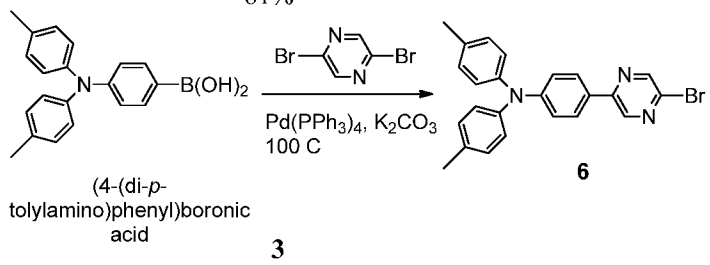
[119] Compound BE-1: A mixture of 4-(5-bromopyrazin-2-yl)-N,N-diphenylaniline (**Compound 1**) (0.99 g, 2.46 mmol), 1-phenyl-2-(5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pyridin-2-yl)-1H-benzo[d]imidazole (**Compound 2**) (1.15 g, 2.9 mmol), $Pd(PPh_3)_4$ (0.22 g, 0.19 mmol) and K_2CO_3 (1.0 g, 7.2 mmol) in

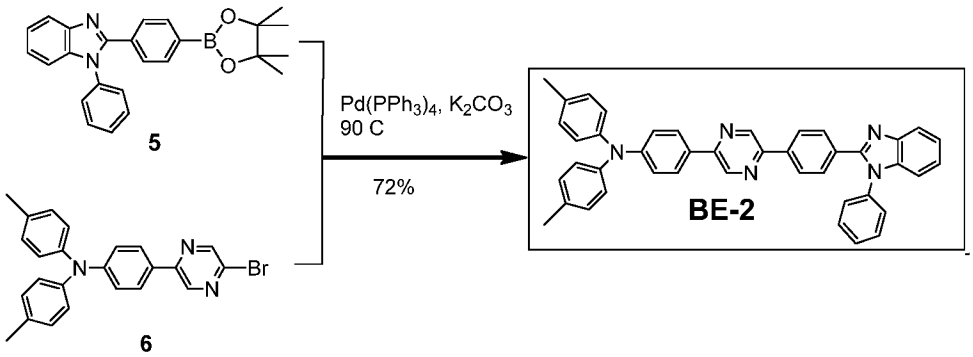
dioxane/water (60 mL/10 mL), was degassed and heated at about 85°C overnight. Yellow precipitate formed. After filtration, the solid was collected and washed with methanol, then hot dichloromethane (500 mL). A yellow solid (**BE-1**) was collected, 1.20 g, in 82% yield. Confirmed by LCMS (APCI+): calcd for $C_{40}H_{29}N_6$ (M+H): 593; found 593.

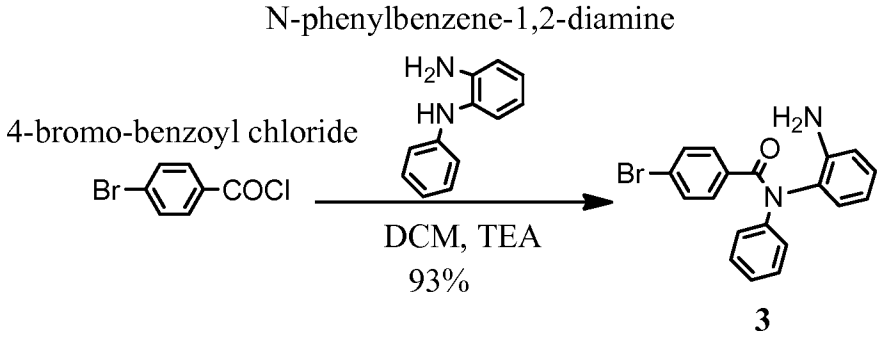
Synthesis of **BE-2**


N-phenylbenzene-1,2-diamine
4-bromo-benzoyl chloride
DCM, TEA
93%
POCl3
100° C
90%
3
4

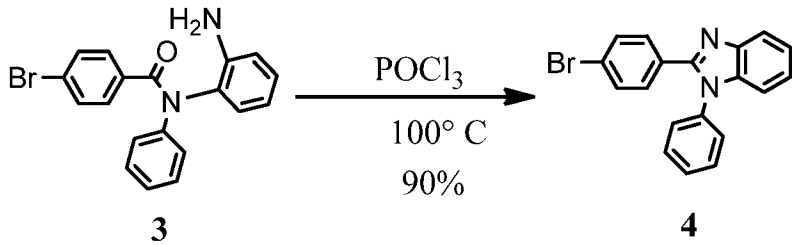

bis(pinacolate)diborane
Pd(dppf)Cl2
KOAc,
80° C
81%
4
5


Pd(PPh3)4, K2CO3
100 C
(4-(di-p-tolylamino)phenyl)boronic acid
3
6

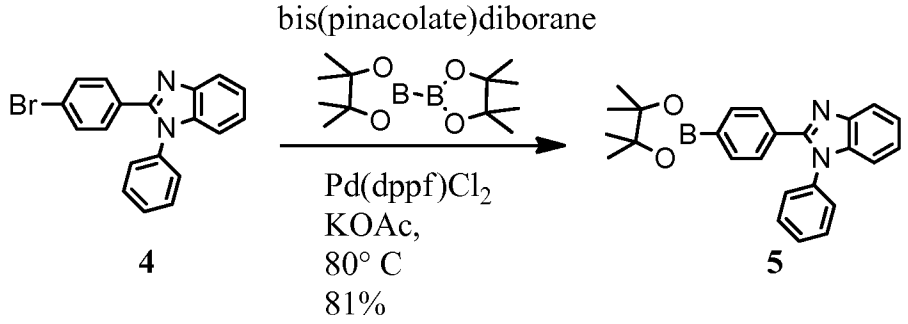

Pd(PPh3)4, K2CO3
90 C
72%
BE-2
5
6



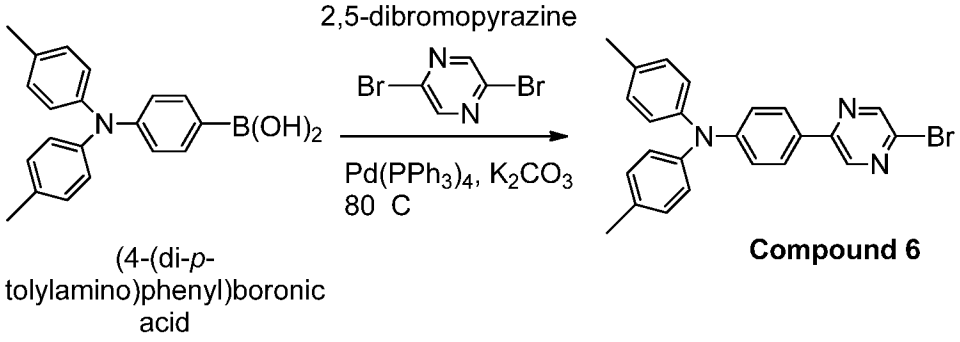
[120] 4-Bromo-N-(2-(phenylamino)phenyl)benzamide (Compound 3): To a solution of 4-bromo-benzoyl chloride (11 g, 50 mmol) in anhydrous dichloromethane (DCM) (100 ml), was added N-phenylbenzene-1,2-diamine (10.2 g, 55 mmol), then triethylamine (TEA) (17 ml, 122 mmol) slowly. The whole was stirred at room temperature (RT) overnight. Filtration gave a white solid **3** (6.5 g). The filtrate was worked up with water (300 ml), then extracted with DCM (300 mL) three times. The organic phase was collected and dried over $MgSO_4$, concentrated and recrystallized in DCM/hexanes to give another portion of white solid **3** (10.6 g). Total amount of product **3** is 17.1 g, in 93% yield.



[121] 2-(4-bromophenyl)-1-phenyl-1H-benzo[d]imidazole (4): To a suspension of amide **3** (9.6 g, 26 mmol) in anhydrous 1,4-dioxane (100 mL) was added phosphorus oxychloride ($POCl_3$) (9.2 mL, 100 mmol) slowly. The whole was then heated at 100° C overnight. After cooling to RT, the mixture was poured into ice (200 g) with stirring. Filtration, followed by recrystallization in DCM/hexanes gave a pale grey solid **4** (8.2 g, in 90% yield).

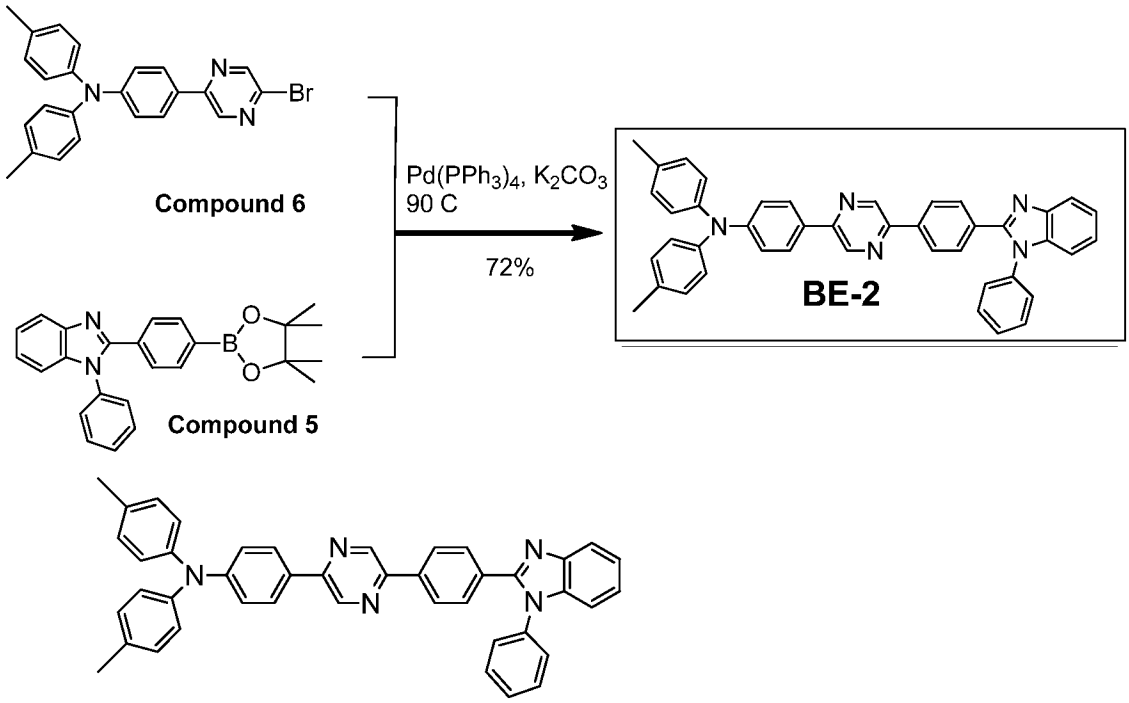


[122] 1-phenyl-2-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)-1H-benzo[d]imidazole (5): A mixture of Compound **4** (0.70 g, 2 mmol), bis(pinacolate)diborane (0.533g, 2.1 mmol), bis(diphenylphosphino)ferrocene]dichloropalladium ($Pd(dppf)Cl_2$) (0.060 g, 0.08 mmol) and anhydrous potassium acetate (KOAc) (0.393 g, 4mmol) in 1,4-dioxane (20 ml) was heated at about 80° C under argon overnight. After cooling to RT, the whole was diluted with ethyl acetate (80 ml) then filtered. The solution was absorbed on silica gel, then purified by column chromatography (hexanes/ethyl acetate 5:1 to 3:1) to give a white solid **5** (0.64 g, in 81% yield).



