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(71)申請人：南韓商ＬＴ素材股份有限公司 (南韓) LT MATERIALS CO., LTD. (KR)
南韓

(72)發明人：蔡雨靜 CHAE, WOO-JEONG (KR) ；牟晙兌 MO, JUN-TAE (KR) ；金東駿 KIM, DONG-JUN (KR)

(74)代理人：葉璟宗；卓俊傑

申請實體審查：無 申請專利範圍項數：15 項 圖式數：4 共 298 頁

(54)名稱

有機發光裝置、其製造方法以及用於有機發光裝置的有機材料層的組合物

(57)摘要

本說明書涉及包含由化學式 1 表示的雜環化合物和由化學式 2 表示的雜環化合物的有機發光裝置、其製造方法和有機材料層的組合物。因此，可以降低裝置的驅動電壓，提高光效率，且特別是通過化合物的熱穩定性提高裝置的使用壽命特性。

The present specification relates to an organic light emitting device including a heterocyclic compound represented by Chemical Formula 1 and a heterocyclic compound represented by Chemical Formula 2, a method for manufacturing the same, and a composition for an organic material layer. Accordingly, it is possible to lower a driving voltage of the device, improve the light efficiency, and particularly improve the service life characteristics of the device by the thermal stability of the compound.

指定代表圖：

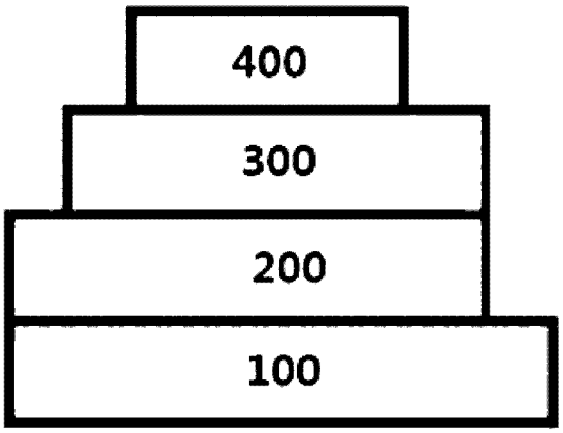
符號簡單說明：

100:基板

200:正極

300:有機材料層

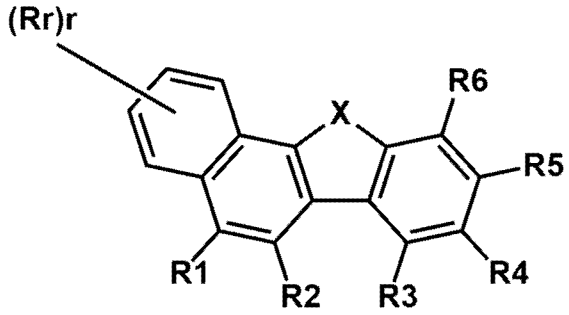
400:負極



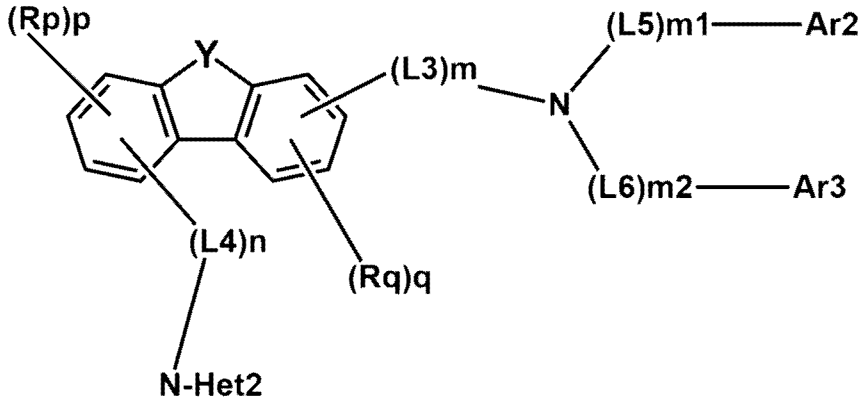
【圖1】

特徵化學式：

[化學式 1]



[化學式 2]



【發明摘要】

【中文發明名稱】有機發光裝置、其製造方法以及用於有機發光裝置的有機材料層的組合物

【英文發明名稱】ORGANIC LIGHT EMITTING DEVICE, MANUFACTURING METHOD OF SAME AND COMPOSITION FOR ORGANIC LAYER OF ORGANIC LIGHT EMITTING DEVICE

【中文】本說明書涉及包含由化學式1表示的雜環化合物和由化學式2表示的雜環化合物的有機發光裝置、其製造方法和有機材料層的組合物。因此，可以降低裝置的驅動電壓，提高光效率，且特別是通過化合物的熱穩定性提高裝置的使用壽命特性。

【英文】The present specification relates to an organic light emitting device including a heterocyclic compound represented by Chemical Formula 1 and a heterocyclic compound represented by Chemical Formula 2, a method for manufacturing the same, and a composition for an organic material layer. Accordingly, it is possible to lower a driving voltage of the device, improve the light efficiency, and particularly improve the service life characteristics of the device by the thermal stability of the compound.

【指定代表圖】圖1。

【代表圖之符號簡單說明】

100:基板

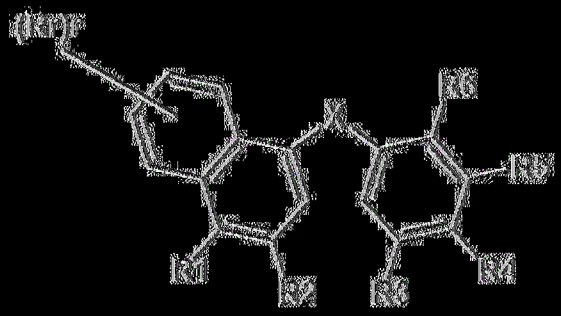
200:正極

300:有機材料層

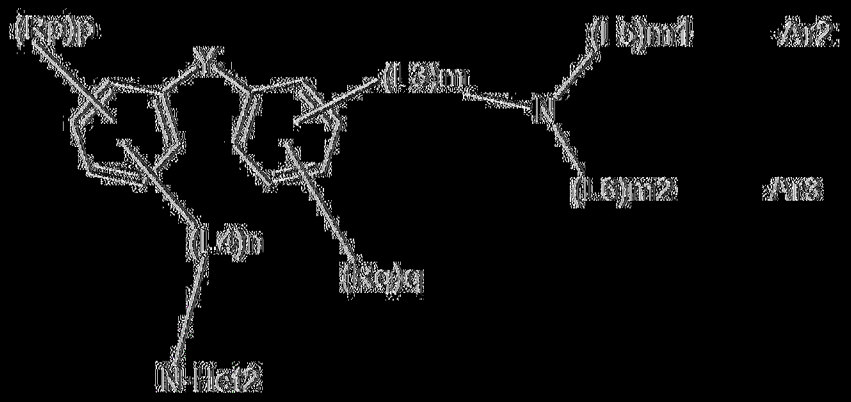
400:負極

【特徵化學式】

[化學式 1]



[化學式 2]



【發明說明書】

【中文發明名稱】有機發光裝置、其製造方法以及用於有機發光裝置的有機材料層的組合物

【英文發明名稱】ORGANIC LIGHT EMITTING DEVICE, MANUFACTURING METHOD OF SAME AND COMPOSITION FOR ORGANIC LAYER OF ORGANIC LIGHT EMITTING DEVICE

【技術領域】

【0001】 本申請涉及一種有機發光裝置、其製造方法和用於有機材料層的組合物。

【0002】 本申請案主張分別於 2022 年 3 月 7 日向韓國智慧財產局提出申請的韓國專利申請案第 10-2022-0028918 號的優先權及利益，所述韓國專利申請案的全部內容併入本案供參考。

【先前技術】

【0003】 電致發光裝置（electroluminescent device）是一種自發光型顯示裝置，且具有視角寬、對比度優異、響應速度快等優點。

【0004】 有機發光裝置具有在兩個電極之間設置有機薄膜的結構。當向具有該結構的有機發光裝置施加電壓時，從兩個電極注入的電子和電洞在有機薄膜中彼此結合以形成一對，然後在熄滅的同時發光。必要時，有機薄膜可以由單層或多層構成。

【0005】 必要時，用於有機薄膜的材料可以具有發光功能。例如，

作為有機薄膜的材料，也可以使用自身單獨構成發光層的化合物，抑或也可以使用能夠作為主體摻雜劑系（host-dopant-based）發光層的主體或摻雜劑的化合物。另外，作為有機薄膜的材料，也可以使用化合物，其可以發揮電洞注入、電洞傳輸、電子阻擋、電洞阻擋、電子傳輸或電子注入等功能。

【0006】 為了提高有機發光裝置的性能、使用壽命或效率，一直需要開發用於有機薄膜的材料。

【0007】 有必要對包括具有化學結構的化合物的有機發光裝置進行研究，其可以滿足可用於有機發光裝置的材料所需的條件，例如合適的能級、電化學穩定性、熱穩定性等，並且可以根據取代基執行有機發光裝置所需的各種功能。

[現有技術文獻]

【0008】 [專利文獻 1] 美國專利第 4,356,429 號

【發明內容】

[發明所欲解決之課題]

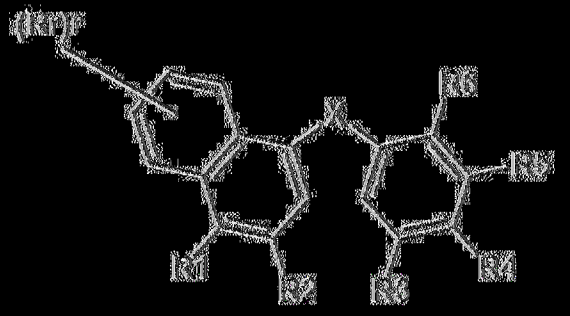
【0009】 本發明致力於提供一種有機發光裝置及其製造方法和用於有機材料層的組合物。

[解決課題之手段]

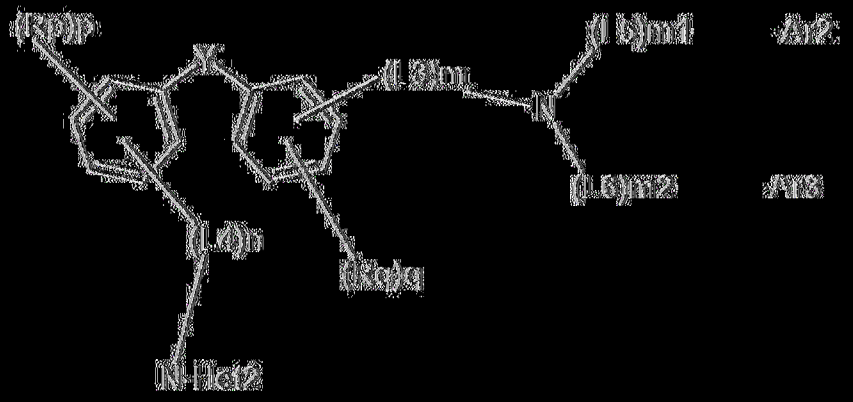
【0010】 提供一種有機發光裝置，包括第一電極、第二電極和具有一層或多層設置在第一電極和第二電極之間的有機材料層，其中有機材料層包括由以下化學式 1 表示的雜環化合物和由以下化

學式 2 表示的雜環化合物。

[0011] [化學式 1]



[0012] [化學式 2]



[0013] 在化學式 1 和 2 中，

X 是 O；或 S，

R1 至 R6 中的一者為 [illegible]，其他中的一者為 [illegible]，其他彼此相同或不同，且各自獨立地選自氫；氘；鹵素；氰基；經取代或未經取代的 C1 至 C60 烷基；經取代或未經取代的 C2 至 C60 烯基；經取代或未經取代的 C2 至 C60 炔基；經取代或未經取代的 C1 至 C60 烷氧基；經取代或未經取代的 C3 至 C60 環烷基；經取代或未經取代的 C2 至 C60 雜環烷基；經取代或未經取代的 C6 至 C60 芳基；經取代或未經取代的 C2 至 C60 雜芳基；-P(=O)RR'；-SiRR'R"和-NRR'，

[illegible]是分別鍵結至 R1 至 R6 的位置，

L1 至 L6 彼此相同或不同，且各自獨立為直接鍵；經取代或未經取代的 C6 至 C60 伸芳基；或經取代或未經取代的 C2 至 C60 伸雜芳基，a、b、m、n、m1 和 m2 各自為 0 至 3 的整數，並且當 a、b、m、n、m1 和 m2 各自為 2 或大於 2 時，括號中的取代基彼此相同或不同，

N-Het1 和 N-Het2 各自獨立地為經取代或未經取代並包括一個或多個 N 的單環或多環雜環基團，

Ar1 為經取代或未經取代的 C6 至 C60 芳基；或經取代或未經取代的 C2 至 C60 雜芳基，

Y 是 O；或 S，

Ar2 和 Ar3 彼此相同或不同，且各自獨立地為經取代或未經取代的 C6 至 C60 的芳基；經取代或未經取代的 C2 至 C60 雜芳基；或-NRR'，

L3、L5、L6、Ar2 和 Ar3 的相鄰取代基可以彼此鍵結以形成經取代或未經取代的脂肪族或芳香族烴環或經取代或未經取代的脂肪族或芳香族雜環，

Rr、Rp 和 Rq 彼此相同或不同，並且各自獨立地選自由以下組成的群組：氫；氘；鹵素；氰基；經取代或未經取代的 C1 至 C60 烷基；經取代或未經取代的 C2 至 C60 烯基；經取代或未經取代的 C2 至 C60 炔基；經取代或未經取代的 C1 至 C60 烷氧基；經取代或未經取代的 C3 至 C60 環烷基；經取代或未經取代的 C2 至 C60 雜環烷基；經取代或未經取代的 C6 至 C60 芳基；經取代或未

經取代的 C2 至 C60 雜芳基；-P(=O)RR’；-SiRR’R”和-NRR’，r 為 0 至 4 的整數，p、q 為 0 至 3 的整數，且當 r、p、q 為 2 或大於 2 時，括號內的取代基為彼此相同或不同，以及

R、R’和 R”彼此相同或不同，且各自獨立地為氫；氘；經取代或未經取代的 C1 至 C60 烷基；經取代或未經取代的 C6 至 C60 芳基；或經取代或未經取代的 C2 至 C60 雜芳基。

【0014】 此外，本申請的另一示例性實施例提供了一種用於有機發光裝置的有機材料層的組合物，包括由化學式 1 表示的雜環化合物；以及由化學式 2 表示的雜環化合物。

【0015】 最後，本申請的一個示例性實施例提供了一種有機發光裝置的製造方法，該方法包括：製備基板；在基板上形成第一電極；在第一電極上形成具有一層或多層的有機材料層；以及在有機材料層上形成第二電極，其中有機材料層的形成包括使用根據本申請的一個示例性實施例的用於有機材料層的組合物形成具有一層或多層的有機材料層。

[發明的效果]

【0016】 本說明書中描述的化合物可以用作有機發光裝置的有機材料層的材料。化合物可作為有機發光裝置中的電洞注入材料、電洞傳輸材料、發光材料、電子傳輸材料、電子注入材料、電子阻擋材料、電洞阻擋材料等。特別地，化合物可以用作有機發光裝置的發光材料。

【0017】 另外，由化學式 1 表示的雜環化合物和由化學式 2 表示

的雜環化合物均可用作有機發光裝置的發光層的材料。在這種情況下，可以降低裝置的驅動電壓，提高光效率，特別是通過化合物的熱穩定性提高裝置的使用壽命特性。

【圖式簡單說明】

【0018】

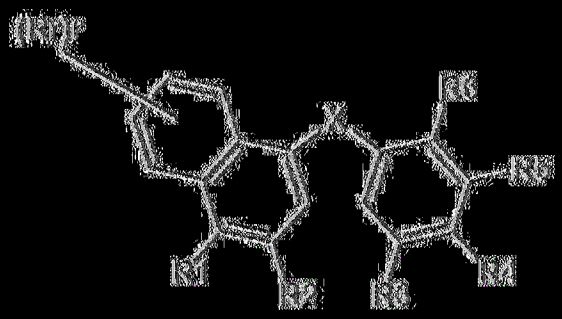
圖 1 至圖 4 均為示意性說明根據本申請的一個示例性實施例的有機發光裝置的堆疊結構的視圖。

【實施方式】

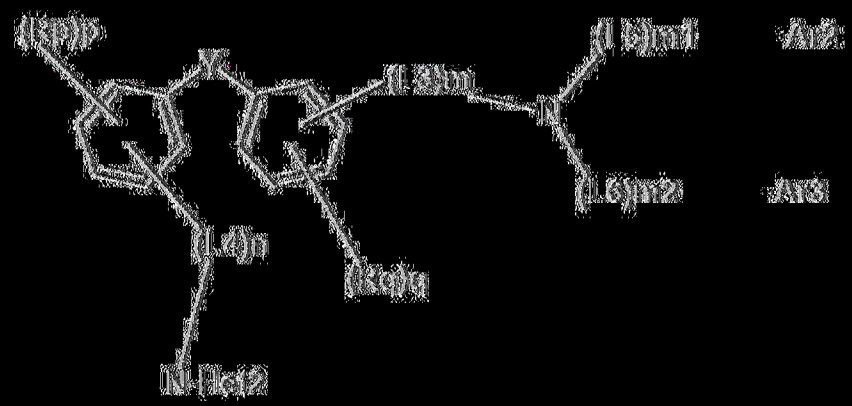
【0019】 在下文中，將詳細描述本申請。

【0020】 提供一種有機發光裝置，包括第一電極、第二電極和具有一層或多層設置在第一電極和第二電極之間的有機材料層，其中有機材料層包括由以下化學式 1 表示的雜環化合物和由以下化學式 2 表示的雜環化合物。

【0021】 [化學式 1]



【0022】 [化學式 2]



[0023] 在化學式 1 和 2 中，

X 是 O；或 S，

R1 至 R6 中的一者為 [illegible]，其他中的一者為 [illegible]，且其他彼此相同或不同，且各自獨立地選自由以下組成的群組：氫；氘；鹵素；氰基；經取代或未經取代的 C1 至 C60 烷基；經取代或未經取代的 C2 至 C60 烯基；經取代或未經取代的 C2 至 C60 炔基；經取代或未經取代的 C1 至 C60 烷氧基；經取代或未經取代的 C3 至 C60 環烷基；經取代或未經取代的 C2 至 C60 雜環烷基；經取代或未經取代的 C6 至 C60 芳基；經取代或未經取代的 C2 至 C60 雜芳基；-P(=O)RR'；-SiRR'R"和-NRR'，

"*"是分別鍵結至 R1 至 R6 的位置，

L1 至 L6 彼此相同或不同，且各自獨立為直接鍵；經取代或未經取代的 C6 至 C60 伸芳基；或經取代或未經取代的 C2 至 C60 伸雜芳基，a、b、m、n、m1 和 m2 各自為 0 至 3 的整數，並且當 a、b、m、n、m1 和 m2 各自為 2 或大於 2 時，括號中的取代基彼此相同或不同，

N-Hc1 和 N-Hc2 各自獨立地為經取代或未經取代並包括一個

或多個 N 的單環或多環雜環基團，

Ar1 為經取代或未經取代的 C6 至 C60 芳基；或經取代或未經取代的 C2 至 C60 雜芳基，

Y 是 O；或 S，

Ar2 和 Ar3 彼此相同或不同，且各自獨立地為經取代或未經取代的 C6 至 C60 的芳基；經取代或未經取代的 C2 至 C60 雜芳基；或-NRR'，

L3、L5、L6、Ar2 和 Ar3 的相鄰取代基可以彼此鍵結以形成經取代或未經取代的脂肪族或芳香族烴環或經取代或未經取代的脂肪族或芳香族雜環，

Rr、Rp 和 Rq 彼此相同或不同，並且各自獨立地選自由以下組成的群組：氫；氘；鹵素；氰基；經取代或未經取代的 C1 至 C60 烷基；經取代或未經取代的 C2 至 C60 烯基；經取代或未經取代的 C2 至 C60 炔基；經取代或未經取代的 C1 至 C60 烷氧基；經取代或未經取代的 C3 至 C60 環烷基；經取代或未經取代的 C2 至 C60 雜環烷基；經取代或未經取代的 C6 至 C60 芳基；經取代或未經取代的 C2 至 C60 雜芳基；-P(=O)RR'；-SiRR'R"和-NRR'，r 為 0 至 4 的整數，p、q 為 0 至 3 的整數，且當 r、p、q 為 2 或大於 2 時，括號內的取代基為彼此相同或不同，以及

R、R'和 R"彼此相同或不同，且各自獨立地為氫；氘；經取代或未經取代的 C1 至 C60 烷基；經取代或未經取代的 C6 至 C60 芳基；或經取代或未經取代的 C2 至 C60 雜芳基。

【0024】 本發明的由化學式 1 表示的雜環化合物具有優異的電子傳輸能力、高熱穩定性和合適的分子量及帶隙（band-gap）。這種合適的帶隙具有良好的電洞傳輸能力，並防止電子損失，從而能夠有效形成復合區（recombination zone）。

【0025】 另外，本發明的由化學式 2 表示的雜環化合物具有優異的電洞遷移率，且通過阻擋電子容易降低漏電流並限制電子。

【0026】 因此，當有機發光裝置的有機材料層包含由化學式 1 表示的雜環化合物和由化學式 2 表示的雜環化合物時，可以提高裝置的效率和使用壽命。特別地，當有機材料層為發光層時，可以進一步提高裝置的效率和使用壽命。

【0027】 在本說明書中，當一個部分「包括」一個組成元素時，除非另有說明，這並不意味著排除另一個組成元素，而是意味著可以進一步包括另一個組成元素。

【0028】 在本說明書中，化學式的 是指組成元素鍵結的位置。

【0029】 術語「取代」是指與化合物的碳原子鍵結的氫原子被改變為另一個取代基，並且被取代的位置不受限制，只要該位置是氫原子被取代的位置（即，取代基可以被取代的位置）即可，並且當兩個或多於兩個取代基被取代時，兩個或多於兩個的取代基可以彼此相同或不同。

【0030】 在本說明書中，「經取代或未經取代的」是指被未經取代或被選自由以下組成的群組中的一或多個取代基取代：氘；鹵素基團；-CN；C1 至 C60 烷基；C2 至 C60 烯基；C2 至 C60 炔基；

C1 至 C60 鹵代烷基；C1 至 C60 烷氧基；C6 至 C60 芳氧基（aryloxy group）；C1 至 C60 烷硫氧基（alkylthioxy group）；C6 至 C60 芳硫氧基（arylthioxy group）；C1 至 C60 烷磺氧基（alkylsulfoxy group）；C6 至 C60 芳磺氧基（arylsulfoxy group）；C3 至 C60 環烷基（cycloalkyl group）；C2 至 C60 雜環烷基（heterocycloalkyl group）；C6 至 C60 芳基；C2 至 C60 雜芳基（heteroaryl group）；-SiRR'R"；-P(=O)RR'；和-NRR'，或從例示的取代基中選擇的兩個或多於兩個取代基連接至其上的取代基，並且 R、R'和 R"各自獨立地是由氫；氘；鹵素基團；烷基；烯基；烷氧基；環烷基；雜環烷基；芳基；和雜芳基中的至少一者組成的取代基。

【0031】 在本說明書中，「Cn」表示碳原子數為 n。例如，C6 表示 6 個碳原子，C60 表示 60 個碳原子。

【0032】 在本說明書中，「當在化學式或化合物的結構中未指明取代基時」是指氫原子與碳原子鍵結。然而，由於氘(^2H)是氫的同位素，一些氫原子可能是氘。

【0033】 在本申請的一個示例性實施例中，「當化學式或化合物的結構中未指明取代基時」可以指取代基可能觸及的所有位置都是氫或氘。即，氘是氫的同位素，且部分氫原子可以是同位素氘，且在此情況下，氘的含量可以為 0%至 100%。

【0034】 在本申請的一個示例性實施例中，在「化學式或化合物的結構中未指明取代基的情況下」，當氘的含量為 0%時，氫的含量為 100%，並且所有的取代基不明確排除氘（例如氫），氫和氘

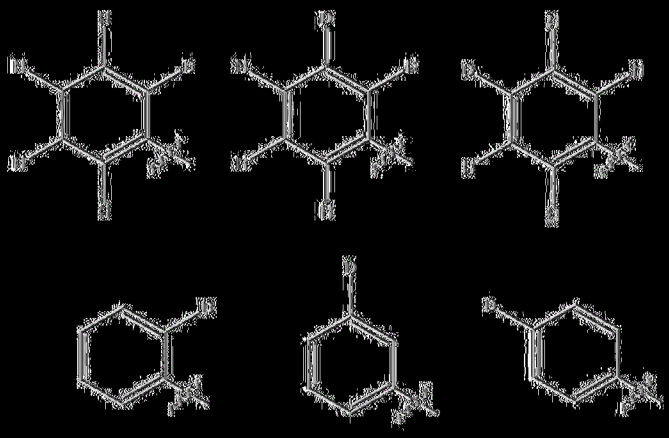
可能在化合物中混合使用。

[0035] 在本申請的一個示例性實施例中，氘是氫的同位素中的一者，是以一個質子和一個中子組成的氘核為原子核的元素，且可以用氫-2表示，且元素符號也可表示為D或^{2}H。

[0036] 在本申請的一個示例性實施例中，同位素是指具有相同原子序數（Z）但不同質量數（A）的原子，且同位素也可以解釋為質子數相同但中子數不相同的元素。

[0037] 在本申請的一個示例性實施例中，當鹼性化合物的取代基總數定義為T1並且取代基中特定取代基的數量定義為T2時，特定取代基的含量T%可以定義為T2/T1×100=T%。

[0038] 即，在一個實例中，當苯基可具有的取代基總數為5(式中的T1)並且取代基中氘的個數為1（式中T2）時， 表示的苯基中的20%的氘含量可以表示為20%。即，苯基中20%的氘含量可由以下結構式表示。



[0039] 此外，在本申請的一個示例性實施例中，「氘含量為0%的苯基」可以指不包括氘原子，即具有五個氫原子的苯基。

【0040】　在本說明書中，鹵素可以是氟、氯、溴或碘。

【0041】　在本說明書中，烷基包括具有 1 至 60 個碳原子的直鏈或支鏈，並且可以另外被另一取代基取代。烷基的碳原子數可為 1 至 60、具體來說 1 至 40 和更具體來說 1 至 20。其具體實例包括甲基、乙基、丙基、正丙基、異丙基、丁基、正丁基、異丁基、叔丁基（tert-butyl group）、仲丁基（sec-butyl group）、1-甲基-丁基、1-乙基-丁基、戊基、正戊基、異戊基、新戊基、叔戊基(tert-pentyl group)、己基、正己基、1-甲基戊基、2-甲基戊基、4-甲基-2-戊基、3,3-二甲基丁基、2-乙基丁基、庚基、正庚基、1-甲基己基、辛基、正辛基、叔辛基（tert-octyl group）、1-甲基庚基、2-乙基己基、2-丙基戊基、正壬基、2,2-二甲基庚基、1-乙基-丙基、1,1-二甲基-丙基、異己基、2-甲基戊基、4-甲基己基、5-甲基己基等，但不限於至此。

【0042】　在本說明書中，烯基包括具有 2 至 60 個碳原子的直鏈或支鏈，並且可以另外被另一個取代基取代。烯基的碳原子數可為 2 至 60、具體來說 2 至 40 和更具體來說 2 至 20。其具體實例包括乙烯基、1-丙烯基、異丙烯基、1-丁烯基、2-丁烯基、3-丁烯基、1-戊烯基、2-戊烯基、3-戊烯基、3-甲基-1-丁烯基、1,3-丁二烯基、烯丙基、1-苯基乙烯基-1-基、2-苯基乙烯基-1-基、2,2-二苯基乙烯基-1-基、2-苯基-2-(萘基-1-基)乙烯基-1-基、2,2-雙(二苯基-1-基)乙烯基-1-基、芪基（stilbenyl group）、苯乙烯基等，但不限於此。

【0043】 在本說明書中，炔基包括具有 2 至 60 個碳原子的直鏈或支鏈，並且可以另外被另一個取代基取代。炔基的碳原子數可為 2 至 60、具體來說 2 至 40 和更具體來說 2 至 20。

【0044】 在本說明書中，鹵代烷基是指被鹵素基團取代的烷基，其具體實例包括-CF_3、-CF_2CF_3等，但不限於此。

【0045】 在本說明書中，烷氧基由-O(R101)表示，上述烷基的實例可適用於 R101。

【0046】 在本說明書中，芳氧基由-O(R102)表示，並且芳基的上述實例可適用於 R102。

【0047】 在本說明書中，烷硫氧基由-S(R103)表示，上述烷基的實例可適用於 R103。

【0048】 在本說明書中，芳硫氧基由-S(R104)表示，並且上述芳基的實例可適用於 R104。

【0049】 在本說明書中，烷磺氧基由-$S(=0)_2$(R105)表示，上述烷基的實例可適用於 R105。

【0050】 在本說明書中，芳磺氧基由-$S(=0)_2$(R106)表示，並且上述芳基的實例可適用於 R106。

【0051】 在本說明書中，環烷基包括具有 3 至 60 個碳原子的單環或多環，並且可以另外被另一個取代基取代。在此，多環是指環烷基與其他環狀基團直接連接或稠合而成的基團。此處，其他環狀基團也可以是環烷基，但也可以是其他種類的環狀基團，例如雜環烷基、芳基、雜芳基等。環烷基的碳原子數可為 3 至 60、

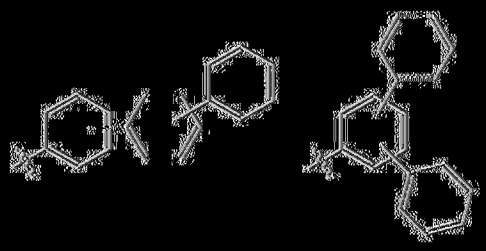
具體來說 3 至 40 和更具體來說 5 至 20。其具體實例包括環丙基、環丁基、環戊基、3-甲基環戊基、2,3-二甲基環戊基、環己基、3-甲基環己基、4-甲基環己基、2,3-二甲基環己基、3,4,5-三甲基環己基、4-叔丁基環己基、環庚基、環辛基等，但不限於此。

【0052】 在本說明書中，雜環烷基包括 O、S、Se、N 或 Si 作為雜原子，包括具有 2 至 60 個碳原子的單環或多環，並且可以另外被另一個取代基取代。在此，多環是指雜環烷基與其他環狀基團直接連接或稠合而成的基團。此處，其他環狀基團也可以是雜環烷基，但也可以是其他種類的環狀基團，例如環烷基、芳基、雜芳基等。雜環烷基的碳原子數可為 2 至 60、具體來說 2 至 40 和更具體來說 3 至 20。

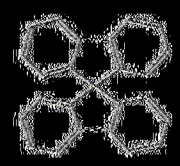
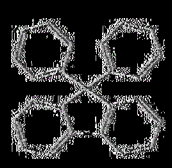
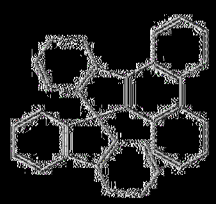
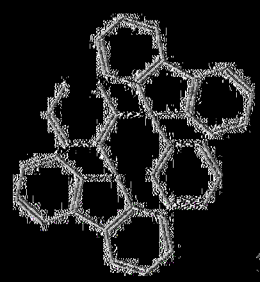
【0053】 在本說明書中，芳基包括具有 6 至 60 個碳原子的單環或多環，並且可以另外被另一取代基取代。在此，多環是指芳基與其他環狀基團直接連接或稠合而成的基團。此處，其他環狀基團也可以是芳基，但也可以是另一種環狀基團，例如環烷基、雜環烷基、雜芳基等。芳基包括螺環基團（spiro group）。芳基的碳原子數可為 6 至 60、具體來說 6 至 40 和更具體來說 6 至 25。芳基的具體實例包括苯基、聯苯基、三苯基（terphenyl group）、萘基、蒽基、䓛基（chrysenyl group）、菲基（phenanthrenyl group）、苝基（perylenyl group）、熒蒽基（fluoranthenyl group）、三亞苯基（triphenylenyl group）、𦯉基（phenalenyl group）、芘基（pyrenyl group）、稠四苯基（tetracenyl group）、稠五苯基、芴基（fluorenyl

group）、茚基（indenyl group）、苊基（acenaphthylenyl group）、苯並芴基（benzofluorenyl group）、螺二芴基（spirobifluorenyl group）、2,3-二氫-1H-茚基（2,3-dihydro-1H-indenyl group）、它們的稠合環基等，但不限於此。

[0054] 在本說明書中，三苯基可以選自以下結構。



[0055] 在本說明書中，芴基可以被取代，並且相鄰的取代基可以彼此鍵結形成環。

[0056] 當芴基被取代時，取代基可以是 、  、 、  、  、  等，但不限於此。

[0057] 在本說明書中，雜芳基包括S、O、Se、N或Si作為雜原子，包括具有2至60個碳原子的單環或多環，並且可以另外被另一個取代基取代。在此，多環是指雜芳基與其他環狀基團直接連接或稠合而成的基團。此處，其他環狀基團也可以是雜芳基，但也可以是另一種環狀基團，例如環烷基、雜環烷基、芳基等。雜芳基的碳原子數可為2至60、具體來說2至40和更具體來說3

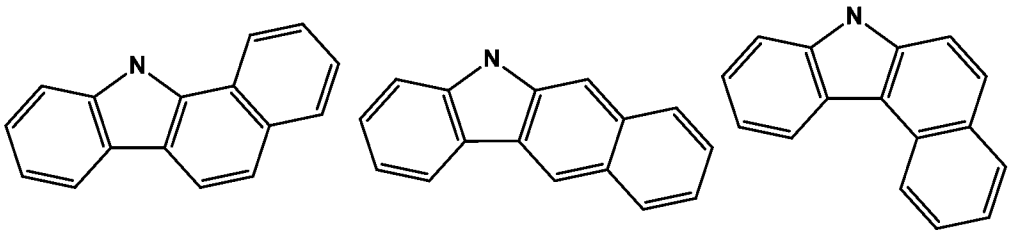
至 25。雜芳基的具體實例包括吡啶基、吡咯基、嘧啶基、噠嗪基、呋喃基、噻吩基、咪唑基、吡唑基、噁唑基、異噁唑基、噻唑基、異噻唑基、三唑基、呋咱基（furazan group）、噁二唑基、噻二唑基、二噻唑基、四唑基、吡喃基、噻喃基（thiopyran group）、二嗪基、噁嗪基、噻嗪基、二噁英基（dioxin group）、三嗪基、四嗪基、喹啉基、異喹啉基、喹唑啉基、異喹唑啉基、喹唑啉基（quinozoline group）、萘啶基、吖啶基、啡啶基（phenanthridine group）、咪唑並吡啶基、二氮雜萘基、三氮雜茚基、吲哚基、吲哚嗪基（indolizine group）、苯並噻唑基、苯並噁唑基、苯並咪唑基、苯並噻吩基、苯並呋喃基、二苯並噻吩基、二苯並呋喃基、哢唑基、苯並哢唑基、二苯並哢唑基、吩嗪基、矽雜芴基（dibenzosilole group）、螺矽芴（spirobi(dibenzosilole)）、二氫吩嗪基、啡噁嗪基（phenoxazine group）、啡啶基（phenanthridine group）、噻吩基、吲哚[2,3-a]哢唑基、吲哚[2,3-b]哢唑基、二氫吲哚基、10,11-二氫-二苯並[b,f]氮呯基（10,11-dihydro-dibenzo[b,f]azepine group）、9,10-二氫吖啶基、菲嗪基（phenanthrazine group）、吩噻嗪基（phenothiazine group）、酞嗪基、菲咯啉基（phenanthroline group）、萘並苯並呋喃基（naphthobenzofuran group）、萘並苯並噻吩基（naphthobenzothiophene group）、苯並[c][1,2,5]噻二唑基（benzo[c][1,2,5]thiadiazole group）、2,3-二氫苯並[b]噻吩基（2,3-dihydrobenzo[b]thiophene group）、2,3-二氫苯並呋喃基

（2,3-dihydrobenzofuran group）、5,10-二氫二苯並[b,e][1,4]氮雜環己基（5,10-dihydrodibenzo[b,e][1,4]azasiline group）、吡唑並[1,5-c]喹唑啉基（pyrazolo[1,5-c]quinazoline group）、吡並[1,2-b]吲唑基（pyrido[1,2-b]indazole group）、吡並[1,2-a]咪唑[1,2]-e]二氫吲哚基（pyrido[1,2-a]imidazo[1,2-e]indoline group）、5,11-二氫茚並[1,2-b]咔唑基（5,11-dihydroindeno[1,2-b]carbazole group）等，但不限於此。

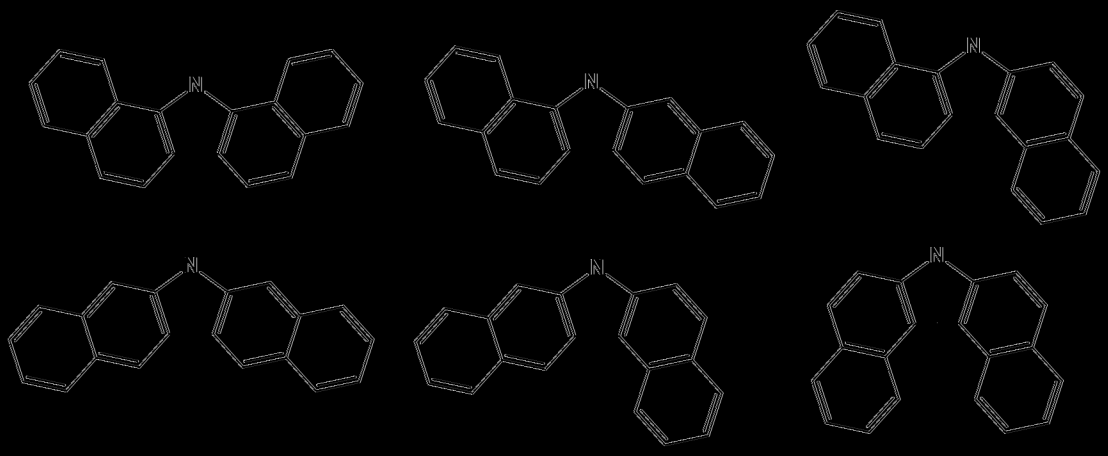
【0058】 在本說明書中，當取代基為咔唑基（carbazole group）時，其表示與咔唑的氮或碳鍵結。

【0059】 在本說明書中，當咔唑基被取代時，額外的取代基可以取代咔唑的氮或碳。

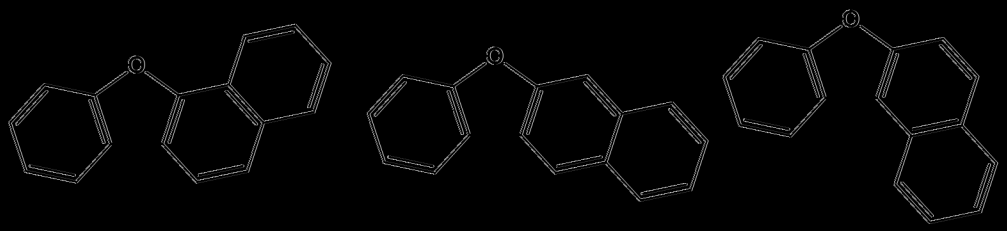
【0060】 在本說明書中，苯並咔唑基（benzocarbazole group）可以是以下結構中的任一種。



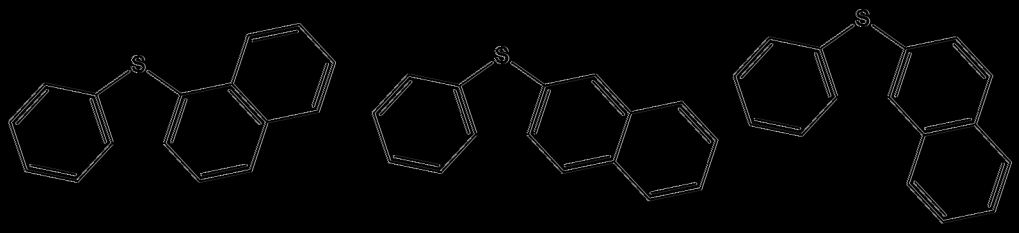
【0061】 在本說明書中，二苯並咔唑基（dibenzocarbazole group）可以是以下結構中的任一種。



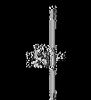
[0062] 在本說明書中，萘並苯並呋喃基可以是以下結構中的任一種。

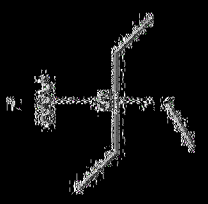
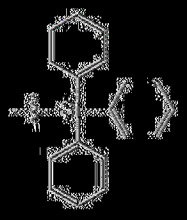
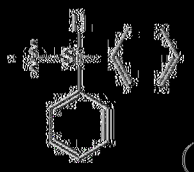


[0063] 在本說明書中，萘並苯並噻吩基可以是以下結構中的任一種。



[0064] 在本說明書中，甲矽烷基（silyl group）包括 Si，是 Si 原子直接連接作為自由基的取代基，且表示為 -Si(R107)(R108)(R109)，R107 至 R109 彼此相同或者不同，並且可以各自獨立地為氫；氘；鹵素基團；烷基；烯基；烷氧基；環烷基；雜環烷基；芳基；和雜芳基等中的至少一者組成的取代基

[0065] 甲矽烷基的具體實例包括  （三甲基甲矽烷基

（trimethyl silyl group））、  （三乙基甲矽烷基（triethylsilyl group））、 （叔丁基二甲基甲矽烷基（t-butyldimethylsilyl group））、 （乙烯基二甲基甲矽烷基（vinyldimethylsilyl group））、 （丙基二甲基甲矽烷基（propyldimethylsilyl group））、  （三苯基甲矽烷基（triphenylsilyl group））、  （二苯基甲矽烷基(diphenylsilyl group））、 （苯基甲矽烷基（phenylsilyl group）），但不限於此。

[0066] 在本說明書中，氧化膦基（phosphine oxide group）由-P(=O)(R110)(R111)表示，R110和R111彼此相同或不同，且可以各自獨立地為由氫；氘；鹵素基團；烷基；烯基；烷氧基；環烷基；雜環烷基；芳基；和雜芳基中的至少一者組成的取代基。具體來說，氧化膦基可以被烷基或芳基取代，並且上述示例可以適用於烷基和芳基。氧化膦基的實例包括二甲基氧化膦基（dimethylphosphine oxide group）、二苯基氧化膦基

（diphenylphosphine oxide group）、二萘基氧化膦基（dinaphthylphosphine oxide group）等，但不限於此。

【0067】 在本說明書中，胺基（amine group）由-N(R112)(R113)表示，R112 和 R113 彼此相同或不同，且可以各自獨立地為由氫；氘；鹵素基團；烷基；烯基；烷氧基；環烷基；雜環烷基；芳基；和雜芳基中的至少一個組成的取代基。胺基可選自由以下組成的群組：$-NH_2$；單烷基胺基；單芳基胺基；單雜芳基胺基；二烷基胺基；二芳基胺基；二雜芳基胺基；烷基芳基胺基；烷基雜芳基胺基；和芳基雜芳基胺基，且其碳原子數沒有特別限制，但優選為 1 至 30。胺基的具體實例包括甲胺基、二甲胺基、乙胺基、二乙胺基、苯胺基、萘胺基、聯苯胺基、二聯苯胺基、蒽基胺基、9-甲基-蒽基胺基、二苯胺基、苯基萘胺基、聯甲苯基胺基（ditolylamine group）、苯基甲苯基胺基、三苯基胺基、聯苯基萘基胺基、苯基聯苯基胺基、聯苯基芴基胺基、苯基三亞苯基胺基（phenyltriphenylenylamine group）、聯苯基三亞苯基胺基（biphenyltriphenylenylamine group）等，但不限於此。

【0068】 在本說明書中，芳基的上述實例可以適用於除了二價伸芳基之外的伸芳基。

【0069】 在本說明書中，雜芳基的上述實例可以適用於除二價伸雜芳基之外的伸雜芳基（heteroarylene group）。

【0070】 在本說明書中，「相鄰的」基團可以指被直接連接到其中相應取代基被取代的原子的原子取代的取代基、佈置在空間上

最接近相應取代基的取代基、或被其中相應的取代基取代的原子取代的另一個取代基。例如，兩個在苯環中鄰位取代的取代基和兩個在脂肪族環中相同碳原子上取代的取代基可被解釋為彼此「相鄰的」基團。

【0071】 相鄰基團可以形成的烴環和雜環包括脂肪族烴環、芳香族烴環、脂肪族雜環和芳香族雜環，以及由上述環烷基、芳基、雜環烷基和雜芳基示例的結構可以應用於環，除了那些不是單價基團的環。

【0072】 在本申請的一個示例性實施例中，由化學式 1 表示的雜環化合物的氘含量可以為 0%或大於 0%且 100%或小於 100%，優選為 20%或大於 20%且 100%或小於 100%，並且更優選為 40%或大於 40%且 100%或小於 100%。

【0073】 特別地，在化學式 1 中，那些沒有被取代基表示的可以是氫或氘。

【0074】 由於本發明的由化學式 1 表示的雜環化合物具有易於調控的帶隙和 T1 值，具有提高的電洞傳輸能力，並且還具有易於調控的分解溫度，因此熱穩定性優異且分子穩定性也得到增強，從而可以降低裝置的驅動電壓，提高光效率，提高裝置的使用壽命特性。

【0075】 在本申請的一個示例性實施例中，化學式 1 的 X 為 O；或 S。

【0076】 在本申請的一個示例性實施例中，X 是 O。

[0077] 在本申請的一個示例性實施例中，X是S。

[0078] 在本申請的一個示例性實施例中，化學式1的R1至R6中的一者為 ，其他中的一者為，其他彼此相同或不同，且可以各自獨立地選自由以下組成的群組：氫；氘；鹵素；氰基；經取代或未經取代的C1至C60烷基；經取代或未經取代的C2至C60烯基；經取代或未經取代的C2至C60炔基；經取代或未經取代的C1至C60烷氧基；經取代或未經取代的C3至C60環烷基；經取代或未經取代的C2至C60雜環烷基；經取代或未經取代的C6至C60芳基；經取代或未經取代的C2至C60雜芳基；-P(=O)RR'；-SiRR'R"和-NRR'。

[0079] 在本申請的一個示例性實施例中，R1至R6中的一者為，其他中的一者為，其他彼此相同或不同，且可以各自獨立地選自由以下組成的群組：氫；氘；經取代或未經取代的C1至C60烷基；經取代或未經取代的C6至C60芳基；和經取代或未經取代的C2至C60雜芳基。

[0080] 在另一個示例性實施例中，R1至R6中的一者為，其他中的一者為，且其他彼此相同或不同，並且可各自獨立地選自由以下組成的群組：氫；氘；C1至C60烷基；C6至C60芳基；和C2至C60雜芳基。

[0081] 在又一示例性實施例中，R1至R6中的一者為，其他中的一者為，且其他彼此相同或不同，且可各自獨立地選自由以下組成的群組：氫；氘；C1至C40

烷基；C6 至 C40 芳基；和 C2 至 C40 雜芳基。

【0082】 在又一個示例性實施例中，R1 至 R6 中的一個是 $-\S-(L1)a-Ar1$，其他中的一者是 $-\S-(L2)b-N\text{-}Het1$，並且其他彼此相同或不同，並且可以各自獨立地選自由以下組成的群組：氫；氘；C1 至 C30 烷基；C6 至 C30 芳基；和 C2 至 C30 雜芳基。

【0083】 在又一示例性實施例中，R1 至 R6 中的一者為 $-\S-(L1)a-Ar1$，其他中的一者為 $-\S-(L2)b-N\text{-}Het1$，其他彼此相同或不同，並且可以各自獨立地為氫；或氘。

【0084】 在本申請的一個示例性實施例中，R1 為 $-\S-(L1)a-Ar1$，R2 為 $-\S-(L2)b-N\text{-}Het1$，且 R3 至 R6 彼此相同或不同，並且可各自獨立地選自由以下組成的群組：氫；氘；鹵素；氰基；經取代或未經取代的 C1 至 C60 烷基；經取代或未經取代的 C2 至 C60 烯基；經取代或未經取代的 C2 至 C60 炔基；經取代或未經取代的 C1 至 C60 烷氧基；經取代或未經取代的 C3 至 C60 環烷基；經取代或未經取代的 C2 至 C60 雜環烷基；經取代或未經取代的 C6 至 C60 芳基；和經取代或未經取代的 C2 至 C60 雜芳基。

【0085】 在本申請的一個示例性實施例中，R1 為 $-\S-(L1)a-Ar1$，R2 為 $-\S-(L2)b-N\text{-}Het1$，且 R3 至 R6 彼此相同或不同，並且可以各自獨立地為氫；或氘。

【0086】 在本申請的一個示例性實施例中，R1 為 $-\S-(L1)a-Ar1$，R3 為 $-\S-(L2)b-N\text{-}Het1$，且 R2 和 R4 至 R6 彼此相同或不同，並且可以各自獨立地選自由以下組成的群組：氫；氘；鹵素基團；氰基；

經取代或未經取代的 C1 至 C60 烷基；經取代或未經取代的 C2 至 C60 烯基；經取代或未經取代的 C2 至 C60 炔基；經取代或未經取代的 C1 至 C60 烷氧基；經取代或未經取代的 C3 至 C60 環烷基；經取代或未經取代的 C2 至 C60 雜環烷基；經取代或未經取代的 C6 至 C60 芳基；經取代或未經取代的 C2 至 C60 雜芳基；-P(=O)RR'；-SiRR'R"和-NRR'。

【0087】 在本申請的一個示例性實施例中，R1 為 $-\S-(L1)a-Ar1$，R3 為 $-\S-(L2)b-N\text{-}Het1$，且 R2 與 R4 至 R6 彼此相同或不同，並且可以各自獨立地為氫；或氘。

【0088】 在本申請的一個示例性實施例中，R1 是 $-\S-(L1)a-Ar1$，R4 是 $-\S-(L2)b-N\text{-}Het1$，且 R2、R3、R5 和 R6 彼此相同或不同，並且可以各自獨立地選自由以下組成的群組：氫；氘；鹵素；氰基；經取代或未經取代的 C1 至 C60 烷基；經取代或未經取代的 C2 至 C60 烯基；經取代或未經取代的 C2 至 C60 炔基；經取代或未經取代的 C1 至 C60 烷氧基；經取代或未經取代的 C3 至 C60 環烷基；經取代或未經取代的 C2 至 C60 雜環烷基；經取代或未經取代的 C6 至 C60 芳基；經取代或未經取代的 C2 至 C60 雜芳基；-P(=O)RR'；-SiRR'R"和-NRR'。

【0089】 在本申請的一個示例性實施例中，R1 為 $-\S-(L1)a-Ar1$，R4 為 $-\S-(L2)b-N\text{-}Het1$，且 R2、R3、R5 和 R6 彼此相同或不同，並且可以各自獨立為氫；或氘。

【0090】 在本申請的一個示例性實施例中，R1 為 $-\S-(L1)a-Ar1$，

R5 為 $-\S-(L2)b-N-Het1$，且 R2 至 R4 和 R6 彼此相同或不同，並且可各自獨立地選自由以下組成的群組：氫；氘；鹵素基團；氰基；經取代或未經取代的 C1 至 C60 烷基；經取代或未經取代的 C2 至 C60 烯基；經取代或未經取代的 C2 至 C60 炔基；經取代或未經取代的 C1 至 C60 烷氧基；經取代或未經取代的 C3 至 C60 環烷基；經取代或未經取代的 C2 至 C60 雜環烷基；經取代或未經取代的 C6 至 C60 芳基；經取代或未經取代的 C2 至 C60 雜芳基；-P(=O)RR'；-SiRR'R"和-NRR'。

【0091】 在本申請的一個示例性實施例中，R1 為 $-\S-(L1)a-Ar1$，R5 為 $-\S-(L2)b-N-Het1$，且 R2 至 R4 和 R6 彼此相同或不同，並且可以各自獨立地為氫；或氘。

【0092】 在本申請的一個示例性實施例中，R1 為 $-\S-(L1)a-Ar1$，R6 為 $-\S-(L2)b-N-Het1$，且 R2 至 R5 彼此相同或不同，並且可各自獨立地選自由以下組成的群組：氫；氘；鹵素；氰基；經取代或未經取代的 C1 至 C60 烷基；經取代或未經取代的 C2 至 C60 烯基；經取代或未經取代的 C2 至 C60 炔基；經取代或未經取代的 C1 至 C60 烷氧基；經取代或未經取代的 C3 至 C60 環烷基；經取代或未經取代的 C2 至 C60 雜環烷基；經取代或未經取代的 C6 至 C60 芳基；經取代或未經取代的 C2 至 C60 雜芳基；-P(=O)RR'；-SiRR'R"和-NRR'。

【0093】 在本申請的一個示例性實施例中，R1 為 $-\S-(L1)a-Ar1$，R6 為 $-\S-(L2)b-N-Het1$，且 R2 至 R5 彼此相同或不同，並且可以各自

獨立地為氫；或氘。

【0094】 在本申請的一個示例性實施例中，R1 為 −§−(L2)b−N-Het1，R2 為 −§−(L1)a−Ar1，且 R3 至 R6 彼此相同或不同，並且可各自獨立地選自由以下組成的群組：氫；氘；鹵素；氰基；經取代或未經取代的 C1 至 C60 烷基；經取代或未經取代的 C2 至 C60 烯基；經取代或未經取代的 C2 至 C60 炔基；經取代或未經取代的 C1 至 C60 烷氧基；經取代或未經取代的 C3 至 C60 環烷基；經取代或未經取代的 C2 至 C60 雜環烷基；經取代或未經取代的 C6 至 C60 芳基；經取代或未經取代的 C2 至 C60 雜芳基；-P(=O)RR'；-SiRR'R"和-NRR'。

【0095】 在本申請的一個示例性實施例中，R1 為 −§−(L2)b−N-Het1，R2 為 −§−(L1)a−Ar1，且 R3 至 R6 彼此相同或不同，並且可以各自獨立地為氫；或氘。

【0096】 在本申請的一個示例性實施例中，R1 為 −§−(L2)b−N-Het1，R3 為 −§−(L1)a−Ar1，且 R2 和 R4 至 R6 彼此相同或不同，並且可以各自獨立地選自由以下組成的群組：氫；氘；鹵素基團；氰基；經取代或未經取代的 C1 至 C60 烷基；經取代或未經取代的 C2 至 C60 烯基；經取代或未經取代的 C2 至 C60 炔基；經取代或未經取代的 C1 至 C60 烷氧基；經取代或未經取代的 C3 至 C60 環烷基；經取代或未經取代的 C2 至 C60 雜環烷基；經取代或未經取代的 C6 至 C60 芳基；經取代或未經取代的 C2 至 C60 雜芳基；-P(=O)RR'；-SiRR'R"和-NRR'。

【0097】 在本申請的一個示例性實施例中，R1 為 -§-(L2)b-N-Het1，R3 為 -§-(L1)a-Ar1，且 R2 與 R4 至 R6 彼此相同或不同，並且可以各自獨立地為氫；或氘。

【0098】 在本申請的一個示例性實施例中，R1 是 -§-(L2)b-N-Het1，R4 是 -§-(L1)a-Ar1，且 R2、R3、R5 和 R6 彼此相同或不同，並且可以各自獨立地選自由以下組成的群組：氫；氘；鹵素；氰基；經取代或未經取代的 C1 至 C60 烷基；經取代或未經取代的 C2 至 C60 烯基；經取代或未經取代的 C2 至 C60 炔基；經取代或未經取代的 C1 至 C60 烷氧基；經取代或未經取代的 C3 至 C60 環烷基；經取代或未經取代的 C2 至 C60 雜環烷基；經取代或未經取代的 C6 至 C60 芳基；經取代或未經取代的 C2 至 C60 雜芳基；-P(=O)RR'；-SiRR'R"和-NRR'。

【0099】 在本申請的一個示例性實施例中，R1 為 -§-(L2)b-N-Het1，R4 為 -§-(L1)a-Ar1，且 R2、R3、R5 和 R6 彼此相同或不同，並且可以各自獨立地為氫；或氘。

【0100】 在本申請的一個示例性實施例中，R1 為 -§-(L2)b-N-Het1，R5 為 -§-(L1)a-Ar1，且 R2 至 R4 和 R6 彼此相同或不同，並且可各自獨立地選自由以下組成的群組：氫；氘；鹵素基團；氰基；經取代或未經取代的 C1 至 C60 烷基；經取代或未經取代的 C2 至 C60 烯基；經取代或未經取代的 C2 至 C60 炔基；經取代或未經取代的 C1 至 C60 烷氧基；經取代或未經取代的 C3 至 C60 環烷基；經取代或未經取代的 C2 至 C60 雜環烷基；經取代或

未經取代的 C6 至 C60 芳基；經取代或未經取代的 C2 至 C60 雜芳基；-P(=O)RR'；-SiRR'R"和-NRR'。

【0101】 在本申請的一個示例性實施例中，R1 為 $-\S-(L2)b-N-Het1$，R5 為 $-\S-(L1)a-Ar1$，且 R2 至 R4 和 R6 彼此相同或不同，並且可以各自獨立地為氫；或氘。

【0102】 在本申請的一個示例性實施例中，R1 為 $-\S-(L2)b-N-Het1$，R6 為 $-\S-(L1)a-Ar1$，且 R2 至 R5 彼此相同或不同，並且可各自獨立地選自由以下組成的群組：氫；氘；鹵素；氰基；經取代或未經取代的 C1 至 C60 烷基；經取代或未經取代的 C2 至 C60 烯基；經取代或未經取代的 C2 至 C60 炔基；經取代或未經取代的 C1 至 C60 烷氧基；經取代或未經取代的 C3 至 C60 環烷基；經取代或未經取代的 C2 至 C60 雜環烷基；經取代或未經取代的 C6 至 C60 芳基；經取代或未經取代的 C2 至 C60 雜芳基；-P(=O)RR'；-SiRR'R"和-NRR'。

【0103】 在本申請的一個示例性實施例中，R1 為 $-\S-(L2)b-N-Het1$，R6 為 $-\S-(L1)a-Ar1$，且 R2 至 R5 彼此相同或不同，並且可以各自獨立地為氫；或氘。

【0104】 在本申請的一個示例性實施例中，化學式 1 的 L1 和 L2 彼此相同或不同，且可以各自獨立地為直接鍵；經取代或未經取代的 C6 至 C60 伸芳基；或經取代或未經取代的 C2 至 C60 伸雜芳基。

【0105】 在另一個示例性實施例中，L1 和 L2 彼此相同或不同，

並且可以各自獨立地為直接鍵；經取代或未經取代的 C6 至 C40 伸芳基；或經取代或未經取代的 C2 至 C40 伸雜芳基。

【0106】 在又一個示例性實施例中，L1 和 L2 彼此相同或不同，並且可以各自獨立地為直接鍵；或經取代或未經取代的 C6 至 C40 伸芳基。

【0107】 在又一個示例性實施例中，L1 和 L2 彼此相同或不同，並且可以各自獨立地為直接鍵；或經取代或未經取代的 C6 至 C40 單環或多環伸芳基。

【0108】 在又一示例性實施例中，L1 和 L2 彼此相同或不同，並且可以各自獨立地為直接鍵；經取代或未經取代的 C6 至 C10 單環伸芳基；或經取代或未經取代的 C10 至 C40 多環伸芳基。

【0109】 在進一步的示例性實施例中，L1 和 L2 彼此相同或不同，並且可以各自獨立地為直接鍵；經取代或未經取代的亞苯基（phenylene group）；經取代或未經取代的亞聯苯基（biphenylene group）；經取代或未經取代的亞萘基（naphthylene group）；或經取代或未經取代的亞蒽基（anthracenylene group）。

【0110】 亞苯基、亞聯苯基、亞萘基和亞蒽基分別是苯基、聯苯基、萘基和蒽基的二價基團。

【0111】 在本申請的一個示例性實施例中，L1 和 L2 可以是未經取代或被氘取代。

【0112】 在本申請的一個示例性實施例中，L1 和 L2 的氘含量可以為 0%或大於 0%且 100%或小於 100%，優選 20%或大於 20%

且 100%或小於 100%，更優選 40%或大於 40%且 100%或小於 100%。

【0113】 在本申請的一個示例性實施例中，a 和 b 各自為 0 至 3 的整數，並且當 a 和 b 各自為 2 或大於 2 時，括號中的取代基彼此相同或不同。

【0114】 在本申請的一個示例性實施例中，a 為 0。a 為 1。a 是 2。a 是 3。當 a 為 2 或大於 2 時，括號內的 L1 彼此相同或不同。

【0115】 在本申請的一個示例性實施例中，b 是 0。b 為 1。b 為 2。b 為 3。當 b 為 2 或大於 2 時，括號內的 L2 彼此相同或不同。

【0116】 在本申請的一個示例性實施例中，Ar1 可以是經取代或未經取代的 C6 至 C60 的芳基；或經取代或未經取代的 C2 至 C60 雜芳基。

【0117】 在本申請的一個示例性實施例中，Ar1 可以是經取代或未經取代的 C6 至 C40 的芳基；或經取代或未經取代的 C2 至 C40 雜芳基。

【0118】 在本申請的一個示例性實施例中，Ar1 可以是經取代或未經取代的 C6 至 C20 的芳基；或經取代或未經取代的 C2 至 C20 雜芳基。

【0119】 在另一個示例性實施例中，Ar1 可以是 C6 至 C40 芳基，其為未經取代或被一個或多個選自由以下組成的群組中的取代基取代：氘、氰基、鹵素基團、C6 至 C40 芳基和 C2 至 C40 雜芳基；或為未經取代或被一個或多個選自由氘、氰基、鹵素基、C6 至 C40

芳基和 C2 至 C40 雜芳基組成的群組中的取代基取代的 C2 至 C40 雜芳基。

【0120】 在又一示例性實施例中，Ar1 可以是 C6 至 C40 芳基，其為未經取代或被一個或多個選自由氘、氰基和鹵素組成的群組中的取代基取代；或 C2 至 C40 雜芳基，其為未經取代或被一個或多個選自由氘、氰基和鹵素基團組成的群組中的取代基取代。

【0121】 在又一示例性實施例中，Ar1 可以是經取代或未經取代的苯基；經取代或未經取代的聯苯基；經取代或未經取代的三聯苯基；經取代或未經取代的萘基；經取代或未經取代的三亞苯基（triphenylenyl group）；經取代或未經取代的菲基；經取代或未經取代的苯蒽基（fluoranthenyl group）；經取代或未經取代的䓛基（chrysenyl group）；經取代或未經取代的二甲基芴基（dimethylfluorenyl group）；經取代或未經取代的苯並[e] 螢蒽基（benzo[e]acephenanthrylene group）；經取代或未經取代的二苯並呋喃基；經取代或未經取代的二苯並噻吩基；經取代或未經取代的咔唑基（carbazole group）；經取代或未經取代的苯環的芴蒽基；經取代或未經取代的苯環稠合的二苯並呋喃基團；經取代或未經取代的苯環稠合的二苯並噻吩基團；或經取代或未經取代的苯環稠合的二甲基芴基。

【0122】 在又一示例性實施例中，Ar1 彼此相同或不同，並且可以各自獨立地為未經取代或被一個或多個選自由氘、氰基和鹵素組成的群組中的取代基取代的苯基；未經取代或被一個或多個選

自由氘、氰基和鹵素基團的取代基取代的聯苯基；未經取代或被一個或多個選自由氘、氰基和鹵素基團組成的群組中的取代基取代的三苯基（terphenyl group）；未經取代或被一個或多個選自由氘、氰基和鹵素基團組成的群組中的取代基取代的萘基；未經取代或被一個或多個選自由氘、氰基和鹵素基團組成的群組中的取代基取代的三亞苯基（triphenylenyl group）；未經取代或被一個或多個選自由氘、氰基和鹵素基團組成的群組中的取代基取代的菲基（phenanthrenyl group）；未經取代或被一個或多個選自由氘、氰基和鹵素基團組成的群組中的取代基取代的芴蒽基；為未經取代或被一個或多個選自由氘、氰基和鹵素基團組成的群組中的取代基取代的熒基；未經取代或被一個或多個選自由氘、氰基和鹵素基團組成的群組中的取代基取代的二甲基芴基；未經取代或被一個或多個選自由氘、氰基和鹵素基團組成的群組中的取代基取代的苯並[e]螢蒽基；未經取代或被一個或多個選自由氘、氰基和鹵素基團組成的群組中的取代基取代的二苯並呋喃基團；未經取代或被一個或多個選自由氘、氰基和鹵素基團組成的群組中的取代基取代的二苯並噻吩基團；未經取代或被一個或多個選自由氘和苯基組成的群組中的取代基取代的咔唑基；未經取代或被一個或多個選自由氘、氰基和鹵素基團組成的群組中的取代基取代的經取代或未經取代的苯環稠合的芴蒽基；未經取代或被一個或多個選自由氘、氰基和鹵素基團組成的群組中的取代基取代的苯環稠合的二苯並呋喃基；未經取代或被一個或多個選自由氘、氰基

和鹵素基團組成的群組中的取代基取代的苯環稠合而成的二苯並噻吩基團；或未經取代或被一個或多個選自由氘、氰基和鹵素基團組成的群組中的取代基取代的苯環稠合的二甲基芴基。

【0123】 在本申請的示例性實施例中，Ar1 的氘含量可以為 0%或大於 0%且 100%或小於 100%，優選為 20%或大於 20%且 100%或小於 100%，並且更優選為 40%或大於 40%且 100%或小於 100%。

【0124】 在本申請的一個示例性實施例中，N-Het1 為單環或多環雜環基團，其經取代或未經取代並且包括一個或多個 N。

【0125】 在本申請的一個示例性實施例中，N-Het1 可以是其中經取代或未經取代且包括一個或多個 N 的單環或多環雜環基團包括一個或多個且三個或少於三個的 N 的 N-Het1。

【0126】 在本申請的一個示例性實施例中，化學式 2 的 L3 和 L4 彼此相同或不同，且可以各自獨立地為直接鍵；經取代或未經取代的 C6 至 C60 伸芳基；或經取代或未經取代的 C2 至 C60 伸雜芳基。

【0127】 在另一個示例性實施例中，L3 和 L4 彼此相同或不同，並且可以各自獨立地為直接鍵；經取代或未經取代的 C6 至 C40 伸芳基；或經取代或未經取代的 C2 至 C40 伸雜芳基。

【0128】 在又一個示例性實施例中，L3 和 L4 彼此相同或不同，並且可以各自獨立地為直接鍵；經取代或未經取代的 C6 至 C20 伸芳基；或經取代或未經取代的 C2 至 C20 伸雜芳基。

【0129】 在又一個示例性實施例中，L3 和 L4 彼此相同或不同，並且可以各自獨立地為直接鍵；經取代或未經取代的亞苯基；經取代或未經取代的亞呋喃基團；經取代或未經取代的亞萘基；或經取代或未經取代的亞蒽基。

【0130】 亞苯基、亞呋喃基、亞萘基和亞蒽基分別是苯基、呋喃基、萘基和蒽基的二價基團。

【0131】 在本申請的示例性實施例中，L3 和 L4 可以是未經取代或被氘取代。

【0132】 在本申請的一個示例性實施例中，L3 和 L4 的氘含量可以為 0%或大於 0%且 100%或小於 100%，優選 20%或大於 20%且 100%或小於 100%，更優選 40%或大於 40%且 100%或小於 100%。

【0133】 在本申請的一個示例性實施例中，m 和 n 各自為 0 至 3 的整數，並且當 m 和 n 各自為 2 或大於 2 時，括號中的取代基彼此相同或不同。

【0134】 在本申請的一個示例性實施例中，m 為 0。m 為 1。m 為 2。m 為 3。當 m 為 2 或大於 2 時，括號內的 L3 彼此相同或不同。

【0135】 在本申請的一個示例性實施例中，n 為 0。n 為 1。n 為 2。n 為 3。當 n 為 2 或大於 2 時，括號內的 L4 彼此相同或不同。

【0136】 在本申請的一個示例性實施例中，N-Het2 為單環或多環雜環基團，其經取代或未經取代且包括一個或多個 N。

[0137] 在本申請的一個示例性實施例中，N-Hct2 可以是其中經取代或未經取代且包括一個或多個 N 的單環或多環雜環基團包括一個或多個且三個或少於三個的 N 的 N-Hct2。

[0138] 在本申請的示例性實施例中，N-Hct1 和 N-Hct2 可以各自獨立地由以下化學式 3 表示。

[0139] [化學式 3]

[0140] 在化學式 3 中，

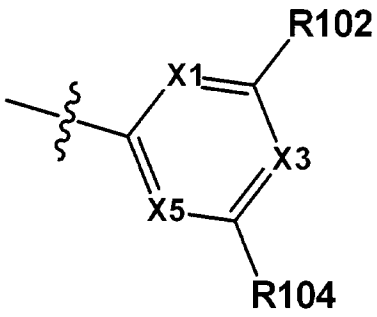
X1 為 CR101 或 N，X2 為 CR102 或 N，X3 為 CR103 或 N，X4 為 CR104 或 N，X5 為 CR105 或 N，且 X1 至 X5 中至少一者為 N，且

R101 至 R105 彼此相同或不同，且各自獨立地選自由以下組成的群組：氫；氘；鹵素；氰基；經取代或未經取代的 C1 至 C60 烷基；經取代或未經取代的 C2 至 C60 烯基；經取代或未經取代的 C2 至 C60 炔基；經取代或未經取代的 C1 至 C20 烷氧基；經取代或未經取代的 C3 至 C60 環烷基；經取代或未經取代的 C2 至 C60 雜環烷基；經取代或未經取代的 C6 至 C60 芳基；經取代或未經取代的 C2 至 C60 雜芳基；經取代或未經取代的氧化膦基；和經取代或未經取代的胺基，或兩個或多於兩個相鄰基團相互鍵結形成經取代或未經取代的脂肪族或芳香族烴環或雜環，且在此， 是

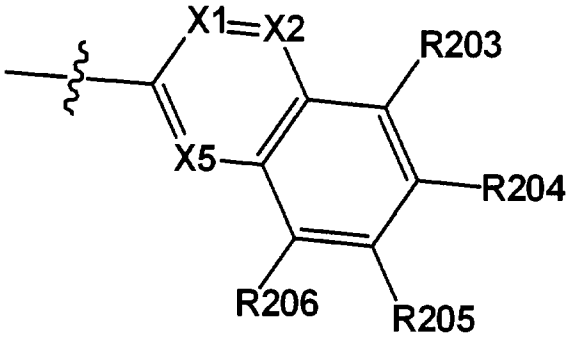
與化學式 1 或 2 連接的部分。

【0141】 在本申請的一個示例性實施例中，化學式 3 可以由以下化學式 4 至 8 中的任何一個表示。

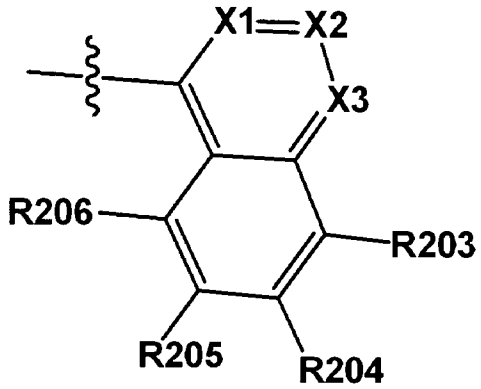
【0142】 [化學式 4]



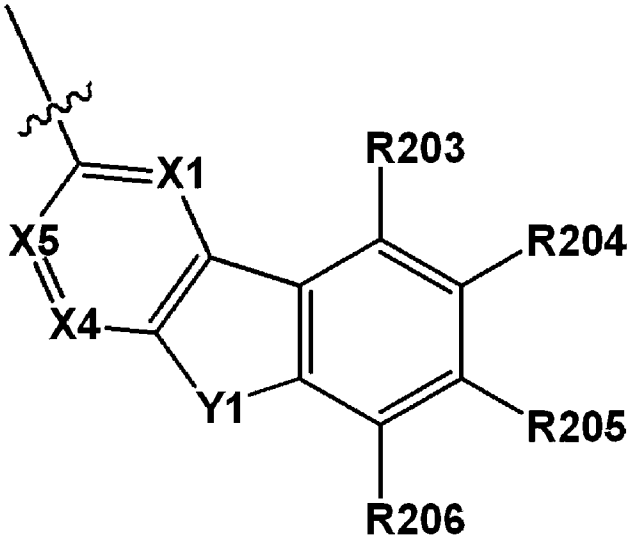
【0143】 [化學式 5]



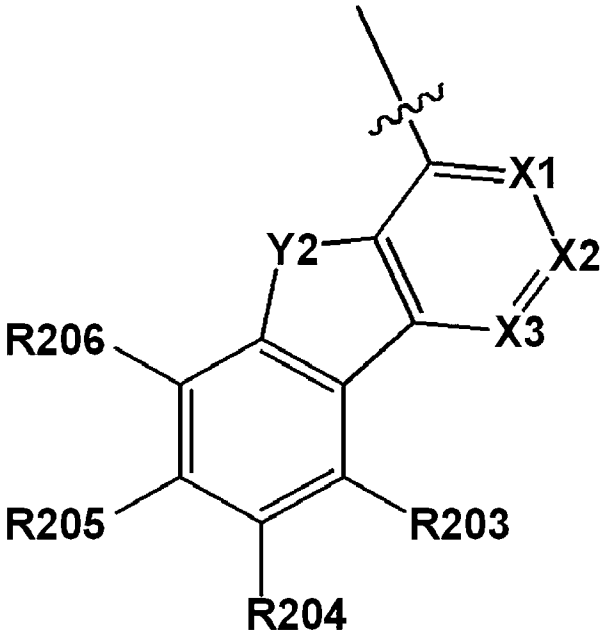
【0144】 [化學式 6]



【0145】 [化學式 7]



【0146】 [化學式 8]



【0147】 在化學分式 4 中，X1、X3、X5 中的一個或多個為 N，其他與化學式 3 中定義相同，

在化學式 5 中，X1、X2、X5 中的一個或多個為 N，其他同化學式 3 中的定義，

在化學式 6 中，X1 至 X3 中的一個或多個為 N，其他與化學式 3 中定義相同，

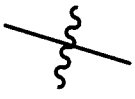
在化學式 7 中，X1、X4、X5 中的一個或多個為 N，其他同

化學式 3 中的定義，

在化學式 8 中，X1 至 X3 中的一個或多個為 N，其他與化學式 3 中定義相同，

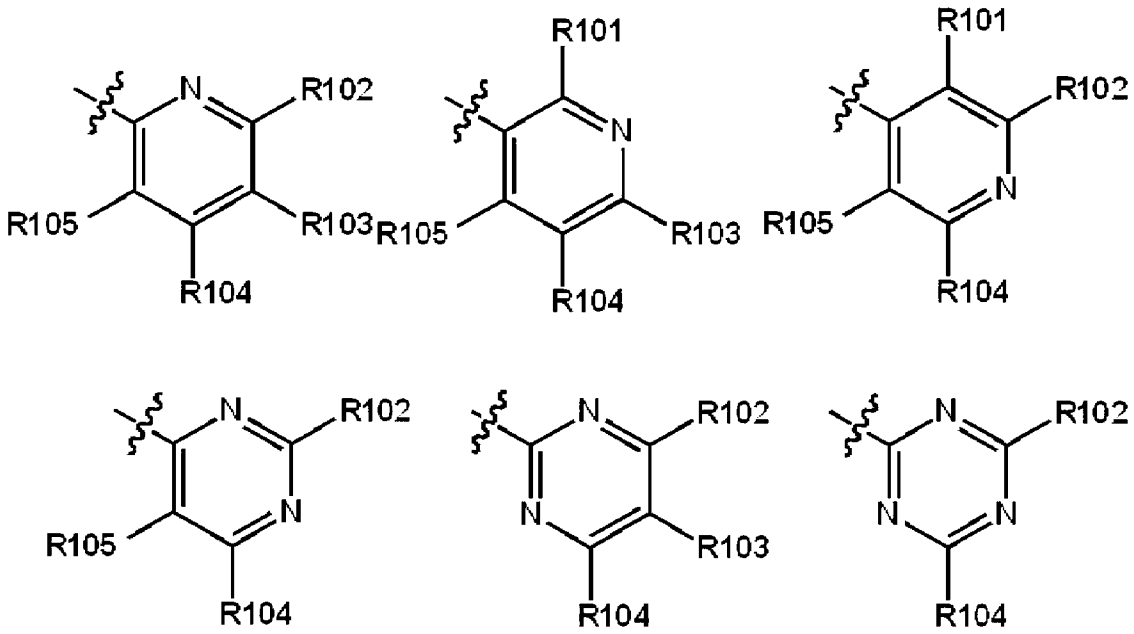
Y1 和 Y2 各自獨立為 O；或 S，

R102、R104、R203 至 R206 彼此相同或不同，且各自獨立地選自由以下組成的群組：氫；氘；鹵素；氰基；經取代或未經取代的 C1 至 C60 烷基；經取代或未經取代的 C2 至 C60 烯基；經取代或未經取代的 C2 至 C60 炔基；經取代或未經取代的 C1 至 C20 烷氧基；經取代或未經取代的 C3 至 C60 環烷基；經取代或未經取代的 C2 至 C60 雜環烷基；經取代或未經取代的 C6 至 C60 芳基；經取代或未經取代的 C2 至 C60 雜芳基；經取代或未經取代的氧化膦基；和經取代或未經取代的胺基，或兩個或多於兩個相鄰的基團彼此鍵結以形成經取代或未經取代的脂肪族或芳香族烴環或雜環，和

 的定義同化學式 3 中的定義。

【0148】 在本申請的一個示例性實施例中，化學式 4 可以選自以下群組 A 結構式中的任一個。

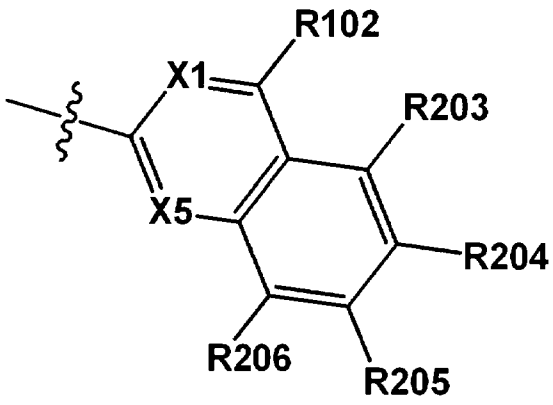
【0149】 [群組 A]



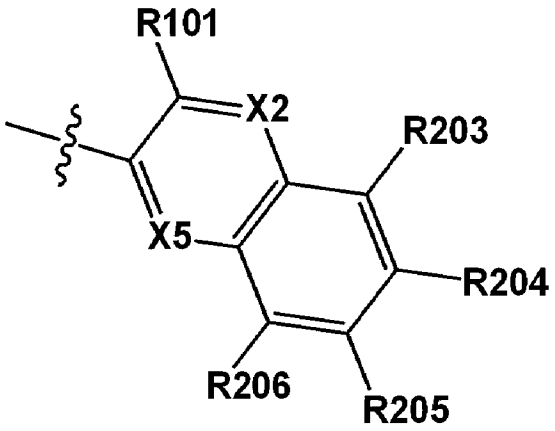
【0150】 群組 A 的結構式中的取代基的定義同化學式 4 中的那些的定義。

【0151】 在本申請的一個示例性實施例中，化學式 5 可以由以下化學式 5-1 或化學式 5-2 表示。

【0152】 [化學式 5-1]



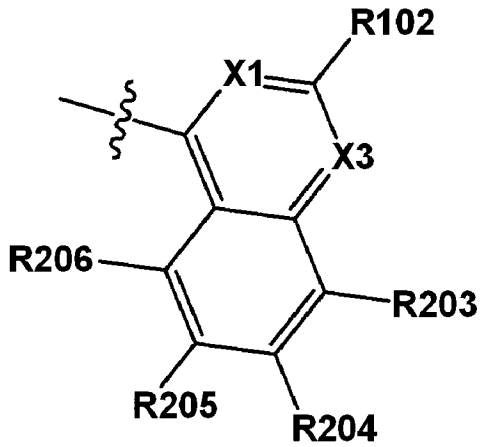
【0153】 [化學式 5-2]



【0154】 化學式 5-1 和 5-2 的取代基與化學式 5 中定義的那些相同。

【0155】 在本申請的一個示例性實施例中，化學式 6 可以由以下化學式 6-1 表示。

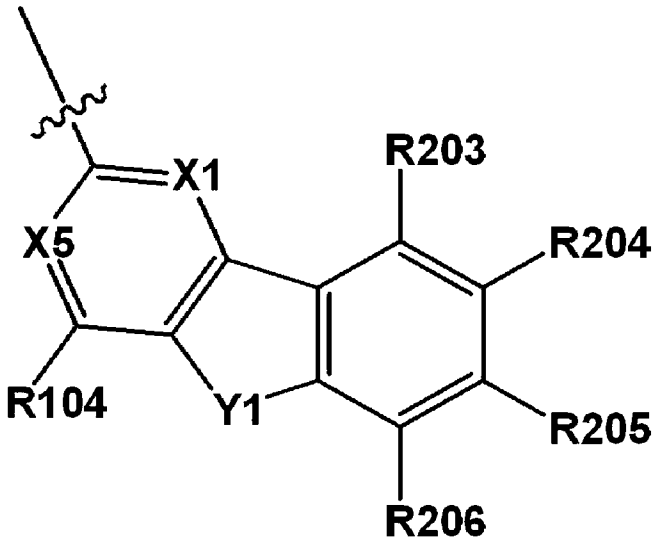
【0156】 [化學式 6-1]



【0157】 化學式 6-1 的取代基與化學式 6 中所定義的那些相同。

【0158】 在本申請的一個示例性實施例中，化學式 7 可以由以下化學式 7-1 表示。

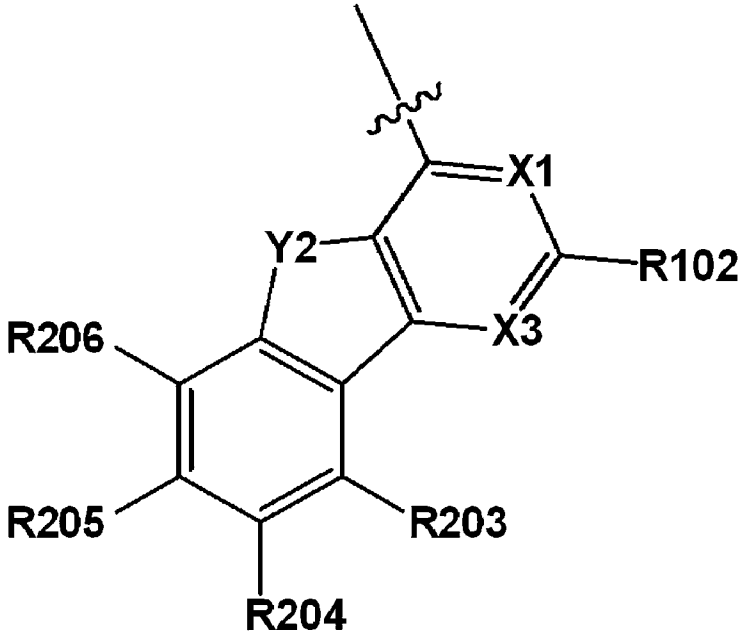
【0159】 [化學式 7-1]



【0160】 化學式 7-1 的取代基與化學式 7 中所定義的那些相同。

【0161】 在本申請的一個示例性實施例中，化學式 8 可以由以下化學式 8-1 表示。

【0162】 [化學式 8-1]



【0163】 化學式 8-1 的取代基與化學式 8 中所定義的那些相同。

【0164】 在本申請的一個示例性實施例中，R101 至 R105 和 R203 至 R206 彼此相同或不同，且可以各自獨立地為氫；氘；鹵素；氰基；經取代或未經取代的 C1 至 C60 烷基；經取代或未經取代的

C6 至 C60 芳基；或經取代或未經取代的 C2 至 C60 雜芳基。

【0165】 在本申請的一個示例性實施例中，R101 至 R105 和 R203 至 R206 彼此相同或不同，且可以各自獨立地為氫；氘；經取代或未經取代的 C6 至 C60 芳基；或經取代或未經取代的 C2 至 C60 雜芳基。

【0166】 在本申請的一個示例性實施例中，R101 至 R105 和 R203 至 R206 彼此相同或不同，且可以各自獨立地為氫；氘；經取代或未經取代的 C6 至 C40 芳基；或經取代或未經取代的 C2 至 C40 雜芳基。

【0167】 在本申請的一個示例性實施例中，R101 至 R105 和 R203 至 R206 彼此相同或不同，且可以各自獨立地為氫；氘；經取代或未經取代的 C6 至 C20 芳基；或經取代或未經取代的 C2 至 C20 雜芳基。

【0168】 在本申請的一個示例性實施例中，化學式 2 的 L5 和 L6 彼此相同或不同，且可以各自獨立地為直接鍵；經取代或未經取代的 C6 至 C60 伸芳基；或經取代或未經取代的 C2 至 C60 伸雜芳基。

【0169】 在另一個示例性實施例中，L5 和 L6 彼此相同或不同，並且可以各自獨立地為直接鍵；經取代或未經取代的 C6 至 C40 伸芳基；或經取代或未經取代的 C2 至 C40 伸雜芳基。

【0170】 在又一個示例性實施例中，L5 和 L6 彼此相同或不同，並且可以各自獨立地為直接鍵；經取代或未經取代的 C6 至 C20

伸芳基；或經取代或未經取代的 C2 至 C20 伸雜芳基。

【0171】 在又一個示例性實施例中，L5 和 L6 彼此相同或不同，並且可以各自獨立地為直接鍵；經取代或未經取代的亞苯基；經取代或未經取代的亞聯苯基；經取代或未經取代的亞萘基；經取代或未經取代的亞蒽基；經取代或未經取代的亞咔唑基（carbazolene group）；經取代或未經取代的稠合的亞咔唑基；經取代或未經取代的亞呋喃基；或經取代或未經取代的亞噻吩基。

【0172】 亞苯基、亞聯苯基、亞萘基、亞蒽基、亞咔唑基、稠合的亞咔唑基、亞呋喃基和亞噻吩基分別為苯基、聯苯基、萘基、蒽基、咔唑基、稠合的咔唑基、呋喃基和噻吩基的二價基團。

【0173】 在本申請的示例性實施例中，L5 和 L6 可以是未經取代或被氘取代。

【0174】 在本申請的一個示例性實施例中，L5 和 L6 的氘含量可以為 0%或大於 0%且 100%或小於 100%，優選 20%或大於 20%且 100%或小於 100%，更優選 40%或大於 40%且 100%或小於 100%。

【0175】 在本申請的一個示例性實施例中，m1 和 m2 各自為 0 至 3 的整數，並且當 m1 和 m2 各自為 2 或大於 2 時，括號中的取代基彼此相同或不同。

【0176】 在本申請的一個示例性實施例中，m1 為 0。m1 為 1。m1 為 2。m1 為 3。當 m1 為 2 或大於 2 時，括號內的 L5 彼此相同或不同。

【0177】 在本申請的一個示例性實施例中，m2 為 0。m2 為 1。m2 為 2。m2 為 3。當 m2 為 2 或大於 2 時，括號內的 L6 彼此相同或不同。

【0178】 在本申請的一個示例性實施例中，化學式 2 的 Y 為 O；或 S。

【0179】 在本申請的一個示例性實施例中，Y 是 O。

【0180】 在本申請的一個示例性實施例中，Y 是 S。

【0181】 在本申請的一個示例性實施例中，化學式 2 的 Ar2 和 Ar3 彼此相同或不同，且各自獨立地為經取代或未經取代的 C6 至 C60 的芳基；經取代或未經取代的 C2 至 C60 雜芳基；或-NRR'。

【0182】 在本申請的一個示例性實施例中，Ar2 和 Ar3 彼此相同或不同，並且可以各自獨立地為經取代或未經取代的 C6 至 C40 的芳基；經取代或未經取代的 C2 至 C40 雜芳基；或-NRR'。

【0183】 在本申請的一個示例性實施例中，Ar2 和 Ar3 彼此相同或不同，並且可以各自獨立地為經取代或未經取代的 C6 至 C20 的芳基；經取代或未經取代的 C2 至 C20 雜芳基；或-NRR'。

【0184】 在本申請的一個示例性實施例中，Ar2 和 Ar3 彼此相同或不同，並且可以各自獨立地為經取代或未經取代的苯基；經取代或未經取代的聯苯基；經取代或未經取代的三聯苯基；經取代或未經取代的萘基；經取代或未經取代的菲基；經取代或未經取代的芘基；經取代或未經取代的苝基；經取代或未經取代的 4,5-二苯基苯並[4,5]環庚[1,2,3-de]萘基

（4,5-diphenylbenzo[4,5]cyclohepta[1,2,3-de]naphthalenyl group）；經取代或未經取代的二甲基芴基；經取代或未經取代的螺二芴基；經取代或未經取代的二苯基芴基（diphenylfluorenyl group）；經取代或未經取代的哢唑基；經取代或未經取代的稠合的哢唑基；經取代或未經取代的芴蒽基（fluoranthene group）；經取代或未經取代的稠合的芴蒽基；經取代或未經取代的二苯並呋喃基團；經取代或未經取代的萘並苯並呋喃基團；經取代或未經取代的二苯並噻吩基團；或-NRR'。

【0185】 在本申請的一個示例性實施例中，L3、L5、L6、Ar2 和 Ar3 的相鄰取代基可以彼此鍵結以形成經取代或未經取代的脂肪族或芳香族烴環或經取代或未經取代的脂肪族或芳香族雜環，L3、L5、L6、Ar2 和 Ar3 的相鄰取代基相互鍵結是指包括除了 Ar2 和 Ar3 相互鍵結的情況之外的所有以下的情況：L3、Ar2 和 Ar3 相互鍵結、L5、L6、Ar2 和 Ar3 相互鍵結以及 L3、L5 和 L6 相互鍵結。

【0186】 在本申請的一個示例性實施例中，Ar2 和 Ar3 可以彼此鍵結以形成經取代或未經取代的脂肪族或芳香族烴環或者經取代或未經取代的脂肪族或芳香族雜環。

【0187】 在本申請的一個示例性實施例中，Ar2 和 Ar3 彼此相同或不同，且各自獨立地為經取代或未經取代的 C6 至 C40 的芳基；經取代或未經取代的 C2 至 C40 雜芳基；或-NRR'，或 Ar2 和 Ar3 可以彼此鍵結以形成經取代或未經取代的脂肪族或芳香族烴環或

經取代或未經取代的脂肪族或芳香族雜環。

【0188】 在本申請的一個示例性實施例中，Ar2 和 Ar3 彼此相同或不同，且各自獨立地為經取代或未經取代的 C6 至 C20 的芳基；經取代或未經取代的 C2 至 C20 雜芳基；或-NRR’，或 Ar2 和 Ar3 可以彼此鍵結以形成經取代或未經取代的脂肪族或芳香族烴環或經取代或未經取代的脂肪族或芳香族雜環。

【0189】 在本申請的一個示例性實施例中，Ar2、Ar3 和 L3 可以彼此鍵結以形成經取代或未經取代的脂肪族或芳香族烴環或者經取代或未經取代的脂肪族或芳香族雜環。在這種情況下，L5 和 L6 可以是直接鍵。關於 Ar2、Ar3 和 L3 相互鍵結形成經取代或未經取代的脂肪族或芳香族烴環或經取代或未經取代的脂肪族或芳香族雜環的情況，可以以下述化學式 A-9 為例，但不限於此。

【0190】 在本申請的示例性實施例中，L5、L6、Ar2 和 Ar3 可以彼此鍵結以形成經取代或未經取代的脂肪族或芳香族烴環或經取代或未經取代的脂肪族或芳香族雜環。

【0191】 在本申請的一個示例性實施例中，L3、L5 和 L6 可以彼此鍵結以形成經取代或未經取代的脂肪族或芳香族烴環或者經取代或未經取代的脂肪族或芳香族雜環。

【0192】 在本申請的一個示例性實施例中，R、R’和 R”彼此相同或不同，並且可以各自獨立地為經取代或未經取代的 C1 至 C60 的烷基；經取代或未經取代的 C6 至 C60 的芳基；或經取代或未經取代的 C2 至 C60 雜芳基。

【0193】 在另一個示例性實施例中，R、R’和 R”彼此相同或不同，並且可以各自獨立地為經取代或未經取代的 C6 至 C60 的芳基。

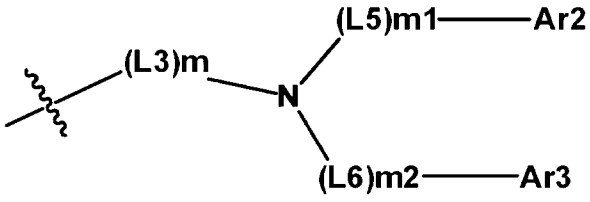
【0194】 在又一個示例性實施例中，R、R’和 R”彼此相同或不同，並且可以各自獨立地是經取代或未經取代的 C6 至 C60 單環或多環芳基。

【0195】 在又一個示例性實施例中，R、R’和 R”彼此相同或不同，並且可以各自獨立地是經取代或未經取代的 C6 至 C40 單環芳基。

【0196】 在又一示例性實施例中，R、R’和 R”彼此相同或不同，並且可以各自獨立地為 C6 至 C20 單環芳基。

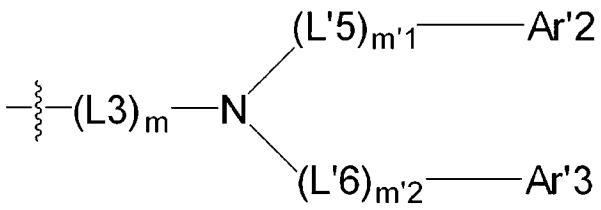
【0197】 在另一個示例性實施例中，R、R’和 R”可以是苯基。

【0198】 在本申請的一個示例性實施例中，

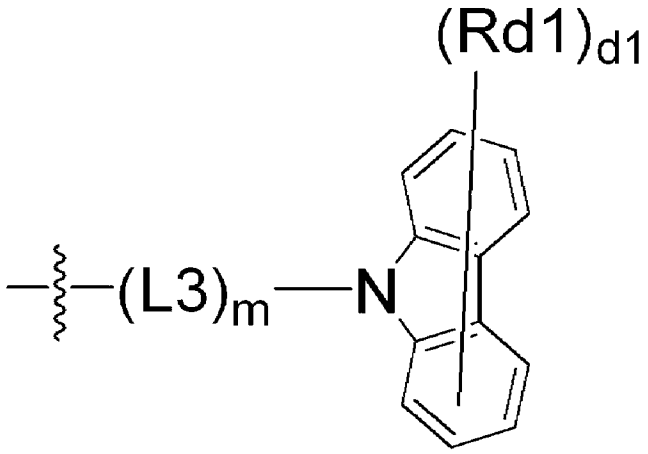


可以由以下化學式 A-1 至 A-12 中的任一個表示。

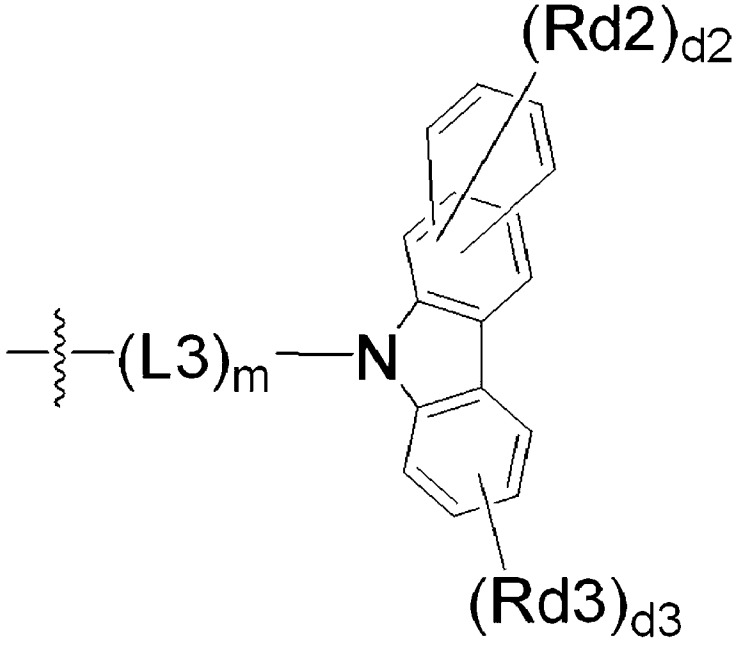
【0199】 [化學式 A-1]



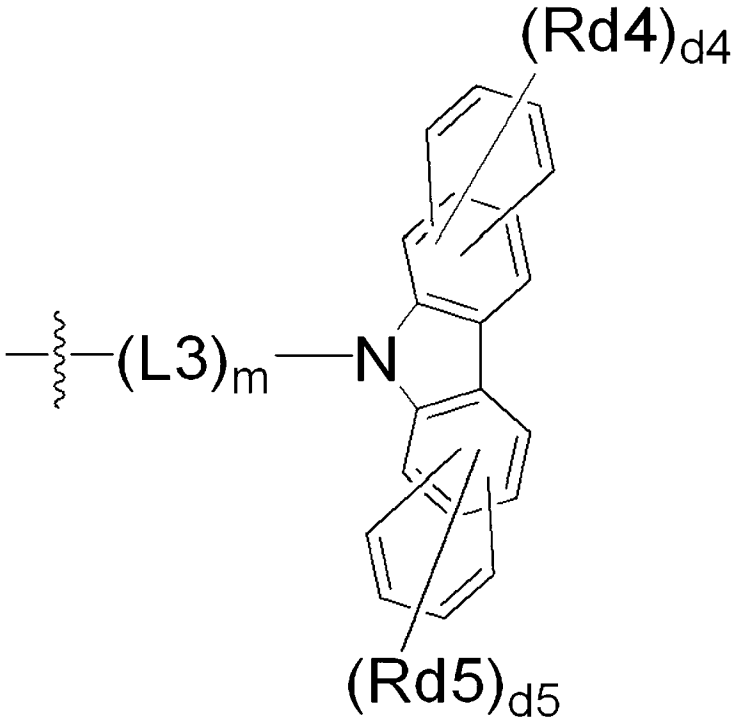
【0200】 [化學式 A-2]



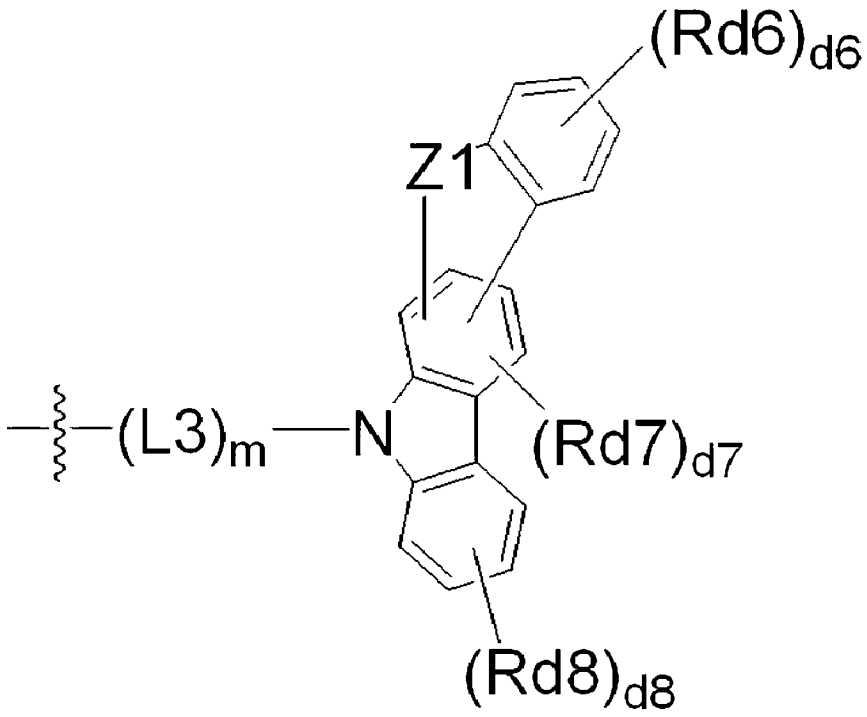
【0201】 [化學式 A-3]