[123] 4-(5-bromopyrazin-2-yl)-N,N-di-*p*-tolylaniline (**Compound 6**): A mixture of (4-(di-***p***-tolylamino)phenyl)boronic acid (0.74 g, 2.33 mmol), 2,5-dibromopyrazine (1.19 g, 5 mmol), $Pd(PPh_3)_4$ (0.14 g, 0.12 mmol) and K_2CO_3 (0.69 g, 5 mmol) in dioxane/water (80 mL/10 mL) was degassed and heated at about 80°C overnight. The whole was diluted with ethyl acetate (250 mL), washed with brine, dried over Na_2SO_4, loaded on silica gel column and purified by flash column using eluents of hexanes to hexanes/dichloromethane (3:1). The desired fraction was

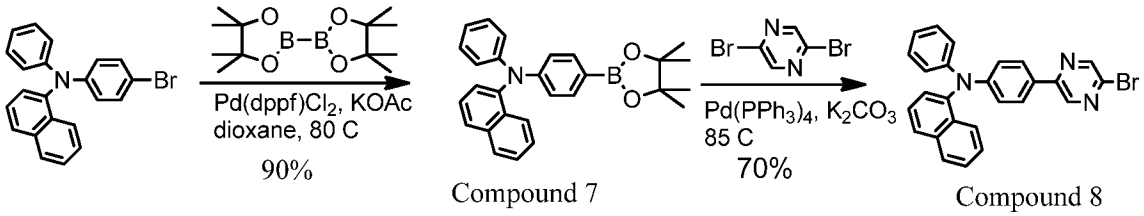
collected, and a yellow solid (**6**) was obtained after removal of solvents, 0.63 g, in 63% yield.

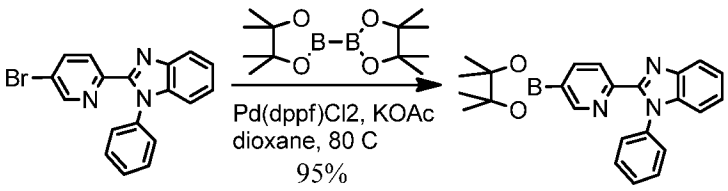


Chemical Formula: $C_{43}H_{33}N_5$
Molecular Weight: 619.76

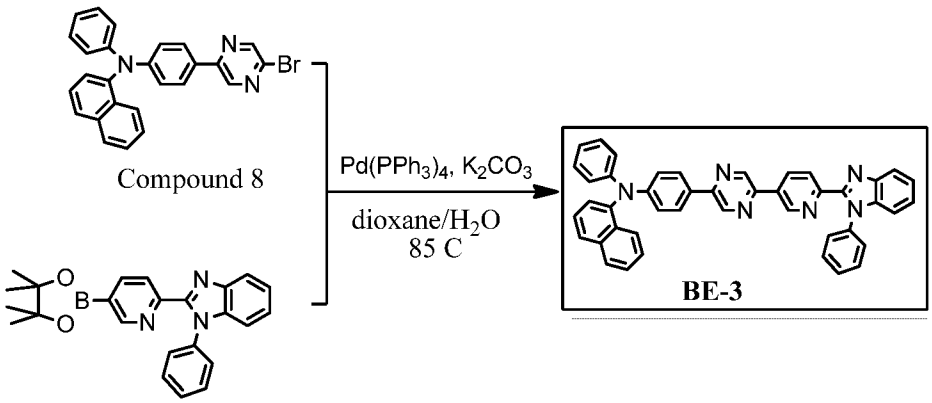
[124] Compound **BE-2**: A mixture of 4-(5-bromopyrazin-2-yl)-N,N-di-***p***-tolylaniline (**Compound 6**) (0.63 g, 1.46 mmol), 1-phenyl-2-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)-1H-benzo[d]imidazole (0.58 g, 1.46 mmol) (**Compound 5**), $Pd(PPh_3)_4$ (0.115 g, 0.1 mmol) and K_2CO_3 (0.414 g, 3 mmol) in dioxane/water (50 mL/10 mL) was degassed and heated at about 90ºC overnight. The resulting solution was diluted with ethyl acetate (250 mL), washed with brine, dried over Na_2SO_4, loaded on silica gel and purified by flash column using eluents of hexanes to dichloromethane to dichloromethane/ethyl acetate 4:1. The desired yellow fraction was collected, concentrated, recrystallized in dichloromethane/hexanes to give a yellow crystalline solid (**Compound 6**) (0.74 g, in 82% yield). Confirmed by LCMS (APCI+): calcd for C43H34N5 (M+H): 620; found: 620.

Synthesis of **BE-3**

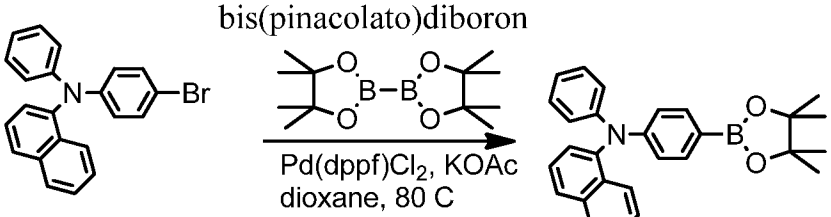




Compound 2



bis(pinacolato)diboron

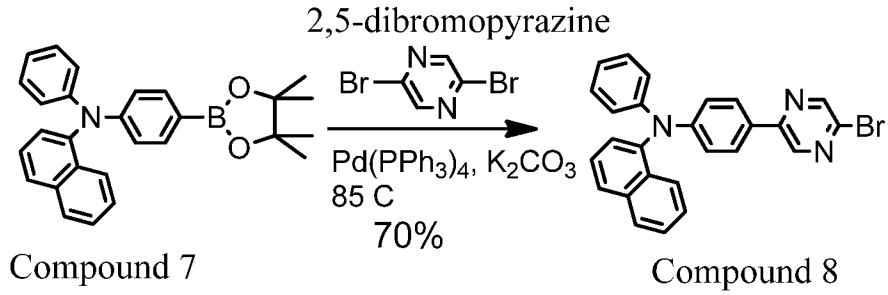


N-(4-bromophenyl)-N-phenylnaphthalen-1-amine 90%

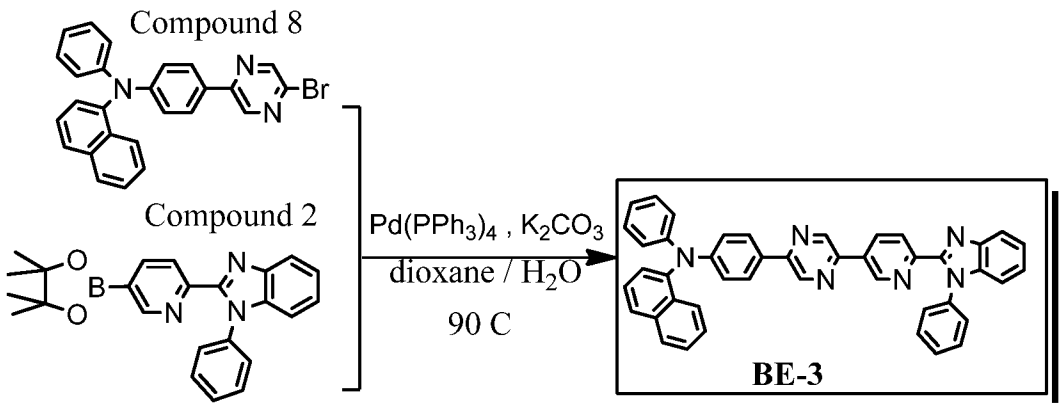
Compound 7

[125] N-phenyl-N-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)naphthalen-1-amine (Compound 7): A mixture of N-(4-bromophenyl)-N-phenylnaphthalen-1-amine (7.14g, 19.1 mmol), bis(pinacolato)diboron (5.08 g, 20 mmol), $Pd(dppf)Cl_2$ (0.73 g, 1.0 mmol) and KOAc (4.9 mmol, 50 mmol) in dioxane

(100 mL) was degassed and heated at about 85ºC for 15 hours. The resulting mixture was poured into ethyl acetate (250 mL), filtered off precipitate, loaded on silica gel and purified by flash column using eluents of hexanes to hexanes/dichloromethane (8:1 to 6:1 to 2:1). The desired fraction was collected, and after removal of solvent to give a white solid (**Compound 7**) (6.0 g, in 75% yield).

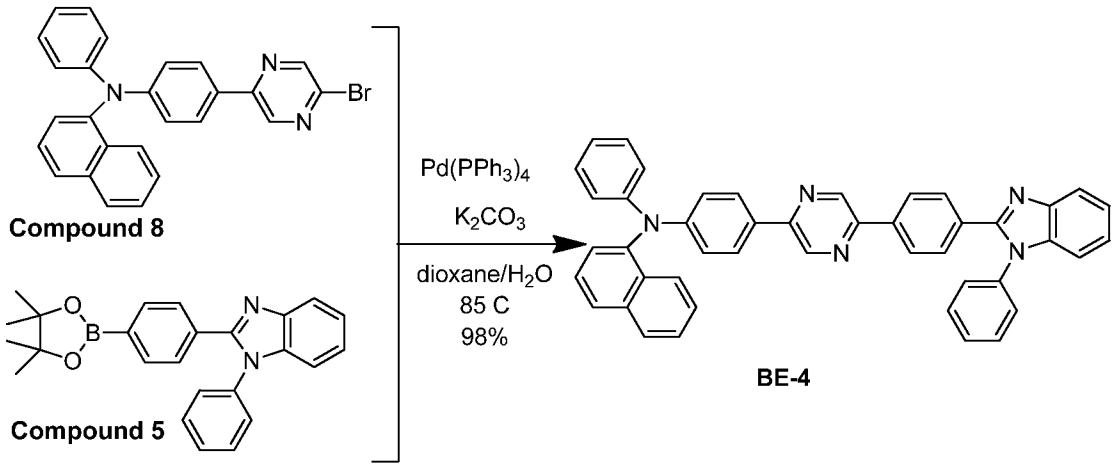


[126] N-**(4-(5-bromopyrazin-2-yl)phenyl)-N-phenylnaphthalen-1-amine** (**Compound 8**): A mixture of N-phenyl-N-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)naphthalen-1-amine (**Compound 7**) (2.91 g, 6.91 mmol), 2,5-dibromopyrazine (3.56 g, 13.8 mmol), $Pd(PPh_3)_4$ (0.346g, 0.3 mmol), K_2CO_3 (1.93 g, 14 mmol) in dioxane/water (80 mL/15 mL), was degassed and heated at about 85ºC overnight. The resulting mixture was diluted with ethyl acetate (250 mL), washed with brine, dried over Na_2SO_4, loaded on silica gel and purified by flash column using eluents of hexanes to hexanes/dichloromethane 4:1 to 2:1 to 3:2). The desired fraction was collected, after removal of solvent to give a yellow solid (**Compound 8**) (2.2 g, in 70.4% yield).



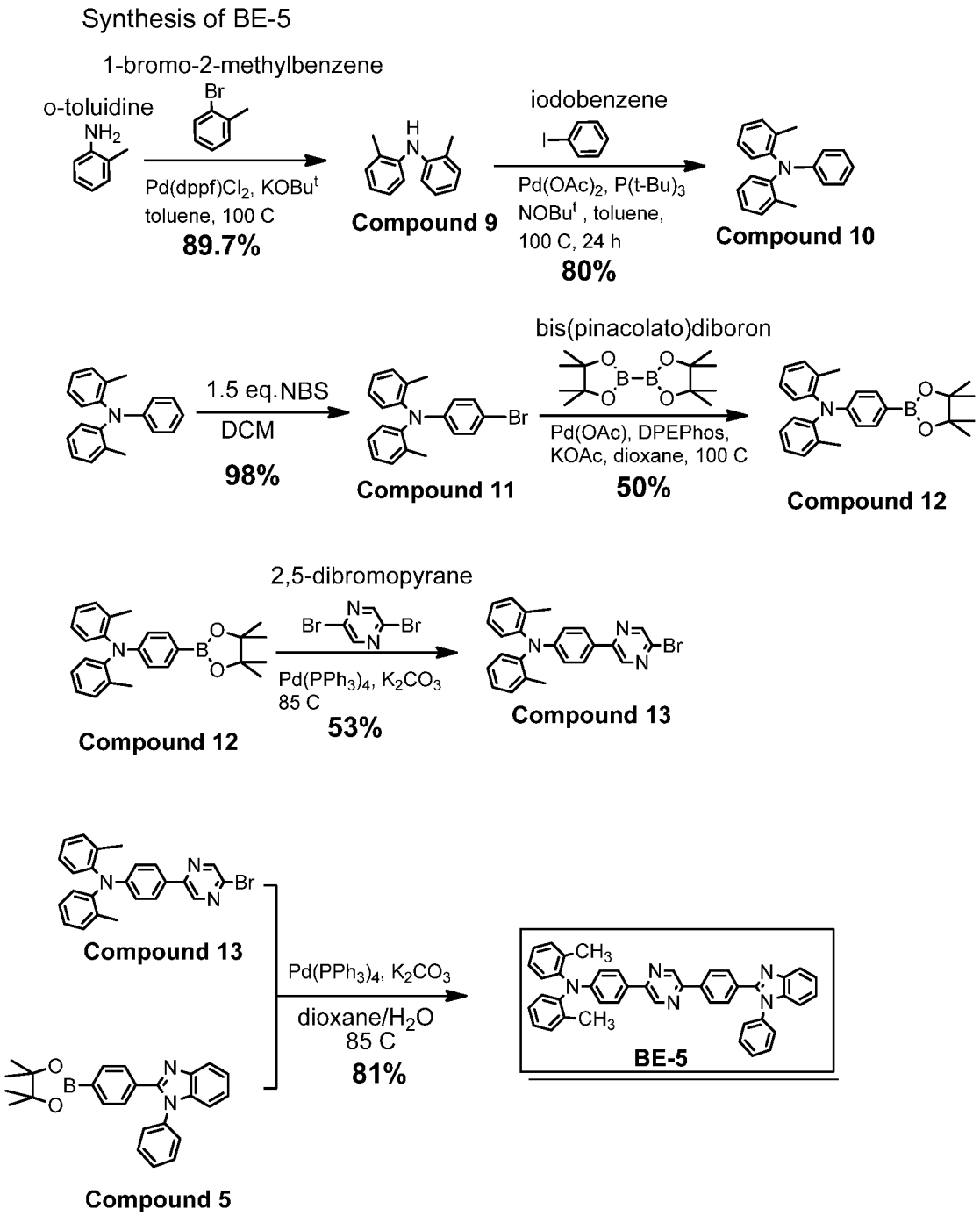
[127] Compound **BE-3**: a mixture of N-(4-(5-bromopyrazin-2-yl)phenyl)-N-phenylnaphthalen-1-amine (**Compound 8**) (1.17 g, 2.6 mmol), 1-phenyl-2-(5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pyridin-2-yl)-1H-benzo[d]imidazole (**Compound 2**) (2.9 mmol), $Pd(PPh_3)_4$ (0.138 g, 0.12 mmol) and K_2CO_3 (0.69 g, 5 mmol) in dioxane/water (70 mL/16 mL) was degassed and heated at about 90°C overnight. The resulting mixture was diluted with ethyl acetate (200 mL), washed with brine, dried over Na_2SO_4, loaded on silica gel and purified by flash column using eluents of hexanes/dichloromethane 1:1 to 1:2 to dichloromethane to dichloromethane/ethyl acetate 10:1 to 4:1. The desired fraction was collected and concentrated to give a yellow solid (1.39 g, in 83% yield). Confirmed by LCMS (APCI+): calcd for $C_{44}H_{31}N_6$ (M+H): 643; found: 643.

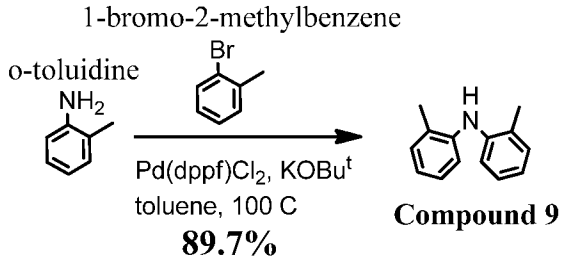
Synthesis of **BE-4**



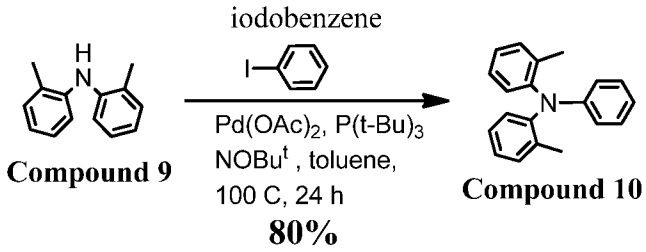
[128] Compound **BE-4**: A mixture of N-(4-(5-bromopyrazin-2-yl)phenyl)-N-phenylnaphthalen-1-amine (**Compound 8**)(1.11 g, 2.46 mmol), 1-phenyl-2-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)-1H-benzo[d]imidazole (**Compound 5**) (0.95 g, 2.4 mmol), $Pd(PPh_3)_4$ (0.14 g, 0.12 mmol) and K_2CO_3 (0.69 g, 5 mmol) in dioxane/water (70 mL/15 mL) was degassed and heated at 85°C overnight. The mixture was diluted with ethyl acetate (200 mL), washed with brine, dried over Na_2SO_4, loaded on silica gel and purified by flash column using eluents of hexanes/dichloromethane 1:1 to dichloromethane to dichloromethane/ethyl acetate 9:1. The desired fraction was collected, concentrated and recrystallized in

dichloromethane/hexanes to give yellow solid (**BE-4**) (1.50 g, in 98% yield). Confirmed by LCMS (APCI+): calcd for $C_{45}H_{32}N_5$ (M+H): 642; Found: 642.

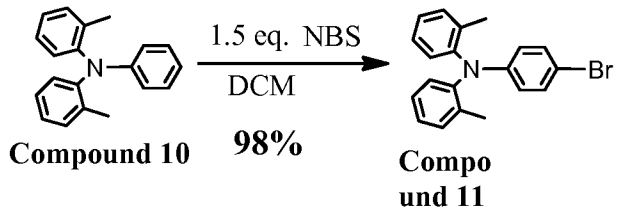




[129] **di-*o*-tolylamine** (**Compound 9**): A mixture of *o*-toluidine (6.05 g, 56.5 mmol), 1-bromo-2-methylbenzene (8.5 g, 50 mmol), $Pd(dppf)Cl_2$ and sodium tert-butoxide (9.6 g, 0.1 mmol) in toluene (120 mL) was degassed and heated at about 100°C overnight. The mixture was purified by flash column using eluents of hexanes/dichloromethane 2:1 to give a white solid (**Compound 9**) (8.84 g, in 89.7% yield).

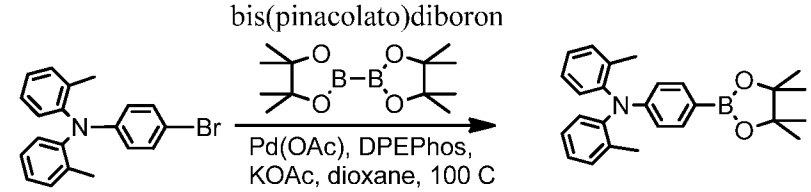


[130] 2-methyl-N-phenyl-N-(o-tolyl)aniline (**Compound 10**): A mixture of di-o-tolylamine (**Compound 9**) (6.00 g, 30.4 mmol), iodobenzene (12.2g, 60 mmol), $Pd(OAc)_2$ (0.34 g, 1.5 mmol), $P(t\text{-}Bu)_3$ (0.6 g, 3 mmol), sodium tert-butoxide (5.76 g, 60 mmol) in toluene (120 mL) was degassed and heated at about 120°C for 40 hours. The resulting mixture was diluted with ethyl acetate (200 mL), washed with brine, dried over Na_2SO_4, loaded on silica gel and purified by flash column using eluents of hexanes to give a white solid (**Compound 10**) (8.2 g, in 98% yield).



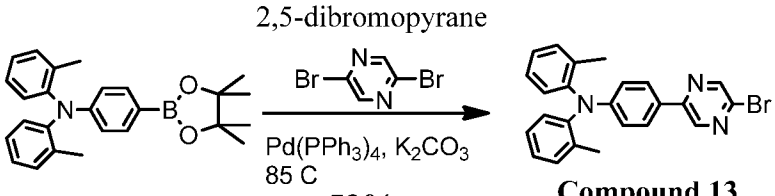
[131] N-(4-bromophenyl)-2-methyl-N-(o-tolyl)aniline (**Compound 11**): To a solution of 2-methyl-N-phenyl-N-(o-tolyl)aniline (**Compound 10**) (8.2 g, 30 mmol) in

dichloromethane (DCM) (100 mL), was added n-bromosuccinimide (NBS) (5.34 g, 30 mmol) at about 0°C and stirred for about 4 hours. The resulting mixture was worked up with dichloromethane/brine, dried over Na_2SO_4, loaded on silica gel and purified by flash column using eluents of hexanes to hexanes/dichloromethane 9:1. The desired fraction was collected, and removal of solvent gave a white solid (**Compound 11**) (10.7 g, in 100% yield).