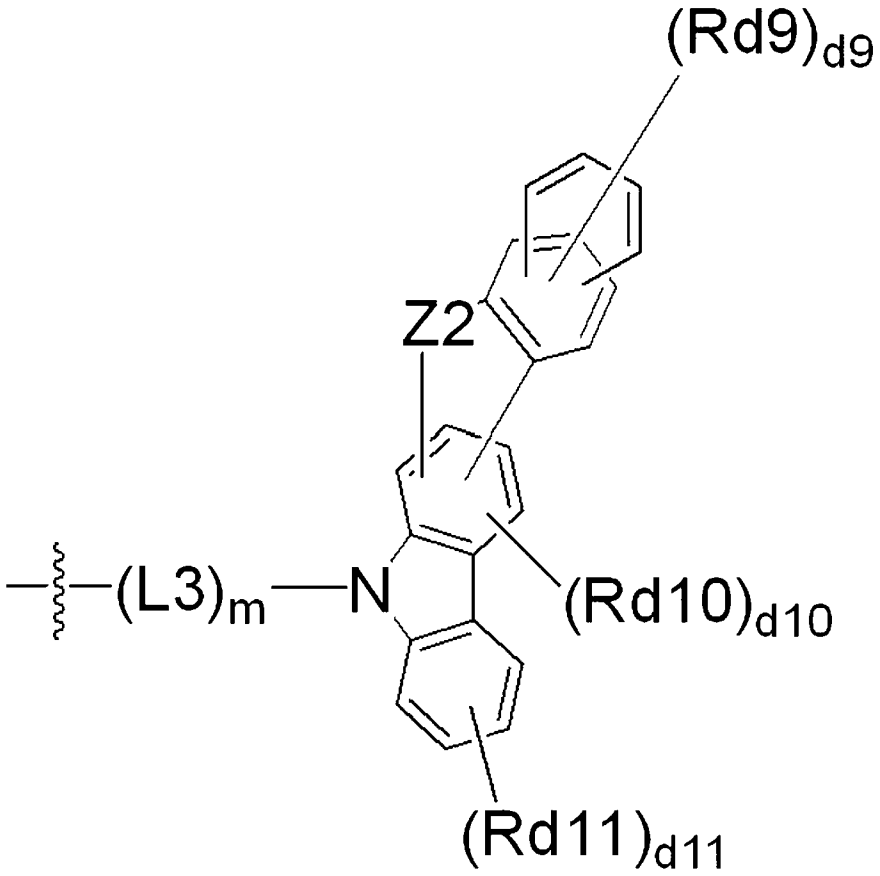
【0202】 [化學式 A-4]



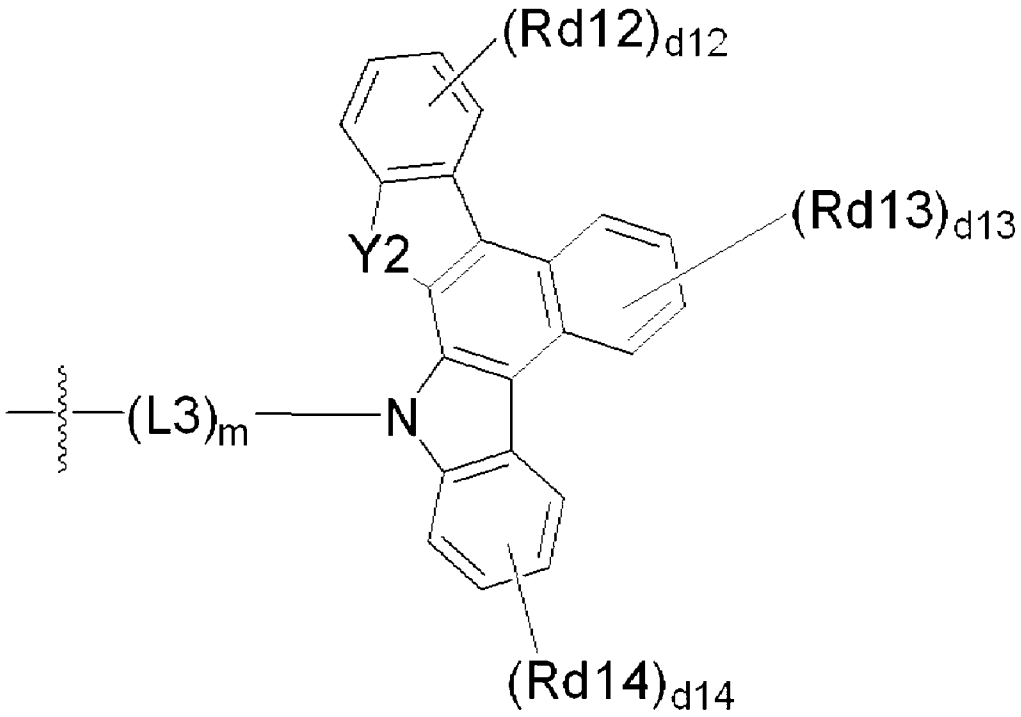
【0203】 [化學式 A-5]



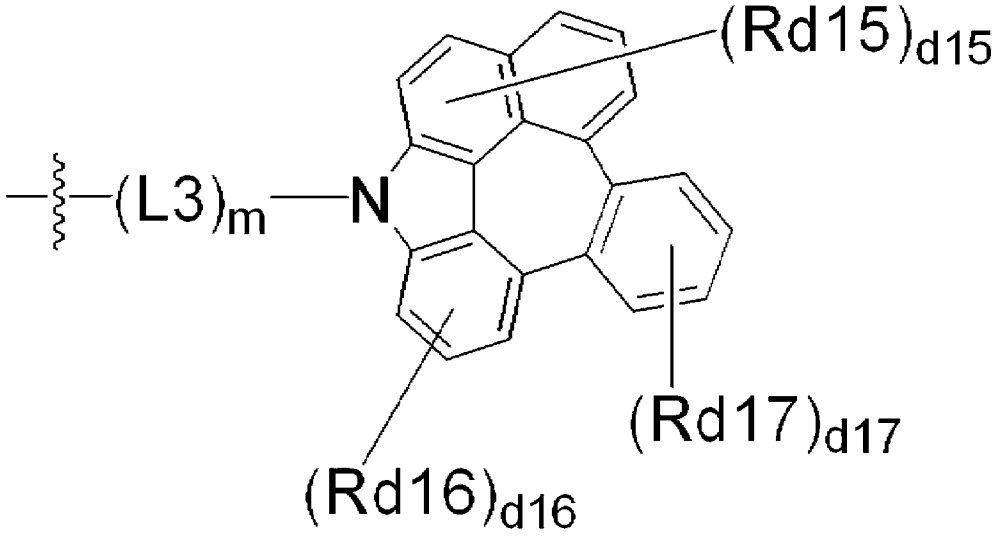
【0204】 [化學式 A-6]



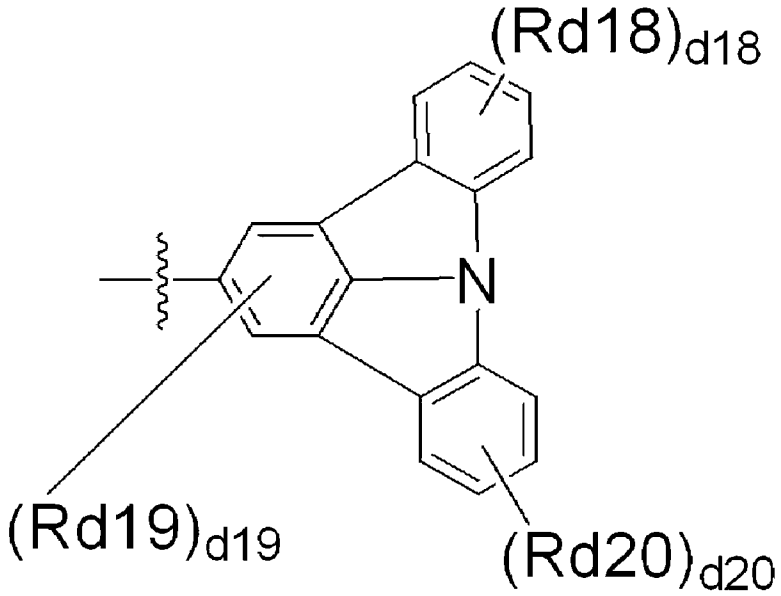
【0205】 [化學式 A-7]



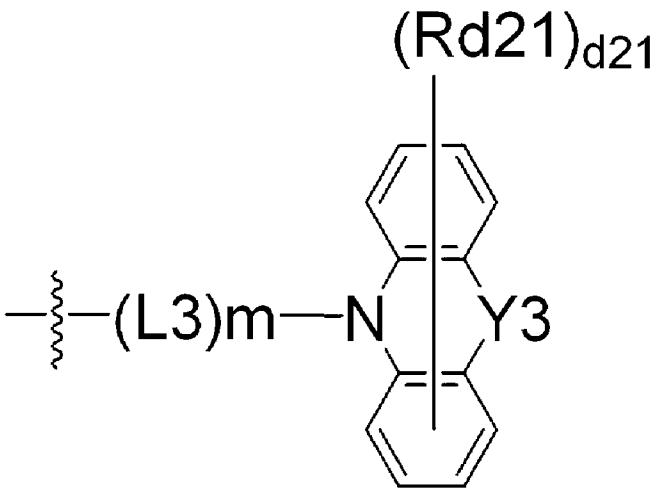
【0206】 [化學式 A-8]



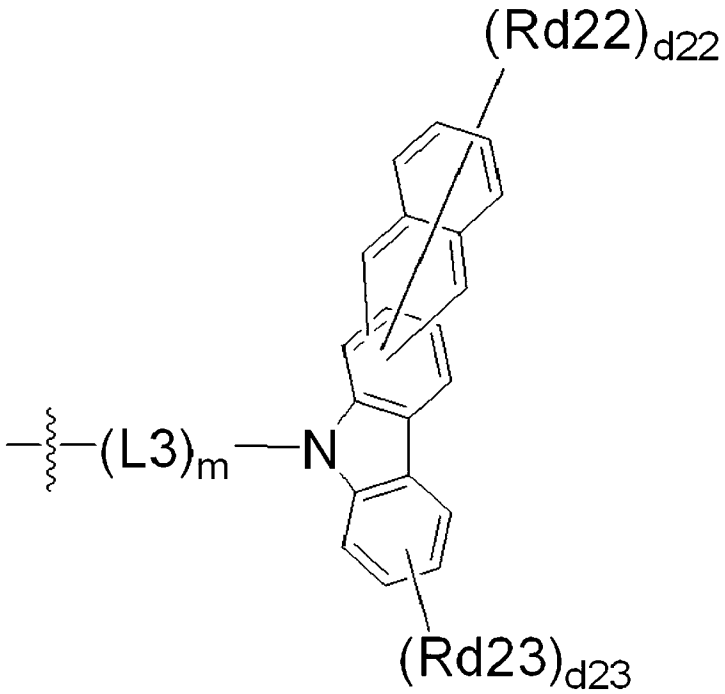
【0207】 [化學式 A-9]



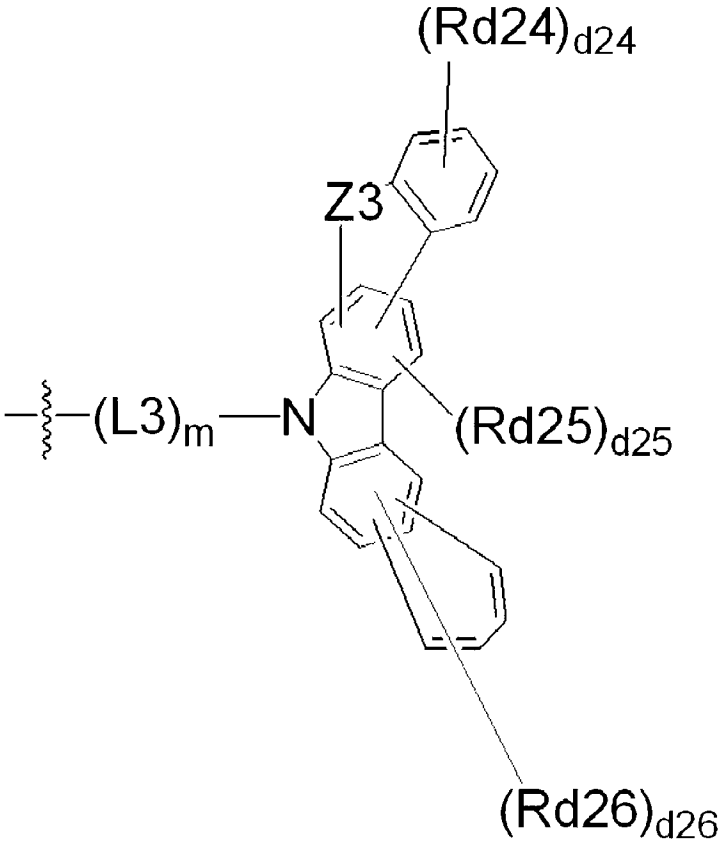
【0208】 [化學式 A-10]



【0209】 [化學式 A-11]



【0210】 [化學式 A-12]



【0211】 在化學式 A-1 至 A-12 中，

L3 和 m 的定義同化學式 2 中的定義，

L’5 和 L’6 彼此相同或不同，且各自獨立為直接鍵；經取代或未經取代的 C6 至 C60 伸芳基；或經取代或未經取代的 C2 至 C60 伸雜芳基，m’1 和 m’2 各自獨立地為 0 至 3 的整數，並且當 m’1 和 m’2 各自為 2 或大於 2 時，括號中的取代基彼此相同或不同，

Ar’2 與 Ar’3 彼此相同或不同，且各自獨立為 NRR’；經取代或未經取代的 C6 至 C60 芳基；或經取代或未經取代的 C2 至 C60 雜芳基，

Z1 至 Z3 各自獨立為 O；S；CRaRb；或 NRc，

Y2 和 Y3 各自獨立為 O；或 S，

R、R’、Ra、Rb、Rc 和 Rd1 至 Rd26 各自獨立地為氫；氘；鹵素基團；氰基；經取代或未經取代的 C1 至 C60 烷基；經取代或未經取代的 C6 至 C60 芳基;或經取代或未經取代的 C2 至 C60 雜芳基，

d1、d21 和 d22 各自獨立地為 0 至 8 的整數，

d2、d4、d5、d9 和 d26 各自獨立地為 0 至 6 的整數，

d3、d6、d8、d11、d12 至 d14、d17、d18、d20、d23 和 d24 各自獨立地為 0 至 4 的整數，

d7、d10、d19 和 d25 各自獨立地為 0 至 2 的整數，

d15 是 0 到 5 的整數，

d16 是 0 到 3 的整數，並且

當 d1 至 d26 為 2 或大於 2 時，括號內的取代基彼此相同或不同。

【0212】 在本申請的一個示例性實施例中，Ar2 和 Ar3 的取代基的定義可以應用於 Ar'2 和 Ar'3，除了在 Ar2 和 Ar3 的取代基的定義中，Ar2 和 Ar3 鍵結形成經取代或未經取代的脂族或芳族烴環或經取代或未經取代的脂族或芳族雜環。

【0213】 在本申請的一個示例性實施例中，Rr、Rp 和 Rq 彼此相同或不同，並且各自獨立地選自由以下組成的群組：氫；氘；鹵素；氰基；經取代或未經取代的 C1 至 C60 烷基；經取代或未經取代的 C2 至 C60 烯基；經取代或未經取代的 C2 至 C60 炔基；經取代或未經取代的 C1 至 C60 烷氧基；經取代或未經取代的 C3 至 C60 環烷基；經取代或未經取代的 C2 至 C60 雜環烷基；經取代或未經取代的 C6 至 C60 芳基；經取代或未經取代的 C2 至 C60 雜芳基；-P(=O)RR'；-SiRR'R"和-NRR'，r 為 0 至 4 的整數，p、q 各自為 0 至 3 的整數，且當 r、p、q 為 2 或大於 2 時，括號內的取代基為彼此相同或不同，且 R、R'和 R"彼此相同或不同，且各自獨立地為氫；氘；經取代或未經取代的 C1 至 C60 烷基；經取代或未經取代的 C6 至 C60 芳基；或經取代或未經取代的 C2 至 C60 雜芳基。

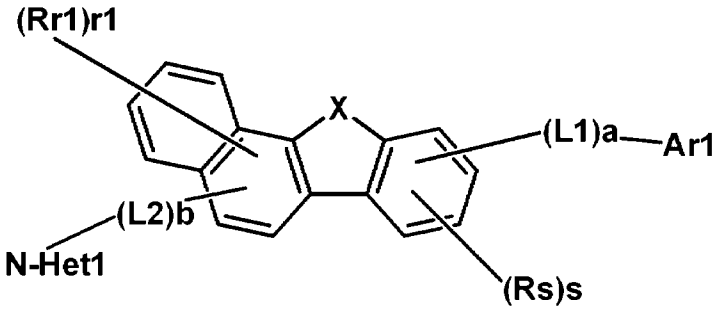
【0214】 在本申請的一個示例性實施例中，Rr、Rp 和 Rq 彼此相同或不同，並且各自獨立地為氫；氘；鹵素；氰基；經取代或未經取代的 C6 至 C60 芳基；或經取代或未經取代的 C2 至 C60 雜芳基。

【0215】 在本申請的一個示例性實施例中，Rr、Rp 和 Rq 彼此相同或不同，並且各自獨立地為氫；氘；鹵素；或氰基。

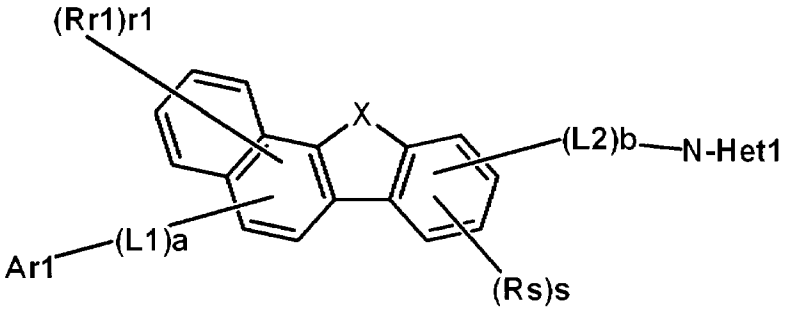
【0216】 在本申請的一個示例性實施例中，Rr、Rp 和 Rq 彼此相同或不同，並且各自獨立地為氫；或氘。

【0217】 在本申請的一個示例性實施例中，化學式 1 可以由以下化學式 1-1 或 1-2 表示。

【0218】 [化學式 1-1]



【0219】 [化學式 1-2]



【0220】 在化學式 1-1 和 1-2 中，

Rr1 和 Rs 彼此相同或不同，且各自獨立為氫；氘；氰基；鹵素基團；或經取代或未經取代的 C1 至 C60 烷基，

r1 為 0 至 5 的整數，且當 r1 為 2 或大於 2 時，括號內的 Rr1 彼此相同或不同，

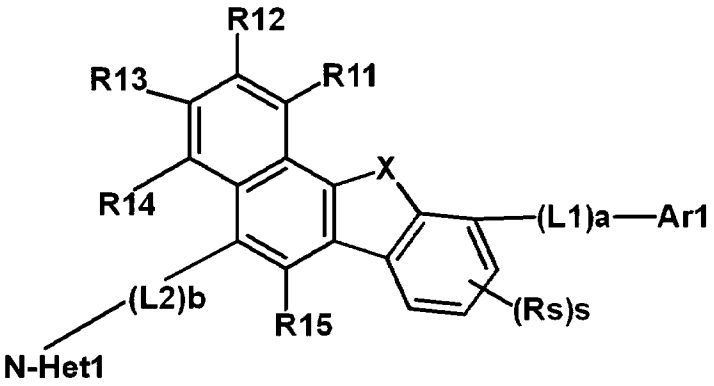
s 為 0 至 3 的整數，且當 s 為 2 或大於 2 時，括號內的 Rs 彼此相同或不同，

X、L1、L2、Ar1、a、b、N-Het1 的定義同化學式 1 中的

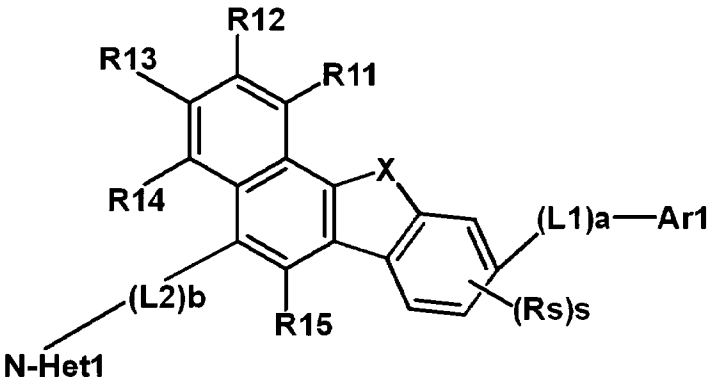
定義。

【0221】 在本申請的一個示例性實施例中，化學式 1-1 可以由以下化學式 1-1-1 至 1-1-4 中的任一個表示。

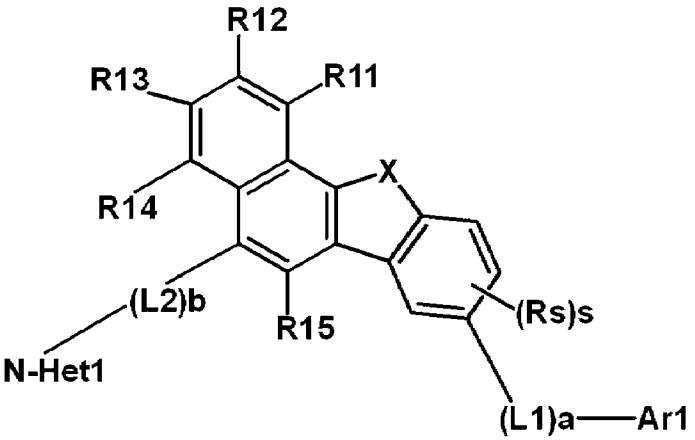
【0222】 [化學式 1-1-1]



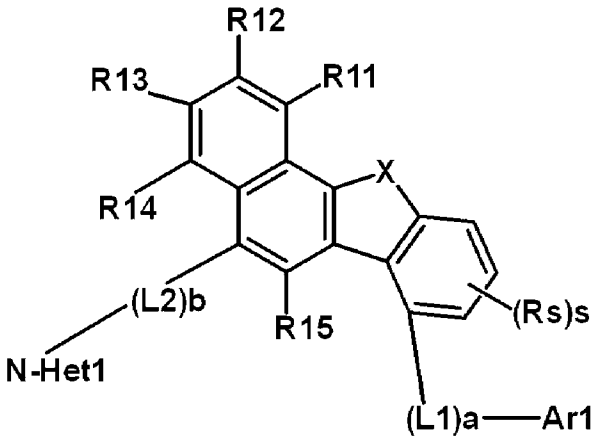
【0223】 [化學式 1-1-2]



【0224】 [化學式 1-1-3]



【0225】 [化學式 1-1-4]



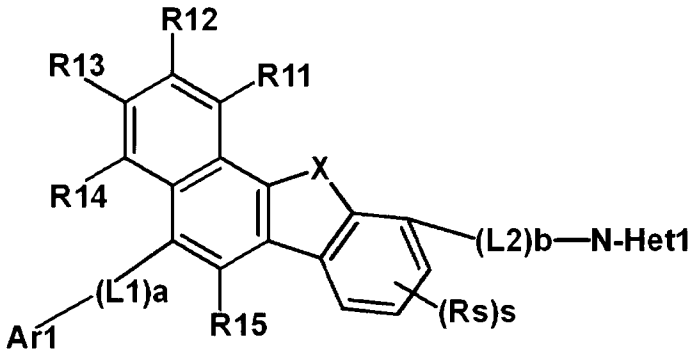
【0226】 在化學式 1-1-1 至 1-1-4 中，

R11 至 R15 彼此相同或不同，且各自獨立為氫；氘；氰基；鹵素基團；或經取代或未經取代的 C1 至 C60 烷基，和

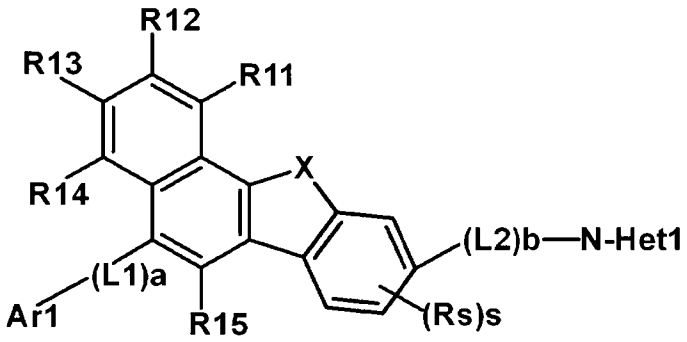
X、Rs、L1、L2、Ar1、a、b、s 和 N-Het1 的定義同化學式 1-1 中的定義。

【0227】 在本申請的一個示例性實施例中，化學式 1-2 可以由以下化學式 1-2-1 至 1-2-4 中的任一個表示。

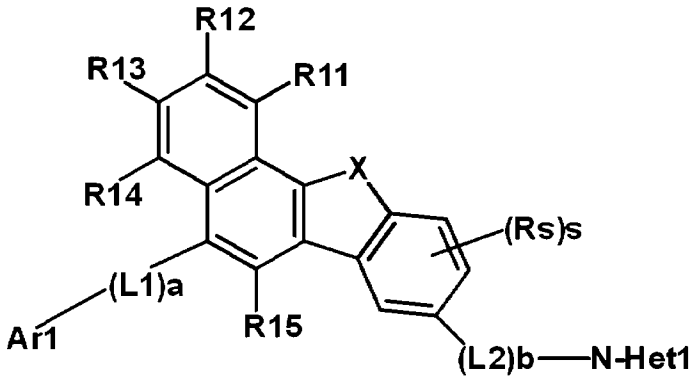
【0228】 [化學式 1-2-1]



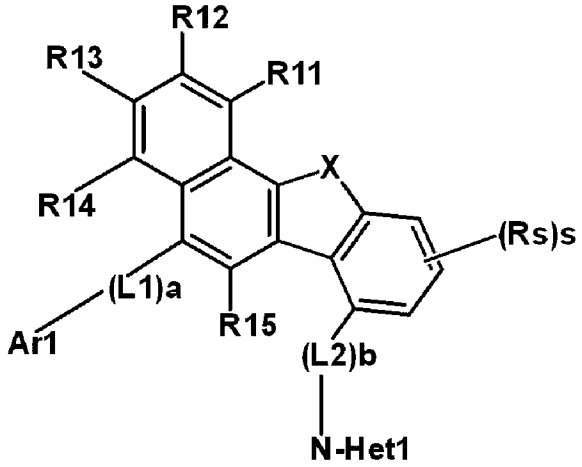
【0229】 [化學式 1-2-2]



【0230】 [化學式 1-2-3]



【0231】 [化學式 1-2-4]



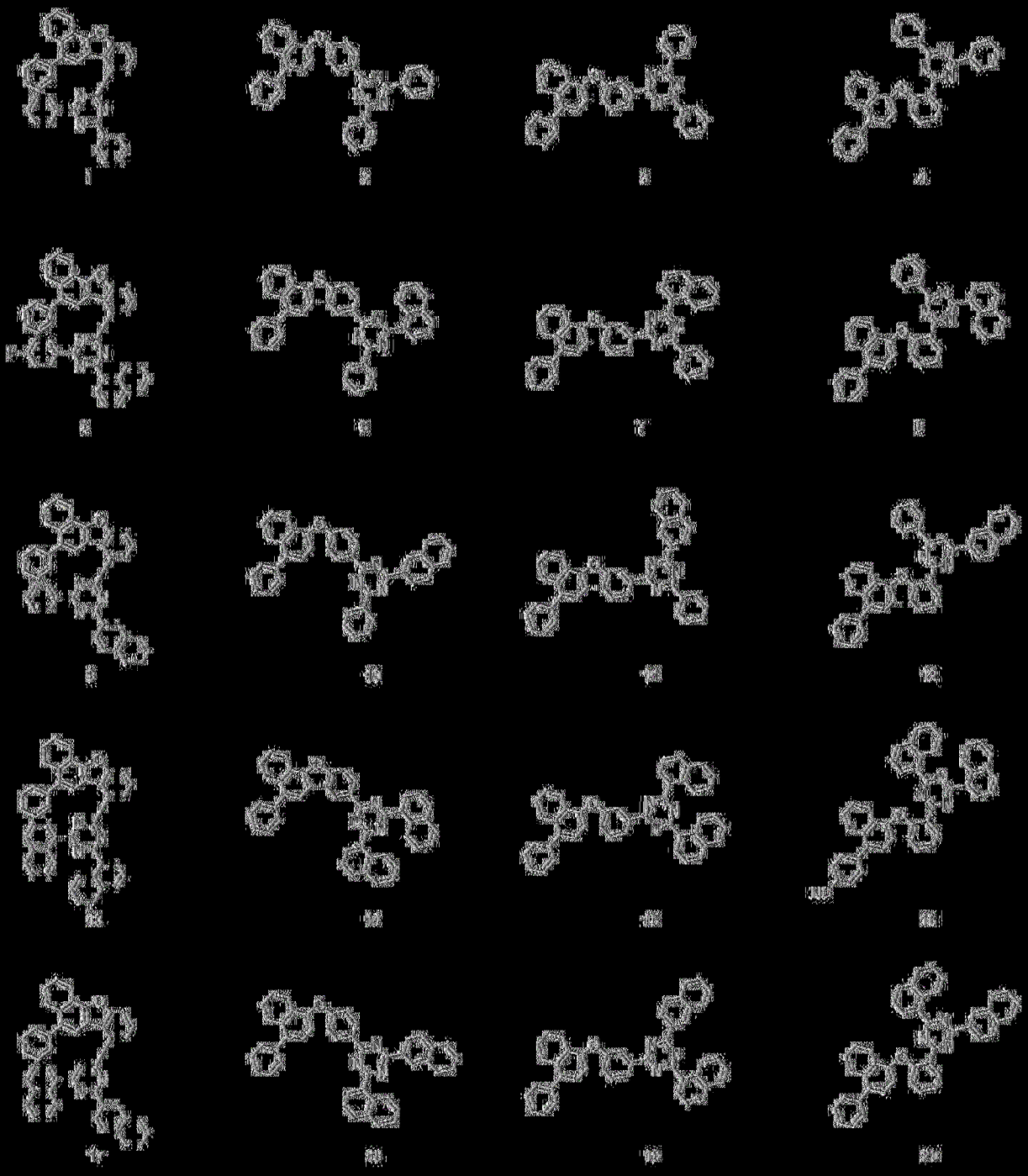
【0232】 在化學式 1-2-1 至 1-2-4 中，

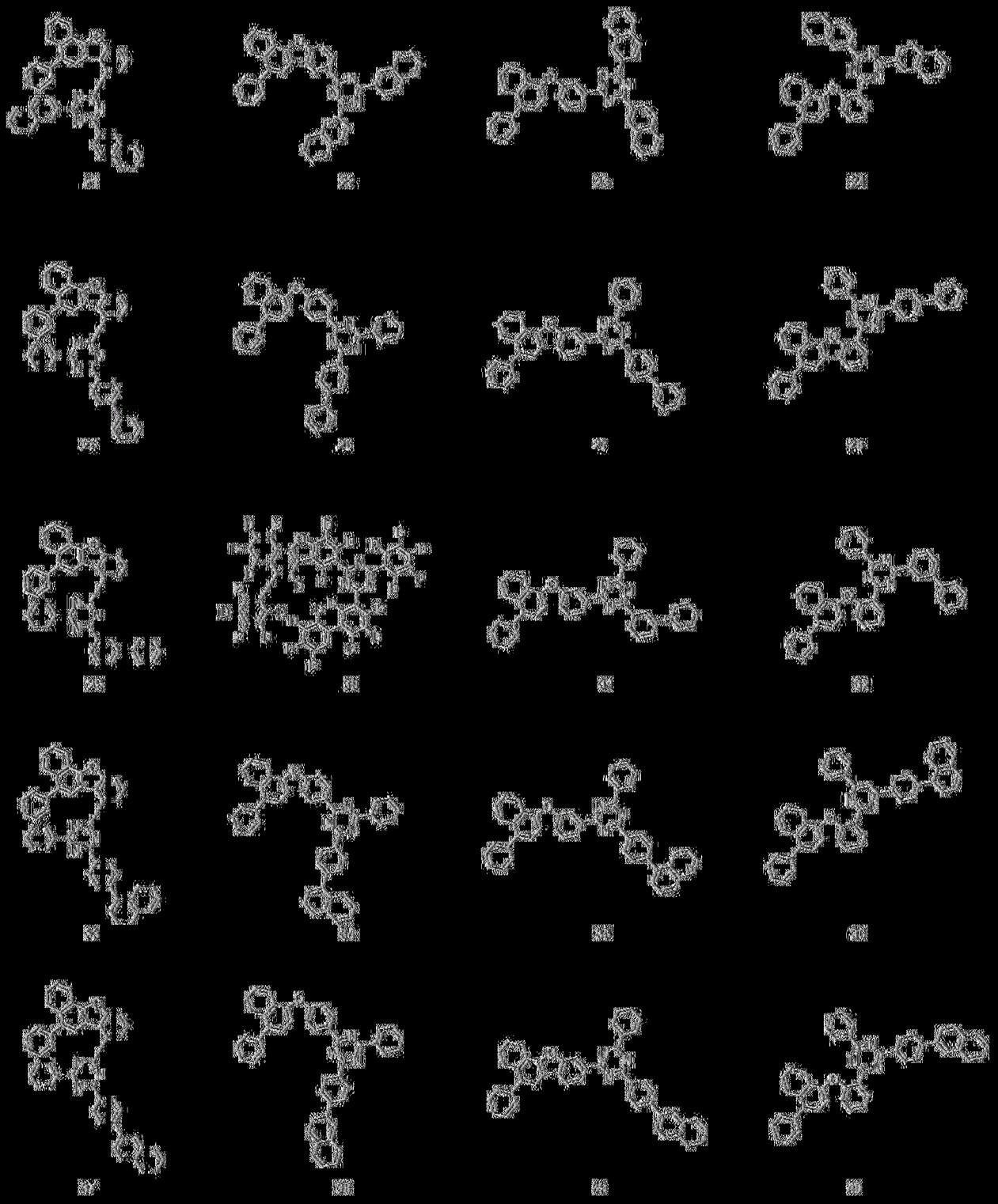
R11 至 R15 彼此相同或不同，且各自獨立為氫；氘；氰基；鹵素基團；或經取代或未經取代的 C1 至 C60 烷基，和

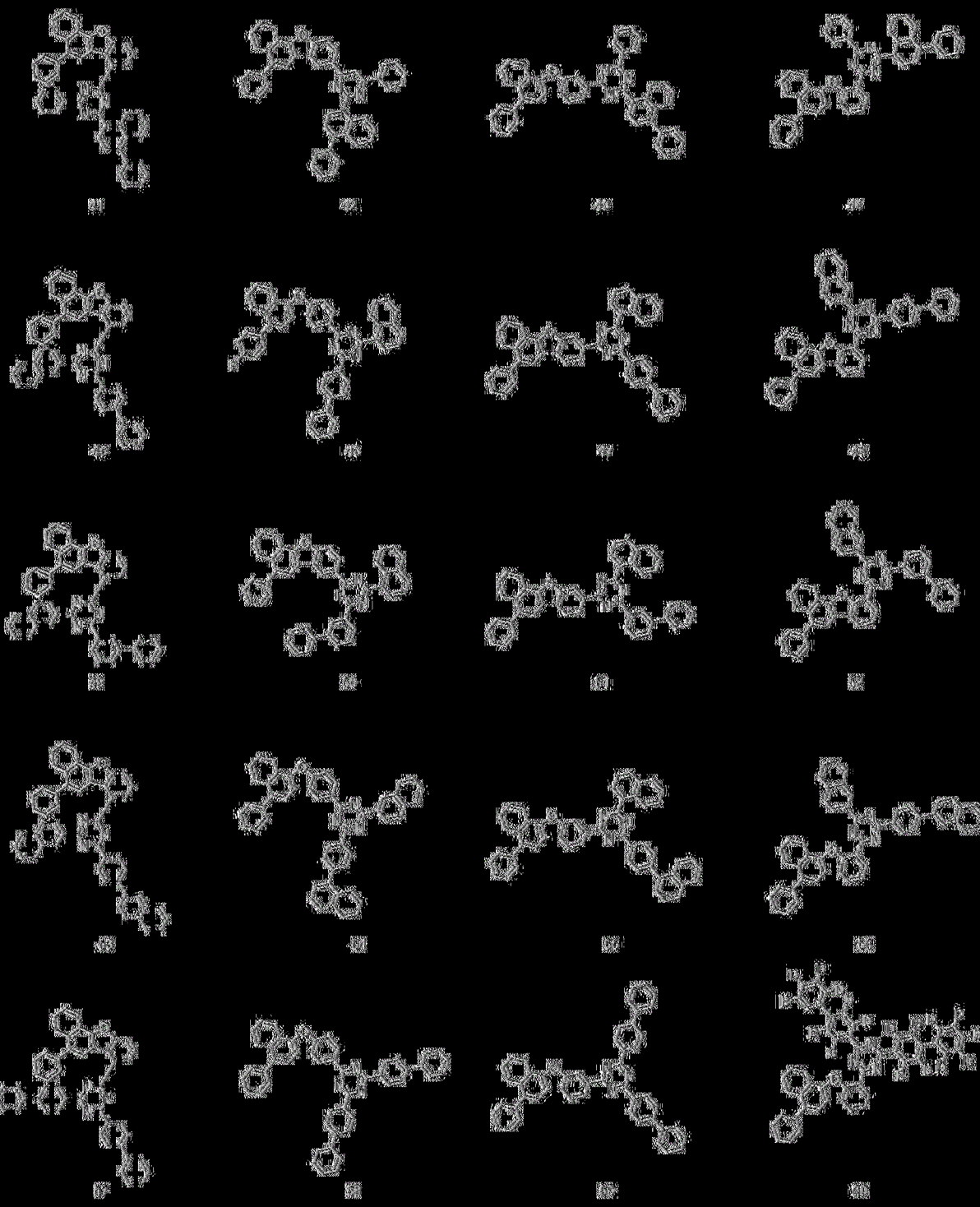
X、Rs、L1、L2、Ar1、a、b、s 和 N-Het1 的定義同化學式 1-2 中的定義。

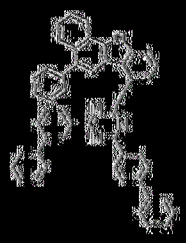
【0233】 根據本申請的一個示例性實施例，化學式 1 可以由以下

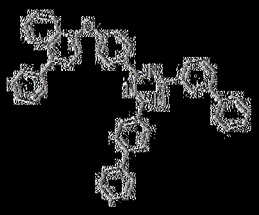
化合物中的任一個表示，但不限於此。

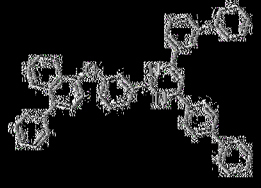


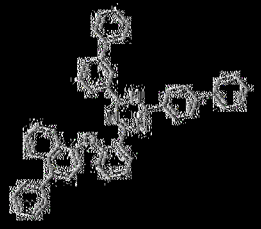


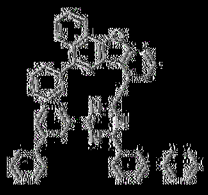


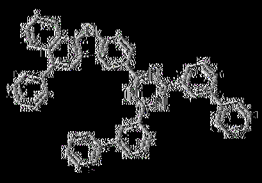


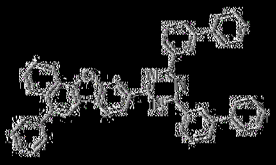


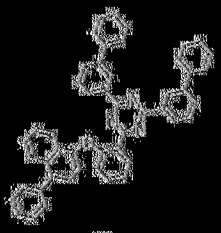


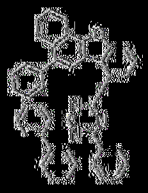


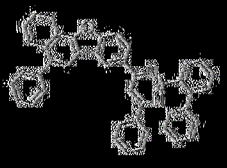


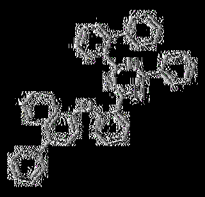


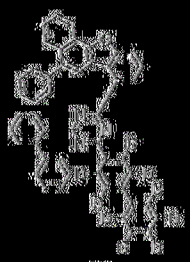


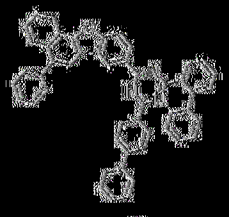


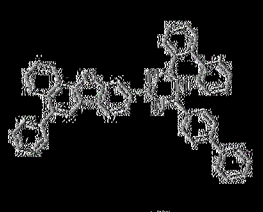


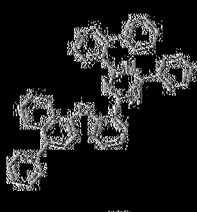


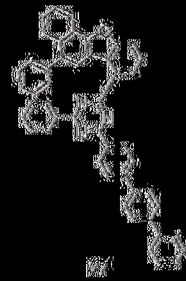


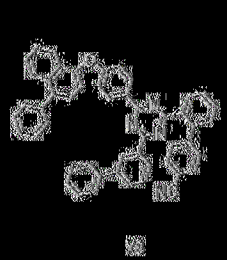


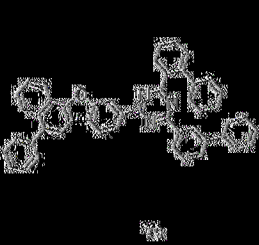


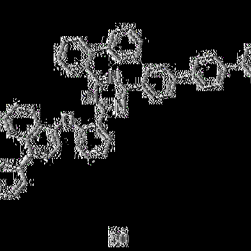


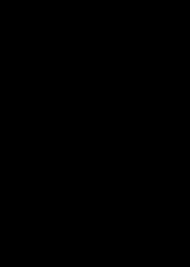


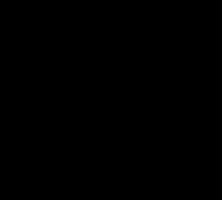


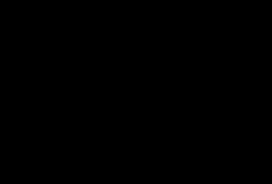


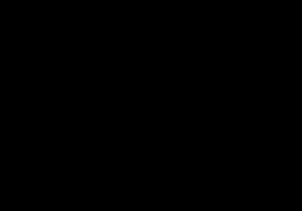


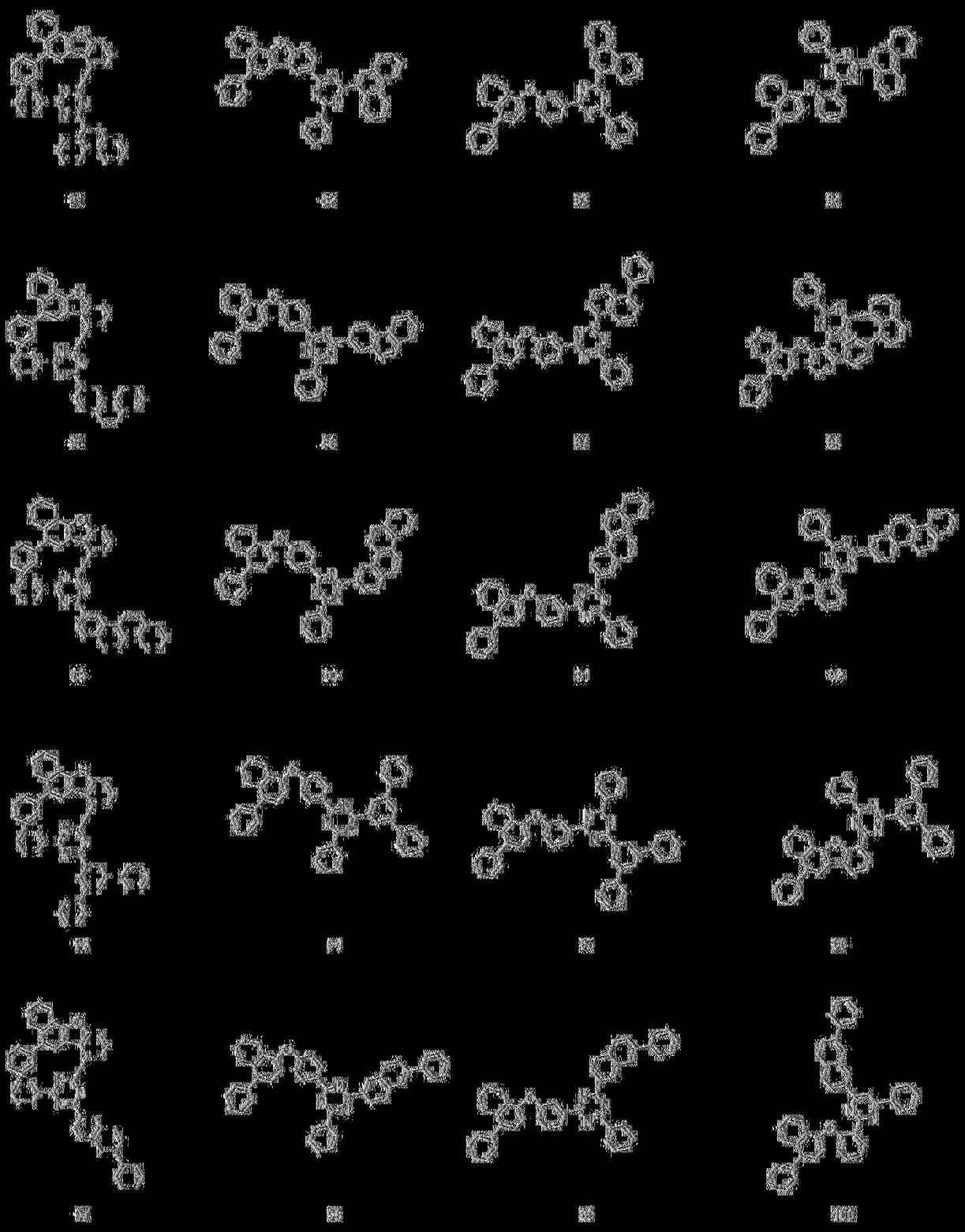


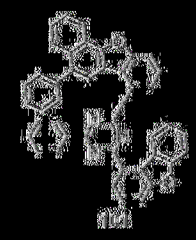


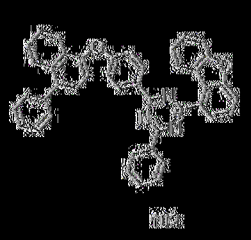


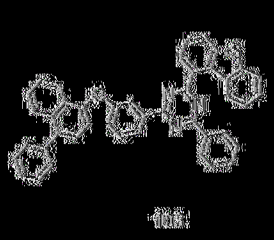


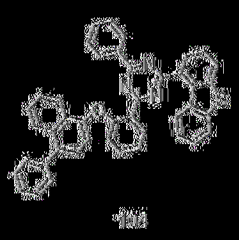


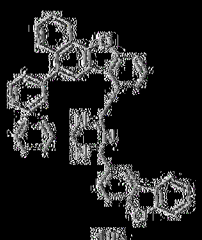


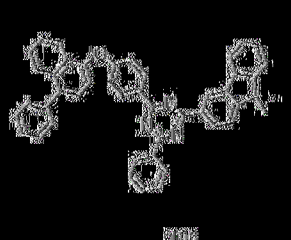


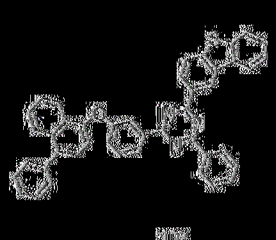


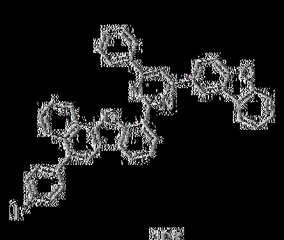


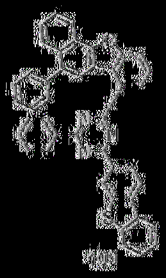


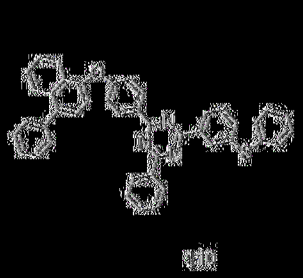


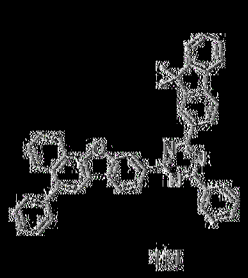


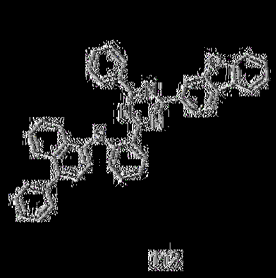


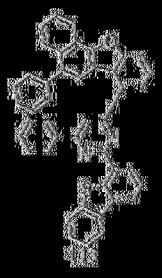


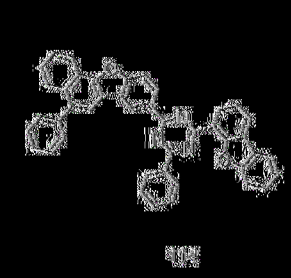


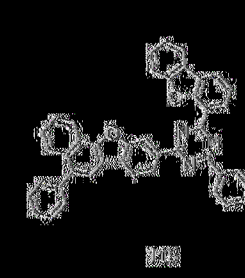


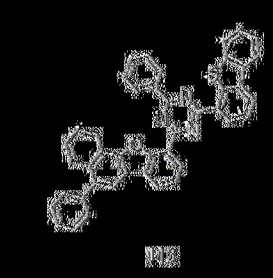


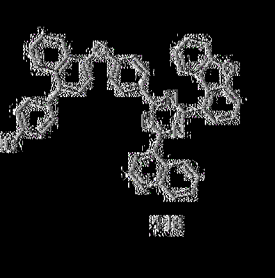


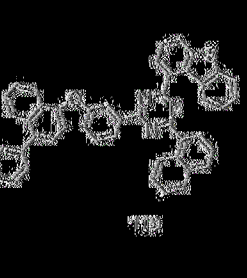


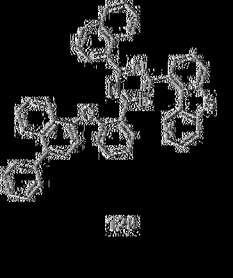


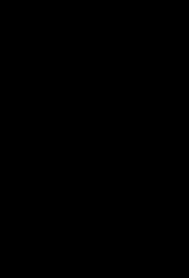


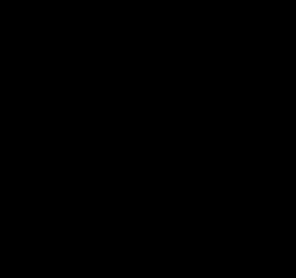


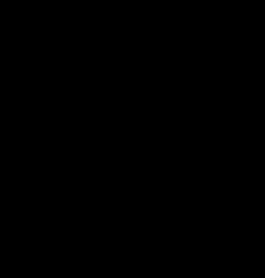


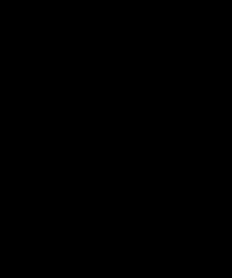


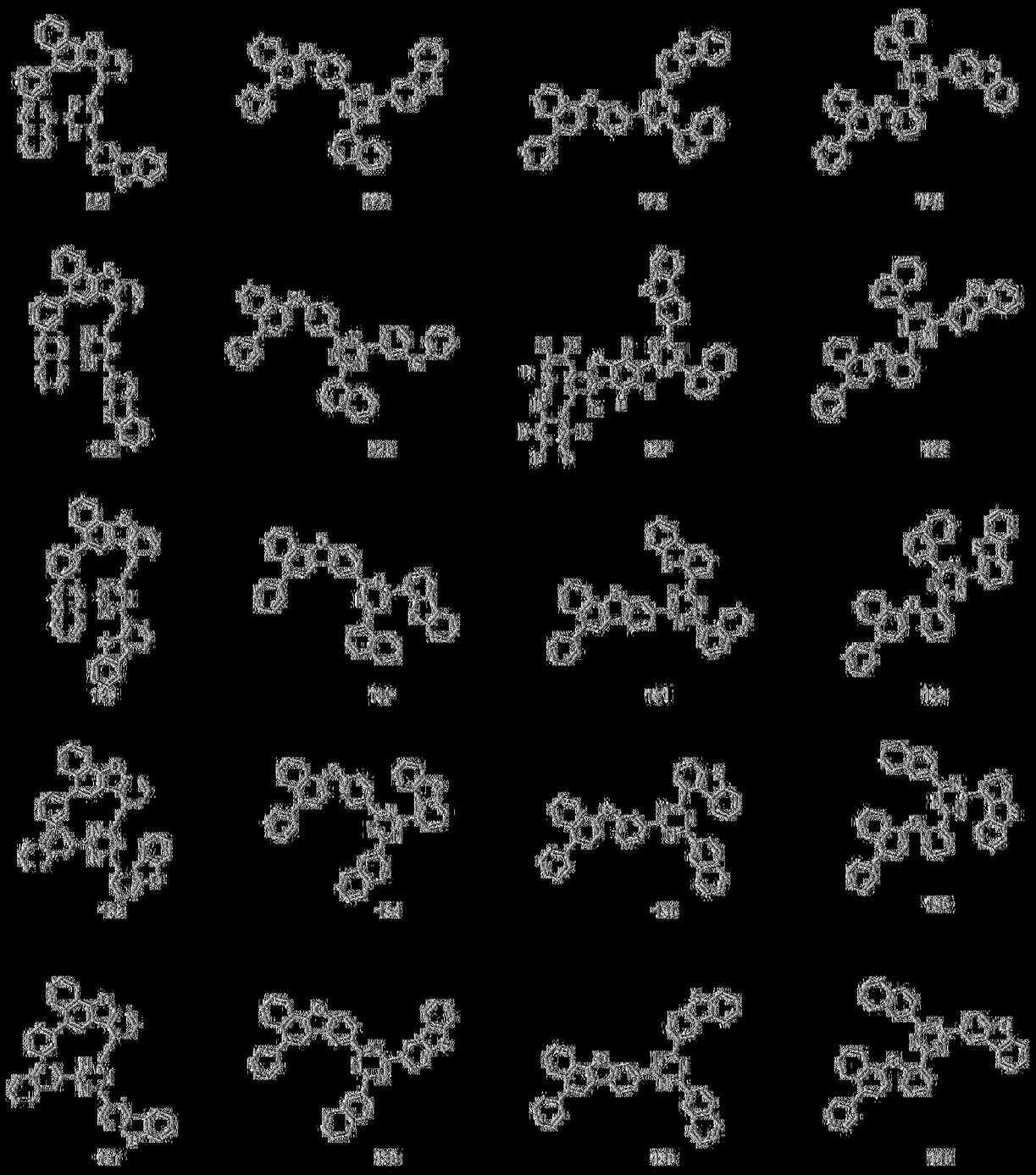


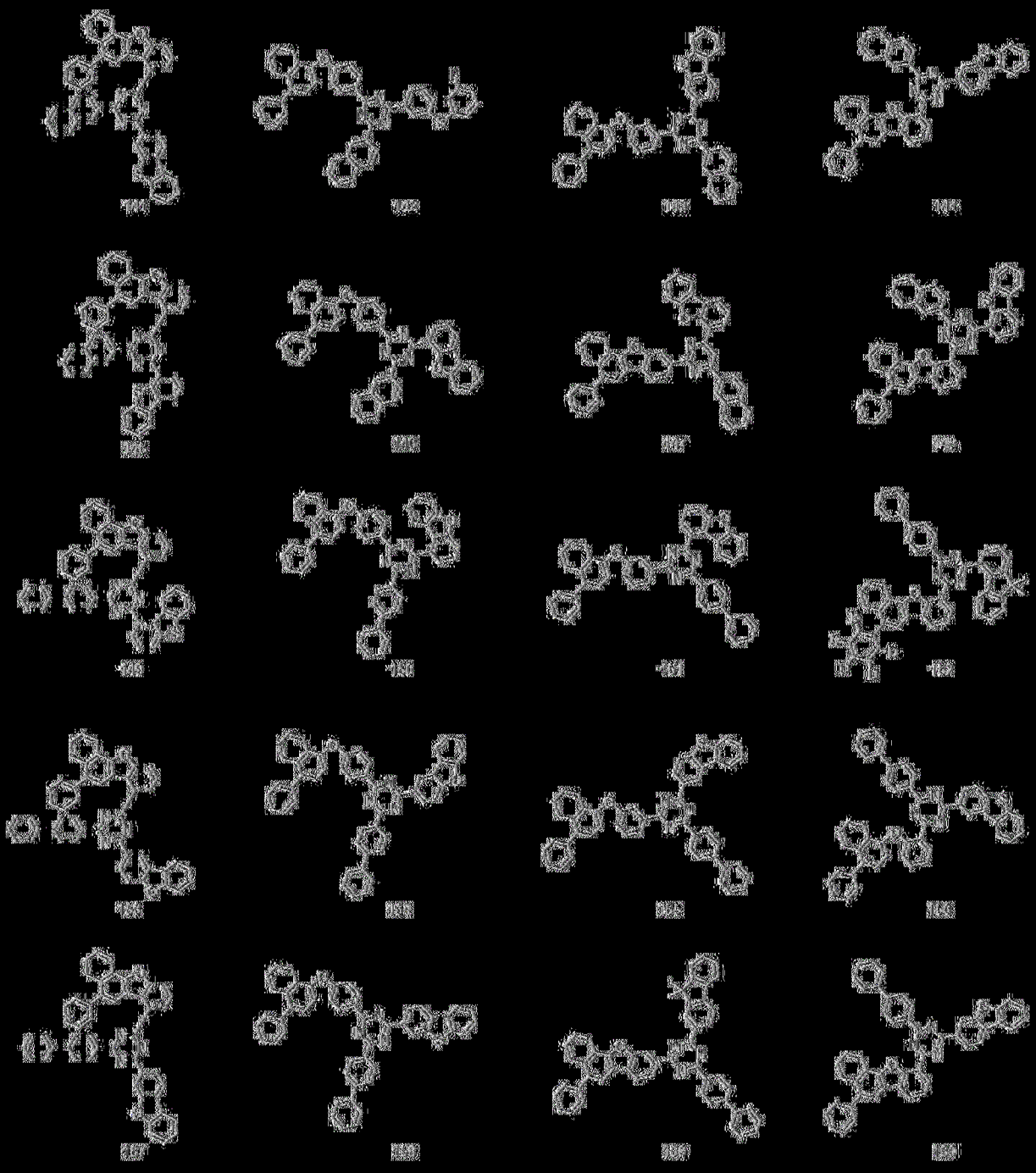


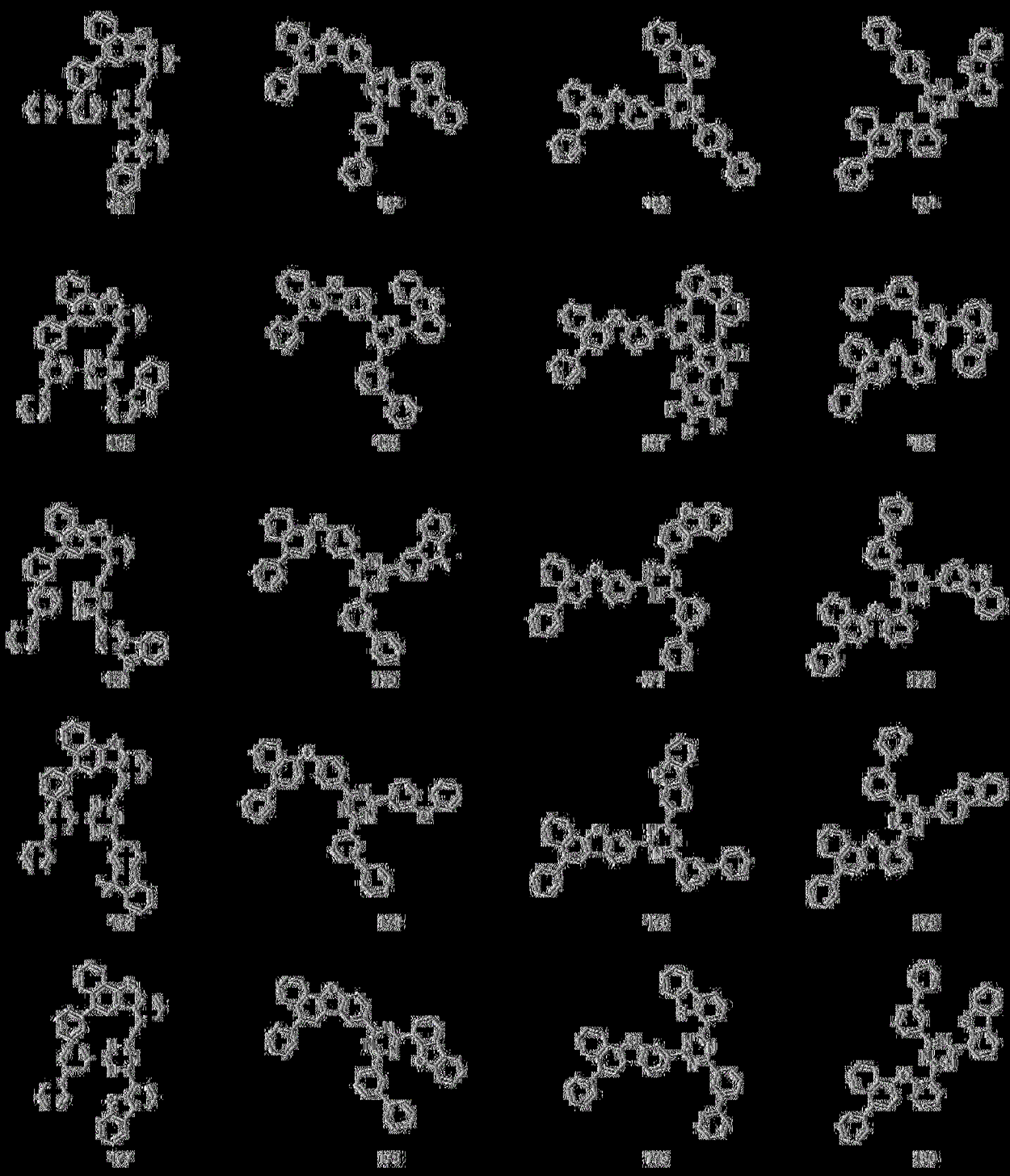


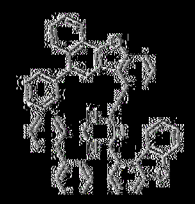


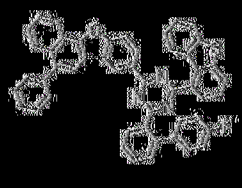


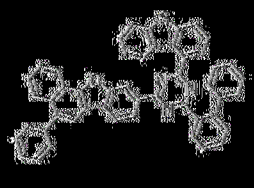


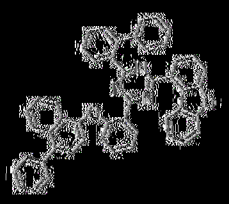


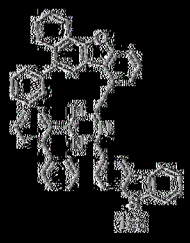


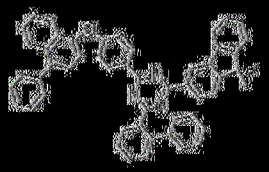


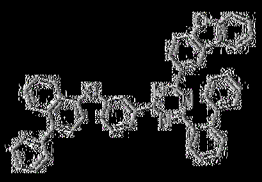


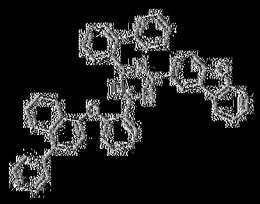


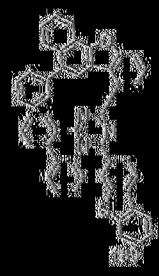


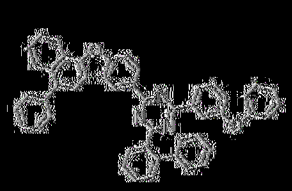


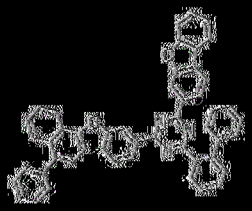


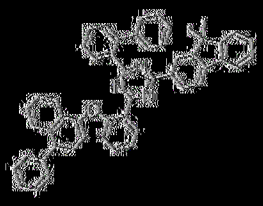


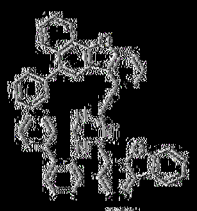


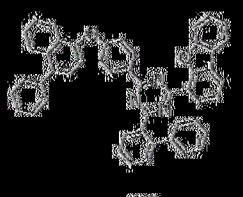


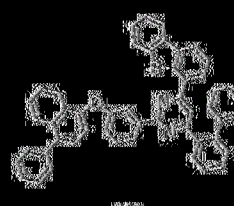


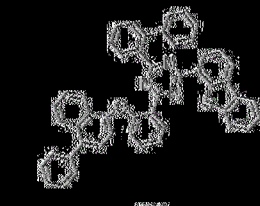


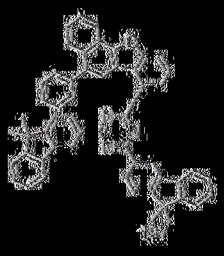


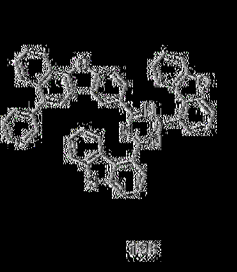


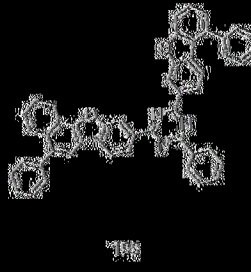


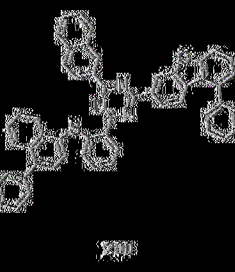


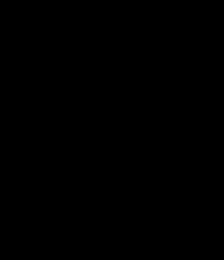


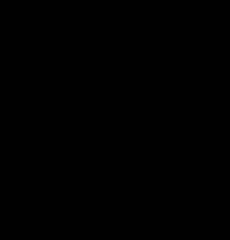


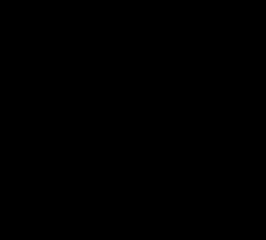


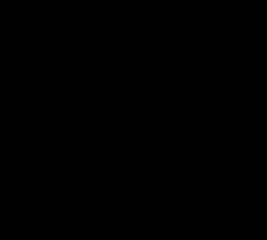


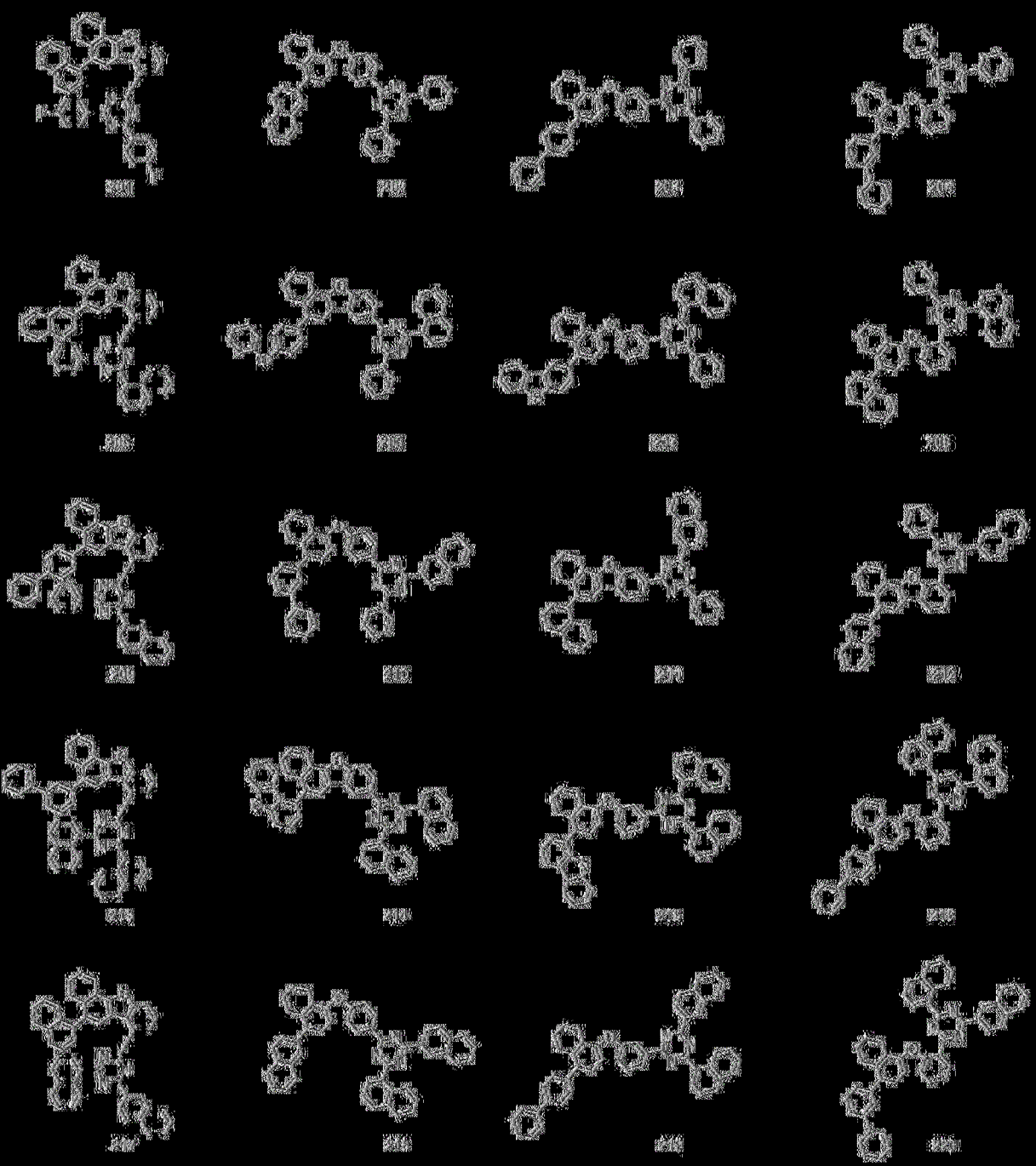


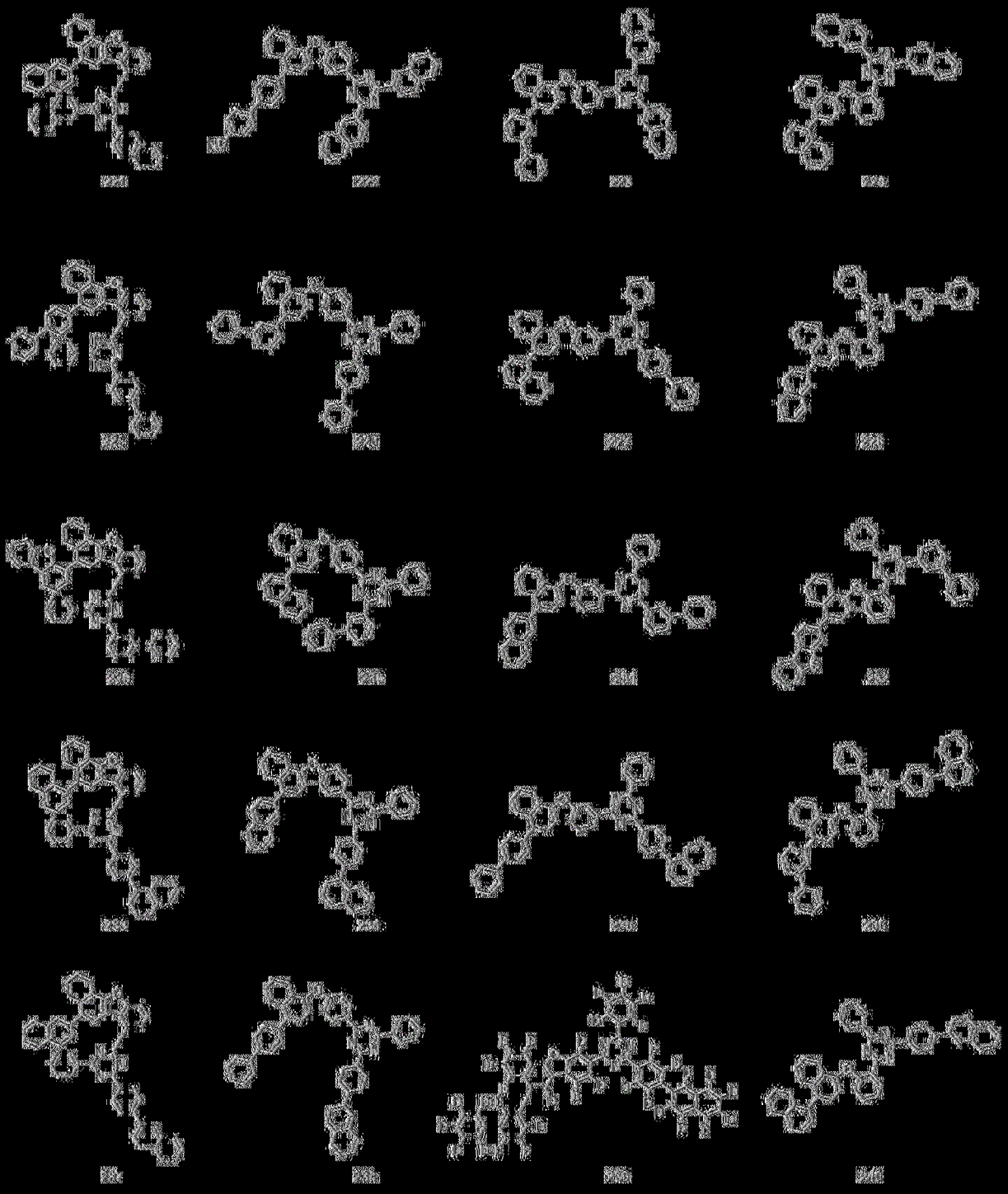


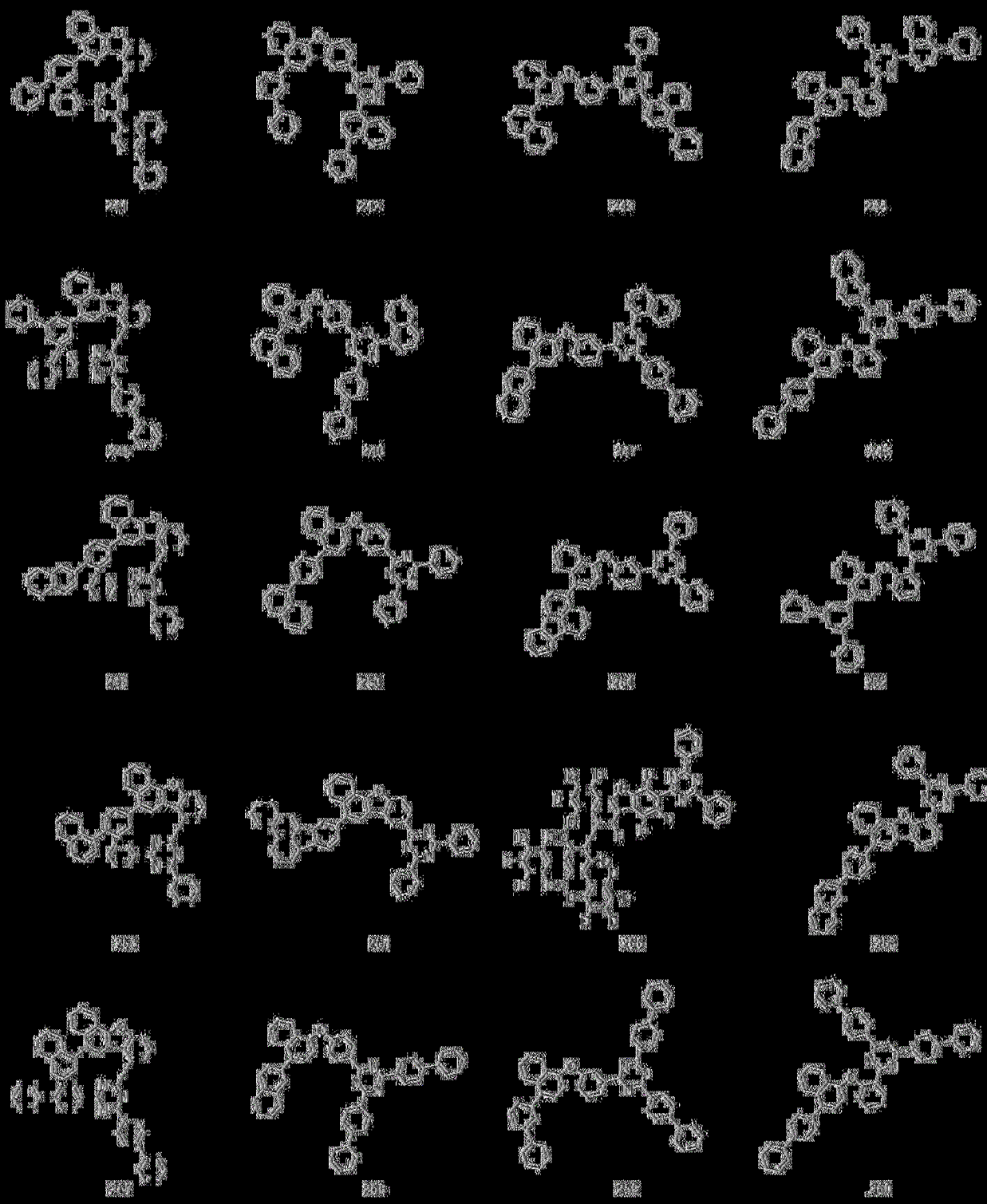












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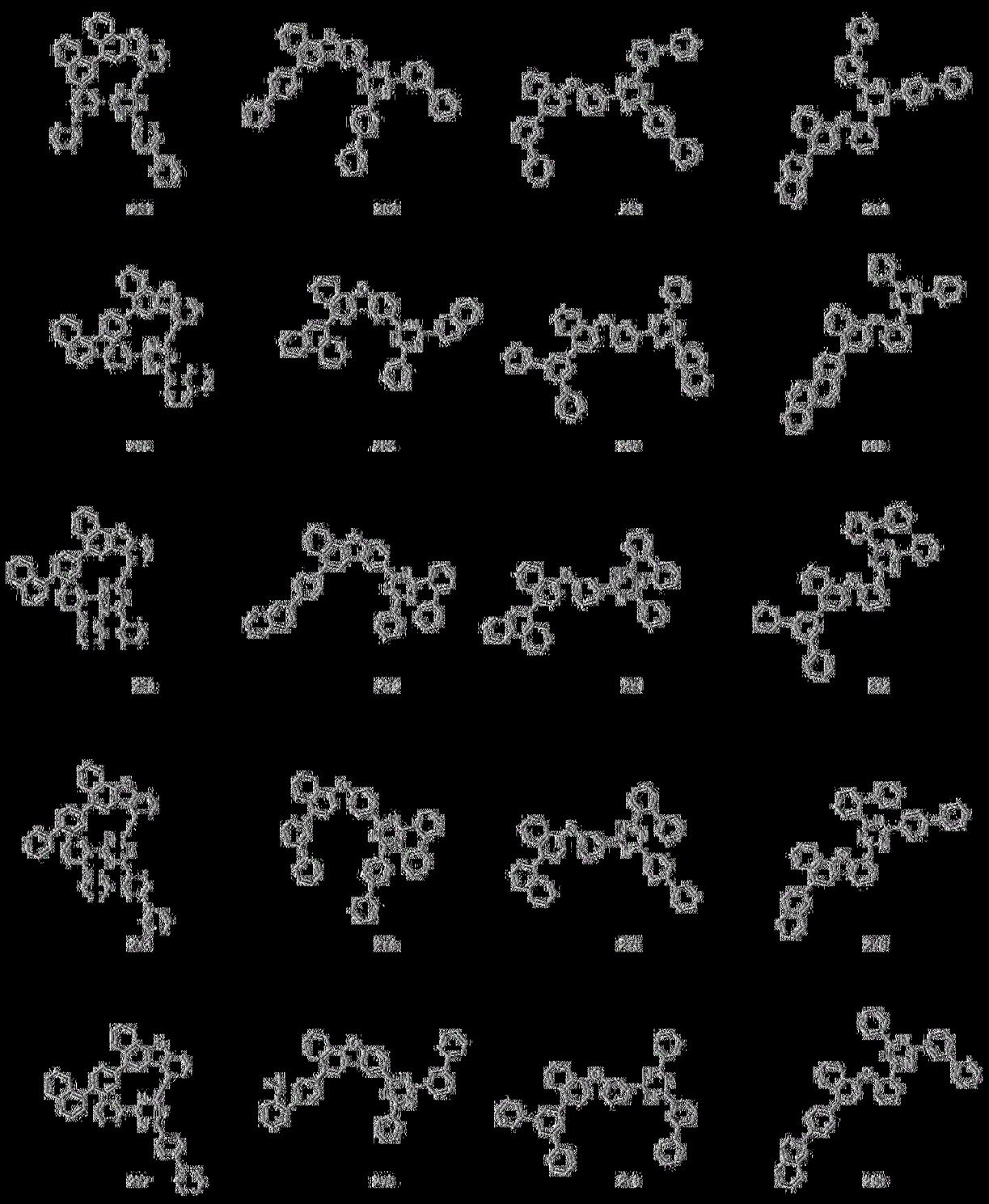
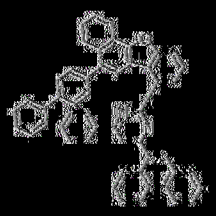
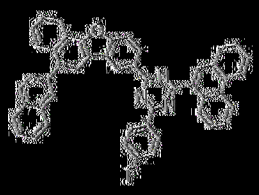
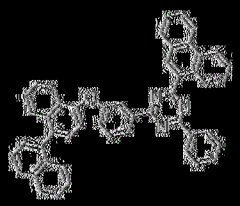
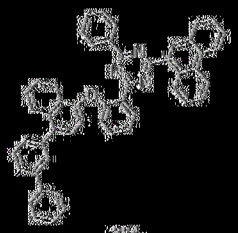
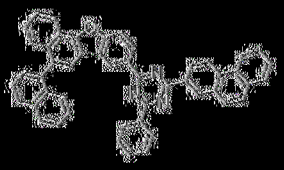