Compound 11 **27%** **Compound 12**

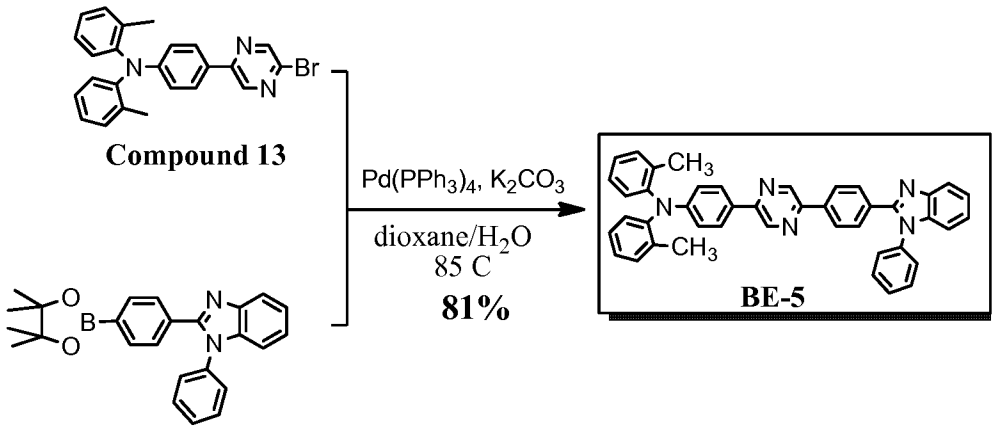
[132] 2-methyl-N-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)-N-(o-tolyl)aniline (**Compound 12**): A mixture of N-(4-bromophenyl)-2-methyl-N-(o-tolyl)aniline (**Compound 11**) (10.7 g, 30.4 mmol), bis(pinacolato)diboron (10.16 g, 40 mmol), KOAc (6.0 g, 0.1 mol), $Pd(OAc)_2$ (0.336 g, 1.5 mmol), Bis(2-diphenylphosphinophenyl)ether (1.614 g, 3 mmol) in dioxane (100 mL) was degassed and heated at about 100°C overnight. The resulting mixture was worked up with ethyl acetate/brine, dried over Na_2SO_4, loaded on silica gel and purified by flash column using eluents of hexanes to hexanes/dichloromethane 4:1. The desired fraction was collected and the solvent was removed to give a colorless oil (**Compound 12**) (3.3 g, in 27% yield).



Compound 12 **53%** **Compound 13**

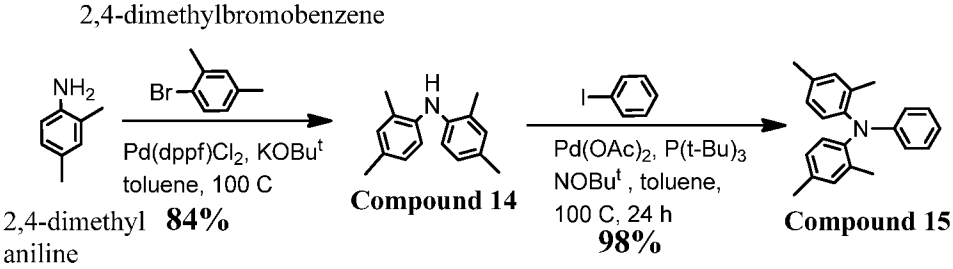
[133] N-(4-(5-bromopyrazin-2-yl)phenyl)-2-methyl-N-(o-tolyl)aniline (**Compound 13**): 2-methyl-N-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)-N-(o-tolyl)aniline (**Compound 12**) (3.3g, 8.3 mmol), 2,5-dibromopyrazine (4.27 g, 16 mmol), $Pd(PPh_3)_4$ (0.46 g, 0.4 mmol), K_2CO_3 (2.21 g, 16 mmol) in dioxane/water

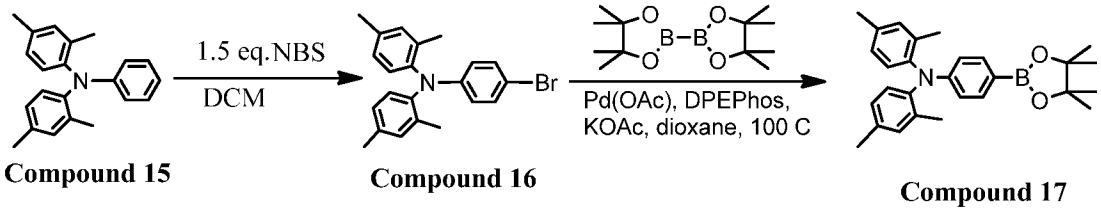
(100 mL/16 mL), was degassed and heated at about 80°C overnight. The resulting mixture was worked up with ethyl acetate/brine, dried over Na_2SO_4, loaded on silica gel, purified by flash column using eluents of hexanes to hexanes/dichloromethane 9:1 to 6:1 to 4:1). The desired fraction was collected, and a yellow solid (**Compound 13**) was obtained after removal of solvents (1.9 g, in 53% yield).

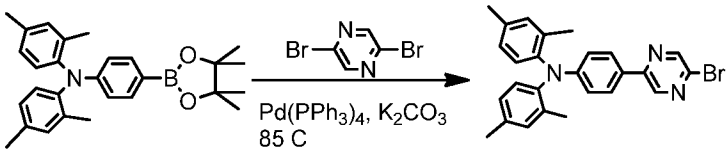


[134] Compound **BE-5**: a mixture of N-(4-(5-bromopyrazin-2-yl)phenyl)-2-methyl-N-(o-tolyl)aniline (**Compound 13**) (1.9 g, 4.4 mmol), 1-phenyl-2-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)-1H-benzo[d]imidazole (**Compound 5**) (1.75 g, 4.4 mmol), $Pd(PPh_3)_4$ (0.25 g, 0.22 mmol), K_2CO_3 (1.38 g, 10 mmol) in dioxane/water (100 mL/16 mL), was degassed and heated at about 90°C overnight. The resulting mixture was worked up with ethyl acetate/brine, dried over Na_2SO_4, loaded on silica gel and purified by flash column using eluents of hexanes to hexanes/dichloromethane 8:1 to 4:1 to dichloromethane/ethyl acetate 9:1. The desired fraction was collected, and after removal of solvent and recrystallization, gave a yellow solid (**Compound BE-5**) (2.2 g, in 80.6% yield). Confirmed by LCMS (APCI+): calcd for $C_{43}H_{34}N_5$ (M+H): 620; found: 620.

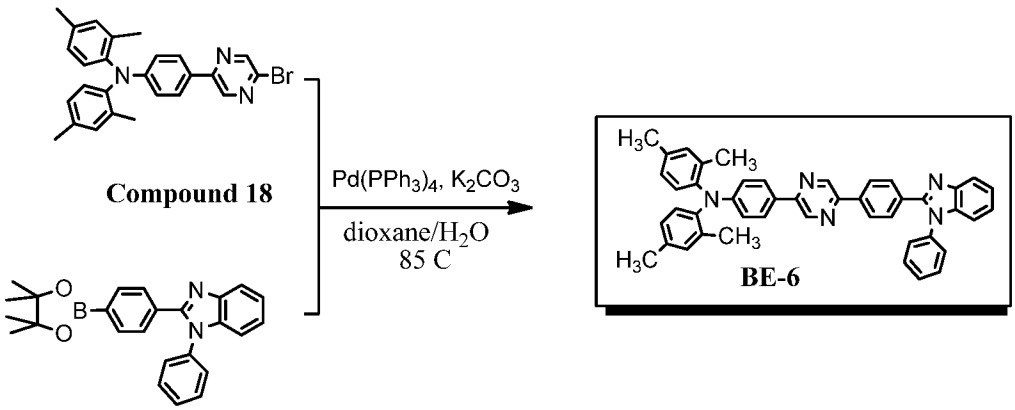
Synthesis of **BE-6**



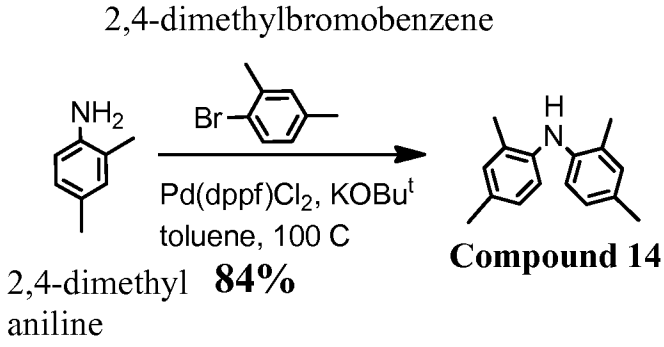




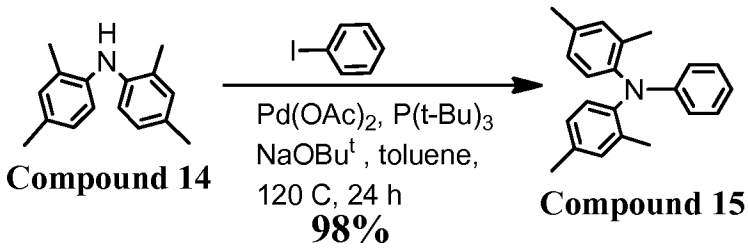
Compound 17



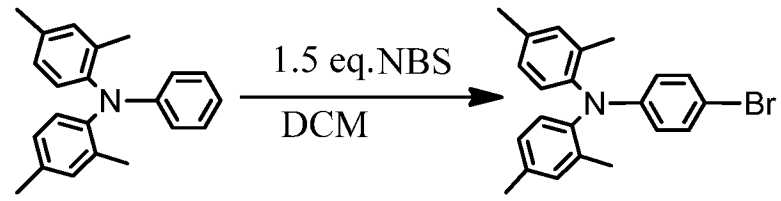
Compound 5



[135] Bis(2,4-dimethylphenyl)amine (Compound 14): A mixture of 2,4-dimethylaniline (6.05 g, 50 mmol), 2,4-dimethylbromobenzene (9.25 g, 50 mmol), $Pd(dppf)Cl_2$ (0.88 g, 1.2 mmol), sodium tert-butoxide ($KOBu^t$) (9.6 g, 0.1 mmol) in toluene (120 mL) was degassed and heated at 100°C overnight. The resulting mixture was worked up with dichloromethane/brine, dried over Na_2SO_4, loaded on silica gel and purified by flash column using eluents of hexanes to hexanes/dichloromethane 9:1. After removal of solvent, a liquid was obtained (9.45 g, in 84% yield).

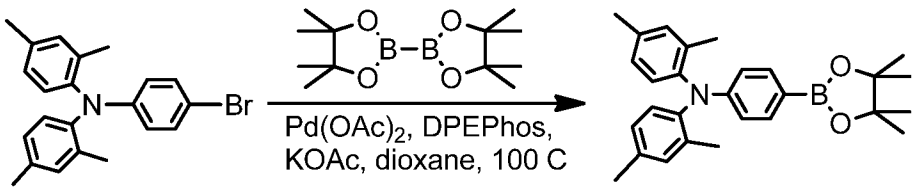


[136] N-(2,4-dimethylphenyl)-2,4-dimethyl-N-phenylaniline (Compound 15): A mixture of bis(2,4-dimethylphenyl)amine (**Compound 14**) (9.4 g, 41.8 mmol), iodobenzene (17.14 g, 84 mmol), Pd(OAc)2 (0.47 g, 2.1 mmol), $P(t\text{-}Bu)_3$ (0.848 g, 4.2 mmol), sodium tert-butoxide (7.68 g, 80 mmol) in toluene (120 mL) was degassed and heated at 120°C for 16 hours. The resulting mixture was poured into ethyl acetate (250 mL), washed with brine, dried over Na_2SO_4, loaded on silicagel and purified by flash column using eluent of hexanes. After removal of solvent, an oil (**Compound 15**) was obtained (12.4 g, in 98.6% yield).



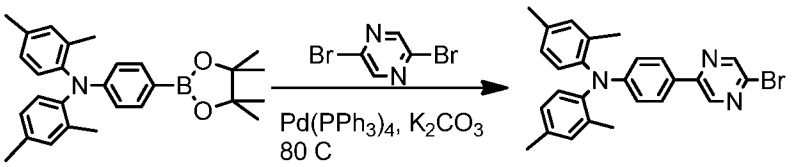
Compound 15 **Compound 16**

[137] **N-(4-bromophenyl)-N-(2,4-dimethylphenyl)-2,4-dimethylaniline** (**Compound 16**): To a solution of N-(2,4-dimethylphenyl)-2,4-dimethyl-N-phenylaniline (**Compound 15**) (12.4 g, 41 mmol) in dichloromethane (200 mL), was added NBS (8.01 g, 45 mmol) at 0°C. The whole was stirred for about 3 hours and worked up with brine. The organic phase was dried over Na_2SO_4, loaded on silica gel and purified by flash column using eluents of hexanes. After removal of solvents, a colorless oil (**Compound 16**) was obtained (15 g, in 96% yield).



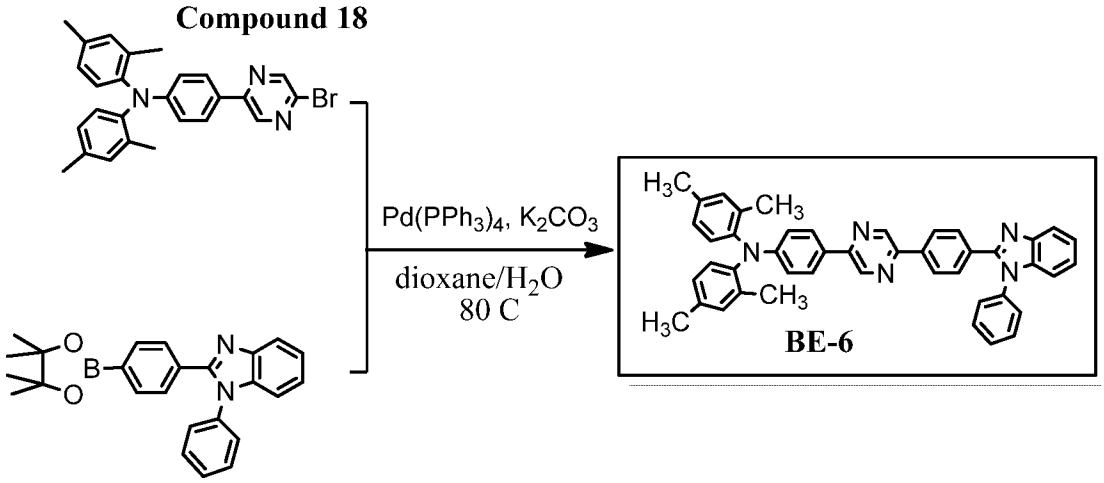
Compound 16 **Compound 17**

[138] N-(2,4-dimethylphenyl)-2,4-dimethyl-N-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)aniline (**Compound 17**): A mixture of N-(4-bromophenyl)-N-(2,4-dimethylphenyl)-2,4-dimethylaniline (**Compound 16**) (15 g, 39.5 mmol), bis(pinacolato)diboron (10.41 g, 41 mmol), KOAc (7.84 g, 80 mmol), Bis(2-diphenylphosphinophenyl)ether (3.23 g, 6 mmol) and $Pd(OAc)_2$ (0.44 g, 2 mmol) in dioxane (100 mL) was degassed and heated at about 100°C overnight. The resulting mixture was poured into ethyl acetate (200 mL), washed with brine, dried over Na_2SO_4, loaded on silica gel and purified by flash column using eluents of hexanes to hexanes/ethyl acetate 18:1. After removal of solvents, a white solid (**Compound 17**) was obtained (14 g, in 83% yield).



Compound 17 **Compound 18**

[139] N-(4-(5-bromopyrazin-2-yl)phenyl)-N-(2,4-dimethylphenyl)-2,4-dimethylaniline (**Compound 18**): A mixture of N-(2,4-dimethylphenyl)-2,4-dimethyl-N-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)aniline (**Compound 17**) (6.0 g, 14 mmol), 2,5-dibromopyrazine (7.74 g, 30 mmol), $Pd(PPh_3)_4$ (0.5 g, 0.43 mmol), K_2CO_3 (4.14 g, 30 mmol) in dioxane/water (80 mL/17 mL) was degassed and heated at about 80°C overnight. The resulting mixture was poured into ethyl acetate (200 mL), washed with brine, dried over Na_2SO_4, then loaded on silica gel and purified by flash column using eluents of hexanes to hexanes/dichloromethane 9:1 to 6:1 to 7:3. The desired yellow fraction was collected, and a yellow solid (**Compound 18**) was obtained after removal of solvents (3.83 g, 60% yield).

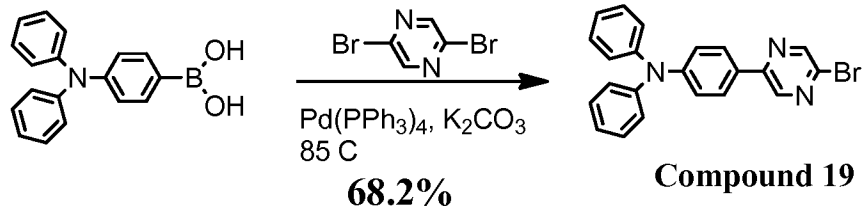


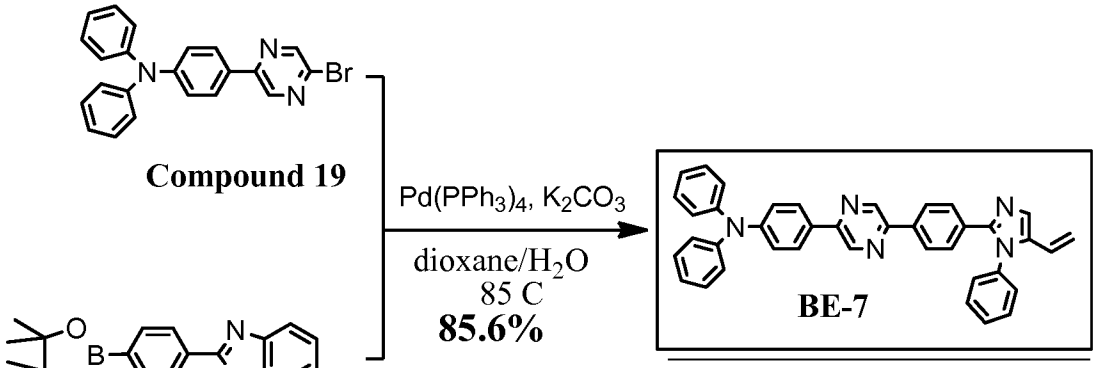
Compound 5

[140] Compound **BE-6**: A mixture of N-(4-(5-bromopyrazin-2-yl)phenyl)-N-(2,4-dimethylphenyl)-2,4-dimethylaniline (**Compound 18**) (1.67 g, 3.65 mmol), 1-phenyl-2-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)-1H-benzo[d]imidazole (**Compound 5**) (1.445 g, 3.65 mmol), $Pd(PPh_3)_4$ (0.21 g, 0.18 mmol), K_2CO_3 (0.966 g, 7mmol) in dioxane/water (50 mL/10 mL) was degassed and

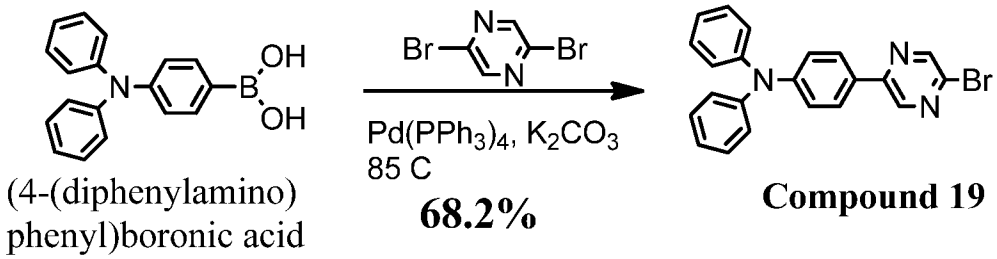
heated at about 100ºC overnight. The resulting mixture was poured into ethyl acetate (200 mL), washed with brine, dried over Na_2SO_4, loaded on silica gel and purified by flash column using eluents of hexanes to hexanes/dichloromethane 1:1 to dichloromethane to dichloromethane/ethyl acetate 90:5.The desired yellow fraction was collected. After removal of solvent, a yellow solid (**BE-6**) was obtained (2.2 g, in 93% yield). Confirmed by LCMS (APCI+): calcd for $C_{45}H_{38}N_5$ (M+H): 648; Found: 648.