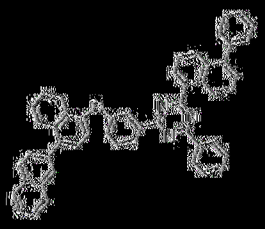


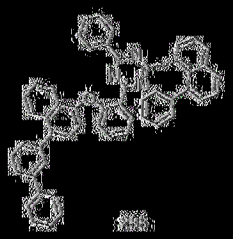


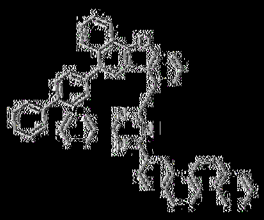


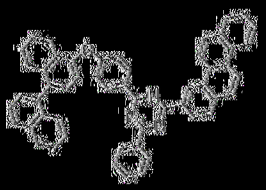


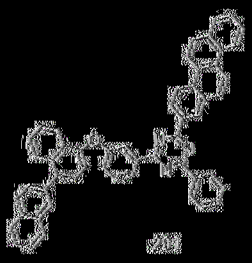


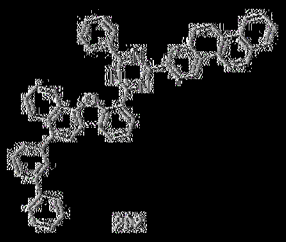


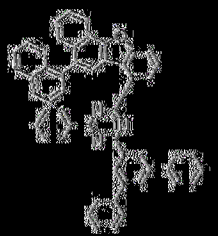


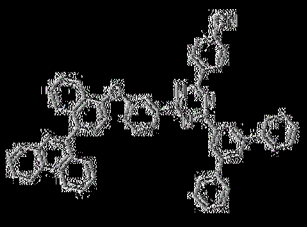


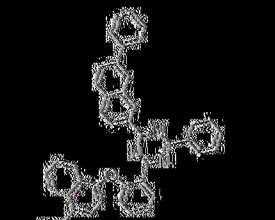


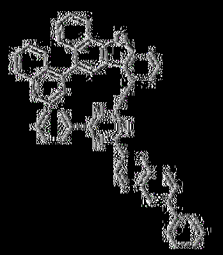


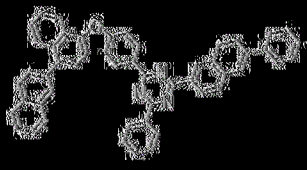


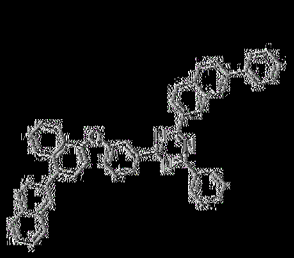


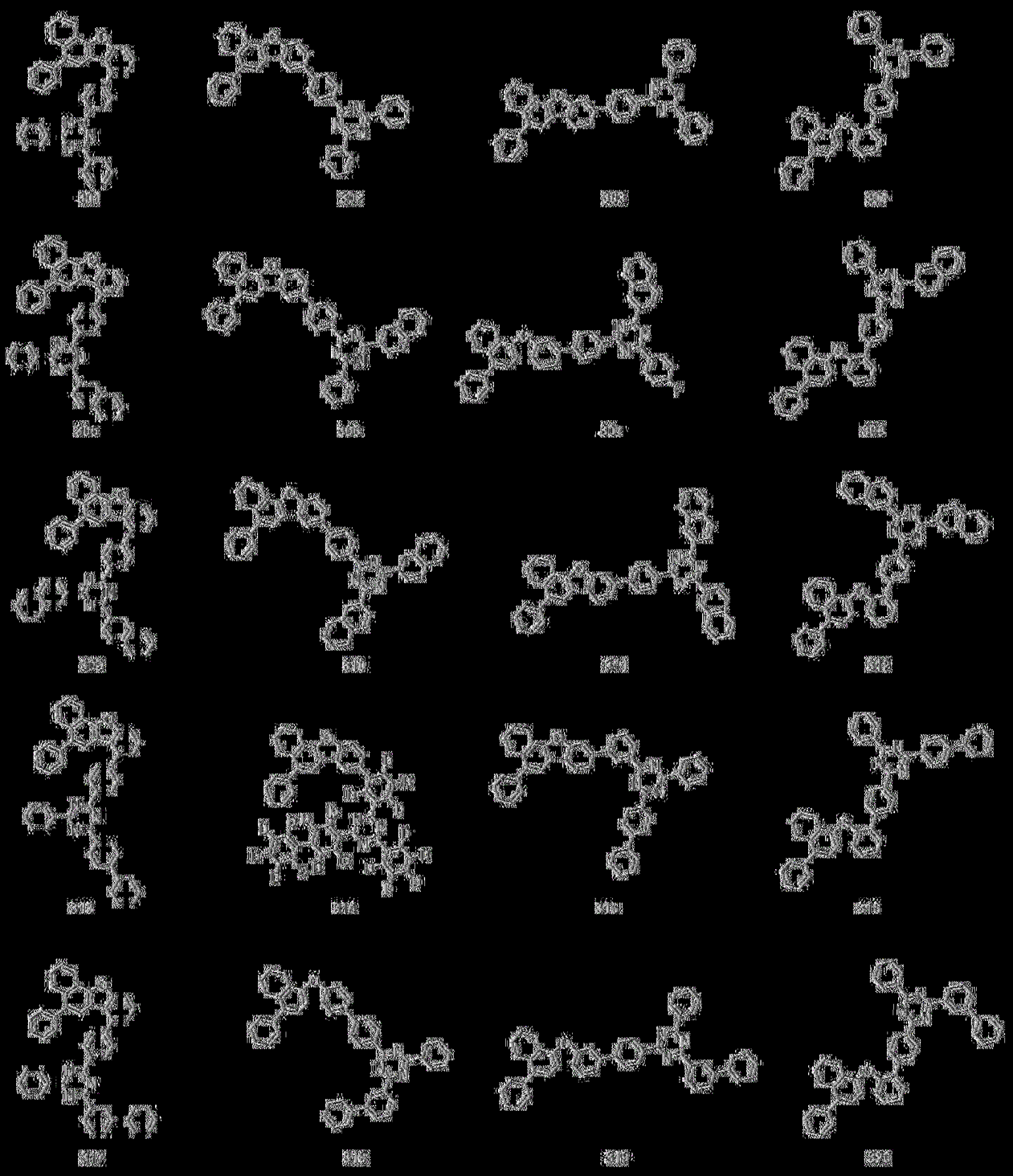


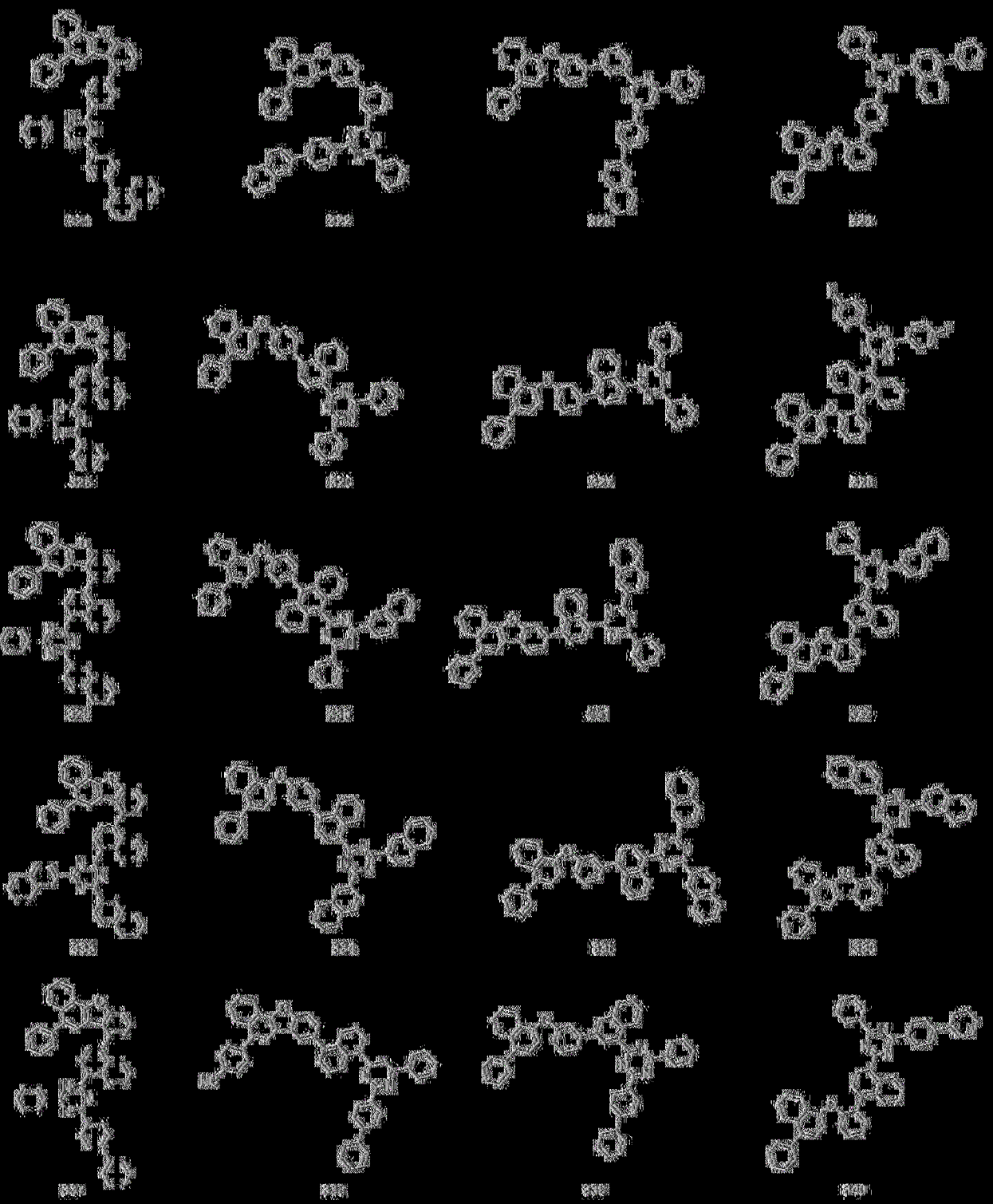


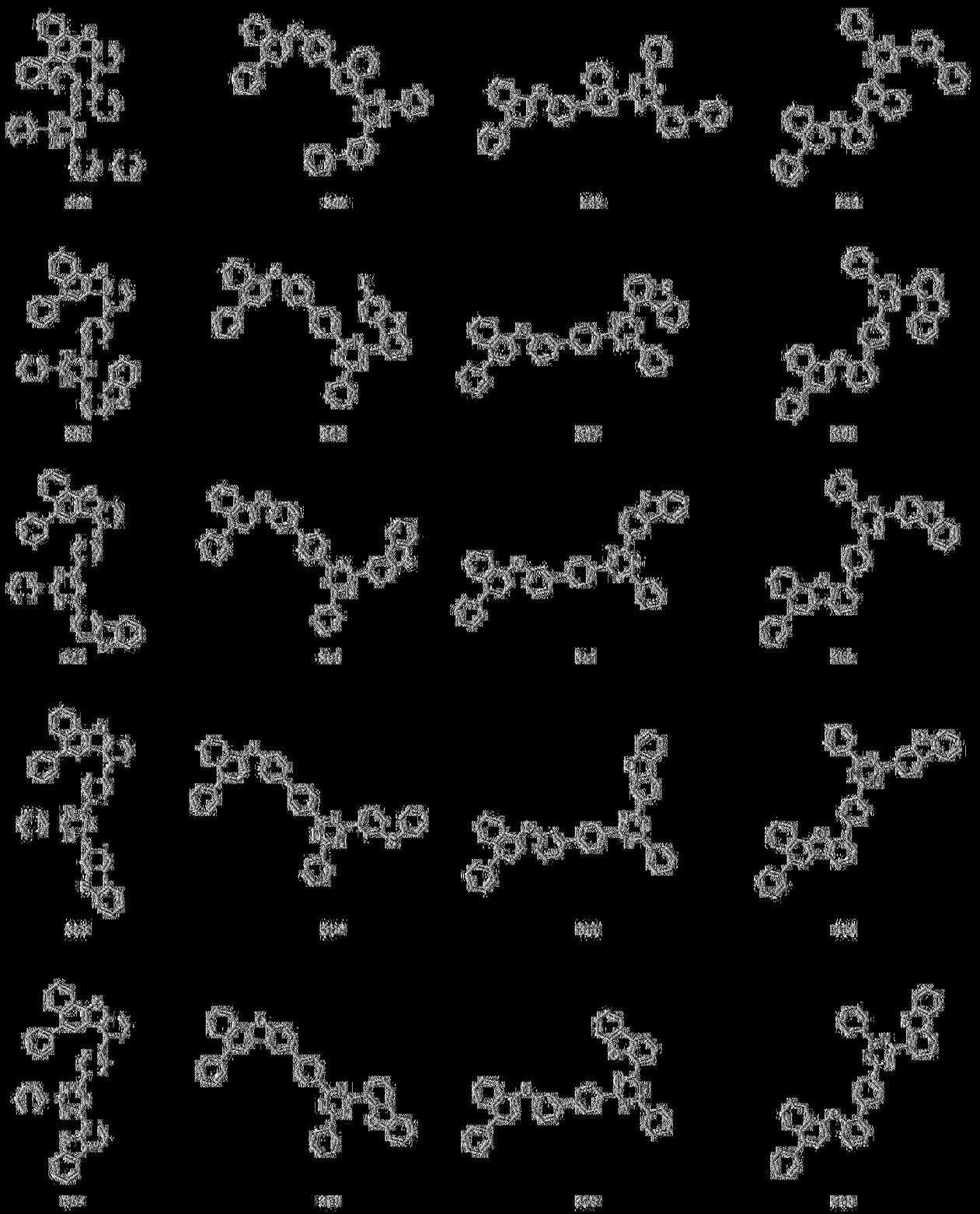


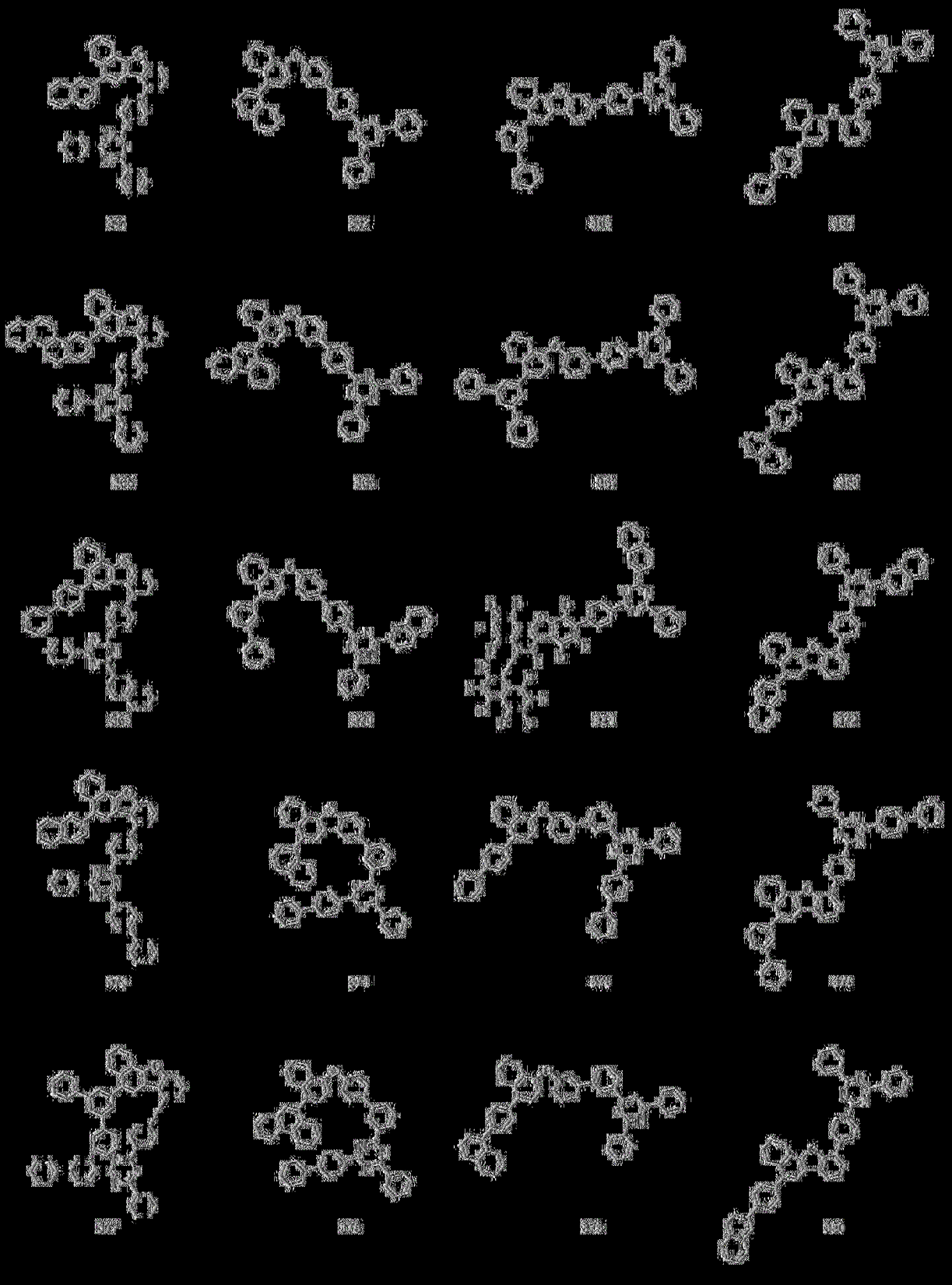


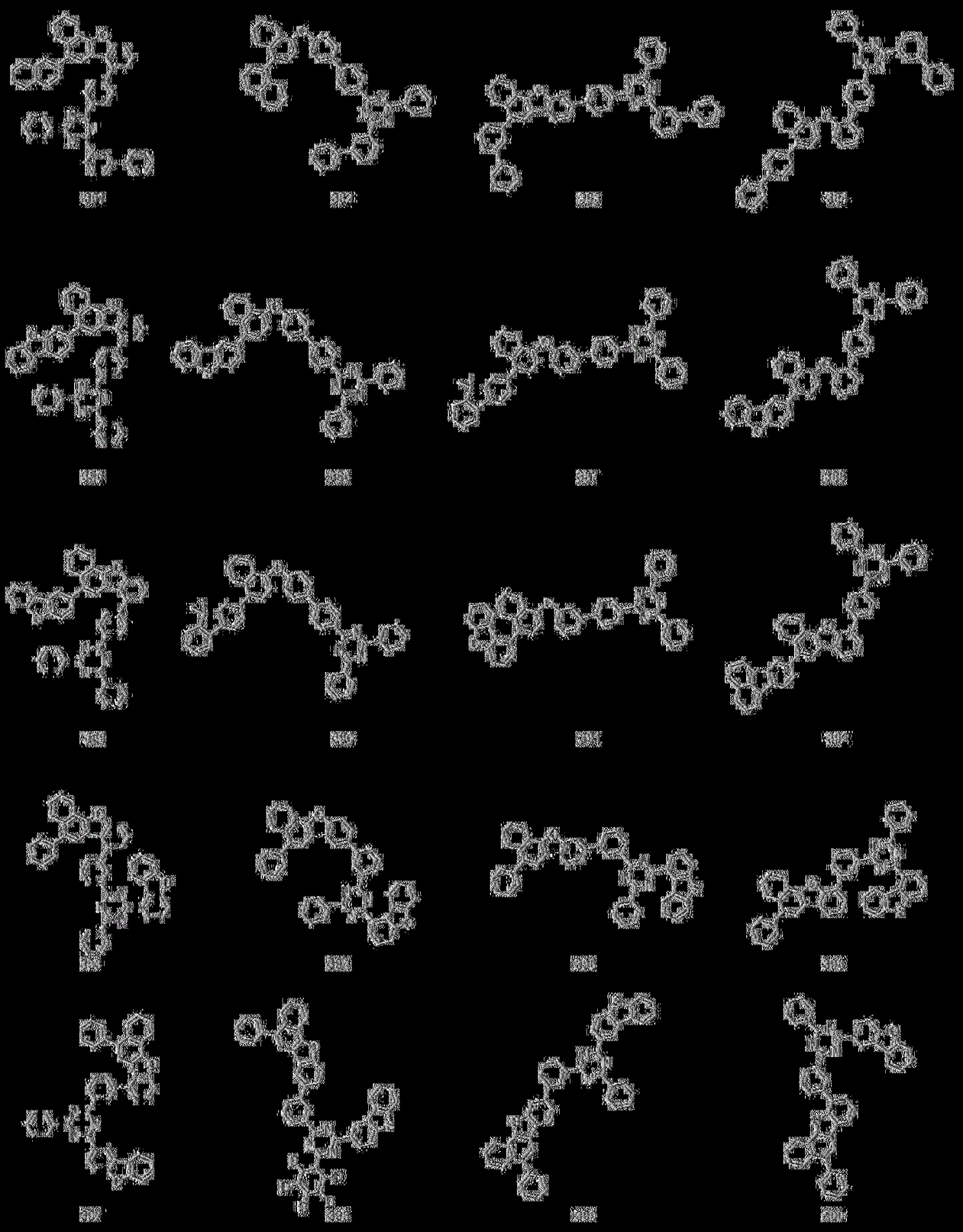


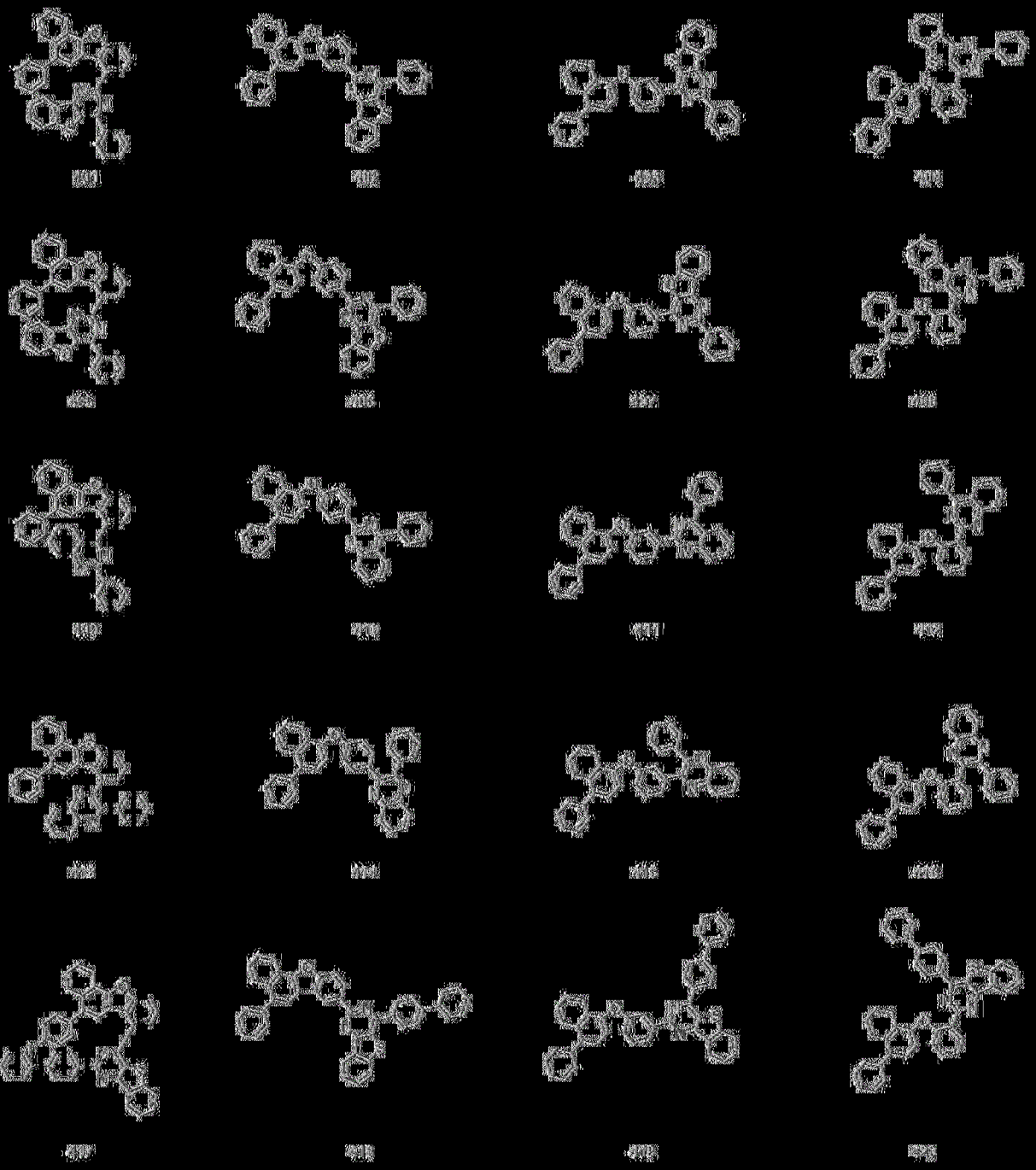


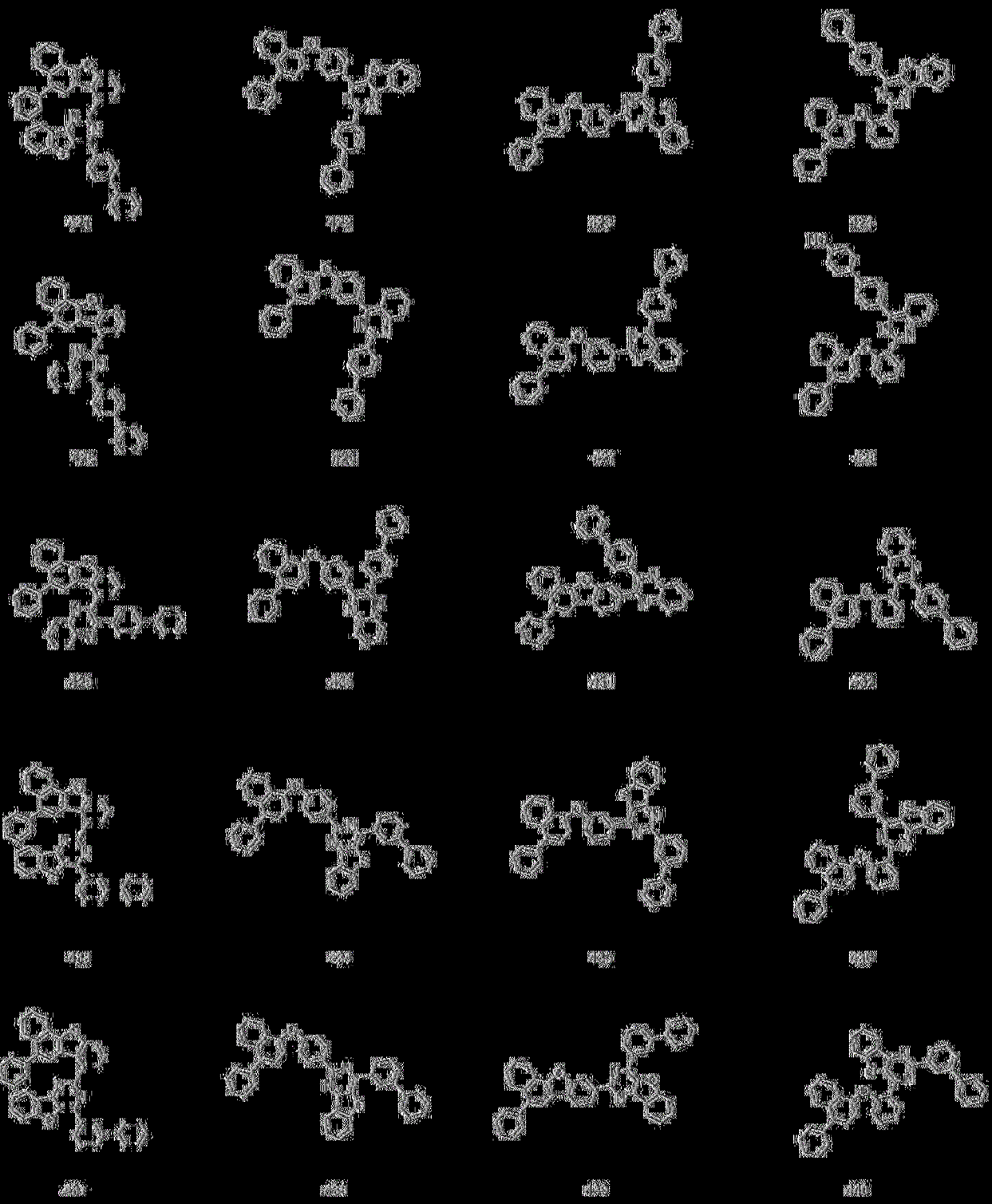


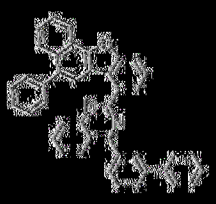


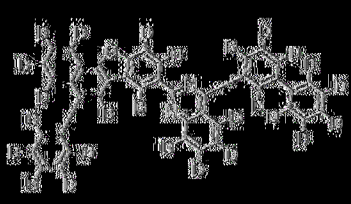


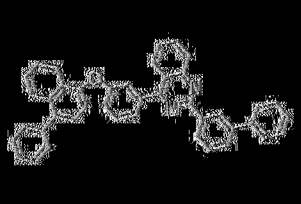


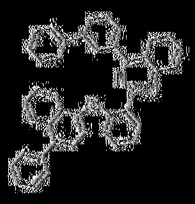


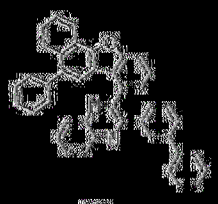


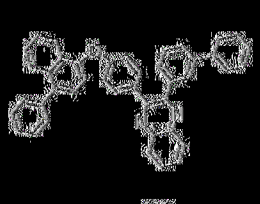


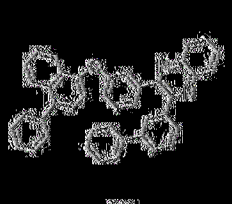


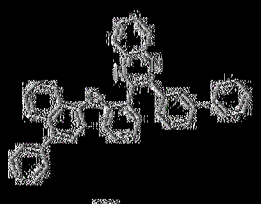


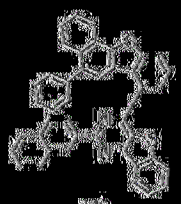


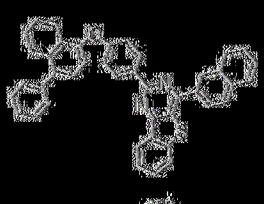


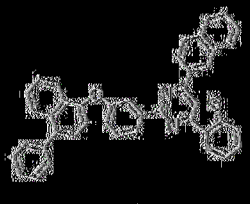


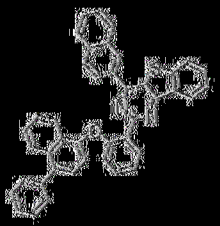


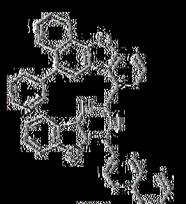


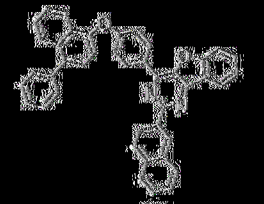


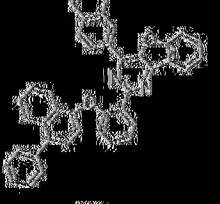


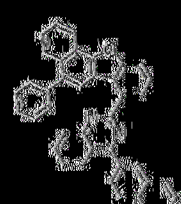


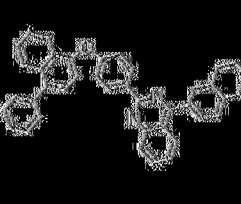


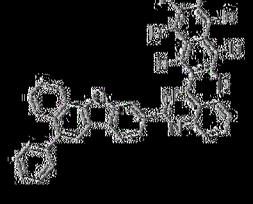


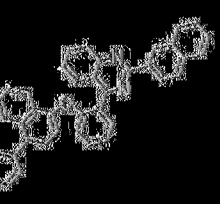


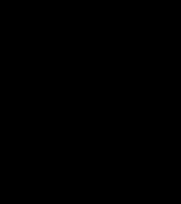


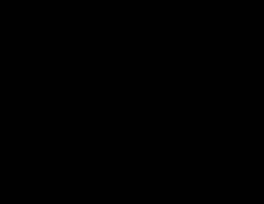


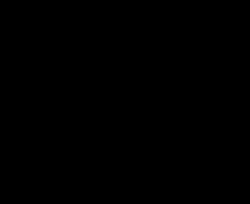


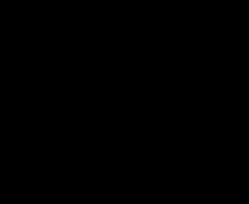


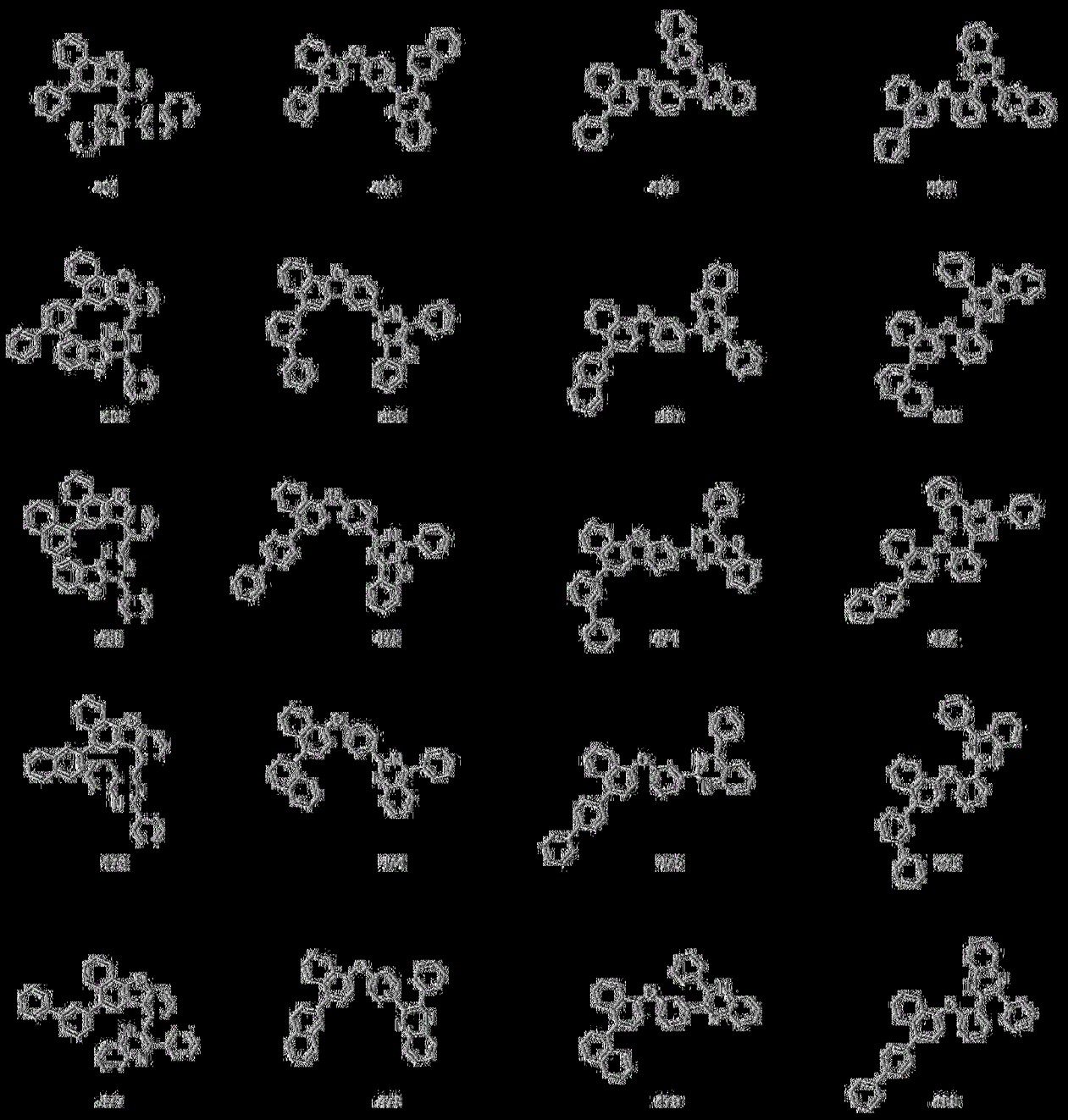


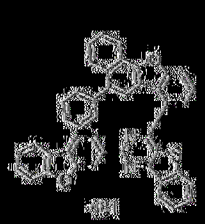


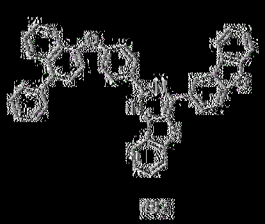


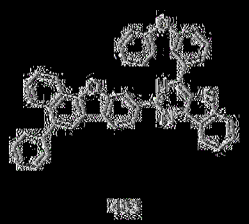


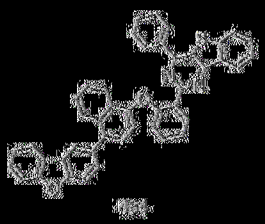


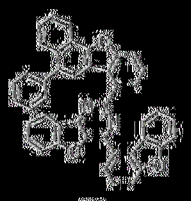


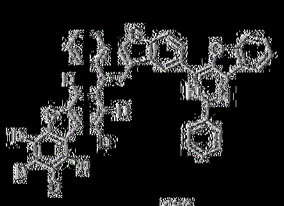


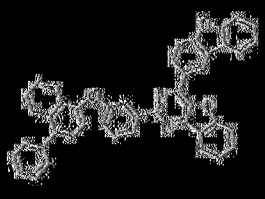


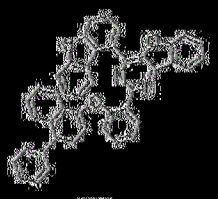


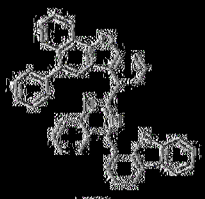


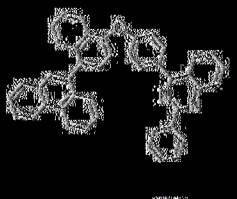


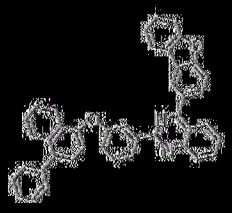


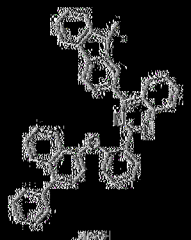


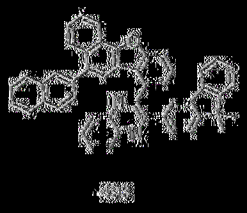


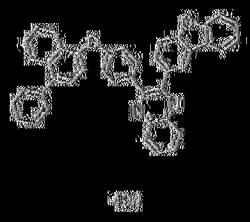


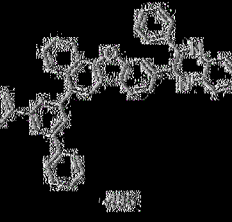


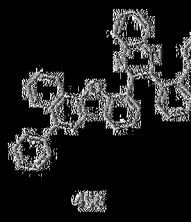


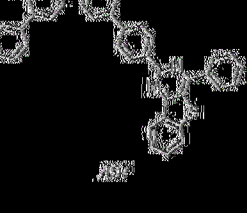


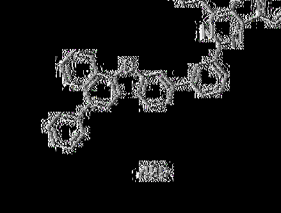


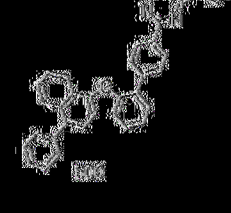


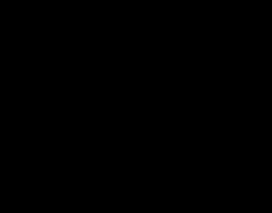


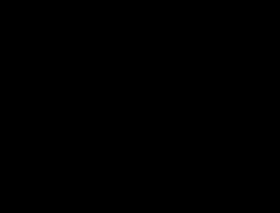


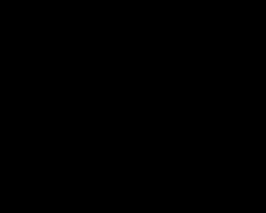


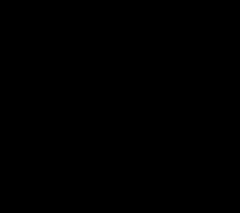


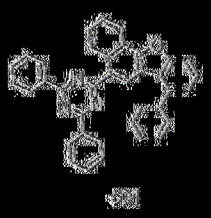


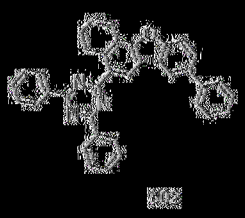


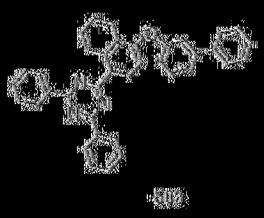


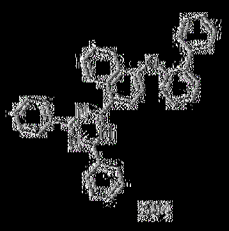


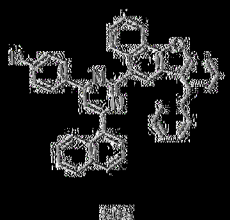


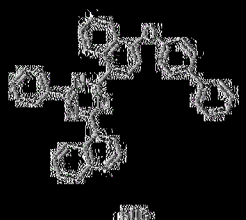


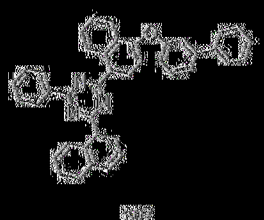


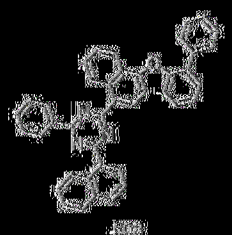


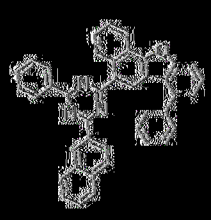


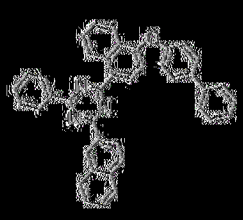


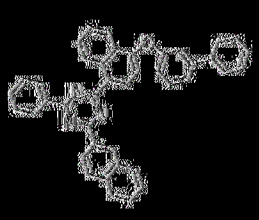


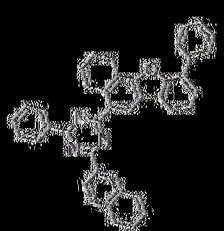


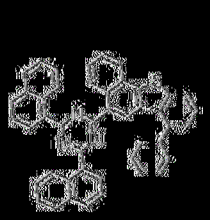


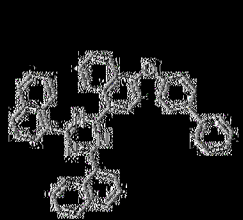


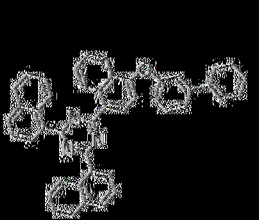


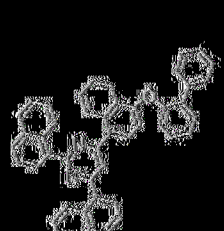


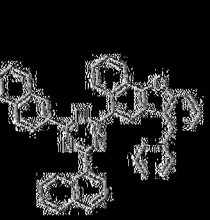


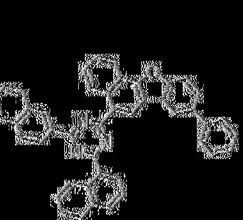


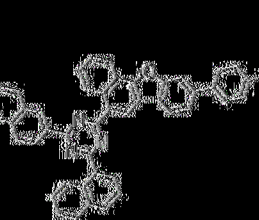


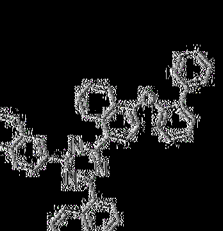


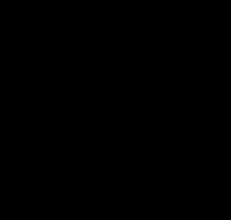


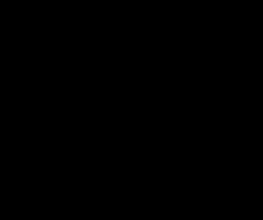


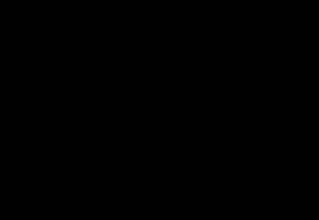


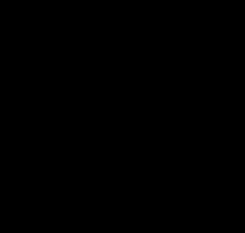


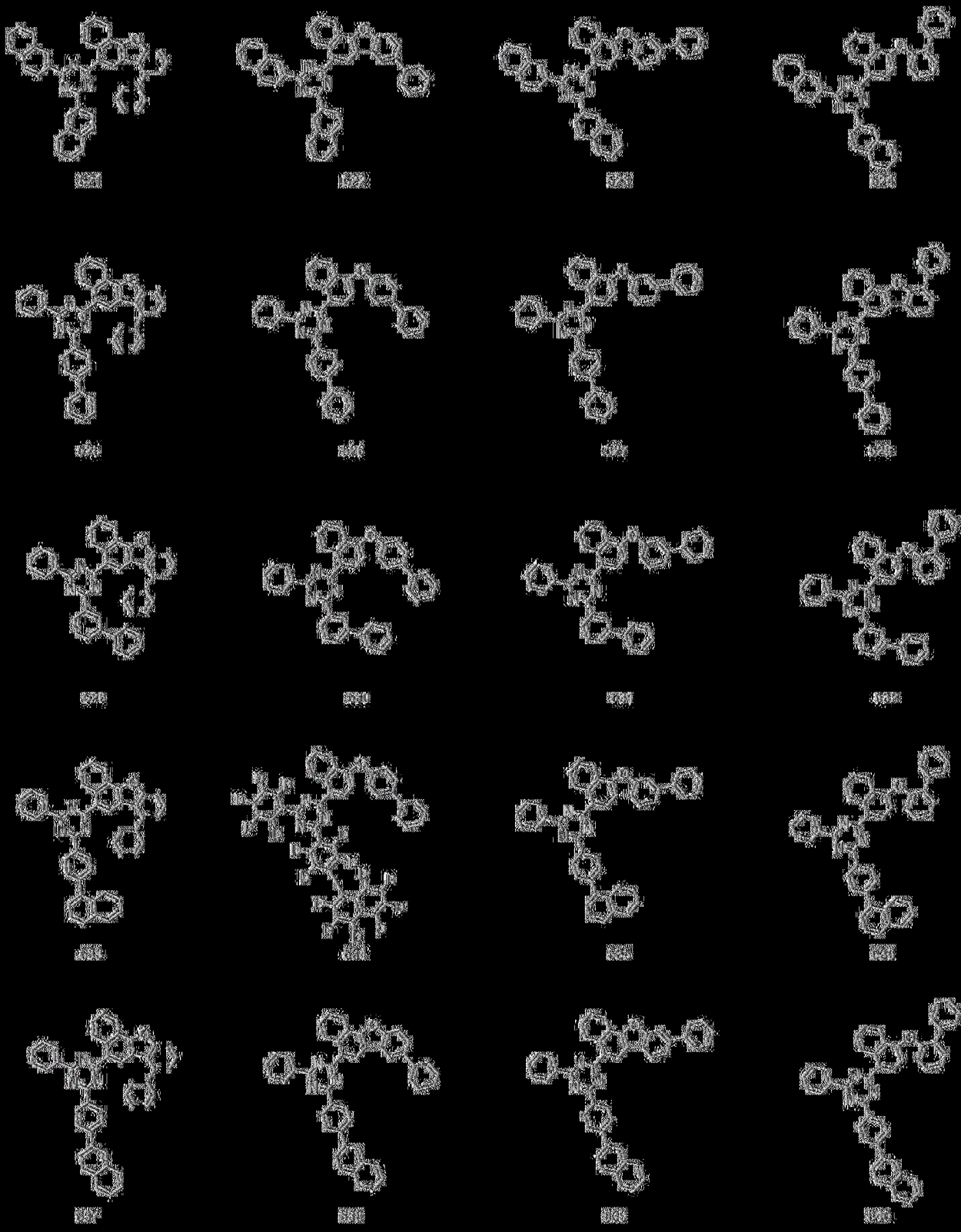


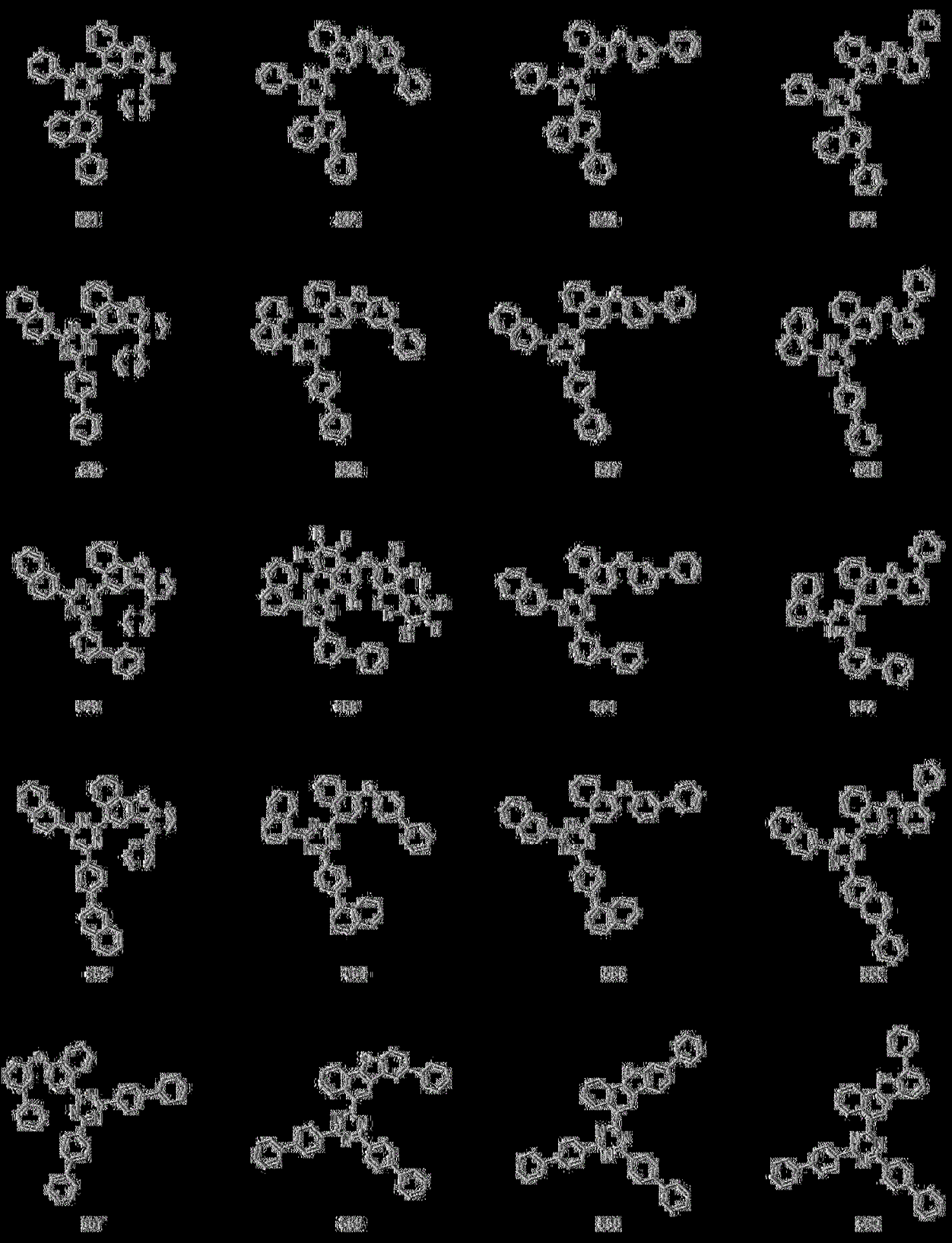


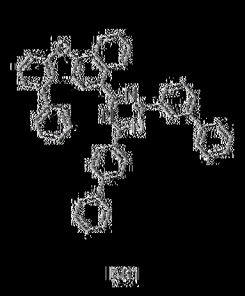


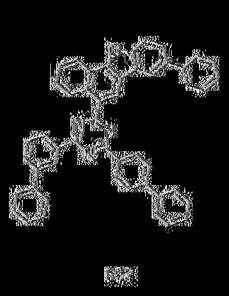


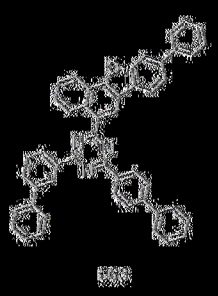


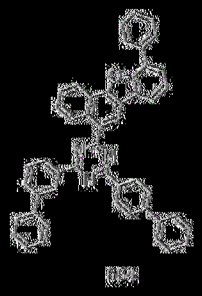


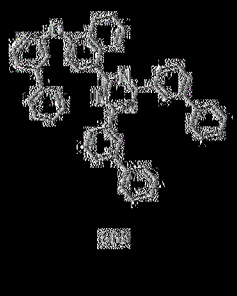


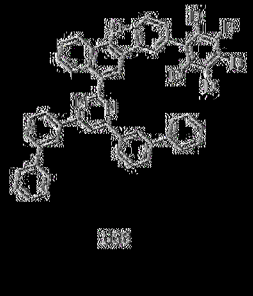


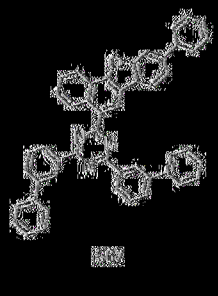


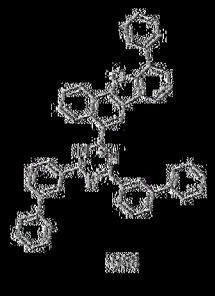


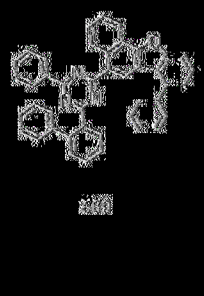


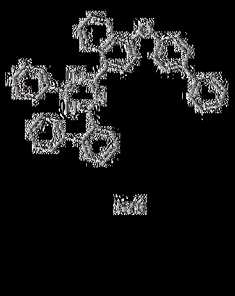


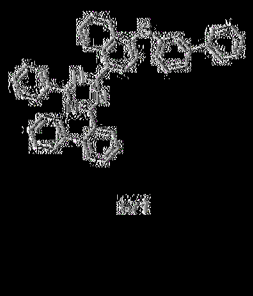


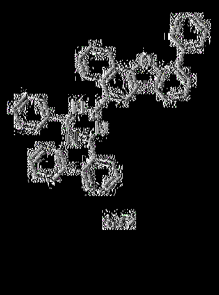


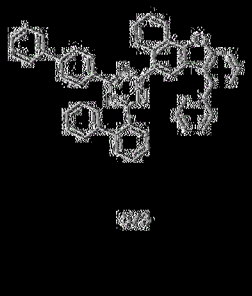


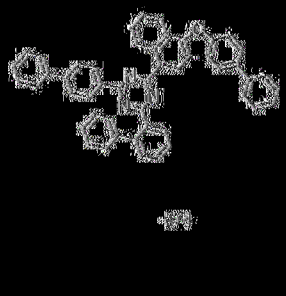


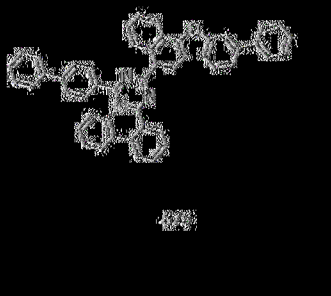


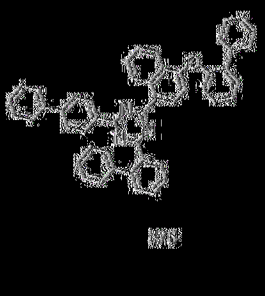


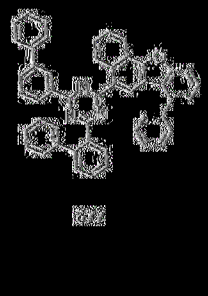


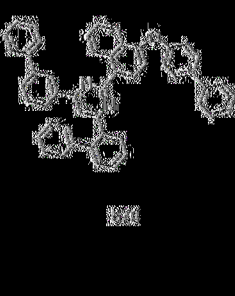


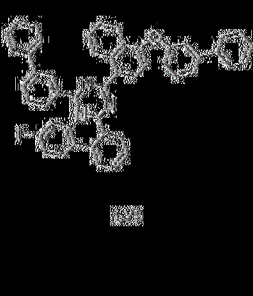


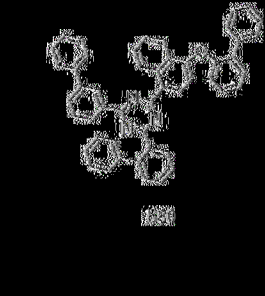


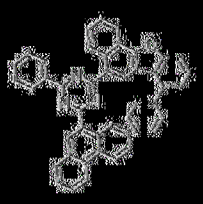


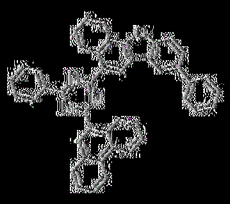


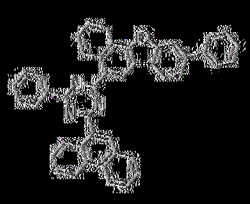


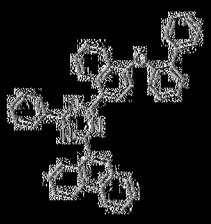


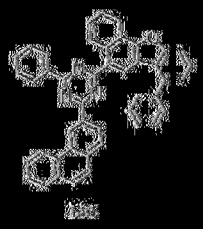


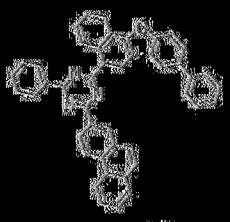


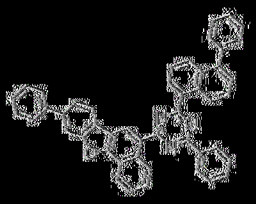


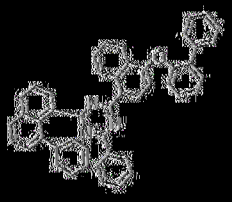


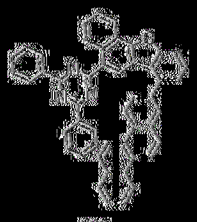


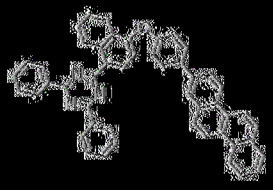


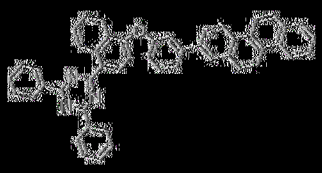


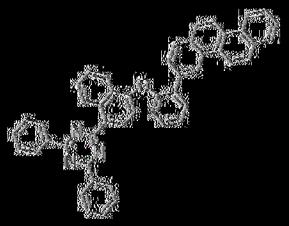


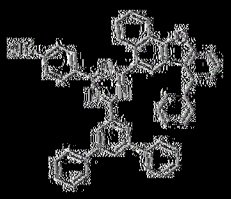


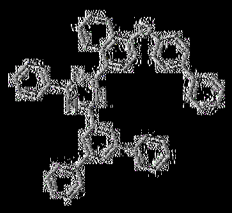


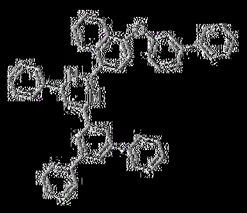


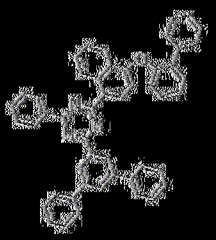


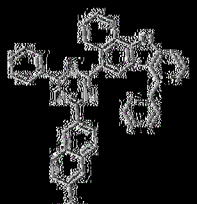


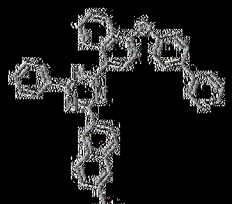


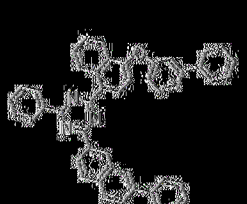


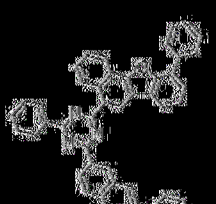


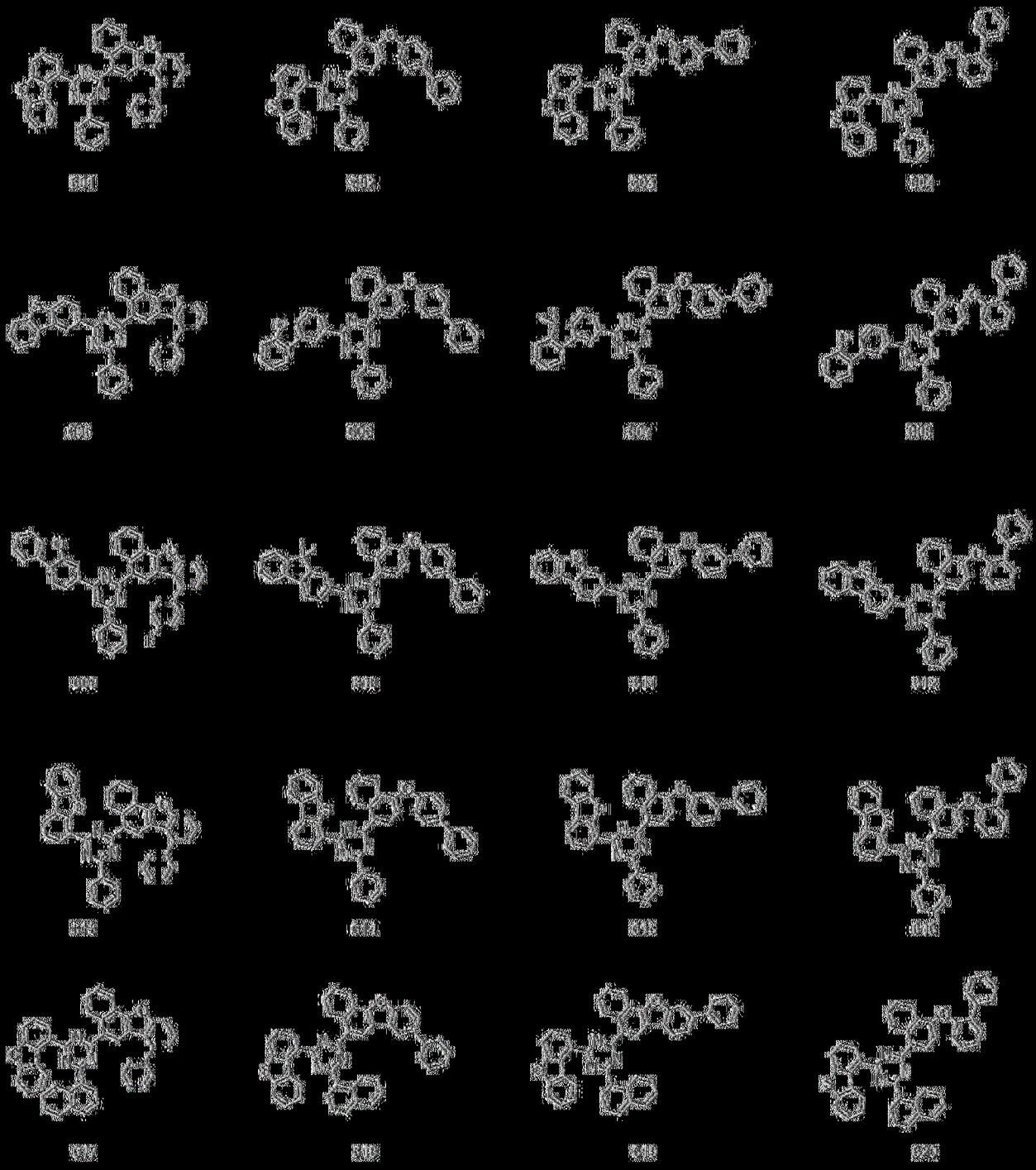


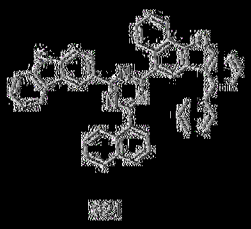


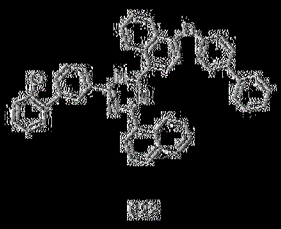


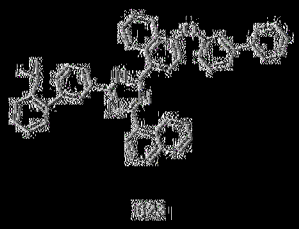


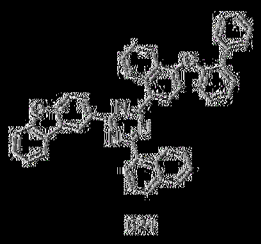


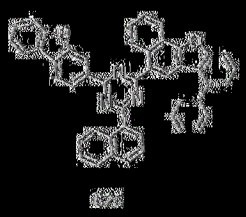


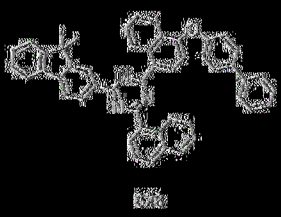


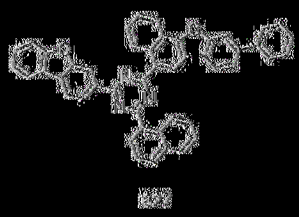


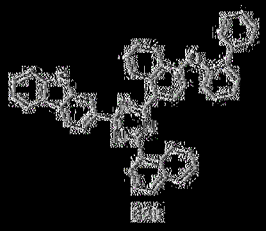


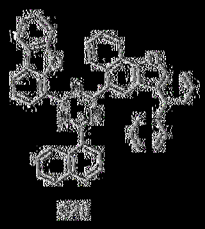


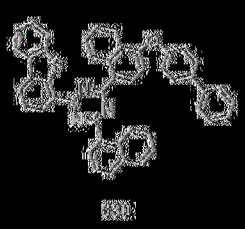


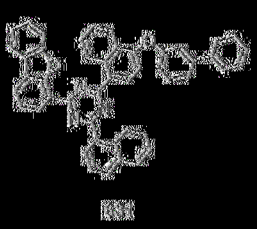


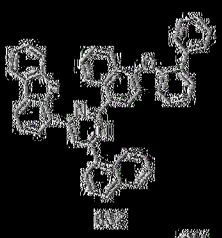


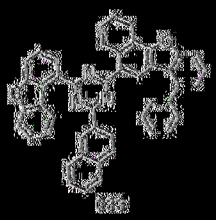


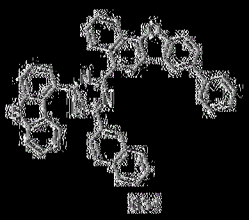


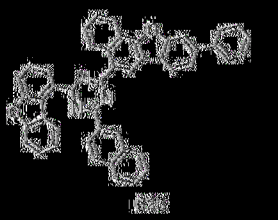


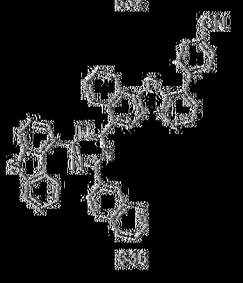


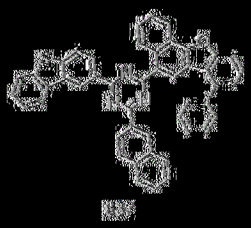


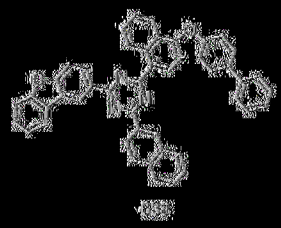


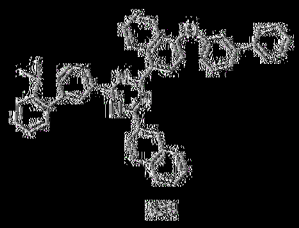


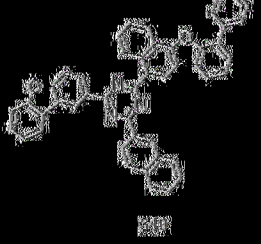


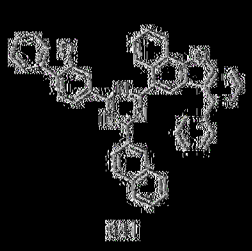


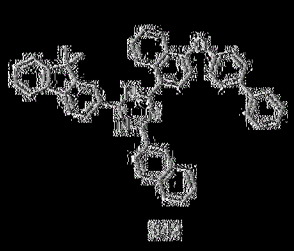


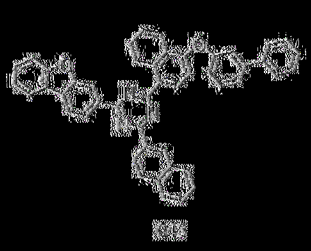


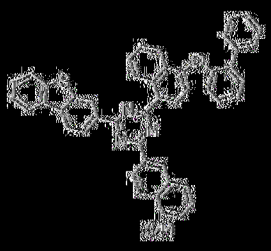


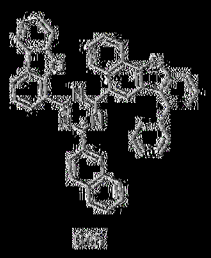


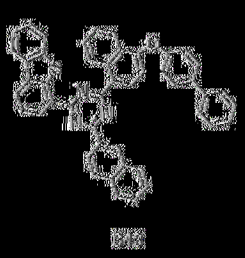


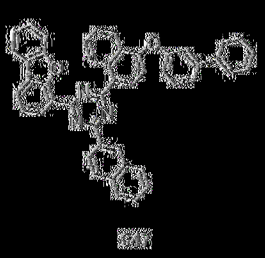


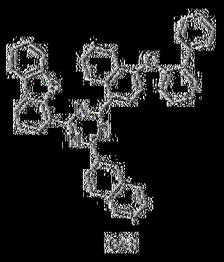


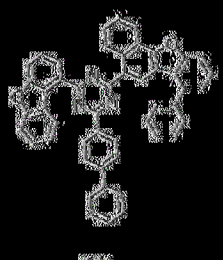


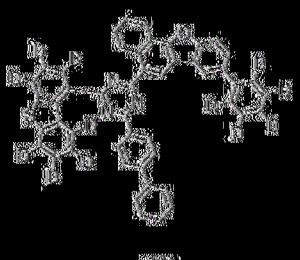


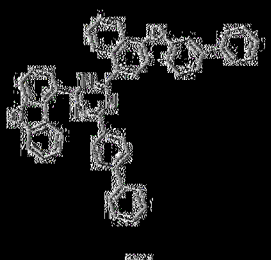


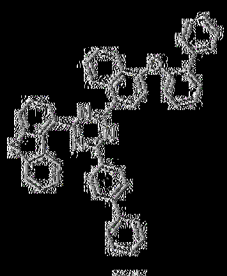


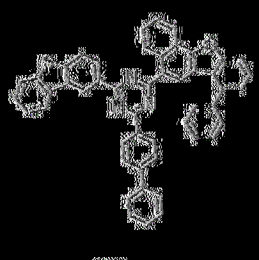


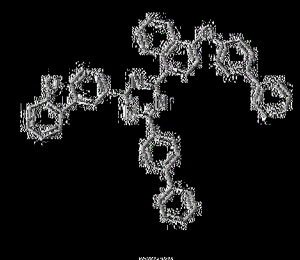


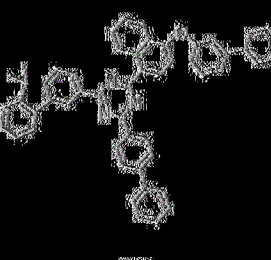


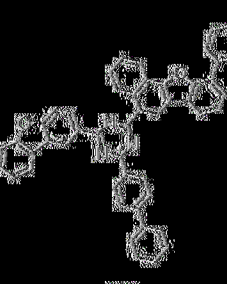


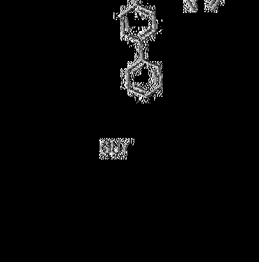


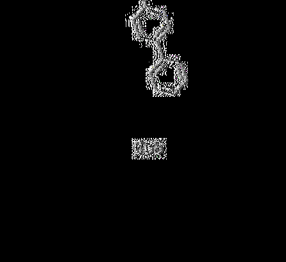


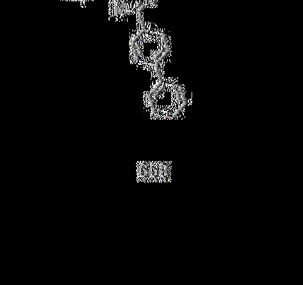


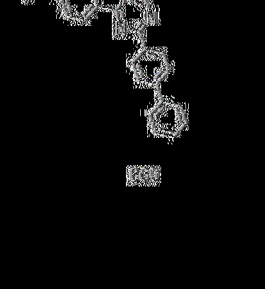


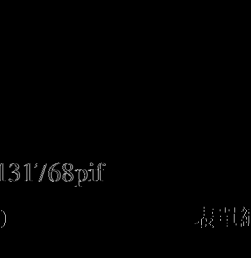


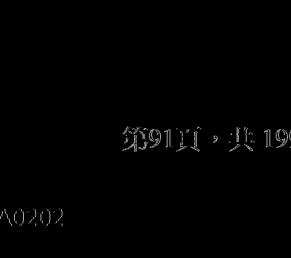


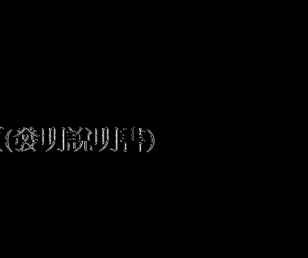


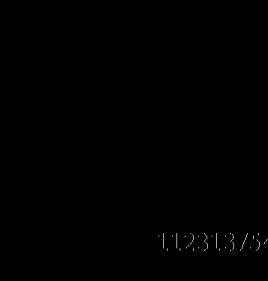


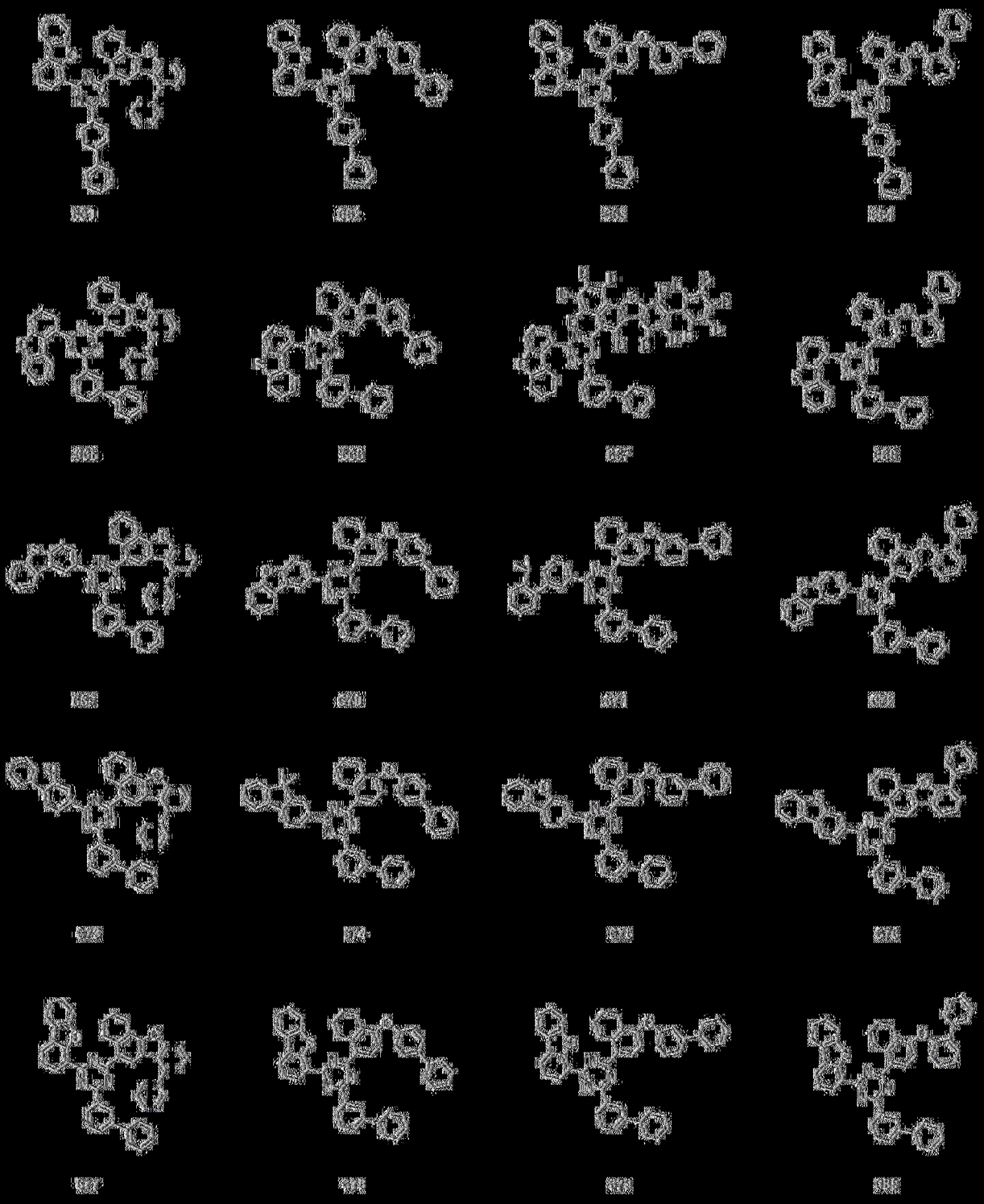


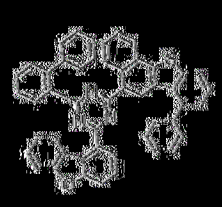


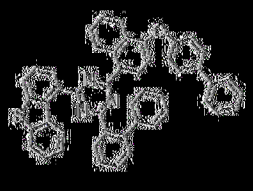


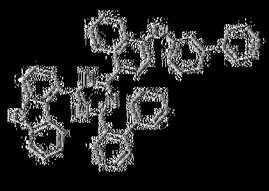


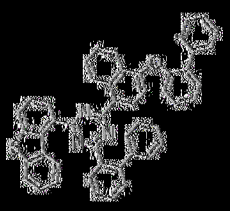


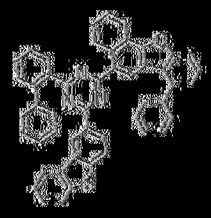


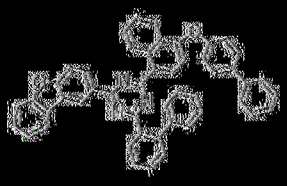


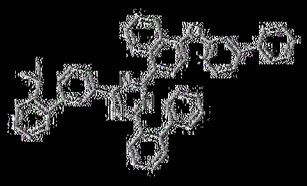


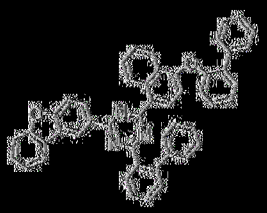


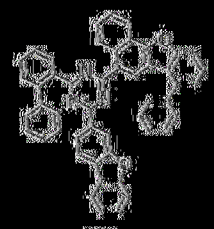


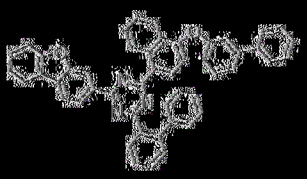


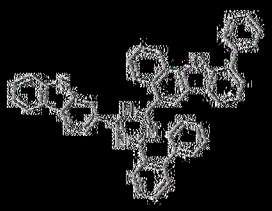


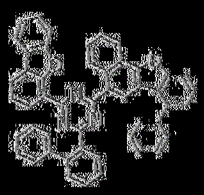


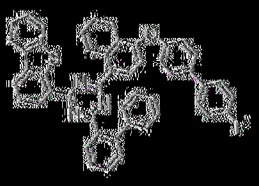


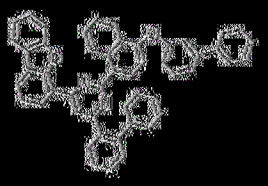


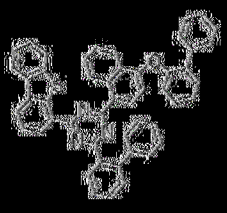


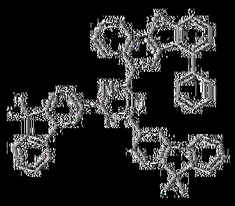


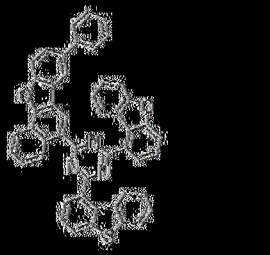


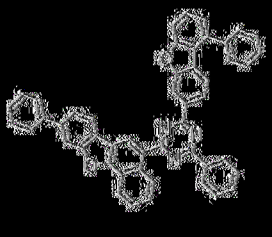


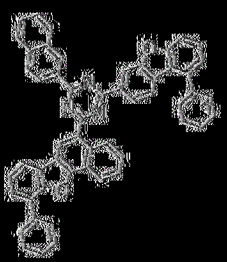


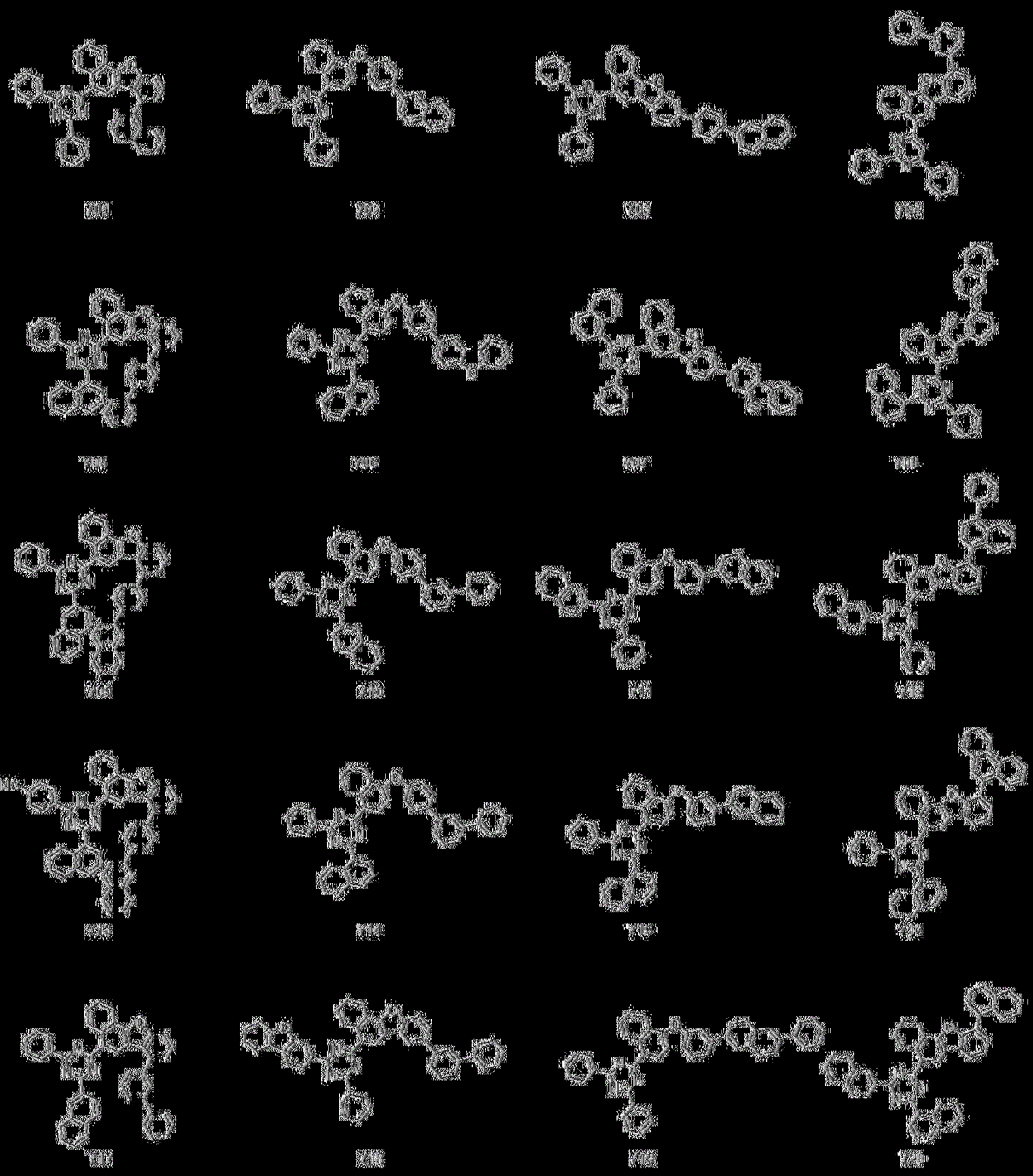


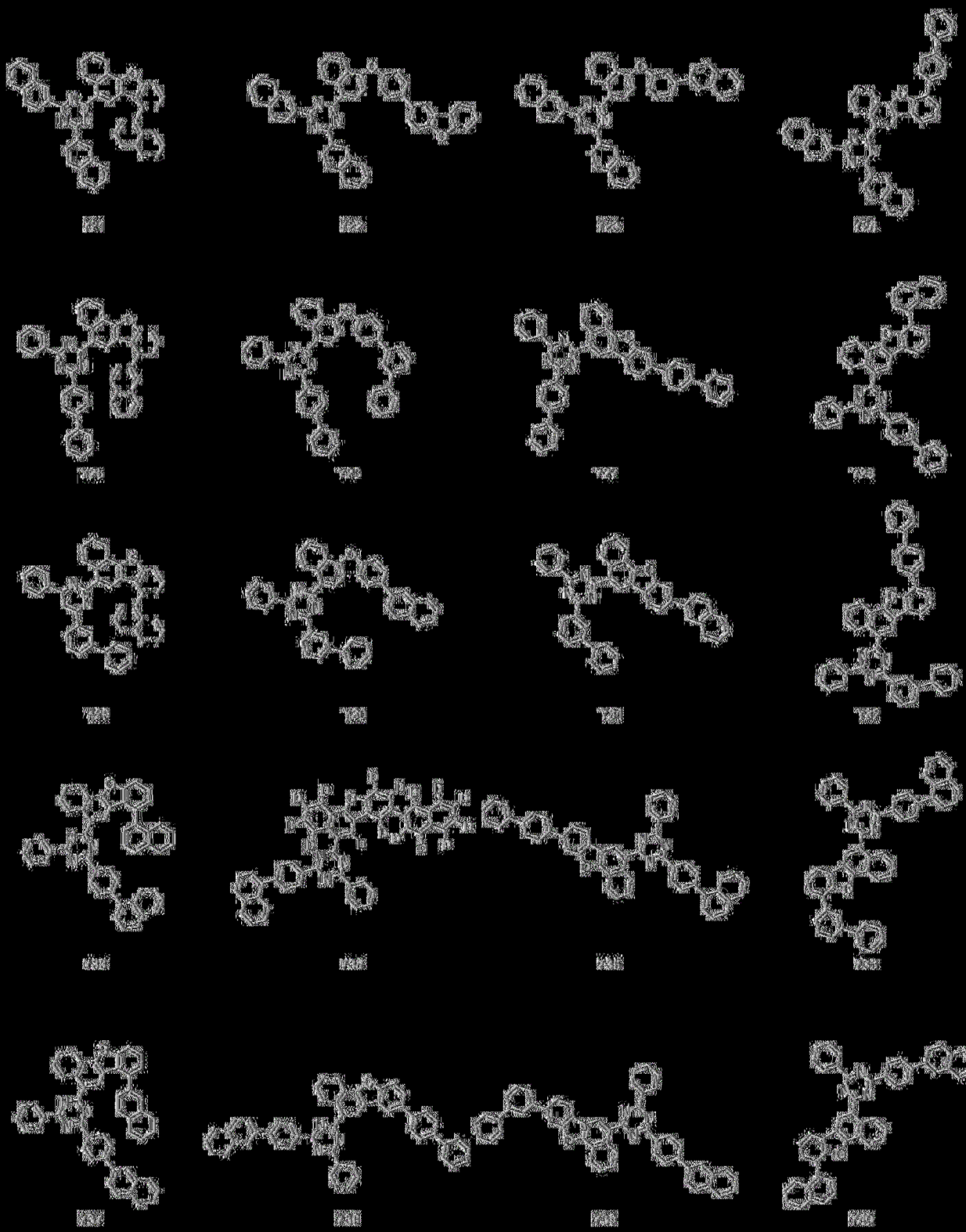


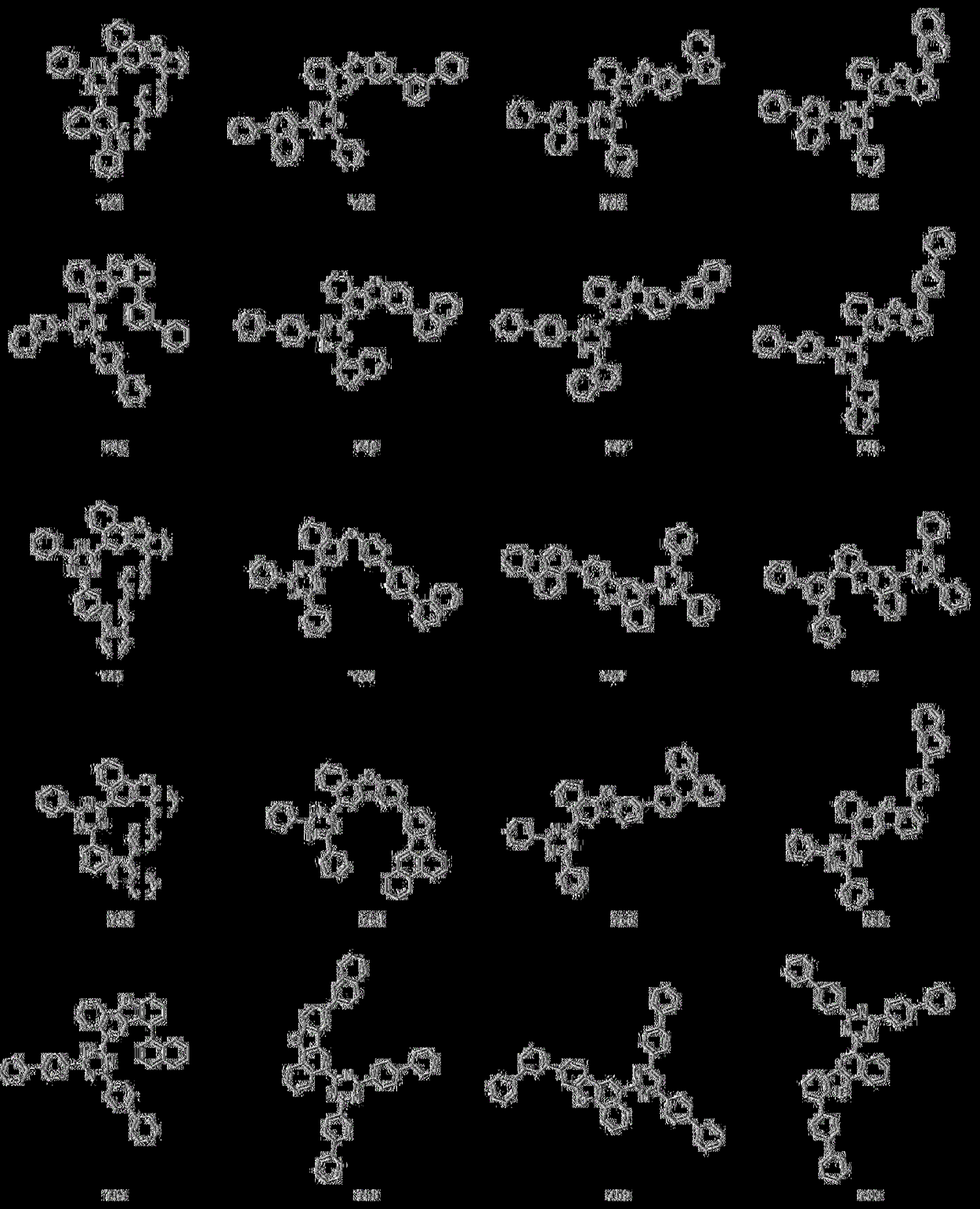


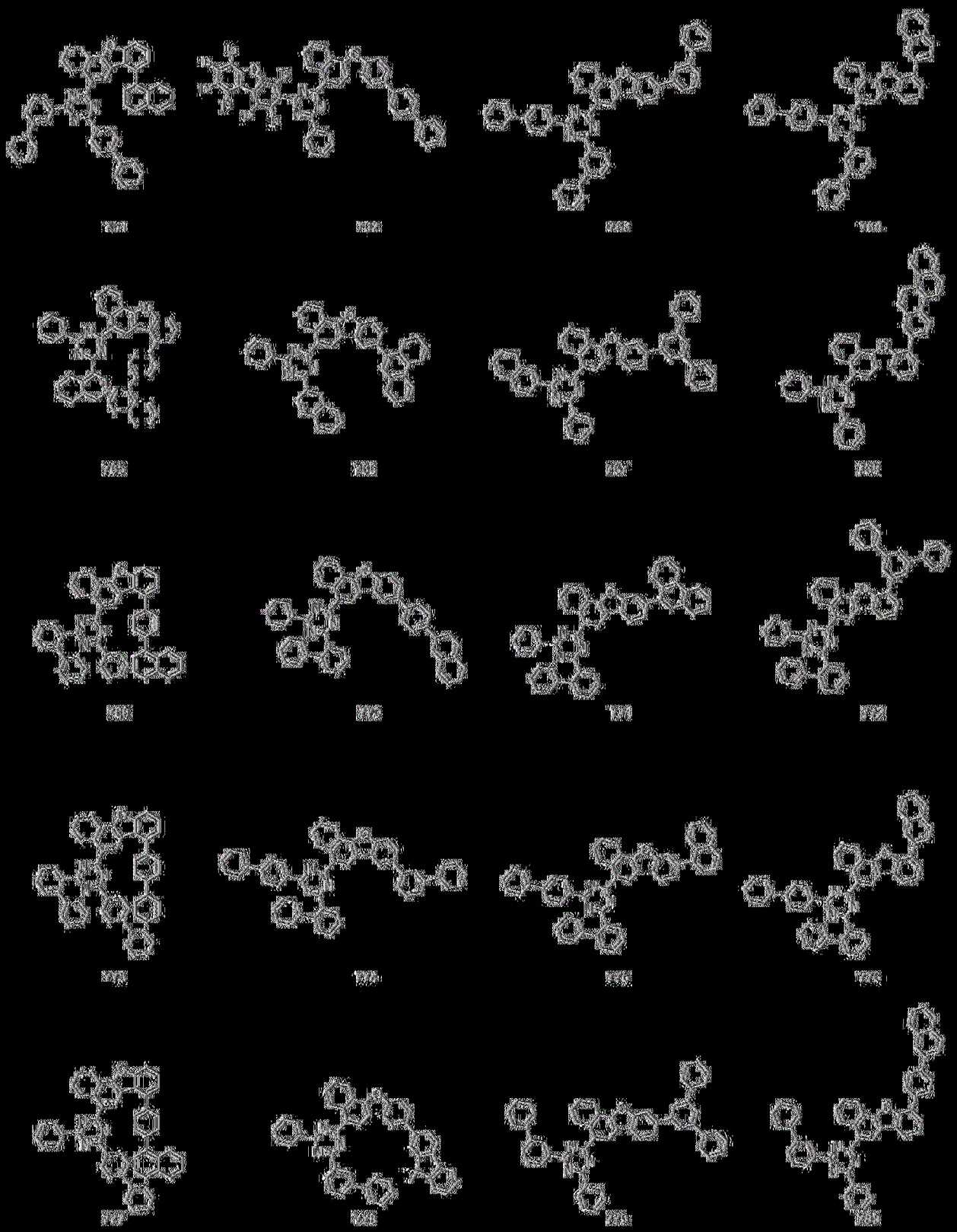


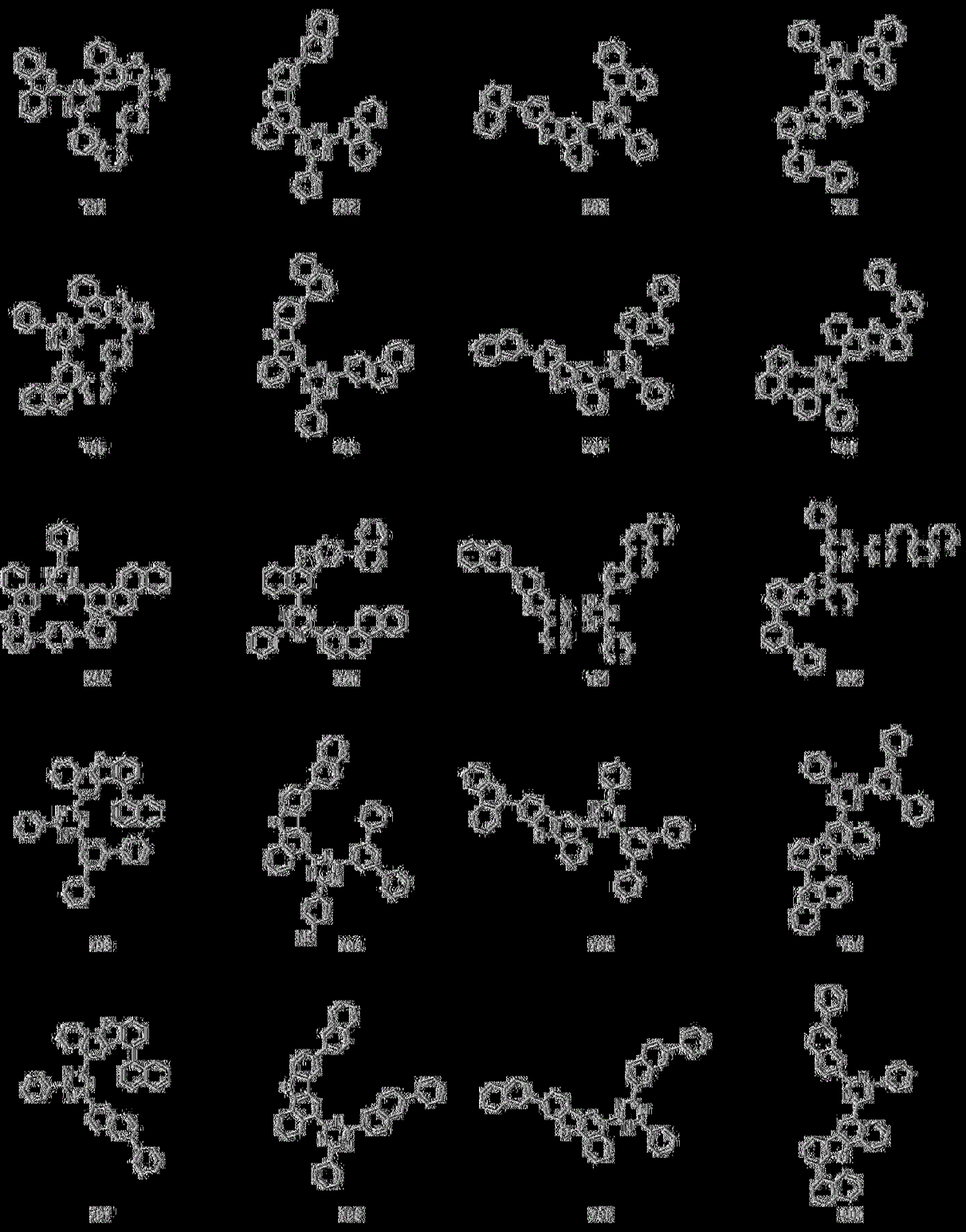


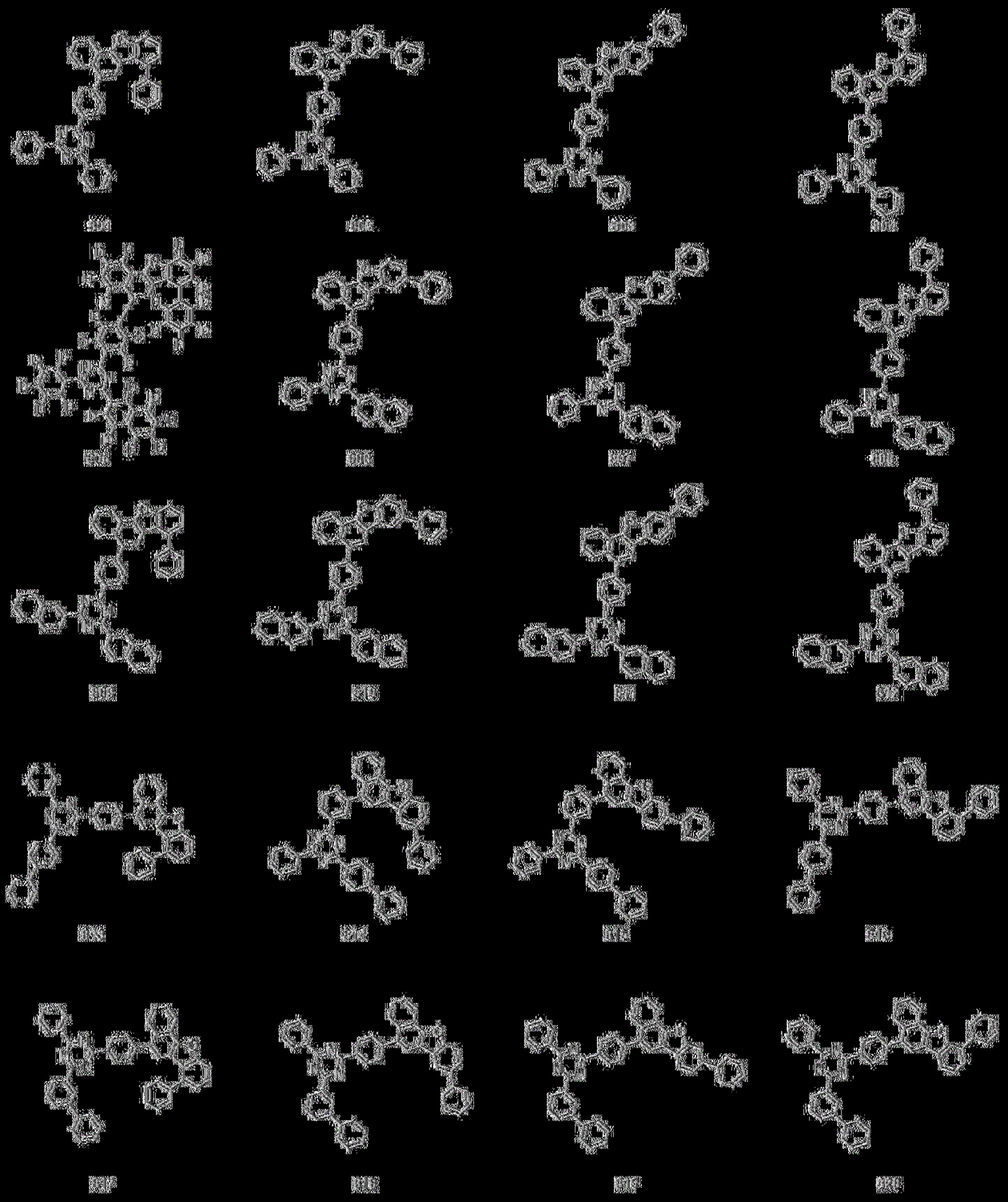


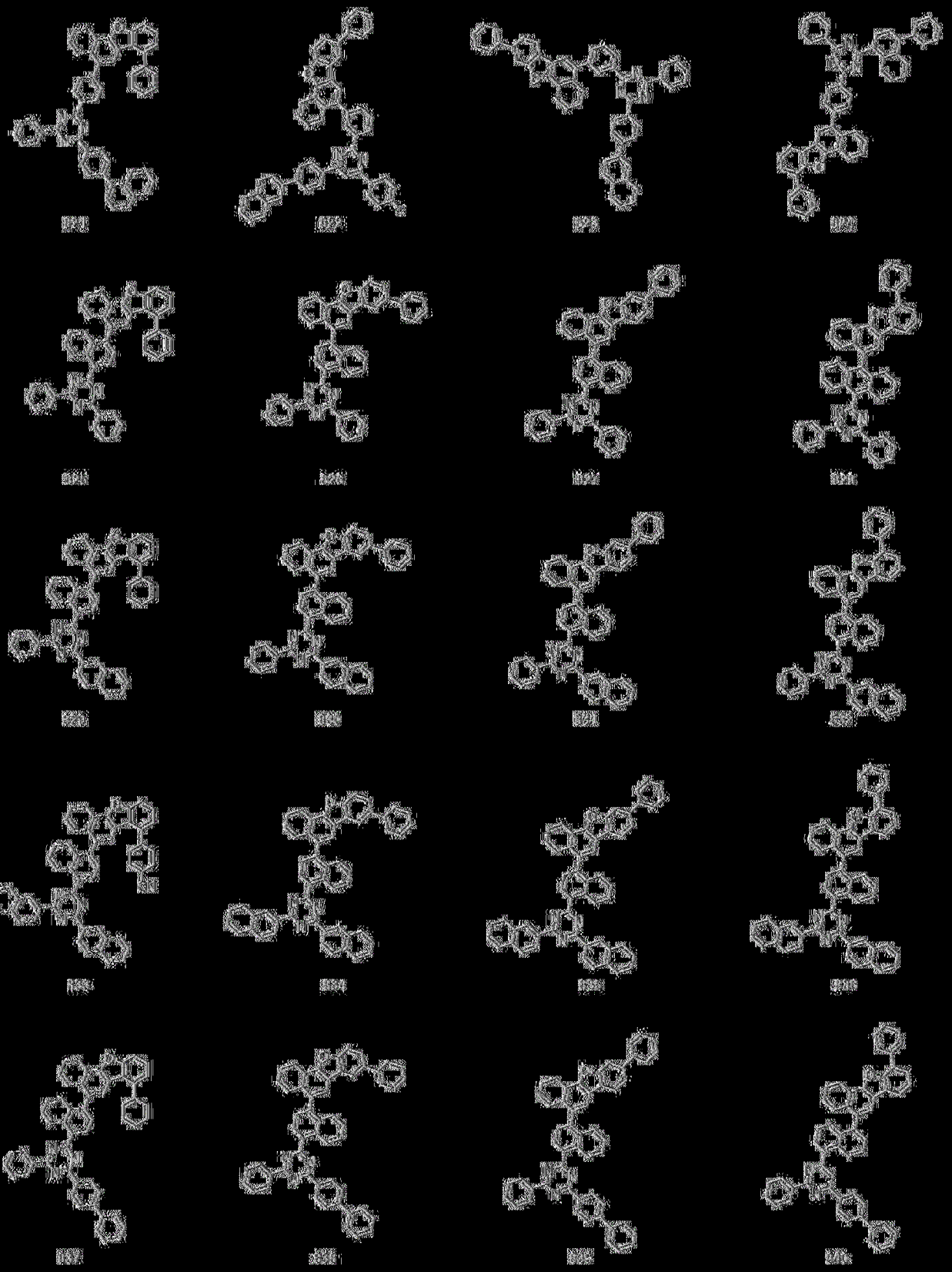


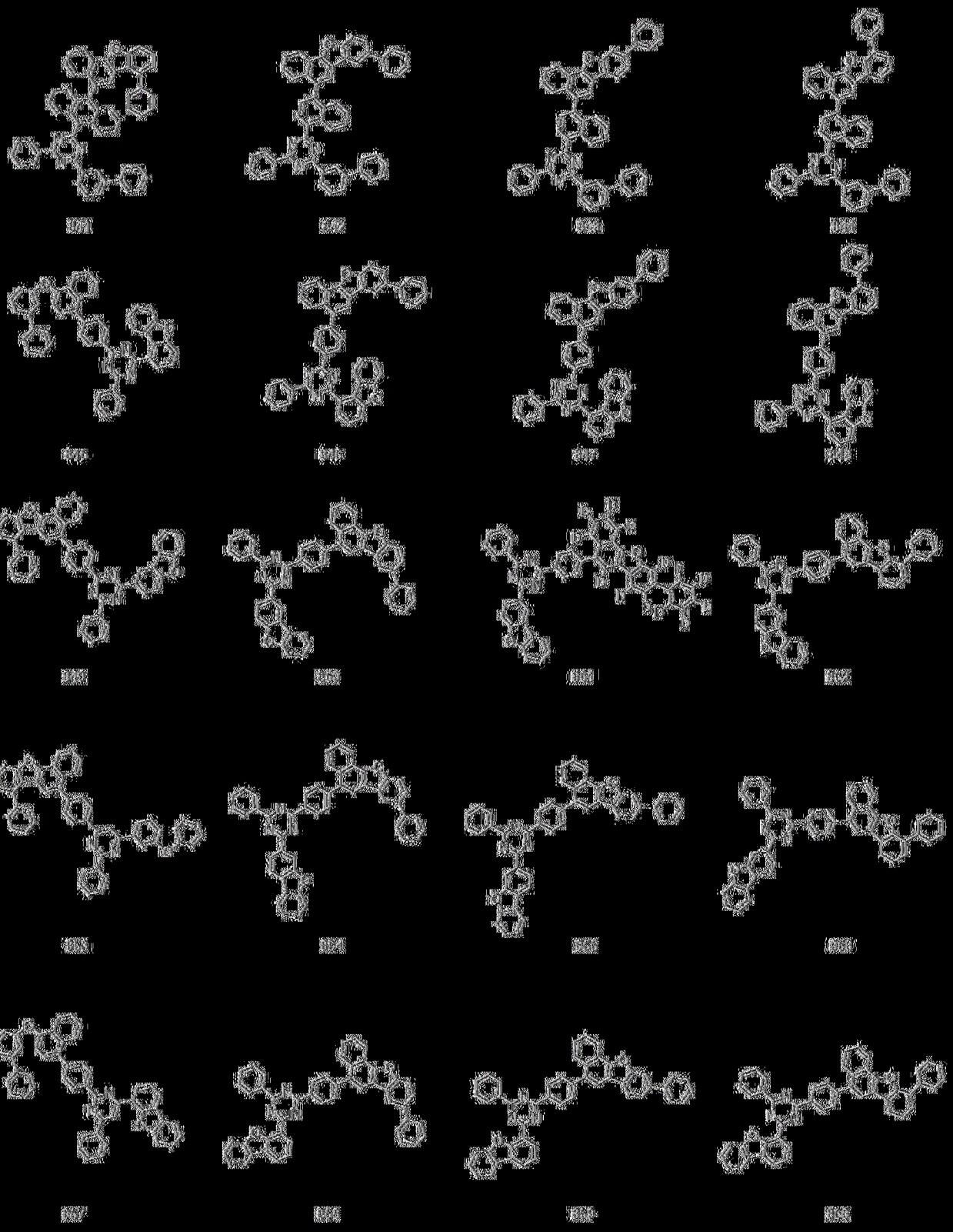


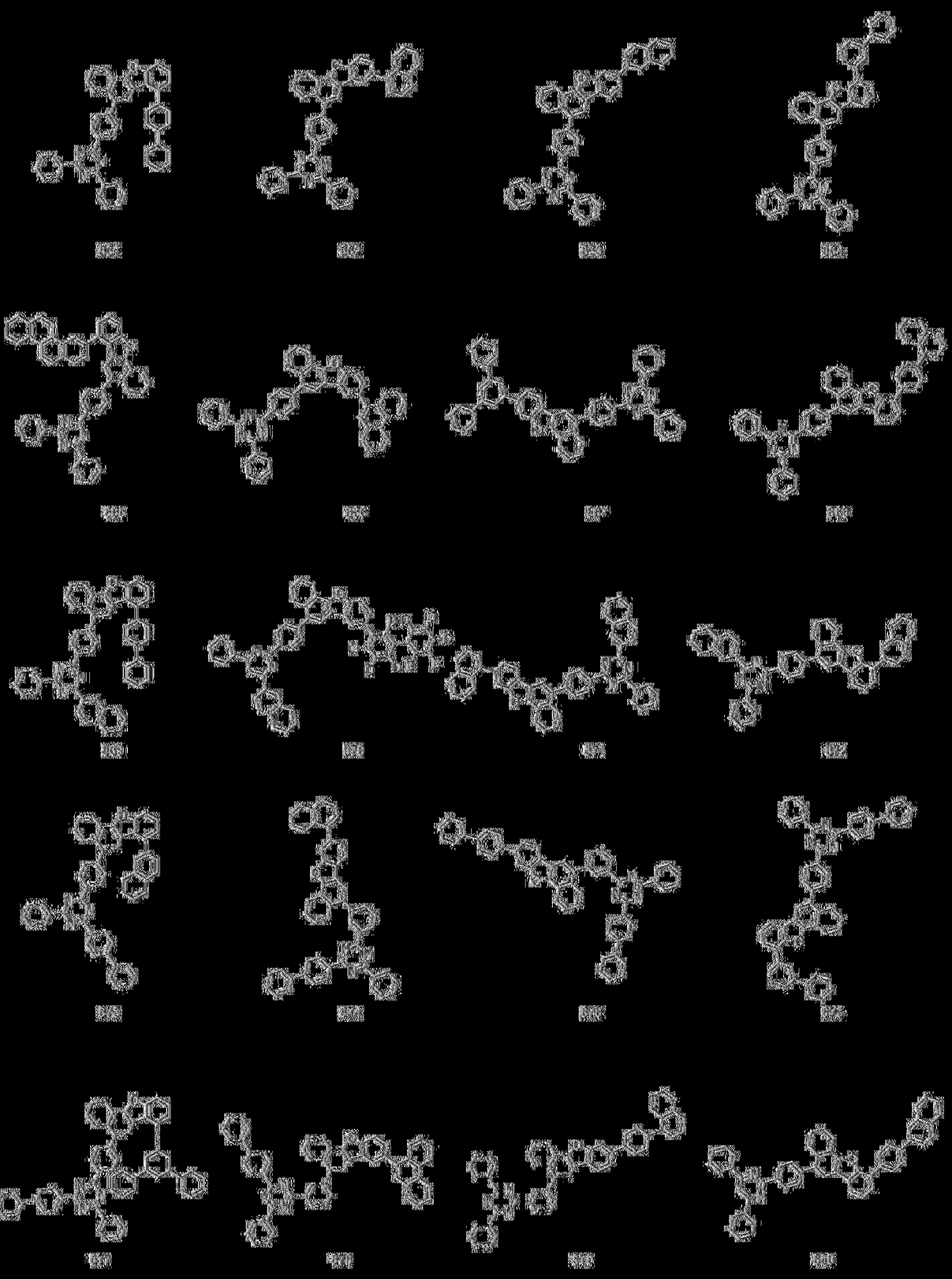


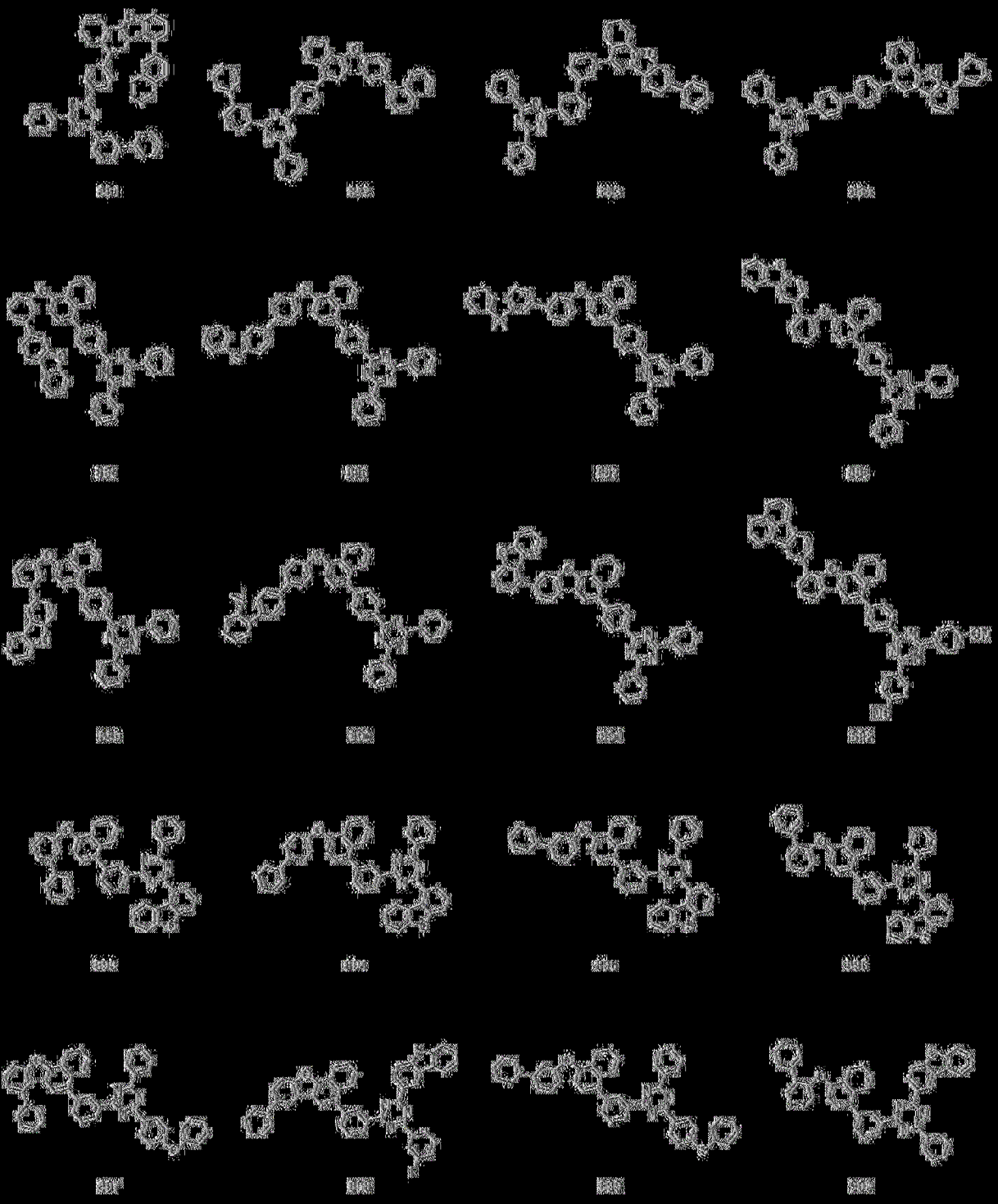


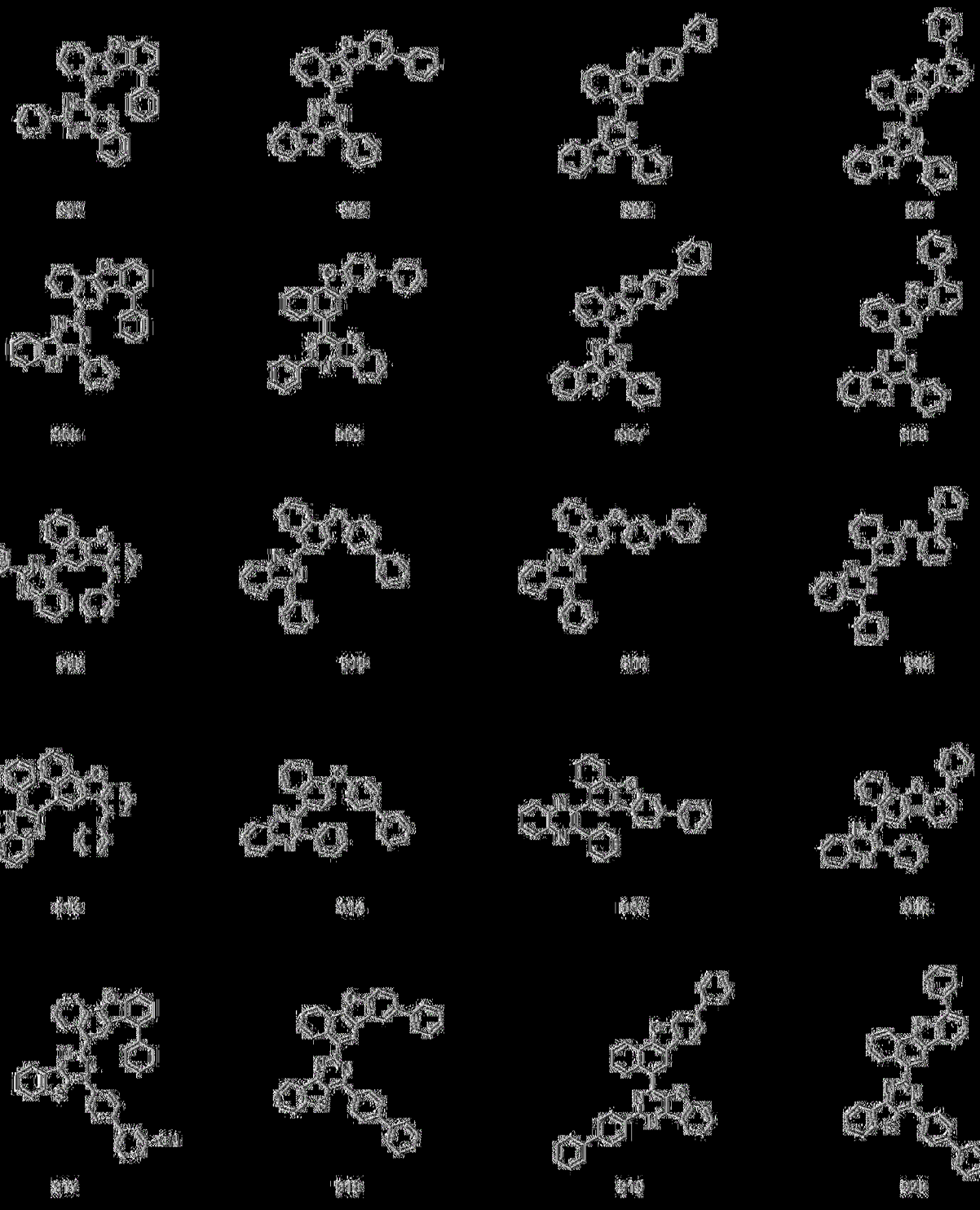


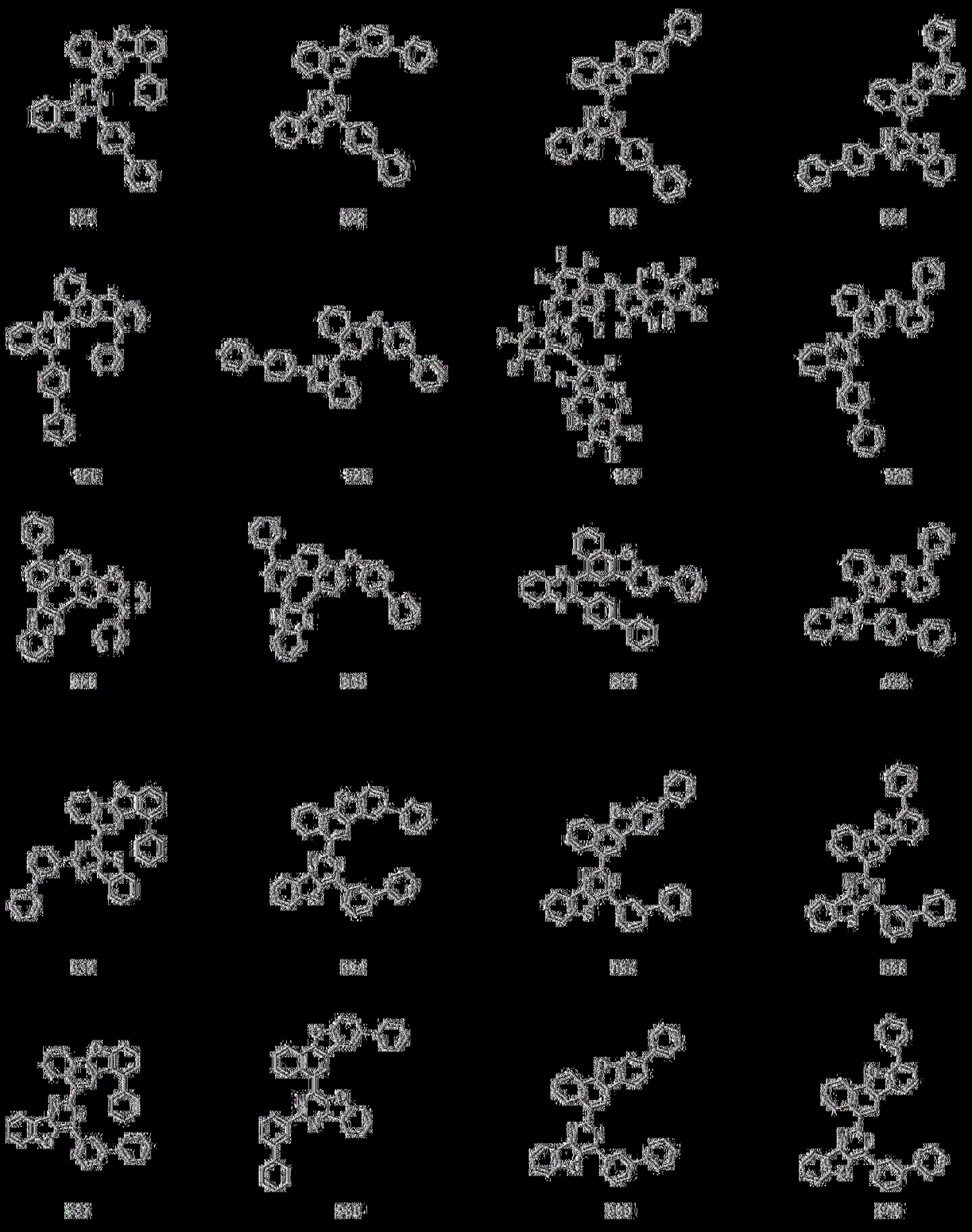


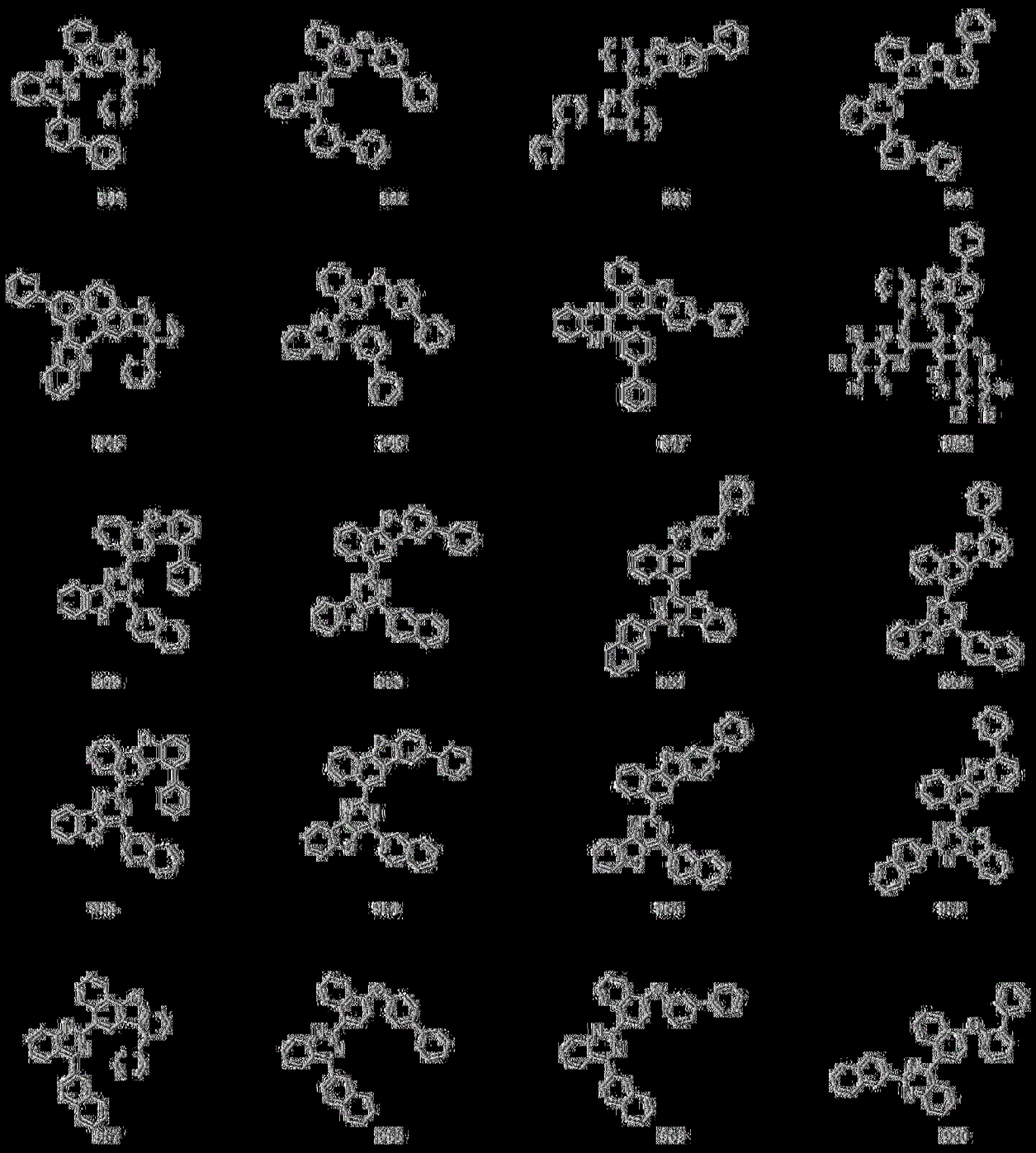


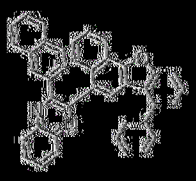


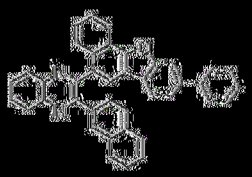


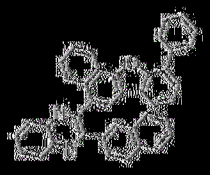


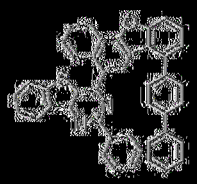


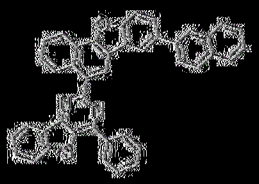


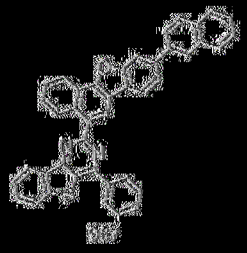


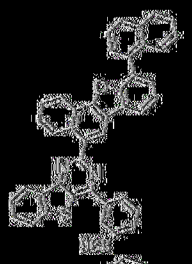


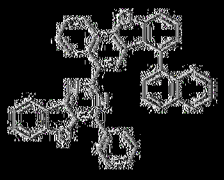


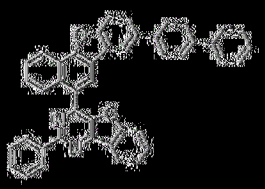


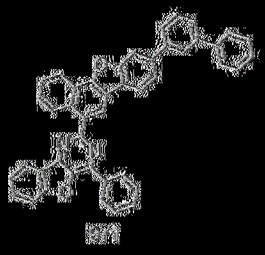


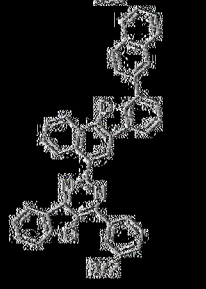


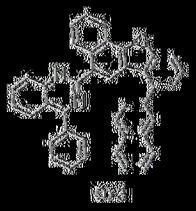


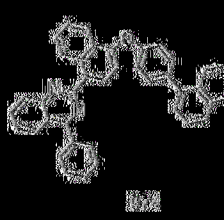


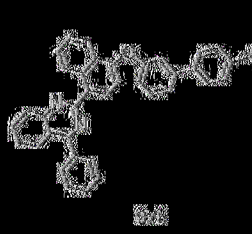


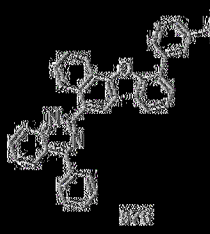


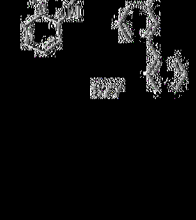


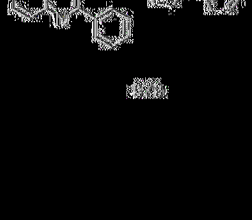


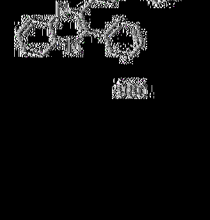


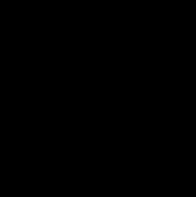


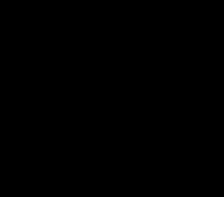


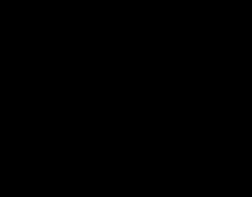


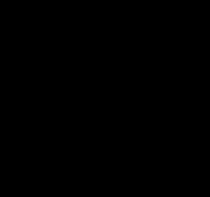


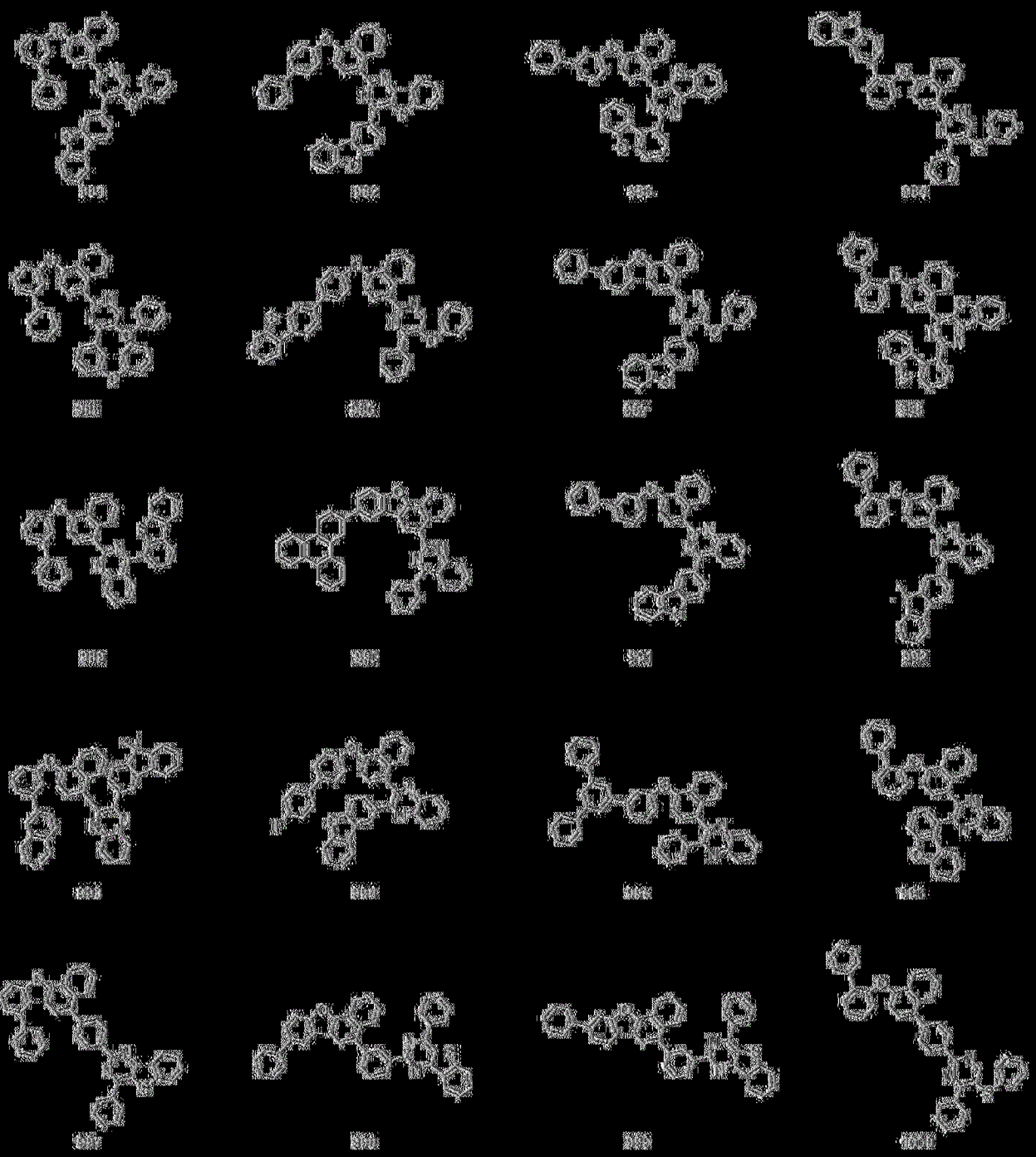




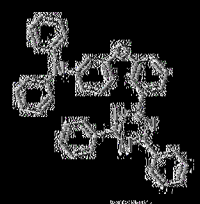


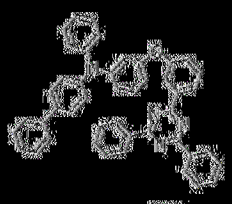


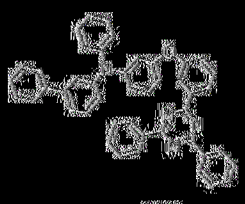


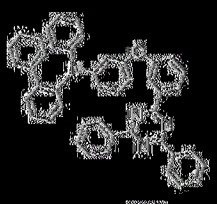


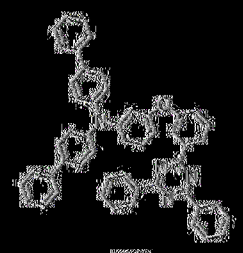
[0234] 根據本申請的一個示例性實施例，化學式 2 可以由以下化合物中的任一個表示，但不限於此。