Synthesis of BE-7

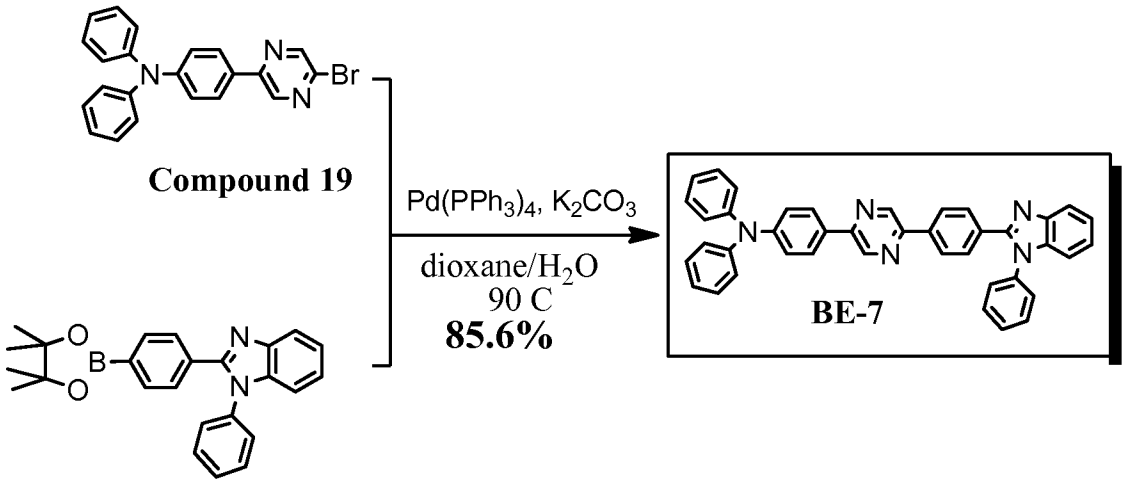




2,5-dibromopyrazine



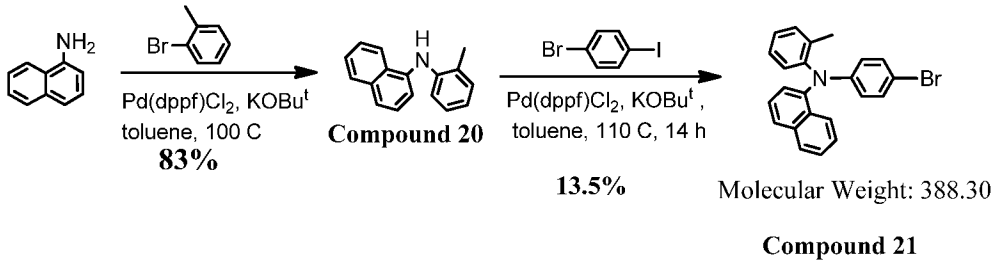
[141] **4-(5-bromopyrazin-2-yl)-N,N-diphenylaniline** (**Compound 19**): A mixture of (4-(diphenylamino)phenyl)boronic acid (3.26 g, 11.3 mmol), 2,5-dibromopyrazine (5.82 g, 22.6 mmol), $Pd(PPh_3)_4$ (0.635 g, 0.55 mmol), K_2CO_3 (3.45 g, 25 mmol) in dioxane/water (100 mL/16 mL) was degassed and heated at about 85ºC for about 20 hours. The resulting mixture was poured into ethyl acetate (250 mL), washed with brine, dried over Na_2SO_4, loaded on silica gel and purified by flash column using eluents of hexanes to hexanes/dichloromethane 4:1. After removal of solvent, a yellow solid (**Compound 19**) was obtained (3.1 g, in 68.2% yield).

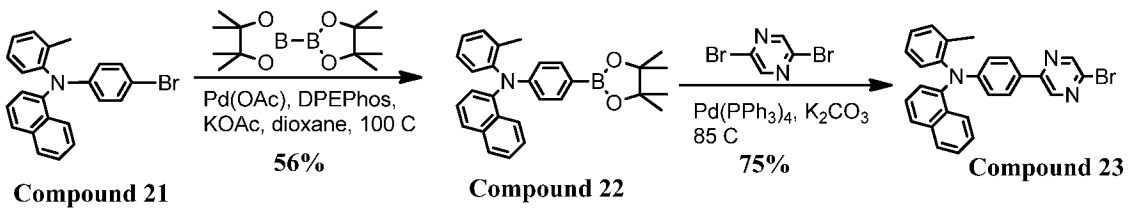


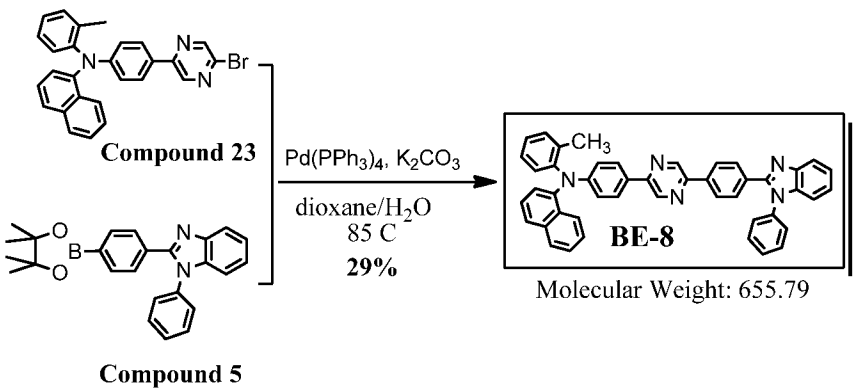
[142] **Compound BE-7**: A mixture of 4-(5-bromopyrazin-2-yl)-N,N-diphenylaniline (**Compound 19**) (1.54 g, 3.83 mmol), 1-phenyl-2-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)-1H-benzo[d]imidazole (**Compound 5**) (1.52 g, 3.83 mmol), $Pd(PPh_3)_4$ (0.22 g, 0.19 mmol), K_2CO_3(1.104 g, 8 mmol) in dioxane/water (100 mL/15 mL) was degassed and heated at about 90ºC for about 16 hours. The resulting mixture was poured into ethyl acetate (250 mL), washed with brine, concentrated and yellow precipitate formed. Filtration and washing with ethyl acetate gave a solid and filtrate. The filtrate was loaded n silica gel was loaded on silica gel and purified by flash column using eluents of hexanes to dichloromethane to dichloromethane/ethyl acetate (9:1 to 4:1). The desired fraction was collected. The solid from the filtration was dissolved in dichloromethane, purified by flash column using eluents of hexanes to dichloromethane to dichloromethane/ethyl acetate 9:1. The desired fraction was collected. Both desired fractions from the chromatography were combined, after removal of solvent, the solid was recrystallized in

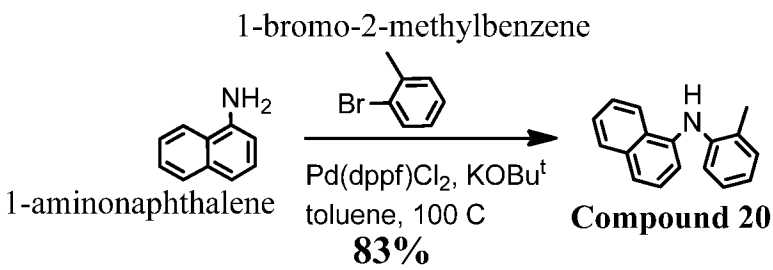
dichloromethane/ethyl acetate to give a yellow solid (**BE-7**), 1.94 g in 85.6% yield. Confirmed by LCMS (APCI+): calcd for $C_{41}H_{30}N_5$ (M+H): 592; found: 592.

Synthesis of **BE-8**

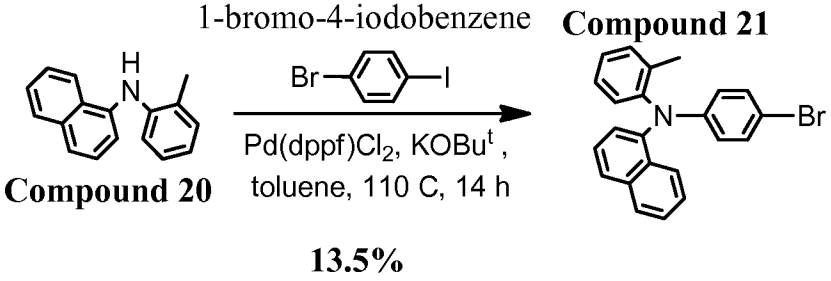




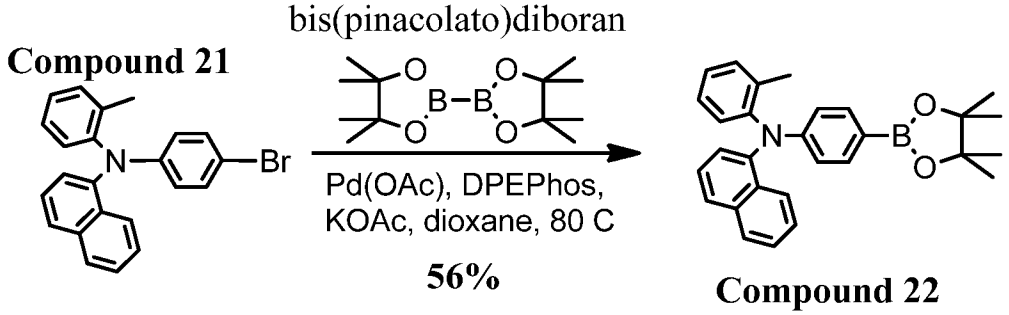




[143] **N-(o-tolyl)naphthalen-1-amine (Compound 20)**: A mixture of 1-aminonaphthalene (7.15 g, 50 mmol), 1-bromo-2-methylbenzene (8.5 g, 50 mmol), $Pd(dppf)Cl_2$ (1.0 g, 1.36 mmol), sodium tert-butoxide (9.6 g, 0.1 mol) in toluene (120 mL) was degassed and heated at about 100°C overnight. The resulting mixture was worked up with ethyl acetate/brine, dried over Na_2SO_4, loaded on silica gel and purified by flash column using eluents of hexanes to hexanes/dichloromethane 9:1. After removal of solvents, an oil (**Compound 20**) was obtained, 10.2 g in 91.5% yield.

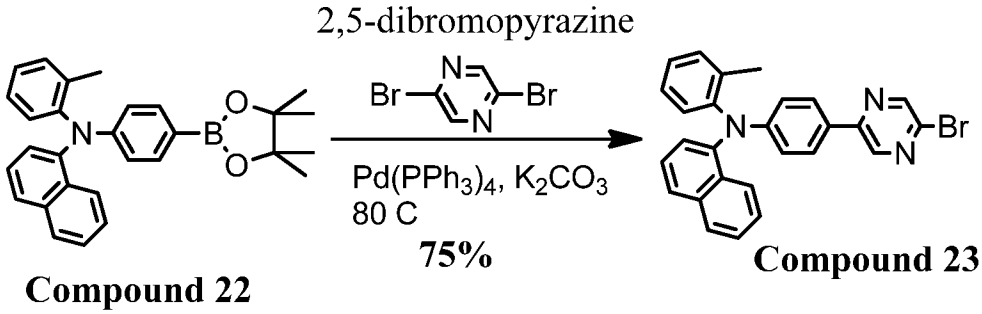


[144] **N-(4-bromophenyl)-N-(o-tolyl)naphthalen-1-amine** (**Compound 21**): A mixture of N-(o-tolyl)naphthalen-1-amine (**Compound 20**) (2.0 g, 8.6 mmol), 1-bromo-4-iodobenzene (8.67 g, 30 mmol), $Pd(dppf)Cl_2$ (0.365 g, 0.5 mmol), potassium tert-butoxide (1.96 g, 20 mmol) in toluene was degassed and heated at 110°C overnight. The resulting mixture was worked up with ethyl acetae/brine, dried over Na_2SO_4, loaded on silica gel and purified by flash column using eluents of hexanes to hexanes/dichloromethane 9:1. After removal of solvents, a yellow solid (**Compound 21**) was obtained, 0.45g in 13.5% yield.

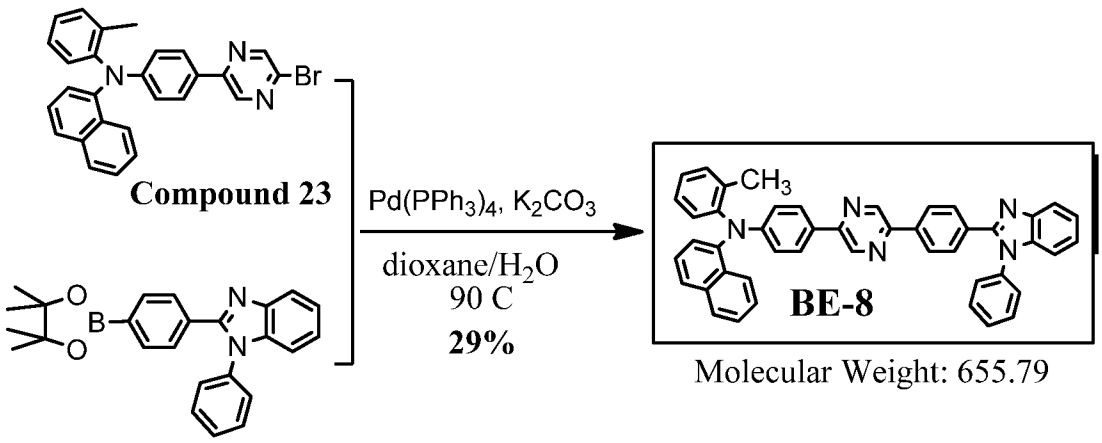


[145] N-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)-N-(o-tolyl)naphthalen-1-amine (**Compound 22**): A mixture of N-(4-bromophenyl)-N-(o-

tolyl)naphthalen-1-amine (**Compound 21**) (0.87 g, 2.24 mmol), bis(pinacolato)diboran (0.635 g, 2.5 mmol), $Pd(dppf)Cl_2$ (81.8 mg, 0.11 mmol), KOAc (0.49g, 5 mmol) in dioxane (50 mL) was degassed and heated at 80°C overnight. The resulting mixture was worked up with ethyl acetate/brine, dried over Na_2SO_4, loaded on silica gel and purified by flash column using eluents of hexanes to hexanes/ethyl acetate 18:1. After removal of solvents, a yellow solid (**Compound 22**) was obtained, 0.55 g in 56% yield.



[146] N-**(4-(5-bromopyrazin-2-yl)phenyl)-N-(o-tolyl)naphthalen-1-amine** (**Compound 23**): A mixture of N-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)-N-(o-tolyl)naphthalen-1-amine (**Compound 22**) (0.55 g, 1.26 mmol), 2,5-dibromopyrazine (0.77 g, 3.0 mmol), $Pd(PPh_3)_4$ (0.1 g, 0.09 mmol), K_2CO_3 (0.414 g, 3 mmol) in dioxane/water (40 mL/8 mL) was degassed and heated at 80°C overnight. The resulting mixture was worked up with ethyl acetate/brine, dried over Na_2SO_4, loaded on silica gel and purified by flash column using eluents of hexanes/dichloromethane 9:1 to 3:2. After removal of solvents, a yellow solid (**Compound 23**) was obtained, 0.44 g in 75% yield.



[147] **Compound BE-8**: A mixture of N-(4-(5-bromopyrazin-2-yl)phenyl)-N-(o-tolyl)naphthalen-1-amine (**Compound 23**) (0.44 g, 0.94 mmol), 1-phenyl-2-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)-1H-benzo[d]imidazole (**Compound 5**) (0.374 g, 0.94 mmol), $Pd(PPh_3)_4$ (0.058 g, 0.05 mmol), K_2CO_3 (0.276 g, 2 mmol) in dioxane/water (40 mL/8 mL) was degassed and heated at about 90ºC for 5 hours. The resulting mixture was worked up with ethyl acetate/brine, dried over Na_2SO_4, loaded on silica gel and purified by flash column using eluents of hexanes to hexanes/dichloromethane 4:1 to 1:1 to dichloromethane/ethyl acetate 10:1. The desired fraction was collected, after removal of solvents, the solid was recrystallized in dichloromethane/hexanes to give a yellow solid (**BE-8**), 0.18 g in 29% yield. Confirmed by LCMS (APCI+): calcd for $C_{46}H_{34}N_5$ (M+H): 656; Found: 656.

Example of OLED device configuration and performance

Example 2

[148] ITO coated glass substrates will be cleaned by ultrasound in water, acetone, and consecutively in 2-propanol, baked at 110 °C for 3 hours, followed by treatment with oxygen plasma for 5 min. A layer of PEDOT: PSS (Baytron P purchased from H.C. Starck) will be spin-coated at 3000 rpm onto the pre-cleaned and O_2-plasma treated (ITO)-substrate and annealed at about 180ºC for 30 min, to yield a thickness of around 55 nm. In a glove-box hosted vacuum deposition system at a pressure of 10^{-7} torr (1 torr=133.322 Pa), DTASi will be first deposited on top of PEDOT/PSS layer at deposition rate of 0.06 nm/s, yielding a 30 nm thick film. Then

the BE-2 will be heated and deposited on top of DTASi, yielding about a 5 nm thick film, followed by co-deposition of BE-2 and $Ir(PIQ)_2(acac)$ at depositions rates of about 0.06 nm/s to form a 5 nm thick layer, and deposition of another BE-2 layer having a thickness of about 5 nm. Then 1,3,5-tris(N-phenylbenzimidizol-2-yl)benzene (TPBI) at deposition rate around 0.06 nm/s will be deposited on the BE-2 layer to form a 40 nm thick film. LiF (1.0 nm) and Al (100 nm) will be then deposited successively at deposition rates of 0.005 and 0.2 nm/s, respectively. Each individual device will have areas of 0.14 cm^2.

Example 3

[149] All spectra will be measured with an Ocean Optics HR 4000 spectrometer and I-V-L characteristics were taken with a Keithley 2400 SourceMeter and Newport 2832-C power meter and 818 UV detector. All device operation will be performed inside a nitrogen-filled glove-box. An example of a configuration of the device (Device-A) is shown in FIG. 4.

[150] It is anticipated that upon determining the luminescent efficiency and power efficiency as a function of luminance of Device-A, a plot of the electroluminescence spectrum of Device-A, and the CRI of Device A, BE-2 will be suitable as a host material in hybrid OLED devices.

[151] Unless otherwise indicated, all numbers expressing quantities of ingredients, properties such as molecular weight, reaction conditions, and so forth used in the specification and claims are to be understood as being modified in all instances by the term “about.” Accordingly, unless indicated to the contrary, the numerical parameters set forth in the specification and attached claims are approximations that may vary depending upon the desired properties sought to be obtained. At the very least, and not as an attempt to limit the application of the doctrine of equivalents to the scope of the claims, each numerical parameter should at least be construed in light of the number of reported significant digits and by applying ordinary rounding techniques.

[152] The terms “a,” “an,” “the” and similar referents used in the context of describing the invention (especially in the context of the following claims) are to be construed to cover both the singular and the plural, unless otherwise indicated herein or clearly contradicted by context. All methods described herein can be performed in any suitable order unless otherwise indicated herein or otherwise clearly contradicted

by context. The use of any and all examples, or exemplary language (e.g., "such as") provided herein is intended merely to better illuminate the invention and does not pose a limitation on the scope of any claim. No language in the specification should be construed as indicating any non-claimed element essential to the practice of the invention.

[153] Groupings of alternative elements or embodiments disclosed herein are not to be construed as limitations. Each group member may be referred to and claimed individually or in any combination with other members of the group or other elements found herein. It is anticipated that one or more members of a group may be included in, or deleted from, a group for reasons of convenience and/or patentability. When any such inclusion or deletion occurs, the specification is deemed to contain the group as modified thus fulfilling the written description of all Markush groups used in the appended claims.

[154] Certain embodiments are described herein, including the best mode known to the inventors for carrying out the invention. Of course, variations on these described embodiments will become apparent to those of ordinary skill in the art upon reading the foregoing description. The inventor expects skilled artisans to employ such variations as appropriate, and the inventors intend for the invention to be practiced otherwise than specifically described herein. Accordingly, the claims include all modifications and equivalents of the subject matter recited in the claims as permitted by applicable law. Moreover, any combination of the above-described elements in all possible variations thereof is contemplated unless otherwise indicated herein or otherwise clearly contradicted by context.

[155] In closing, it is to be understood that the embodiments disclosed herein are illustrative of the principles of the claims. Other modifications that may be employed are within the scope of the claims. Thus, by way of example, but not of limitation, alternative embodiments may be utilized in accordance with the teachings herein. Accordingly, the claims are not limited to embodiments precisely as shown and described.

WHAT IS CLAIMED IS:

1. A compound represented by a formula:

HT—[Ph^1]$_r$—Py—Het—ET

wherein HT is optionally substituted diphenylamine or optionally substituted phenyl(naphthyl)amine,

each Ph^1 is independently optionally substituted *p*-phenylene, wherein the *p*-phenylene directly bonded to HT may optionally form a bond to a phenyl of HT to form a three ring system;

Py is optionally substituted pyrazin-2,5-ylene;

Het is optionally substituted *p*-phenylene or optionally substituted pyridin-2,5-ylene;

ET is optionally substituted benzimidazol-2-yl, optionally substituted benzoxazol-2-yl, or optionally substituted benzothiazol-2-yl; and

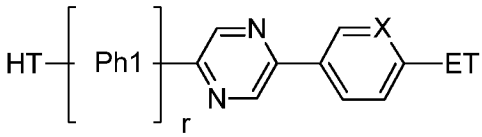
r is 1, 2, 3.

2. The compound of claim 1, further represented by a formula:

HT—Ph^{1a}— Ph^{1b}—Ph^{1c}—Py—Het—ET

wherein Ph^{1a} is optionally substituted *p*-phenylene, or HT—Ph^{1a} is 9-phenylcarbazol-3-yl; and Ph^{1b} and Ph^{1c} are independently a bond or optionally substituted *p*-phenylene.

3. The compound of claim 1, further represented by a formula:

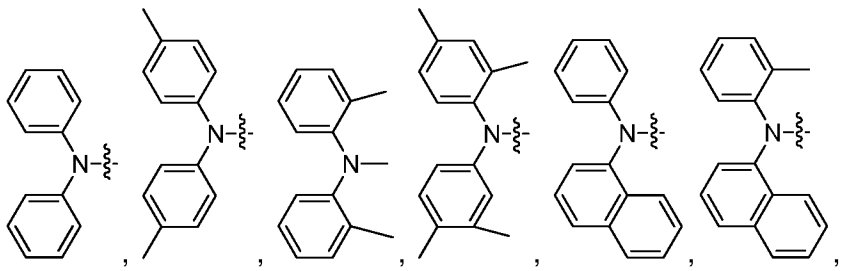


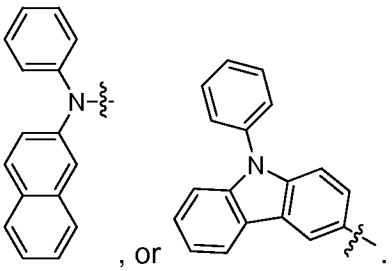
wherein X is C or N.