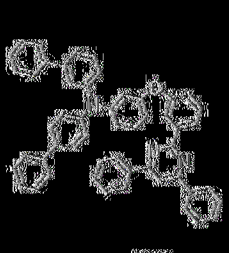


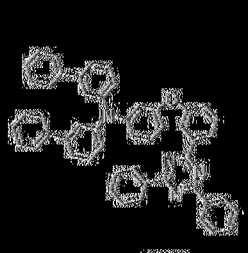


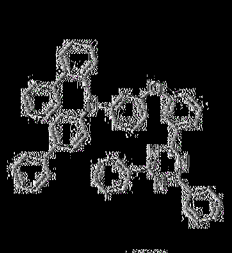


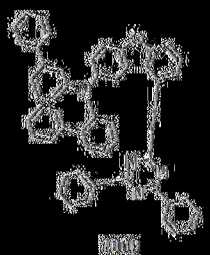


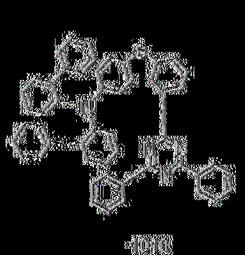


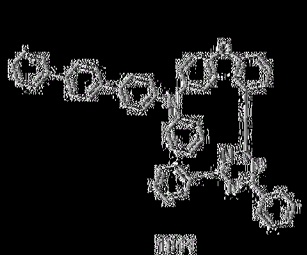


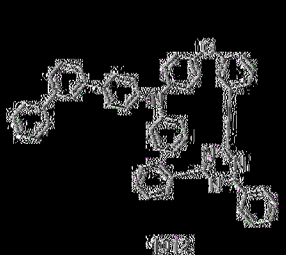


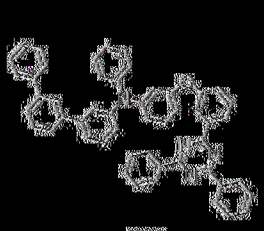


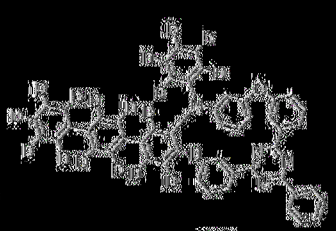


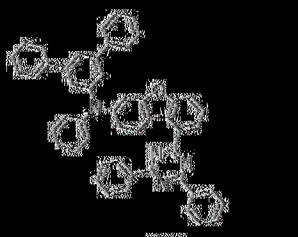


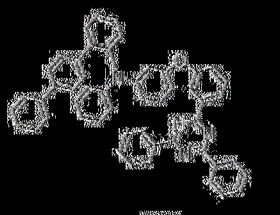


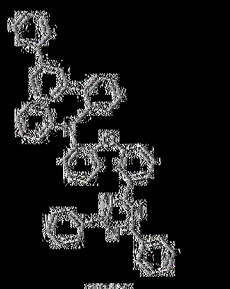


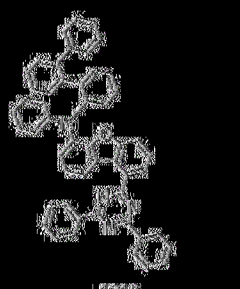


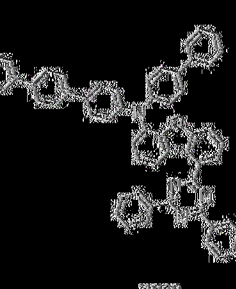


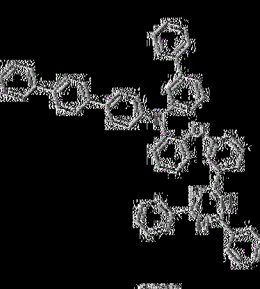


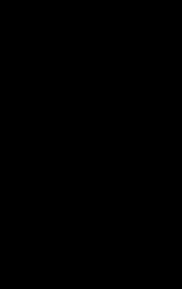


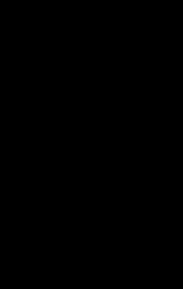


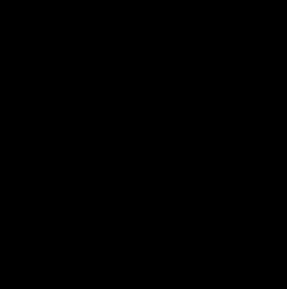


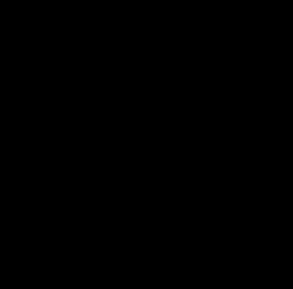


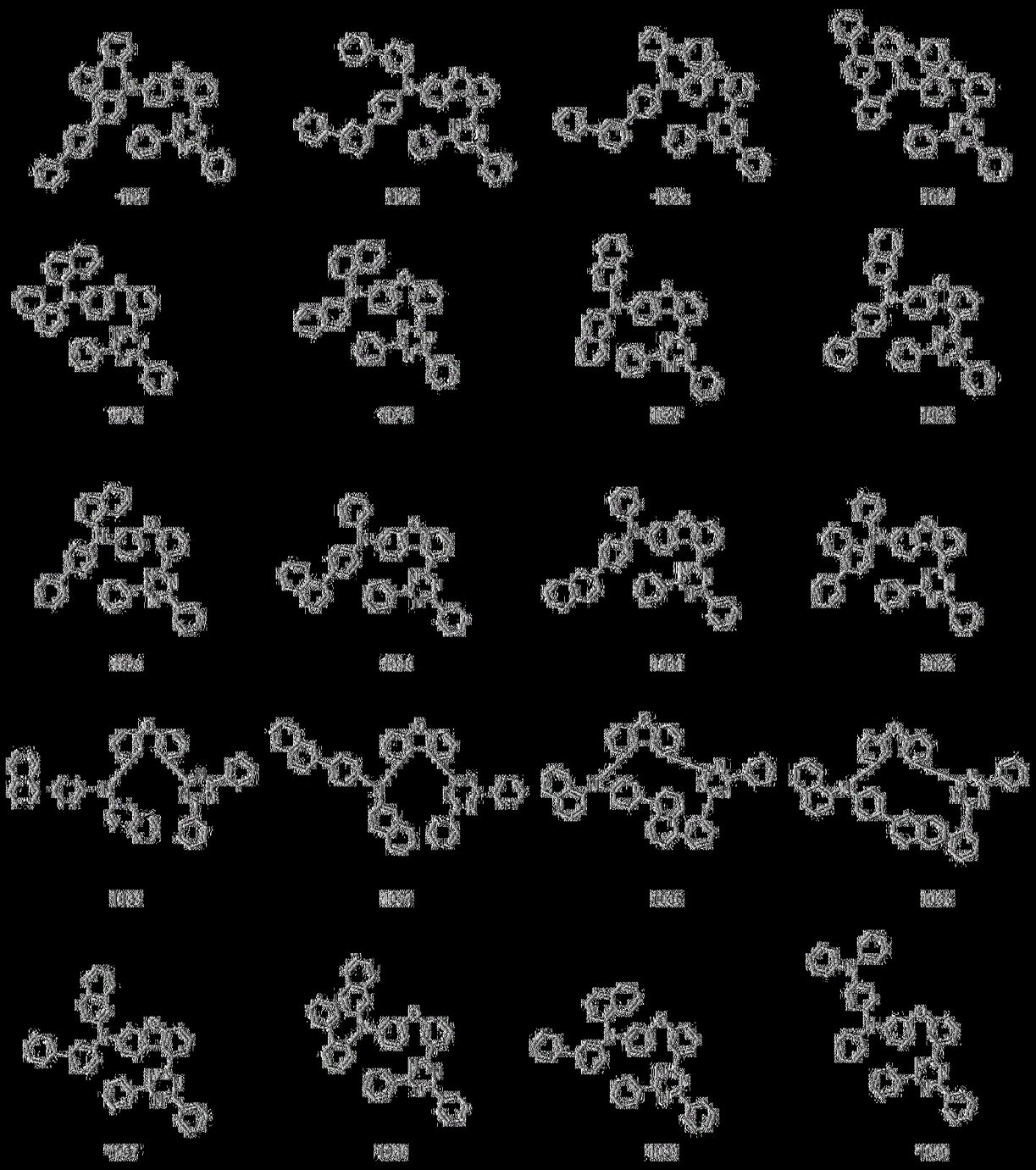


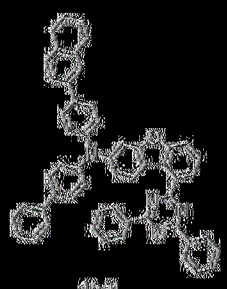


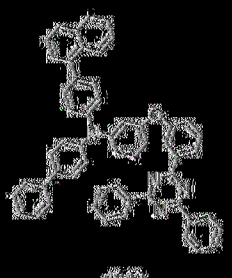


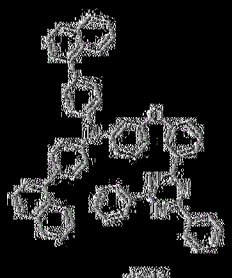


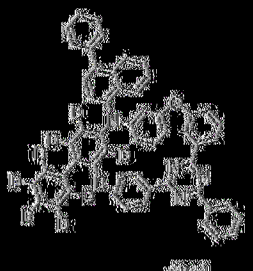


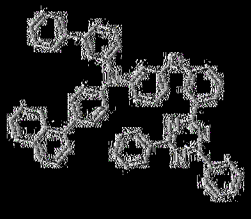


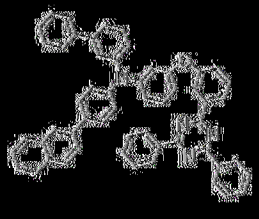


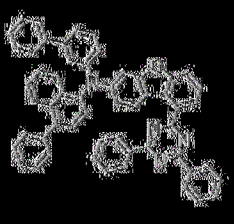


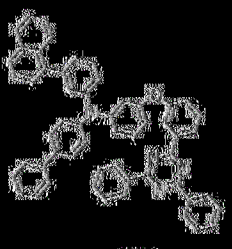


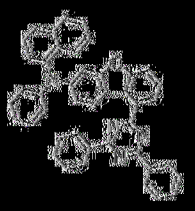


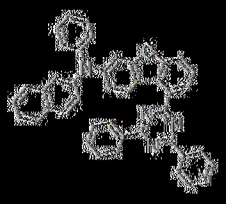


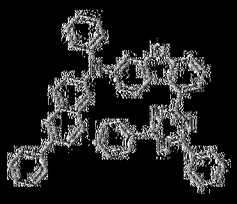


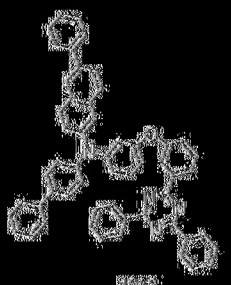


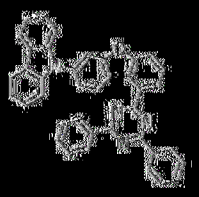


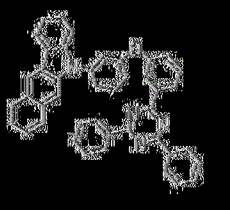


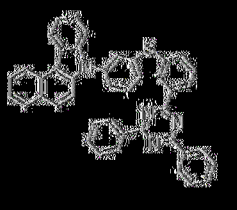


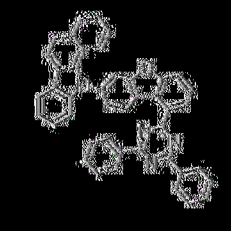


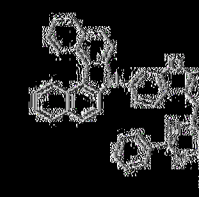


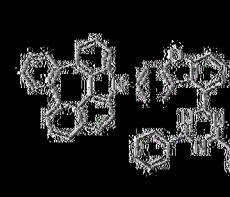


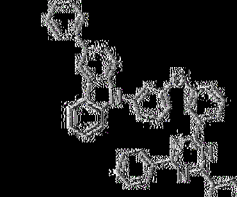


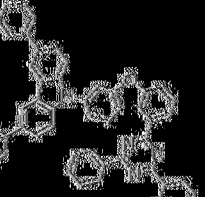


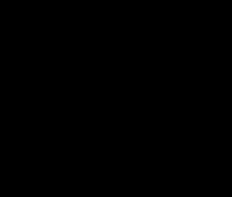


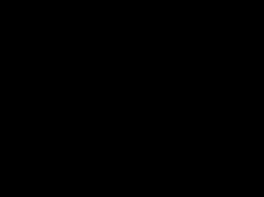


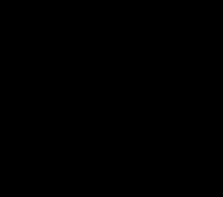


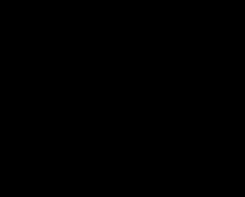


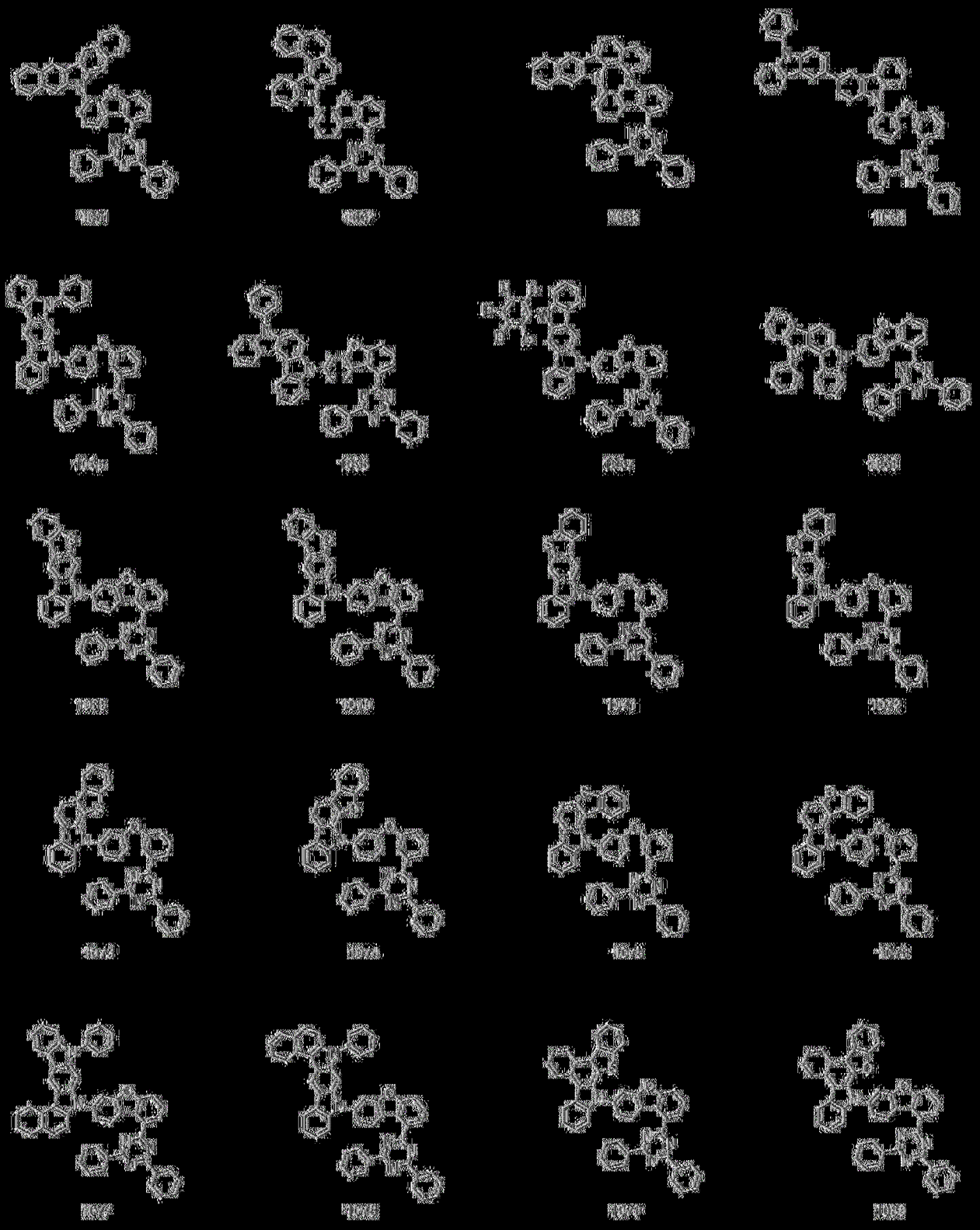


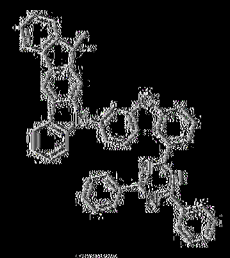


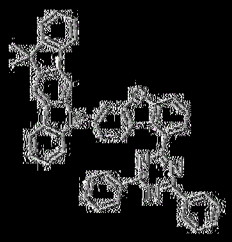


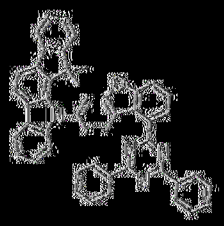


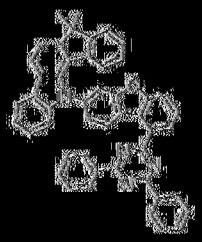


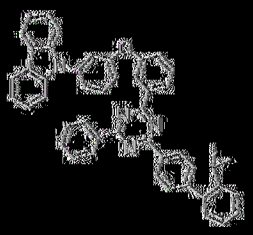


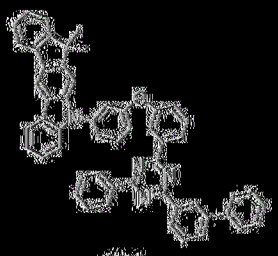


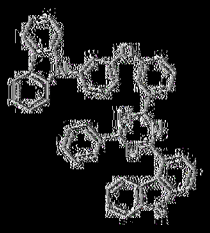


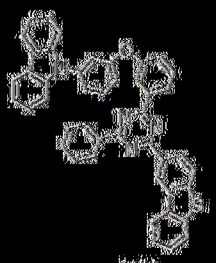


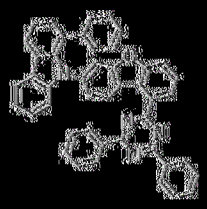


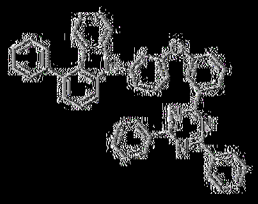


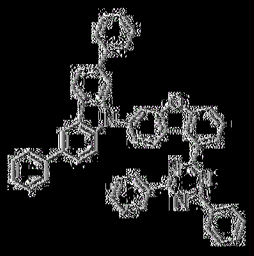


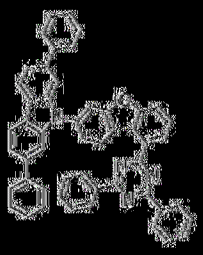


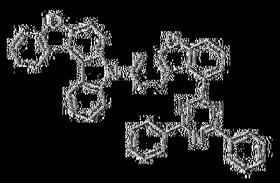


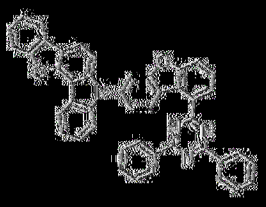


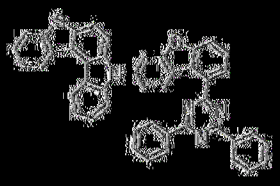


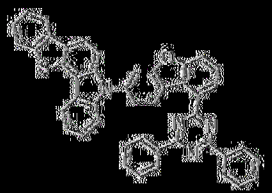


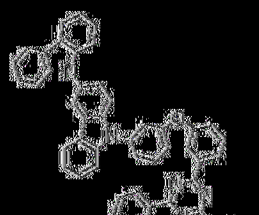


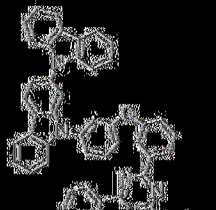


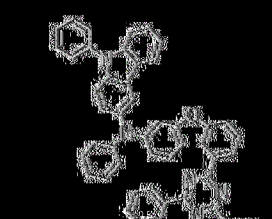


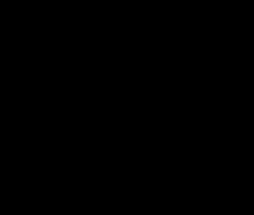


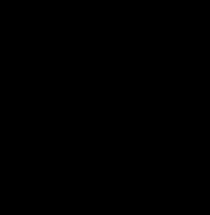


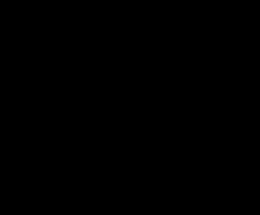


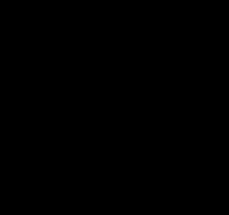


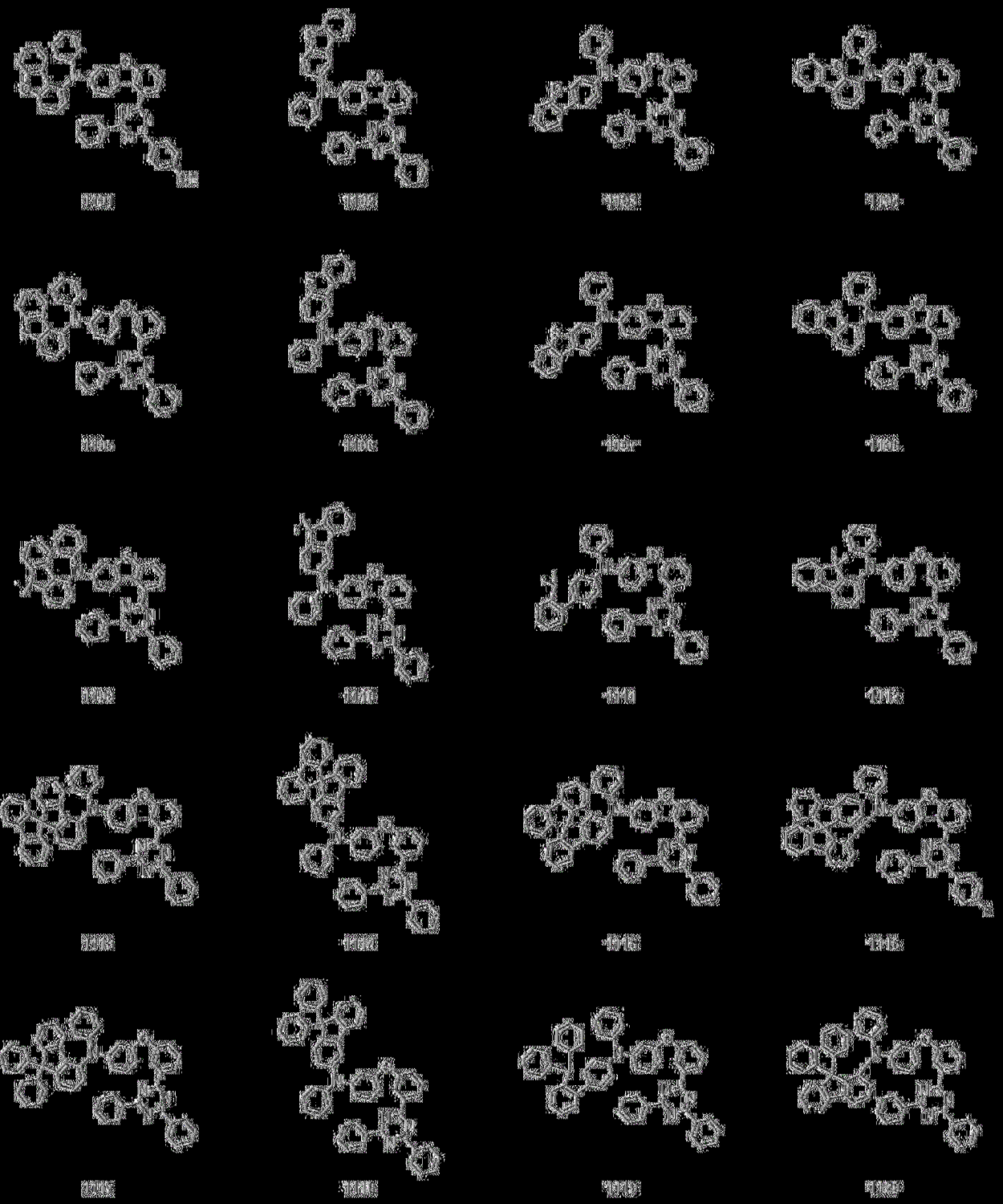


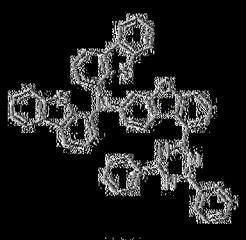


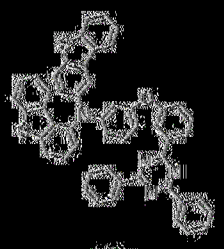


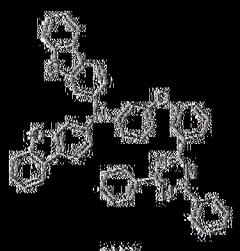


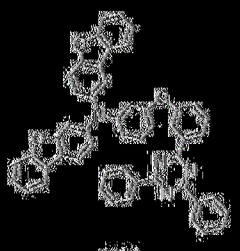


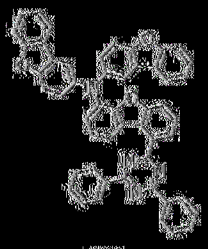


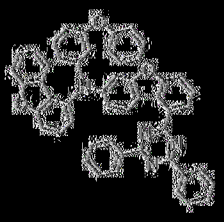


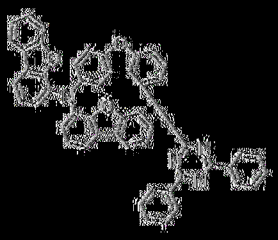


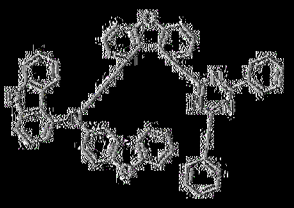


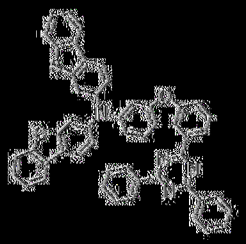


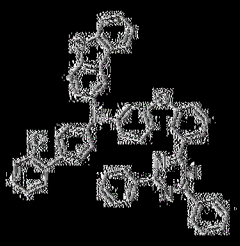


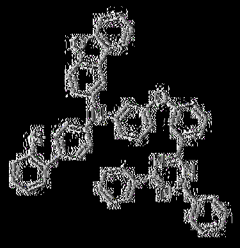


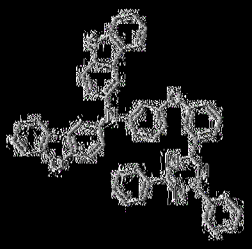


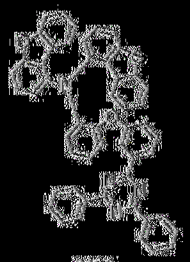


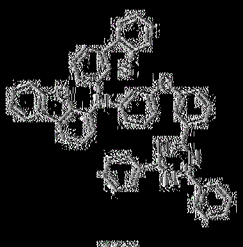


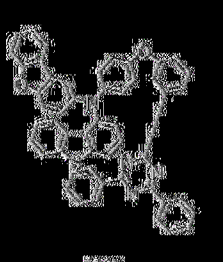


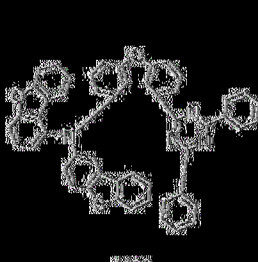


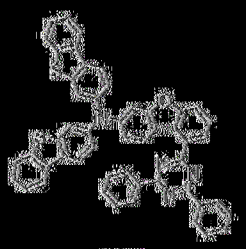


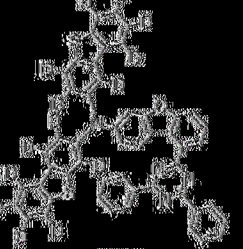


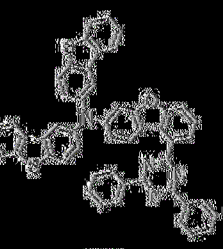


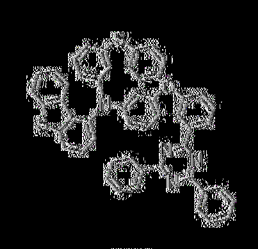


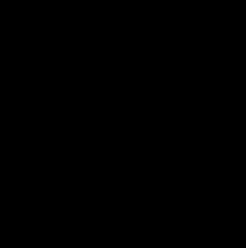


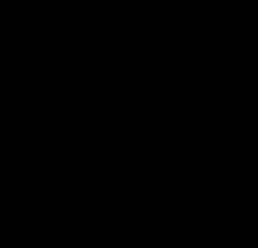


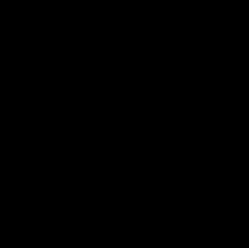


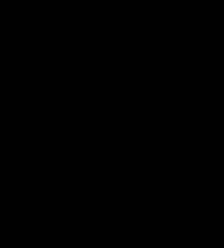


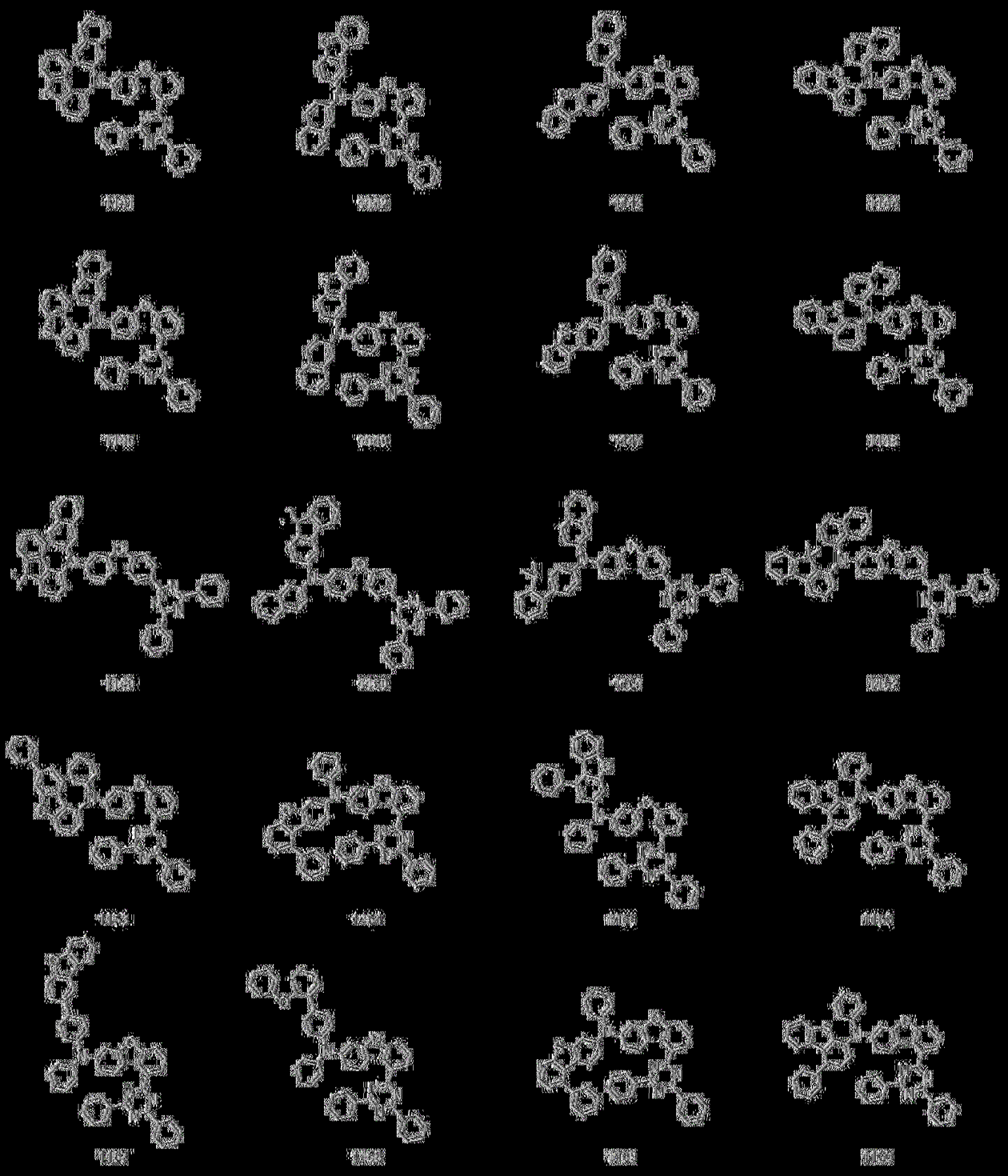


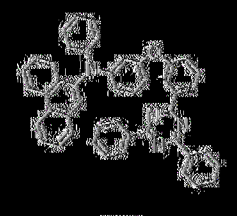


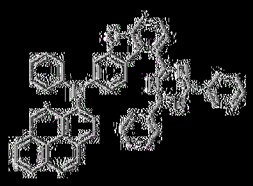


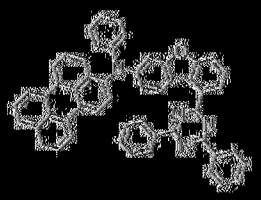


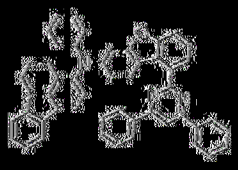


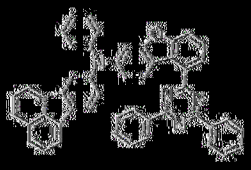


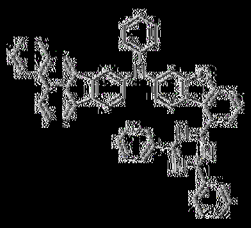


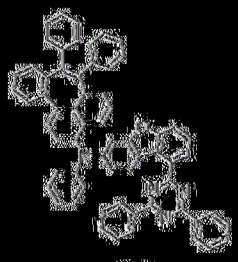


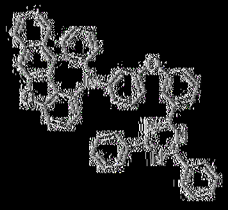


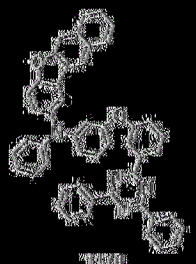


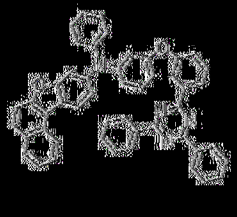


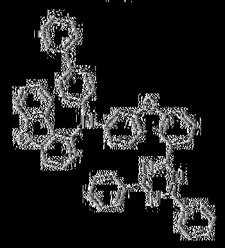


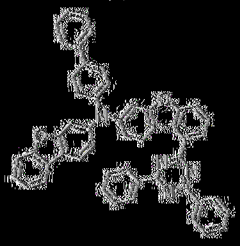


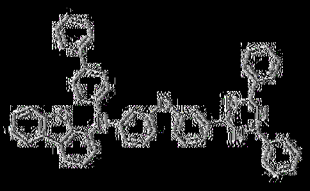


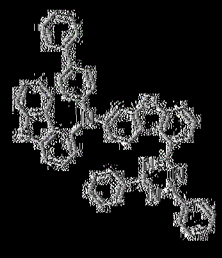


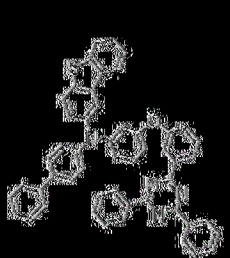


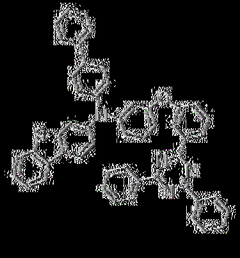


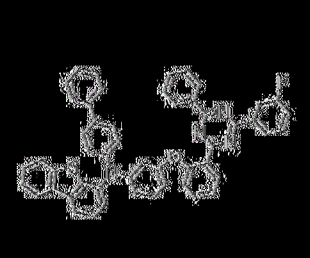


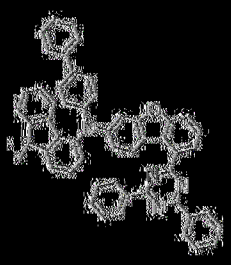


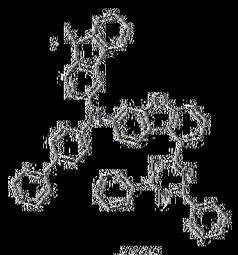


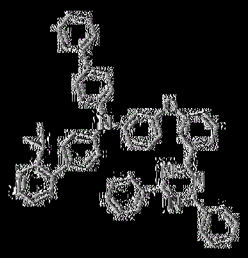


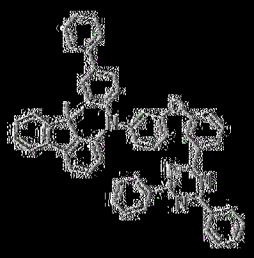


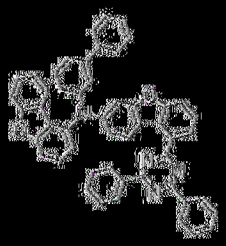


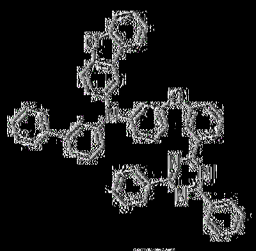


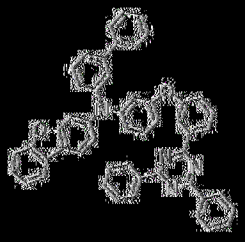


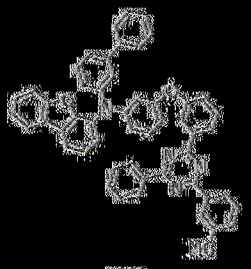


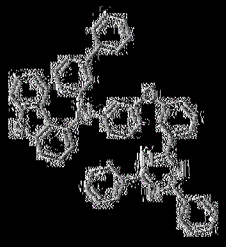


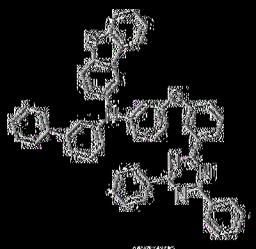


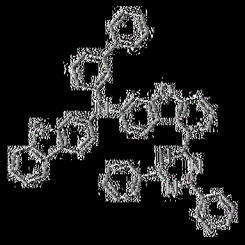


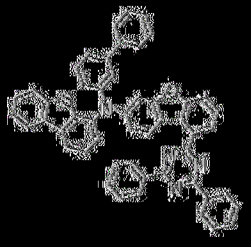


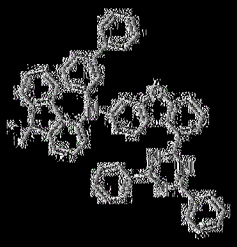


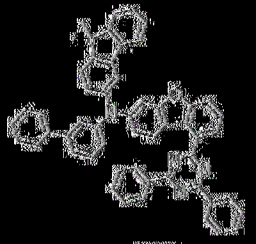


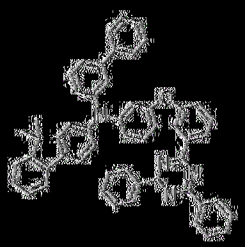


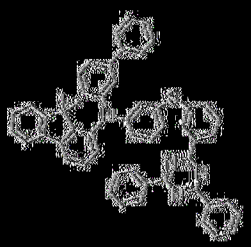


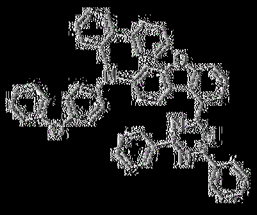


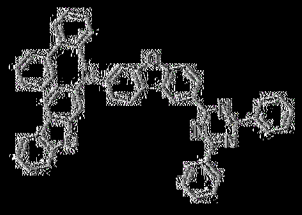


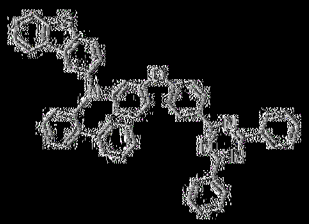


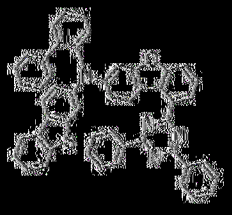


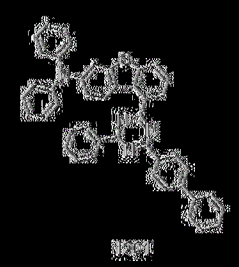


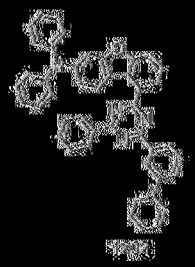


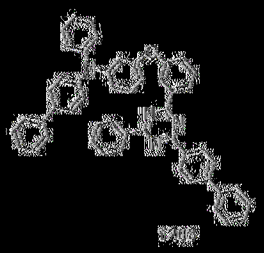


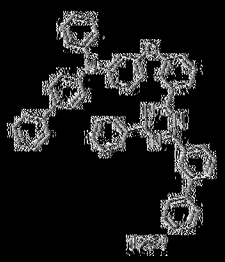


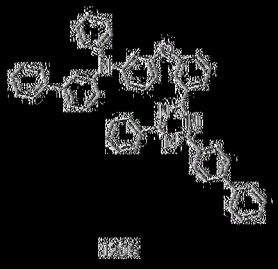


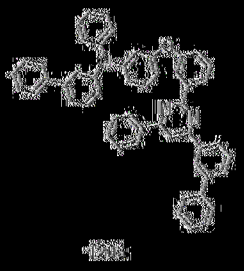


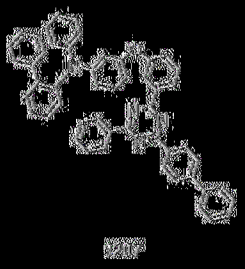


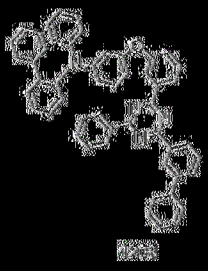


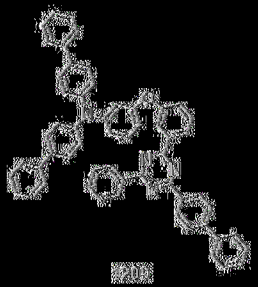


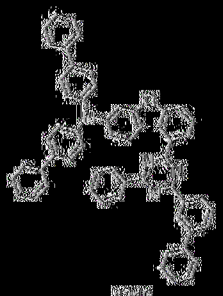


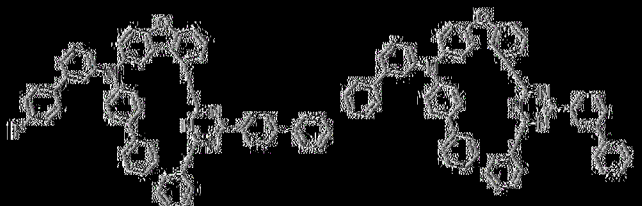


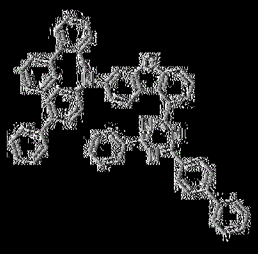


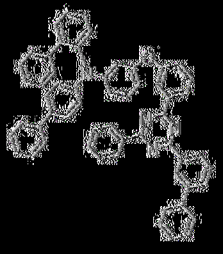


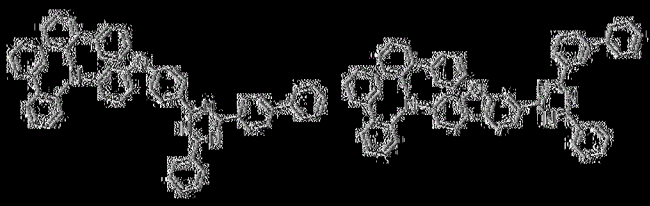


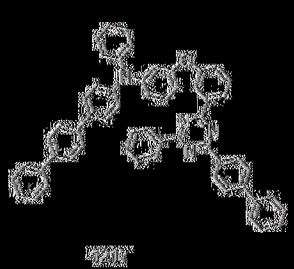


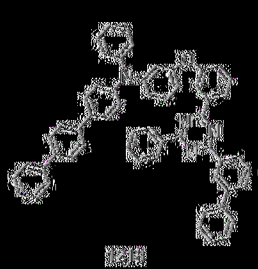


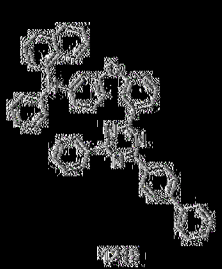


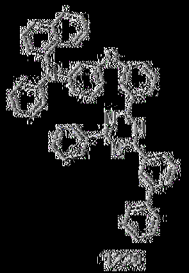


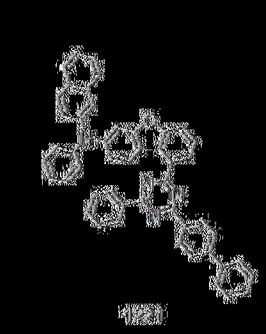


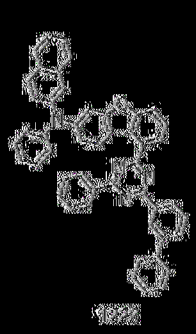


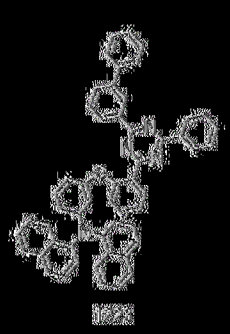


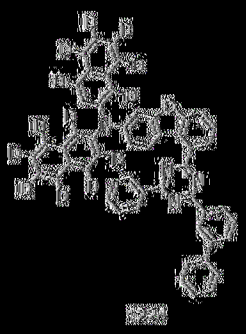


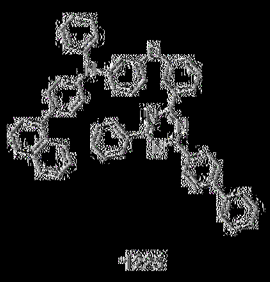


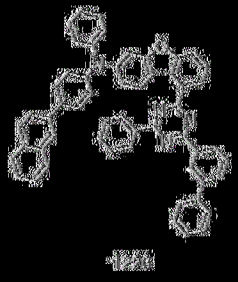


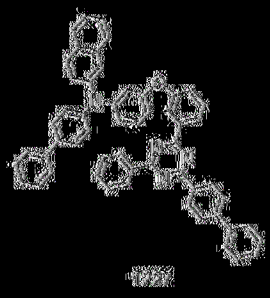


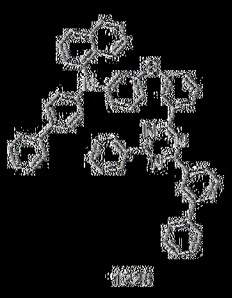


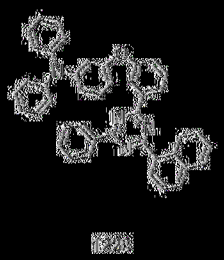


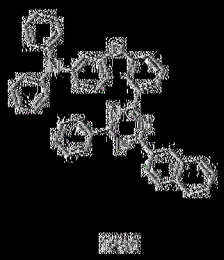


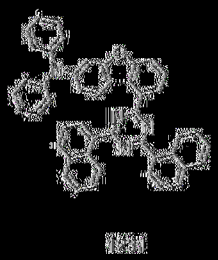


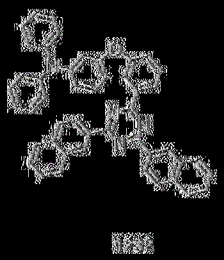


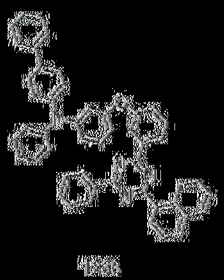


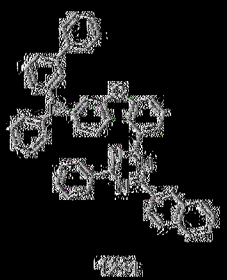


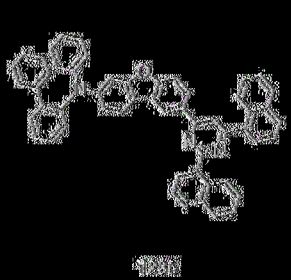


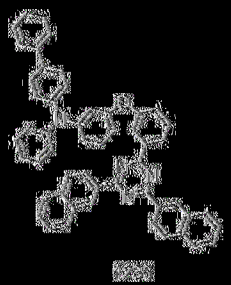


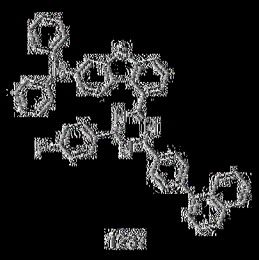


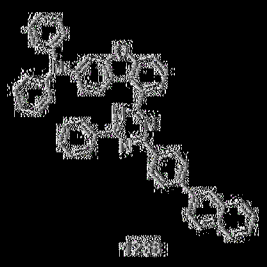


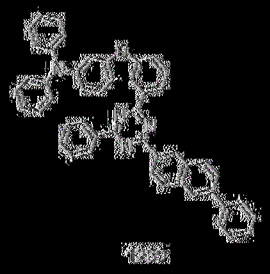


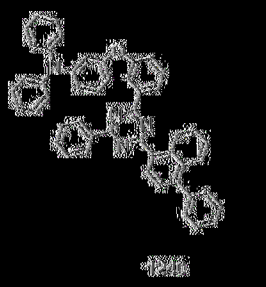


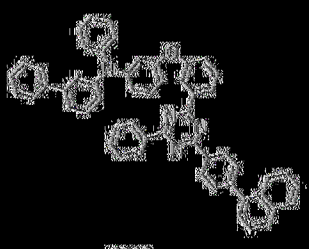


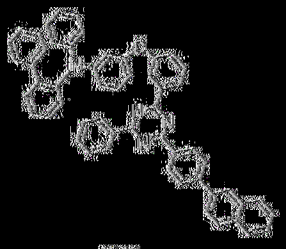


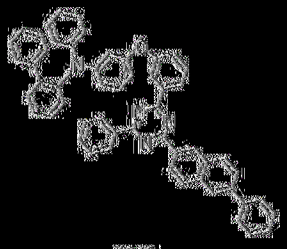


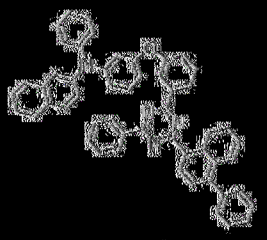


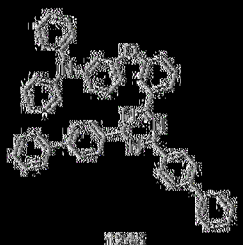


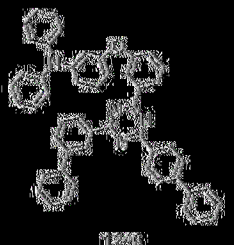


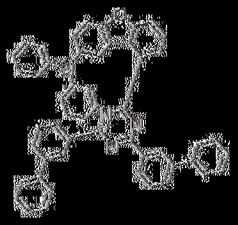


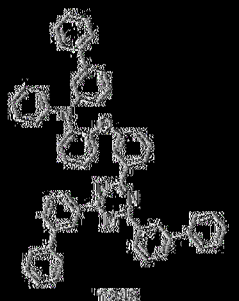


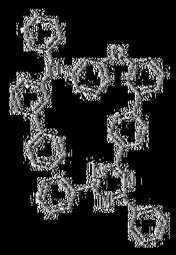


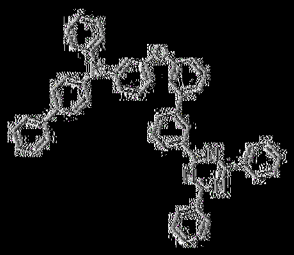


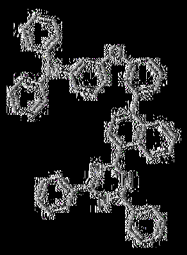


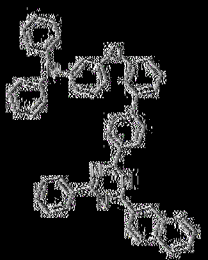


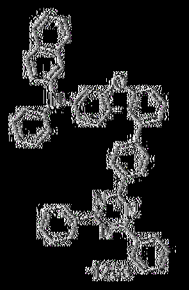


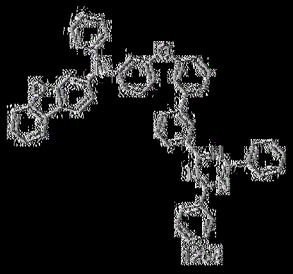


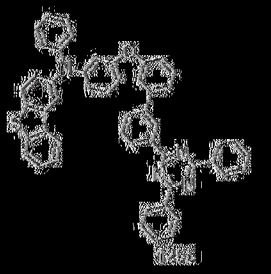


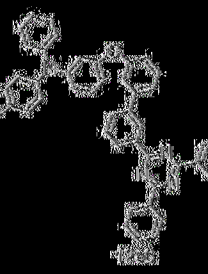


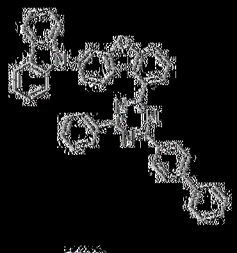


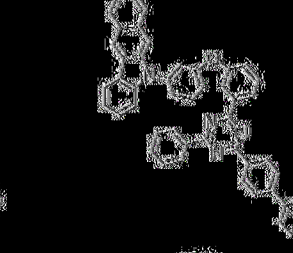


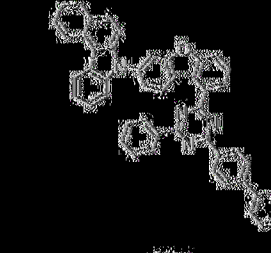


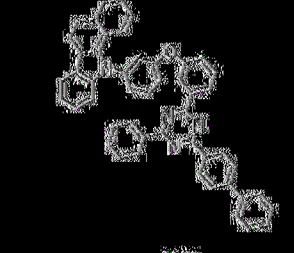


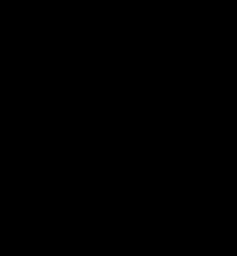


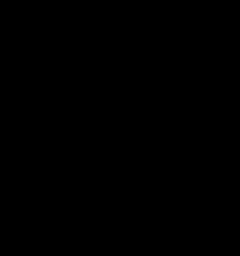


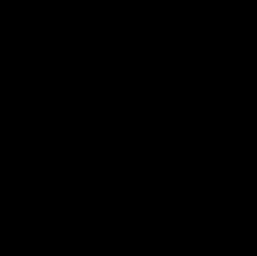


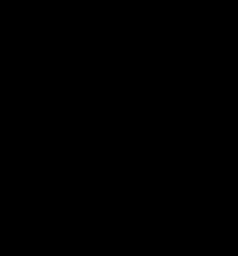


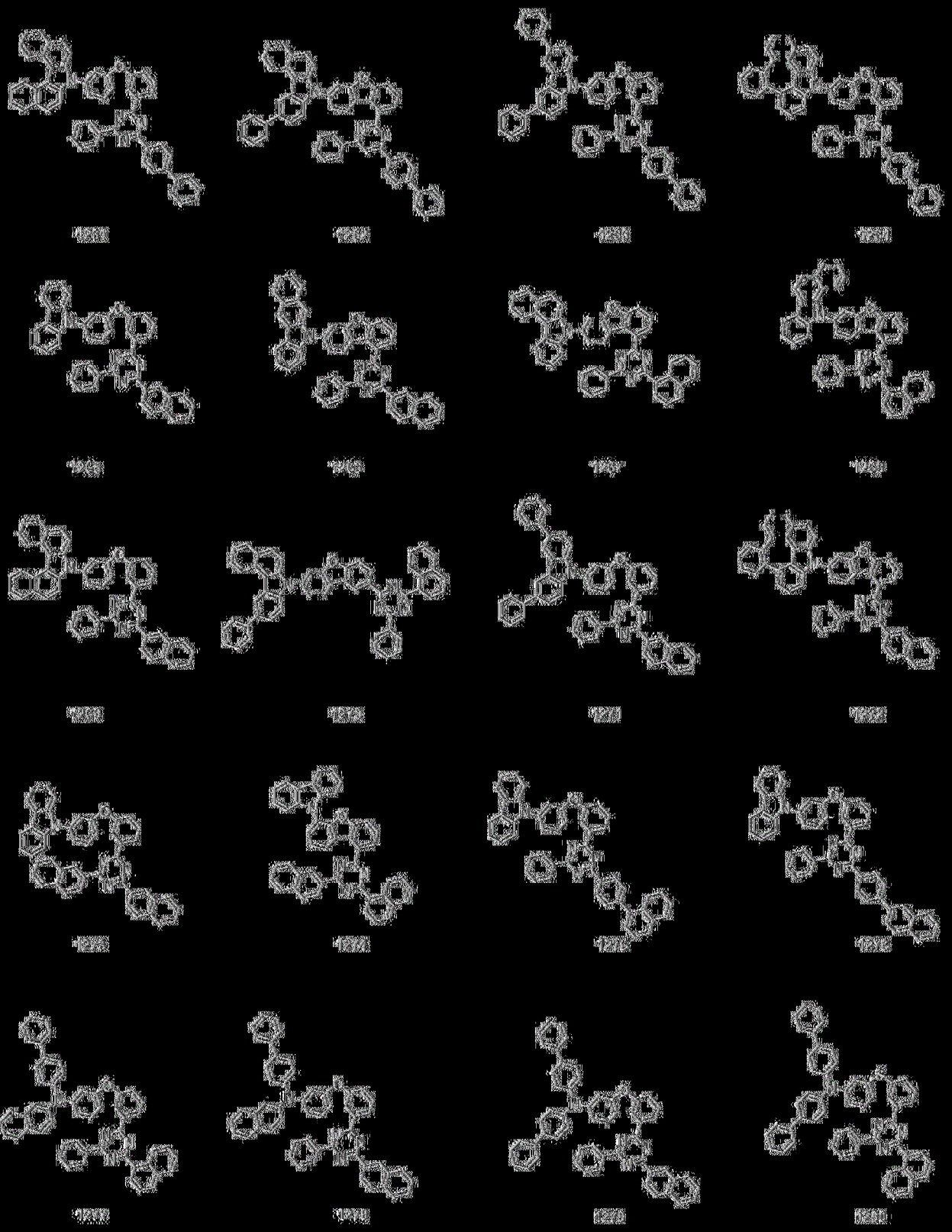


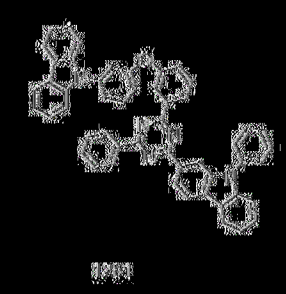


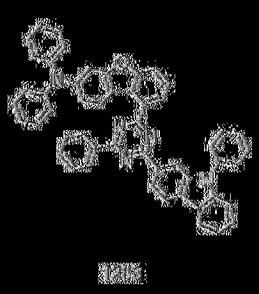


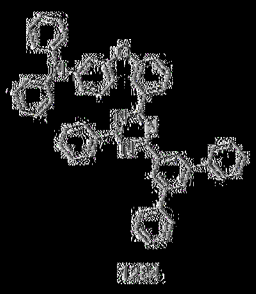


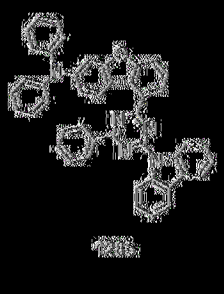


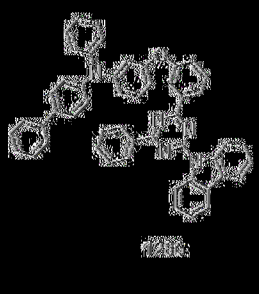


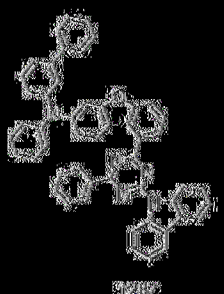


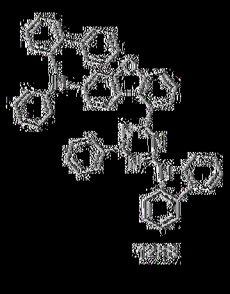


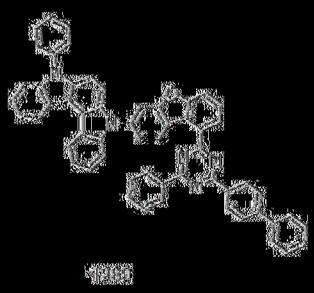


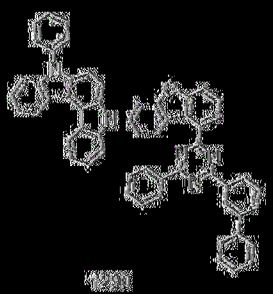


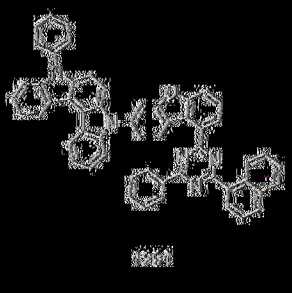


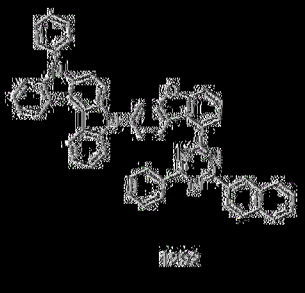


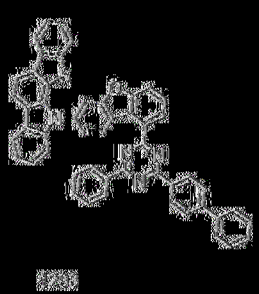


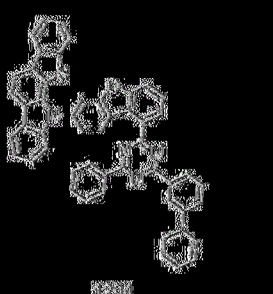


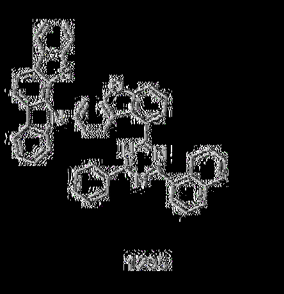


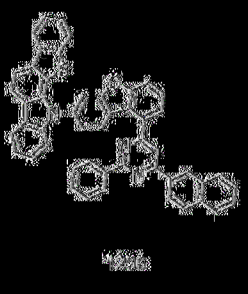


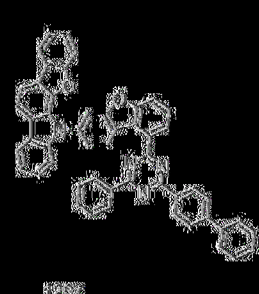


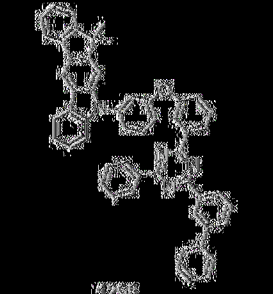


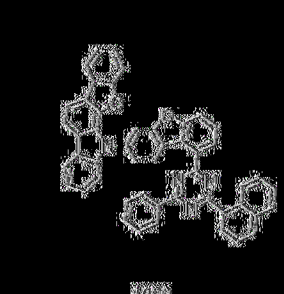


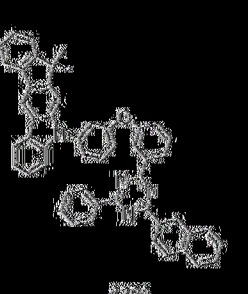


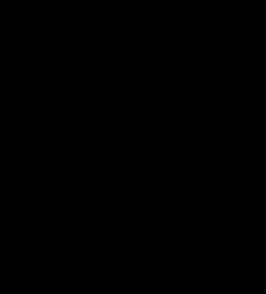


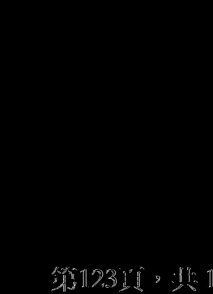


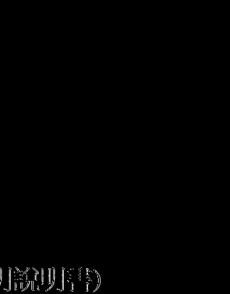


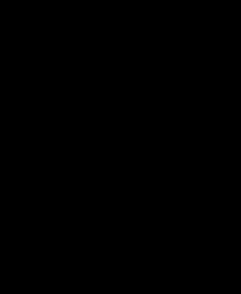


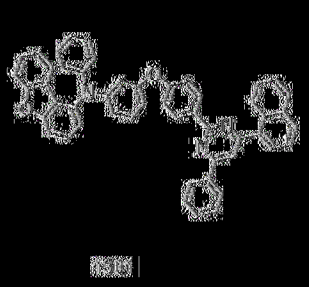


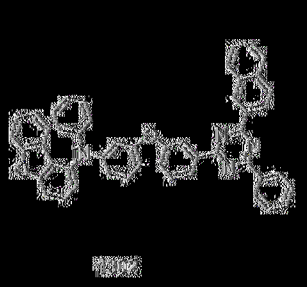


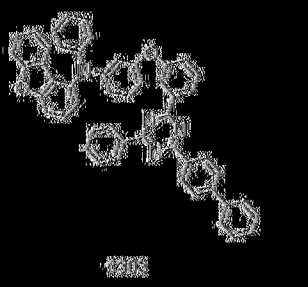


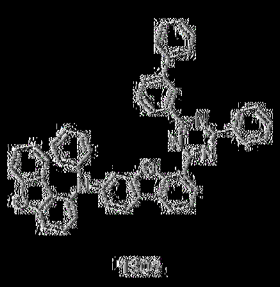


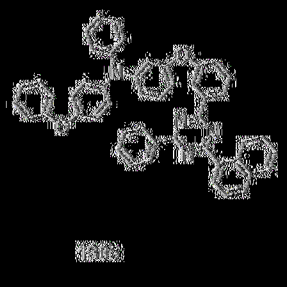


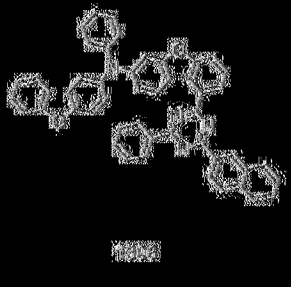


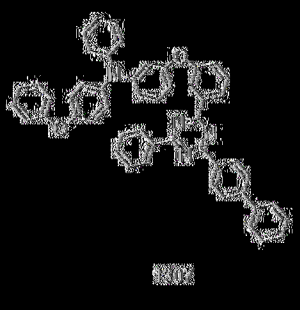


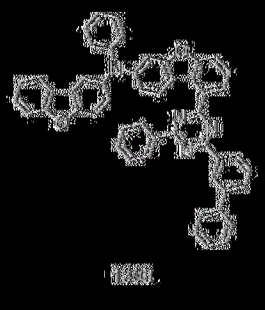


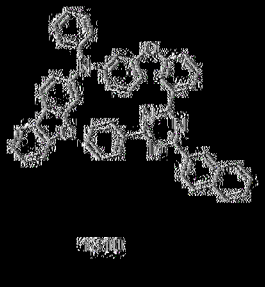


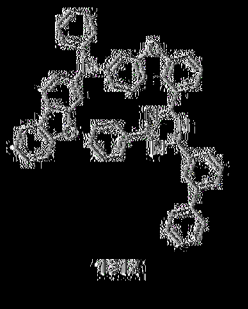


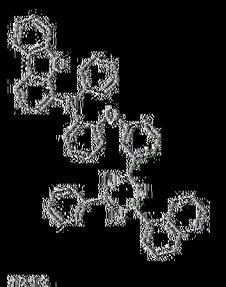


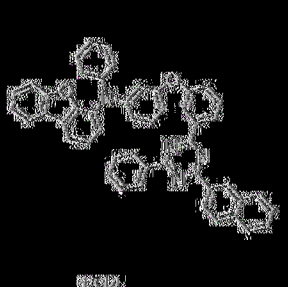


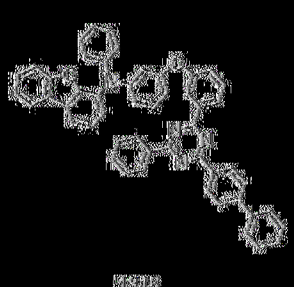


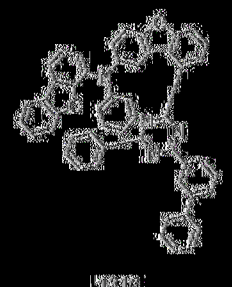


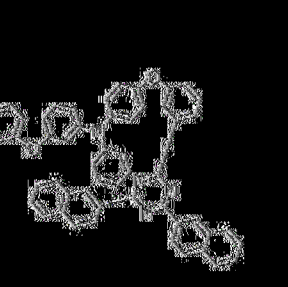


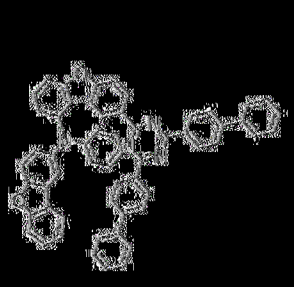


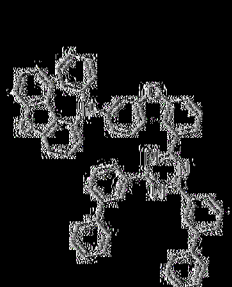


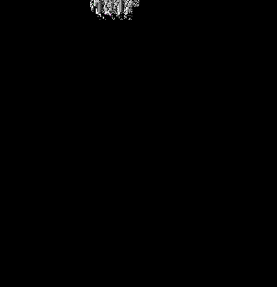


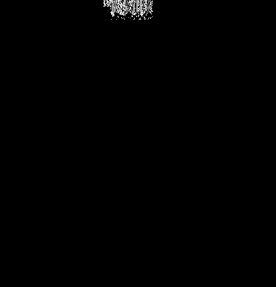


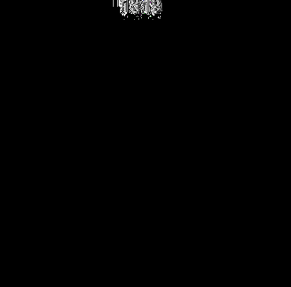


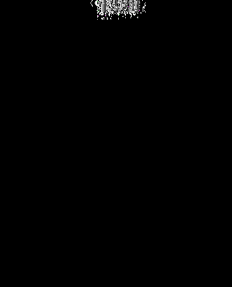


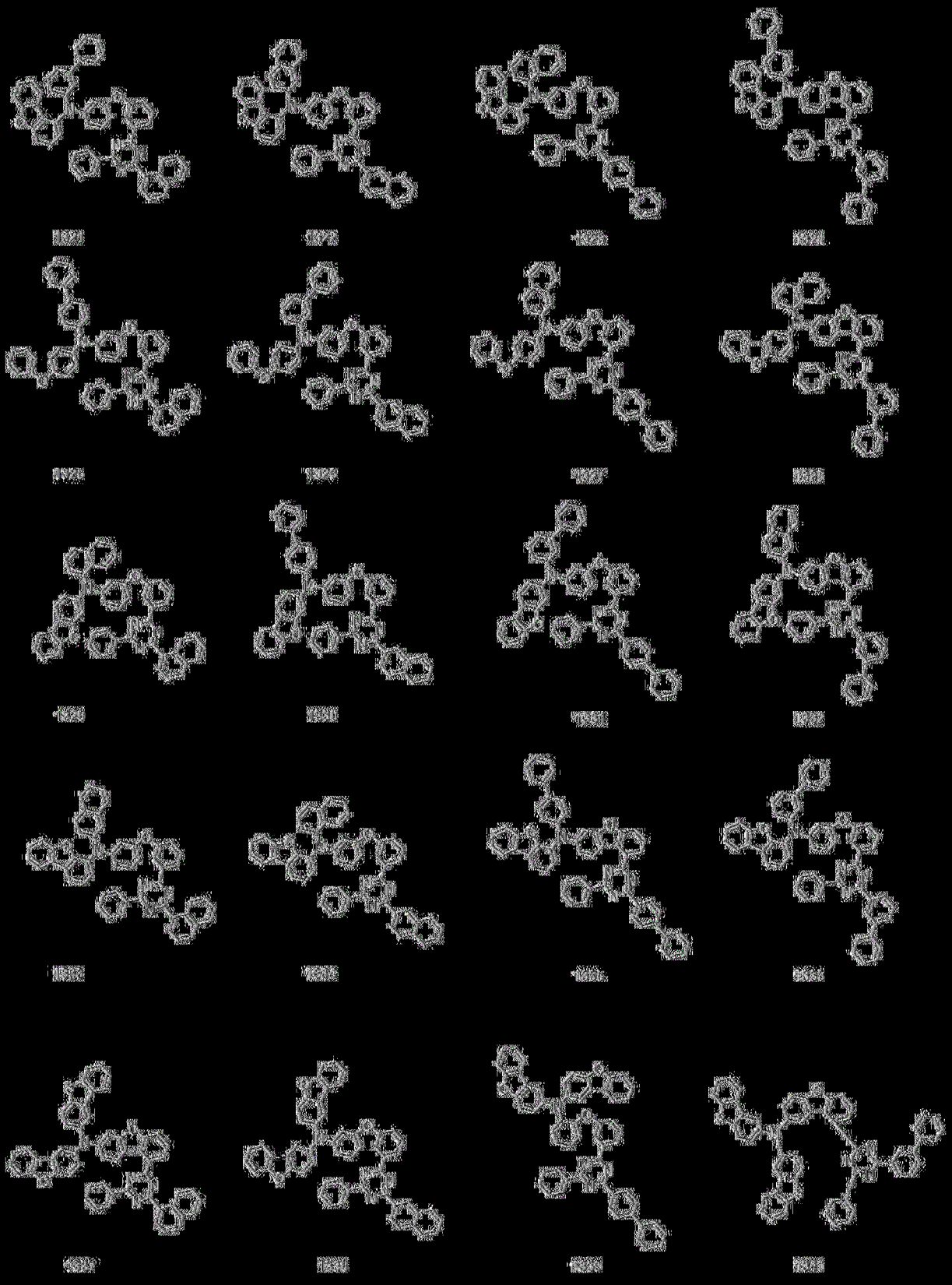


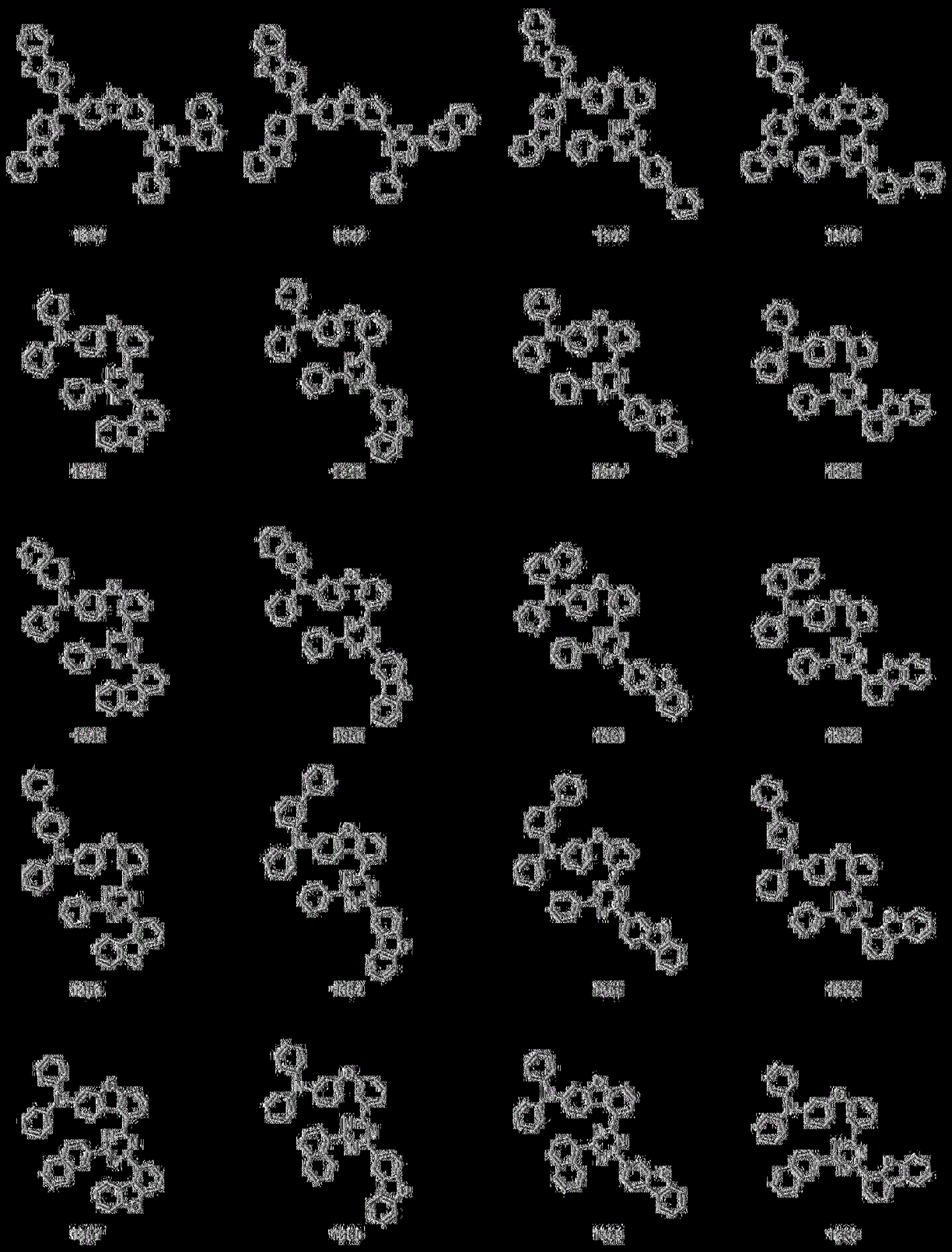


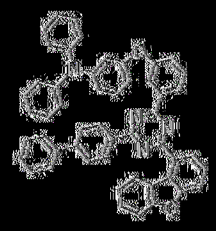


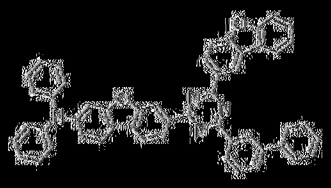


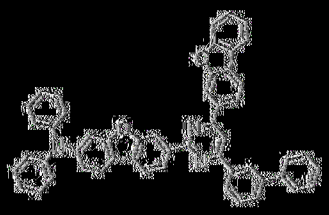


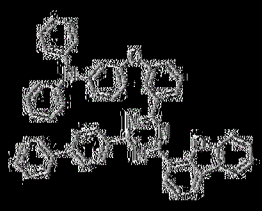


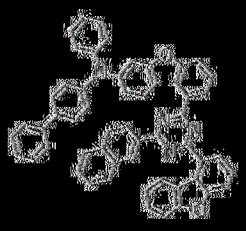


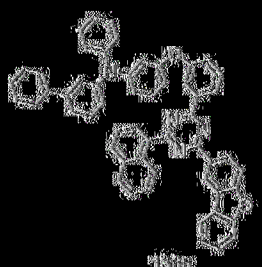


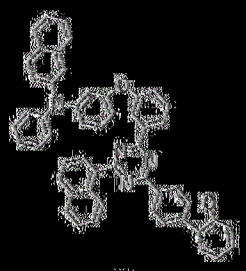


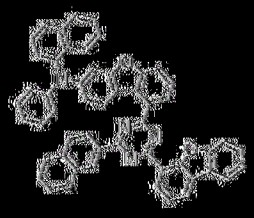


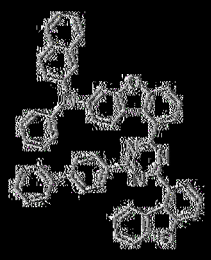


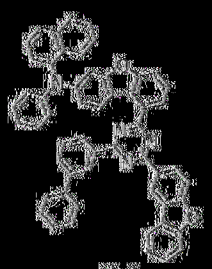


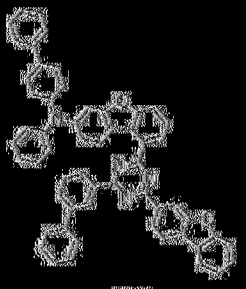


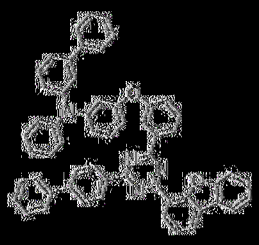


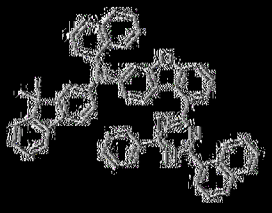


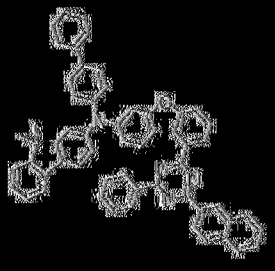


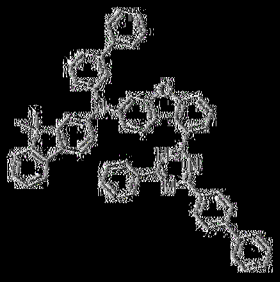


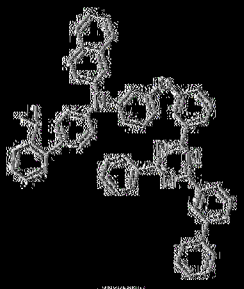


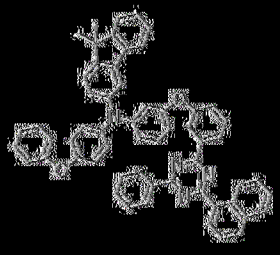


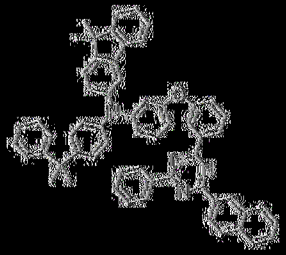


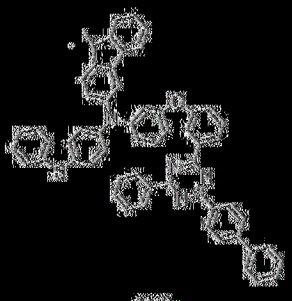


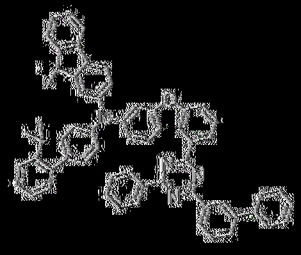


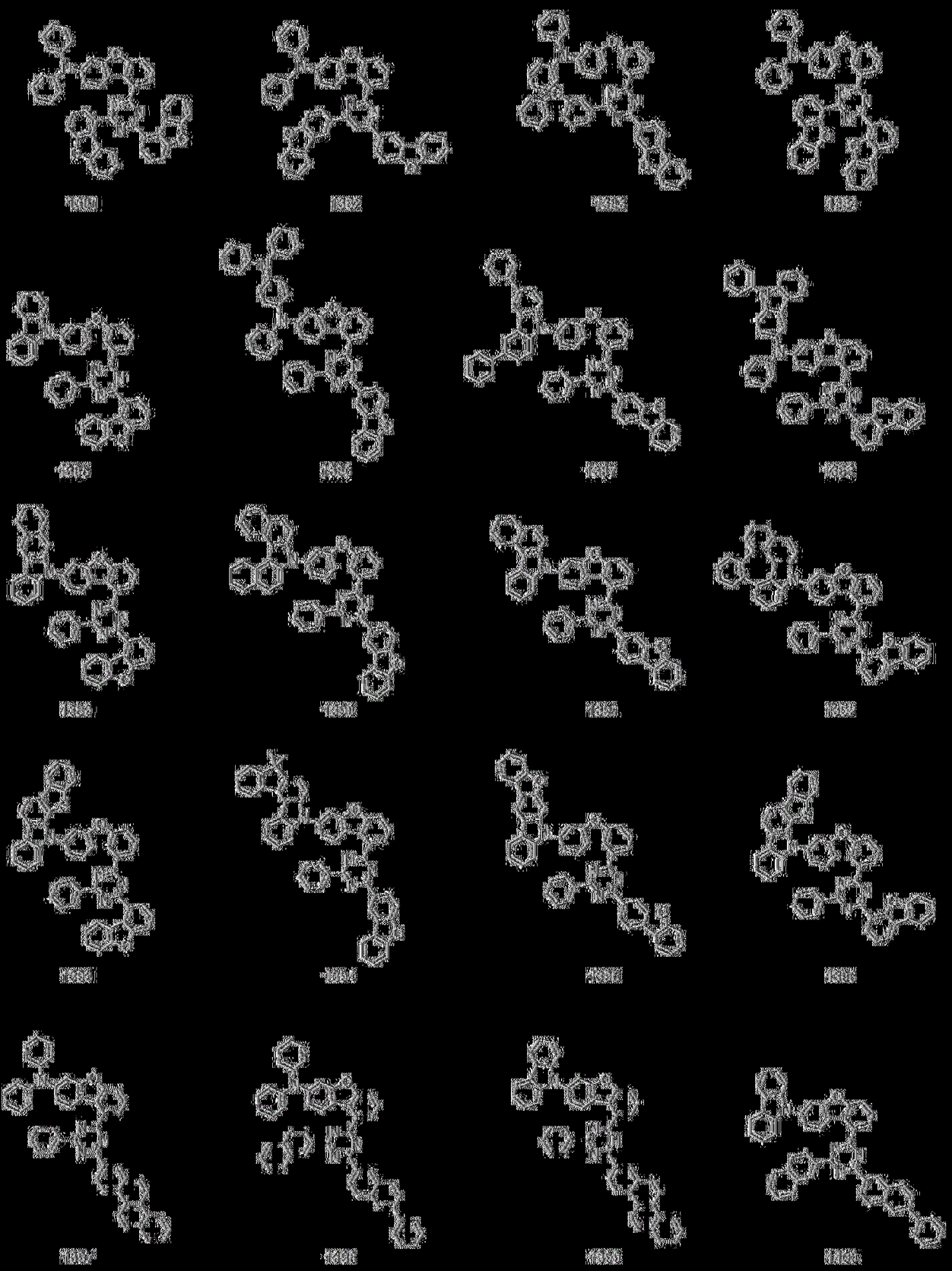


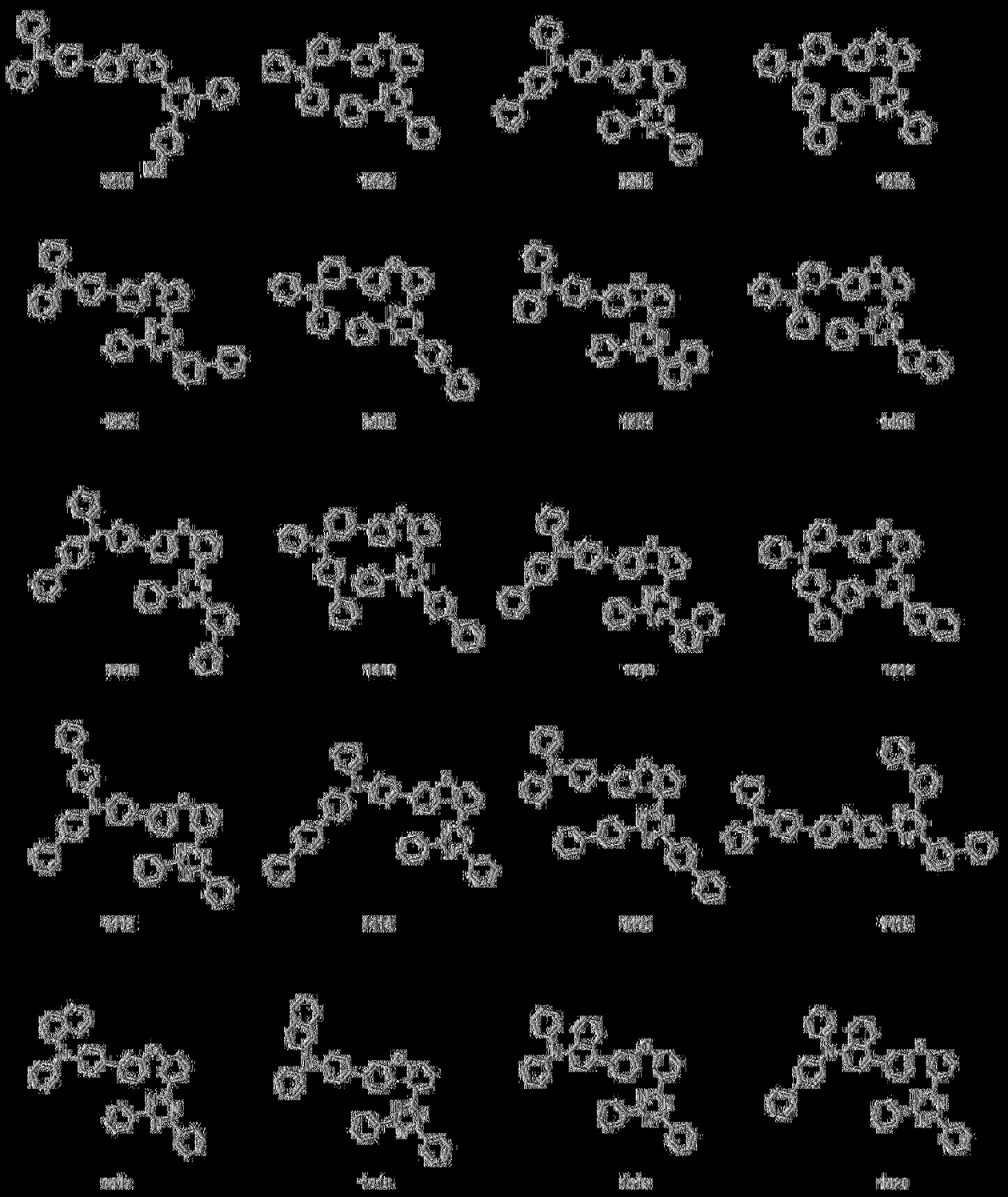


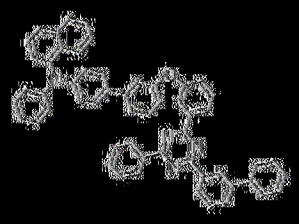


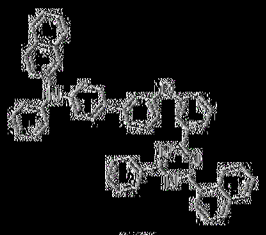


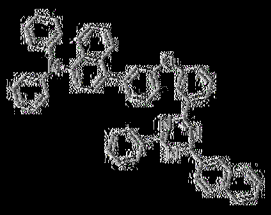


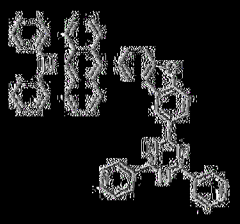


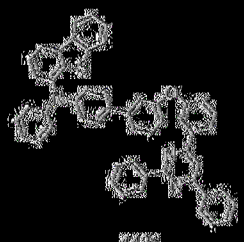


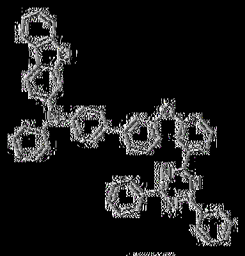


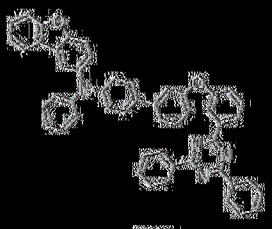


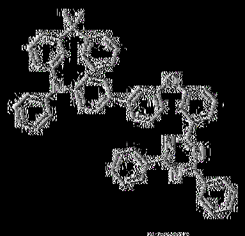


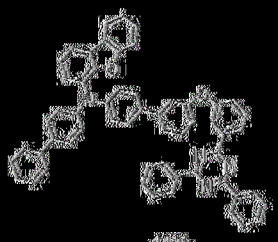


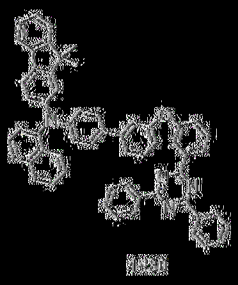


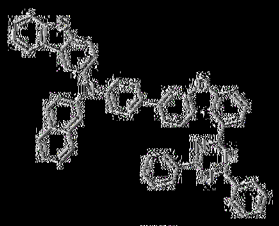


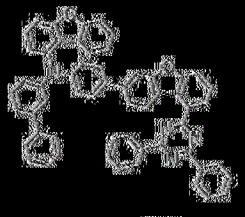


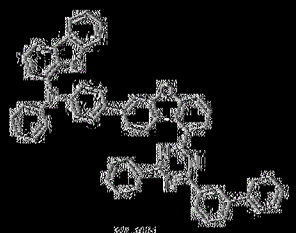


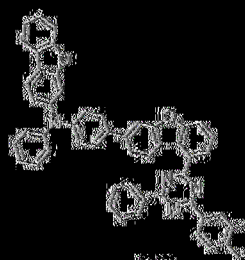


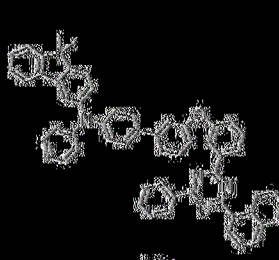


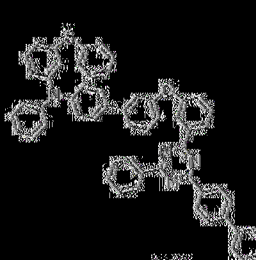


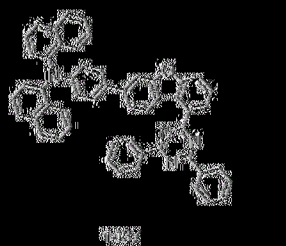


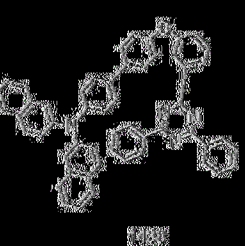


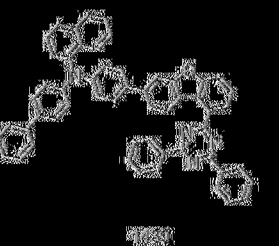


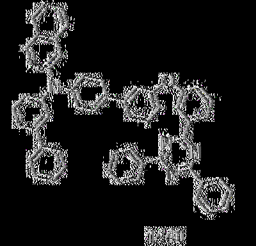


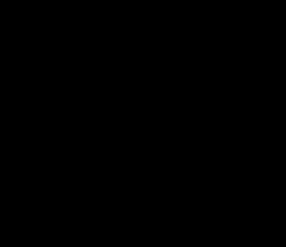


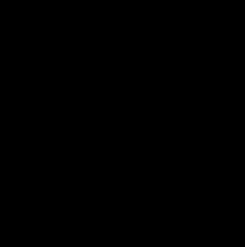


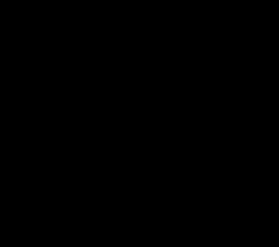


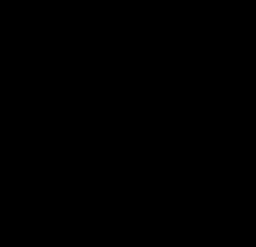


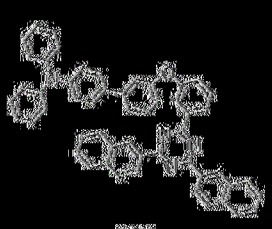


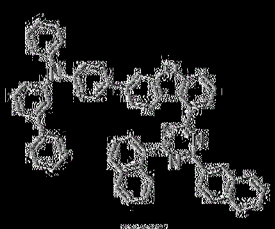


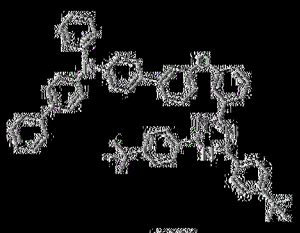


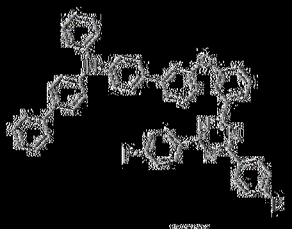


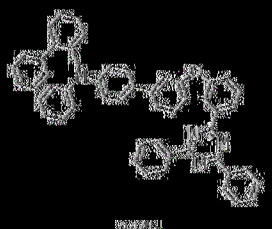


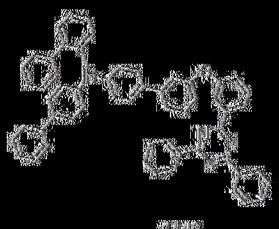


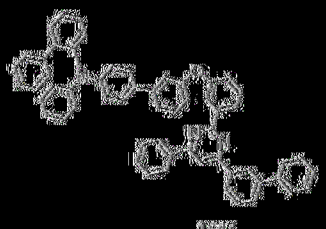


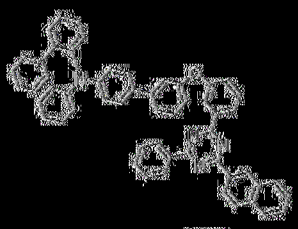


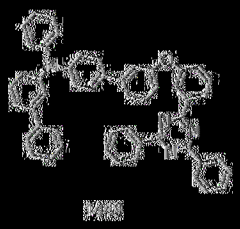


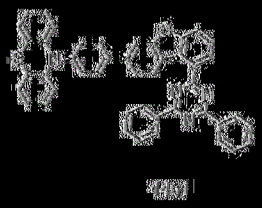


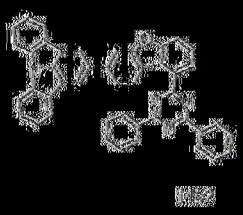


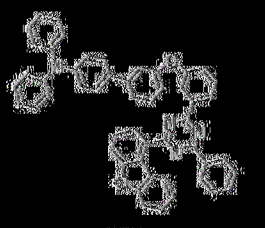


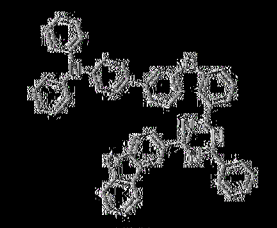


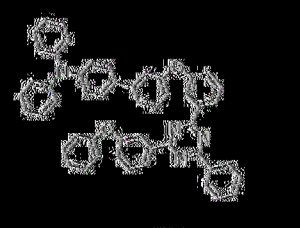


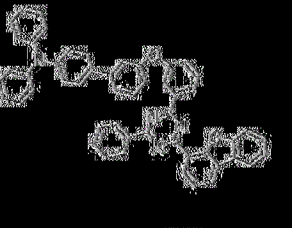


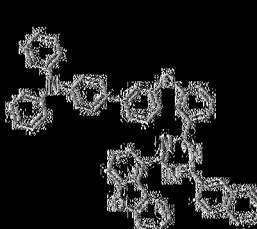


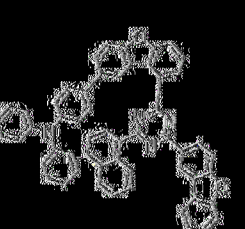


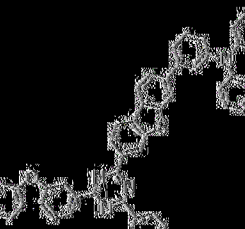


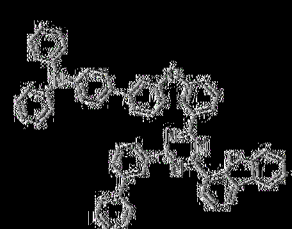


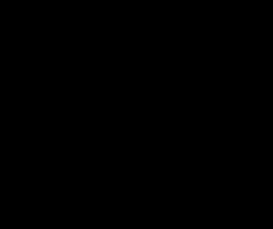


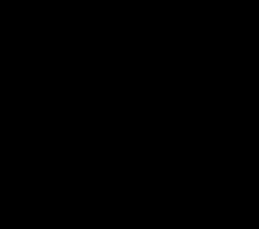


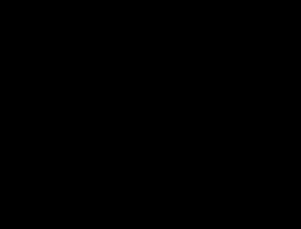


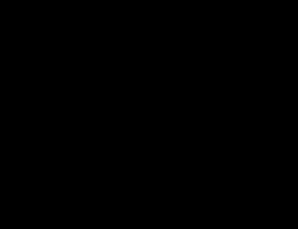


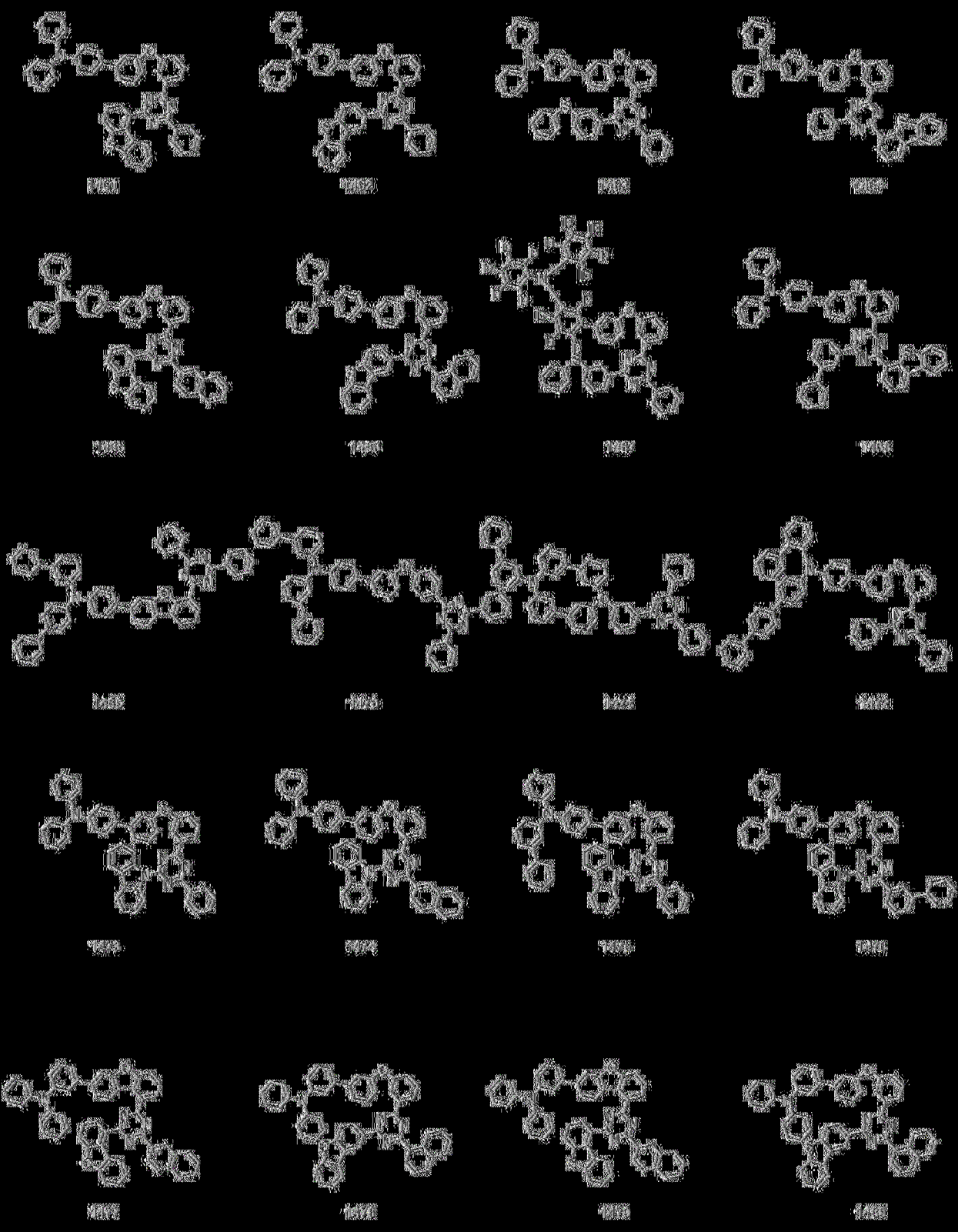


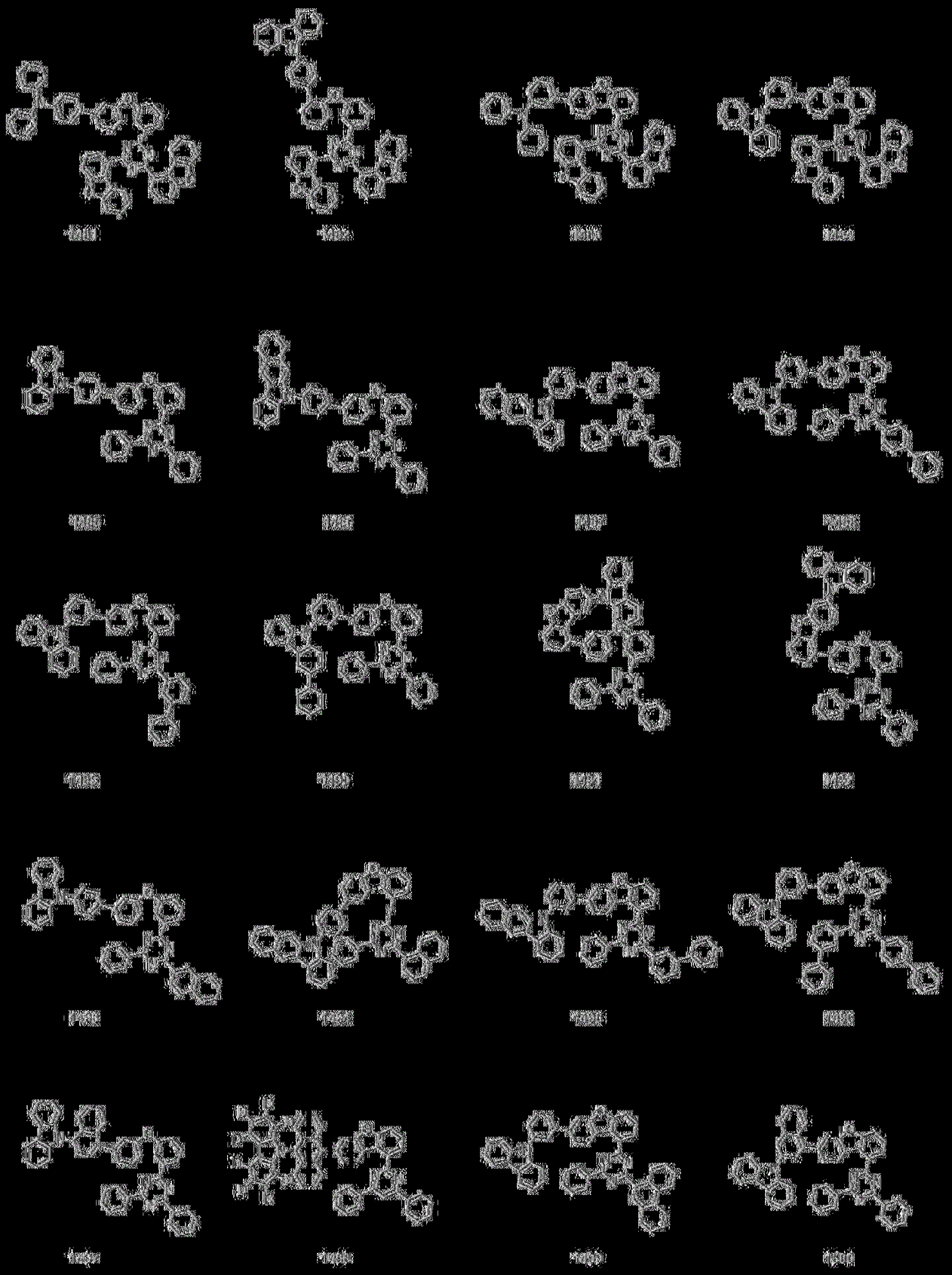


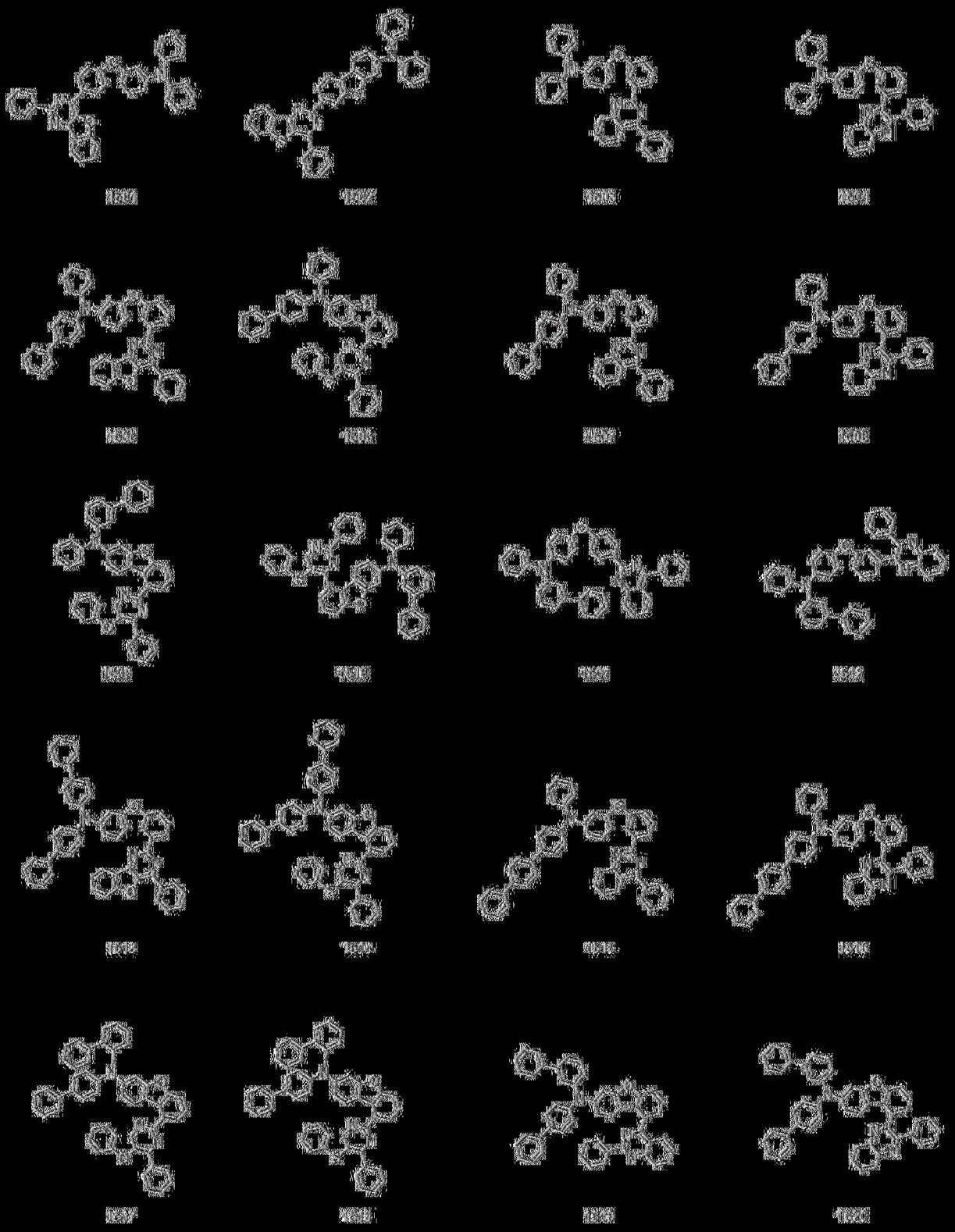


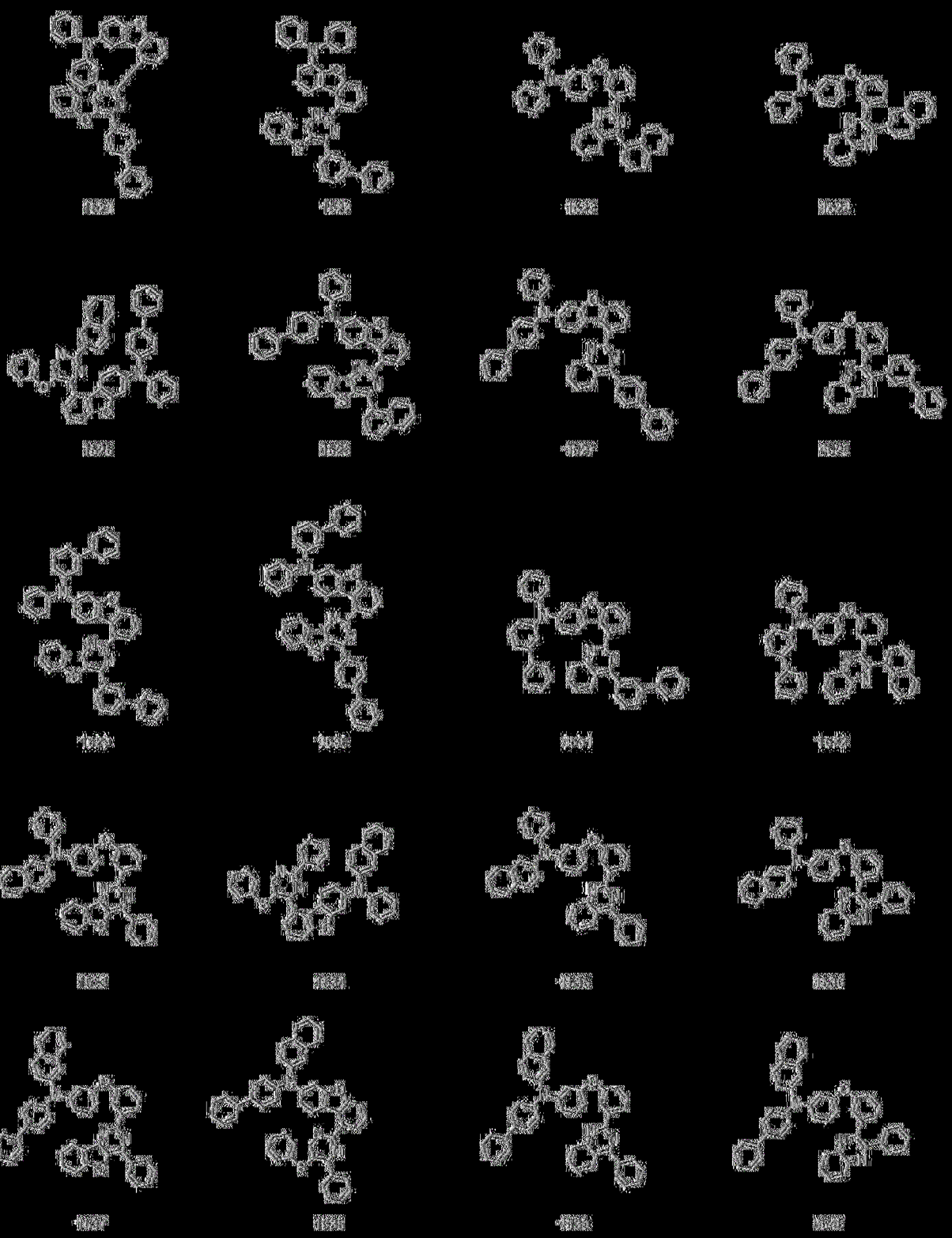


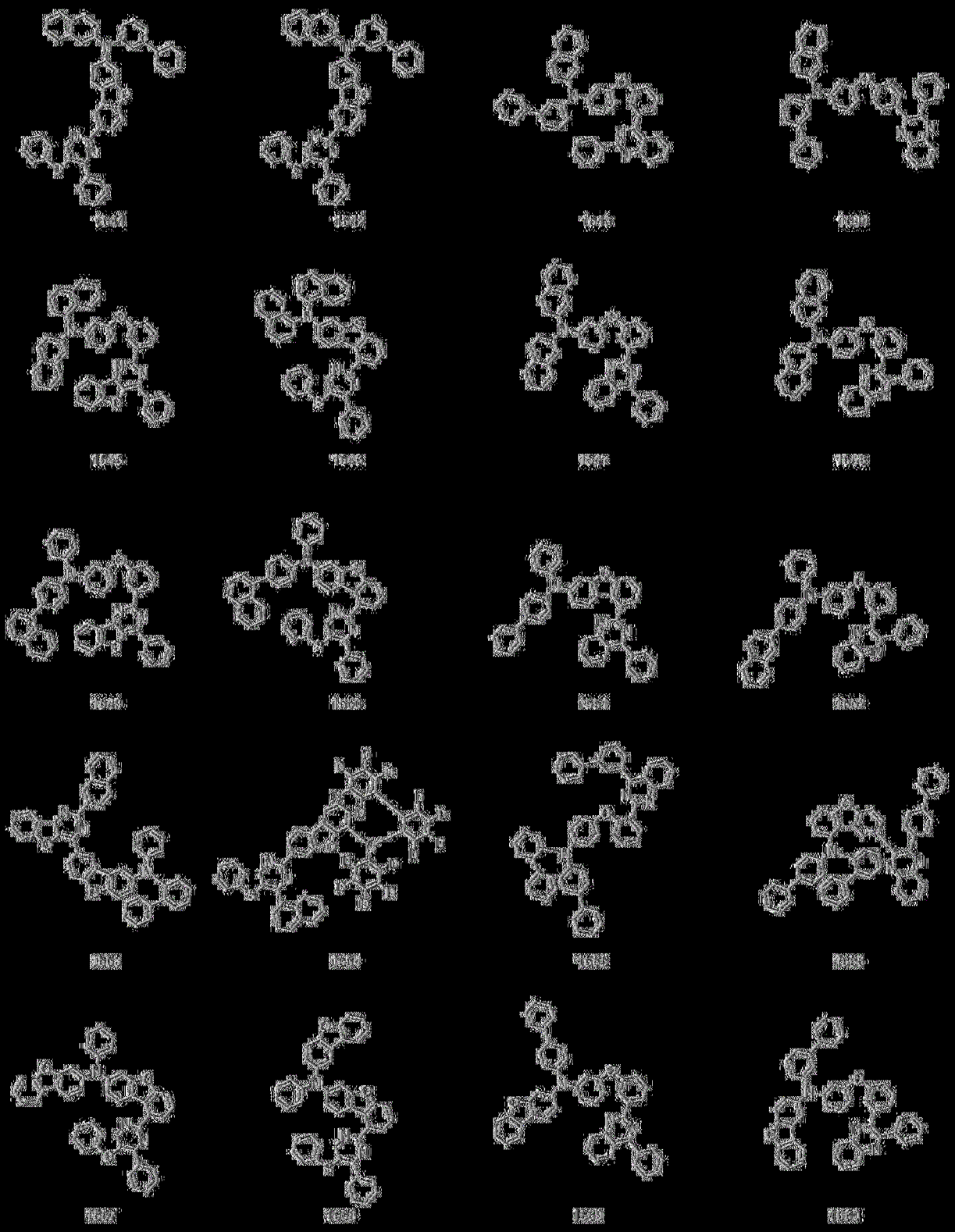


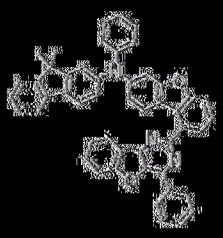


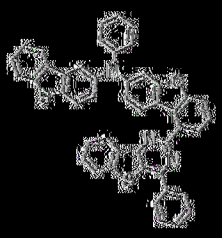


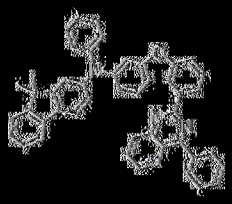


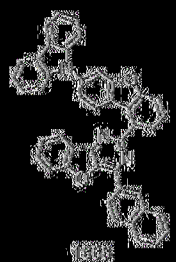


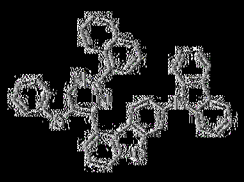


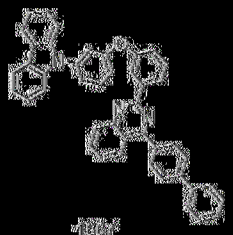


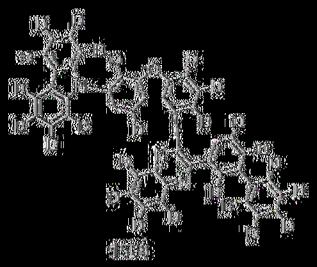


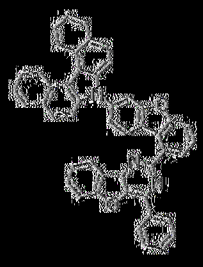


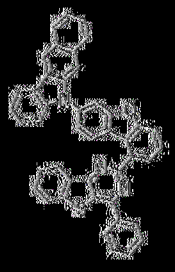


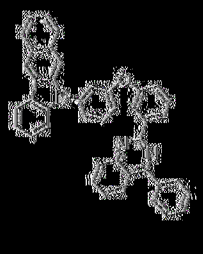


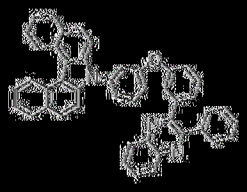


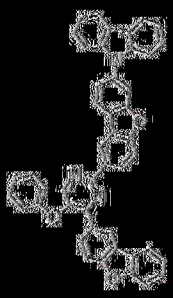


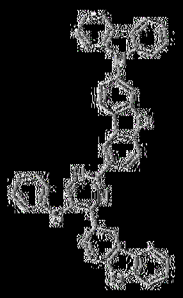


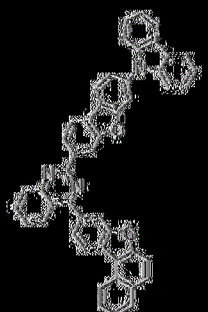


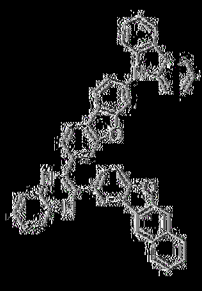


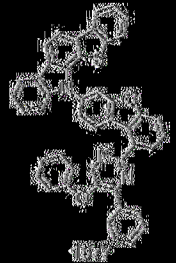


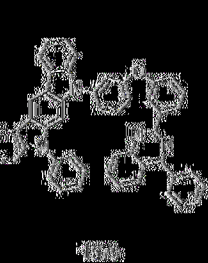


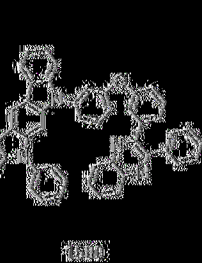


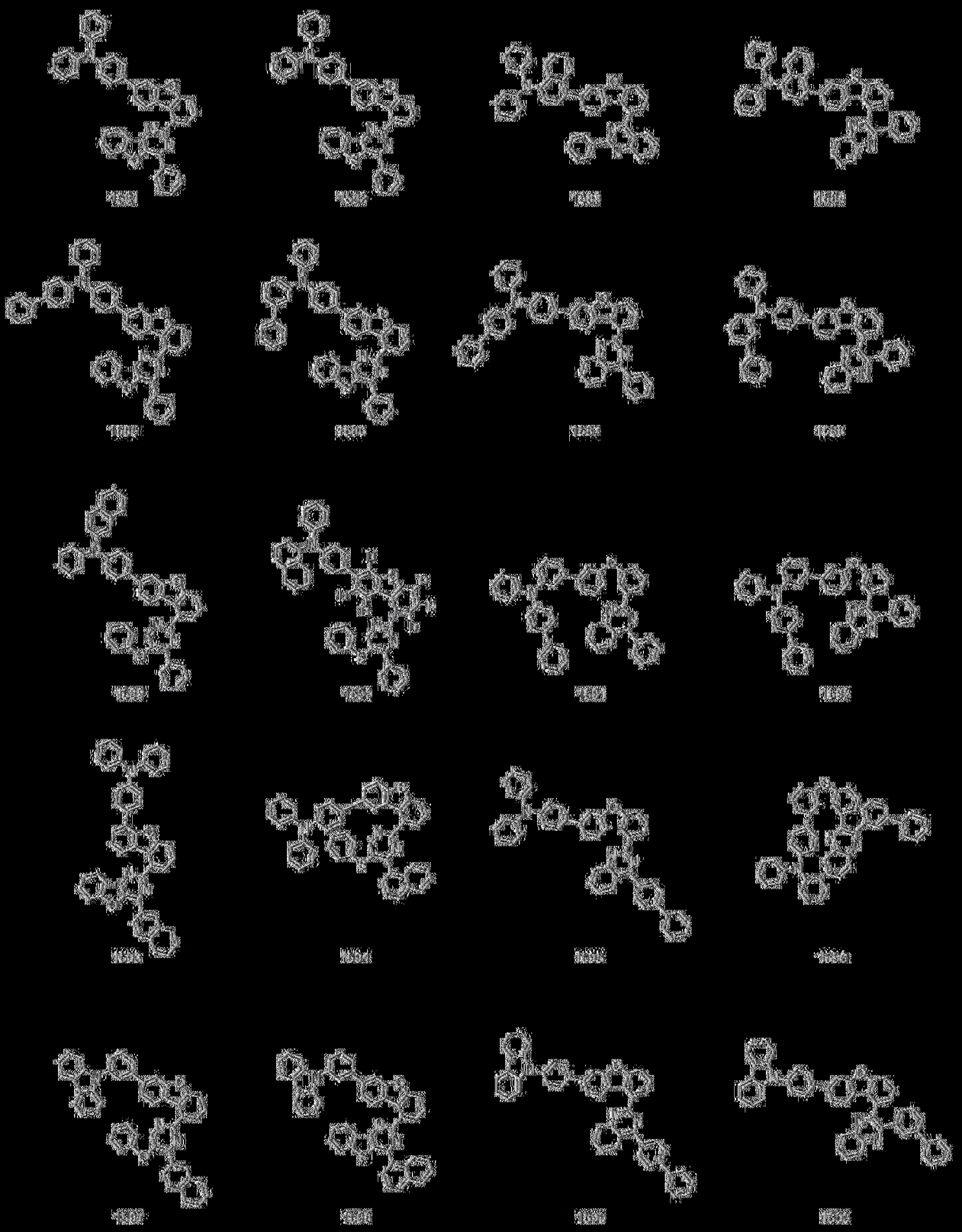












[0235] 通過在化學式 1 和 2 的結構中引入各種取代基，可以合成具有引入的取代基的固有特性的化合物。例如，可以通過引入通常用於製備有機發光裝置的電洞注入層材料、用於傳輸電洞的

材料、發光層材料、電子傳輸層材料和電荷產生層材料的取代基至核心結構來合成滿足每個有機材料層所需條件的材料。

【0236】 此外，可以通過將各種取代基引入化學式 1 和 2 的結構中來微調能帶隙，同時，可以改善有機材料之間界面處的特性並使材料的用途多樣化。

【0237】 同時，化合物具有高玻璃化轉變溫度(Tg)，因此具有優異的熱穩定性。熱穩定性的提高成為為裝置提供驅動穩定性的重要因素。

【0238】 在本申請的一個示例性實施例中，第一電極可以是正極（positive electrode），第二電極可以是負極（negative electrode）。

【0239】 在另一個示例性實施例中，第一電極可以是負極，第二電極可以是正極。

【0240】 在本申請的一個示例性實施例中，有機發光裝置可以是藍色有機發光裝置，並且根據化學式 1 的雜環化合物可以用作藍色有機發光裝置的材料。

【0241】 在本申請的一個示例性實施例中，有機發光裝置可以是綠色有機發光裝置，並且可以使用化學式 1 表示的雜環化合物作為綠色有機發光裝置的材料。

【0242】 在本申請的一個示例性實施例中，有機發光裝置可以是紅色有機發光裝置，並且可以使用化學式 1 表示的雜環化合物作為紅色有機發光裝置的材料。

【0243】 在本申請的一個示例性實施例中，有機發光裝置可以是

藍色有機發光裝置，並且根據化學式 1 的雜環化合物可以用作藍色有機發光裝置的發光層的材料。

【0244】 在本申請的一個示例性實施例中，有機發光裝置可以是綠色有機發光裝置，並且化學式 1 表示的雜環化合物可以作為綠色有機發光裝置的發光層的材料。

【0245】 在本申請的一個示例性實施例中，有機發光裝置可以是紅色有機發光裝置，並且可以使用化學式 1 表示的雜環化合物作為紅色有機發光裝置的發光層的材料。

【0246】 除了上述雜環化合物用於形成具有一層或多層的有機材料層之外，本發明的有機發光裝置可以使用有機發光裝置的典型製造方法和材料來製造。

【0247】 在製造有機發光裝置時，雜環化合物不僅可以通過真空沉積法還可以通過溶液塗佈法形成為有機材料層。這裡，溶液塗佈方法是指旋塗、浸塗、噴墨印刷（inkjet printing）、絲網印刷（screen printing）、噴塗法、輥塗等，但不限於此。

【0248】 本發明的有機發光裝置的有機材料層可以由單層結構構成，也可以由兩個或多於兩個的有機材料層層疊而成的多層結構構成。例如，本發明的有機發光裝置可以具有包括電洞注入層、電洞傳輸層、發光層、電子傳輸層、電子注入層等作為有機材料層的結構。然而，有機發光裝置的結構不限於此，並且可以包括更少數量的有機材料層。

【0249】 在本發明的有機發光裝置中，有機材料層包括發光層，

並且發光層可以包括由化學式 1 表示的雜環化合物和由化學式 2 表示的雜環化合物。

【0250】 在另一個示例性實施例中，發光層可以包括主體材料，並且主體材料可以包括由化學式 1 表示的雜環化合物和由化學式 2 表示的雜環化合物。

【0251】 在本發明的有機發光裝置中，有機材料層包括發光層，並且發光層可以包括由化學式 1 表示的雜環化合物和由化學式 2 表示的雜環化合物作為發光層的主體。

【0252】 在又一示例性實施例中，主體材料可以包括兩種或多於兩種主體材料，並且在兩種或多於兩種主體材料中，由化學式 1 表示的雜環化合物為 N 型主體材料，由化學式 2 表示的雜環化合物可以為 P 型主體材料。

【0253】 在這種情況下，為由於兩個分子之間的電子交換，受體（N 型主體）的最低佔據分子軌域（LUMO）能級和供體（P 型主體）的最高佔據分子軌域（HOMO）能級之間的能量差異導致的發射現象的激發錯合體（exciplex）現象發生得更頻繁。

【0254】 也就是說，當化學式 1 的雜環化合物和化學式 2 的雜環化合物包含在有機發光裝置的有機材料層中時，表現出更好的效率和使用壽命效果。從這個結果可以預期，當包含兩個化合物時，將發生激發錯合體現象。

【0255】 激發錯合體現像是由於兩個分子之間的電子交換而釋放具有供體（p-主體）的 HOMO 能級和受體（n-主體）的 LUMO

能級大小的能量的現象。當兩個分子之間發生激發錯合體現象時，就會發生逆向系統間跨越（reverse intersystem crossing，RISC），且由於 RISC，螢光（fluorescence）的內量子效率（internal quantum efficiency）可以提高到 100%。當具有良好電洞傳輸能力的供體（p-主體）和具有良好電子傳輸能力的受體（n-主體）作為發光層的主體時，電洞注入 p-主體且電子注入 n-主體，使得可以降低驅動電壓，有利於提高使用壽命。

【0256】 在本發明的有機發光裝置中，主體材料可以包括兩種或多於兩種主體材料，並且可以將兩種或多於兩種主體材料預先混合使用。

【0257】 此外，本申請的另一示例性實施例提供了一種用於有機發光裝置的有機材料層的組合物，包括由化學式 1 表示的雜環化合物；以及由化學式 2 表示的雜環化合物。

【0258】 由化學式 1 表示的雜環化合物和由化學式 2 表示的雜環化合物的具體內容同上。

【0259】 組合物中由化學式 1 表示的雜環化合物與由化學式 2 表示的雜環化合物的重量比可以為 1:10 至 10:1、1:8 至 8:1、1:5 至 5:1 和 1:2 比 2:1，但不限於此。

【0260】 該組合物可以在形成用於有機發光裝置的有機材料時使用，特別地，可以更優選在形成發光層的主體時使用。

【0261】 在本申請的一個示例性實施例中，有機材料層包括：由化學式 1 表示的雜環化合物；以及由化學式 2 表示的雜環化合物

且也可以與磷光摻雜劑並用。

【0262】 在本申請的一個示例性實施例中，有機材料層包括：由化學式 1 表示的雜環化合物；和由化學式 2 表示的雜環化合物，並且可以與銥類的摻雜劑一起使用。

【0263】 作為磷光摻雜劑的材料，可以使用本領域已知的材料。

【0264】 例如，可以使用由 LL'MX'、LL'L"M、LMX'X"、L2MX' 和 L3M 表示的磷光摻雜劑，但本發明的範圍不受這些例子的限制。

【0265】 此處，L、L'、L"、X'、X"是互不相同的雙齒配體（bidentate ligand），且 M 是形成八面體錯合物（octahedral complex）的金屬。

【0266】 M 可以是銥（iridium）、鉑（platinum）、鋨（osmium）等。

【0267】 L 是通過 sp2 碳和雜原子通過銥類的摻雜劑在 M 上配位的陰離子雙齒配體，且 X 可以執行捕獲電子或電洞的功能。L 的非限制性實例包括 2-(1-萘基)苯並噁唑

（2-(1-naphthyl)benzoxazole）、(2-苯基苯並噁唑)

（(2-phenylbenzoxazole)）、(2-苯基苯並噻唑)

（(2-phenylbenzothiazole)）、(2-苯基苯並噻唑)

（(2-phenylbenzothiazole)）、(7,8-苯並喹啉)

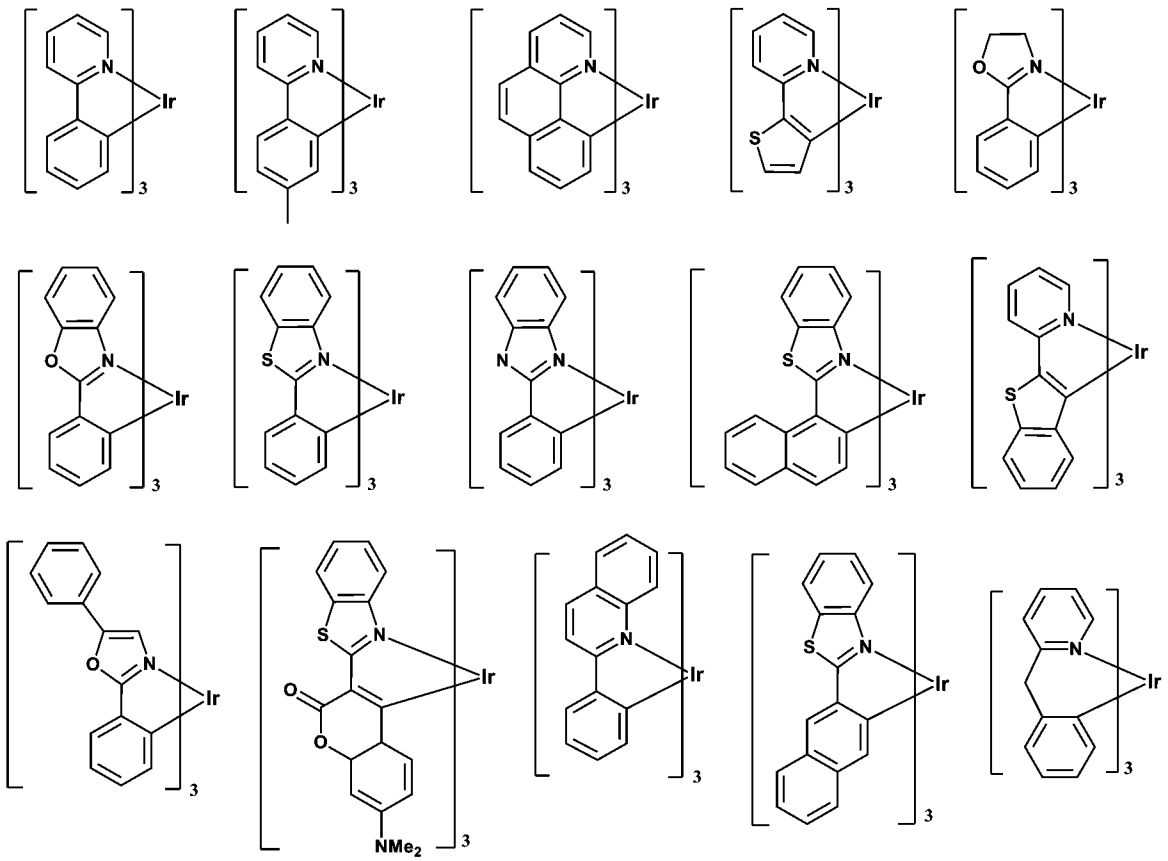
（(7,8-benzoquinoline)）、(噻吩基吡嗪)（(thiophene group pyrizine)）、苯基吡啶（phenylpyridine）、苯並噻吩基吡嗪

（benzothiophene group pyrizine）、3-甲氧基-2-苯基吡啶

（3-methoxy-2-phenylpyridine）、噻吩基吡嗪（thiophene group

pyrizine）、甲苯基吡啶（tolylpyridine）等。X’和 X”的非限制性實例包括乙醯丙酮酸鹽（acetylacetonate，acac）、六氟乙醯丙酮酸鹽（hexafluoroacetylacetonate）、亞水楊基（salicylidene）、吡啶甲酸鹽（picolinate）、8-羥基喹啉酸鹽（8-hydroxyquinolinate）等。

【0268】 下面將給出其更具體的例子，但本申請不僅限於這些例子。



【0269】 在本申請的一個示例性實施例中，作為銥類的摻雜劑，可以使用作為綠色磷光摻雜劑的 $Ir(ppy)_3$。

【0270】 在本申請的一個示例性實施例中，基於整個發光層，摻雜劑的含量可以為 1%至 15%，優選 3%至 10%，更優選 5%至 10%。含量可以指重量比。

【0271】 本發明的有機發光裝置還可以包括選自由以下組成的群組中的一層或兩層或多層：發光層、電洞注入層、電洞傳輸層、電子注入層、電子傳輸層、電子阻擋層，和電洞阻擋層。

【0272】 圖 1 至圖 4 例示了根據本申請一個示例性實施例的有機發光裝置的多個電極和有機材料層堆疊順序。然而，本申請的範圍不旨在受限於這些附圖，並且本領域已知的有機發光裝置的結構也可以應用於本申請。

【0273】 根據圖 1，示出了有機發光裝置，其中正極 200、有機材料層 300 和負極 400 依次堆疊在基板 100 上。然而，有機發光裝置並不僅限於這種結構，還可以實現如圖 2 中負極、有機材料層和正極依次堆疊在基板上的有機發光裝置。

【0274】 圖 3 舉例說明瞭有機材料層是多層的情況。根據圖 3 的有機發光裝置包括電洞注入層 301、電洞傳輸層 302、發光層 303、電洞阻擋層 304、電子傳輸層 305 和電子注入層 306。然而，本申請的範圍不限於上述堆疊結構，並且必要時，可以省略除發光層之外的其他層，並且可以進一步添加其他必要的功能層。

【0275】 此外，根據本申請的一個示例性實施例的有機發光裝置包括第一電極、設置在第一電極上並包括第一發光層的第一堆疊、設置在第一堆疊上的電荷產生層、設置在電荷產生層上並且包括第二發光層的第二疊層，以及設置在第二疊層上的第二電極。

【0276】 在本申請的一個示例性實施例中，第一發光層和第二發光層可以分別包括由化學式 1 表示的雜環化合物和由化學式 2 表

示的雜環化合物。

【0277】 作為根據本申請的一個示例性實施例的有機發光裝置，具有 2 堆疊串聯結構（2-stack tandem structure）的有機發光裝置示例性地示於下圖 4 中。

【0278】 在這種情況下，可以根據情況省略下圖 4 中描述的第一電子阻擋層、第一電洞阻擋層、第二電洞阻擋層等。

【0279】 在本申請的一個示例性實施例中，化學式 1 的化合物可以摻雜有鹼金屬（alkali metal）或鹼土金屬（alkaline earth metal）。在這種情況下，由於間隙態的形成，可以降低有機發光裝置的驅動電壓並且可以進一步提高效率和使用壽命。

【0280】 在本申請的一個示例性實施例中，提供了一種在化學式 1 的化合物中包含鹼金屬或鹼土金屬的組合物。組合物中鹼金屬或鹼土金屬的含量可以為 0.01 重量%至 30 重量%，優選 0.01 重量%至 25 重量%，更優選 0.01 重量%至 20 重量%，基於整個組合物的重量。

【0281】 在本申請的一個示例性實施例中，鹼金屬或鹼土金屬可以是鋰(Li)、銣(Rb)、銫(Cs)或鎂(Mg)。然而，鹼金屬或鹼土金屬不限於此。

【0282】 在本申請的一個示例性實施例中，提供了一種有機發光裝置的製造方法，該方法包括：製備基板；在基板上形成第一電極；在第一電極上形成具有一層或多層的有機材料層；以及在有機材料層上形成第二電極，其中有機材料層的形成包括使用根據

本申請的一個示例性實施例的用於有機材料層的組合物形成具有一層或多層的有機材料層。

【0283】 在本申請的一個示例性實施例中，提供了一種用於製造有機發光裝置的方法，其中有機材料層的形成通過將由化學式 1 表示的雜環化合物和由化學式 2 表示的雜環化合物預混合，以及採用熱真空沉積法而形成有機材料層。

【0284】 預混合是指在化學式 1 的雜環化合物和化學式 2 的雜環化合物沉積到有機材料層上之前，將材料先混合，且將混合物裝在一個共同的容器中混合。

【0285】 根據本申請的一個示例性實施例，預混材料可稱為用於有機材料層的組合物。

【0286】 包括由化學式 1 表示的雜環化合物；以及由化學式 2 表示的雜環化合物的有機材料層可以根據需要進一步包含其他材料。

【0287】 在根據本申請的一個示例性實施例的有機發光裝置中，除了由化學式 1 表示的雜環化合物；以及由化學式 2 表示的雜環化合物之外的材料將於下面舉例說明，但這些材料只是為了舉例說明，並不限制本申請的範圍，且可以用本領域公知的材料代替。

【0288】 作為正極材料，可以使用具有相對高的功函數的材料，並且可以使用透明導電氧化物、金屬或導電聚合物等。正極材料的具體實例包括：金屬（如釩、鉻、銅、鋅和金，或其合金）；金

屬氧化物（如氧化鋅、氧化銦、氧化銦錫（indium tin oxide，ITO）、氧化銦鋅（indium zinc oxide，IZO））；金屬和氧化物的組合（例如 ZnO:Al 或 SnO_2:Sb）；導電聚合物（如聚(3-甲基噻吩)、聚[3,4-(伸乙-1,2-二氧基)噻吩]（poly[3,4-(ethylene-1,2-dioxy)thiophene]，PEDOT）、聚吡咯、聚苯胺）；及其類似物，但不限於此。

【0289】 作為負極材料，可以使用相對低的功函數的材料，可以使用金屬、金屬氧化物、導電性聚合物等。負極材料的具體實例包括：金屬（如鎂、鈣、鈉、鉀、鈦、銦、釔、鋰、釕、鋁、銀、錫和鉛，或其合金）；多層結構材料（例如 LiF/Al 或 LiO_2/Al）；及其類似物，但不限於此。

【0290】 作為電洞注入材料，也可以使用公知的電洞注入材料，例如，酞菁化合物，例如在美國專利第 4,356,429 號中揭露的銅酞菁；或文獻[先進材料（Advanced Material），6，P.677（1994）]中描述的星爆型（starburst-type）胺衍生物，例如三（4-肼甲醯基-9-基苯基）胺（tris(4-carbazoyl-9-ylphenyl)amine，TCTA），4,4',4”-三[苯基（間甲苯基）胺基]三苯基胺（4,4',4"-tri[phenyl(m-tolyl)amino]triphenylamine，m-MTDATA），1,3,5-三[4-(3-甲基苯基苯基胺基)苯基]苯（1,3,5-tris[4-(3-methylphenylphenylamino)phenyl]benzene，m-MTDAPB），作為具有溶解性的導電聚合物的聚苯胺/十二烷基苯磺酸或聚(3,4-伸乙二氧噻吩)/聚(4-苯乙烯磺酸酯)、聚苯胺/樟腦磺酸或聚苯胺/聚(4-苯乙烯-磺酸鹽)等。

【0291】 作為電洞傳輸材料，可以使用吡唑啉衍生物、芳胺類衍生物、二苯乙烯衍生物（stilbene derivative）、三苯基二胺衍生物（triphenyldiamine derivative）等，且也可以使用低分子或聚合物材料。

【0292】 作為電子傳輸材料，可以使用噁二唑衍生物、蒽醌二甲烷 anthraquinodimethane）及其衍生物、苯醌及其衍生物、萘醌及其衍生物、蒽醌及其衍生物、四氰基蒽醌二甲烷及其衍生物、芴酮衍生物、二苯基二氰基乙烯及其衍生物、聯苯醌衍生物、8-羥基喹啉的金屬錯合物及其衍生物等，且也可以使用低分子材料、聚合物材料。

【0293】 作為電子注入材料，例如，LiF 在本領域中具有代表性，但本申請不限於此。

【0294】 作為發光材料，可以使用紅色、綠色或藍色的發光材料，且必要時，可以混合使用兩種或多兩種發光材料。在這種情況下，兩種或多兩種發光材料被沉積或用作單獨的供應源，或者預混合以被沉積並用作一個供應源。此外，螢光材料也可以用作發光材料，但也可以用作磷光材料。作為發光材料，也可以單獨使用通過將從正極和負極分別注入的電洞和電子結合而發光的材料，但是亦可使用具有一起參與發光的主體材料及摻雜劑材料的材料。

【0295】 當發光材料的主體混合使用時，可以是同系列的主體混合使用，且也可以是不同系列的主體混合使用。例如，可以使用

選自 n 型主體材料或 p 型主體材料中的兩種或多於兩種材料作為發光層的主體材料。

【0296】 根據本申請的一個示例性實施例的有機發光裝置可以根據所使用的材料為頂面發射型（top emission type）、底面發射型（bottom emission type）或雙面發射型（dual emission type）。

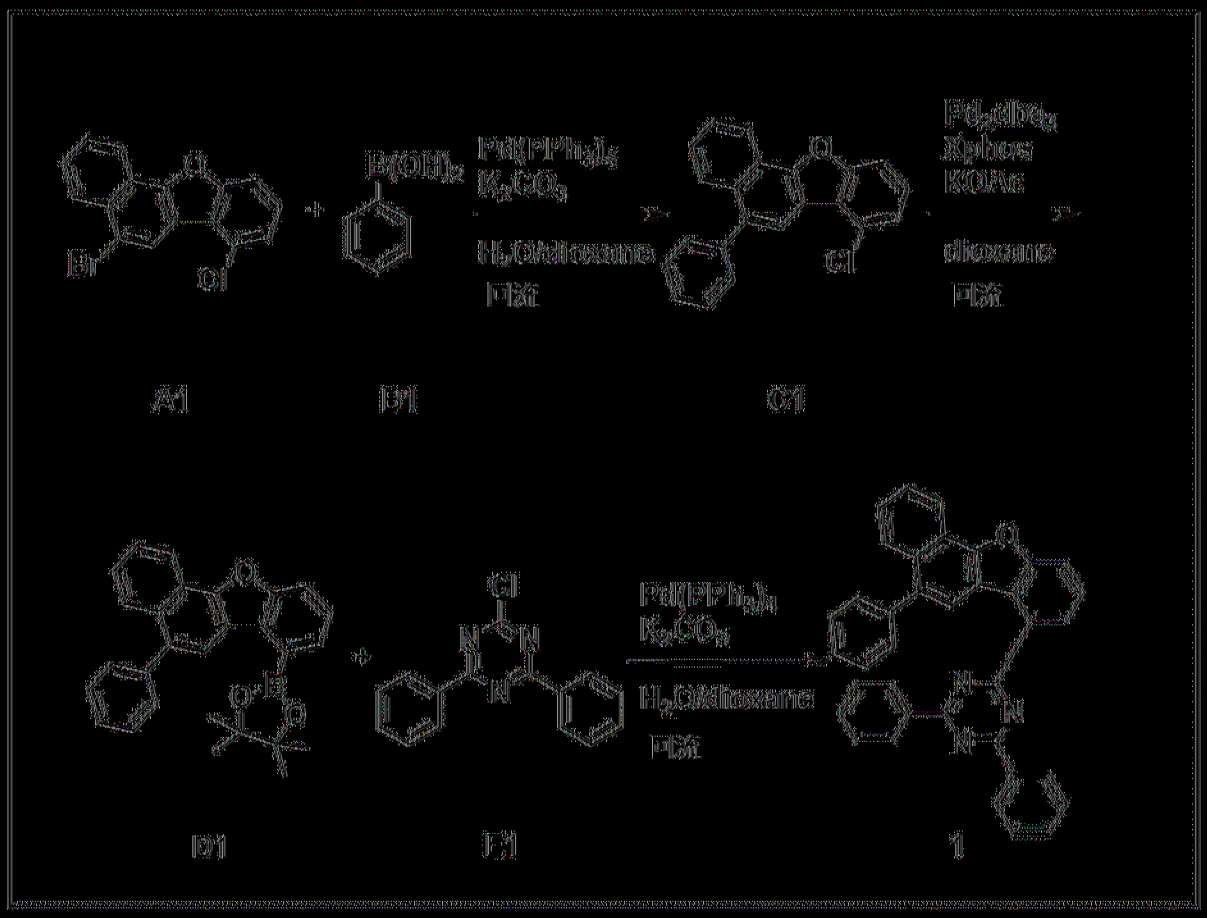
【0297】 基於與應用於有機發光裝置的原理類似的原理，根據本申請的一個示例性實施例的雜環化合物甚至可以在包括有機太陽能電池、有機光導體、有機電晶體等的有機電子裝置中起作用。

【0298】 以下，將通過實例對本說明書進行更詳細的說明，但這些實例僅用於舉例說明本申請，並不用於限製本申請的範圍。

【0299】 **< 製備例>**

【0300】 **<製備例 1>化合物 1 的製備**

【0301】



|(0302)| 1）化合物 C1 的製備

|(0303)| 將化合物 A1(50.0g，151mmol)、化合物 B1(22.1g，181mmol)、$Pd(PPh_3)_4$(8.72g，7.56mmol)和 K_2CO_3(41.7g，302mmol)溶於蒸餾水/1,4-二噁烷(dioxane)(H_2O/1,4-二噁烷)(150mL/500mL)中後，將所得溶液回流 3 小時。反應終止後，室溫下用二氯甲烷/蒸餾水(二氯甲烷/H_2O)萃取。將反應產物通過管柱層析法（ column chromatography)(DCM:Hex：1:5)純化並用甲醇再結晶以獲得化合物 C1(45.1g，137mmol，91%)。

|(0304)| DCM 表示二氯甲烷，Hex 表示己烷。

|(0305)| 2)化合物 D1 的製備

|(0306)| 將化合物 C1(45.1g，137mmol)、Pd_2dba_3(6.27g，

6.85mmol)、Xphos(6.53g，13.7mmol)和 KOAc(26.9g，274mmol)溶解在二噁烷(450mL)中後，將所得溶液回流 4 小時。反應終止後，反應產物減壓過濾濾除鹽分，然後濃縮。經濃縮的反應產物通過管柱層析法(DCM:Hex＝1:3)純化並用甲醇再結晶以獲得化合物 D1(36.3g，86.4mmol，63%)。

【0307】 **3)化合物 1 的製備**

【0308】 將化合物 D1(7.0g，16.7mmol)、化合物 E1(4.34g，16.3mmol)、$Pd(PPh_3)_4$(0.96g，0.84mmol)和 K_2CO_3(4.62g，33.4mmol)溶於蒸餾水/1,4-二噁烷(H_2O/1,4-二噁烷)(21mL/70mL)中後，將所得溶液回流 2 小時。反應終止後，用水和丙酮洗滌反應產物，以得到固體。將經乾燥的固體通過管柱層析法(DCB)純化並用 DCB 再結晶以獲得化合物 1(8.16g，15.5mmol，93%)。

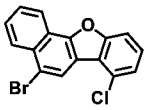
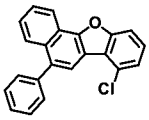
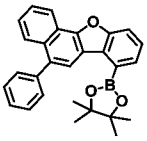
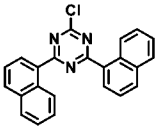
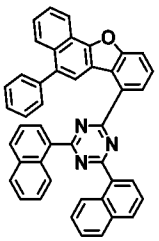
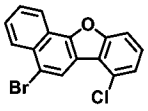
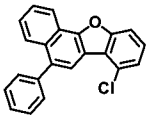
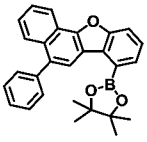
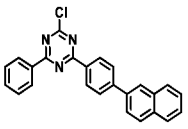
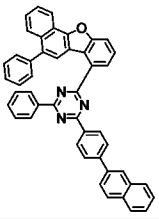
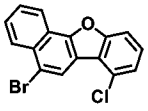
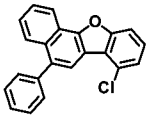
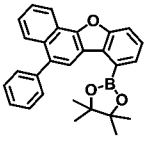
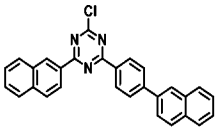
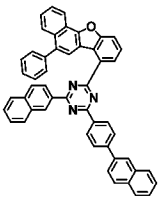
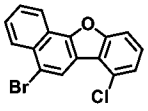
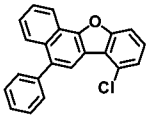
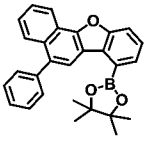
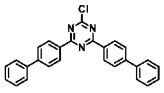
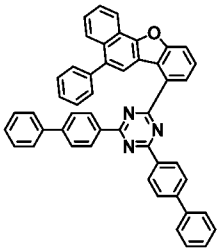
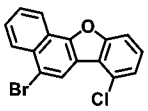
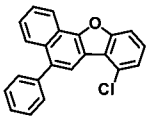
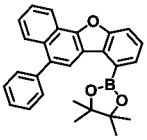
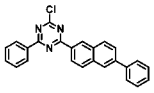
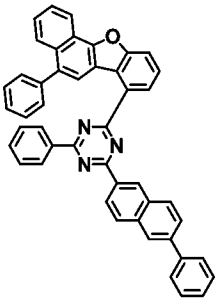
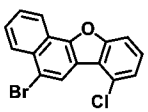
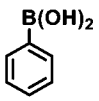
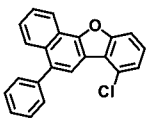
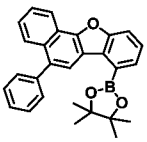
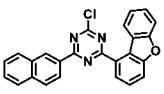
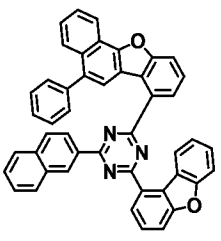
【0309】 DCB 表示二氯苯。

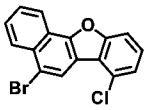
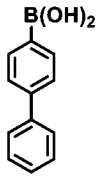
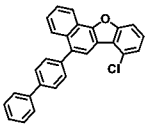
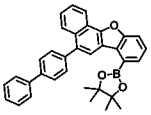
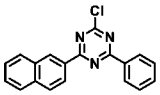
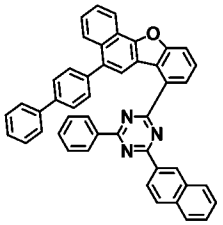
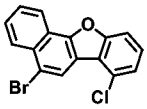
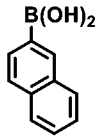
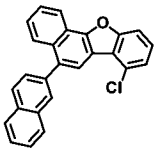
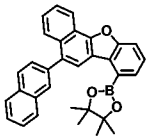
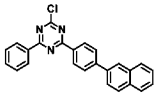
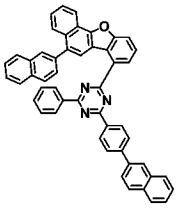
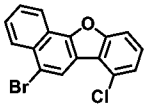
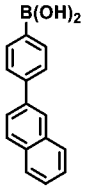
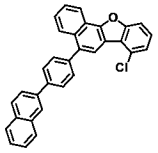
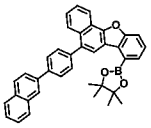
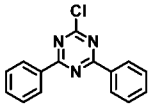
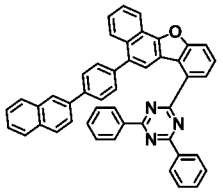
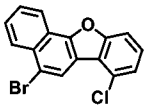
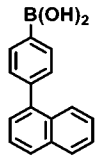
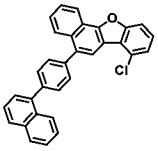
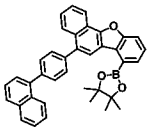
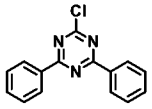
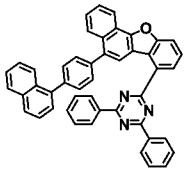
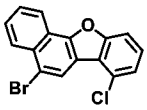
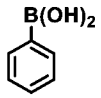
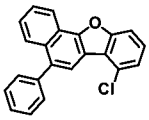
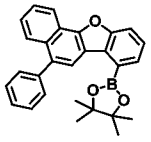
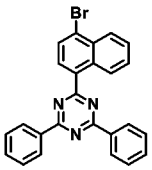
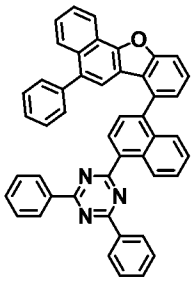
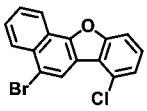
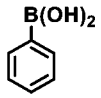
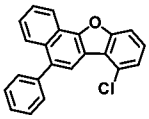
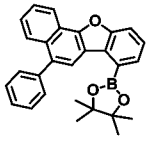
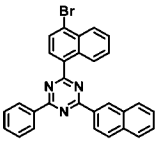
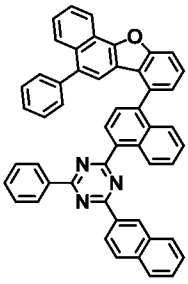
【0310】 **<製備例 2>化合物 13、37、53、57、97、133、209、237、249、253、325 和 329 的製備**

【0311】 化合物 13、37、53、57、97、133、209、237、249、253、325 和 329 的合成方法與製備例 1 中的製備方法相同，不同之處在於製備例 2 中，化合物 A 至 E 使用了以下表 1。

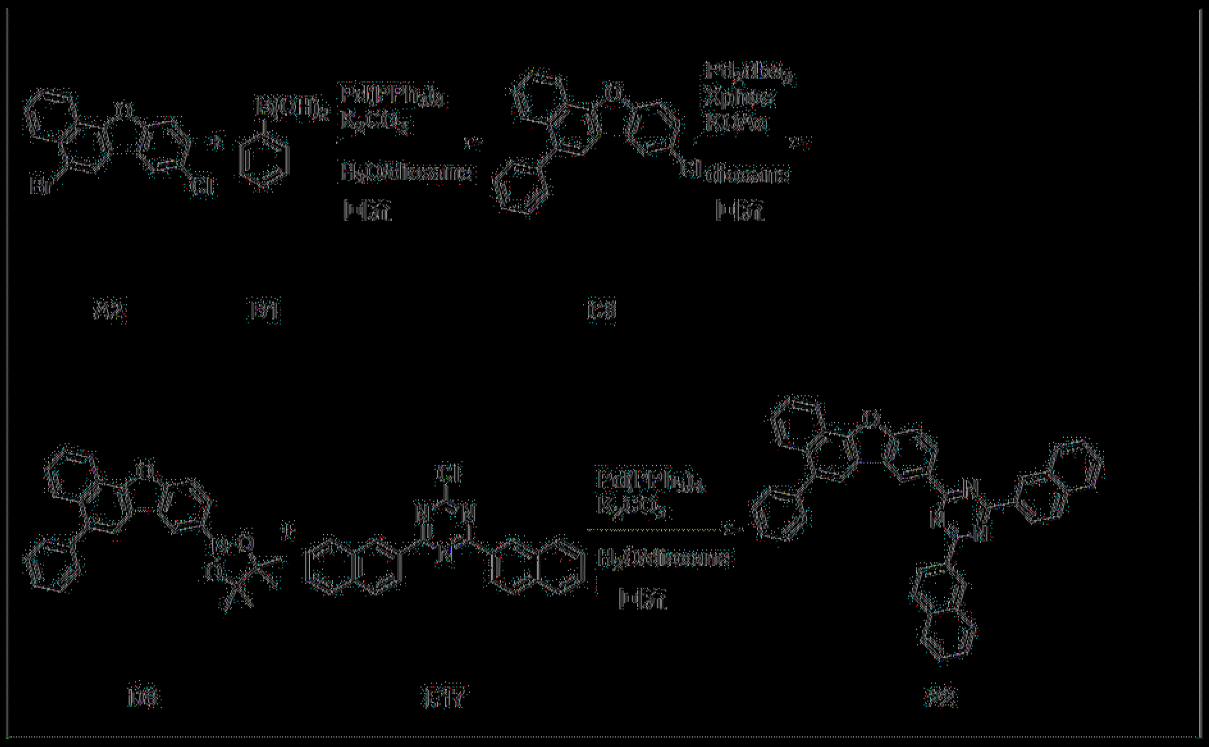
【0312】 表 1

化合物 A	化合物 B	化合物 C	化合物 D	化合物 E	產物	產物產率

A1 	B1	C1 	D1 	E2 	13 	49%
A1 	B1	C1 	D1 	E3 	37 	54%
A1 	B1	C1 	D1 	E4 	53 	55%
A1 	B1	C1 	D1 	E5 	57 	51%
A1 	B1	C1 	D1 	E6 	97 	55%
A1 	B1 	C1 	D1 	E9 	133 	50%

A1 	B2 	C2 	D2 	E10 	209 	52%
A1 	B4 	C4 	D4 	E3 	237 	54%
A1 	B5 	C5 	D5 	E1 	249 	49%
A1 	B6 	C6 	D6 	E1 	253 	48%
A1 	B1 	C1 	D1 	E12 	325 	51%
A1 	B1 	C1 	D1 	E13 	329 	53%

【0313】 <製備例 3>化合物 22 的製備



|(0314)|

|(0315)| 1）化合物 C8 的製備

|(0316)| 將化合物 A2(50.0g，151mmol)、化合物 B1(22.1g，181mmol)、$Pd(PPh_3)_4$(8.72g，7.56mmol)和 K_2CO_3(41.7g，302mmol)溶於蒸餾水/1,4-二噁烷(H_2O/1,4-二噁烷)(150mL/500mL)中後，將所得溶液回流 3 小時。反應終止後，室溫下用二氯甲烷/蒸餾水(二氯甲烷/H_2O)萃取。將反應產物通過管柱層析法(DCM:Hex：1:5)純化並用甲醇再結晶以獲得化合物 C8(44.7g，136mmol，90%)。

|(0317)| 2)化合物 D8 的製備

|(0318)| 將化合物 C8（44.7g，136mmol）、Pd_2dba_3（6.27g，6.80mmol）、Xphos（6.48g，13.6mmol）和 KOAc（26.7g，272mmol）溶解在二噁烷（450mL）中後，將所得溶液回流 4 小時。反應終止後，反應產物減壓過濾濾除鹽分，然後濃縮。經濃縮的反應產物通過管柱層析法(DCM:Hex：1:3)純化並用甲醇再結晶以獲得化合

物 D8(37.2g，88.4mmol，65%)。

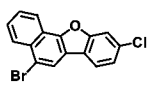
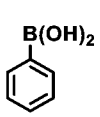
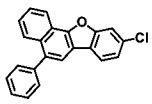
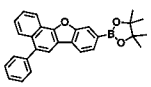
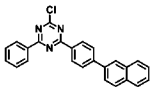
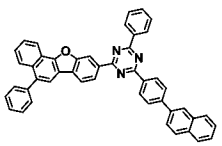
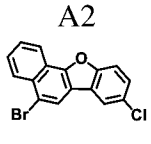
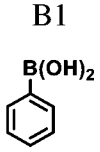
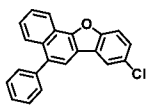
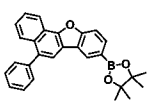
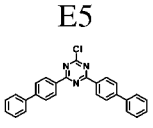
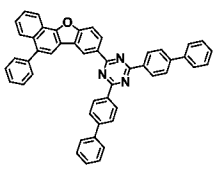
【0319】 **3)化合物 22 的製備**

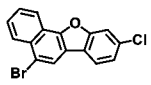
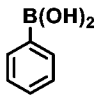
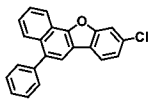
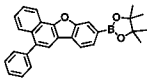
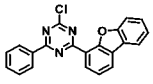
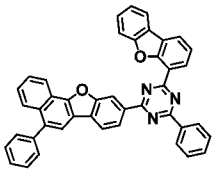
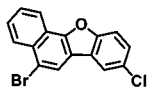
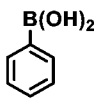
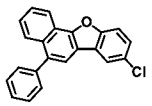
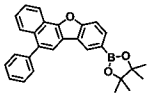
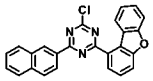
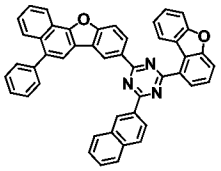
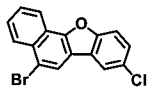
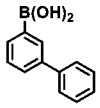
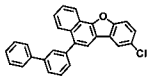
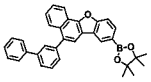
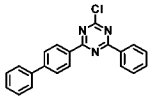
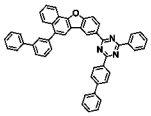
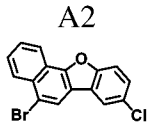
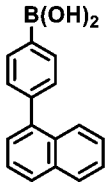
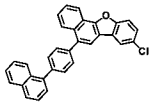
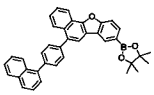
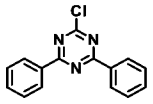
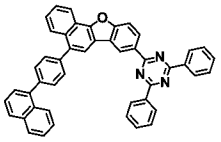
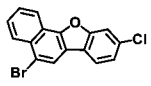
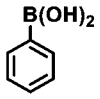
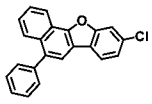
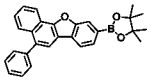
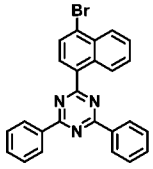
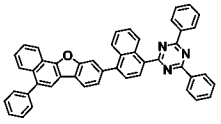
【0320】 將化合物 D8(7.0g，16.7mmol)、化合物 E17(6.00g，16.3mmol)、$Pd(PPh_3)_4$(0.96g，0.84mmol)和 K_2CO_3(4.62g，33.4mmol)溶於蒸餾水/1,4-二噁烷(H_2O/1,4-二噁烷)(21mL/70mL)中後，將所得溶液回流 2 小時。反應終止後，用水和丙酮洗滌反應產物，以得到固體。將經乾燥的固體通過管柱層析法(DCB)純化並用 DCB 再結晶以獲得化合物 22(10.0g，15.6mmol，96%)。

【0321】 **<製備例 4>化合物 39、58、115、134、226、250 和 327 的製備**

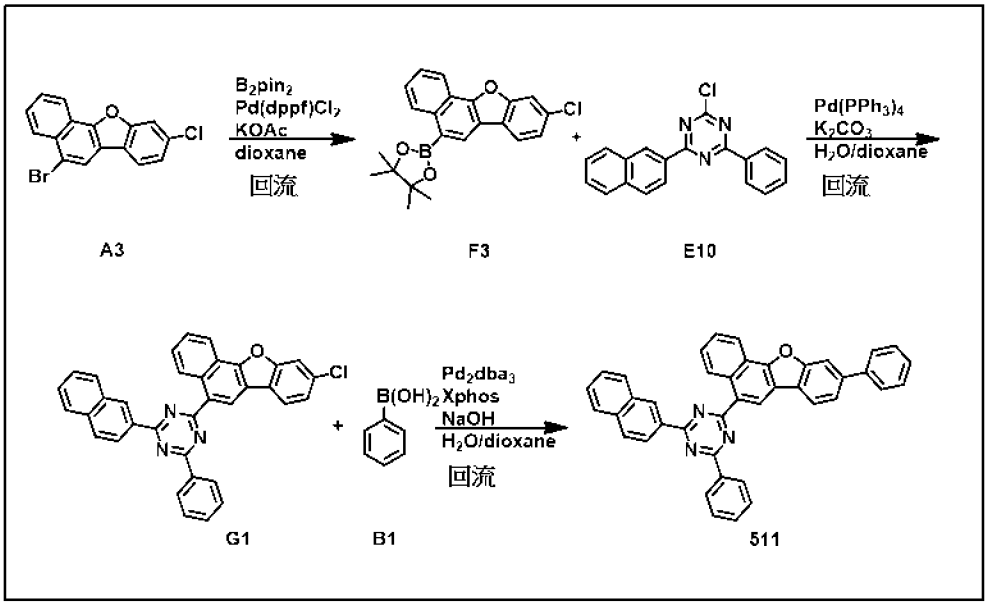
【0322】 化合物 39、58、115、134、226、250 和 327 以與製備例 3 中的製備方法相同的方式合成，除了在製備例 4 中，使用以下表 2 中的化合物 A 至 E。

【0323】 表 2

化合物 A	化合物 B	化合物 C	化合物 D	化合物 E	產物	產物產率
A3 	B1 	C9 	D9 	E3 	39 	58%
A2 	B1 	C8 	D8 	E5 	58 	55%

A3 	B1 	C9 	D9 	E8 	115 	56%
A2 	B1 	C8 	D8 	E9 	134 	53%
A2 	B3 	C10 	D10 	E11 	226 	51%
A2 	B6 	C11 	D11 	E1 	250 	54%
A3 	B1 	C9 	D9 	E12 	327 	56%

【0324】 **<製備例 5>化合物 511 的製備**



【0325】

【0326】 **1）化合物 F3 的製備**

【0327】 將化合物 A3(50.0g，151mmol)、B_2pin_2(60.0g，158mmol)、$Pd(dppf)Cl_2$(5.52g，7.55mmol)和 KOAc(29.6g，302mmol)溶解在二噁烷(500mL)中後，將所得溶液回流 4 小時。反應終止後，反應產物減壓過濾濾除鹽分，然後濃縮。經濃縮的反應產物通過管柱層析法(DCM:Hex＝1:4)純化並用甲醇再結晶以獲得化合物 F3(46.3g，122mmol，81%)。

【0328】 **2)化合物 G1 的製備**

【0329】 將化合物 F3(46.3g，122mmol)、化合物 E10(38.0g，120mmol)、$Pd(PPh_3)_4$(7.05g，6.10mmol)和 K_2CO_3(33.7g，244mmol)溶於蒸餾水/1,4-二噁烷(H_2O/1,4-二噁烷)(140mL/460mL)中後，將所得溶液回流 2 小時。反應終止後，用水和丙酮洗滌反應產物，以得到固體。將經乾燥的固體通過管柱層析法(DCB)純化並用 DCB 再結晶以獲得化合物 G1(59.3g，111mmol，91%)。

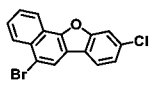
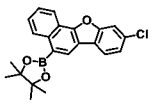
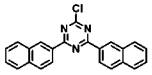
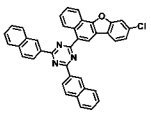
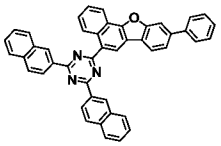
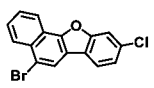
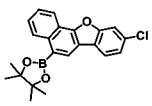
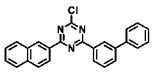
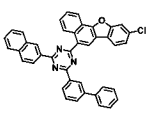
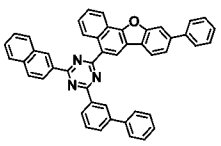
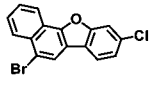
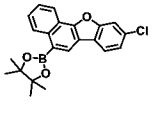
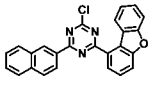
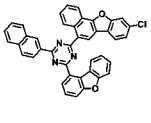
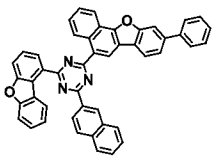
【0330】 **3)化合物 511 的製備**

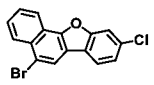
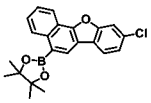
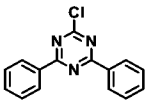
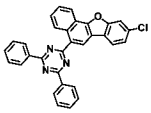
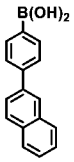
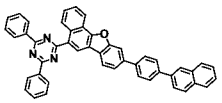
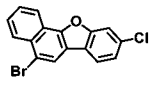
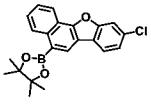
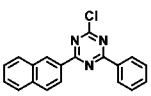
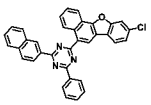
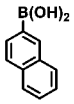
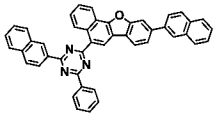
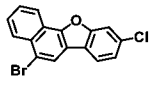
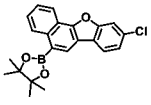
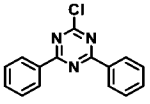
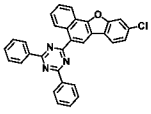
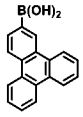
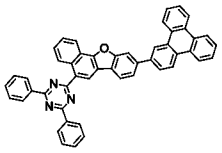
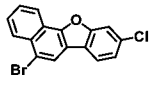
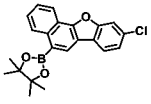
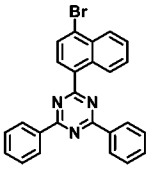
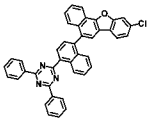
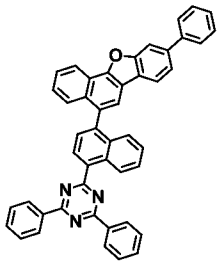
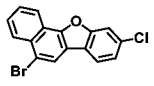
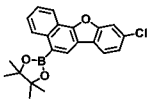
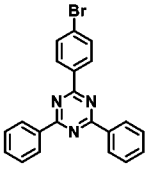
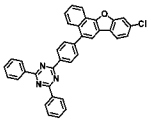
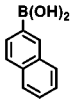
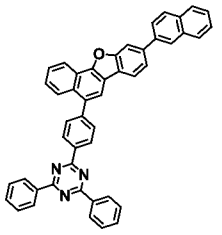
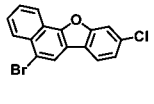
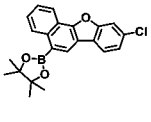
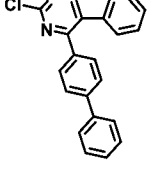
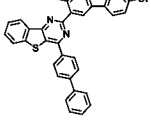
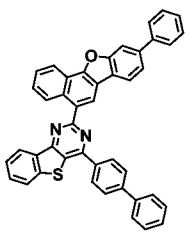
【0331】 將化合物 G1(7.0g，13.1mmol)、化合物 B1(1.92g，15.7mmol)、$Pd(PPh_3)_4$(0.76g，0.66mmol)和 K_2CO_3(3.62g，26.2mmol)溶於蒸餾水/1,4-二噁烷(H_2O/1,4-二噁烷)(21mL/70mL)中後，將所得溶液回流 4 小時。反應終止後，用水和丙酮洗滌反應產物，以得到固體。將經乾燥的固體通過管柱層析法(DCB)純化並用 DCB 再結晶以獲得化合物 511(7.09g，12.3mmol，94%)。

【0332】 **<製備例 6>化合物 523、551、635、703、711、755、827、863、919 的製備**

【0333】 化合物 523、551、635、703、711、755、827、863 和 919 以與製備例 5 中的製備方法相同的方式合成，不同之處在於在製備例 6 中，使用了以下表 3 的化合物 A、F、E、G 和 B。

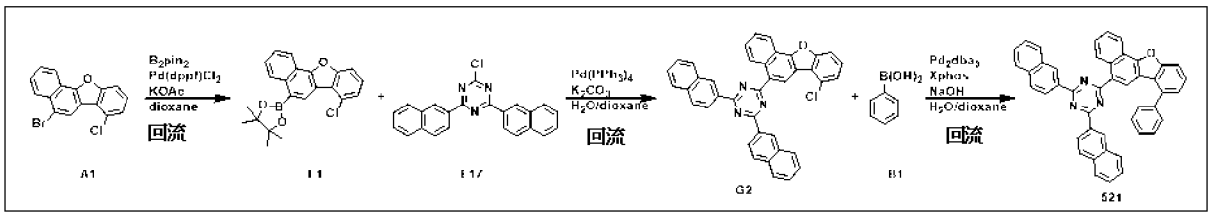
【0334】 表 3

化合物 A	化合物 F	化合物 E	化合物 G	化合物 B	產物	產物產率
A3 	F3 	E17 	G3 	B1	523 	70%
A3 	F3 	E14 	G5 	B1	551 	66%
A3 	F3 	E9 	G9 	B1	635 	69%

A3 	F3 	E1 	G10 	B5 	703 	71%
A3 	F3 	E10 	G1 	B4 	711 	73%
A3 	F3 	E1 	G10 	B7 	755 	74%
A3 	F3 	E12 	G14 	B1	827 	68%
A3 	F3 	E16 	G15 	B4 	863 	69%
A3 	F3 	E18 	G16 	B1	919 	71%

【0335】 **<製備例 7>化合物 521 的製備**

【0336】



【0337】 **1）化合物 F1 的製備**

【0338】 將化合物 A1（50.0g，151mmol）、B_2pin_2（60.0g，158mmol）、$Pd(dppf)Cl_2$（5.52g，7.55mmol）和 KOAc（29.6g，302mmol）溶解在二噁烷（500mL）中後，將所得溶液回流 4 小時。反應終止後，反應產物減壓過濾濾除鹽分，然後濃縮。經濃縮的反應產物通過管柱層析法(DCM:Hex＝1:4)純化並用甲醇再結晶以獲得化合物 F1(47.5g，125mmol，83%)。

【0339】 **2)化合物 G2 的製備**

【0340】 將化合物 F1(7.0g，18.5mmol)、化合物 E17(6.66g，18.1mmol)、$Pd(PPh_3)_4$(1.07g，0.93mmol)和 K_2CO_3(5.11g，37.0mmol)溶於蒸餾水/1,4-二噁烷(H_2O/1,4-二噁烷)(21mL/70mL)中後，將所得溶液回流 2 小時。反應終止後，用水和丙酮洗滌反應產物，以得到固體。將經乾燥的固體通過管柱層析法(DCB)純化並用 DCB 再結晶以獲得化合物 G2(10.1g，17.3mmol，94%)。