4. The compound of claim 1 or 3, wherein r is 1.

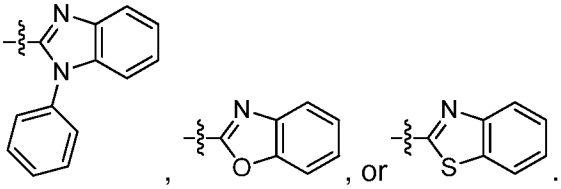
5. The compound of claim 1, 2, or 3, wherein ET is optionally substituted 1-phenyl-1H-benzo[d]imidazol-2-yl.

6. The compound of claim 1, 2, 3, 4, or 5, wherein HT is





7. The compound of claim 1, 2, 3, 4, 5, or 6, wherein ET is



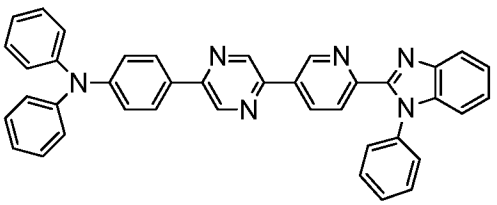
8. The compound of claim 1, 2, 4, 5, 6, or 7, wherein Het is optionally substituted *p*-phenylene.

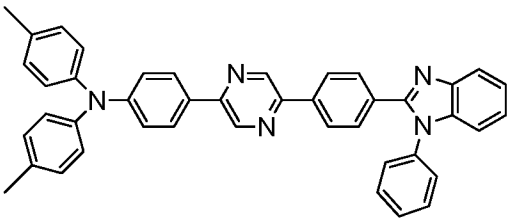
9. The compound of claim 1, 2, 4, 5, 6, or 7, wherein Het is optionally substituted pyridin-2,5-ylene.

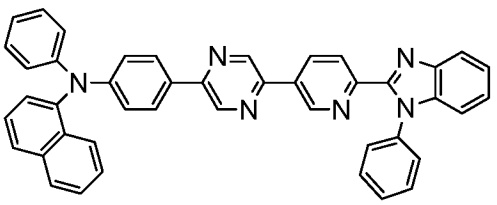
10. The compound of claim 1, 3, 5, 6, 7, 8, or 9, wherein r is 2.

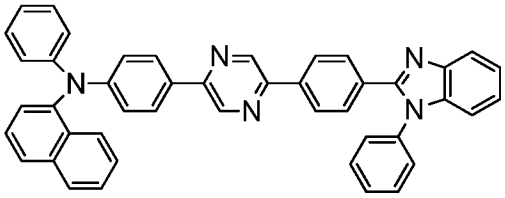
11. The compound of claim 1, 3, 5, 6, 7, 8, or 9, wherein r is 3.

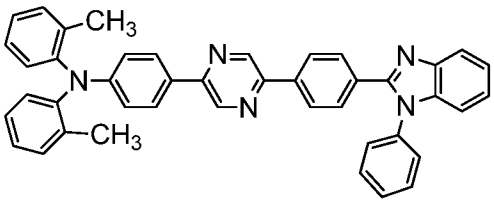
12. The compound of claim 1, wherein the compound is:

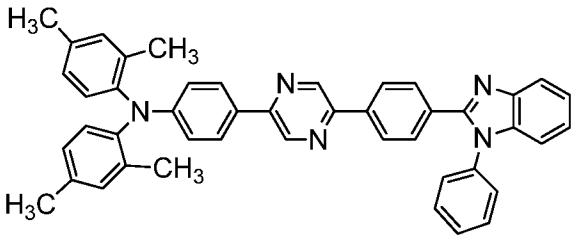


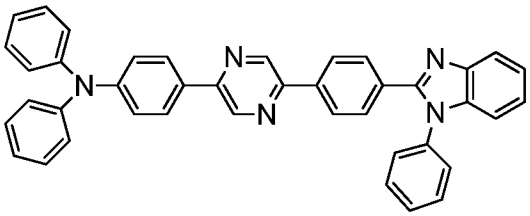


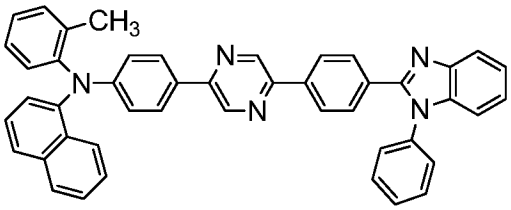


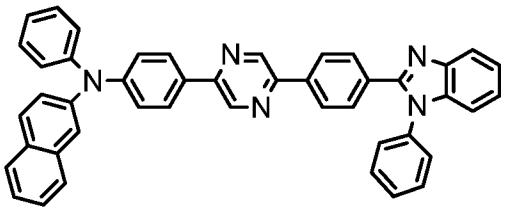

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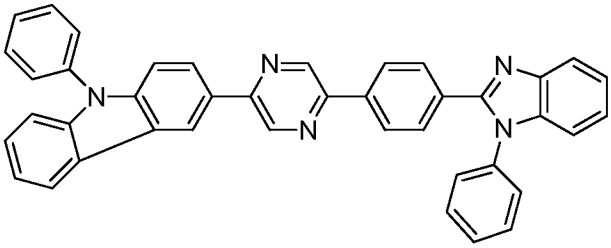

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, or


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13. The compound of claim 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, or 12, wherein the compound is electroluminescent.

14. The compound of claim 13, wherein the compound has a lowest energy triplet having an energy of about 2.5 eV to about 4 eV.

15. A light emitting layer comprising the compound of any of claims 1-14.

16. A light emitting device, comprising:

an anode layer comprising a high work function metal;

a cathode layer comprising a low work function metal; and

a light emitting layer comprising an compound of any of claims 1-14.

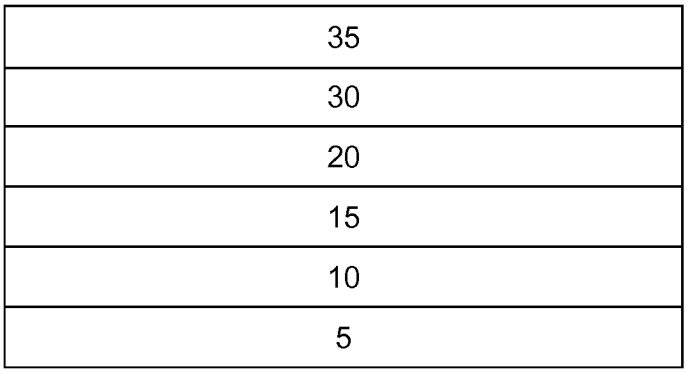

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FIG.1

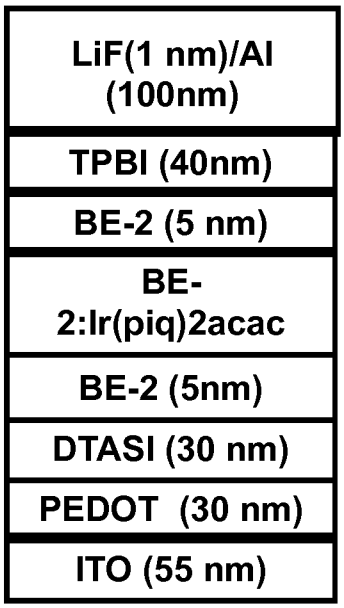

LiF(1 nm)/Al (100nm)
TPBI (40nm)
BE-2 (5 nm)
BE-2:Ir(piq)2acac
BE-2 (5nm)
DTASI (30 nm)
PEDOT (30 nm)
ITO (55 nm)

FIG.2

INTERNATIONAL SEARCH REPORT

International application No
PCT/US2013/074144

A. CLASSIFICATION OF SUBJECT MATTER
INV. C07D401/14 C07D403/10 H01L51/50
ADD.

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)
C07D H01L

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practicable, search terms used)
EPO-Internal, CHEM ABS Data, WPI Data

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
A	WO 2012/037269 A1 (NITTO DENKO CORP [JP]; SISK DAVID T [US]; KHAN SAZZADUR RAHMAN [US]; M) 22 March 2012 (2012-03-22) claims 1-8, 13-18, 27-33; examples 3-5, 9-11; compounds 10, 12, 14, 19, 20, 21	1-16
A	WO 2012/088294 A1 (NITTO DENKO CORP [JP]; ZHENG SHIJUN [US]; MA LIPING [US]; MOCHIZUKI AM) 28 June 2012 (2012-06-28) claims 1-10; compounds X, Host 1-4	1-16
A	WO 2010/027004 A1 (SEMICONDUCTOR ENERGY LAB [JP]; SEO SATOSHI [JP]; KAWAKAMI SACHIKO; NOM) 11 March 2010 (2010-03-11) claims 1-11, 21, 2, 24; compounds 101-294	1-16

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[X] Further documents are listed in the continuation of Box C.

[X] See patent family annex.

* Special categories of cited documents :

"A" document defining the general state of the art which is not considered to be of particular relevance

"E" earlier application or patent but published on or after the international filing date

"L" document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified)

"O" document referring to an oral disclosure, use, exhibition or other means

"P" document published prior to the international filing date but later than the priority date claimed

"T" later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention

"X" document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone

"Y" document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art

"&" document member of the same patent family

Date of the actual completion of the international search	Date of mailing of the international search report
24 January 2014	03/02/2014

Name and mailing address of the ISA/	Authorized officer
European Patent Office, P.B. 5818 Patentlaan 2 NL - 2280 HV Rijswijk Tel. (+31-70) 340-2040, Fax: (+31-70) 340-3016	Sotoca Usina, E

INTERNATIONAL SEARCH REPORT

International application No
PCT/US2013/074144

C(Continuation). DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
A	WO 2010/126270 A1 (DOW ADVANCED DISPLAY MATERIALS [KR]; EUM SUNG JIN [KR]; KIM CHI SIK [K) 4 November 2010 (2010-11-04) claims 1-9; compounds 40-42 -----	1-16

INTERNATIONAL SEARCH REPORT

Information on patent family members

International application No
PCT/US2013/074144

Patent document cited in search report	Publication date	Patent family member(s)	Publication date
WO 2012037269 A1	22-03-2012	CN 103209975 A	17-07-2013
		EP 2616457 A1	24-07-2013
		JP 2013541526 A	14-11-2013
		TW 201300502 A	01-01-2013
		US 2012179089 A1	12-07-2012
		WO 2012037269 A1	22-03-2012
WO 2012088294 A1	28-06-2012	CN 103502223 A	08-01-2014
		EP 2655338 A1	30-10-2013
		US 2011140093 A1	16-06-2011
		US 2013146856 A1	13-06-2013
		WO 2012088294 A1	28-06-2012
WO 2010027004 A1	11-03-2010	CN 102144313 A	03-08-2011
		EP 2321862 A1	18-05-2011
		JP 2010083876 A	15-04-2010
		KR 20110063749 A	14-06-2011
		US 2010060155 A1	11-03-2010
		US 2013112961 A1	09-05-2013
		WO 2010027004 A1	11-03-2010
WO 2010126270 A1	04-11-2010	KR 20100118690 A	08-11-2010
		TW 201100522 A	01-01-2011
		WO 2010126270 A1	04-11-2010