【0341】 **3)化合物 521 的製備**

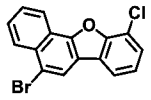
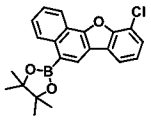
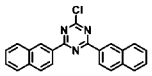
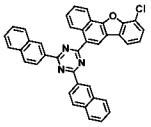
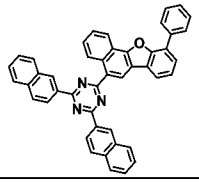
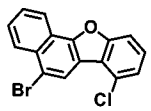
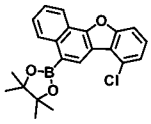
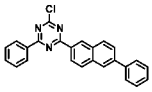
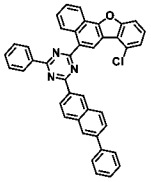
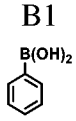
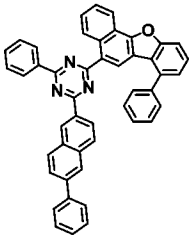
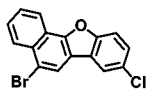
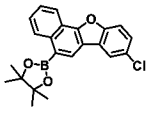
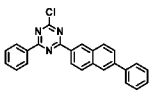
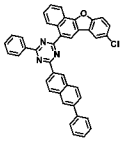
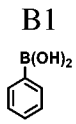
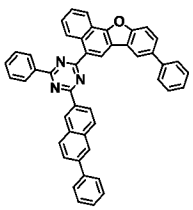
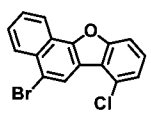
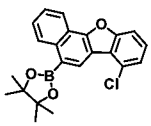
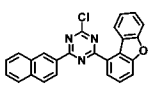
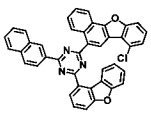
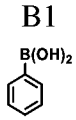
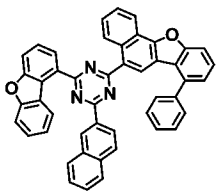
【0342】 將化合物 G2(10.1g，17.3mmol)、化合物 B1(2.53g，20.8mmol)、$Pd(PPh_3)_4$(1.01g，0.87mmol)和 K_2CO_3(4.78g，34.6mmol)溶於蒸餾水/1,4-二噁烷(H_2O/1,4-二噁烷)(30mL/100mL)中後，將所得溶液回流 4 小時。反應終止後，用水和丙酮洗滌反應產物，以

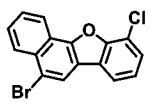
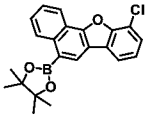
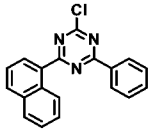
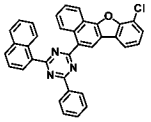
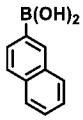
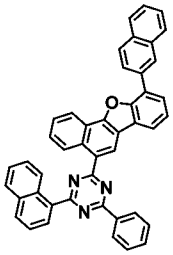
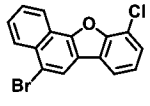
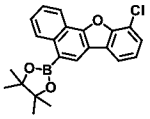
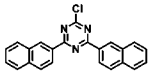
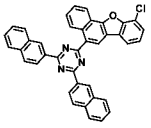
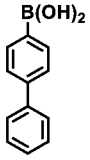
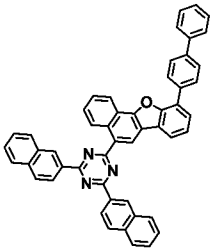
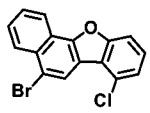
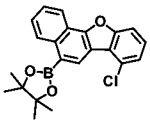
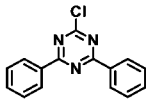
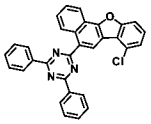
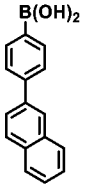
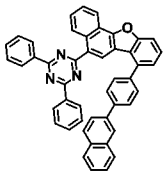
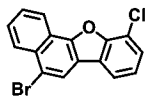
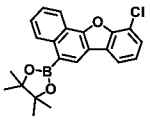
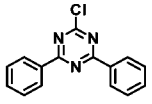
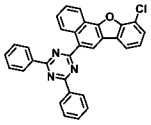
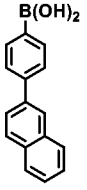
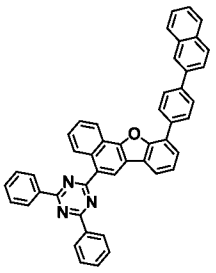
得到固體。將經乾燥的固體通過管柱層析法(DCB)純化並用 DCB 再結晶以獲得化合物 521(9.63g，15.4mmol，89%)。

【0343】 **<製備例 8>化合物 524、597、598、633、708、724、749、756 的製備**

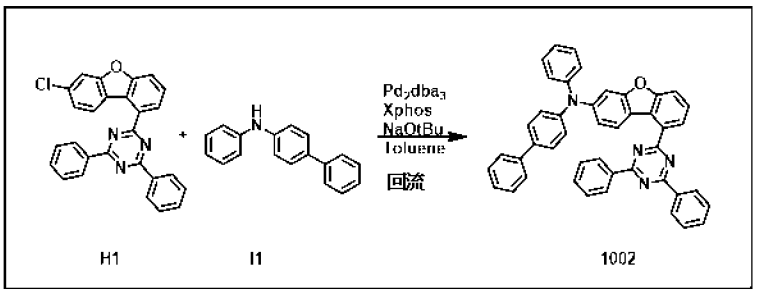
【0344】 化合物 524、597、598、633、708、724、749 和 756 的合成方法與製備例 7 中的製備方法相同，不同之處在於在製備例 8 中，使用了以下表 4 的化合物 A、F、E、G 和 B。

【0345】 表 4

化合物 A	化合物 F	化合物 E	化合物 G	化合物 B	產物	產物產率
A4 	F4 	E17 	G4 	B1	524 	68%
A1 	F1 	E6 	G6 	B1 	597 	65%
A2 	F2 	E6 	G7 	B1 	598 	64%
A1 	F1 	E9 	G8 	B1 	633 	69%

A4 	F4 	E15 	G11 	B4 	708 	65%
A4 	F4 	E17 	G4 	B2 	724 	66%
A1 	F1 	E1 	G12 	B5 	749 	70%
A4 	F4 	E1 	G13 	B5 	756 	65%

【0346】 **<製備例 9>化合物 1002 的製備**

【0347】 

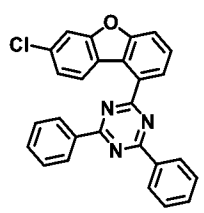
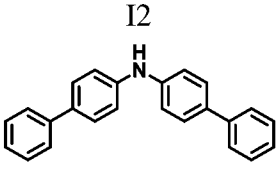
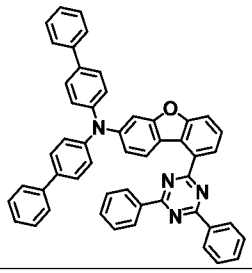
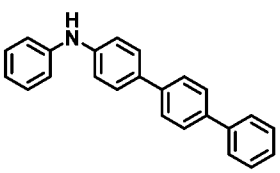
【0348】 將化合物 H1（7.0g，16.1mmol）、化合物 I1（3.96g，16.1mmol）、Pd_2dba_3（0.74g，0.81mmol）、Xphos（0.77g，1.61mmol）

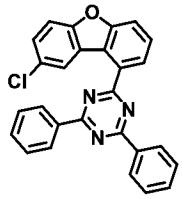
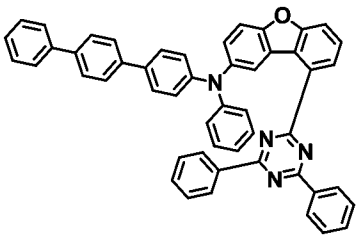
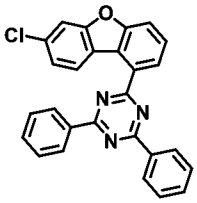
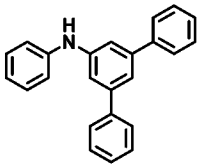
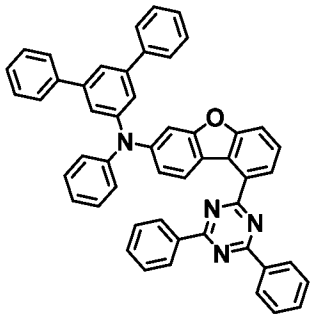
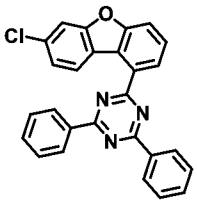
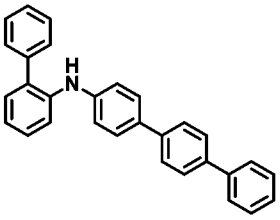
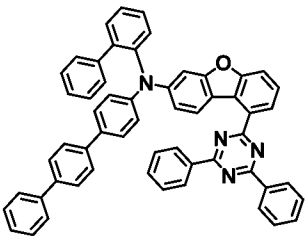
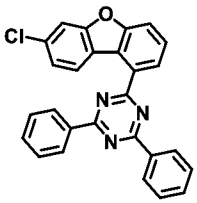
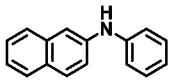
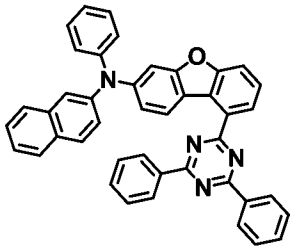
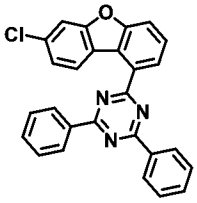
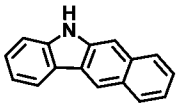
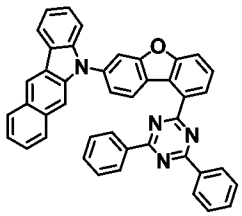
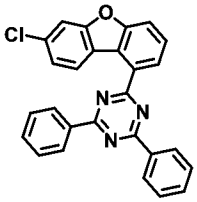
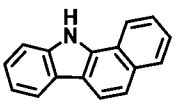
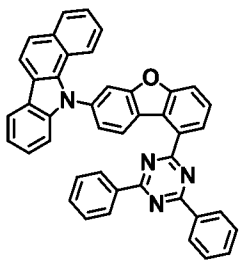
和 NaOtBu（3.10g，32.2mmol）溶解在甲苯 (70mL) 中後，將所得溶液回流 3 小時。反應完成後，將反應產物冷卻至室溫並用 DCM 通過矽藻土過濾器（Celite filter）過濾。濾液濃縮後，經濃縮的濾液在 DCM:Hex=1:2 條件下經過管柱分離，以得到化合物 1002(9.15g，14.7mmol，91%)。

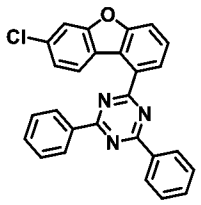
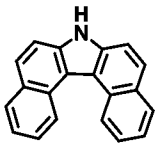
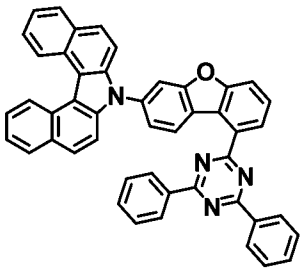
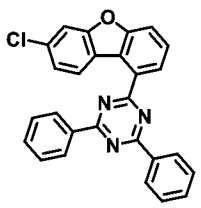
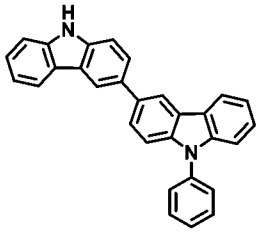
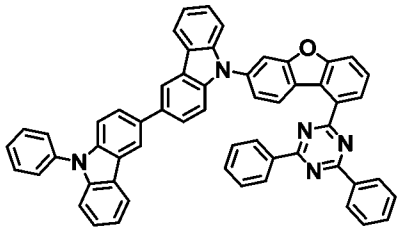
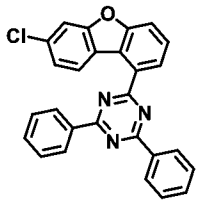
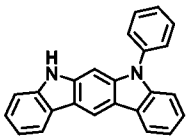
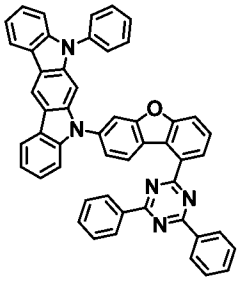
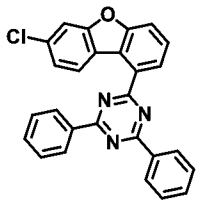
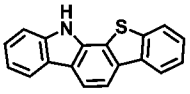
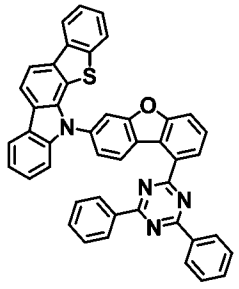
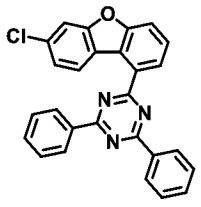
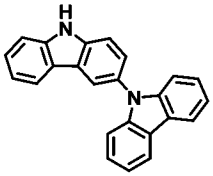
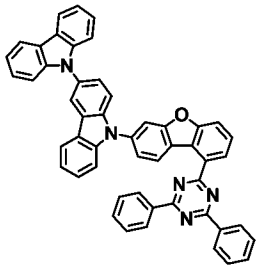
【0349】 **<製備例 10>化合物 1005、1011、1015、1021、1050、1054、1056、1057、1064、1065、1073、1097、1100、1123、1124、1142、1146、1157、1158、1174、1175、1176、1186 和 1187 的製備**

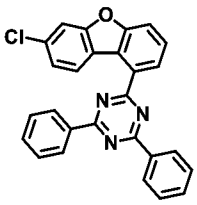
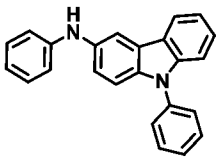
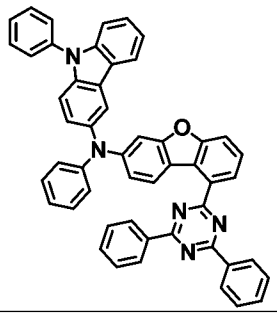
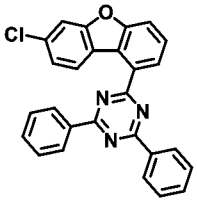
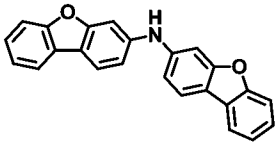
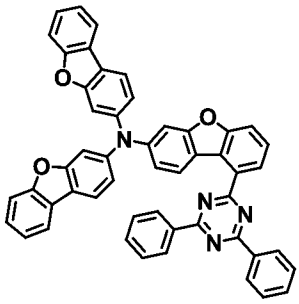
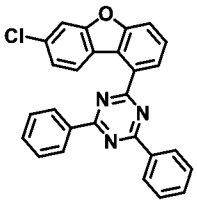
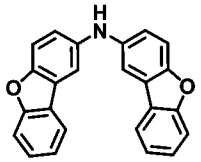
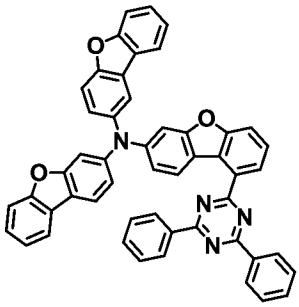
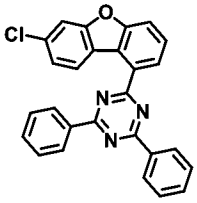
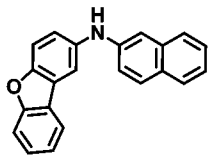
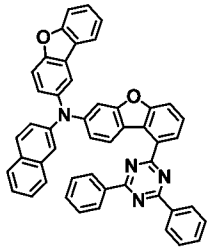
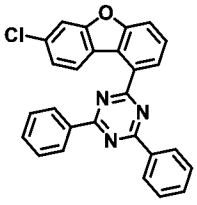
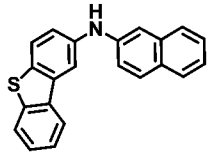
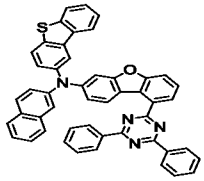
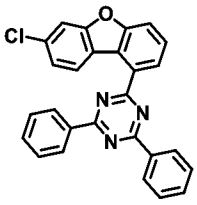
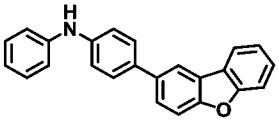
【0350】 化合物 1005、1011、1015、1021、1050、1054、1056、1057、1064、1065、1073、1097、1100、1123、1124、1142、1146、1157、1158、1174、1175、1176、1186 和 1187 以與製備例 9 中的製備方法相同的方式合成，除了在製備例 10 中，使用下述表 5 的化合物 H 和 I 以外。

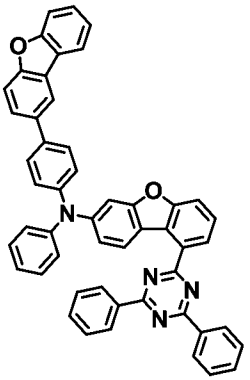
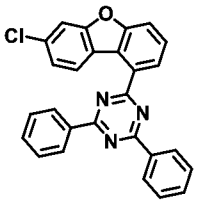
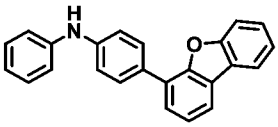
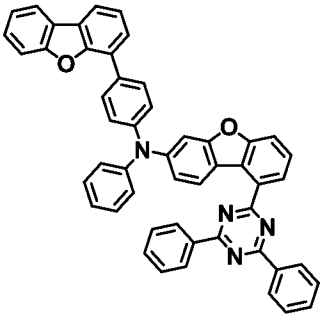
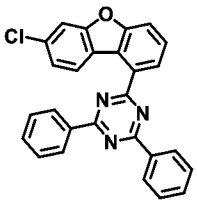
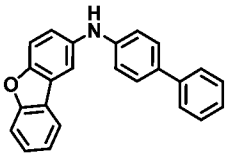
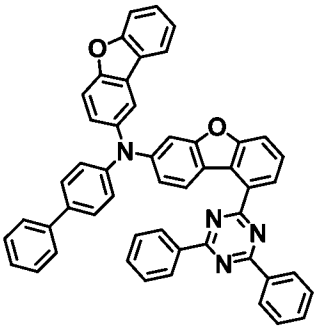
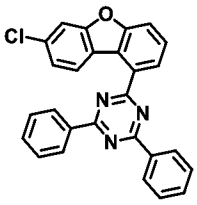
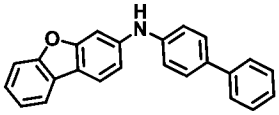
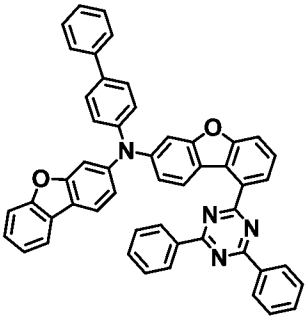
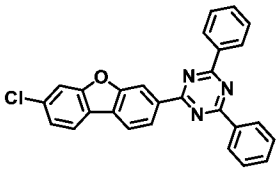
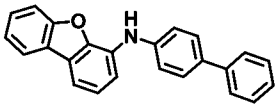
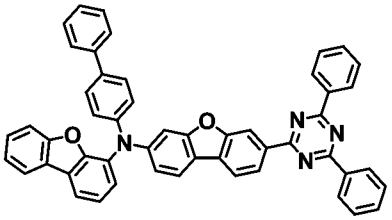
【0351】 表 5

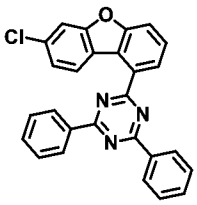
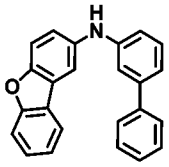
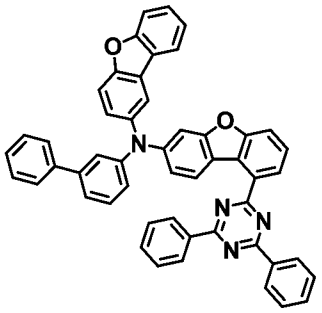
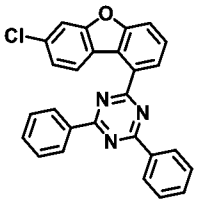
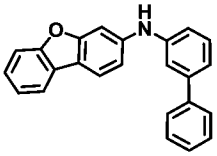
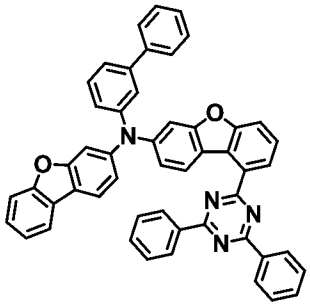
化合物 H	化合物 I	產物	產物產率
H1 	I2 	1005 	89%
H16	I27 	1011	80%

			
H1 	I3 	1015 	85%
H1 	I4 	1021 	84%
H1 	I5 	1050 	85%
H1 	I6 	1054 	88%
H1 	I7 	1056 	86%

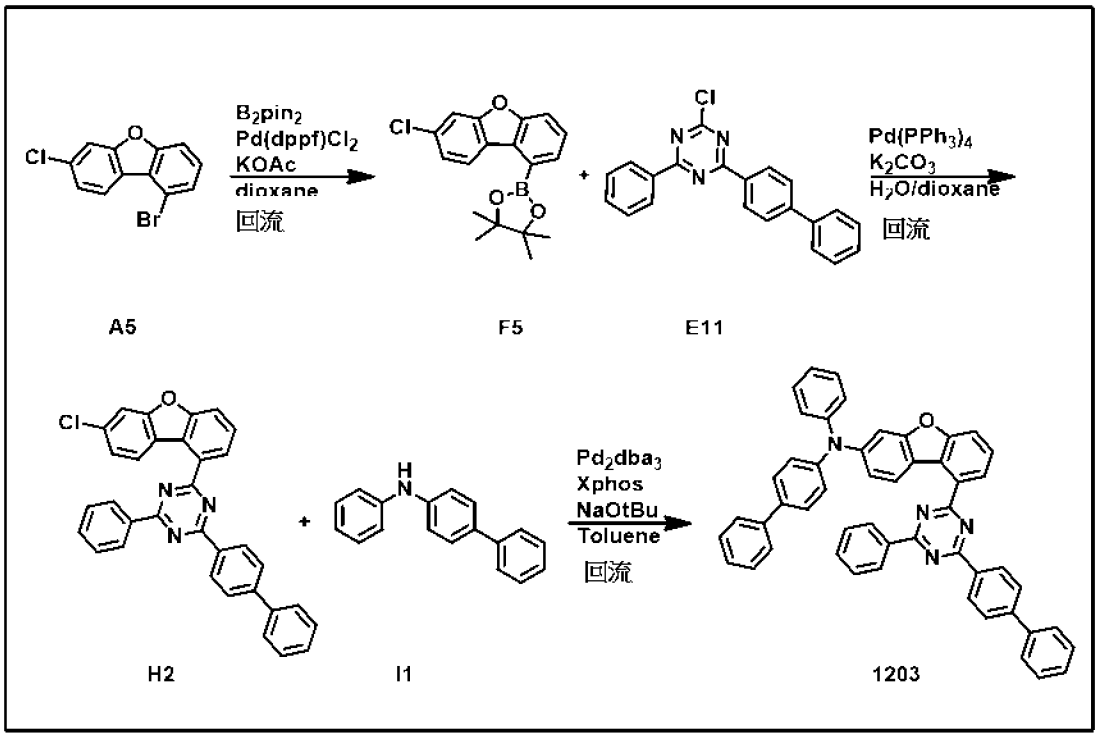
H1 	I8 	1057 	89%
H1 	I9 	1064 	91%
H1 	I10 	1065 	92%
H1 	I11 	1073 	87%
H1 	I12 	1097 	83%

H1 	I13 	1100 	81%
H1 	I14 	1123 	79%
H1 	I15 	1124 	82%
H1 	I16 	1142 	86%
H1 	I17 	1146 	79%
H1 	I18 	1157	82%

			
H1 	I19 	1158 	86%
H1 	I20 	1174 	91%
H1 	I21 	1175 	85%
H17 	I28 	1176 	83%

H1 	I22 	1186 	81%
H1 	I23 	1187 	84%

【0352】 **<製備例 11>化合物 1203 的製備**

【0353】 

【0354】 **1）化合物 F5 的製備**

【0355】 將化合物 A5(50.0g，178mmol)、B_2pin_2(54.1g，213mmol)、$Pd(dppf)Cl_2$(6.51g，8.90mmol)和 KOAc(34.9g，356mmol)溶解在二

噁烷(500mL)中後，將所得溶液回流 4 小時。反應終止後，反應產物減壓過濾濾除鹽分，然後濃縮。經濃縮的反應產物通過管柱層析法(DCM:Hex＝1:4)純化並用甲醇再結晶以獲得化合物 F5(44.0g，134mmol，75%)。

【0356】 **2）化合物 H2 的製備**

【0357】 將化合物 F5(7.0g，21.3mmol)、化合物 E11(7.18g，20.9mmol)、$Pd(PPh_3)_4$(1.23g，1.07mmol)和 K_2CO_3(5.89g，42.6mmol)溶於蒸餾水/1,4-二噁烷(H_2O/1,4-二噁烷(21mL/70mL)中後，將所得溶液回流 2 小時。反應終止後，用水和丙酮洗滌反應產物，以得到固體。將經乾燥的固體通過管柱層析法(DCB)純化並用 DCB 再結晶以獲得化合物 H2(10.4g，20.4mmol，96%)。

【0358】 **3）化合物 1203 的製備**

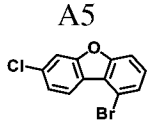
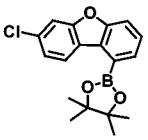
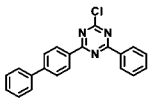
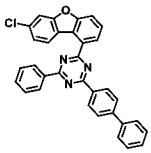
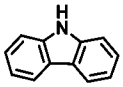
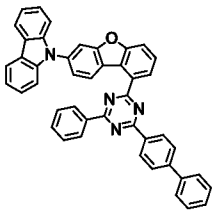
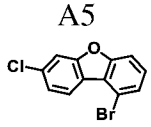
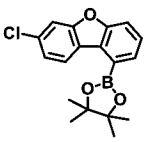
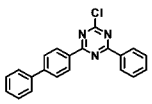
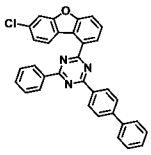
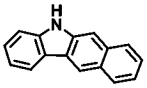
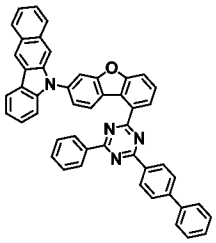
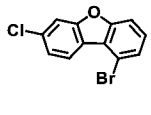
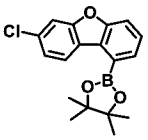
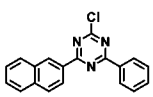
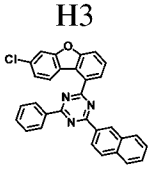
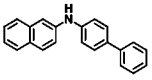
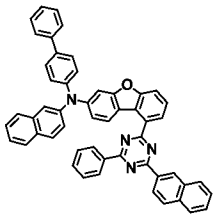
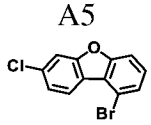
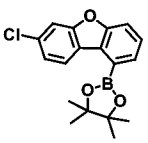
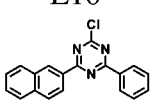
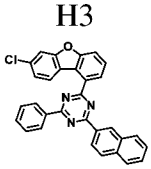
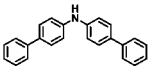
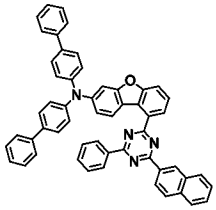
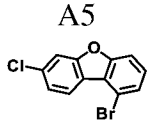
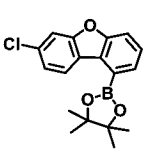
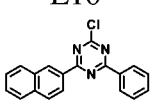
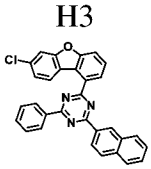
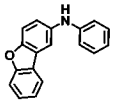
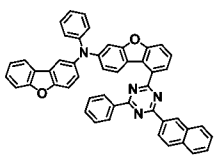
【0359】 將化合物 H2（10.4g，20.4mmol）、化合物 I1（5.00g，20.4mmol）、Pd_2dba_3（0.93g，1.02mmol）、Xphos（0.97g，2.04mmol）和 NaOtBu（3.92g，40.8mmol）溶解在甲苯 (100mL) 中後，將所得溶液回流 3 小時。反應完成後，將反應產物冷卻至室溫並用 DCM 通過矽藻土過濾器過濾。濾液濃縮後，經濃縮的濾液在 DCM:Hex=1:2 條件下經過管柱分離，以得到化合物 1203（11.6g，16.1mmol，76%）。

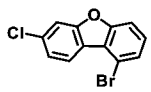
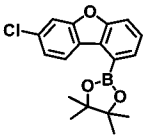
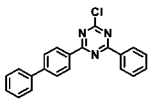
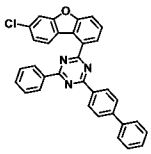
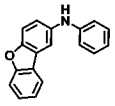
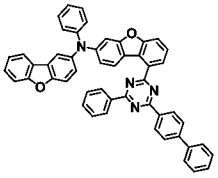
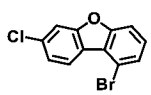
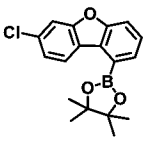
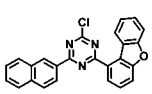
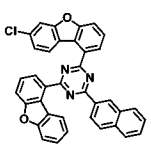
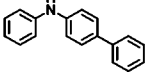
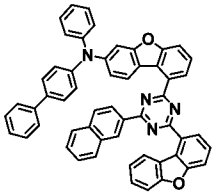
【0360】 **<製備例 12>化合物 1257、1258、1278、1279、1306、1307 和 1365 的製備**

【0361】 化合物 1257、1258、1278、1279、1306、1307 和 1365

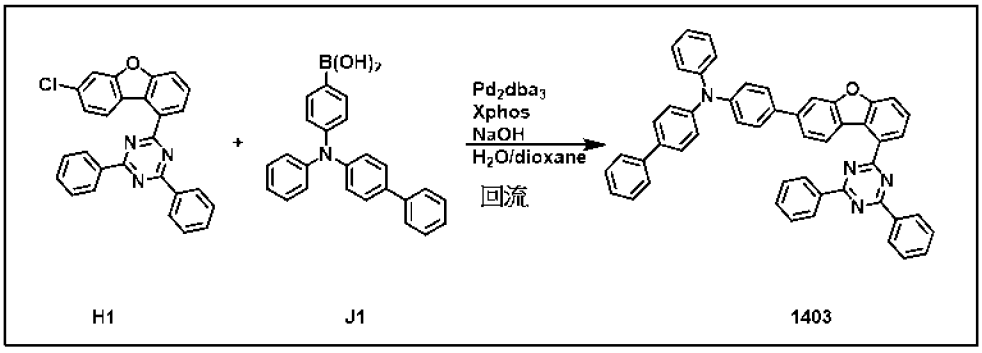
的合成方法與製備例 11 中的製備方法相同，不同之處在於在製備例 12 中，使用了下表 6 中的化合物 A、F、E、H 和 I。

【0362】 表 6

化合物 A	化合物 F	化合物 E	化合物 H	化合物 I	產物	產物產率
A5 	F5 	E11 	H2 	I24 	1257 	55%
A5 	F5 	E11 	H2 	I6 	1258 	57%
A5 	F5 	E10 	H3 	I25 	1278 	51%
A5 	F5 	E10 	H3 	I2 	1279 	53%
A5 	F5 	E10 	H3 	I26 	1306 	54%

A5 	F5 	E11 	H2 	I26 	1307 	56%
A5 	F5 	E9 	H4 	I1 	1365 	49%

【0363】 **<製備例 13>化合物 1403 的製備**

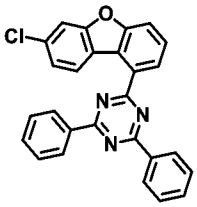
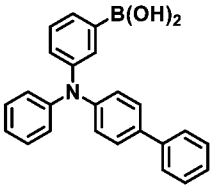
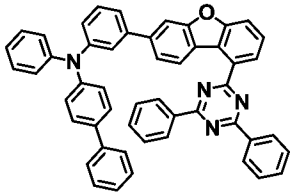
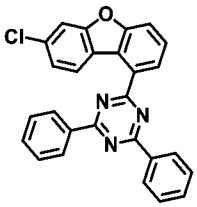
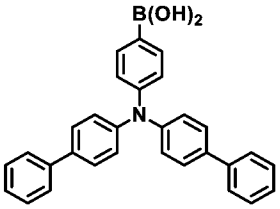
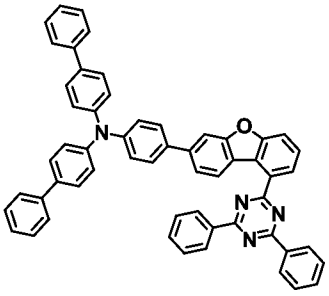
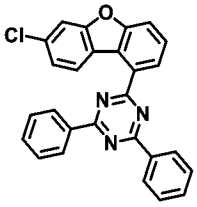
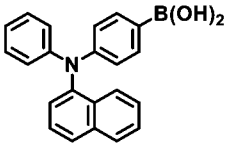
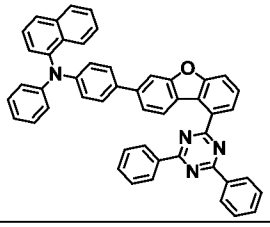
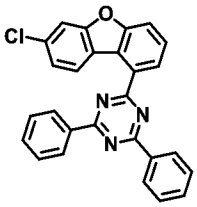
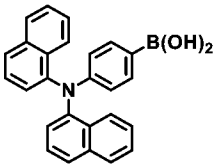
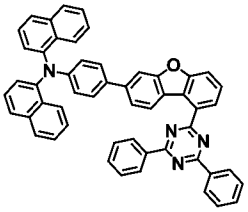
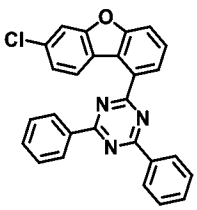
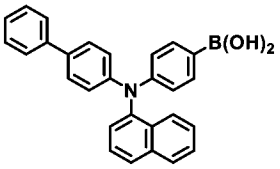
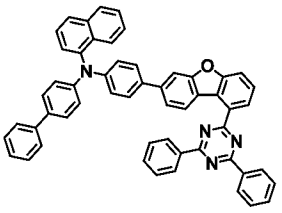
【0364】 

【0365】 將化合物 H1（7.0g，16.1mmol）、化合物 J1（6.50g，16.9mmol）、Pd_2dba_3（0.74g，0.81mmol）、Xphos（0.77g，1.61mmol）和 NaOH（1.29g，32.2mmol）溶解在蒸餾水/1,4-二噁烷(H_2O/1,4-二噁烷(21mL/70mL)中後，將所得溶液回流 3 小時。反應完成後，將反應產物冷卻至室溫並用 DCM 通過矽藻土過濾器過濾。濾液濃縮後，經濃縮的濾液在 DCM:Hex=1:3 條件下經過管柱分離，以得到化合物 1403（9.95g，13.8mmol，86%）。

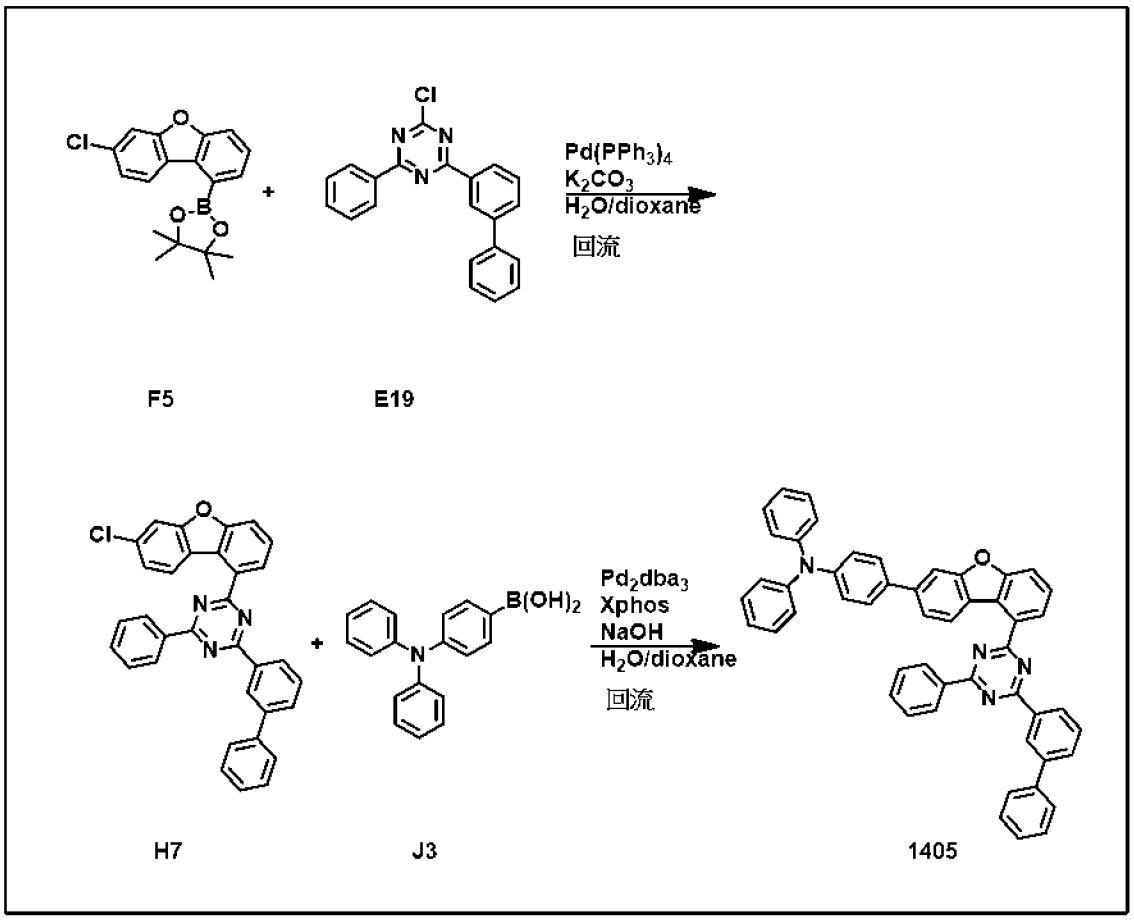
【0366】 **<製備例 14>化合物 1404、1413、1417、1437 和 1439 的製備**

【0367】 化合物 1404、1413、1417、1437 和 1439 除了在製備例 14 中使用下述表 7 中的化合物 H、J 以外，以與製備例 13 的製備方法相同的方式合成。

【0368】 表 7

化合物 H	化合物 J	產物	產物產率
H1 	J2 	1404 	85%
H1 	J4 	1413 	81%
H1 	J5 	1417 	80%
H1 	J6 	1437 	82%
H1 	J7 	1439 	86%

【0369】 **<製備例 15>化合物 1405 的製備**



【0370】

【0371】 **1）化合物 H7 的製備**

【0372】 將化合物 F5(7.0g，21.3mmol)、化合物 E19(7.18g，20.9mmol)、$Pd(PPh_3)_4$(1.23g，1.07mmol)和 K_2CO_3(5.89g，42.6mmol)溶於蒸餾水/1,4-二噁烷(H_2O/1,4-二噁烷)(21mL/70mL)中後，將所得溶液回流 2 小時。反應終止後，用水和丙酮洗滌反應產物，以得到固體。將經乾燥的固體通過管柱層析法(DCB)純化並用 DCB 再結晶以獲得化合物 H7(10.2g，20.0mmol，94%)。

【0373】 **2）化合物 1405 的製備**

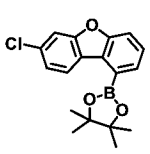
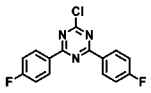
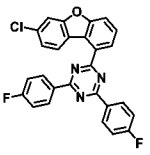
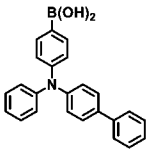
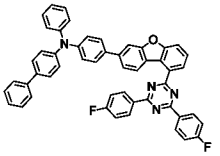
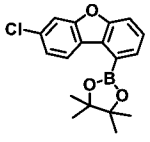
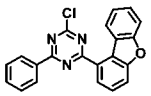
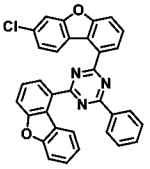
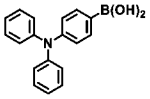
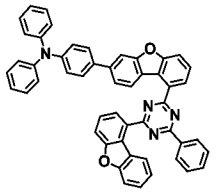
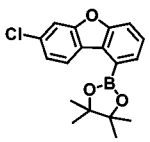
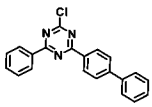
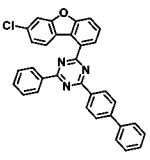
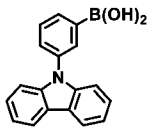
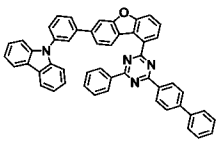
【0374】 將化合物 H7（10.2g，20.0mmol）、化合物 J3（6.07g，21.0mmol）、Pd_2dba_3（0.92g，1.00mmol）、Xphos（0.95g，2.00mmol）和 NaOH（1.60g，40.0mmol）溶解在蒸餾水/1,4-二噁烷(H_2O/1,4-

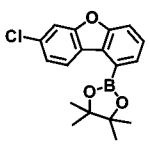
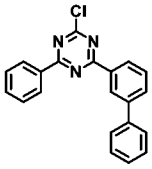
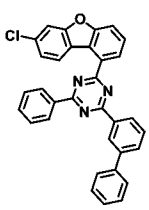
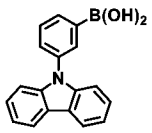
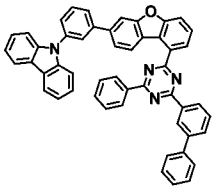
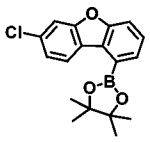
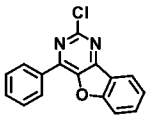
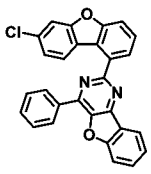
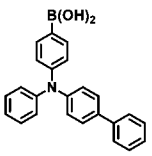
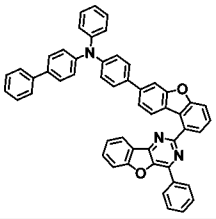
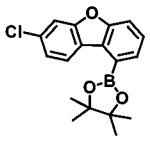
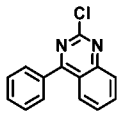
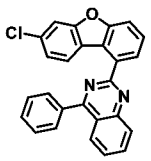
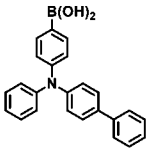
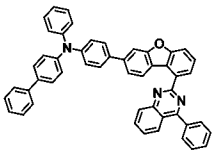
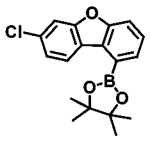
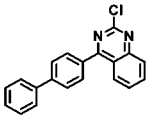
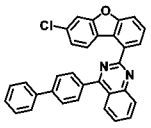
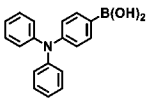
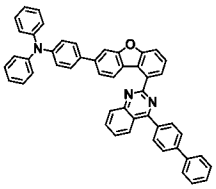
二噁烷)(21mL/70mL)中後，將所得溶液回流 3 小時。反應完成後，將反應產物冷卻至室溫並用 DCM 通過矽藻土過濾器過濾。濾液濃縮後，經濃縮的濾液在 DCM:Hex=1:3 條件下經過管柱分離，以得到化合物 1405(11.8g，16.4mmol，82%)。

【0375】 <製備例 16>化合物 1444、1453、1488、1489、1585、1587 和 1595 的製備

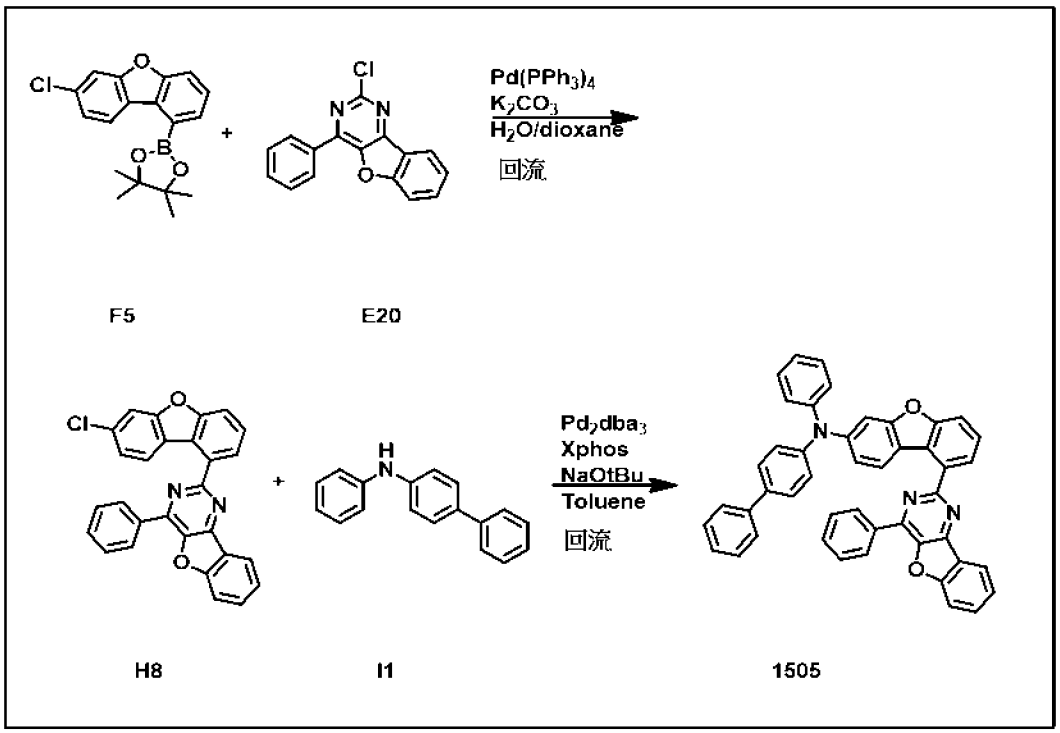
【0376】 化合物 1444、1453、1488、1489、1585、1587 和 1595 以與製備例 15 中的製備方法相同的方式合成，除了在製備例 16 中，使用以下表 8 中的化合物 F、E、H 和 J。

【0377】 表 8

化合物 F	化合物 E	化合物 H	化合物 J	產物	產物產率
F5 	E20 	H5 	J1 	1444 	72%
F5 	E21 	H6 	J3 	1453 	75%
F5 	E11 	H2 	J8 	1488 	79%

F5 	E19 	H7 	J8 	1489 	76%
F5 	E20 	H8 	J1 	1585 	73%
F5 	E22 	H10 	J1 	1587 	74%
F5 	E23 	H11 	J3 	1595 	77%

【0378】 **<製備例 17>化合物 1505 的製備**



【0379】

【0380】 **1）化合物 H8 的製備**

【0381】 將化合物 F5(7.0g，21.3mmol)、化合物 E20(5.86g，20.9mmol)、$Pd(PPh_3)_4$(1.23g，1.07mmol)和 K_2CO_3(5.89g，42.6mmol)溶於蒸餾水/1,4-二噁烷(H_2O/1,4-二噁烷)(21mL/70mL)中後，將所得溶液回流 2 小時。反應終止後，用水和丙酮洗滌反應產物，以得到固體。將經乾燥的固體通過管柱層析法(DCB)純化並用 DCB 再結晶以獲得化合物 H8(8.47g，19.0mmol，89%)。

【0382】 **2）化合物 1505 的製備**

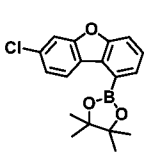
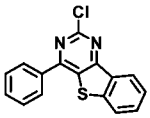
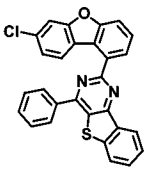
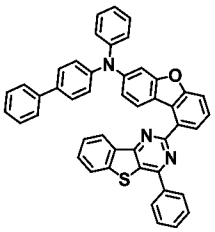
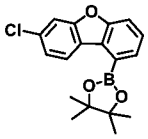
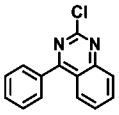
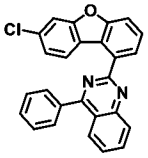
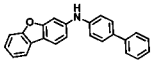
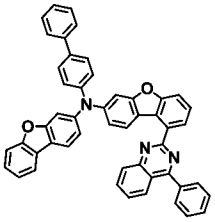
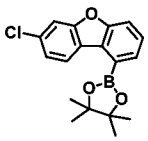
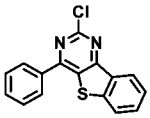
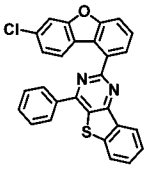
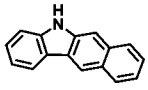
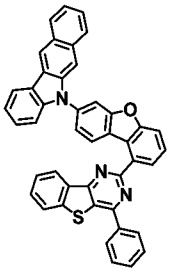
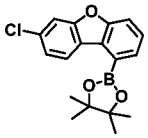
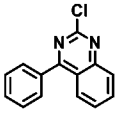
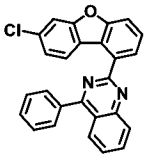
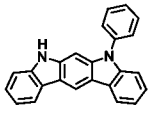
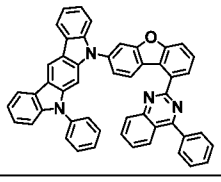
【0383】 將化合物 H8（8.47g，19.0mmol）、化合物 I1（4.66g，19.0mmol）、Pd_2dba_3（0.87g，0.95mmol）、Xphos（0.91g，1.90mmol）和 NaOH（1.52g，38.0mmol）溶解在蒸餾水/1,4-二噁烷(H_2O/1,4-二噁烷)(25mL/85mL)中後，將所得溶液回流 3 小時。反應完成後，將反應產物冷卻至室溫並用 DCM 通過矽藻土過濾器過濾。濾液濃

縮後，經濃縮的濾液在 DCM:Hex=1:2 條件下經過管柱分離，以得到化合物 1505（10.1g，15.4mmol，81%）。

【0384】 **<製備例 18>化合物 1506、1559、1570 和 1579 的製備**

【0385】 化合物 1506、1559、1570 和 1579 以與製備例 17 中的製備方法相同的方式合成，除了在製備例 18 中，使用以下表 9 中的化合物 F、E、H 和 I。

【0386】 表 9

化合物 F	化合物 E	化合物 H	化合物 I	產物	產物產率
F5 	E21 	H9 	I1	1506 	71%
F5 	E22 	H10 	I21 	1559 	73%
F5 	E21 	H9 	I6 	1570 	69%
F5 	E22 	H10 	I10 	1579 	72%

【0387】 製備例 1 至 18 和表 1 至 9 中描述的化合物的合成結果顯示在以下表 10 和 11 中。以下表 10 為 ^{1}H NMR($CDCl_3$，300Mz)的測量值，且以下表 11 為場解吸質譜（field desorption mass spectrometry，FD-MS）的測量值。

【0388】 表 10

化合物	^{1}H NMR($CDCl_3$, 300Mz)
1	δ = 8.81~8.79 (d, 4H), 8.65~8.63 (d, 1H), 8.61 (s, 1H), 8.54~8.52 (d, 1H), 8.06~8.03 (m, 2H), 7.98~7.96 (d, 1H), 7.75~7.73 (d, 1H), 7.70~7.67 (t, 1H), 7.61~7.52 (m, 4H), 7.46~7.40 (m, 3H), 7.38~7.34 (m, 2H), 7.24~7.22 (d, 2H)
13	δ = 9.31 (s, 1H), 9.20~9.18 (d, 1H), 8.78~8.76 (d, 1H), 8.62~8.54 (m, 4H), 8.10~8.08 (d, 1H), 8.03~7.93 (m, 6H), 7.75~7.50 (m, 8H), 7.05~7.01 (m, 3H), 6.86~6.83 (t, 2H)
22	δ = 9.29 (s, 1H), 9.19~9.17 (d, 1H), 8.77~8.75 (d, 1H), 8.64 (s, 2H), 8.60~8.52 (m, 4H), 8.09~8.07 (d, 1H), 8.02~7.94 (m, 6H), 7.74~7.52 (m, 7H), 7.36~7.32 (m, 2H), 7.24~7.22 (t, 2H)
37	δ = 8.83~8.81 (d, 4H), 8.65~8.63 (d, 1H), 8.63 (s, 1H), 8.59 (s, 1H), 8.49~8.47 (d, 1H), 8.04~8.00(t, 1H), 7.86~7.74 (m, 9H), 7.56~7.52 (m, 4H), 7.48~7.45 (m, 2H), 7.39~7.37 (d, 2H), 7.21~7.18 (m, 3H)
39	δ = 9.22 (s, 1H), 8.97~8.95 (d, 1H), 8.94~8.89 (d, 1H), 8.88~8.86 (d, 1H), 8.62~8.60 (d, 1H), 8.20 (s, 1H), 8.19~8.17 (d, 1H), 8.03~7.97 (m, 6H), 7.93~7.91 (d, 1H), 7.90~7.88 (d, 1H), 7.75~7.71 (t, 1H), 7.66~7.50 (m, 13H)
53	δ = 8.82~8.80 (d, 4H), 8.64~8.62 (d, 1H), 8.62 (s, 1H), 8.51~8.49 (d, 1H), 8.03~7.99 (t, 1H), 7.84~7.72 (m, 10H), 7.58~7.51 (m, 5H), 7.46~7.44 (m, 2H), 7.38~7.37 (d, 2H), 7.16~7.11 (m, 4H)
57	δ = 8.80~8.78 (d, 4H), 8.64~8.62 (d, 1H), 8.60 (s, 1H), 8.52~8.50 (d, 1H), 8.04~8.02 (m, 2H), 7.99~7.97 (d, 1H), 7.76~7.74 (d, 1H), 7.69~7.65 (t, 1H), 7.62~7.51 (m, 6H), 7.47~7.41 (m, 5H), 7.39~7.35 (m, 3H), 7.25~7.23 (d, 3H)
58	δ = 9.28 (s, 1H), 9.18~9.16 (d, 1H), 8.78~8.76 (d, 1H), 8.62~8.54 (m, 4H), 8.10~8.08 (d, 1H), 8.03~7.95 (m, 8H), 7.72~7.54 (m, 9H), 7.37~7.30 (m, 3H), 7.23~7.18 (t, 3H)
115	δ = 9.25 (s, 1H), 8.97~8.95 (d, 1H), 8.94~8.92 (d, 2H), 8.87~8.85 (d, 1H), 8.62~8.60 (d, 1H), 8.23~8.21 (d, 1H), 8.17~8.15 (d, 1H), 8.06~8.04 (d, 1H), 8.02~8.00 (m, 2H), 7.87~7.75 (d, 1H), 7.73~7.70 (t, 1H), 7.66~7.44 (m, 11H), 7.46~7.41 (t, 1H)

133	δ = 8.81~8.79 (d, 2H), 8.74~8.72 (d, 1H), 8.61 (s, 1H), 8.49~8.47 (d, 1H), 8.01~7.97 (t, 1H), 7.82~7.70 (m, 9H), 7.59~7.50 (m, 4H), 7.47~7.44 (m, 2H), 7.39~7.37 (d, 2H), 7.15~7.10 (m, 4H)
134	δ = 8.79~8.77 (d, 2H), 8.72~8.70 (d, 1H), 8.58 (s, 1H), 8.47~8.45 (d, 1H), 8.12~7.98 (t, 1H), 7.84~7.75 (m, 9H), 7.62~7.55 (m, 4H), 7.50~7.46 (m, 2H), 7.42~7.38 (d, 2H), 7.25~7.20 (m, 4H)
209	δ = 9.31 (s, 1H), 8.80~8.78 (d, 3H), 8.65~8.63 (d, 1H), 8.62 (s, 1H), 8.53~8.51 (d, 1H), 8.10~8.08 (d, 1H), 8.05~8.01 (m, 2H), 7.97~7.95 (d, 1H), 7.91~7.88 (d, 1H), 7.76~7.74 (d, 1H), 7.71~7.69 (t, 1H), 7.60~7.50 (m, 6H), 7.45~7.42 (m, 4H), 7.37~7.33 (m, 3H), 7.20~7.18 (d, 2H)
226	δ = 9.30 (s, 1H), 9.19~9.17 (d, 1H), 8.76~8.74 (d, 1H), 8.64 (s, 1H), 8.61~8.55 (m, 4H), 8.23~8.22 (d, 1H), 8.13~8.01 (m, 8H), 7.75~7.56 (m, 8H), 7.35~7.29 (m, 3H), 7.24~7.19 (t, 3H)
237	δ = 8.80~8.78 (d, 2H), 8.75~8.72 (m, 3H), 8.65~8.63 (d, 1H), 8.49~8.47 (d, 1H), 8.05~8.01 (m, 2H), 7.99~7.96 (d, 1H), 7.93~7.90 (m, 3H), 7.83 (s, 1H), 7.73~7.65 (m, 7H), 7.58~7.43 (m, 8H), 7.30~7.27 (m, 2H)
249	δ = 8.76~8.74 (d, 4H), 8.67 (s, 1H), 8.65~8.63 (d, 1H), 8.51~8.49 (d, 1H), 8.16~8.13 (d, 1H), 8.03~7.90 (m, 3H), 7.75~7.70 (m, 4H), 7.62~7.59 (t, 1H), 7.57~7.44 (m, 13H)
250	δ = 9.20 (s, 1H), 8.92~8.90 (d, 1H), 8.86~8.84 (d, 4H), 8.64~8.62 (d, 1H), 8.21~8.17 (m, 2H), 8.13~8.11 (m, 2H), 8.79~7.96 (d, 1H), 7.94~7.92 (d, 1H), 7.77~7.55 (m, 16H)
253	δ = 8.78~8.76 (d, 4H), 8.69 (s, 1H), 8.66~8.64 (d, 1H), 8.49~8.47 (d, 1H), 8.18~8.16 (d, 1H), 8.01~7.99 (d, 1H), 7.96~7.94 (d, 1H), 7.92~90 (d, 1H), 7.88~7.85 (d, 2H), 7.75~7.66 (m, 2H), 7.64~7.43 (m, 12H), 7.38~7.36 (d, 2H)
325	δ = 9.34 (s, 1H), 9.23~9.21 (d, 1H), 8.81~8.79 (d, 1H), 8.65~8.57 (m, 4H), 8.13~8.11 (d, 1H), 8.05~7.91 (m, 7H), 7.76~7.52 (m, 8H), 7.12~7.05 (m, 4H), 6.89~6.85 (t, 2H)
327	δ = 9.21 (s, 1H), 8.83~8.81 (d, 4H), 8.60~8.58 (d, 2H), 8.17~8.15 (d, 2H), 8.03~8.01 (m, 2H), 7.93 (s, 1H), 7.67~7.45 (m, 17H)
329	δ = 9.34 (s, 1H), 9.21~9.19 (d, 1H), 8.79~8.77 (d, 1H), 8.66 (s, 1H), 8.63~8.55 (m, 4H), 8.11~8.09 (d, 1H), 8.04~7.92 (m, 8H), 7.74~7.49 (m, 8H), 7.08~7.01 (m, 4H), 6.87~6.84 (t, 2H)
511	δ = 9.41 (s, 1H), 9.38~9.36 (d, 1H), 9.17 (s, 1H), 8.94~8.92 (d, 2H), 8.66~8.64 (d, 1H), 8.26~8.24 (d, 1H), 8.17~8.15 (d, 2H), 8.11~8.09 (d, 2H), 8.03 (s, 1H), 7.99~7.97 (d, 2H), 7.82~7.74 (m, 4H), 7.64~7.58 (m, 4H), 7.56~7.52 (m, 2H), 7.46~7.42 (t, 1H)
521	δ = 9.46~9.44 (d, 1H), 9.33 (s, 2H), 8.94 (s, 1H), 8.82~8.80 (d, 2H), 8.66~8.64 (d, 1H), 8.16~8.14 (d, 2H), 8.10~8.08 (d, 2H), 8.00~7.98 (d, 2H), 7.85~7.80 (m, 5H), 7.69~7.59 (m, 7H), 7.48~7.46 (t, 1H), 7.44~7.42 (d, 1H)
523	δ = 9.42 (s, 2H), 9.39~9.36 (d, 1H), 9.18 (s, 1H), 8.93~8.90 (d, 2H), 8.65~8.63 (d, 1H), 8.24~8.22 (d, 1H), 8.16~8.14 (d, 2H), 8.09~8.07 (d, 2H), 8.01 (s, 1H), 7.98~7.96 (d, 2H), 7.81~7.72 (m, 5H), 7.65~7.59 (m, 4H), 7.55~7.51 (m, 2H),

	7.44~7.41 (t, 1H)
524	δ = 9.41~9.36 (m, 3H), 9.20 (s, 1H), 8.91~8.89 (d, 2H), 8.61~8.60 (d, 1H), 8.17~8.13 (m, 3H), 8.09~8.06 (m, 4H), 7.97~7.95 (d, 2H), 7.77~7.70 (m, 3H), 7.66~7.50 (m, 8H)
551	δ = 9.43 (s, 1H), 9.39~9.37 (d, 1H), 9.21 (s, 1H), 9.15 (s, 1H), 8.93~8.91 (d, 2H), 8.69~8.67 (d, 1H), 8.31~8.29 (d, 1H), 8.21~8.19 (d, 2H), 8.15~8.11 (d, 2H), 8.04 (s, 1H), 7.98~7.94 (d, 3H), 7.83~7.74 (m, 5H), 7.65~7.56 (m, 5H), 7.54~7.51 (m, 2H), 7.45~7.41 (t, 1H)
597	δ = 9.42~9.40 (d, 1H), 9.32 (s, 1H), 8.92 (s, 1H), 8.84~8.82 (d, 2H), 8.65~8.63 (d, 1H), 8.15~8.11 (m, 3H), 8.09~8.07 (d, 2H), 8.02~7.99 (d, 2H), 7.87~7.82 (m, 6H), 7.71~7.60 (m, 8H), 7.49~7.45 (t, 1H), 7.43~7.41 (d, 1H)
598	δ = 9.41~9.39 (d, 1H), 9.31 (s, 1H), 8.91 (s, 1H), 8.82~8.80 (d, 2H), 8.63~8.61 (d, 1H), 8.17~8.12 (m, 3H), 8.08~8.06 (d, 2H), 7.93~7.91 (d, 2H), 7.82~7.70 (m, 6H), 7.65~7.51 (m, 8H), 7.43~7.41 (t, 1H), 7.23~7.21 (d, 1H)
633	δ = 9.38~9.36 (d, 2H), 9.28 (s, 1H), 8.84~8.82 (d, 1H), 8.64 (s, 1H), 8.58~8.56 (d, 1H), 8.15~8.11 (t, 1H), 7.92~7.80 (m, 8H), 7.65~7.58 (m, 4H), 7.48~7.44 (m, 2H), 7.38~7.36 (d, 2H), 7.18~7.11 (m, 4H)
635	δ = 9.39~9.37 (d, 2H), 9.29 (s, 1H), 8.83~8.81 (d, 1H), 8.62 (s, 1H), 8.59~8.57 (d, 1H), 8.24~8.20 (t, 1H), 7.98~7.82 (m, 8H), 7.67~7.59 (m, 4H), 7.51~7.47 (m, 2H), 7.42~7.40 (d, 2H), 7.35~7.28 (m, 4H)
703	δ = 9.35~9.33 (d, 1H), 9.15 (s, 1H), 8.86~8.84 (d, 4H), 8.64~8.62 (d, 1H), 8.23~8.21 (d, 1H), 8.15 (s, 1H), 8.07 (s, 1H), 7.98~7.84 (m, 8H), 7.80~7.69 (m, 3H), 7.69~7.61 (m, 6H), 7.56~7.49 (m, 2H)
708	δ = 9.39~9.35 (m, 2H), 9.21~9.19 (d, 1H), 8.88~8.86 (d, 3H), 8.60~8.58 (d, 1H), 8.55 (s, 1H), 8.19~8.17 (m, 2H), 8.13~8.05 (m, 4H), 7.97~7.95 (m, 2H), 7.83~7.81 (d, 1H), 7.75~7.73 (m, 2H), 7.66~7.59 (m, 8H)
711	δ = 9.40 (s, 1H), 9.37~9.35 (d, 1H), 9.17 (s, 1H), 8.90~8.88 (d, 3H), 8.66~8.64 (d, 1H), 8.27~8.25 (d, 1H), 8.21 (s, 1H), 8.13~8.11 (m, 2H), 8.08~8.06 (d, 2H), 8.07~7.96 (m, 3H), 7.90~7.87 (m, 2H), 7.85~7.83 (d, 1H), 7.79~7.77 (m, 2H), 7.67~7.53 (m, 6H)
724	δ = 9.37~9.35 (d, 1H), 9.20 (s, 1H), 8.87~8.85 (d, 3H), 8.81~8.79 (d, 1H), 8.65~8.63 (d, 1H), 8.25~8.23 (m, 3H), 8.19~8.17 (d, 1H), 8.05~7.99 (m, 3H), 7.94~7.92 (m, 2H), 7.81~7.75 (m, 3H), 7.68~7.54 (m, 8H)
749	δ = 9.44~9.42 (d, 1H), 9.31 (s, 1H), 8.93 (s, 1H), 8.86~8.84 (d, 2H), 8.63~8.61 (d, 1H), 8.17~8.13 (m, 3H), 8.08~8.06 (d, 2H), 8.03~7.98 (d, 2H), 7.88~7.77 (m, 6H), 7.73~7.62 (m, 8H), 7.51~7.47 (t, 1H), 7.44~7.42 (d, 1H)
755	Not measurable due to poor solubility
756	δ = 9.36~9.33 (d, 1H), 9.19 (s, 1H), 8.86~8.84 (d, 4H), 8.66~8.64 (d, 1H), 8.23~8.21 (m, 3H), 8.18~8.16 (d, 1H), 8.12~7.99 (m, 4H), 7.92~7.90 (m, 2H), 7.79~7.77 (m, 3H), 7.69~7.53 (m, 9H)
827	δ = 9.38~9.36 (d, 1H), 9.18 (s, 1H), 8.91~8.89 (d, 4H), 8.64~8.62 (d, 1H), 8.25~8.23 (d, 1H), 8.19 (s, 1H), 8.14~8.12 (m, 2H), 8.09~8.07 (d, 2H), 8.05~7.99 (m, 3H), 7.91~7.86 (m, 2H), 7.82~7.80 (d, 2H), 7.77~7.74 (m, 3H), 7.68~7.56

	(m, 6H)
863	δ = 9.37~9.35 (d, 1H), 9.20 (s, 1H), 8.92~8.90 (d, 4H), 8.66 (s, 1H), 8.65~8.63 (d, 1H), 8.27~8.25 (d, 1H), 8.21 (s, 1H), 8.16~8.14 (m, 2H), 8.10~8.08 (d, 2H), 8.04~7.98 (m, 3H), 7.92~7.89 (m, 2H), 7.86~7.81 (d, 2H), 7.78~7.75 (m, 2H), 7.66~7.54 (m, 6H)
919	δ = 9.21~9.19 (d, 1H), 8.52~8.50 (d, 1H), 8.48~8.46 (d, 1H), 8.42~8.40 (d, 1H), 8.22~8.20 (d, 1H), 8.18~8.16 (d, 1H), 8.10~8.08 (d, 1H), 8.03~8.01 (d, 1H), 7.92~7.86 (m, 9H), 7.80~7.75 (m, 9H)
1002	δ = 8.80~8.78 (d, 4H), 8.51~8.49 (d, 1H), 8.44~8.42 (d, 1H), 7.77~7.75 (d, 1H), 7.64~7.55 (m, 13H), 7.47~7.40 (m, 4H), 7.36~7.34 (d, 1H), 7.32~7.27 (m, 5H)
1005	δ = 8.81~8.79 (d, 4H), 8.50~8.48 (d, 1H), 8.42~8.40 (d, 1H), 7.75~7.73 (d, 1H), 7.65~7.53 (m, 15H), 7.46~7.42 (m, 4H), 7.37~7.35 (d, 1H), 7.33~7.26 (m, 7H)
1011	δ = 8.81~8.79 (d, 4H), 8.49~8.46 (d, 1H), 8.41~8.39 (d, 1H), 7.74~7.72 (d, 1H), 7.67~7.55 (m, 15H), 7.48~7.44 (t, 2H), 7.37~7.30 (m, 4H), 7.26~7.24(m, 4H), 7.12~7.08 (t, 1H), 7.03~7.00 (d, 1H)
1015	δ = 8.77~8.75 (d, 4H), 8.48~8.46 (s, 2H), 8.40~8.38 (d, 1H), 7.86~7.84 (d, 4H), 7.63~7.61 (m, 6H), 7.48~7.42 (m, 6H), 7.35~7.33 (d, 2H), 7.30~7.15 (m, 8H), 7.13~7.09 (t, 1H)
1021	δ = 8.79~8.77 (d, 4H), 8.37~8.35 (d, 1H), 8.38~8.25 (d, 1H), 7.69~7.51 (m, 14H), 7.47~7.33 (m, 9H), 7.22~7.20 (m, 2H), 7.13~7.04 (m, 6H), 6.80~6.78 (d, 1H)
1050	δ = 8.81~8.79 (d, 4H), 8.65 (s, 1H), 8.49~8.47 (d, 1H), 8.42~8.40 (d, 1H), 7.79~7.77 (d, 1H), 7.66~7.48 (m, 11H), 7.45~7.39 (m, 4H), 7.37~7.35 (d, 1H), 7.33~7.26 (m, 4H)
1054	δ = 8.93~8.91 (d, 1H), 8.86~8.84 (d, 4H), 8.64 (s, 1H), 8.55~8.53 (d, 1H), 8.30~8.28 (d, 1H), 8.09~8.07 (d, 1H), 7.97 (s, 1H), 7.91~7.85 (m, 3H), 7.76~7.72 (t, 1H), 7.66~7.54 (m, 8H), 7.52~7.41 (m, 3H), 7.37~7.33 (t, 1H)
1056	δ = 8.90~8.88 (d, 1H), 8.83~8.81 (d, 4H), 8.56~8.54 (d, 1H), 8.26~8.24 (d, 1H), 8.23~8.21 (d, 1H), 8.01~7.99 (d, 1H), 7.93~7.91 (d, 1H), 7.91 (s, 1H), 7.79~7.74 (t, 2H), 7.63~7.54 (m, 6H), 7.52~7.50 (d, 1H), 7.45~7.33 (m, 5H), 7.22~7.18 (t, 1H)
1057	δ = 9.28~9.26 (d, 2H), 8.95~8.93 (d, 1H), 8.85~8.83 (d, 4H), 8.56~8.54 (d, 1H), 8.07~8.05 (d, 1H), 7.93~7.87 (m, 4H), 7.78~7.69 (m, 5H), 7.64~7.50 (m, 9H), 7.49~7.47 (d, 1H)
1064	δ = 8.91~8.89 (d, 1H), 8.85~8.83 (d, 4H), 8.54~8.52 (d, 1H), 8.47 (s, 2H), 8.27~8.24 (m, 2H), 7.93 (s, 1H), 7.90~7.88 (d, 1H), 7.82~7.78 (m, 2H), 7.75~7.71 (t, 1H), 7.64~7.54 (m, 12H), 7.53~7.43 (m, 6H), 7.37~7.30 (m, 2H)
1065	δ = 8.85 (s, 1H), 8.82~8.80 (d, 5H), 8.51~8.49 (d, 1H), 8.28~8.25 (d, 2H), 7.87 (s, 1H), 7.87~7.85 (d, 1H), 7.72~7.68 (t, 1H), 7.63~7.51 (m, 10H), 7.48~7.25 (m, 9H)
1073	δ = 8.96~8.94 (d, 1H), 8.87~8.85 (d, 4H), 8.58~8.56 (d, 1H), 8.29~8.24 (m, 3H), 8.16~8.14 (d, 1H), 7.94~7.92 (d, 1H), 7.92 (s, 1H), 7.80~7.76 (t, 1H), 7.70~7.68 (d, 1H), 7.61~7.55 (m, 6H), 7.49~7.45 (m, 4H), 7.39~7.36 (t, 2H)

1097	δ = 8.81~8.79 (d, 4H), 8.44~8.41 (m, 2H), 8.12~8.10 (d, 1H), 8.09~8.07 (d, 1H), 7.73~7.71 (d, 1H), 7.65~7.49 (m, 13H), 7.36~7.30 (m, 3H), 7.28~7.23 (m, 3H), 7.20~7.18 (d, 2H), 7.15~7.13 (d, 1H), 7.07~7.03 (t, 1H), 6.99~6.97 (d, 1H)
1100	δ = 8.79~8.77 (d, 4H), 8.42~8.37 (m, 2H), 8.09~8.07 (d, 1H), 8.06~8.04 (d, 1H), 7.71~7.69 (d, 1H), 7.63~7.47 (m, 13H), 7.37~7.34 (m, 3H), 7.30~7.25 (m, 3H), 7.21~7.19 (d, 2H), 7.13~7.11 (d, 1H), 7.05~7.02 (t, 1H), 6.98~6.96 (d, 1H)
1123	δ = 8.79~8.77 (d, 4H), 8.46~8.44 (d, 1H), 8.41~8.39 (d, 1H), 7.83~7.81 (m, 4H), 7.51~7.49 (d, 1H), 7.48~7.42 (m, 11H), 7.36~7.34 (m, 2H), 7.29~7.27 (d, 2H), 7.25~7.23 (m, 2H), 7.22 (s, 1H), 7.00~6.98 (d, 1H)
1124	δ = 8.80~8.78 (d, 4H), 8.45~8.43 (d, 1H), 8.39~8.37 (d, 1H), 7.82~7.80 (m, 4H), 7.53~7.51 (d, 1H), 7.49~7.43 (m, 11H), 7.38~7.35 (m, 2H), 7.30~7.28 (d, 2H), 7.26~7.24 (m, 2H), 7.22~7.20 (d, 1H), 6.99~6.97 (d, 1H)
1142	δ = 8.81~8.79 (d, 4H), 8.45~8.43 (d, 1H), 8.41~8.39 (d, 1H), 7.83 (s, 1H), 7.81~7.76 (m, 3H), 7.73~7.71 (d, 1H), 7.62~7.51 (m, 11H), 7.48~7.33 (m, 5H), 7.30~7.25 (m, 2H), 7.05~7.03 (d, 1H)
1146	δ = 8.80~8.78 (d, 4H), 8.51~8.49 (d, 1H), 8.43~8.41 (d, 1H), 8.03 (s, 1H), 7.97~7.95 (d, 1H), 7.86~7.84 (d, 1H), 7.81~7.74 (m, 3H), 7.72~7.70 (d, 1H), 7.63~7.53 (m, 9H), 7.46~7.26 (m, 7H), 7.09~7.06 (d, 1H)
1157	δ = 8.81~8.79 (d, 4H), 8.51~8.49 (d, 1H), 8.42~8.40 (d, 1H), 8.00~7.98 (d, 1H), 7.93~7.91 (d, 1H), 7.88~7.86 (d, 2H), 7.75~7.73 (d, 1H), 7.64~7.56 (m, 9H), 7.49~7.40 (m, 2H), 7.38~7.28 (m, 8H), 7.14~7.10 (t, 1H), 7.07~7.05 (d, 1H)
1158	δ = 8.82~8.80 (d, 4H), 8.49~8.47 (d, 1H), 8.42~8.40 (d, 1H), 8.14 (s, 1H), 8.01~7.99 (d, 1H), 7.75~7.73 (d, 1H), 7.69~7.57 (m, 10H), 7.50~7.46 (t, 1H), 7.39~7.26 (m, 10H), 7.13~7.09 (t, 1H), 7.04~7.02 (d, 1H)
1174	δ = 8.80~8.78 (d, 4H), 8.49~8.46 (d, 1H), 8.41~8.39 (d, 1H), 7.85~7.83 (m, 2H), 7.73~7.71 (d, 1H), 7.61~7.52 (m, 13H), 7.48~7.42 (m, 3H), 7.39~7.26 (m, 6H), 7.04~7.02 (d, 1H)
1175	δ = 8.81~8.79 (d, 4H), 8.52~8.50 (d, 1H), 8.43~8.41 (d, 1H), 7.90~7.88 (d, 1H), 7.85~7.83 (d, 1H), 7.75~7.73 (d, 1H), 7.62~7.51 (m, 11H), 7.46~7.41 (m, 4H), 7.39~7.29 (m, 6H), 7.24~7.22 (d, 1H), 7.08~7.06 (d, 1H)
1176	δ = 9.40 (s, 1H), 8.94~8.92 (d, 1H), 8.85~8.83 (d, 4H), 8.28~8.26 (d, 1H), 8.22~8.18 (m, 3H), 7.88 (s, 1H), 7.68~7.60 (m, 9H), 7.56~7.54 (d, 2H), 7.48~7.44 (m, 5H), 7.37~7.32 (m, 4H), 7.23~7.21 (d, 1H)
1186	δ = 8.79~8.77 (d, 4H), 8.47~8.44 (d, 1H), 8.41~8.39 (d, 1H), 7.86~7.83 (m, 2H), 7.72~7.70 (d, 1H), 7.60~7.44 (m, 13H), 7.41~7.28 (m, 8H), 7.18~7.16 (d, 1H), 7.06~7.03 (d, 1H)
1187	δ = 8.80~8.78 (d, 4H), 8.50~8.47 (d, 1H), 8.42~8.40 (d, 1H), 7.90~7.88 (d, 1H), 7.85~7.83 (d, 1H), 7.74~7.72 (d, 1H), 7.60~7.52 (m, 10H), 7.48 (s, 1H), 7.42~7.79 (m, 9H), 7.26~7.24 (d, 1H), 7.21~7.19 (d, 1H), 7.08~7.06 (d, 1H)
1203	δ = 8.82~8.80 (d, 4H), 8.51~8.49 (d, 1H), 8.43~8.41 (d, 1H), 7.78~7.76 (d, 1H), 7.62~7.57 (m, 13H), 7.48~7.39 (m, 6H), 7.36~7.34 (d, 2H), 7.31~7.25 (m, 6H)
1257	δ = 8.91~8.89 (d, 1H), 8.85~8.83 (d, 4H), 8.53~8.51 (d, 1H), 8.32~8.30 (d, 1H), 8.11~8.09 (d, 1H), 7.98 (s, 1H), 7.92~7.85 (m, 4H), 7.77~7.73 (t, 1H), 7.68~7.52

	(m, 9H), 7.50~7.42 (m, 4H), 7.38~7.34 (t, 1H)
1258	δ = 8.90~8.88 (d, 1H), 8.84~8.82 (d, 4H), 8.54~8.53 (d, 1H), 8.31~8.29 (d, 1H), 8.10~8.08 (d, 1H), 7.97 (s, 1H), 7.91~7.82 (m, 5H), 7.79~7.75 (t, 1H), 7.69~7.53 (m, 9H), 7.51~7.43 (m, 5H), 7.40~7.36 (t, 1H)
1278	δ = 9.35 (s, 1H), 8.86~8.84 (m, 3H), 8.59~8.57 (d, 1H), 8.48~8.46 (d, 1H), 8.02~8.00 (d, 2H), 7.92~7.90 (d, 1H), 7.80~7.75 (m, 3H), 7.66~7.53 (m, 11H), 7.48~7.40 (m, 7H), 7.35~7.28 (m, 3H), 7.08~7.06 (d, 1H)
1279	δ = 9.36 (s, 1H), 8.86~8.84 (m, 3H), 8.57~8.55 (d, 1H), 8.48~8.46 (d, 1H), 8.05~8.01 (m, 2H), 7.93~7.91 (d, 1H), 7.77~7.75 (d, 1H), 7.65~7.50 (m, 14H), 7.46~7.42 (m, 5H), 7.35~7.29 (m, 6H), 7.06~7.04 (d, 1H)
1306	δ = 9.34 (s, 1H), 8.84~8.82 (m, 3H), 8.53~8.51 (d, 1H), 8.46~8.44 (d, 1H), 8.00~7.98 (d, 2H), 7.89~7.87 (d, 1H), 7.84~7.82 (d, 1H), 7.81 (s, 1H), 7.74~7.72 (d, 1H), 7.60~7.51 (m, 7H), 7.47~7.43 (t, 2H), 7.36~7.28 (m, 5H), 7.23~7.21 (m, 2H), 7.08~7.04 (t, 1H), 6.99~6.96 (d, 1H)
1307	δ = 8.86~8.84 (d, 2H), 8.81~8.79 (d, 2H), 8.47~8.45 (d, 1H), 8.42~8.40 (d, 1H), 7.84~7.82 (d, 2H), 7.79~7.77 (d, 2H), 7.73~7.71 (d, 1H), 7.67~7.65 (d, 2H), 7.60~7.53 (m, 5H), 7.51~7.39 (m, 5H), 7.35~7.22 (m, 7H), 7.08~7.05 (t, 1H), 7.01~6.96 (d, 1H)
1365	δ = 9.40 (s, 1H), 8.86~8.84 (d, 1H), 8.75~8.73 (d, 1H), 8.65~8.63 (d, 1H), 8.57~8.54 (t, 2H), 8.04~8.02 (d, 1H), 8.00~7.98 (d, 1H), 7.96~7.94 (d, 1H), 7.87~7.85 (d, 1H), 7.79~7.77 (d, 1H), 7.68~7.65 (m, 2H), 7.62~7.49 (m, 8H), 7.45~7.42 (t, 2H), 7.35~7.29 (m, 4H), 7.22~7.20 (d, 4H), 7.16~7.12 (t, 1H), 7.11~7.07 (t, 1H), 6.93~6.90 (d, 1H)
1403	δ = 8.83~8.81 (d, 4H), 8.63~8.60 (d, 1H), 8.44~8.42 (d, 1H), 7.84~7.82 (d, 1H), 7.79~7.77 (d, 1H), 7.69~7.58 (m, 9H), 7.53~7.49 (m, 3H), 7.45~7.40 (m, 3H), 7.38~7.36 (m, 2H), 7.34~7.29 (m, 3H), 7.25~7.23 (d, 4H), 7.21~7.17 (t, 1H), 7.15~7.11 (t, 1H)
1404	δ = 8.82~8.80 (d, 4H), 8.61~8.59 (d, 1H), 8.42~8.40 (d, 1H), 7.82~7.80 (d, 1H), 7.77 (s, 1H), 7.67~7.56 (m, 9H), 7.52~7.48 (m, 3H), 7.44~7.39 (m, 3H), 7.37~7.36 (m, 2H), 7.33~7.29 (m, 3H), 7.23~7.21 (d, 4H), 7.15~7.13 (t, 1H), 7.09~7.05 (t, 1H)
1405	δ = 9.01 (s, 1H), 8.80~8.78 (d, 2H), 8.75~8.73 (d, 1H), 8.70~8.68 (d, 1H), 8.49~8.47 (d, 1H), 8.15~8.13 (d, 2H), 7.92 (s, 1H), 7.84~7.80 (m, 4H), 7.78~7.76 (d, 1H), 7.74~7.56 (m, 9H), 7.52~7.43 (m, 10H), 7.35~7.31 (t, 1H)
1413	δ = 8.85~8.83 (d, 4H), 8.64~8.62 (d, 1H), 8.45~8.43 (d, 1H), 7.83~7.81 (d, 1H), 7.78~7.76 (d, 1H), 7.70~7.54 (m, 9H), 7.52~7.44 (m, 4H), 7.41~7.35 (m, 3H), 7.33~7.30 (m, 3H), 7.28~7.22 (m, 4H), 7.20~7.12 (d, 5H), 7.10~7.08 (t, 2H)
1417	δ = 8.84~8.82 (d, 4H), 8.61~8.59 (d, 1H), 8.44~8.42 (d, 1H), 7.82~7.80 (d, 1H), 7.77~7.74 (d, 1H), 7.68~7.53 (m, 8H), 7.51~7.46 (m, 4H), 7.44~7.40 (m, 3H), 7.38~7.35 (m, 2H), 7.33~7.30 (m, 2H), 7.27~7.23 (d, 3H), 7.21~7.17 (t, 1H)
1437	δ = 8.86~8.84 (d, 4H), 8.62~8.60 (d, 1H), 8.45~8.43 (d, 1H), 7.84~7.82 (d, 1H), 7.76~7.74 (d, 1H), 7.69~7.54 (m, 8H), 7.49~7.47 (m, 4H), 7.43~7.39 (m, 3H), 7.37~7.34 (m, 2H), 7.32~7.29 (m, 3H), 7.26~7.22 (m, 4H), 7.20~7.16 (t, 1H)

1439	δ = 8.84~8.82 (d, 4H), 8.63~8.61 (d, 1H), 8.43~8.41 (d, 1H), 7.83~7.81 (d, 1H), 7.78~7.76 (d, 1H), 7.67~7.52 (m, 8H), 7.50~7.47 (m, 5H), 7.44~7.39 (m, 4H), 7.37~7.34 (m, 2H), 7.31~7.28 (m, 2H), 7.26~7.22 (d, 3H), 7.19~7.15 (t, 1H)
1444	δ = 8.83~8.80 (d, 4H), 8.55~8.53 (d, 1H), 8.39~8.37 (d, 1H), 7.84 (s, 1H), 7.83~7.81 (d, 1H), 7.66~7.58 (m, 5H), 7.53~7.51 (d, 2H), 7.48~7.41 (m, 3H), 7.34~7.20 (m, 13H), 7.10~7.07 (t, 1H)
1453	δ = 8.85~8.84 (d, 2H), 8.75~8.73 (d, 1H), 8.72~8.70 (d, 1H), 8.55~8.53 (d, 1H), 8.52~8.50 (d, 1H), 7.87~7.83 (m, 3H), 7.69~7.56 (m, 9H), 7.52~7.48 (t, 1H), 7.42~7.40 (d, 1H), 7.31~7.29 (m, 3H), 7.18~7.15 (m, 7H), 7.07~7.03 (t, 2H)
1488	δ = 8.86~8.84 (d, 2H), 8.82~8.80 (d, 2H), 8.69~8.67 (d, 1H), 8.43~8.41 (d, 1H), 8.17~8.15 (d, 2H), 7.91~7.89 (d, 2H), 7.82~7.78 (m, 4H), 7.70~7.58 (m, 8H), 7.56~7.46 (m, 5H), 7.44~7.38 (m, 3H), 7.31~7.28 (t, 2H)
1489	δ = 9.05 (s, 1H), 8.84~8.82 (d, 2H), 8.81~8.79 (d, 1H), 8.74~8.72 (d, 1H), 8.48~8.46 (d, 1H), 8.19~8.17 (d, 2H), 7.91 (s, 1H), 7.86~7.82 (m, 3H), 7.78~7.76 (d, 1H), 7.72~7.58 (m, 9H), 7.50~7.30 (m, 9H), 7.25~7.23 (t, 1H)
1505	δ = 8.79~8.77 (d, 2H), 8.48~8.46 (d, 1H), 8.40~8.38 (d, 1H), 8.25~8.23 (d, 1H), 7.80~7.75 (m, 2H), 7.68~7.48 (m, 8H), 7.46~7.42 (t, 2H), 7.37~7.20 (m, 10H), 7.09~7.00 (m, 2H)
1506	δ = 8.67~8.65 (d, 2H), 8.42~8.40 (d, 1H), 8.35~8.33 (d, 1H), 8.21~8.19 (d, 1H), 7.71~7.68 (m, 2H), 7.63~7.47 (m, 8H), 7.43~7.39 (t, 2H), 7.36~7.18 (m, 10H), 7.05~7.02 (m, 2H)
1559	δ = 8.58~5.56 (d, 1H), 8.34~8.32 (d, 1H), 8.25~8.23 (d, 1H), 8.21~8.19 (d, 1H), 7.96~7.91 (m, 3H), 7.85~7.83 (d, 1H), 7.83 (s, 1H), 7.65~7.51 (m, 12H), 7.48~7.43 (m, 3H), 7.41~7.29 (m, 4H), 7.26~7.24 (d, 2H), 7.09~7.07 (d, 1H)
1570	δ = 9.03~8.99 (t, 1H), 8.79~8.75 (t, 1H), 8.65~8.63 (d, 1H), 8.53~8.44 (m, 3H), 8.32~8.38 (t, 1H), 8.11~8.07 (t, 1H), 8.04~7.99 (t, 1H), 7.97~7.95 (d, 1H), 7.88~7.82 (m, 2H), 7.77~7.60 (m, 6H), 7.53~7.40 (m, 5H), 7.38~7.32 (t, 1H), 7.26~7.24 (d, 1H)
1579	δ = 8.79~8.77 (d, 1H), 8.65 (s, 1H), 8.60 (s, 1H), 8.84~8.82 (d, 1H), 8.27~8.25 (d, 1H), 8.06~7.98 (m, 4H), 7.95~7.93 (d, 1H), 7.87 (s, 1H), 7.79~7.65 (m, 7H), 7.62~7.37 (m, 8H), 7.33~7.23 (m, 4H)
1585	δ = 8.80~8.78 (d, 2H), 8.48 (s, 1H), 8.43~8.41 (d, 1H), 7.92 (s, 1H), 7.84~7.77 (m, 2H), 7.72~7.70 (d, 2H), 7.64~7.60 (m, 5H), 7.59~7.55(t, 1H), 7.49~7.45 (m, 2H), 7.31~7.19 (m, 14H), 7.07~7.04 (t, 2H)
1587	δ = 8.56~8.54 (m, 2H), 8.30~8.28 (d, 1H), 8.26~8.24 (d, 1H), 8.03~7.99 (t, 1H), 7.96~7.93 (m, 3H), 7.72~7.67 (m, 3H), 7.62~7.59 (m, 6H), 7.53~7.48 (m, 2H), 7.45~7.42 (m, 3H), 7.34~7.30 (m, 3H), 7.26~7.21 (m, 7H), 7.10~7.06 (t, 1H)
1595	δ = 8.57~8.55 (m, 2H), 8.31~8.29 (d, 1H), 8.27~8.25 (d, 1H), 8.04~8.00 (t, 1H), 7.97~7.94 (m, 2H), 7.73~7.68 (m, 3H), 7.63~7.61 (m, 5H), 7.52~7.47 (m, 2H), 7.44~7.41 (m, 4H), 7.35~7.29 (m, 4H), 7.25~7.19 (m, 7H), 7.12~7.08 (t, 1H)

【0389】 表 11

化合物	FD-Mass	化合物	FD-Mass

1	m/z=525.2012(C37H23N3O, 525.1841)	1054	m/z=614.2082(C43H26N4O, 614.2107)
13	m/z=625.2178(C45H27N3O, 625.2154)	1056	m/z=614.2074(C43H26N4O, 614.2107)
22	m/z=625.2146(C45H27N3O, 625.2154)	1057	m/z=664.2318(C47H28N4O, 664.2263)
37	m/z=651.2102(C47H29N3O, 651.2311)	1064	m/z=805.2941(C57H35N5O, 805.2842)
39	m/z=651.2183(C47H29N3O, 651.2311)	1065	m/z=729.2518(C51H31N5O, 729.2529)
53	m/z=701.2589(C51H31N3O, 701.2467)	1073	m/z=670.1769(C45H26N4OS, 670.1827)
57	m/z=677.2515(C49H31N3O, 677.2467)	1097	m/z=729.2615(C51H31N5O, 729.2529)
58	m/z=677.3152(C49H31N3O, 677.2467)	1100	m/z=731.2721(C51H33N5O, 731.2685)
97	m/z=651.2279(C47H29N3O, 651.2311)	1123	m/z=746.2348(C51H30N4O3, 746.2318)
115	m/z=615.1824(C43H25N3O2, 615.1947)	1124	m/z=746.2482(C51H30N4O3, 746.2318)
133	m/z=655.2200(C47H27N3O2, 665.2103)	1142	m/z=706.2417(C49H30N4O2, 706.2369)
134	m/z=665.2021(C47H27N3O2, 665.2103)	1146	m/z=722.2153(C49H30N4OS, 722.2140)
209	m/z=651.2284(C47H29N3O, 651.2311)	1157	m/z=732.2671(C51H32N4O2, 732.2525)
226	m/z=677.2551(C49H31N3O, 677.2467)	1158	m/z=732.2715(C51H32N4O2, 732.2525)
237	m/z=701.2569(C51H31N3O, 701.2467)	1174	m/z=732.2618(C51H32N4O2, 732.2525)
249	m/z=651.2137(C47H29N3O, 651.2311)	1175	m/z=732.2639(C51H32N4O2, 732.2525)
250	m/z=651.2154(C47H29N3O, 651.2311)	1176	m/z=732.1952(C51H32N4O2, 732.2525)
253	m/z=651.2318(C47H29N3O, 651.2311)	1186	m/z=732.2617(C51H32N4O2, 732.2525)
325	m/z=651.2513(C47H29N3O, 651.2311)	1187	m/z=732.2492(C51H32N4O2, 732.2525)
327	m/z=651.2317(C47H29N3O, 651.2311)	1203	m/z=718.2489(C51H34N4O, 718.2733)
329	m/z=701.2514(C51H31N3O, 701.2467)	1257	m/z=640.2671(C45H28N4O, 640.2263)
511	m/z=575.1958(C41H25N3O,	1258	m/z=690.2418(C49H30N4O,

	575.1998)		690.2420)
521	m/z=625.2155(C45H27N3O, 625.2154)	1278	m/z=742.2715(C53H34N4O, 742.2733)
523	m/z=625.2192(C45H27N3O, 625.2154)	1279	m/z=768.2781(C55H36N4O, 768.2889)
524	m/z=625.1986(C45H27N3O, 625.2154)	1306	m/z=706.2446(C49H30N4O2, 706.2369)
551	m/z=651.2417(C47H29N3O, 651.2311)	1307	m/z=732.2413(C51H32N4O2, 732.2525)
597	m/z=651.2318(C47H29N3O, 651.2311)	1365	m/z=782.2649(C55H34N4O2, 782.2682)
598	m/z=651.2183(C47H29N3O, 651.2311)	1403	m/z=718.2731(C51H34N4O, 718.2733)
633	m/z=665.2095(C47H27N3O2, 665.2103)	1404	m/z=718.2492(C51H34N4O, 718.2733)
635	m/z=665.2069(C47H27N3O2, 665.2103)	1405	m/z=718.2519(C51H34N4O, 718.2733)
703	m/z=651.2182(C47H29N3O, 651.2311)	1413	m/z=794.3186(C57H38N4O, 794.3046)
708	m/z=625.2217(C45H27N3O, 625.2154)	1417	m/z=692.1964(C49H32N4O, 692.2576)
711	m/z=625.2133(C45H27N3O, 625.2154)	1437	m/z=742.2485(C53H34N4O, 742.2733)
724	m/z=701.2518(C51H31N3O, 701.2467)	1439	m/z=768.2945(C55H36N4O, 768.2889)
749	m/z=651.2178(C47H29N3O, 651.2311)	1444	m/z=754.2468(C51H32F2N4O,754.2544)
755	m/z=675.2347(C49H29N3O, 675.2311)	1453	m/z=732.2429(C51H32N4O2, 732.2525)
756	m/z=651.2129(C47H29N3O, 651.2311)	1488	m/z=716.2558(C51H32N4O, 716.2576)
827	m/z=651.2354(C47H29N3O, 651.2311)	1489	m/z=716.2514(C51H32N4O, 716.2576)
863	m/z=651.2316(C47H29N3O, 651.2311)	1505	m/z=655.2182(C46H29N3O2, 655.2260)
919	m/z=630.1842(C44H26N2OS, 630.1766)	1506	m/z=671.1956(C46H29N3OS, 671.2031)
1002	m/z=642.2408(C45H30N4O, 642.2420)	1559	m/z=705.2408(C50H31N3O2, 705.2416)
1005	m/z=718.2185(C51H34N4O, 718.2733)	1570	m/z=643.1682(C44H25N3OS, 643.1718)
1011	m/z=718.1583(C51H34N4O, 718.2733)	1579	m/z=702.2183(C50H30N4O, 702.2420)

1015	m/z=718.2463(C51H34N4O, 718.2733)	1585	m/z=731.2427(C52H33N3O2, 731.2573)
1021	m/z=794.3152(C57H38N4O, 794.3046)	1587	m/z=691.2716(C50H33N3O, 691.2624)
1050	m/z=616.2315(C43H28N4O, 616.2263)	1595	m/z=691.2820(C50H33N3O, 691.2624)

【0390】 **<實驗例 1>**

【0391】 **1)有機發光裝置的製造（紅色主體，單個）**

【0392】 用蒸餾水對其中薄塗 ITO 以具有 1,500 埃(Å)的厚度的玻璃基板進行超聲波清洗。蒸餾水清洗結束後，用丙酮、甲醇、異丙醇等溶劑對玻璃基板進行超聲波清洗，乾燥後，在 UV 清洗機中使用 UV 進行 5 分鐘紫外線臭氧（ultraviolet ozone，UVO）處理。其後，將基板轉移到電漿清洗機（plasma washing machine，PT），然後在真空狀態下進行用於 ITO 表面處理並去除殘留膜的電漿處理，並將基板轉移到用於有機沈積的熱沉積裝置。

【0393】 在 ITO 透明電極（正極）上，形成作為通用層的電洞注入層 4,4',4"-三[2-萘基(苯基) 胺基]三苯基胺（4,4´,4´´-tris[2-naphthyl(phenyl)amino]triphenylamine，2-TNATA）和電洞傳輸層 N,N'-二苯基-(1,1'-聯苯)-4,4'-二胺（N,N'-diphenyl-(1,1'-biphenyl)-4,4'-diamine，NPB）。

【0394】 如下在其上熱真空沉積發光層。通過從單一供應源沉積以下表 12 中描述的化合物作為紅色主體並使用$(piq)_2(Ir)(acac)$作為紅色磷光摻雜劑來向主體以 3wt%的 Ir 化合物進行摻雜而將發光層沉積為具有 400Å 的厚度。此後，沉積作為電洞阻擋層的紅菲

咯啉（bathophenanthroline）（以下稱為 Bphen）以具有 30Å 的厚度，並且在其上沉積具有 250Å 的厚度作為電子傳輸層的 Alq_3。最後，通過在電子傳輸層上沉積厚度為 10Å 的氟化鋰（LiF）以形成電子注入層，然後在電子注入層上沉積厚度為 1,200Å 的鋁（A1）負極，以形成負電極，從而製造了有機電致發光裝置。

【0395】 同時，將製造 OLED 裝置所需的所有有機化合物對每種材料在 10^{-6} 至 10^{-8} 托下進行真空昇華純化，並用於製造 OLED。

【0396】 2)有機發光裝置的性能評價（紅色主體，單個）

【0397】 對於如上所述製造的有機電致發光裝置，電致發光（electroluminescent，EL）特性通過由麥克賽恩斯有限公司（McScience Inc.）製造的 M7000 測量，並且基於其測量結果，通過由麥克賽恩斯有限公司製造的壽命測量裝置（M6000）測量標準亮度（reference luminance）為 6,000 坎德拉/平方米（cd/m^2）時的 T_{90}。

【0398】 測量結果示於以下表 12 中。

【0399】 表 12

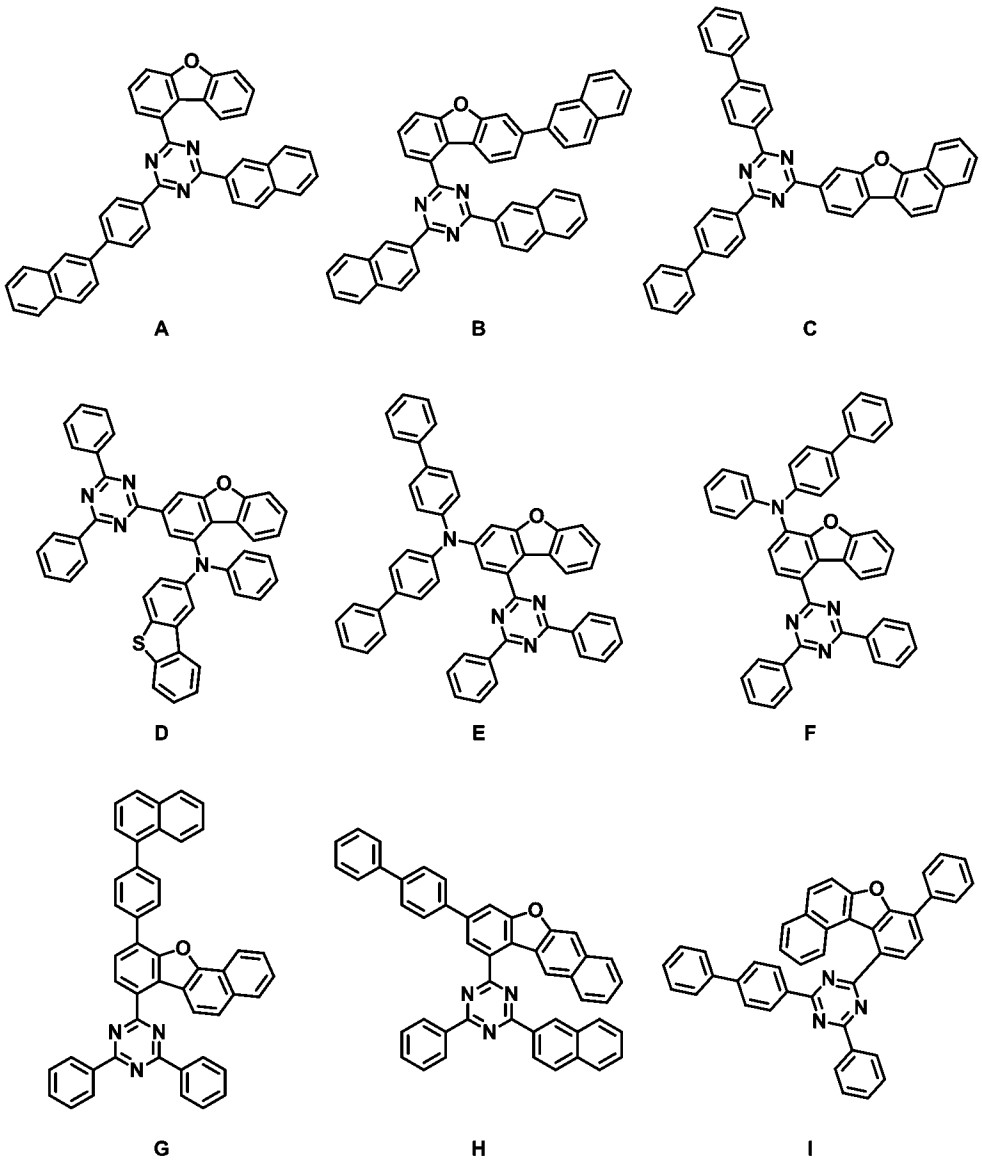
	發光層	驅動電壓 (V)	效率 (cd/A)	彩色座標 (x, y)	壽命 (T_{90})
比較例 1	A	5.90	31.5	(0.685, 0.315)	21
比較例 2	B	5.49	29.5	(0.685, 0.315)	25
比較例 3	C	5.32	35.1	(0.685, 0.315)	11
比較例 4	D	5.94	21.9	(0.685, 0.315)	10
比較例 5	E	5.90	20.8	(0.685, 0.315)	15
比較例 6	F	5.91	28.8	(0.685, 0.315)	18
比較例 7	G	5.81	33.5	(0.685, 0.315)	20
比較例 8	H	5.75	32.7	(0.685, 0.315)	25
比較例 9	I	5.33	31.1	(0.685, 0.315)	19

比較例 10	1	3.87	34.9	(0.685, 0.315)	27
比較例 11	13	3.91	35.5	(0.685, 0.315)	20
比較例 12	22	3.79	40.3	(0.685, 0.315)	15
比較例 13	30	3.85	32.2	(0.685, 0.315)	19
比較例 14	37	3.75	34.7	(0.685, 0.315)	29
比較例 15	39	3.81	34.8	(0.685, 0.315)	21
比較例 16	48	3.72	34.6	(0.685, 0.315)	20
比較例 17	53	3.64	32.7	(0.685, 0.315)	26
比較例 18	57	3.78	33.6	(0.685, 0.315)	27
比較例 19	58	4.09	39.8	(0.685, 0.315)	16
比較例 20	97	4.02	32.4	(0.685, 0.315)	19
比較例 21	115	4.14	32.5	(0.685, 0.315)	22
比較例 22	133	3.80	34.4	(0.685, 0.315)	10
比較例 23	134	3.85	35.3	(0.685, 0.315)	24
比較例 24	206	3.84	36.2	(0.685, 0.315)	25
比較例 25	209	3.38	43.2	(0.685, 0.315)	38
比較例 26	215	3.56	33.8	(0.685, 0.315)	30
比較例 27	226	3.75	36.1	(0.685, 0.315)	13
比較例 28	237	3.71	35.2	(0.685, 0.315)	16
比較例 29	239	3.82	36.1	(0.685, 0.315)	21
比較例 30	249	3.33	48.7	(0.685, 0.315)	41
比較例 31	250	4.26	24.6	(0.685, 0.315)	22
比較例 32	253	4.13	27.6	(0.685, 0.315)	20
比較例 33	280	4.01	32.5	(0.685, 0.315)	25
比較例 34	316	3.92	35.2	(0.685, 0.315)	32
比較例 35	325	3.41	49.9	(0.685, 0.315)	22
比較例 36	327	4.02	30.8	(0.685, 0.315)	25
比較例 37	329	3.34	48.2	(0.685, 0.315)	30
比較例 38	438	3.65	39.5	(0.685, 0.315)	10
比較例 39	447	3.75	38.7	(0.685, 0.315)	15
比較例 40	505	3.60	40.2	(0.685, 0.315)	16
比較例 41	511	3.74	49.8	(0.685, 0.315)	36
比較例 42	521	3.61	48.7	(0.685, 0.315)	29
比較例 43	523	3.62	50.8	(0.685, 0.315)	30
比較例 44	524	3.96	49.3	(0.685, 0.315)	35
比較例 45	551	3.84	47.7	(0.685, 0.315)	35
比較例 46	597	3.75	47.1	(0.685, 0.315)	28
比較例 47	598	3.70	45.2	(0.685, 0.315)	31
比較例 48	633	3.89	41.3	(0.685, 0.315)	25
比較例 49	635	3.65	49.8	(0.685, 0.315)	21
比較例 50	681	3.71	49.2	(0.685, 0.315)	25
比較例 51	703	3.86	47.5	(0.685, 0.315)	20

比較例 52	708	3.61	38.4	(0.685, 0.315)	19
比較例 53	711	3.65	49.0	(0.685, 0.315)	30
比較例 54	724	3.74	39.8	(0.685, 0.315)	23
比較例 55	749	3.68	40.1	(0.685, 0.315)	20
比較例 56	755	3.65	49.5	(0.685, 0.315)	26
比較例 57	756	3.74	37.4	(0.685, 0.315)	23
比較例 58	827	3.61	49.3	(0.685, 0.315)	35
比較例 59	863	3.62	50.2	(0.685, 0.315)	26
比較例 60	919	3.73	45.1	(0.685, 0.315)	27
比較例 61	942	3.85	39.6	(0.685, 0.315)	35
比較例 62	1002	4.14	34.8	(0.685, 0.315)	49
比較例 63	1005	4.13	35.7	(0.685, 0.315)	50
比較例 64	1011	4.34	21.6	(0.685, 0.315)	38
比較例 65	1015	4.01	32.0	(0.685, 0.315)	63
比較例 66	1021	4.05	48.2	(0.685, 0.315)	87
比較例 67	1050	3.91	37.9	(0.685, 0.315)	45
比較例 68	1054	3.85	33.5	(0.685, 0.315)	86
比較例 69	1056	3.81	31.4	(0.685, 0.315)	81
比較例 70	1057	3.91	30.9	(0.685, 0.315)	97
比較例 71	1064	4.05	23.5	(0.685, 0.315)	81
比較例 72	1065	4.12	39.4	(0.685, 0.315)	85
比較例 73	1073	4.03	34.8	(0.685, 0.315)	99
比較例 74	1097	3.84	38.7	(0.685, 0.315)	90
比較例 75	1100	3.68	34.6	(0.685, 0.315)	92
比較例 76	1123	3.59	42.3	(0.685, 0.315)	91
比較例 77	1124	3.65	43.5	(0.685, 0.315)	84
比較例 78	1142	3.71	40.4	(0.685, 0.315)	86
比較例 79	1146	3.82	41.5	(0.685, 0.315)	78
比較例 80	1157	3.77	35.2	(0.685, 0.315)	56
比較例 81	1158	3.79	35.9	(0.685, 0.315)	64
比較例 82	1174	3.64	48.5	(0.685, 0.315)	80
比較例 83	1175	3.73	45.4	(0.685, 0.315)	90
比較例 84	1176	4.35	23.6	(0.685, 0.315)	41
比較例 85	1186	4.10	46.8	(0.685, 0.315)	94
比較例 86	1187	4.01	45.7	(0.685, 0.315)	92
比較例 87	1203	3.65	44.1	(0.685, 0.315)	89
比較例 88	1257	3.64	35.5	(0.685, 0.315)	70
比較例 89	1258	3.78	37.3	(0.685, 0.315)	75
比較例 90	1278	3.87	38.4	(0.685, 0.315)	81
比較例 91	1279	3.69	35.6	(0.685, 0.315)	72
比較例 92	1306	4.12	41.7	(0.685, 0.315)	125
比較例 93	1307	4.01	43.8	(0.685, 0.315)	115

比較例 94	1365	3.42	48.9	(0.685, 0.315)	123
比較例 95	1403	3.21	50.4	(0.685, 0.315)	100
比較例 96	1404	3.85	47.5	(0.685, 0.315)	90
比較例 97	1405	3.64	48.7	(0.685, 0.315)	135
比較例 98	1413	3.76	49.8	(0.685, 0.315)	120
比較例 99	1417	3.55	46.0	(0.685, 0.315)	115
比較例 100	1437	3.74	41.2	(0.685, 0.315)	101
比較例 101	1439	3.65	39.6	(0.685, 0.315)	125
比較例 102	1444	3.69	45.7	(0.685, 0.315)	132
比較例 103	1453	3.67	47.8	(0.685, 0.315)	104
比較例 104	1488	3.52	35.6	(0.685, 0.315)	96
比較例 105	1489	3.61	38.4	(0.685, 0.315)	85
比較例 106	1505	4.04	35.9	(0.685, 0.315)	71
比較例 107	1506	3.90	36.7	(0.685, 0.315)	98
比較例 108	1559	3.81	37.5	(0.685, 0.315)	104
比較例 109	1570	3.59	35.1	(0.685, 0.315)	77
比較例 110	1579	3.65	37.2	(0.685, 0.315)	88
比較例 111	1585	3.74	35.3	(0.685, 0.315)	90
比較例 112	1587	3.65	35.8	(0.685, 0.315)	74
比較例 113	1595	3.86	21.4	(0.685, 0.315)	68

【0400】 表 12 中的化合物 A 至 I 如下。



【0401】 **<實驗例 2>**

【0402】 **1)有機發光裝置的製造（預混、紅色主體）**

【0403】 用蒸餾水對其中薄塗 ITO 以具有 1,500 Å 的厚度的玻璃基板進行超聲波清洗。蒸餾水清洗結束後，用丙酮、甲醇、異丙醇等溶劑對玻璃基板進行超聲波清洗，乾燥後，在 UV 清洗機中使用 UV 進行 5 分鐘 UVO 處理。此後，將基板轉移到電漿清洗機（PT），然後在真空狀態下進行用於 ITO 功函數並去除殘留膜的電漿處理，並將基板轉移到用於有機沉積的熱沉積裝置。

【0404】 在 ITO 透明電極（正極）上，形成作為通用層的電洞注入層 4,4',4''-三[2-萘基(苯基)氨基]三苯基胺（2-TNATA），電洞傳輸層 N,N'-二苯基-(1,1'-聯苯)-4,4'-二胺（NPB）和電子阻擋層環己基二[N,N-雙(4-甲基苯基)苯胺]（cyclohexylidenebis[N,N-bis(4-methylphenyl)benzenamine]，TAPC）或激子阻擋層（exciton blocking layer）三（4-肼甲醯基-9-基苯基）胺（TCTA）。

【0405】 如下在其上熱真空沉積發光層。通過從單一供應源沉積以下表 13 中描述的兩種類型的化合物作為紅色主體，並使用 $(piq)_2(Ir)(acac)$作為紅色磷光摻雜劑在主體中摻雜 3wt%的 Ir 化合物，而沉積發光層以具有 400Å 的厚度。此後，沉積作為電洞阻擋層的 Bphen 以具有 30 Å 的厚度，並且在其上沉積具有 250Å 的厚度作為電子傳輸層的 1,3,5-三（N-苯基苯並咪唑-2-基）苯（1,3,5-tris(N-phenylbenzimidazole-2-yl)benzene，TPBI）。最後，通過在電子傳輸層上沉積厚度為 10Å 的氟化鋰（LiF）以形成電子注入層，然後在電子注入層上沉積厚度為 1,200Å 的鋁（A1）負極，以形成負電極，從而製造了有機電致發光裝置。

【0406】 同時，將製造 OLED 裝置所需的所有有機化合物對每種材料在 10^{-6} 至 10^{-8} 托下進行真空昇華純化，並用於製造 OLED。

【0407】 2)有機發光裝置的性能評價（預混、紅色主體）

【0408】 對於如上所述製造的有機電致發光裝置，電致發光（electroluminescent，EL）特性通過由麥克賽恩斯有限公司

（McScience Inc.）製造的 M7000 測量，並且基於其測量結果，通過由麥克賽恩斯有限公司製造的壽命測量裝置（M6000）測量標準亮度為 6,000 坎德拉/平方米（cd/m^2）時的 T_{90}。

【0409】 測量結果示於以下表 13 中。

【0410】 表 13

	發光層	比例 (P:N)	驅動電壓 (V)	效率 (cd/A)	彩色座標 (x, y)	壽命 (T_{90})
比較例 104	A:D	1:2	4.56	38.7	(0.685, 0.315)	59
比較例 105		1:1	4.72	39.9	(0.685, 0.315)	64
比較例 106		2:1	4.91	37.1	(0.685, 0.315)	49
比較例 107	G:E	1:2	3.91	48.7	(0.685, 0.315)	56
比較例 108		1:1	3.89	46.8	(0.685, 0.315)	52
比較例 109		2:1	3.88	46.6	(0.685, 0.315)	49
比較例 110	22:D	1:2	4.34	45.1	(0.685, 0.315)	40
比較例 111		1:1	4.21	48.4	(0.685, 0.315)	51
比較例 112		2:1	4.45	46.8	(0.685, 0.315)	39
比較例 113	A:1005	1:2	3.98	44.7	(0.685, 0.315)	76
比較例 114		1:1	3.92	42.9	(0.685, 0.315)	87
比較例 115		2:1	4.02	39.1	(0.685, 0.315)	68
比較例 116	H:1203	1:2	3.86	48.6	(0.685, 0.315)	50
比較例 117		1:1	3.87	49.1	(0.685, 0.315)	61
比較例 118		2:1	3.90	49.8	(0.685, 0.315)	73
實例 1	30:1002	1:2	3.61	53.5	(0.685, 0.315)	91
實例 2		1:1	3.62	58.9	(0.685, 0.315)	88
實例 3		2:1	3.65	61.3	(0.685, 0.315)	82
實例 4	37:1005	1:2	3.56	52.8	(0.685, 0.315)	79
實例 5		1:1	3.51	61.2	(0.685, 0.315)	88
實例 6		2:1	3.69	63.9	(0.685, 0.315)	87
實例 7	58:1021	1:8	3.79	67.8	(0.685, 0.315)	102
實例 8		1:5	3.85	69.3	(0.685, 0.315)	121
實例 9		1:2	3.77	72.9	(0.685, 0.315)	119
實例 10		1:1	3.68	68.5	(0.685, 0.315)	130
實例 11		2:1	3.59	71.8	(0.685, 0.315)	134
實例 12		5:1	3.76	75.9	(0.685, 0.315)	123
實例 13		8:1	3.81	71.2	(0.685, 0.315)	105
實例 14	97:1054	1:2	3.25	74.9	(0.685, 0.315)	248
實例 15		1:1	3.40	75.7	(0.685, 0.315)	224
實例 16		2:1	3.45	78.6	(0.685, 0.315)	181

實例 17	133:1124	1:8	3.51	80.8	(0.685, 0.315)	155
實例 18		1:5	3.83	76.0	(0.685, 0.315)	138
實例 19		1:2	3.89	73.3	(0.685, 0.315)	169
實例 20		1:1	3.63	81.8	(0.685, 0.315)	154
實例 21		2:1	3.77	85.5	(0.685, 0.315)	135
實例 22		5:1	3.78	90.7	(0.685, 0.315)	113
實例 23		8:1	3.87	61.1	(0.685, 0.315)	109
實例 24	206:1142	1:2	3.61	62.3	(0.685, 0.315)	125
實例 25		1:1	3.66	64.8	(0.685, 0.315)	140
實例 26		2:1	3.68	65.4	(0.685, 0.315)	156
實例 27	249:1175	1:2	3.59	69.5	(0.685, 0.315)	183
實例 28		1:1	3.62	74.1	(0.685, 0.315)	204
實例 29		2:1	3.78	79.9	(0.685, 0.315)	195
實例 30	280:1100	1:2	3.60	66.8	(0.685, 0.315)	135
實例 31		1:1	3.58	67.9	(0.685, 0.315)	146
實例 32		2:1	3.55	68.1	(0.685, 0.315)	151
實例 33	316:1186	1:2	3.61	62.8	(0.685, 0.315)	162
實例 34		1:1	3.63	63.7	(0.685, 0.315)	167
實例 35		2:1	3.64	64.1	(0.685, 0.315)	145
實例 36	325:1187	1:2	3.77	81.7	(0.685, 0.315)	173
實例 37		1:1	3.75	84.4	(0.685, 0.315)	144
實例 38		2:1	3.86	70.6	(0.685, 0.315)	128
實例 39	438:1278	1:2	3.69	65.1	(0.685, 0.315)	154
實例 40		1:1	3.71	67.5	(0.685, 0.315)	160
實例 41		2:1	3.74	67.9	(0.685, 0.315)	135
實例 42	447:1307	1:2	3.70	61.2	(0.685, 0.315)	128
實例 43		1:1	3.68	63.5	(0.685, 0.315)	134
實例 44		2:1	3.63	64.8	(0.685, 0.315)	149
實例 45	505:1365	1:2	3.75	65.1	(0.685, 0.315)	172
實例 46		1:1	3.72	62.8	(0.685, 0.315)	183
實例 47		2:1	3.69	61.5	(0.685, 0.315)	149
實例 48	523:1203	1:8	3.65	69.8	(0.685, 0.315)	187
實例 49		1:5	3.78	74.7	(0.685, 0.315)	203
實例 50		1:2	3.79	77.4	(0.685, 0.315)	189
實例 51		1:1	3.82	78.5	(0.685, 0.315)	195
實例 52		2:1	3.85	82.6	(0.685, 0.315)	143
實例 53		5:1	3.87	84.9	(0.685, 0.315)	135
實例 54		8:1	3.91	86.2	(0.685, 0.315)	129
實例 55	597:1453	1:8	3.52	74.7	(0.685, 0.315)	261
實例 56		1:5	3.66	73.6	(0.685, 0.315)	252
實例 57		1:2	3.79	77.2	(0.685, 0.315)	229
實例 58		1:1	3.40	70.1	(0.685, 0.315)	279

實例 59		2:1	3.33	71.0	(0.685, 0.315)	278
實例 60		5:1	3.35	60.0	(0.685, 0.315)	267
實例 61		8:1	3.45	57.5	(0.685, 0.315)	231
實例 62	635:1488	1:2	3.35	63.1	(0.685, 0.315)	225
實例 63		1:1	3.55	55.5	(0.685, 0.315)	219
實例 64		2:1	3.30	60.8	(0.685, 0.315)	229
實例 65	703:1404	1:2	3.25	68.3	(0.685, 0.315)	235
實例 66		1:1	3.40	58.1	(0.685, 0.315)	225
實例 67		2:1	3.32	65.0	(0.685, 0.315)	261
實例 68	711:1506	1:8	3.45	63.1	(0.685, 0.315)	324
實例 69		1:5	3.36	67.0	(0.685, 0.315)	348
實例 70		1:2	3.35	71.1	(0.685, 0.315)	352
實例 71		1:1	3.35	71.0	(0.685, 0.315)	366
實例 72		2:1	3.20	71.9	(0.685, 0.315)	409
實例 73		5:1	3.35	71.5	(0.685, 0.315)	325
實例 74		8:1	3.48	71.0	(0.685, 0.315)	281
實例 75	827:1585	1:2	3.34	70.6	(0.685, 0.315)	236
實例 76		1:1	3.55	58.7	(0.685, 0.315)	212
實例 77		2:1	3.35	70.9	(0.685, 0.315)	184
實例 78	863:1505	1:2	3.88	65.5	(0.685, 0.315)	282
實例 79		1:1	3.90	70.1	(0.685, 0.315)	205
實例 80		2:1	3.95	74.9	(0.685, 0.315)	251
實例 81	919:1559	1:2	3.41	68.1	(0.685, 0.315)	273
實例 82		1:1	3.50	67.5	(0.685, 0.315)	246
實例 83		2:1	3.55	60.4	(0.685, 0.315)	227
實例 84	942:1587	1:2	3.62	62.1	(0.685, 0.315)	154
實例 85		1:1	3.60	63.8	(0.685, 0.315)	138
實例 86		2:1	3.59	62.7	(0.685, 0.315)	129

【0411】 由表 12 和 13 的結果可知，可以確認與比較例的有機發光裝置相比，在以本發明的由化學式 1 表示的雜環化合物和由化學式 2 表示的雜環化合物作為用於有機發光裝置的有機材料層，特別是發光層的主體的實施例 1 至 86 的情況下，驅動電壓、效率和壽命得到改善。

【0412】 本發明的化學式 1 的雜環化合物具有高的熱穩定性和合適的分子量和帶隙。發光層的這種合適的帶隙具有良好的電洞傳

輸能力，防止電子損失，有助於復合區的有效形成。

【0413】 可以確認，通過在有機發光裝置的有機材料層中包含本發明的由化學式 2 表示的化合物，由於電洞遷移率的增加，驅動電壓和壽命可以顯著提高。此外，可以確認通過電子阻擋和電子限制減少電流洩漏也提高了效率。

【0414】 在發光層中化學式 1 和化學式 2 組合的情況下，提高了驅動電壓、效率和使用壽命。當以具有良好電洞傳輸能力的供體（p-主體，由化學式 2 表示的雜環化合物）和具有良好電子傳輸能力的受體（n-主體，由化學式 1 表示的雜環化合物）作為發光層的主體時，可以降低注入電子和電洞的驅動電壓，且通過有效形成復合區提高效率和使用壽命。

【0415】 這些是由激發錯合體現象更頻繁地發生引起的，該現像是由於兩個分子之間的電子交換，受體（N 型主體）的 LUMO 能級和供體（P 型主體）的 HOMO 能級之間的能量差異導致的發射現象。當具有良好電洞傳輸能力的供體（P 型主體）和具有良好電子傳輸能力的受體（N 型主體）通過激發錯合體現象作為發光層的主體時，電洞被注入到 P-型主體和電子被注入到 N 型主體中，從而促進電子和電洞在發光層中的結合。

【符號說明】

【0416】

100:基板

200:正極

300:有機材料層

301:電洞注入層

302:電洞傳輸層

303:發光層

304:電洞阻擋層

305:電子傳輸層

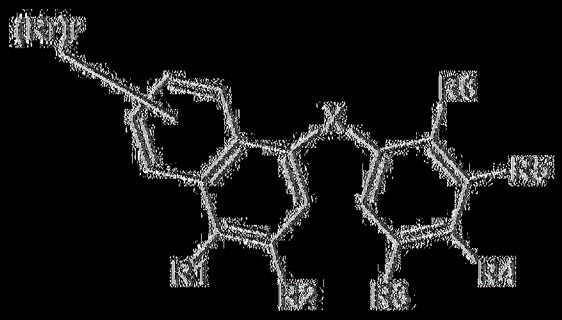
306:電子注入層

400:負極

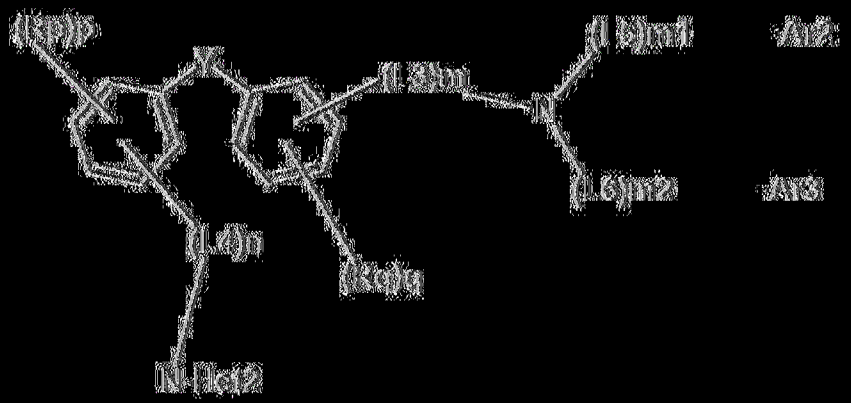
【發明申請專利範圍】

【請求項1】一種有機發光裝置，包括第一電極、第二電極和在所述第一電極和所述第二電極之間具有一層或多層的有機材料層，其中所述有機材料層包括由以下化學式1表示的雜環化合物和由以下化學式2表示的雜環化合物：

[化學式 1]



[化學式 2]



其中，在化學式 1 和 2 中，

X 是 O；或 S，

R1 至 R6 中的一者為 $-\frac{1}{2}(L1)_{n}-Ar1$，其他中的一者為 $-\frac{1}{2}(L2)_{n}-N-Hc1$，且其他彼此相同或不同，且各自獨立地選自由以下組成的群組：氫；氘；鹵素；氰基；經取代或未經取代的 C1 至 C60 烷基；經取代或未經取代的 C2 至 C60 烯基；經取代或未經取代的 C2 至 C60 炔基；經取代或未經取代的 C1 至 C60 烷氧基；經

取代或未經取代的 C3 至 C60 環烷基；經取代或未經取代的 C2 至 C60 雜環烷基；經取代或未經取代的 C6 至 C60 芳基；經取代或未經取代的 C2 至 C60 雜芳基；-P(=O)RR’；-SiRR’R”和-NRR’，

是分別鍵結至 R1 至 R6 的位置，

L1 至 L6 彼此相同或不同，且各自獨立為直接鍵；經取代或未經取代的 C6 至 C60 伸芳基；或經取代或未經取代的 C2 至 C60 伸雜芳基，a、b、m、n、m1 和 m2 各自為 0 至 3 的整數，並且當 a、b、m、n、m1 和 m2 各自為 2 或大於 2 時，括號中的取代基彼此相同或不同，

N-Het1 和 N-Het2 各自獨立地為經取代或未經取代並包括一個或多個 N 的單環或多環雜環基團，

Ar1 為經取代或未經取代的 C6 至 C60 芳基;或經取代或未經取代的 C2 至 C60 雜芳基，

Y 是 O；或 S，

Ar2 和 Ar3 彼此相同或不同，且各自獨立地為經取代或未經取代的 C6 至 C60 的芳基;經取代或未經取代的 C2 至 C60 雜芳基;或-NRR’，

L3、L5、L6、Ar2 和 Ar3 的相鄰取代基可以彼此鍵結以形成經取代或未經取代的脂肪族或芳香族烴環或經取代或未經取代的脂肪族或芳香族雜環，

Rr、Rp 和 Rq 彼此相同或不同，並且各自獨立地選自由以下組成的群組：氫；氘；鹵素；氰基；經取代或未經取代的 C1 至

C60 烷基；經取代或未經取代的 C2 至 C60 烯基；經取代或未經取代的 C2 至 C60 炔基；經取代或未經取代的 C1 至 C60 烷氧基；經取代或未經取代的 C3 至 C60 環烷基；經取代或未經取代的 C2 至 C60 雜環烷基；經取代或未經取代的 C6 至 C60 芳基；經取代或未經取代的 C2 至 C60 雜芳基；-P(=O)RR'；-SiRR'R"和-NRR'，r 為 0 至 4 的整數，p、q 為 0 至 3 的整數，且當 r、p、q 為 2 或大於 2 時，括號內的取代基為彼此相同或不同，以及

R、R'和 R"彼此相同或不同，且各自獨立地為氫；氘；經取代或未經取代的 C1 至 C60 烷基；經取代或未經取代的 C6 至 C60 芳基；或經取代或未經取代的 C2 至 C60 雜芳基。

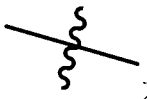
[請求項2] 如請求項1所述的有機發光裝置，其中所述N-Hc11和N-Hc12各自獨立地由以下化學式3表示：

[化學式 3]

在化學式 3 中，

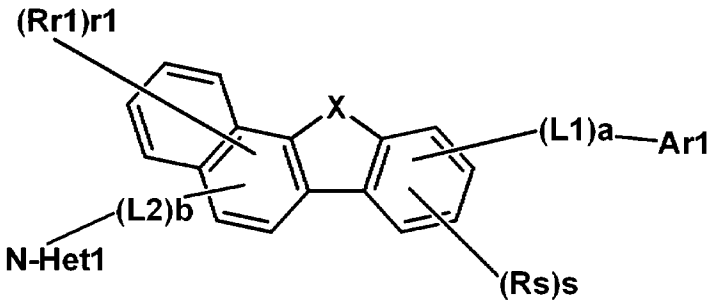
X1 為 CR101 或 N，X2 為 CR102 或 N，X3 為 CR103 或 N，X4 為 CR104 或 N，X5 為 CR105 或 N，且 X1 至 X5 中至少一者為 N，以及

R101 至 R105 彼此相同或不同，且各自獨立地選自氫；氘；鹵素；氰基；經取代或未經取代的 C1 至 C60 烷基；經取代或未經

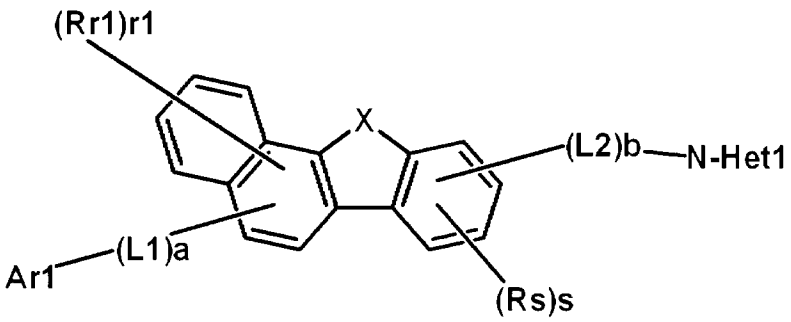
取代的 C2 至 C60 烯基；經取代或未經取代的 C2 至 C60 炔基；經取代或未經取代的 C1 至 C20 烷氧基；經取代或未經取代的 C3 至 C60 環烷基；經取代或未經取代的 C2 至 C60 雜環烷基；經取代或未經取代的 C6 至 C60 芳基；經取代或未經取代的 C2 至 C60 雜芳基；經取代或未經取代的氧化膦基；和經取代或未經取代的胺基，或兩個或多於兩個相鄰基團相互鍵結形成經取代或未經取代的脂肪族或芳香族烴環或雜環，且  是與化學式 1 或 2 連接的部分。

【請求項3】 如請求項1所述的有機發光裝置，其中化學式1是由以下化學式1-1或1-2表示的雜環化合物：

[化學式 1-1]



[化學式 1-2]



在化學式 1-1 至 1-2 中，

Rr1 和 Rs 彼此相同或不同，且各自獨立為氫；氘；氰基；鹵

素基團；或經取代或未經取代的 C1 至 C60 烷基，

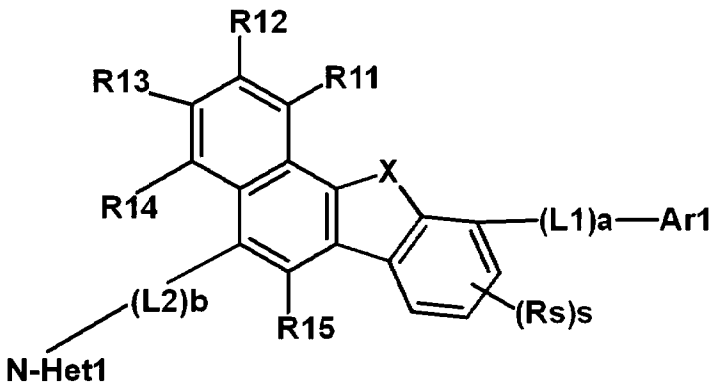
r1 為 0 至 5 的整數，且當 r1 為 2 或大於 2 時，括號內的 Rr1 彼此相同或不同，

s 為 0 至 3 的整數，且當 s 為 2 或大於 2 時，括號內的 Rs 彼此相同或不同，以及

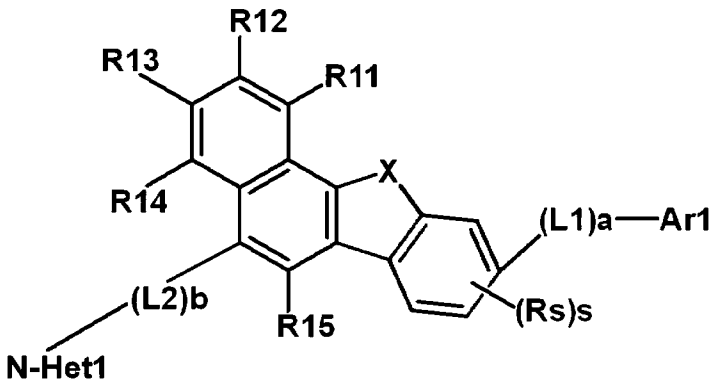
X、L1、L2、Ar1、a、b 和 N-Het1 的定義同化學式 1 中的定義。

【請求項4】 如請求項3所述的有機發光裝置，其中化學式1-1由以下化學式1-1-1至1-1-4中的任一者表示：

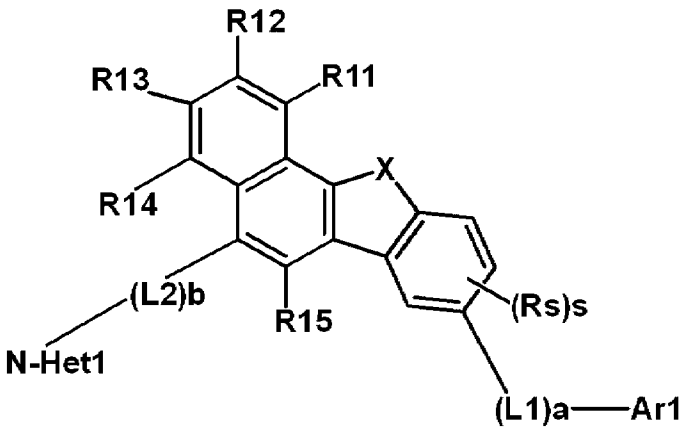
[化學式 1-1-1]



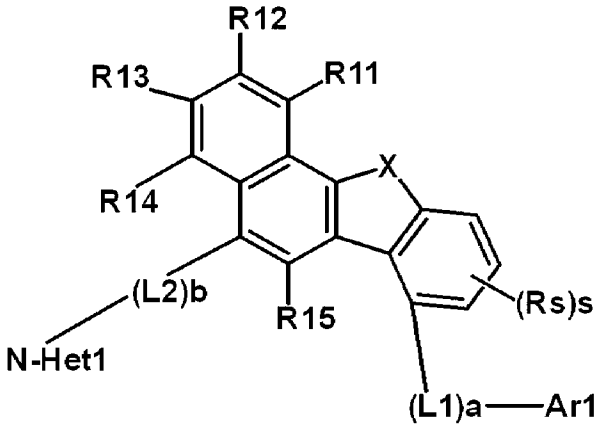
[化學式 1-1-2]



[化學式 1-1-3]



[化學式 1-1-4]



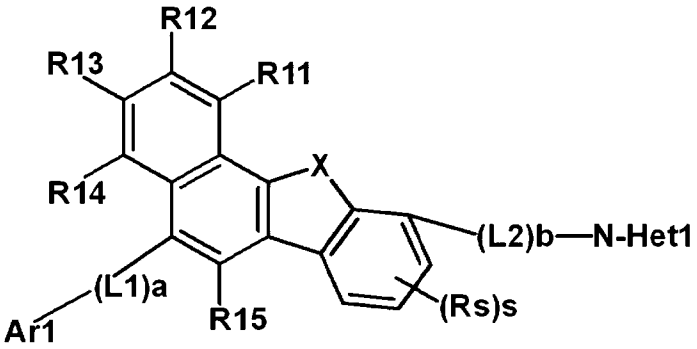
在化學式 1-1-1 至 1-1-4 中，

R11 至 R15 彼此相同或不同，且各自獨立為氫；氘；氰基；鹵素基團；或經取代或未經取代的 C1 至 C60 烷基，以及

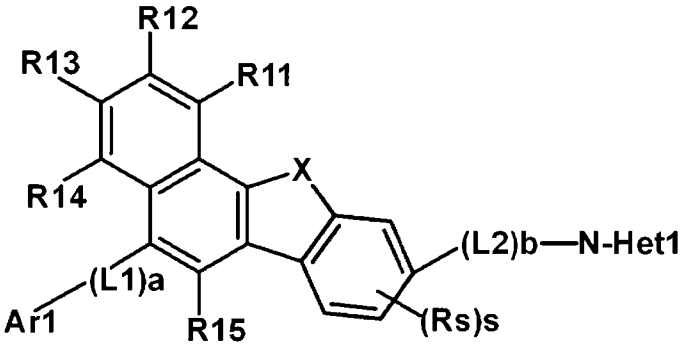
X、Rs、L1、L2、Ar1、a、b、s 和 N-Het1 的定義同化學式 1-1 中的定義。

【請求項5】 如請求項3所述的有機發光裝置，其中化學式1-2由以下化學式1-2-1至1-2-4中的任一者表示：

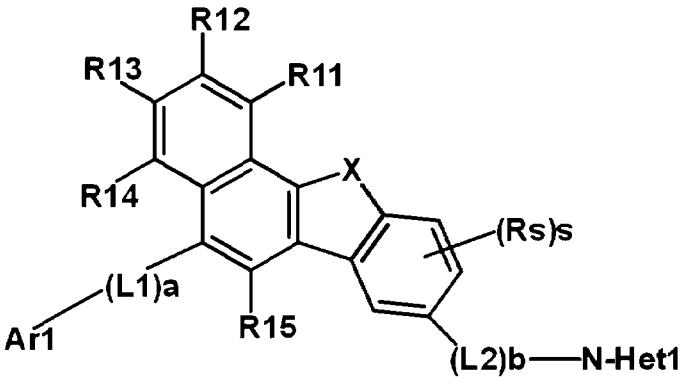
[化學式 1-2-1]



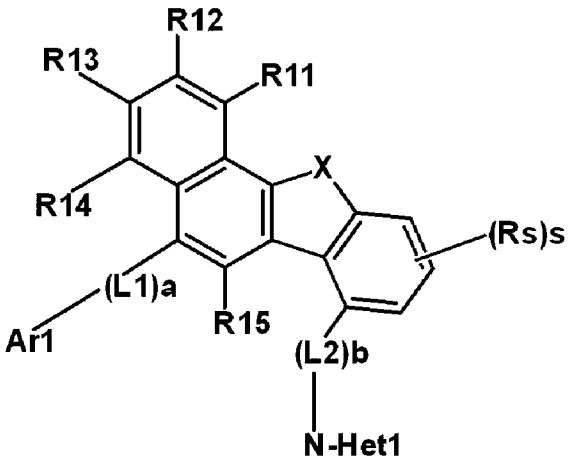
[化學式 1-2-2]



[化學式 1-2-3]



[化學式 1-2-4]

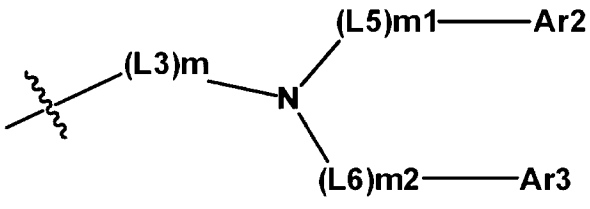


在化學式 1-2-1 至 1-2-4 中，

R11 至 R15 彼此相同或不同，且各自獨立為氫；氘；氰基；鹵素基團；或經取代或未經取代的 C1 至 C60 烷基，以及

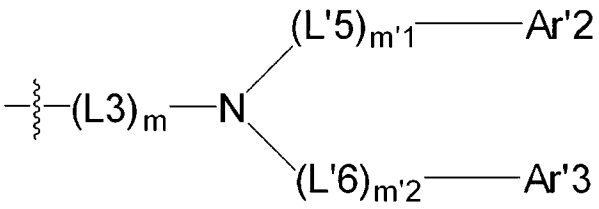
X、Rs、L1、L2、Ar1、a、b、s 和 N-Het1 的定義同化學式 1-2 中的定義。

【請求項6】 如請求項1所述的機發光裝置，其中

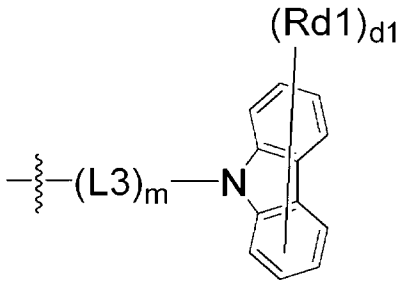


由以下化學式A-1至A-12中的任一個表示：

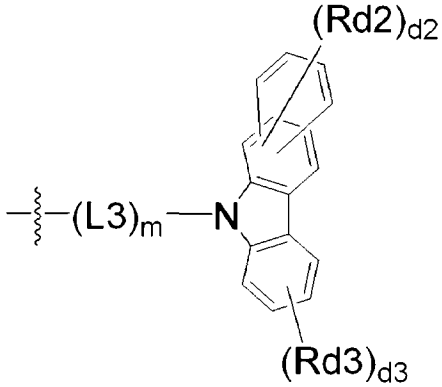
[化學式 A-1]



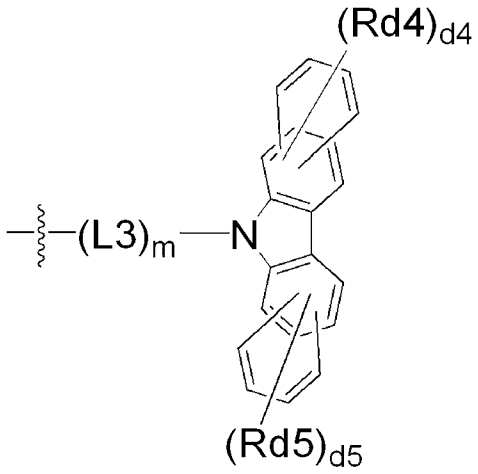
[化學式 A-2]



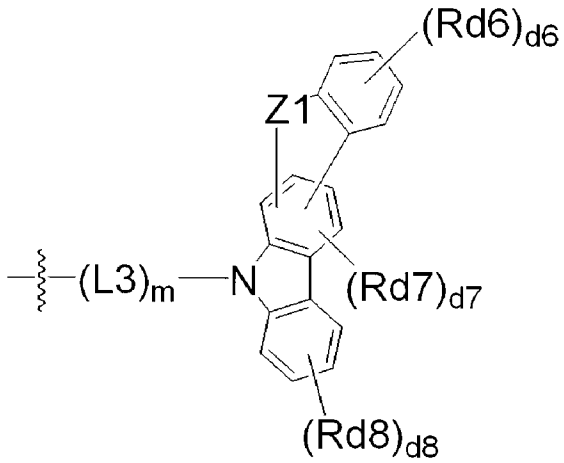
[化學式 A-3]



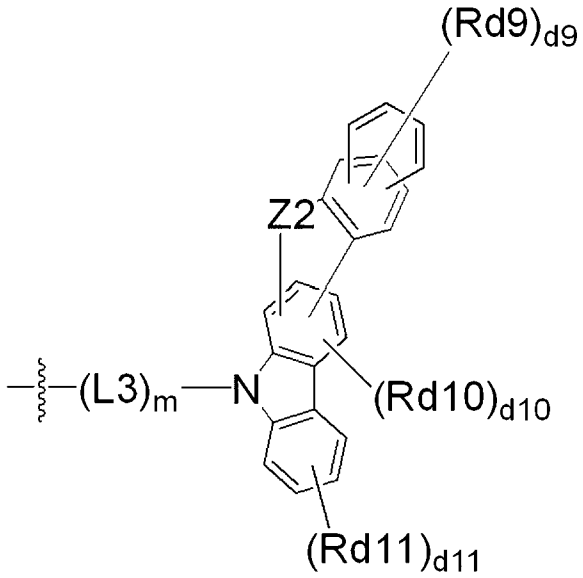
[化學式 A-4]



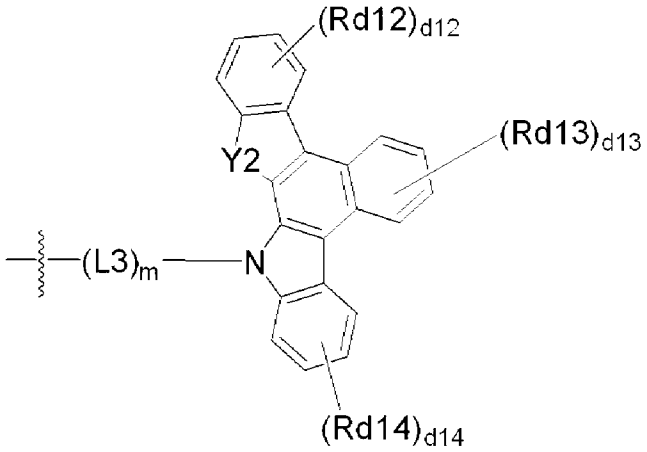
[化學式 A-5]



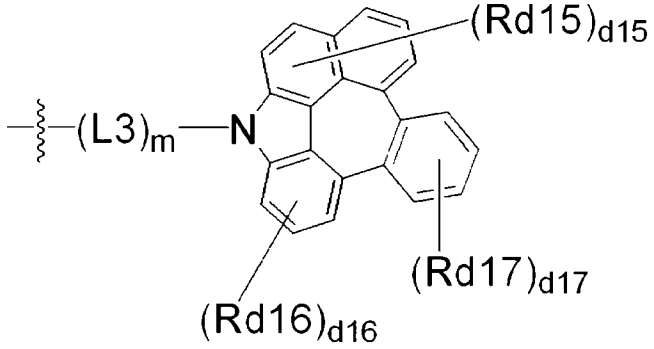
[化學式 A-6]



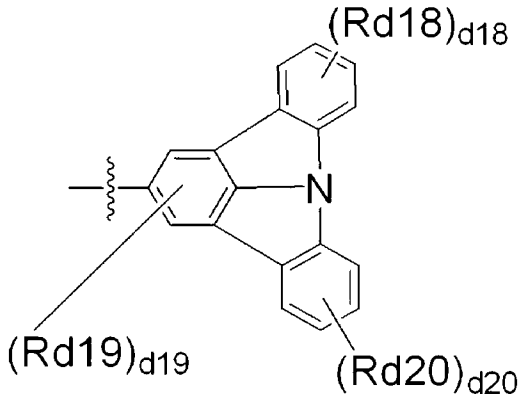
[化學式 A-7]



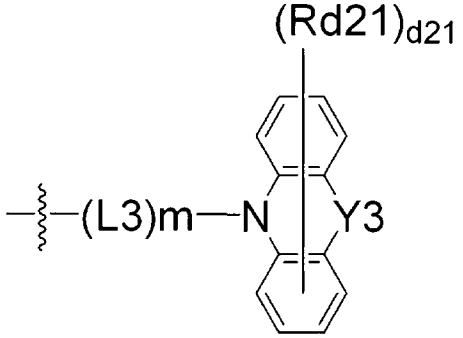
[化學式 A-8]



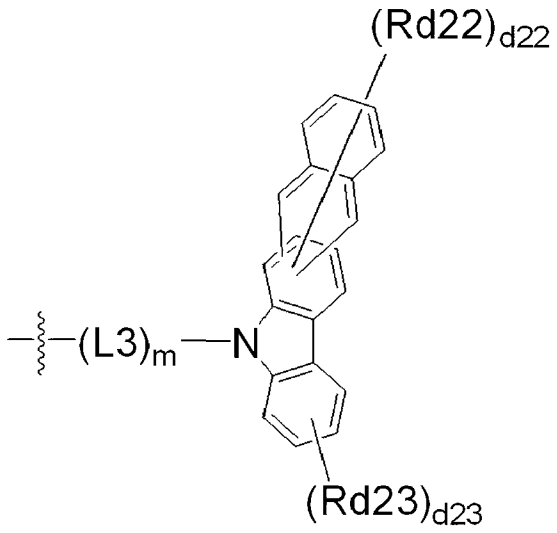
[化學式 A-9]



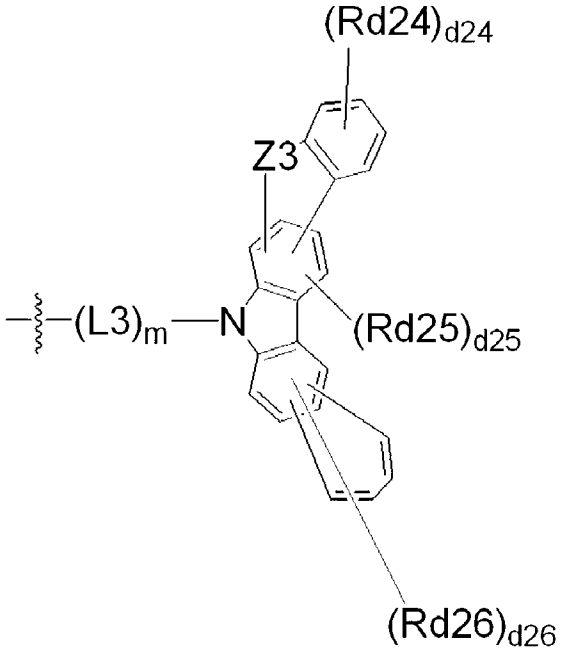
[化學式 A-10]



[化學式 A-11]



[化學式 A-12]



在化學式 A-1 至 A-12 中，

L3 和 m 的定義同化學式 2 中的定義，

L’5 和 L’6 彼此相同或不同，且各自獨立為直接鍵；經取代或未經取代的 C6 至 C60 伸芳基；或經取代或未經取代的 C2 至 C60 伸雜芳基，m’1 和 m’2 各自獨立地為 0 至 3 的整數，並且當 m’1 和 m’2 各自為 2 或大於 2 時，括號中的取代基彼此相同或不同，

Ar’2 與 Ar’3 彼此相同或不同，且各自獨立為 NRR’；經取代或未經取代的 C6 至 C60 芳基；或經取代或未經取代的 C2 至 C60 雜芳基，

Z1 至 Z3 各自獨立為 O；S；CRaRb；或 NRc，

Y2 和 Y3 各自獨立為 O；或 S，

R、R’、Ra、Rb、Rc 和 Rd1 至 Rd26 各自獨立地為氫；氘；鹵素基團；氰基；經取代或未經取代的 C1 至 C60 烷基；經取代或未經取代的 C6 至 C60 芳基；或經取代或未經取代的 C2 至 C60 雜芳基，

d1、d21 和 d22 各自獨立地為 0 至 8 的整數，

d2、d4、d5、d9 和 d26 各自獨立地為 0 至 6 的整數，

d3、d6、d8、d11、d12 至 d14、d17、d18、d20、d23 和 d24 各自獨立地為 0 至 4 的整數，

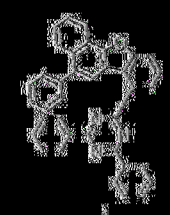
d7、d10、d19 和 d25 各自獨立地為 0 至 2 的整數，

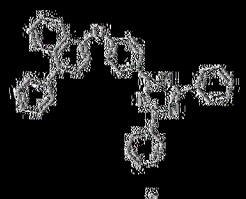
d15 是 0 到 5 的整數，

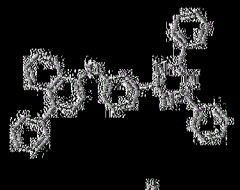
d16 是 0 到 3 的整數，以及

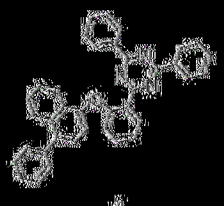
d1 至 d26 為 2 或大於 2 時，括號內的取代基彼此相同或不同。

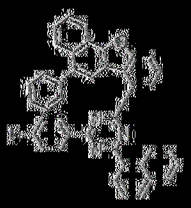
【請求項7】 如請求項1所述的有機發光裝置，其中化學式1由以下化合物中的任一個表示：

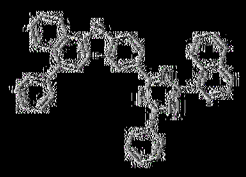


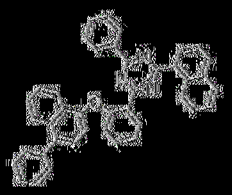


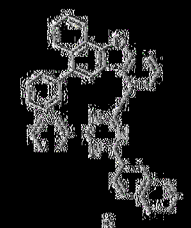


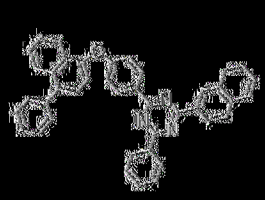


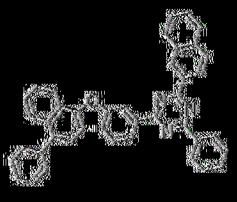


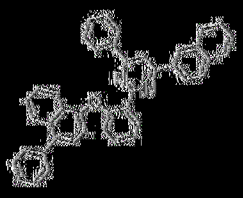


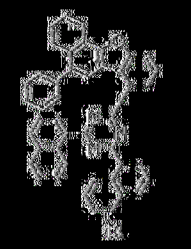


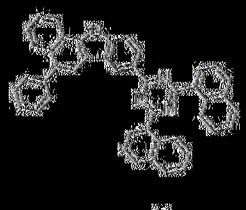


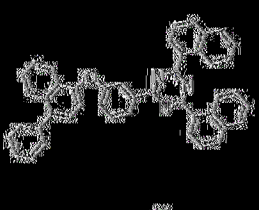


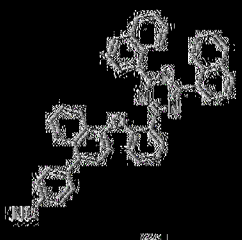


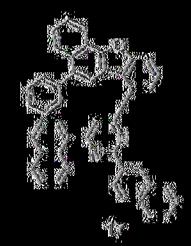


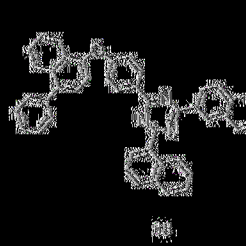


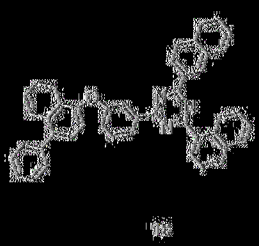


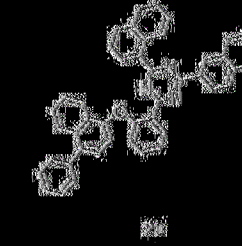


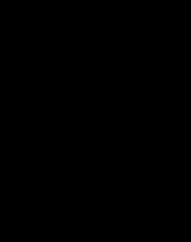


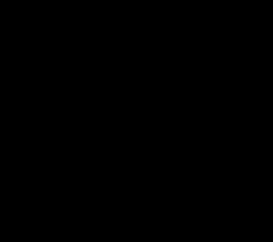


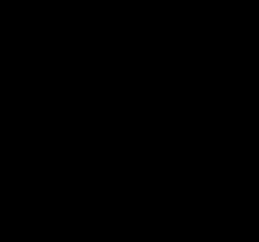


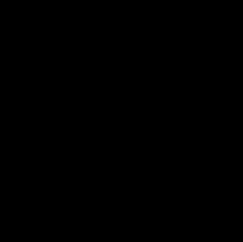


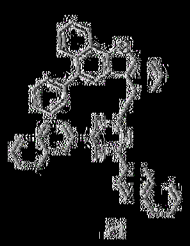


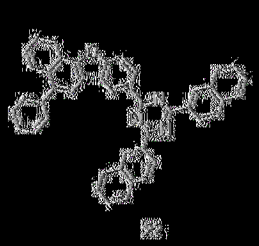


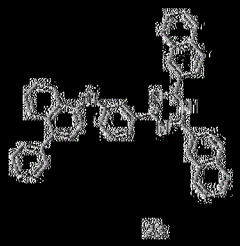


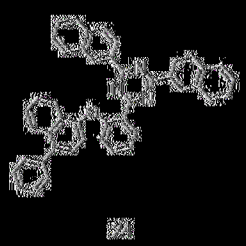


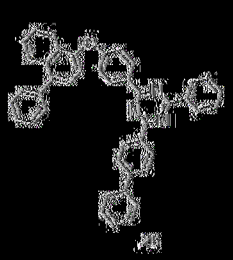


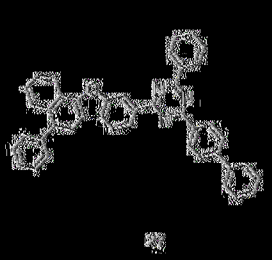


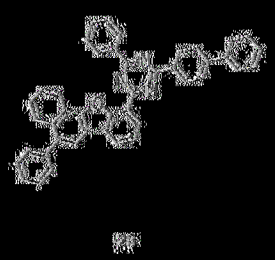


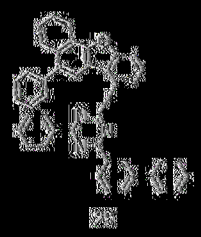


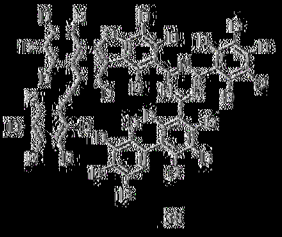


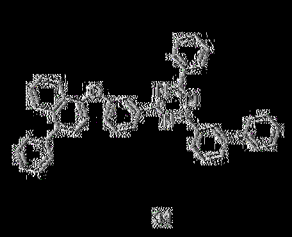


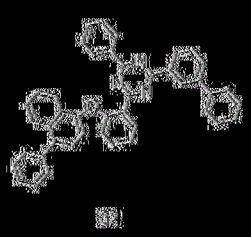


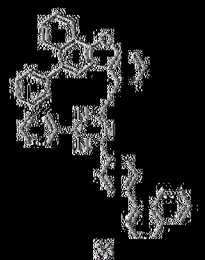


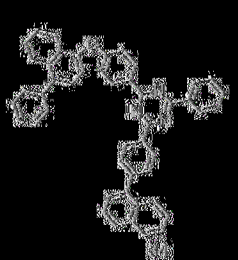


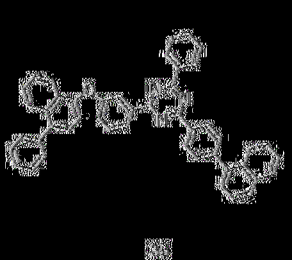


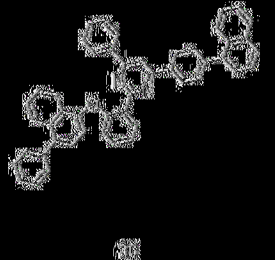


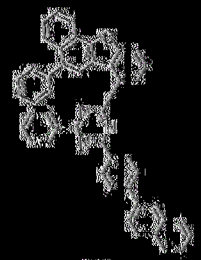


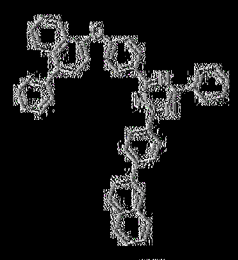


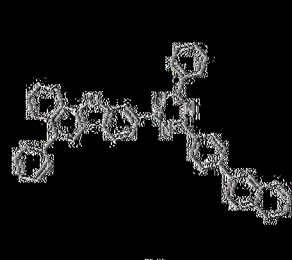


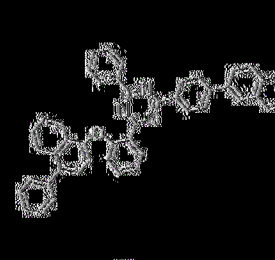


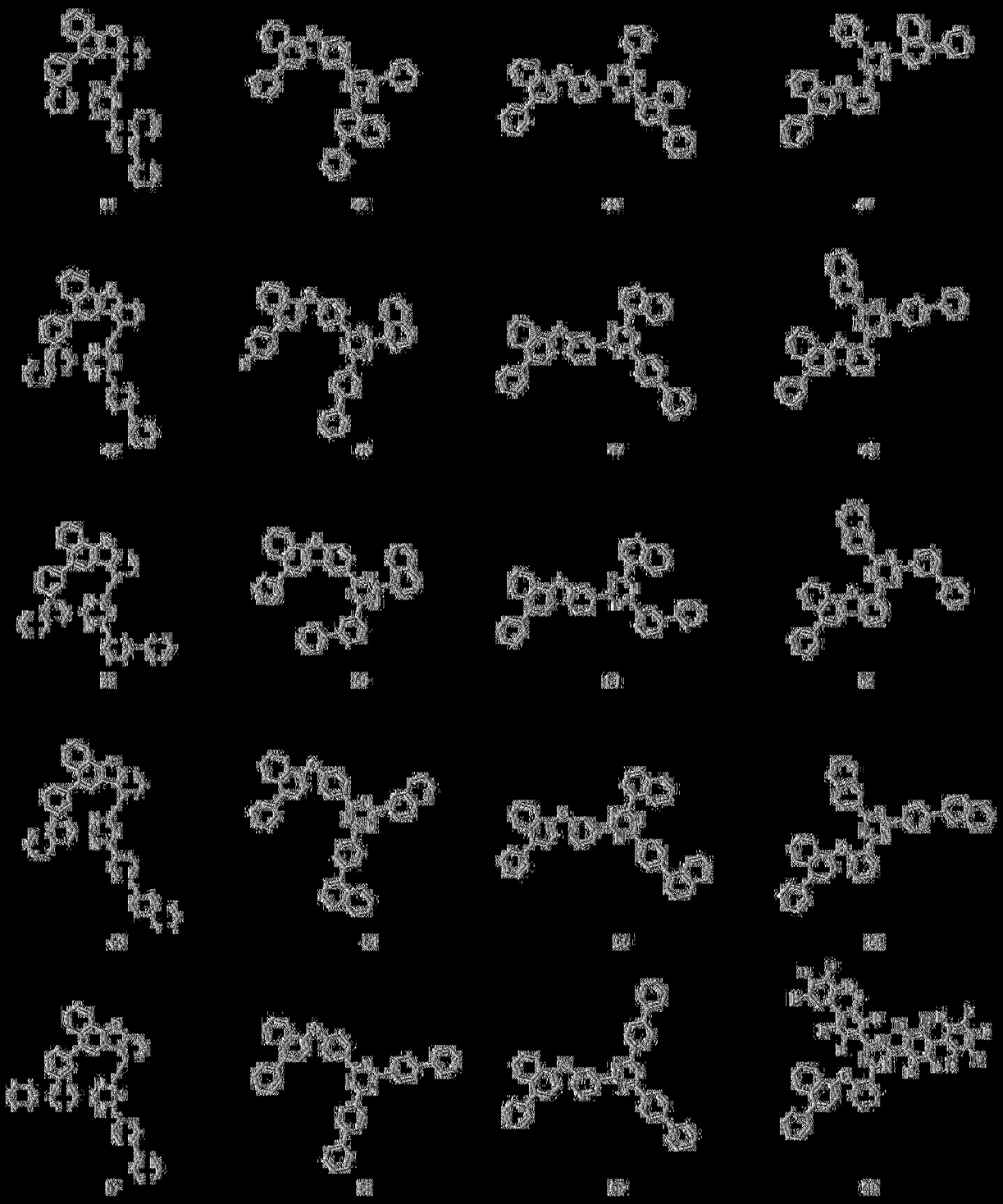


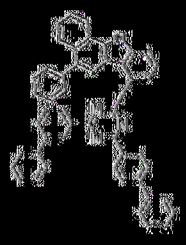


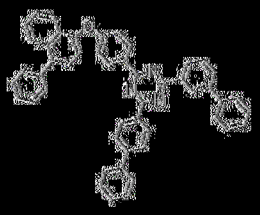


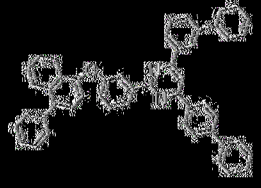


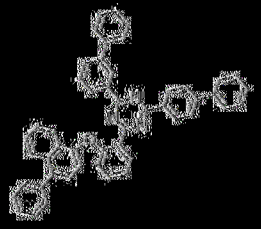


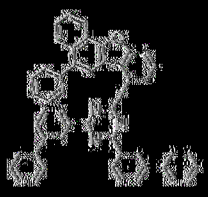


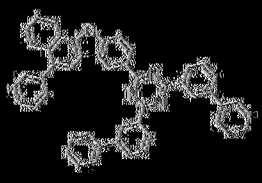


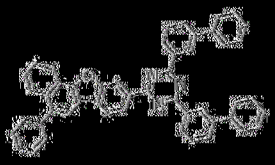


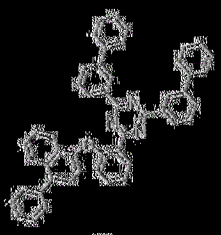


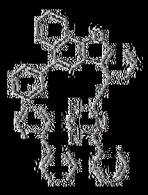


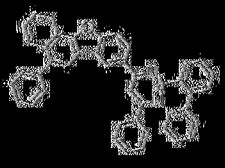


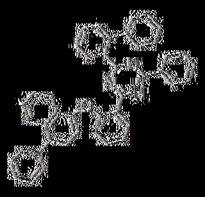


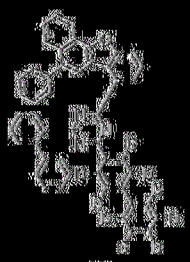


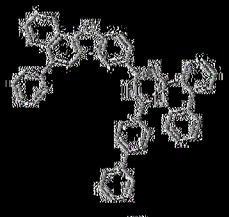


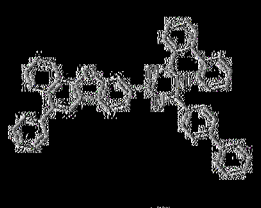


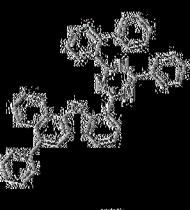


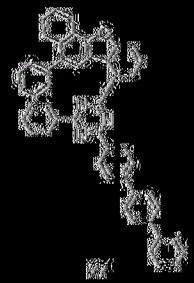


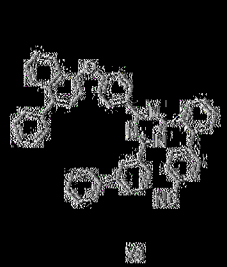


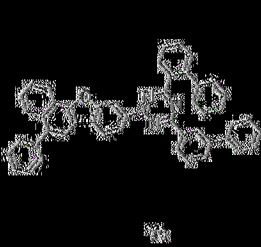


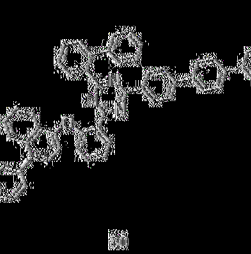


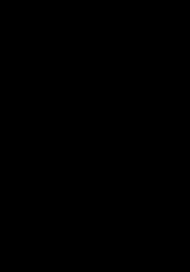


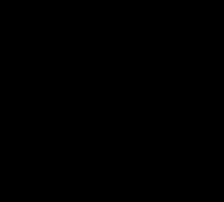


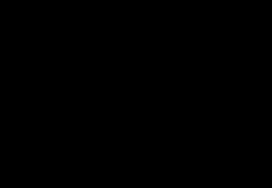


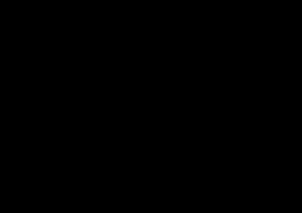


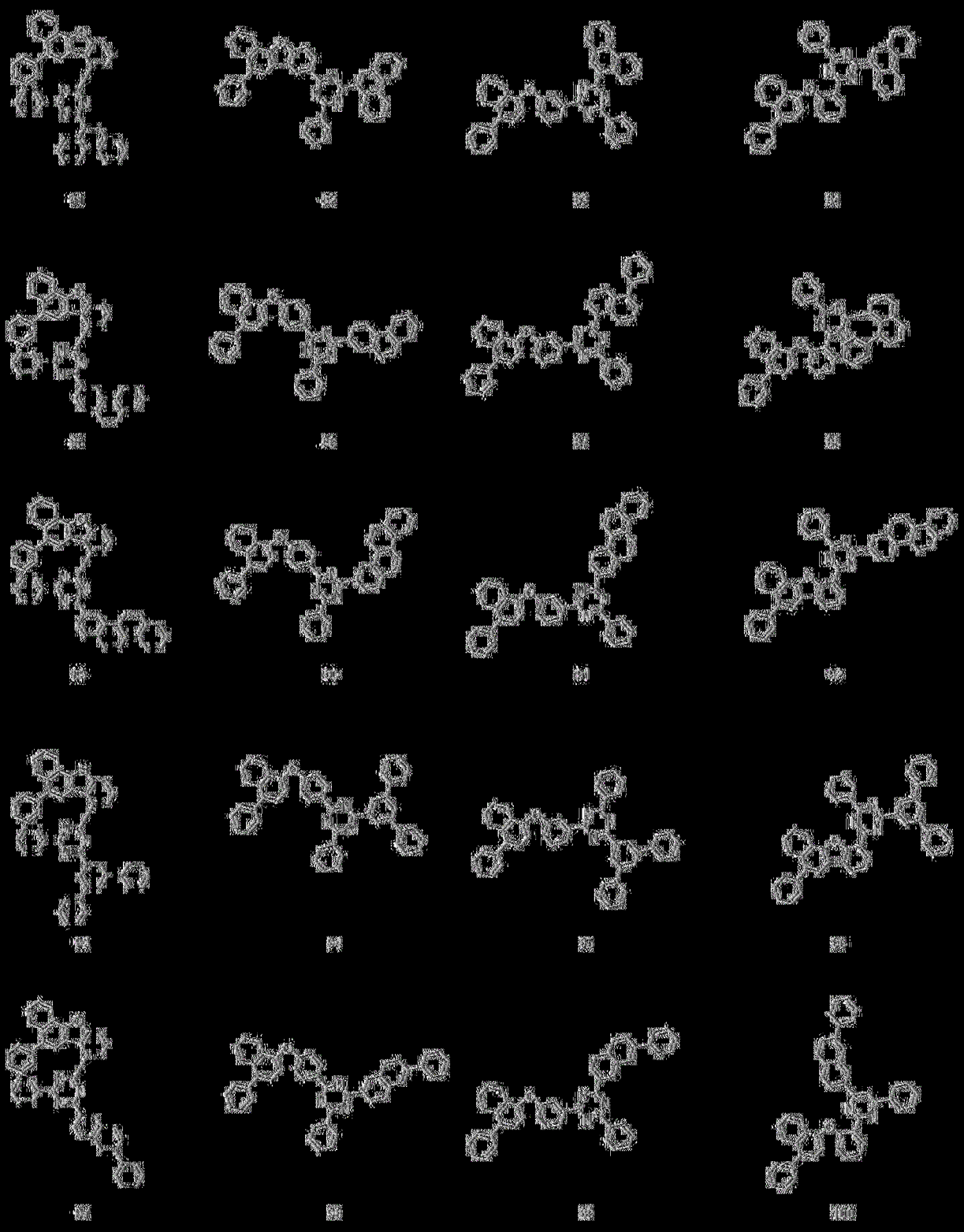


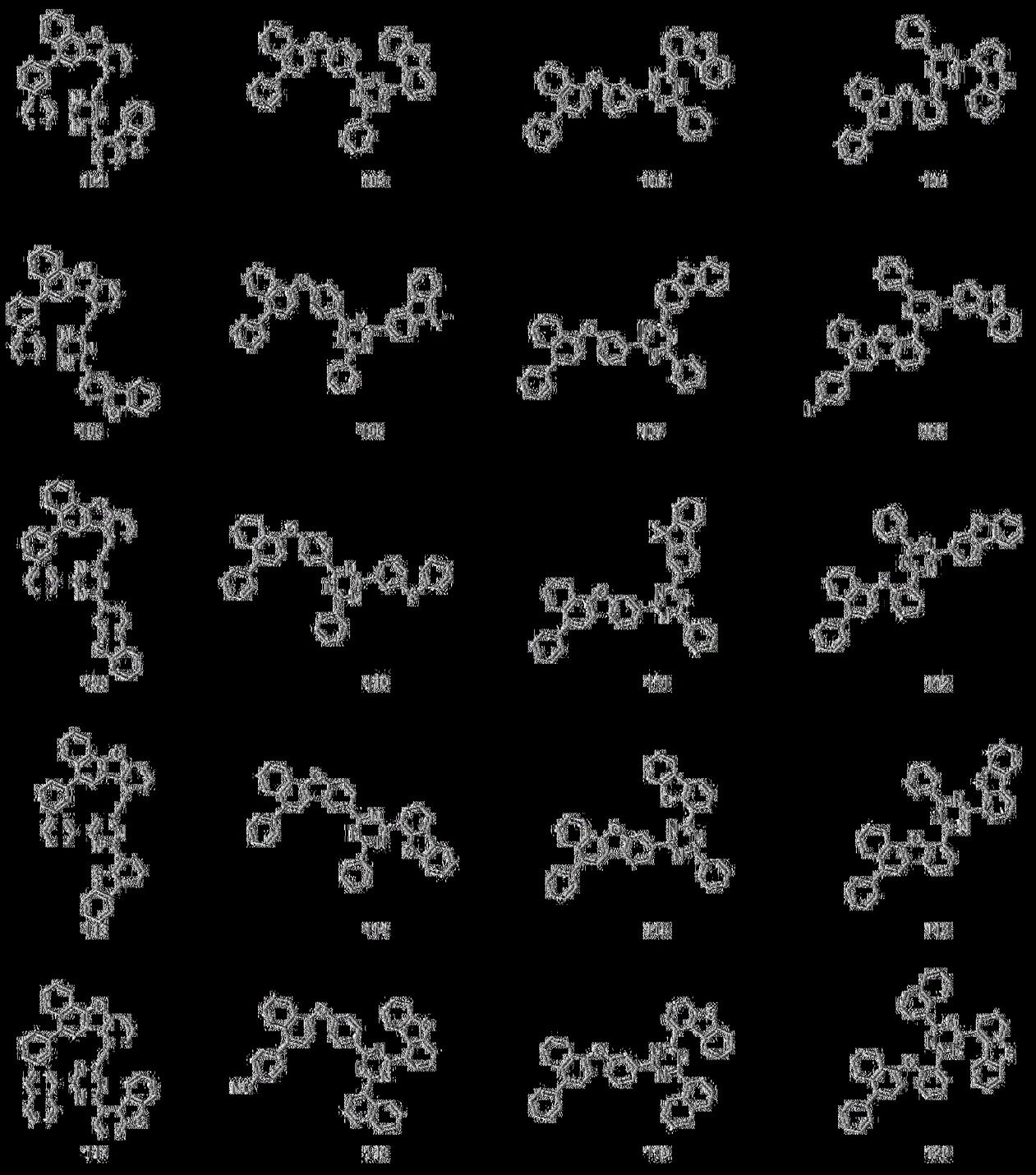


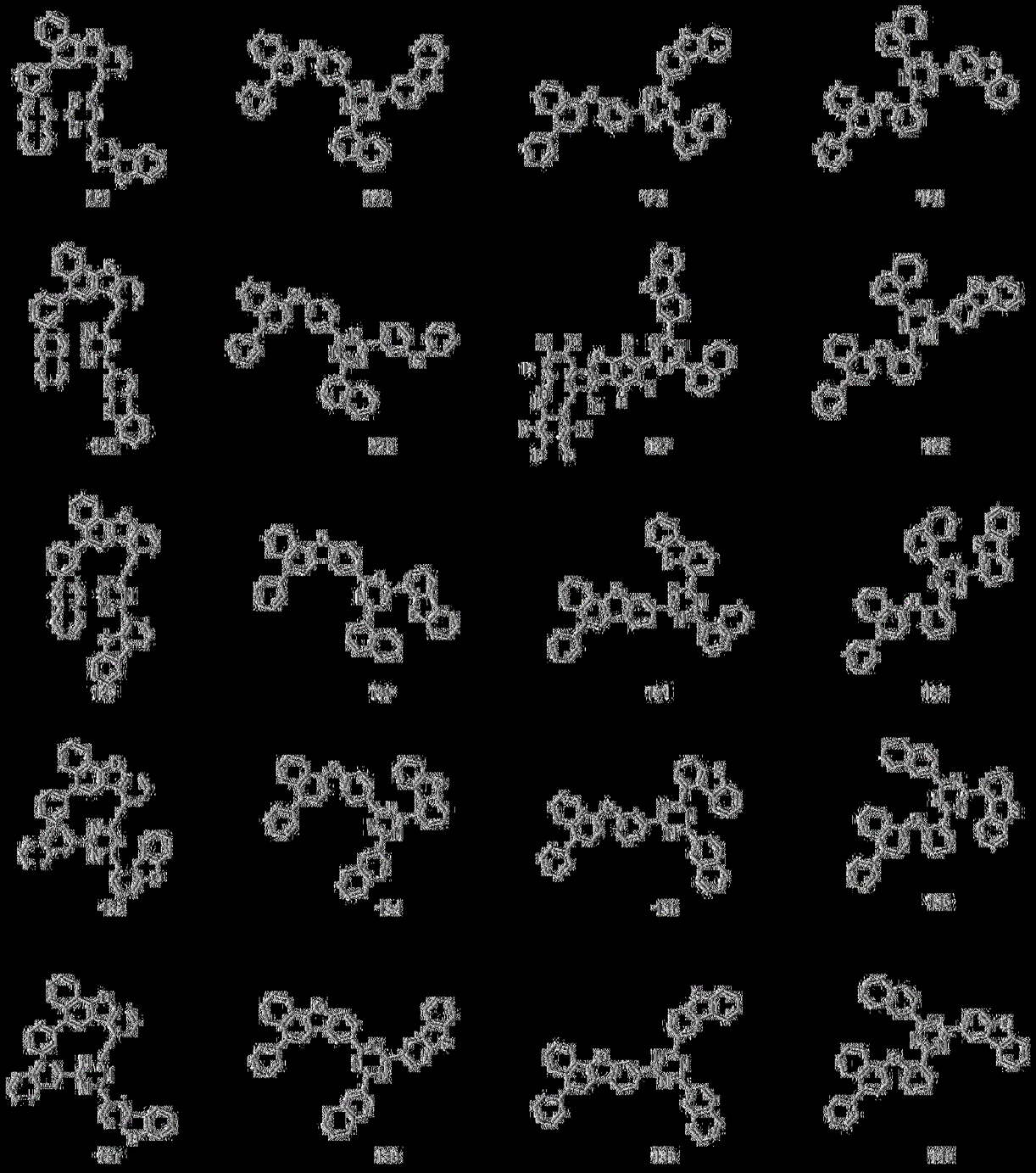


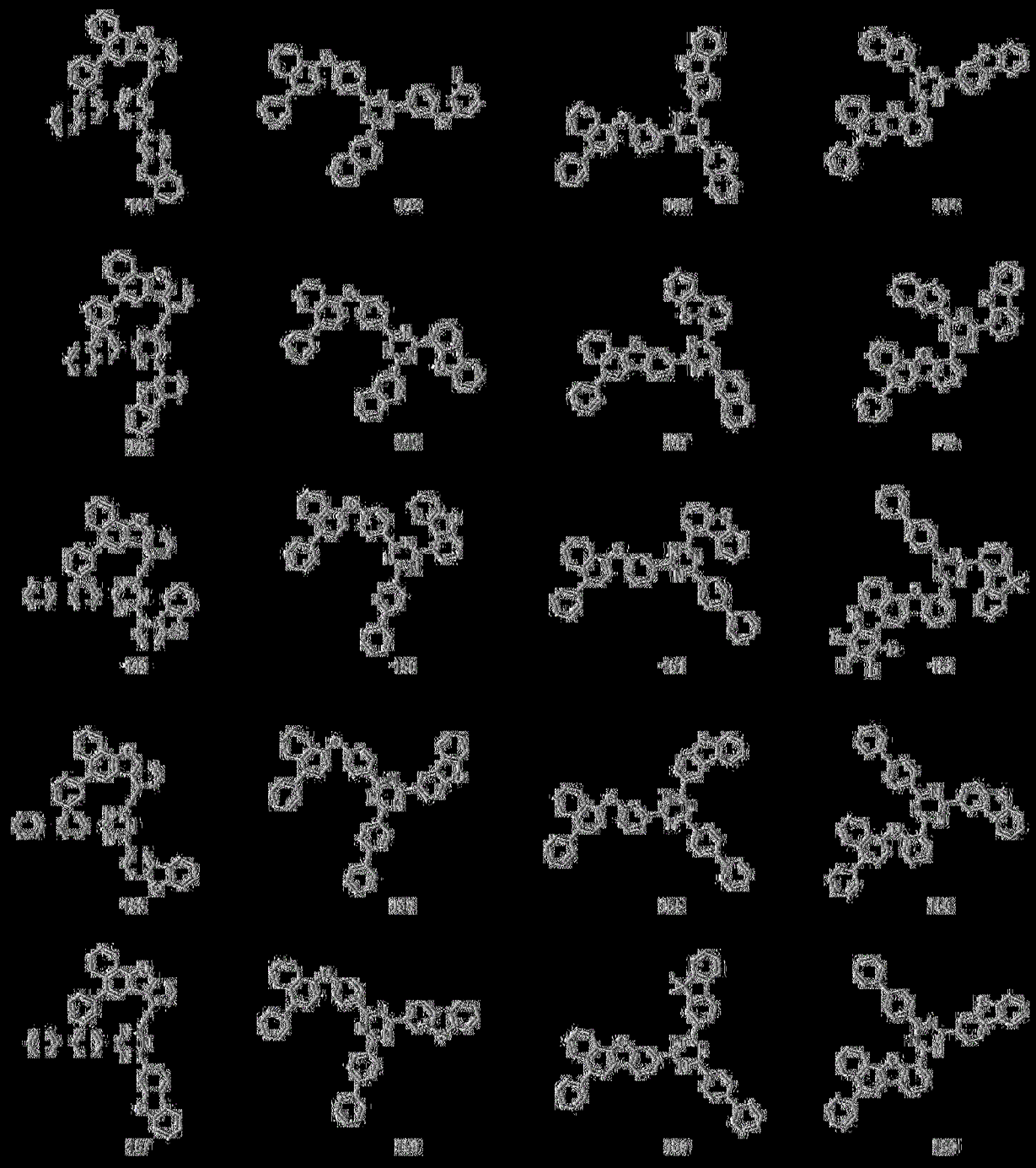


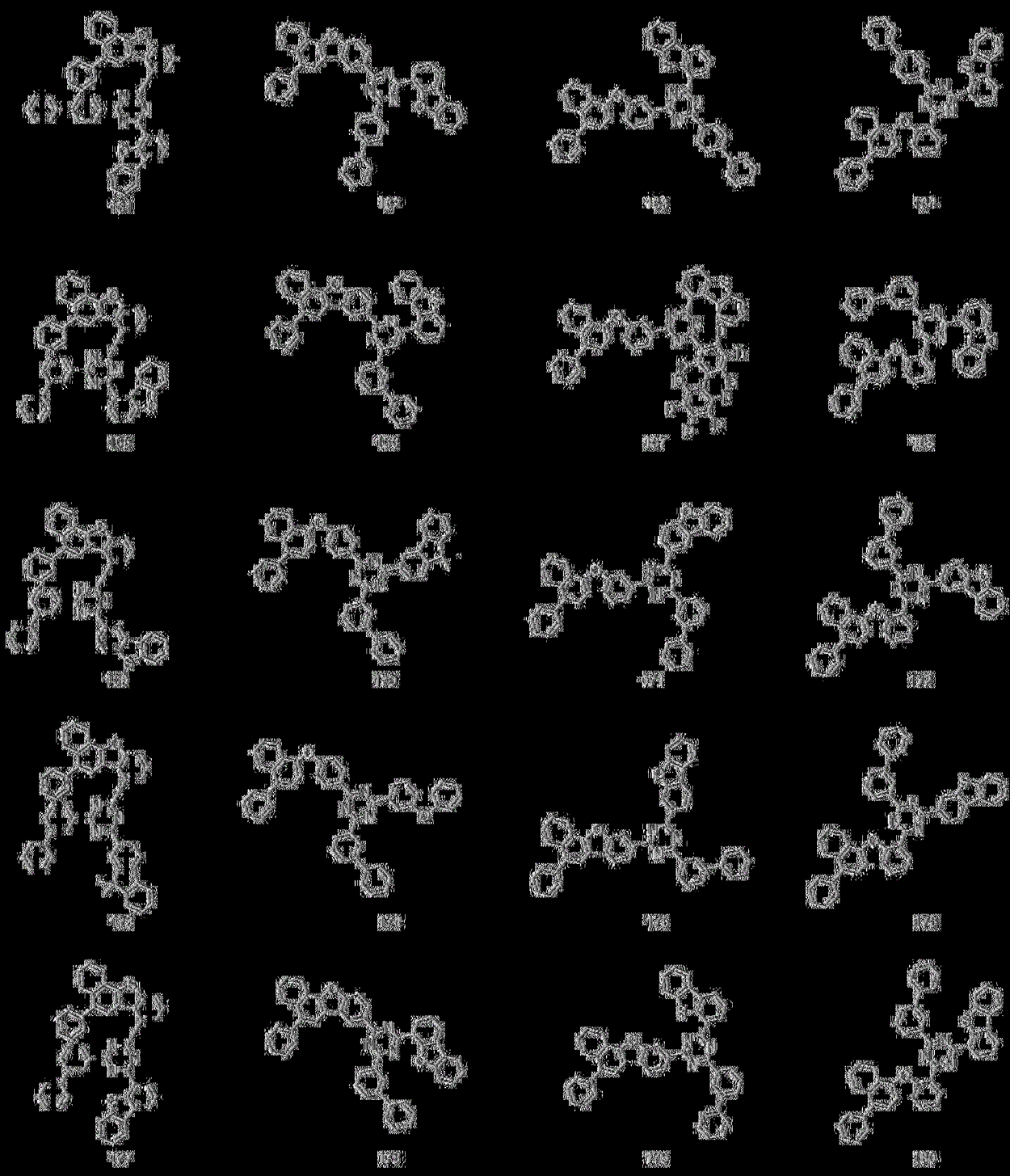


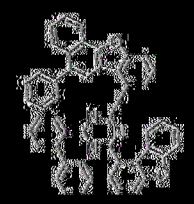


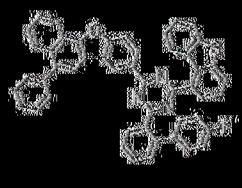


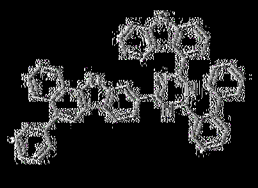


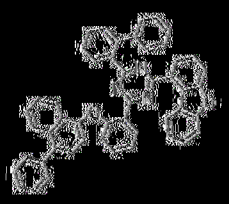


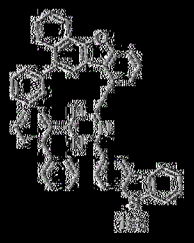


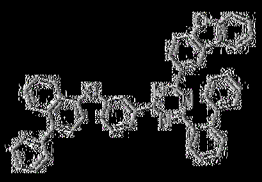


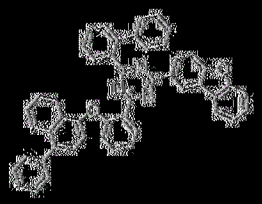


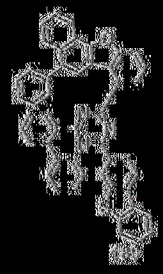


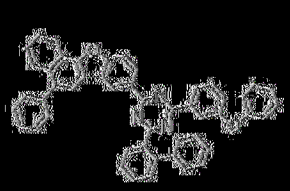


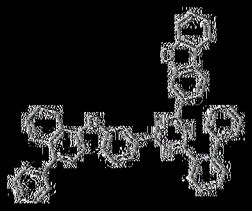


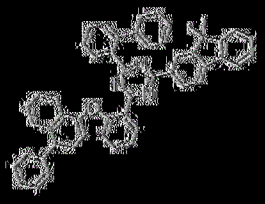


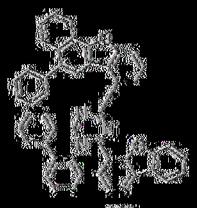


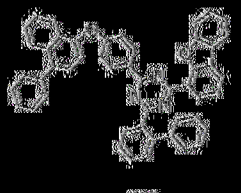


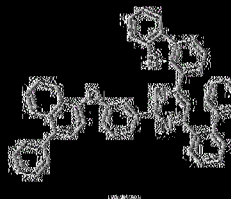


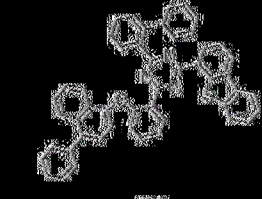


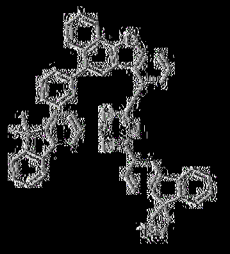


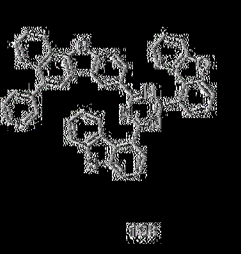


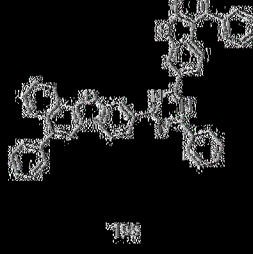


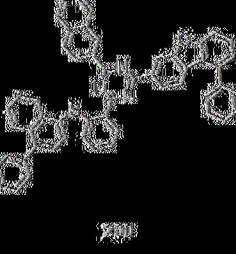


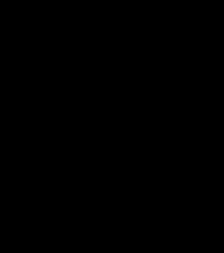


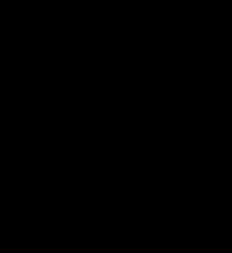


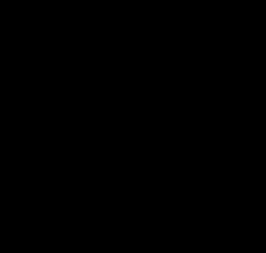


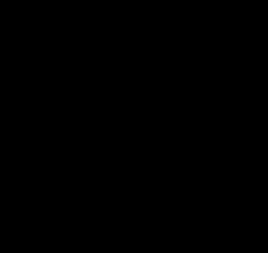


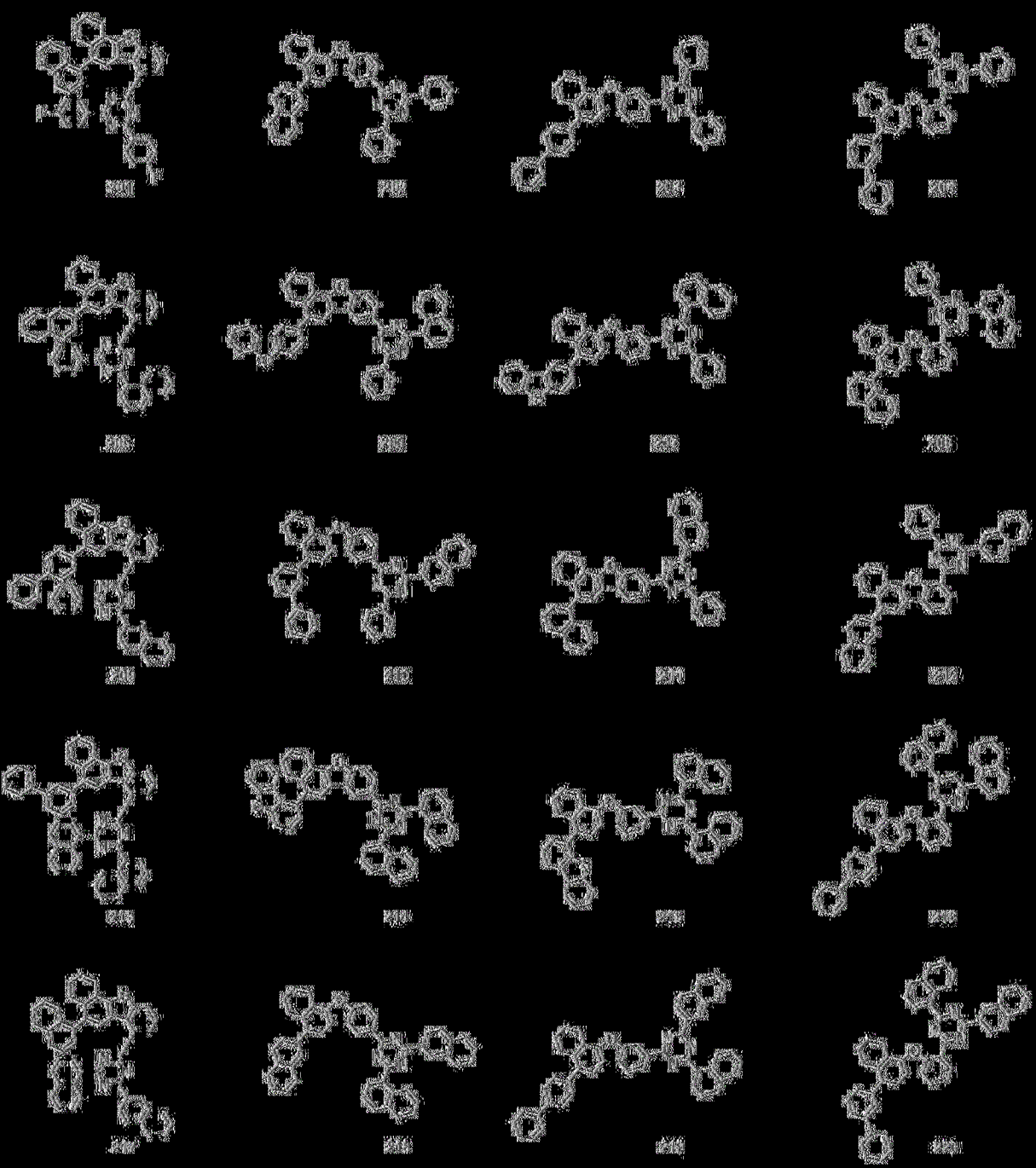


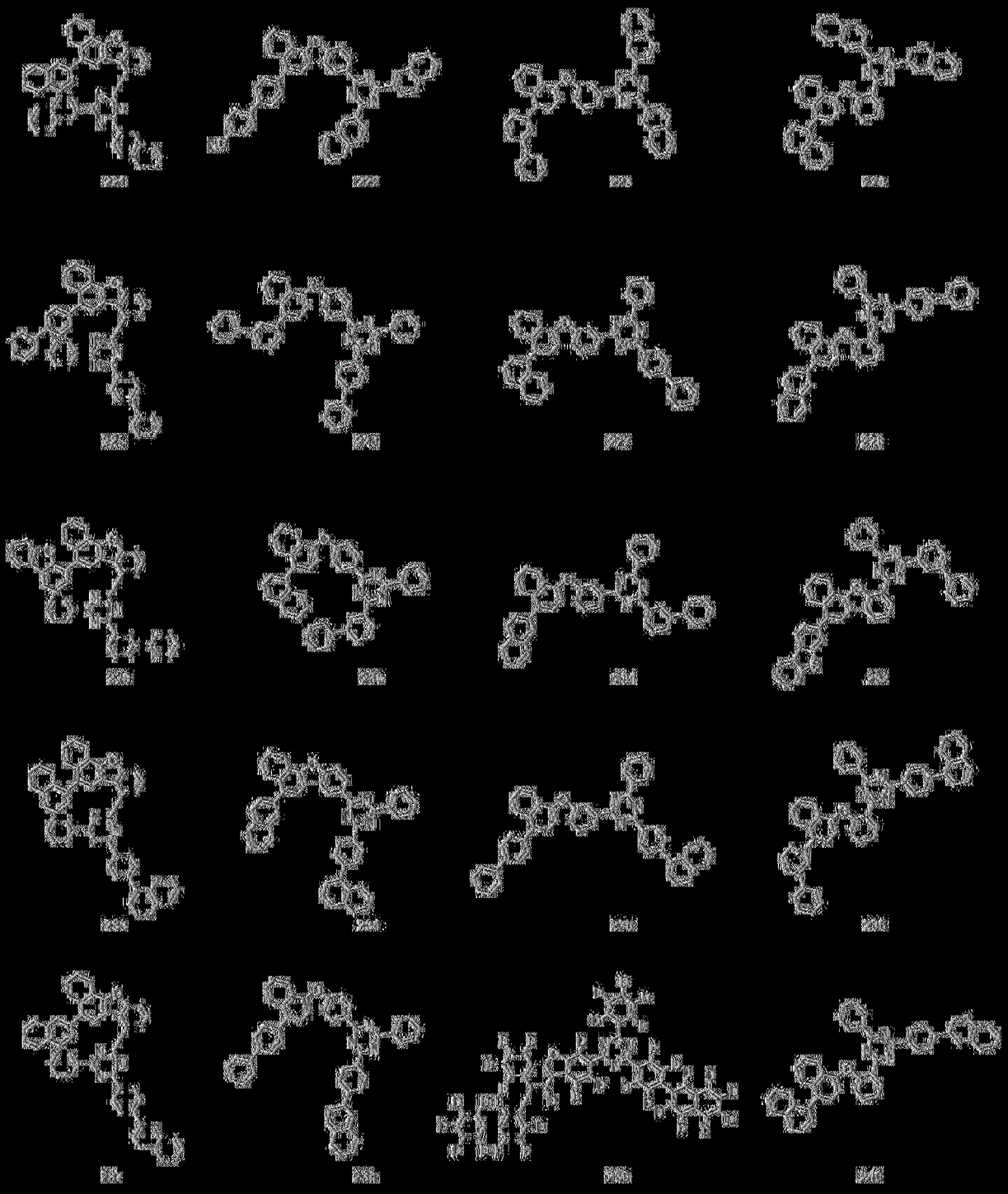


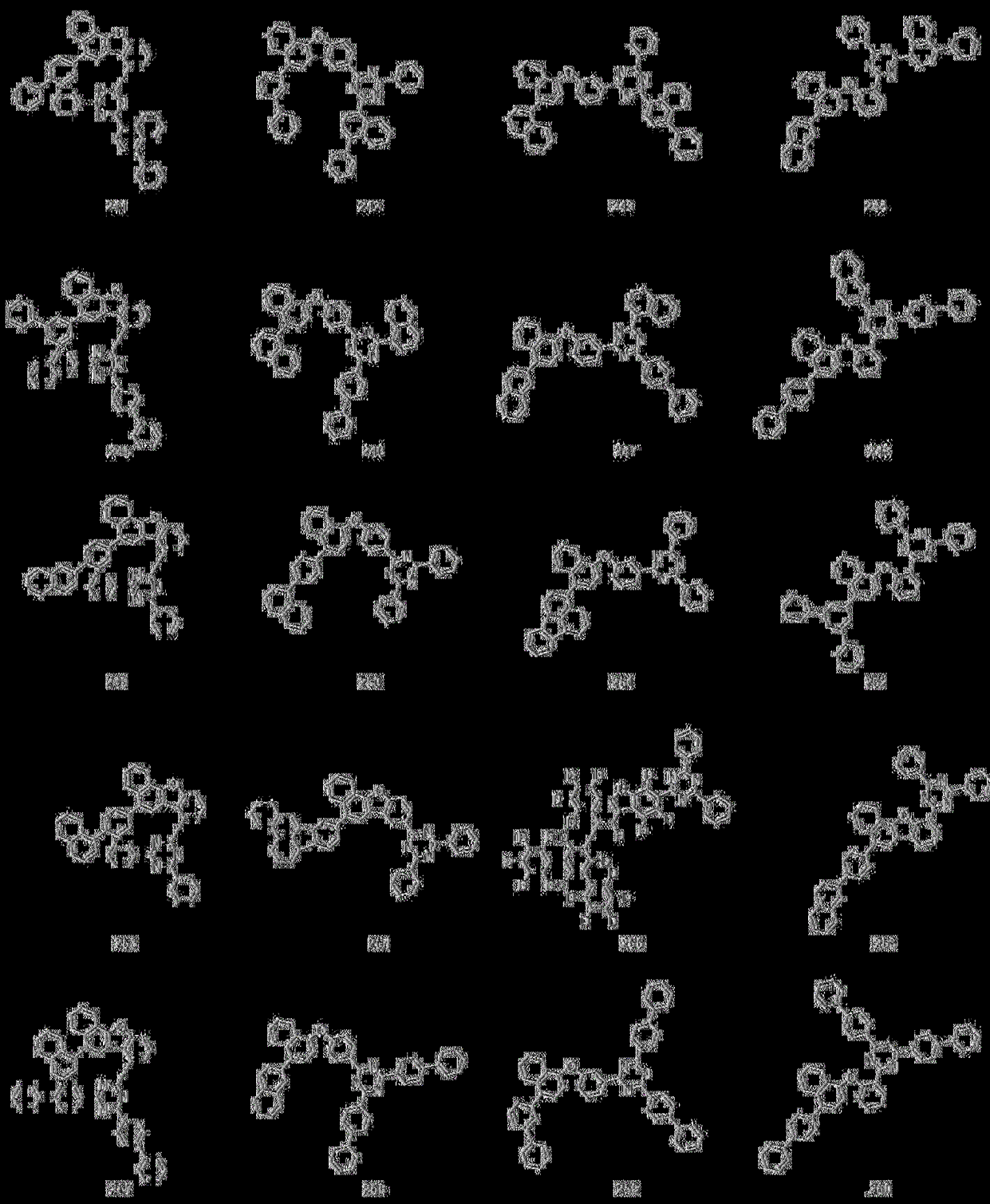


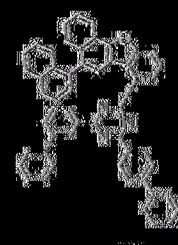


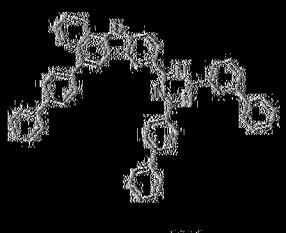


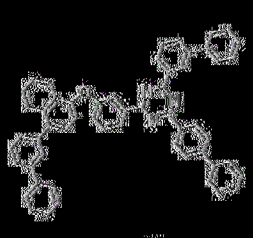


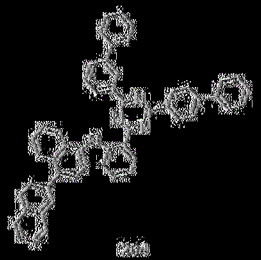


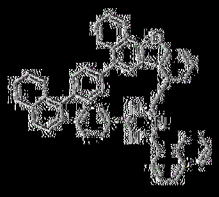


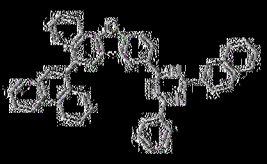


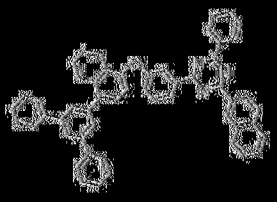


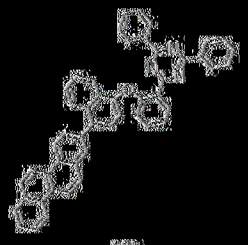


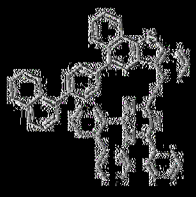


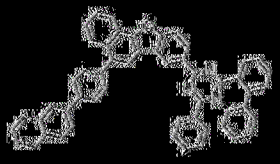


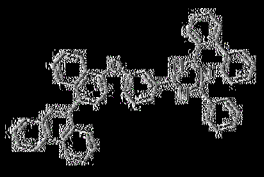


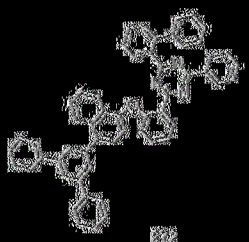


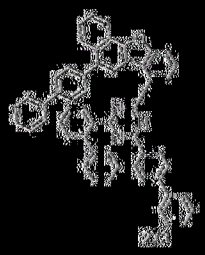


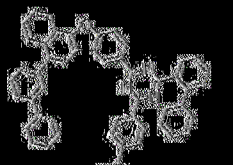


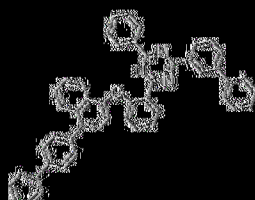


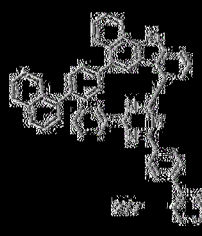


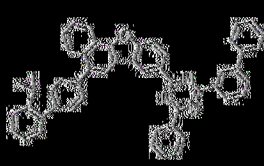


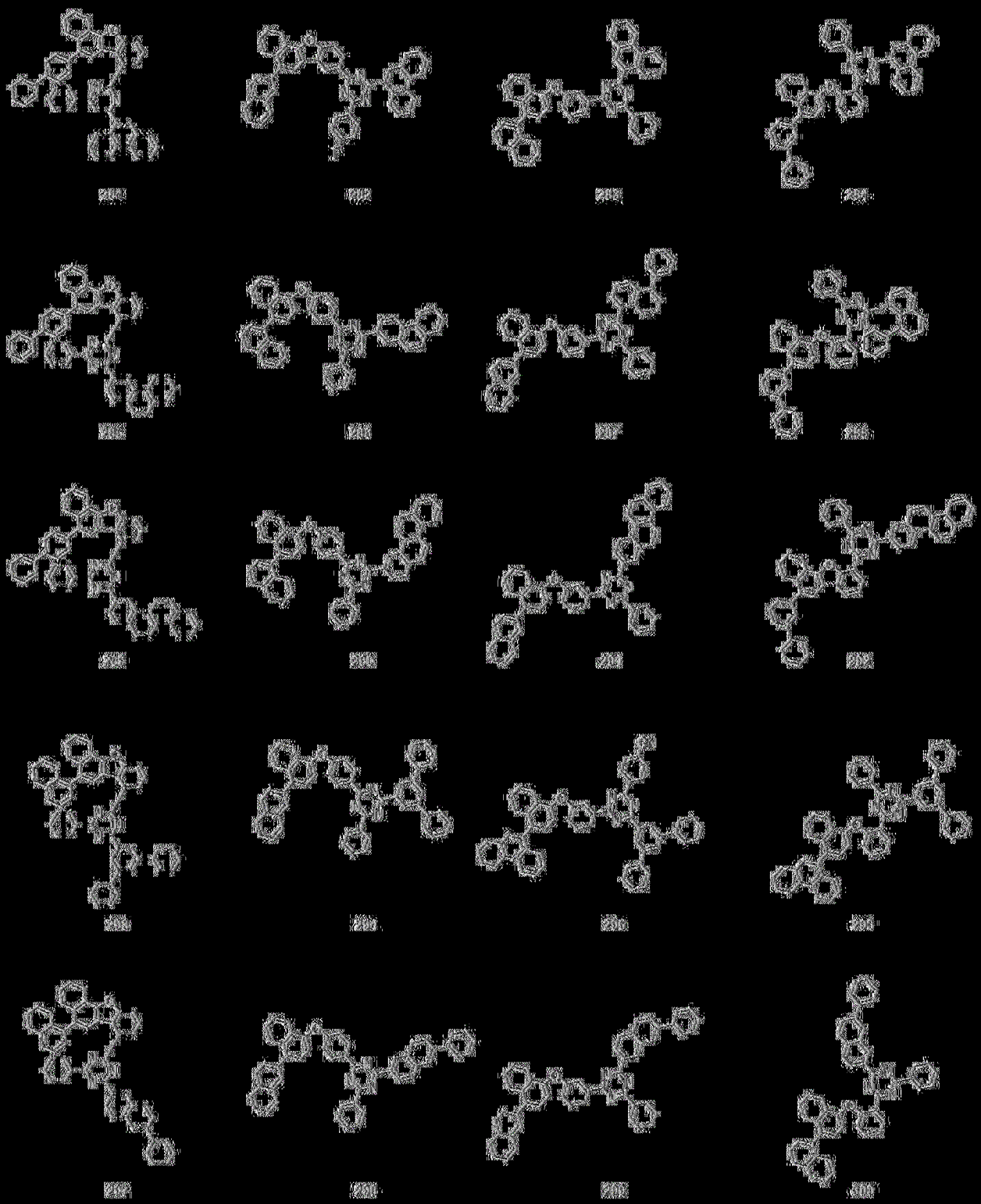


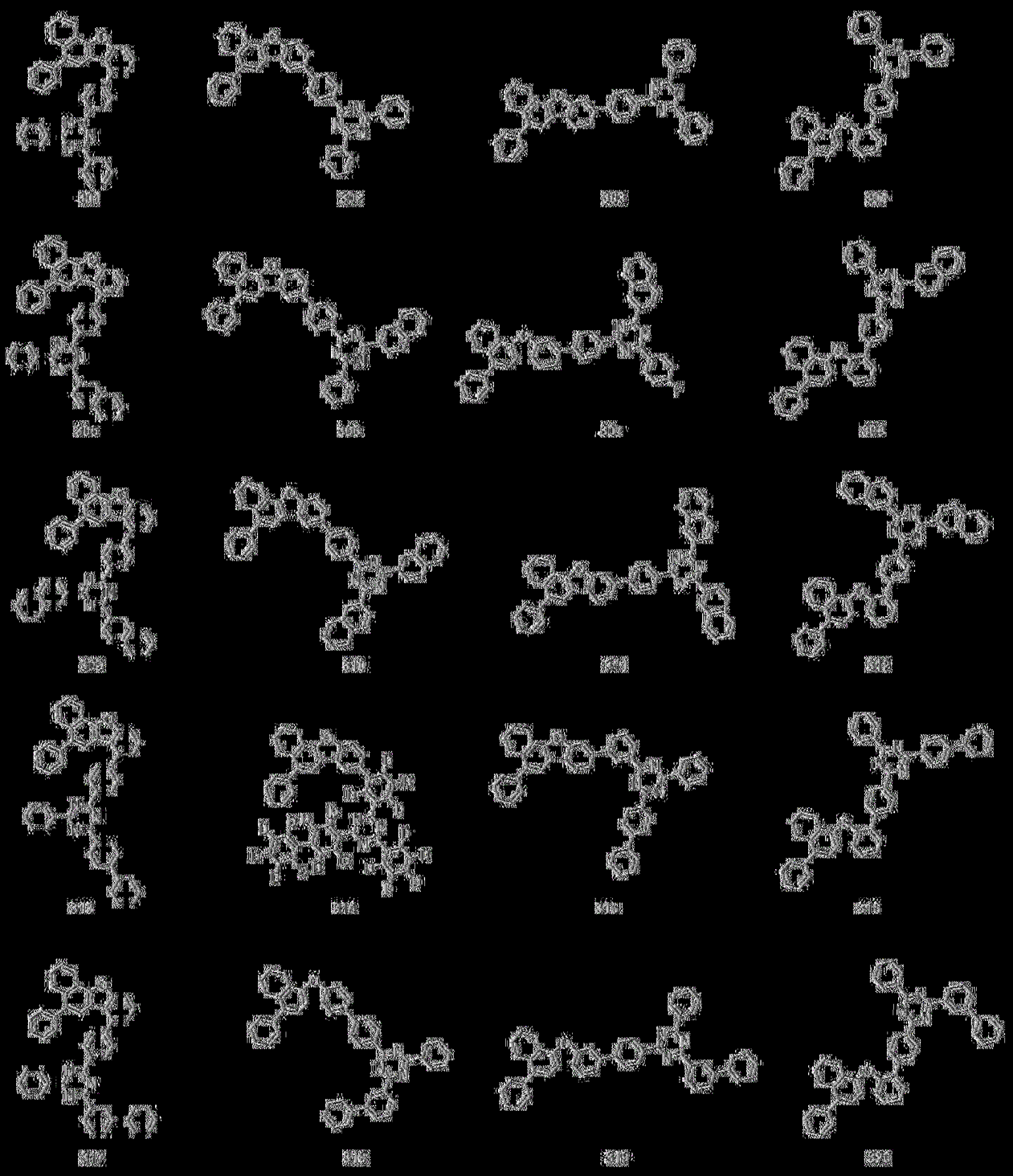


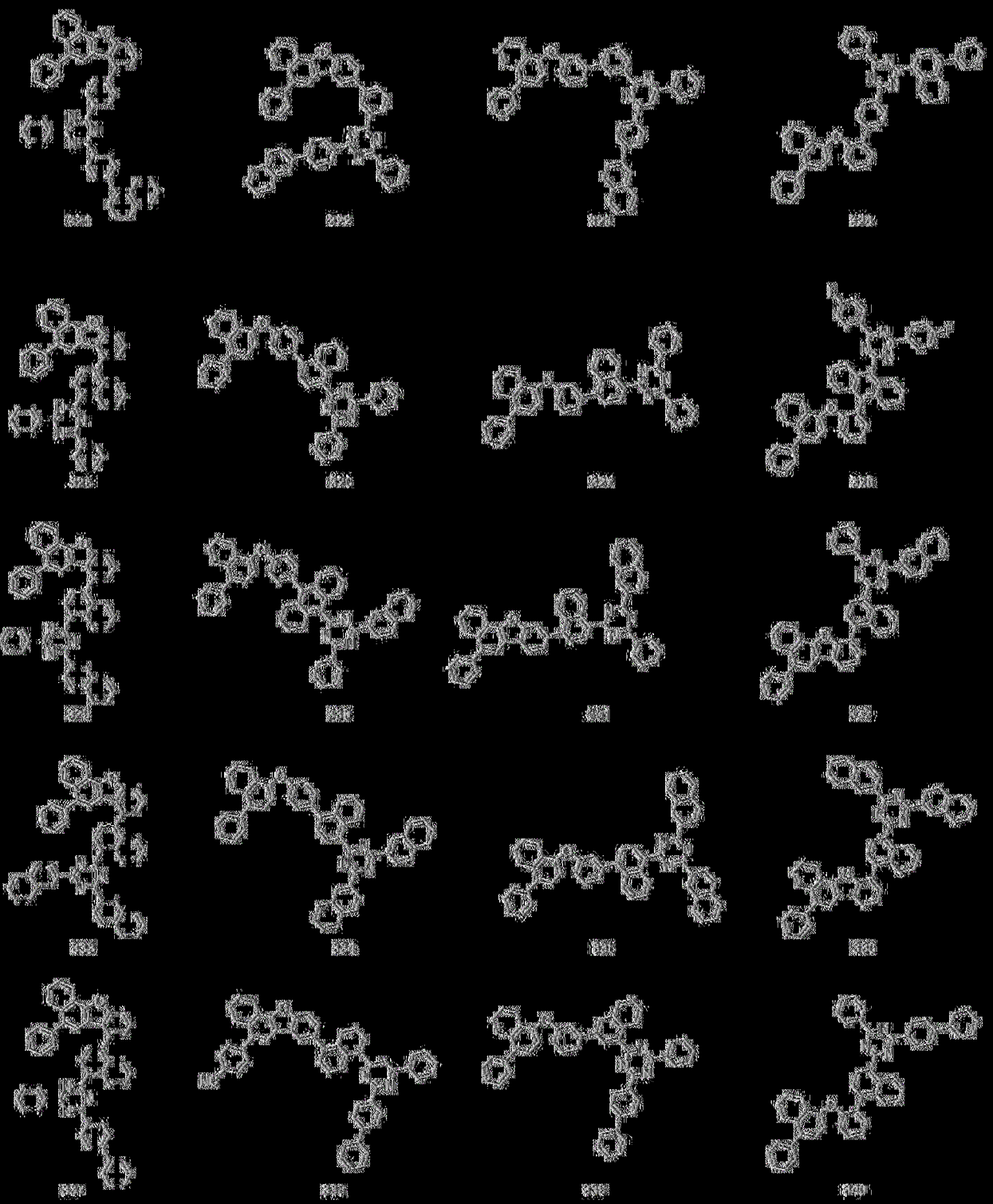


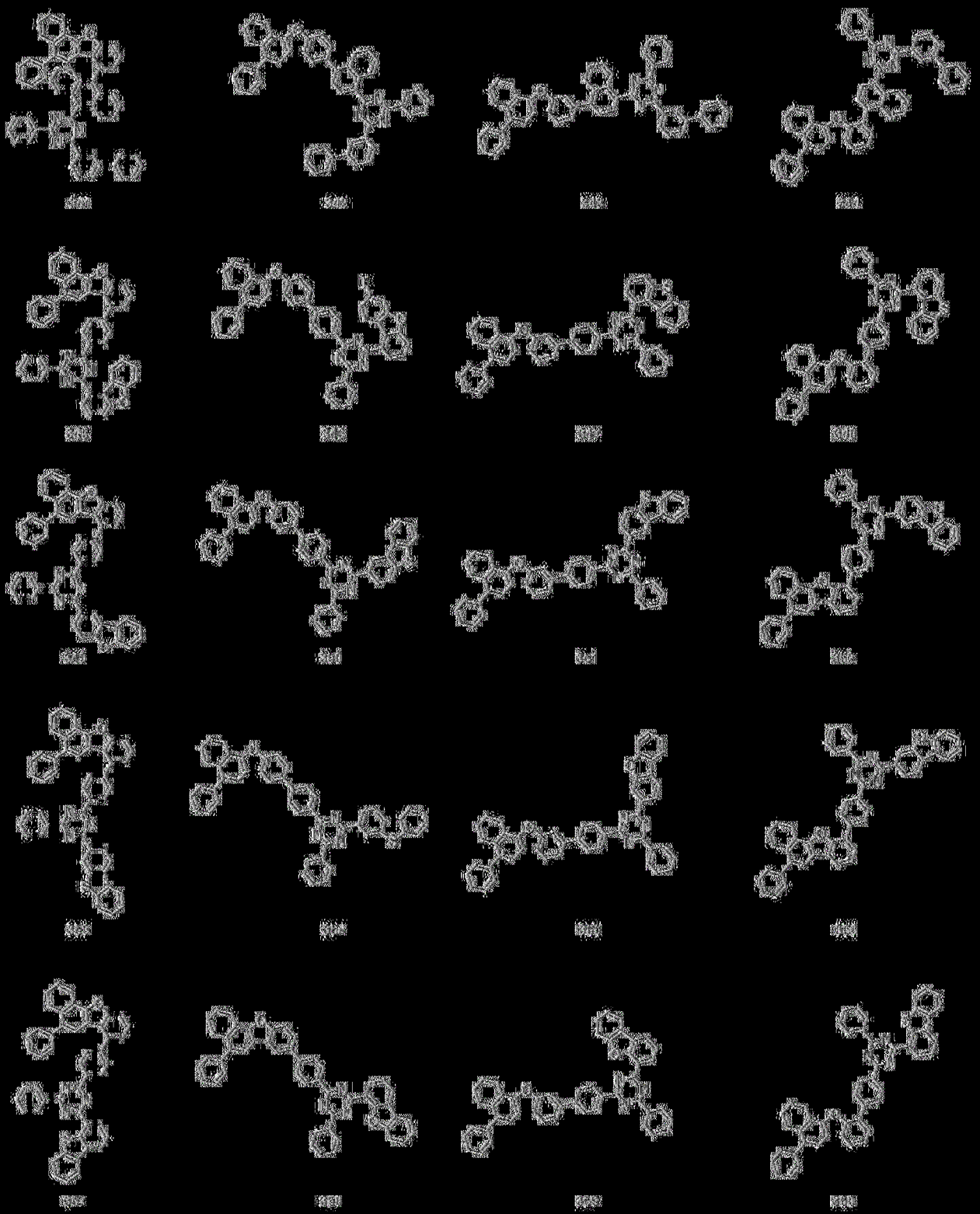


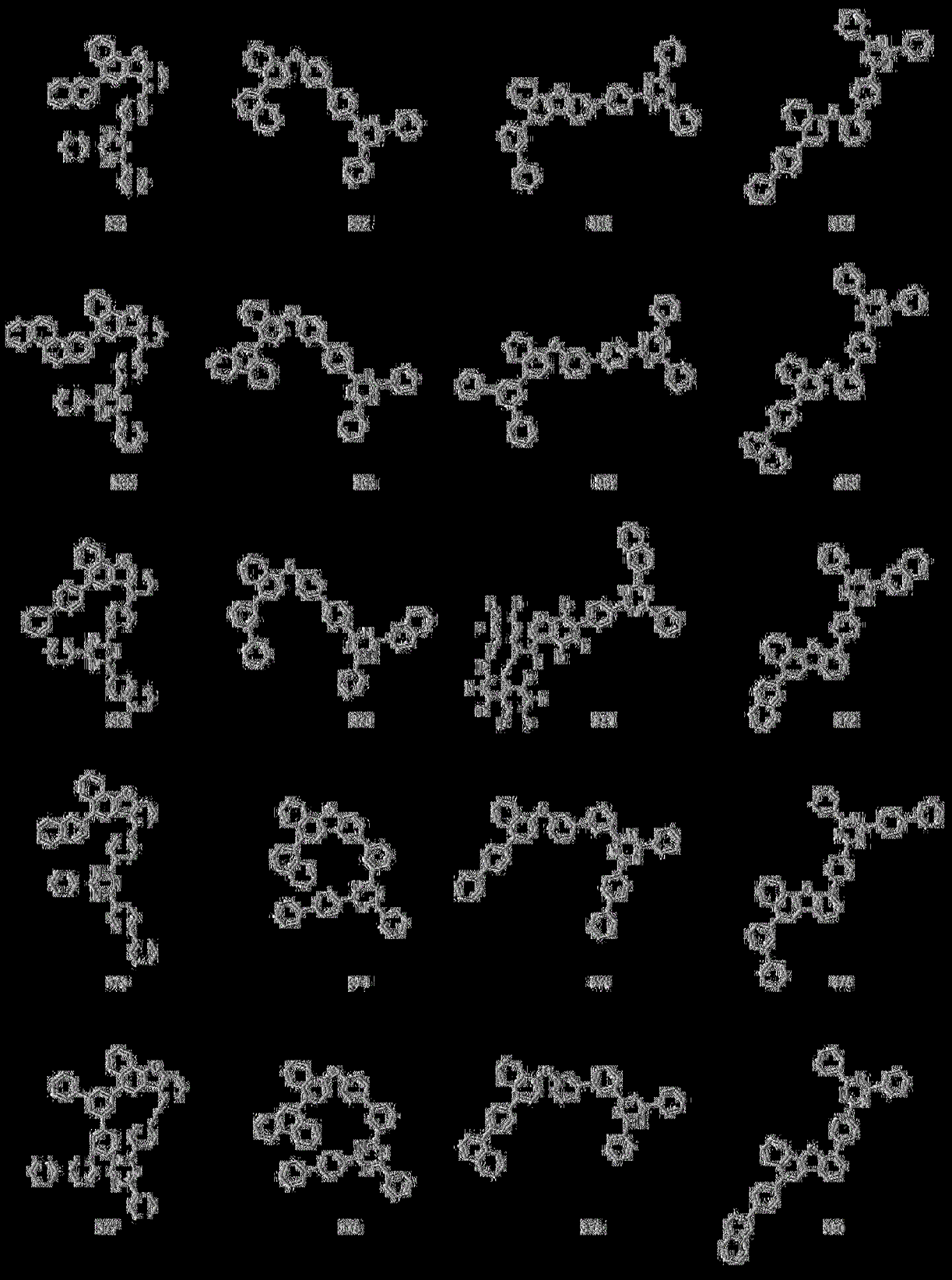


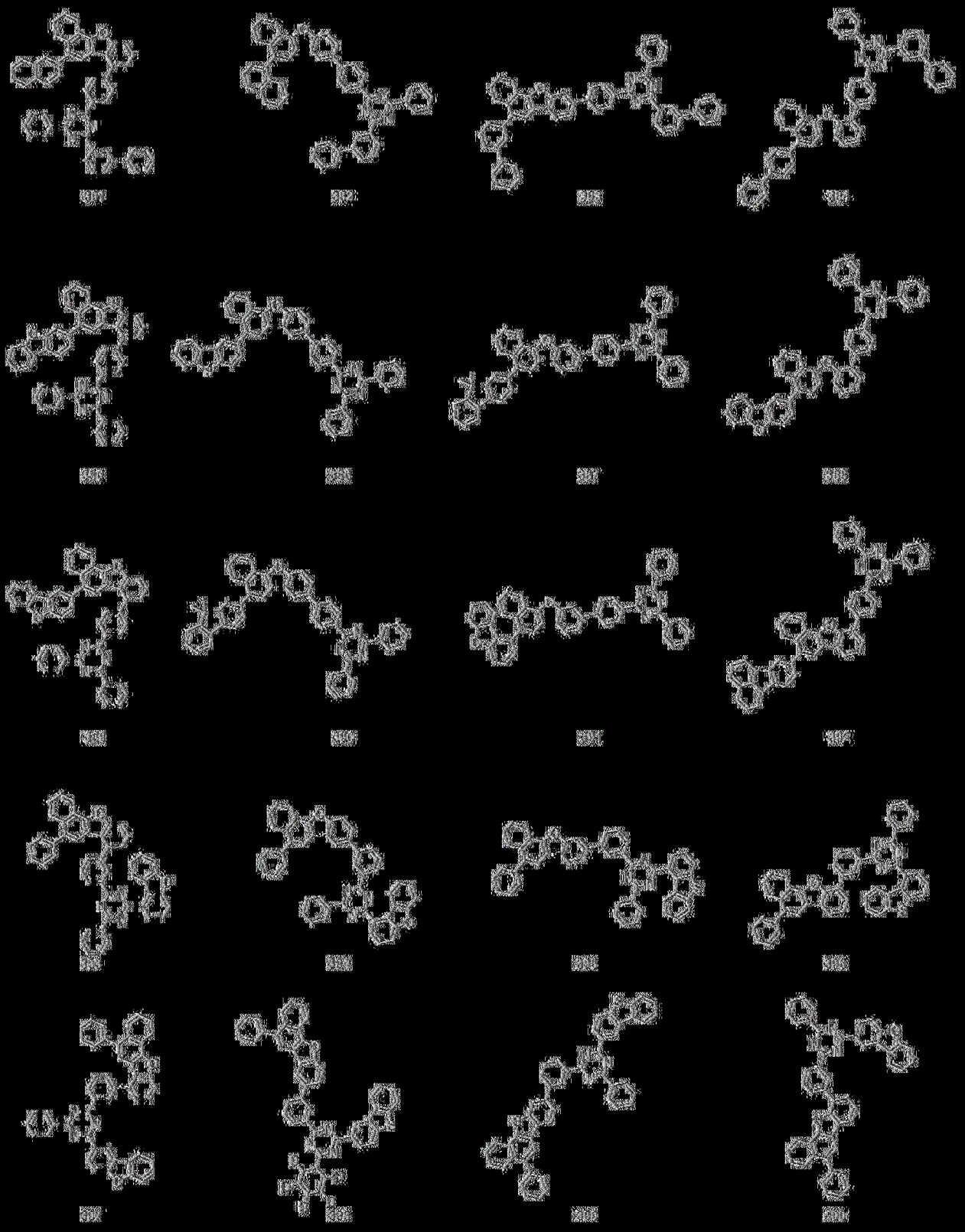


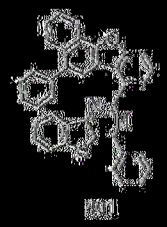


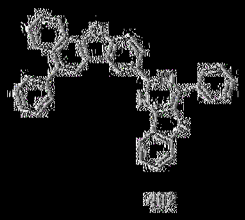


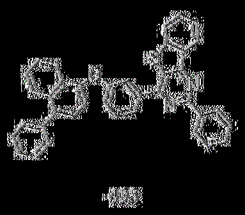


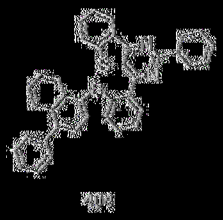


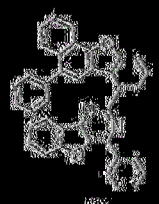


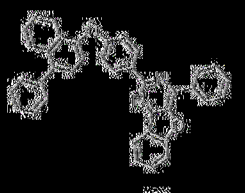


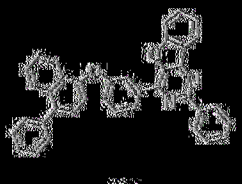


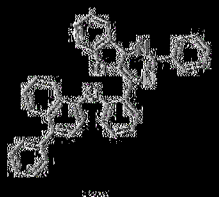


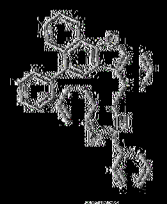


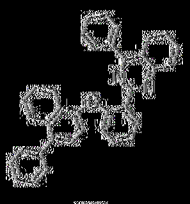


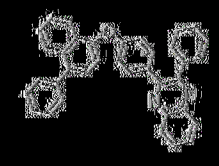


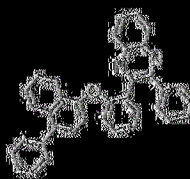


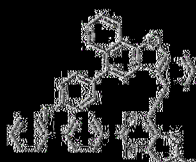


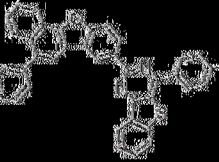


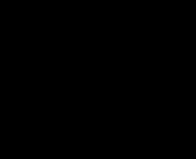


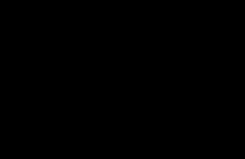


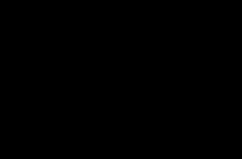


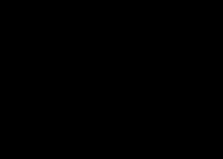


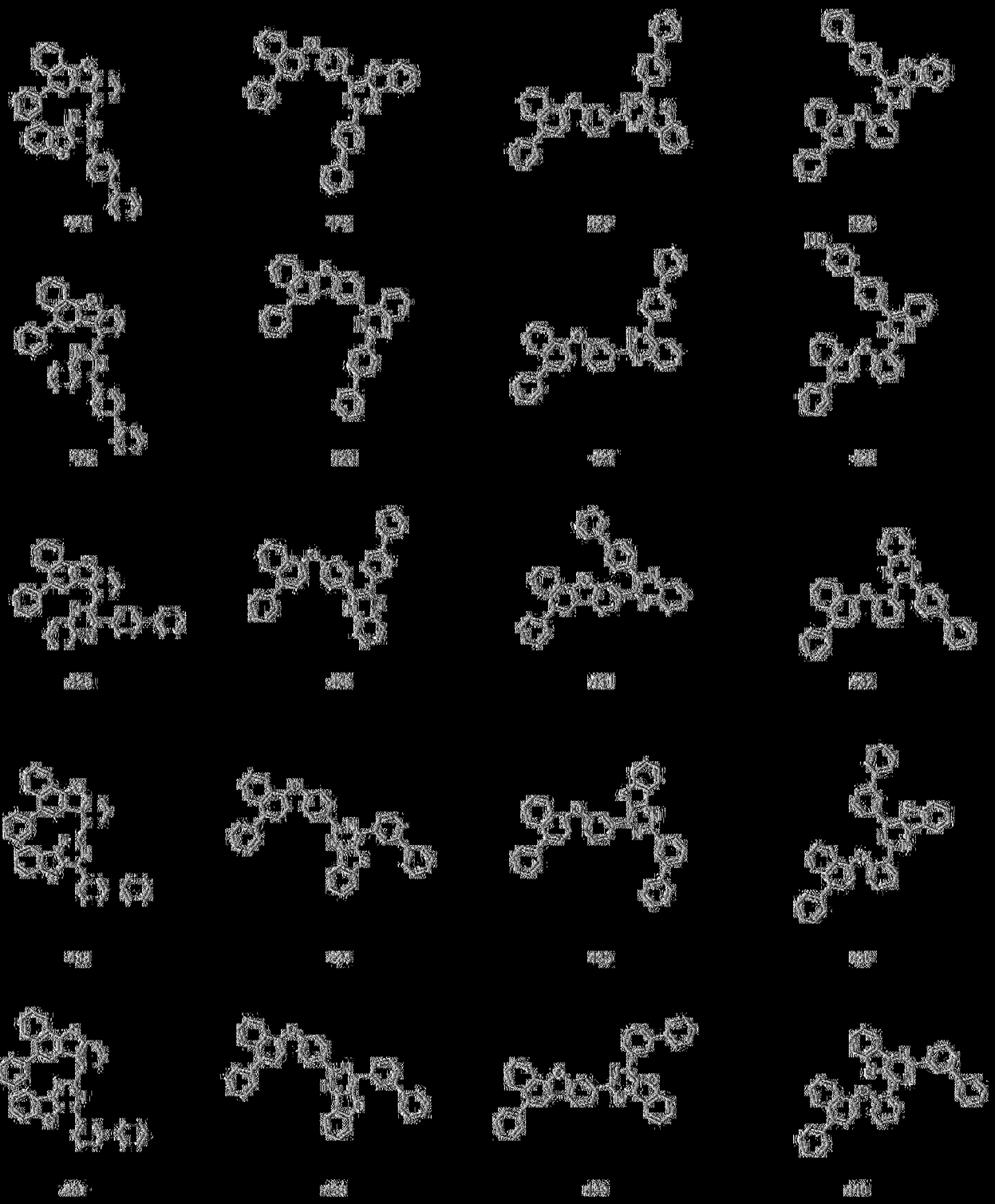


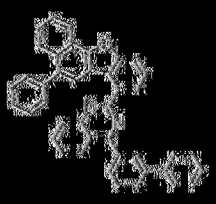


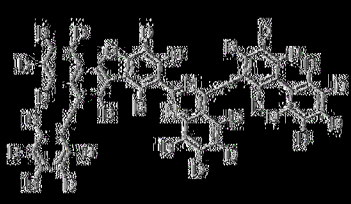


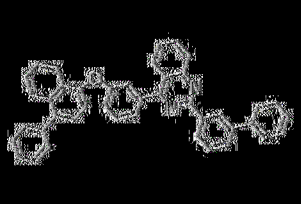


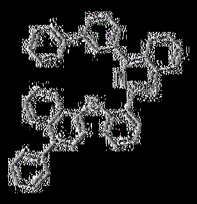


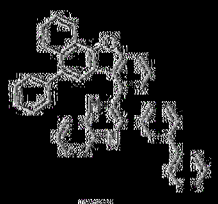


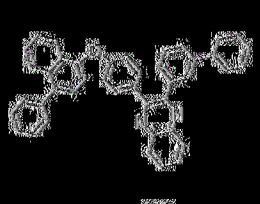


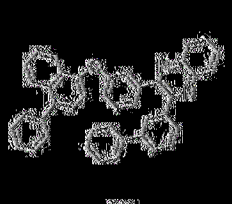


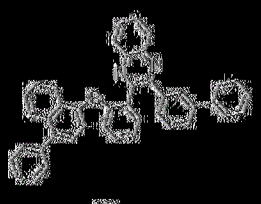


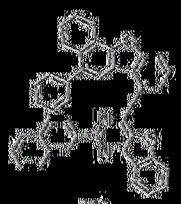


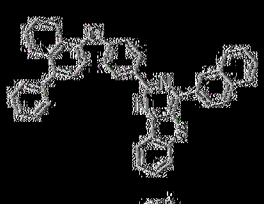


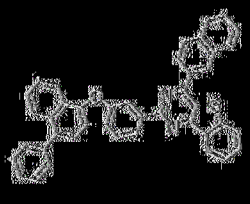


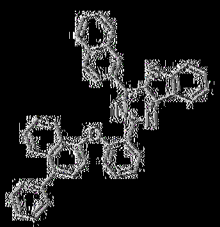


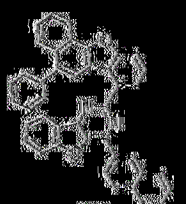


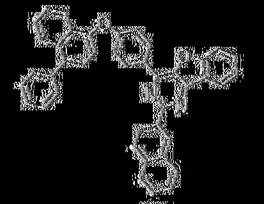


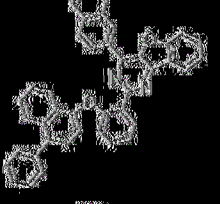


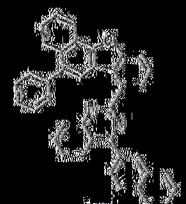


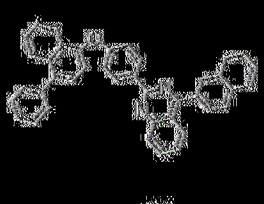


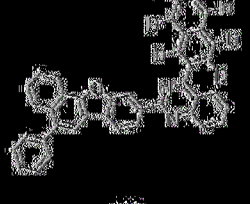


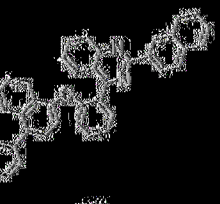


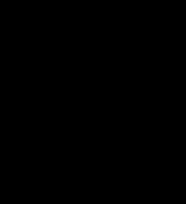


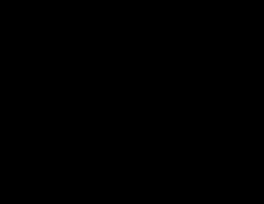


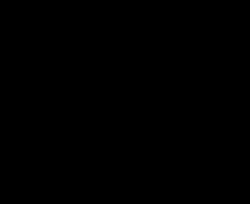


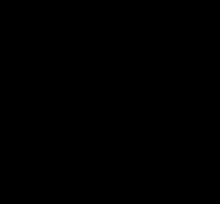


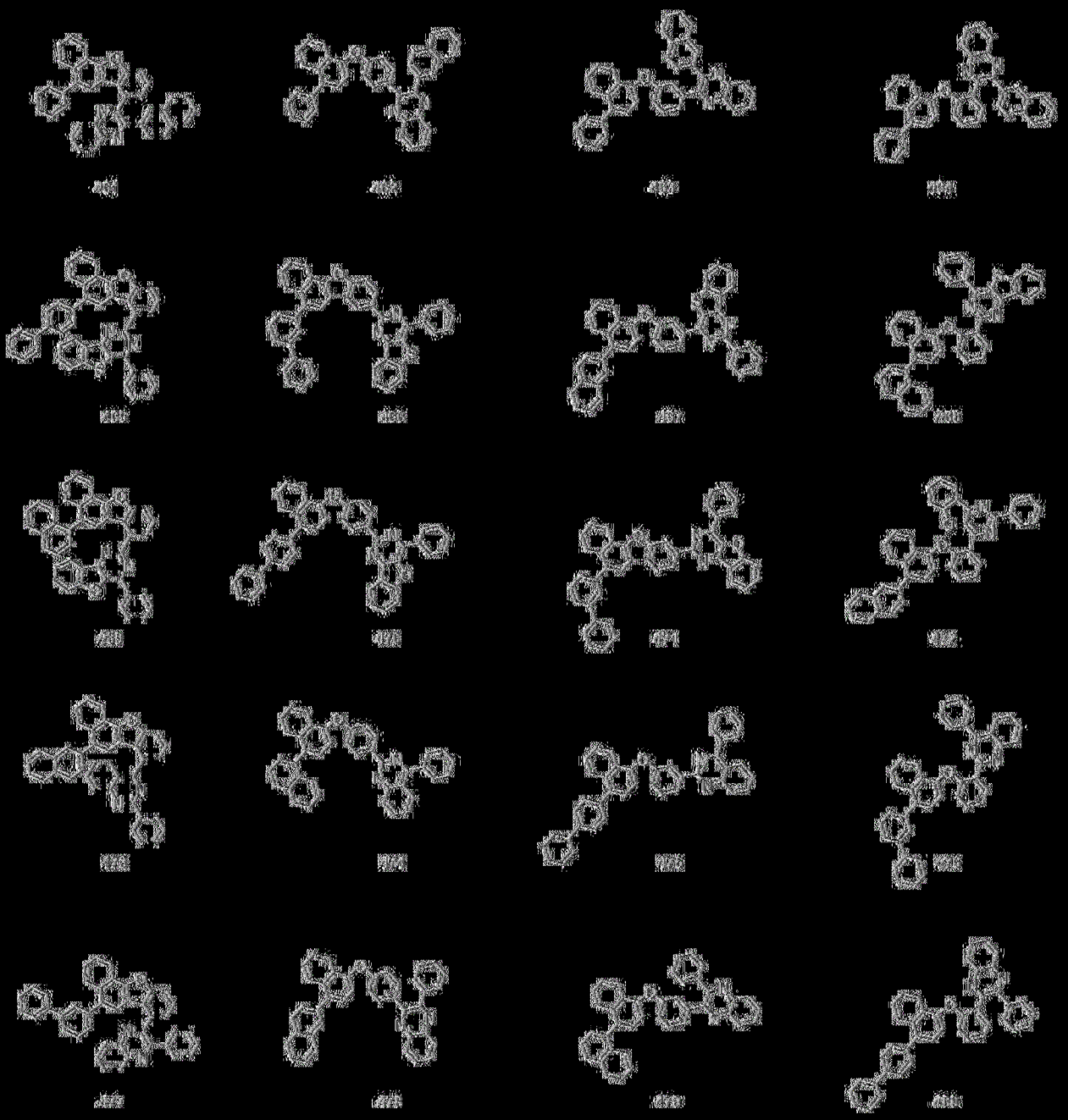


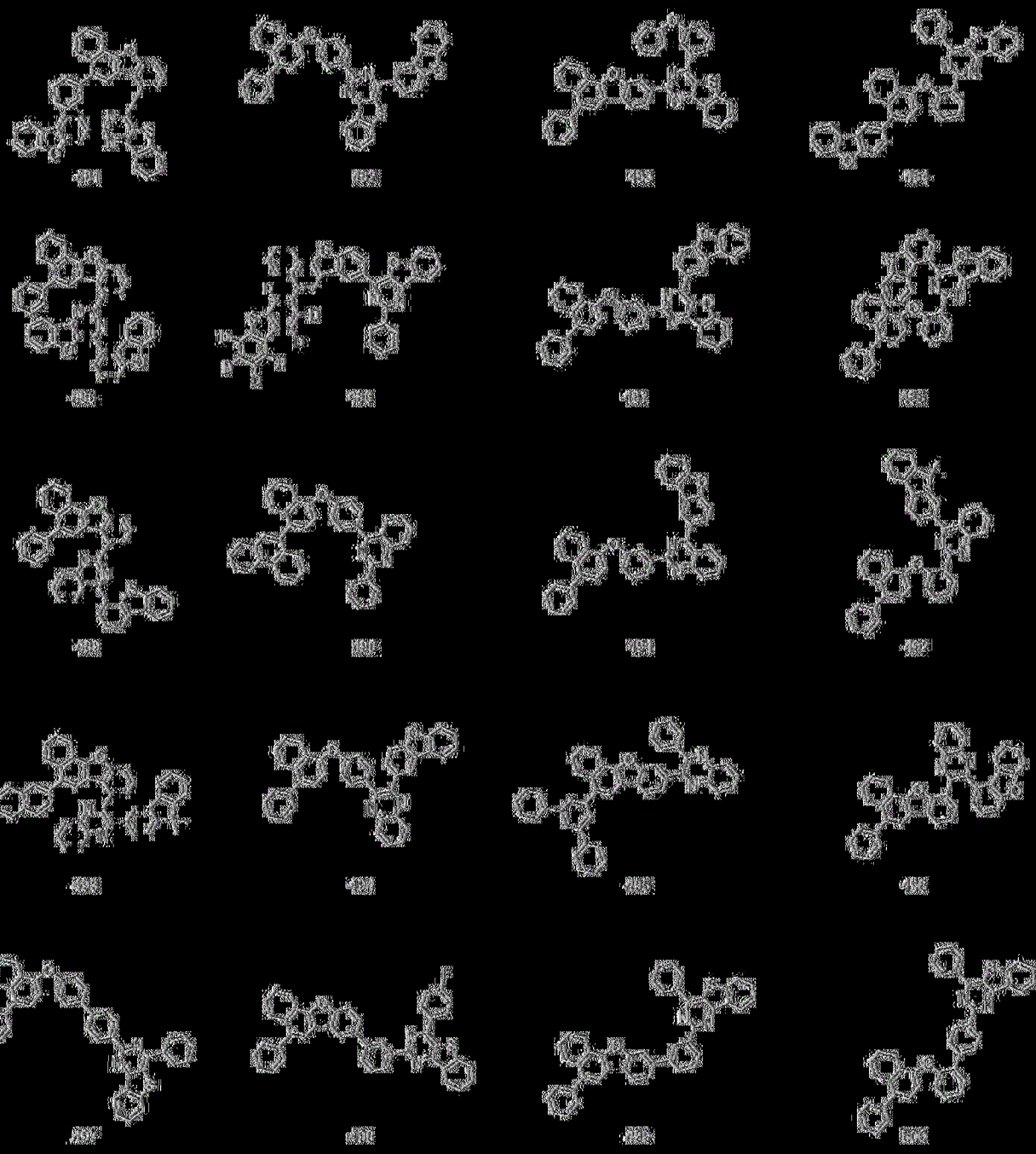


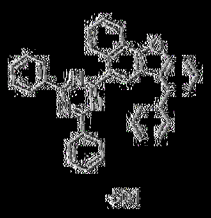


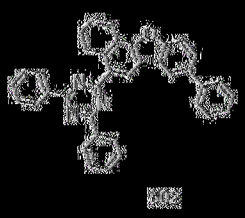


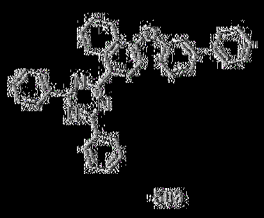


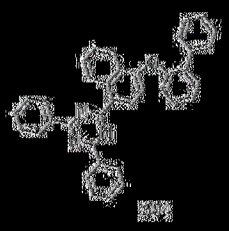


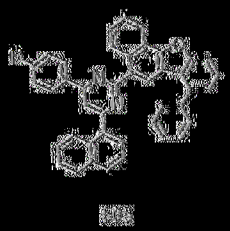


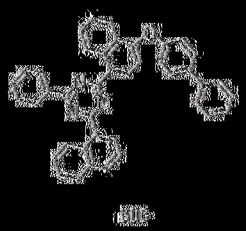


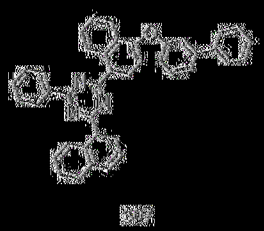


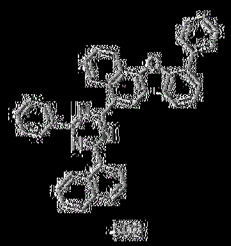


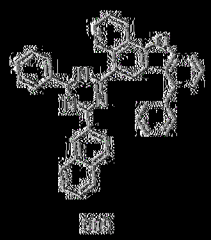


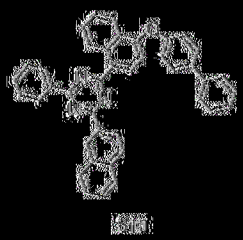


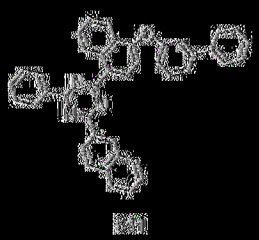


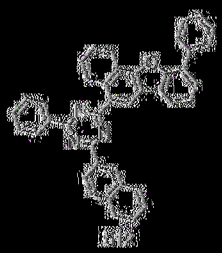


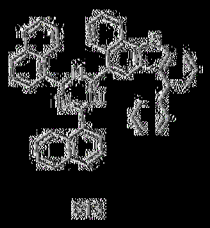


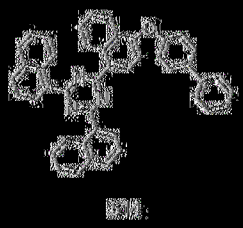


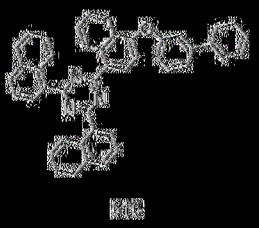


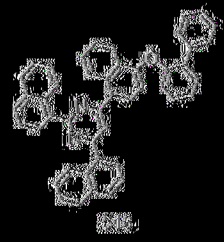


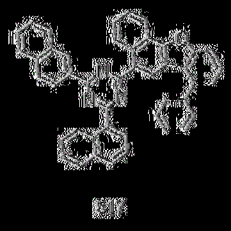


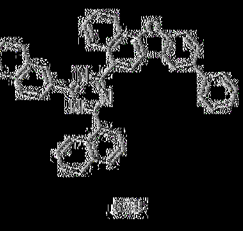


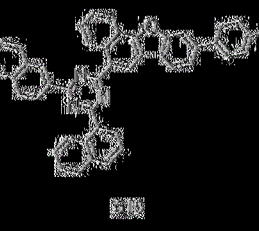


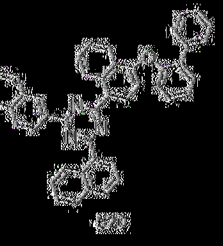


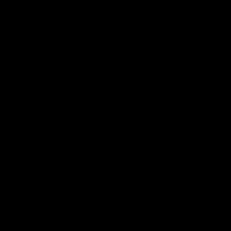


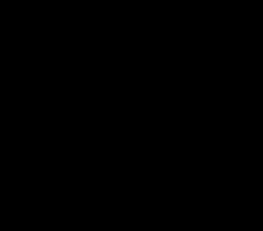


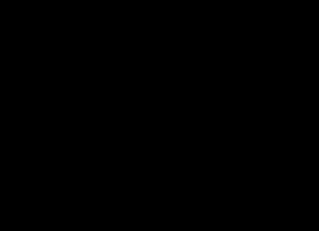


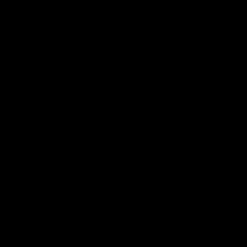


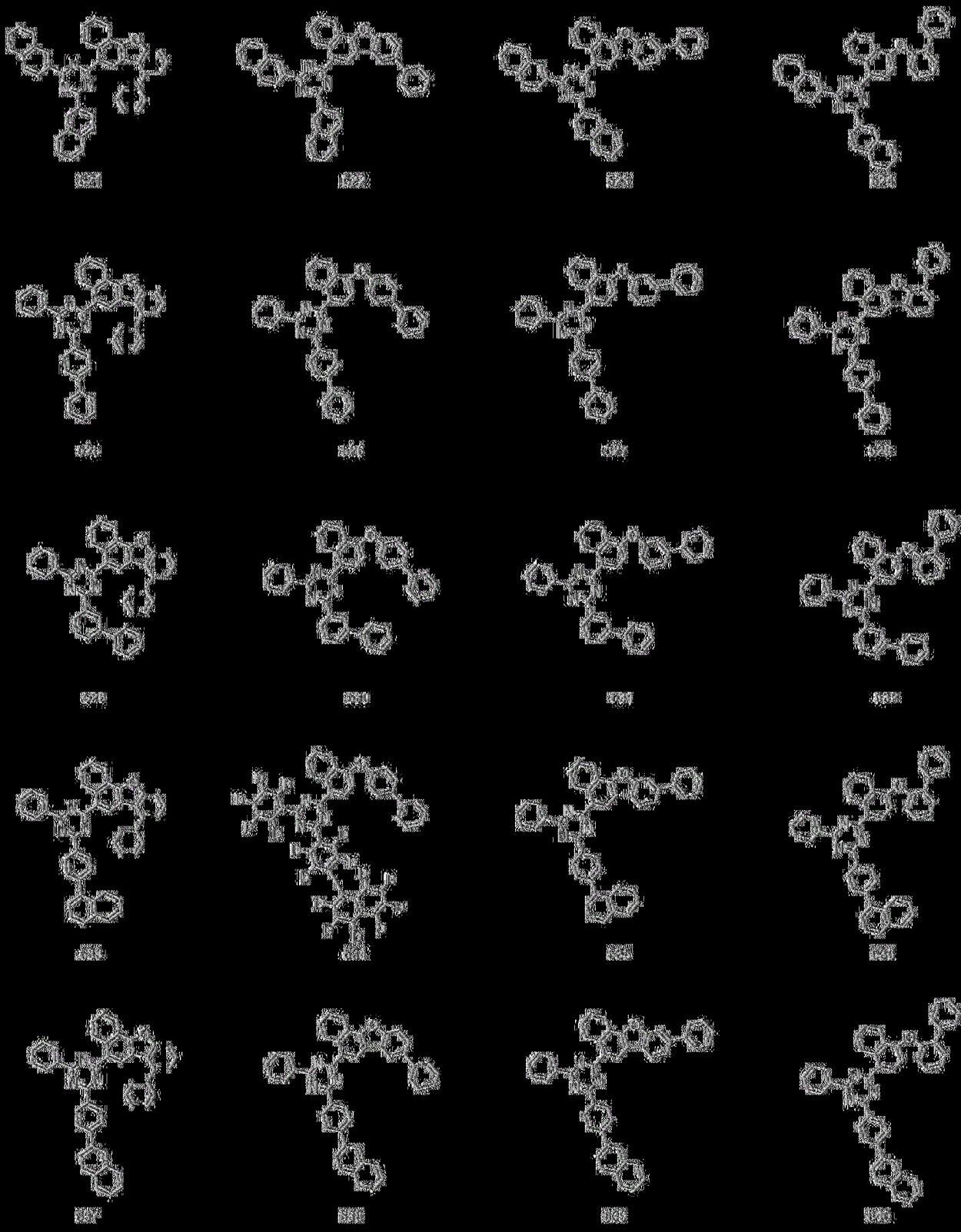


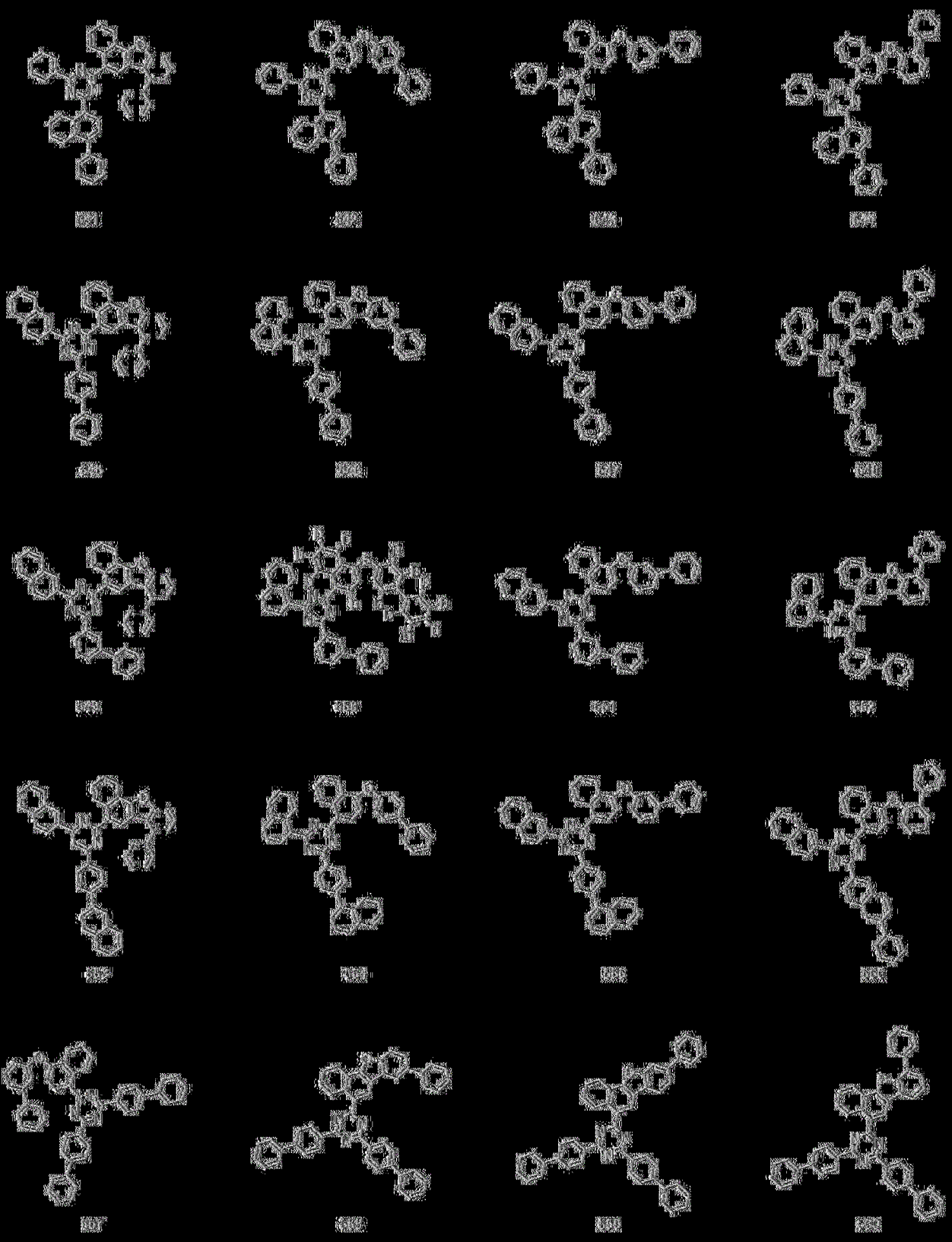


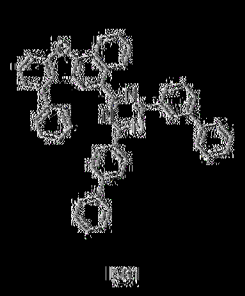


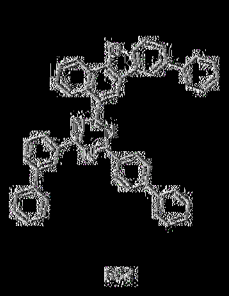


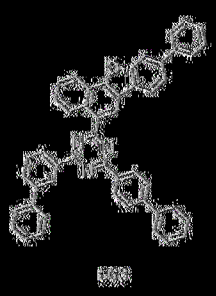


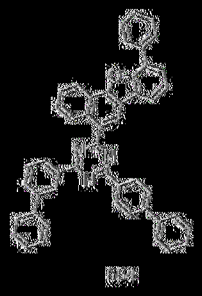


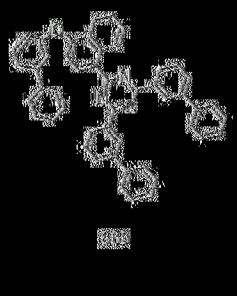


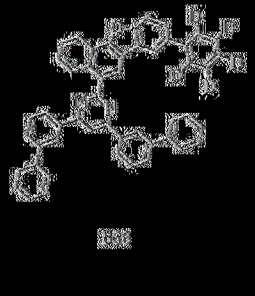


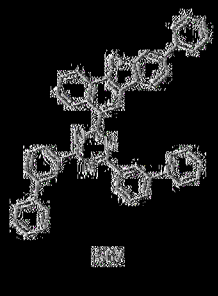


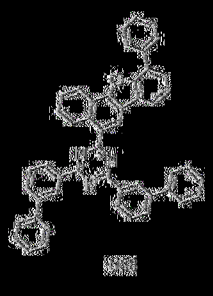


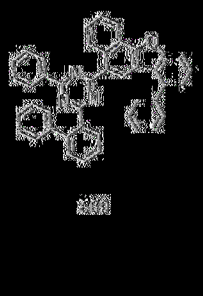


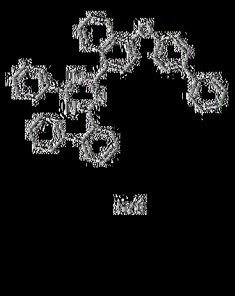


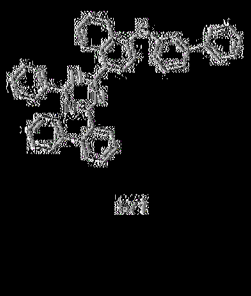


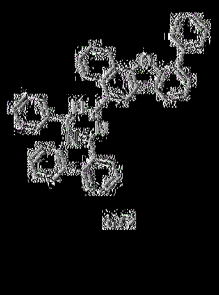


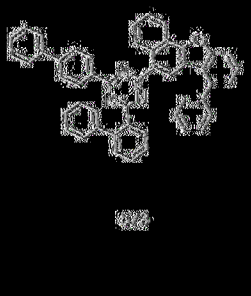


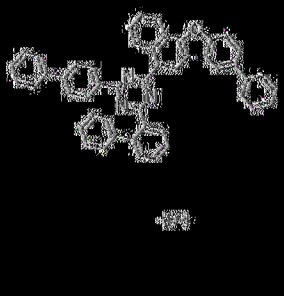


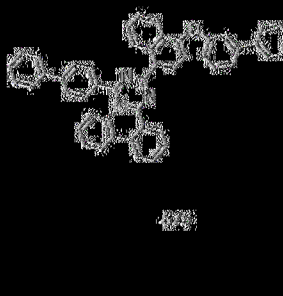


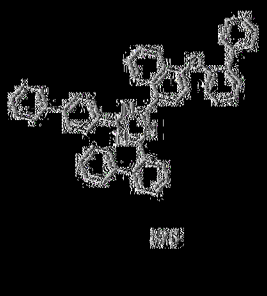


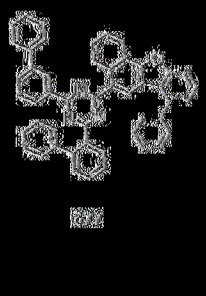


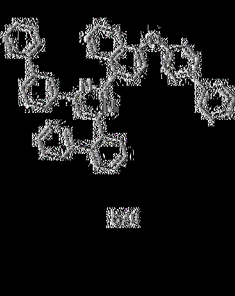


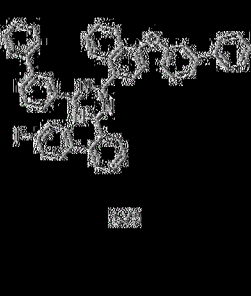


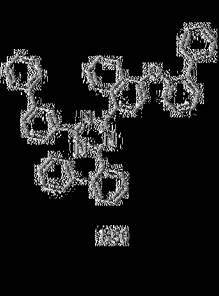


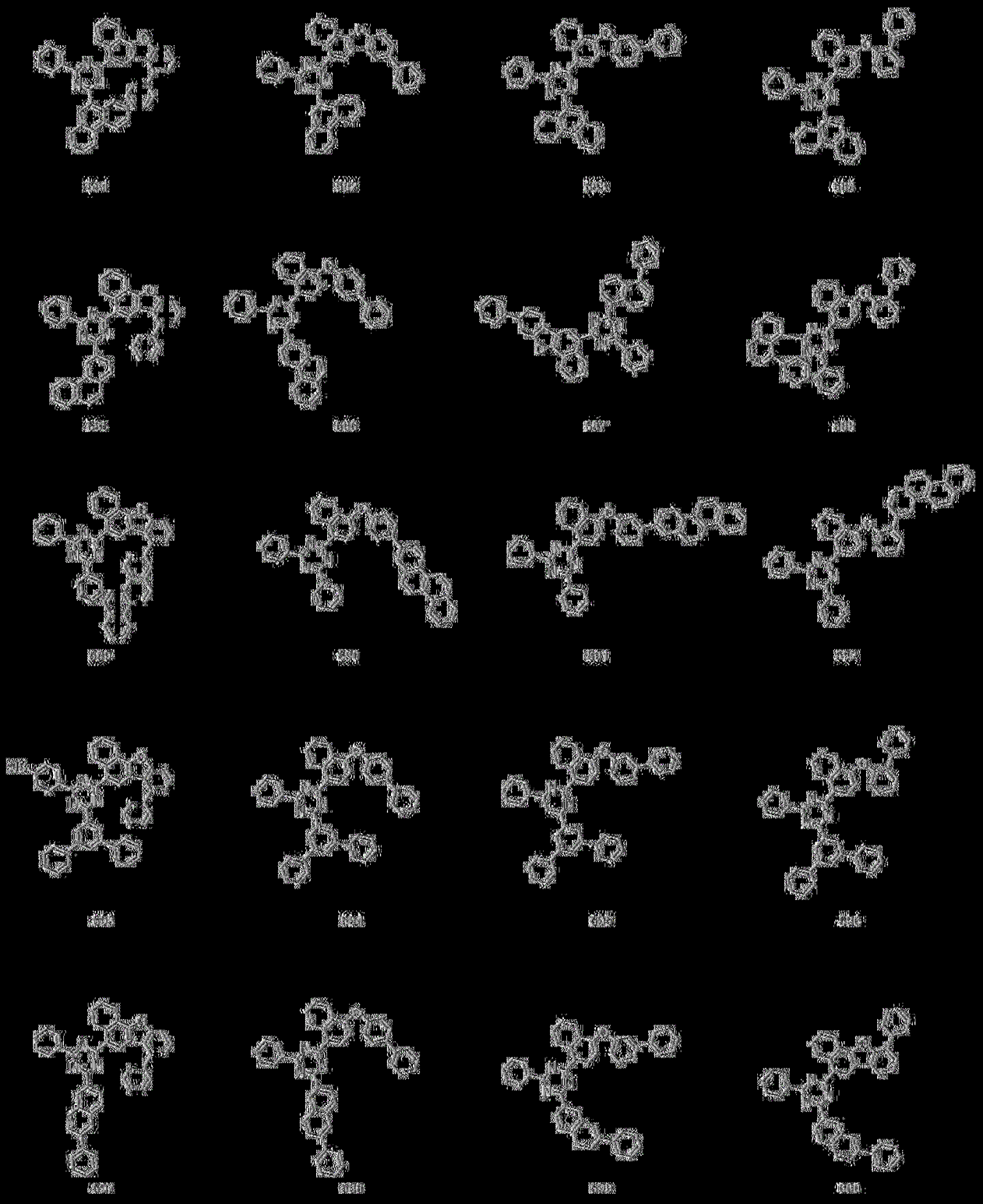


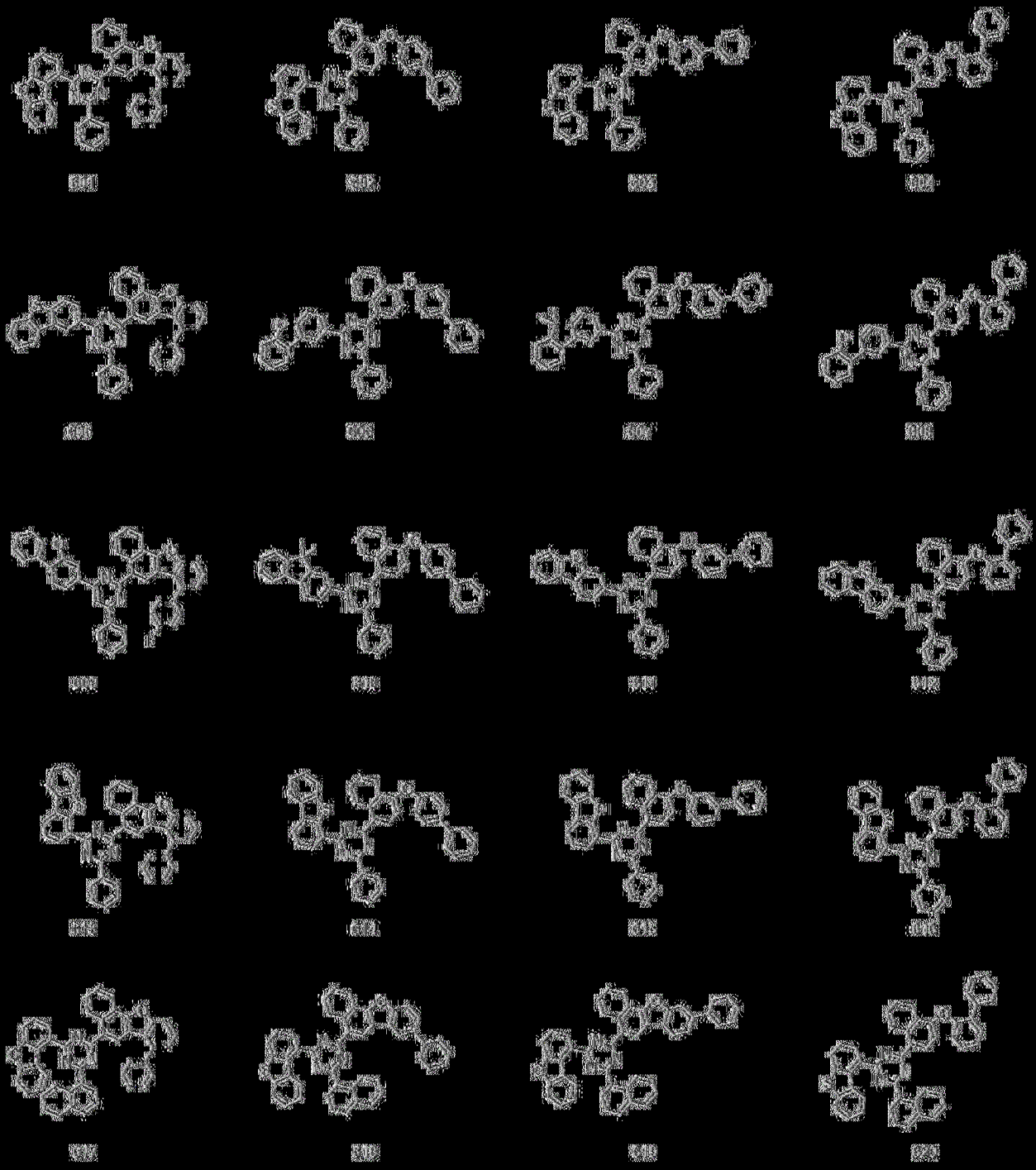


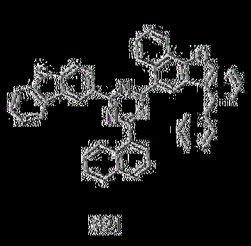


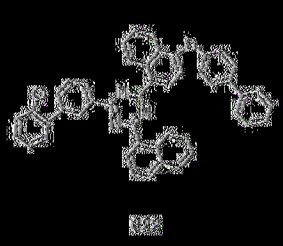


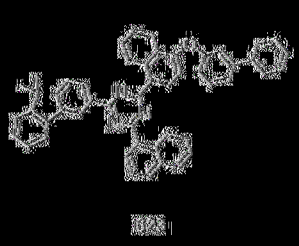


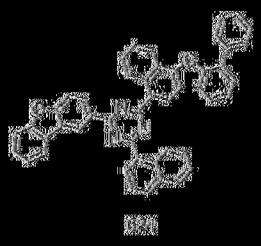


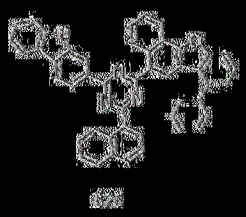


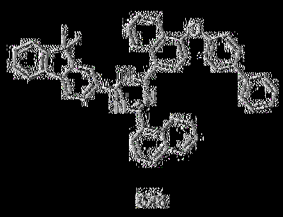


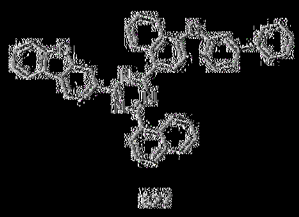


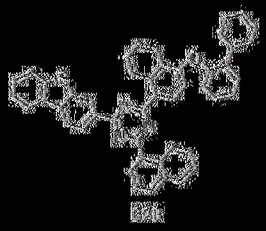


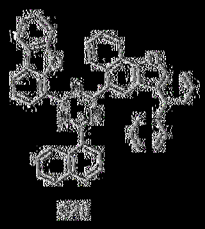


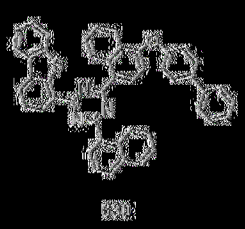


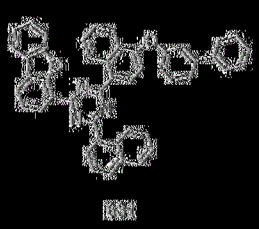


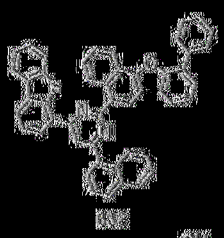


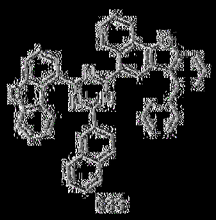


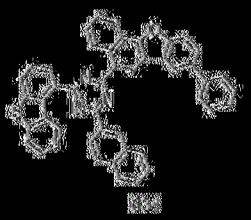


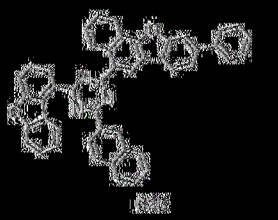


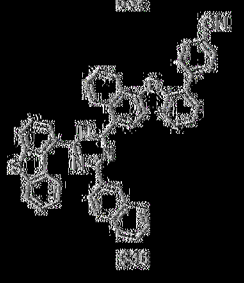


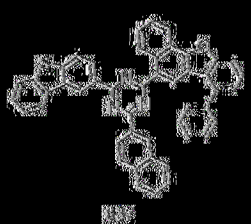


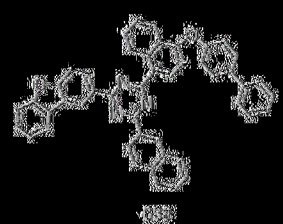


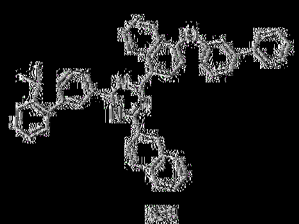


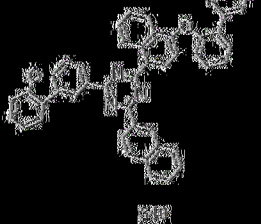


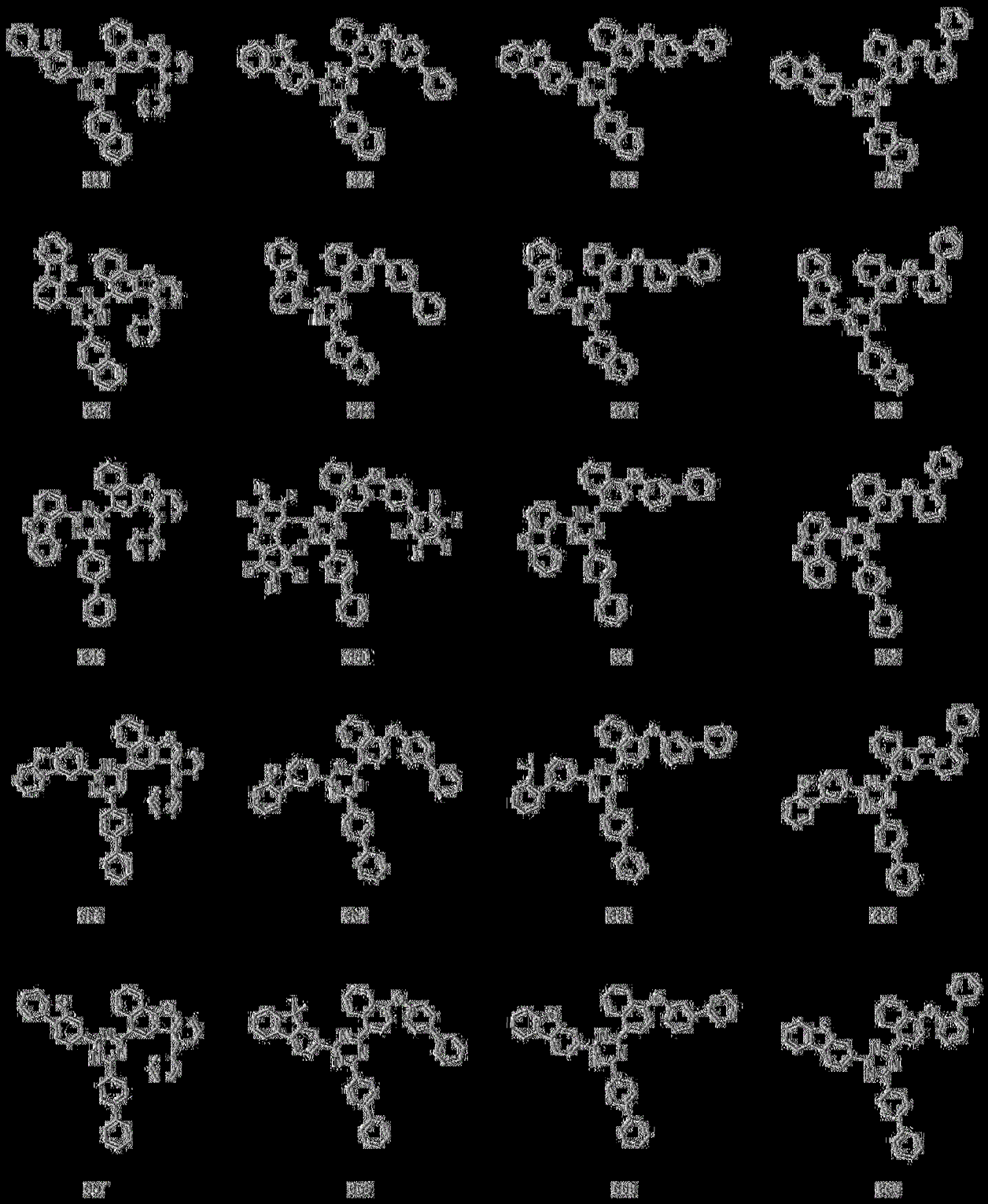


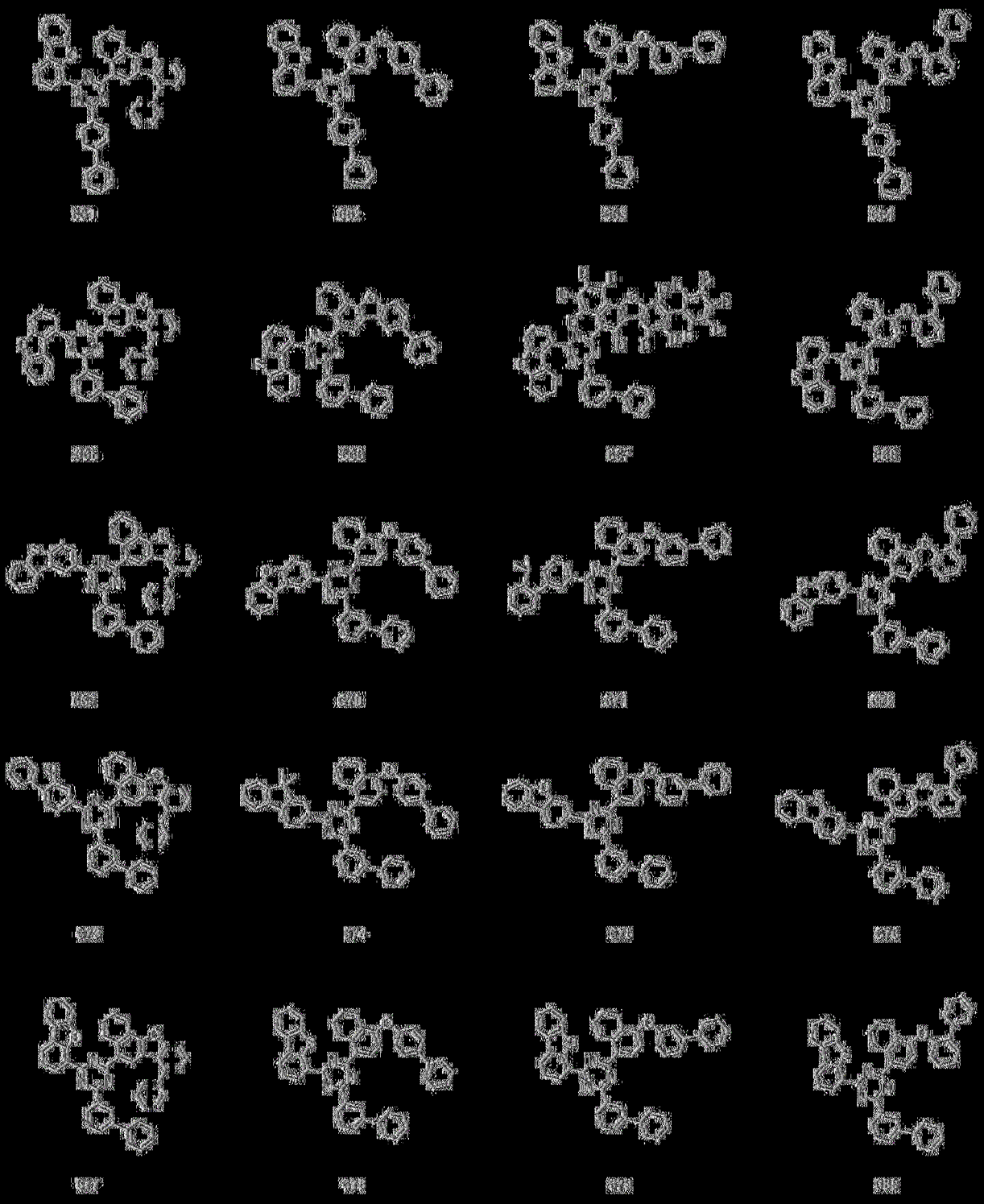


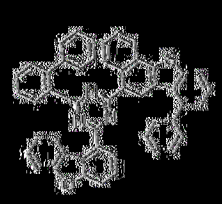


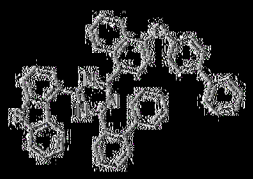


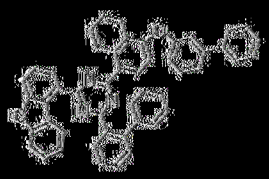


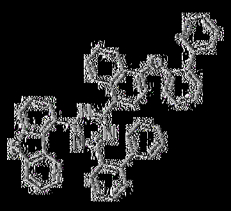


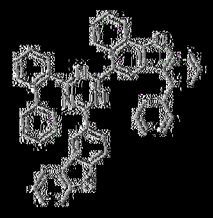


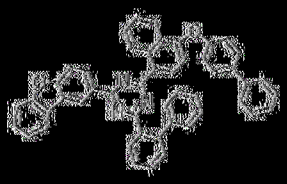


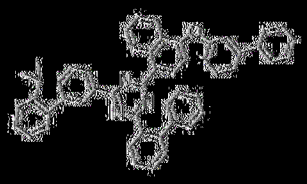


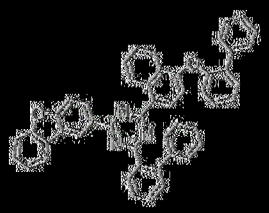


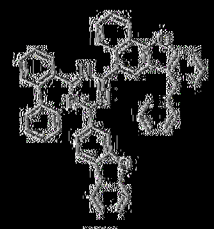


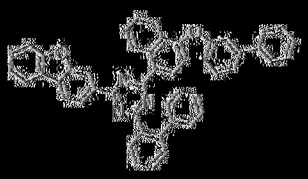


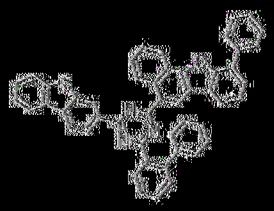


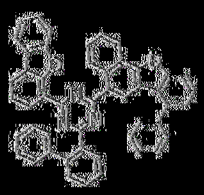


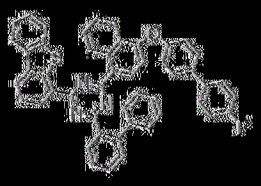


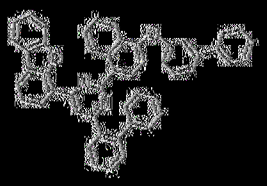


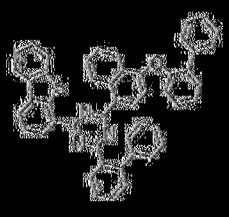


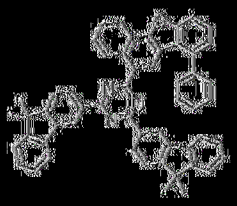


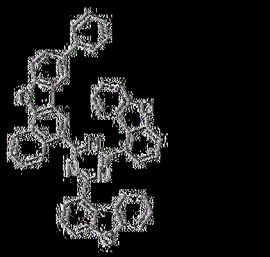


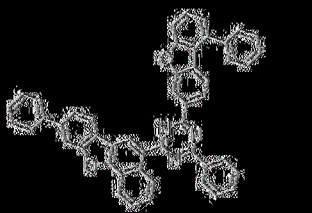


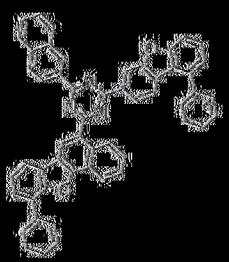


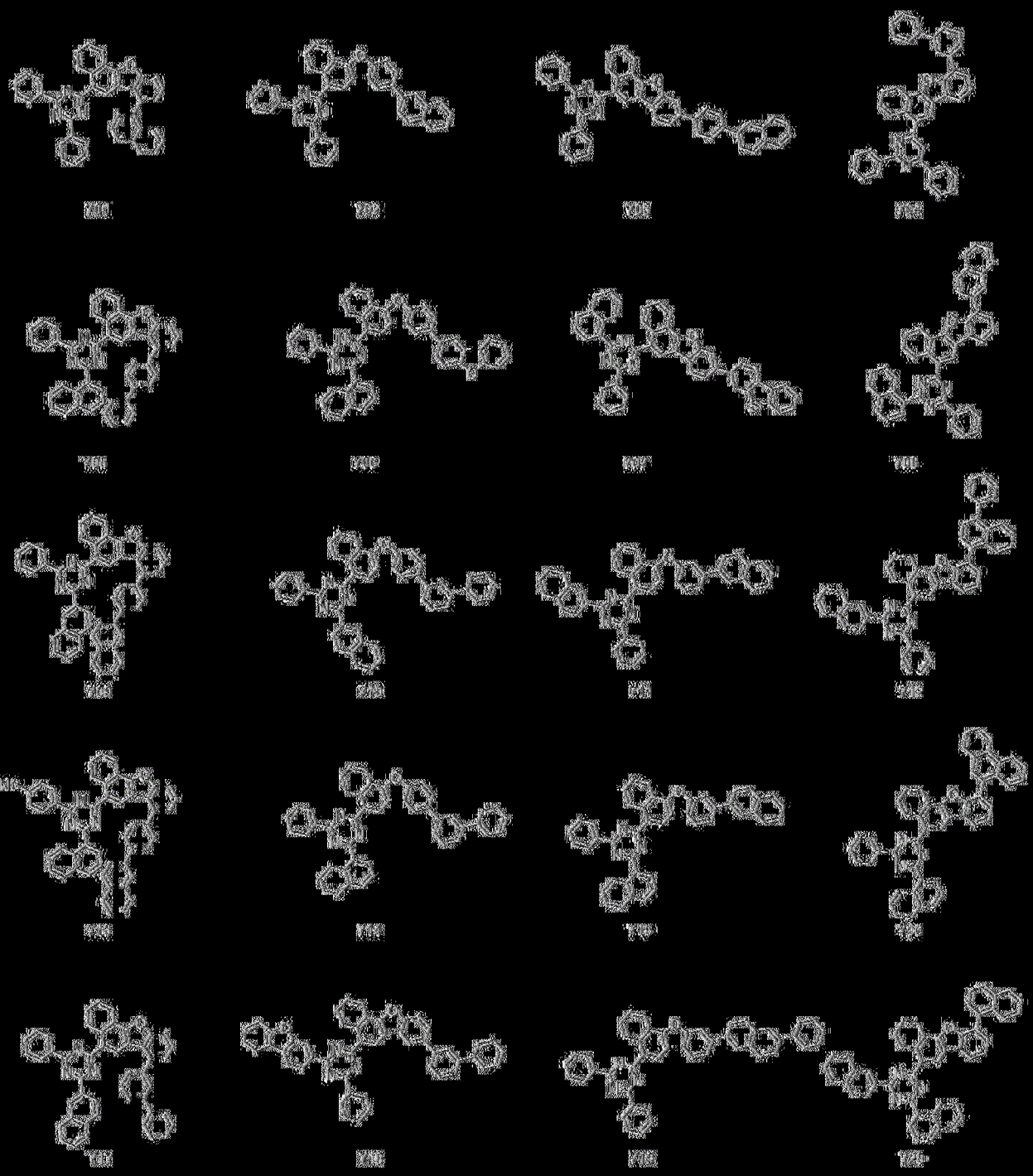


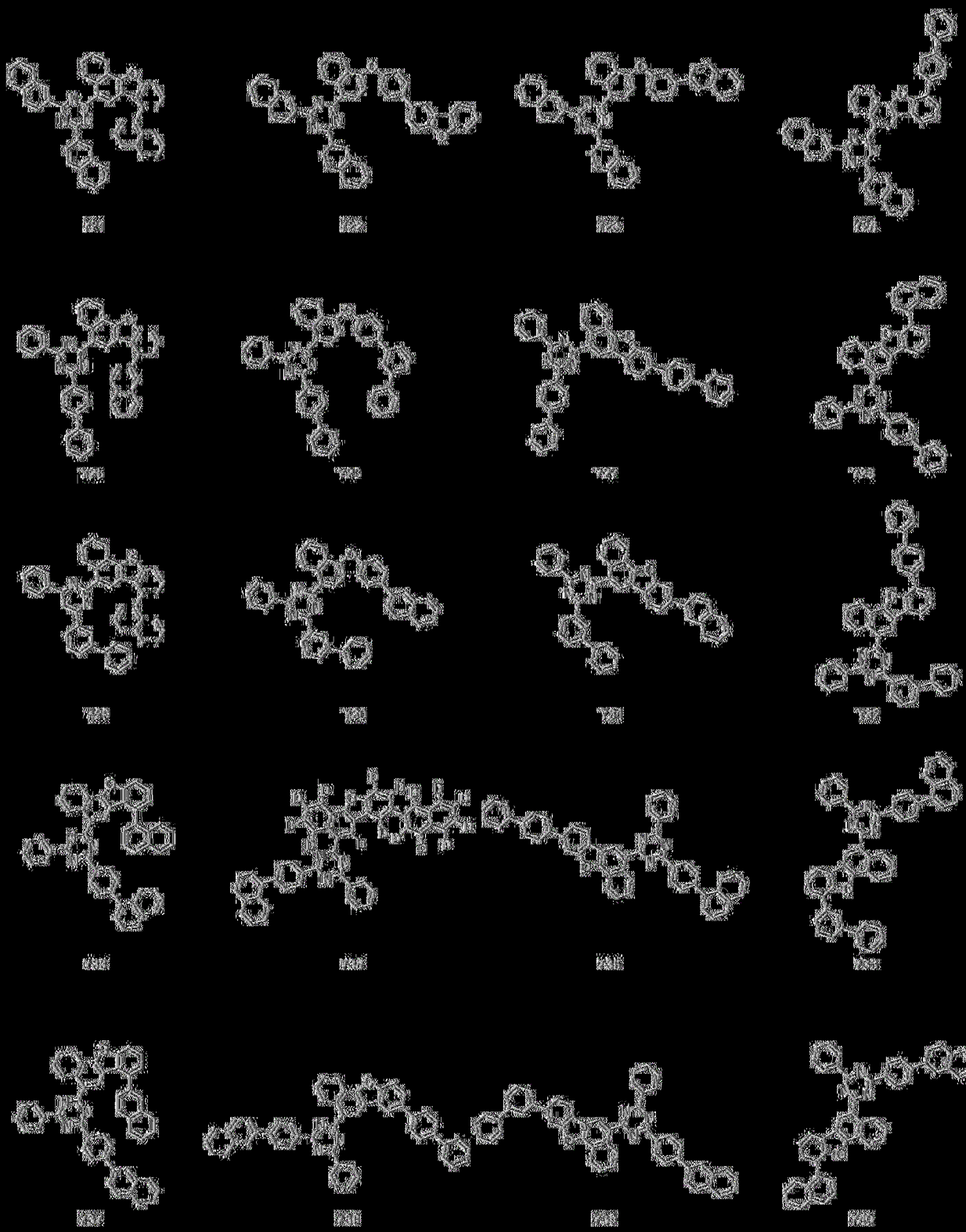


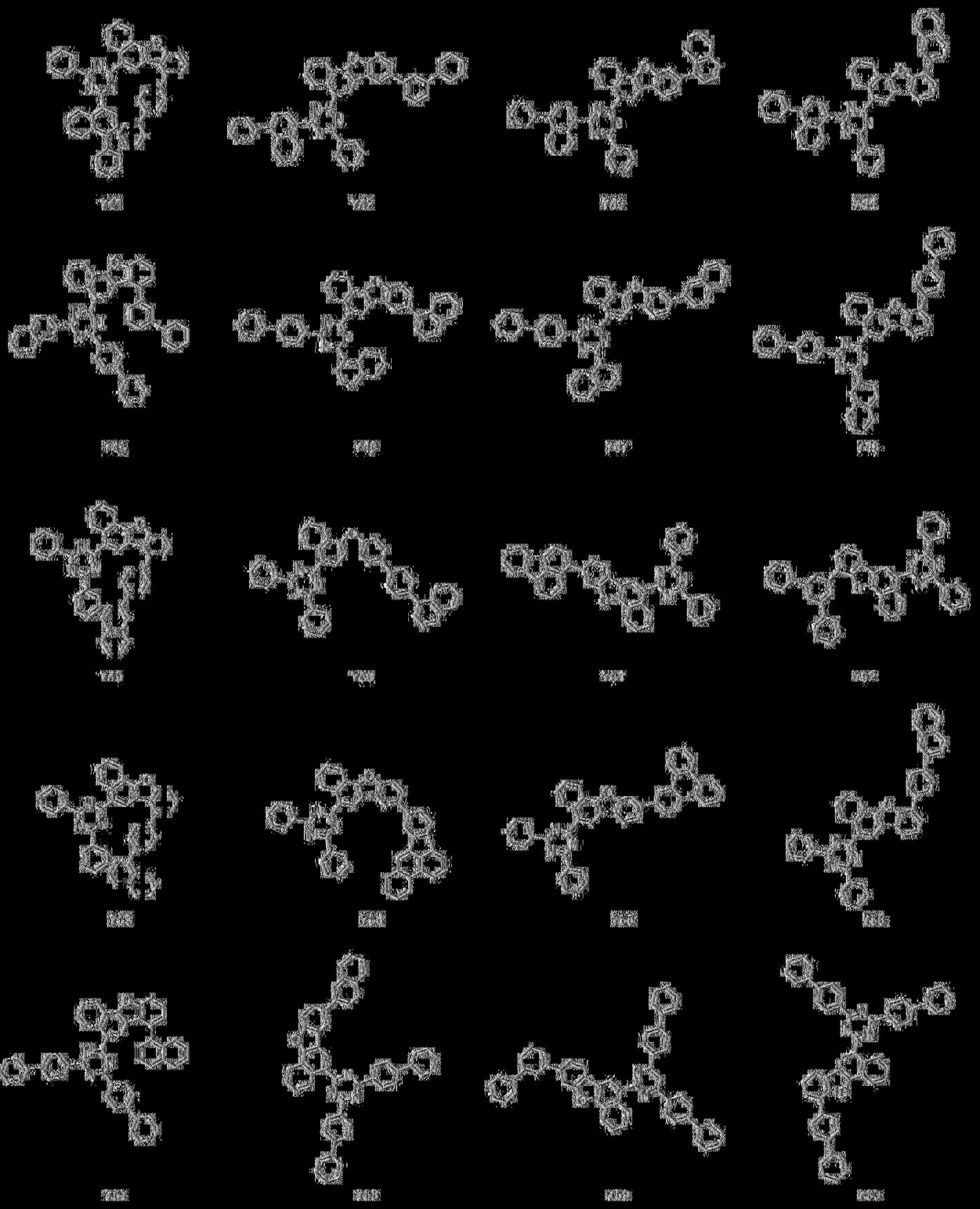


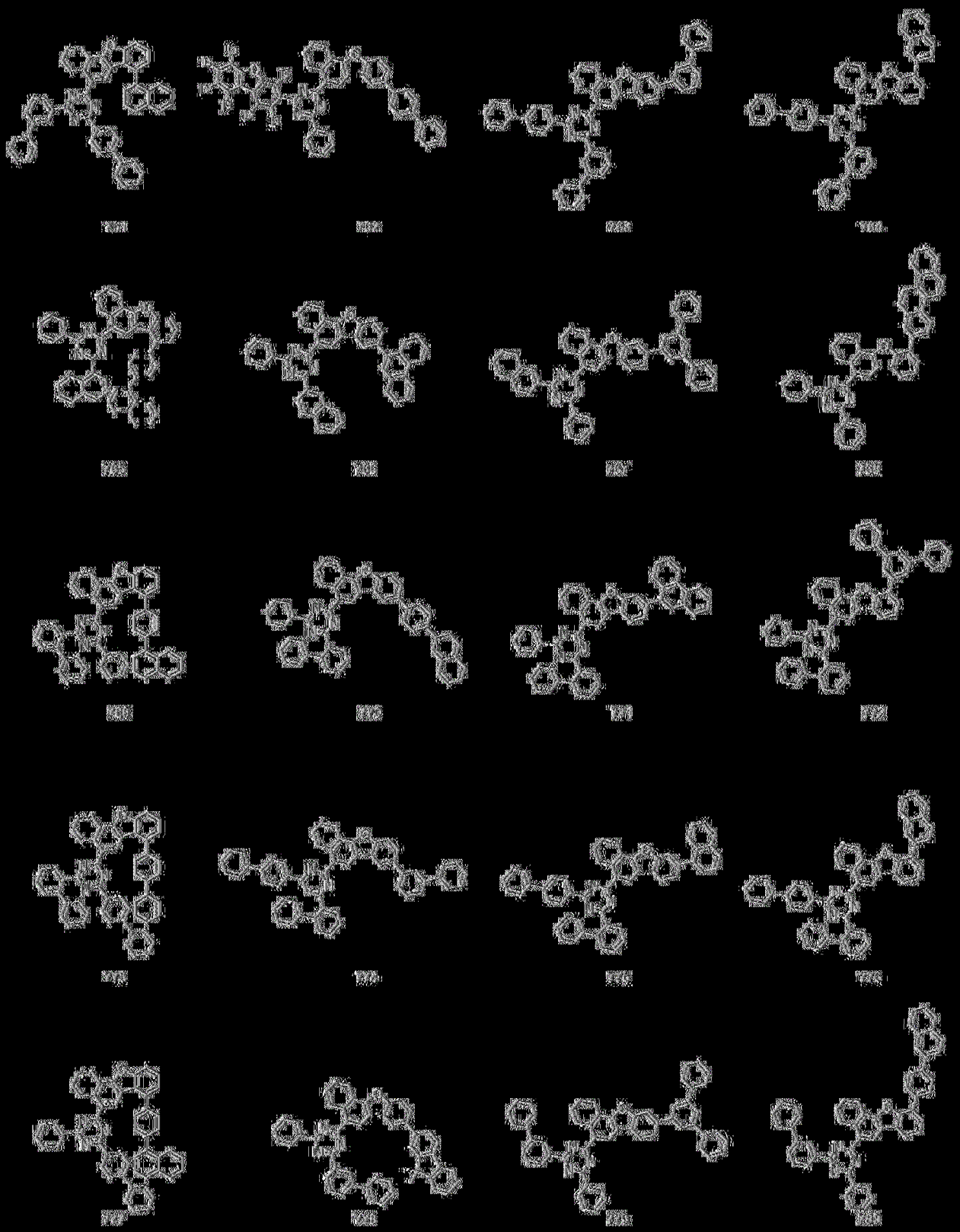


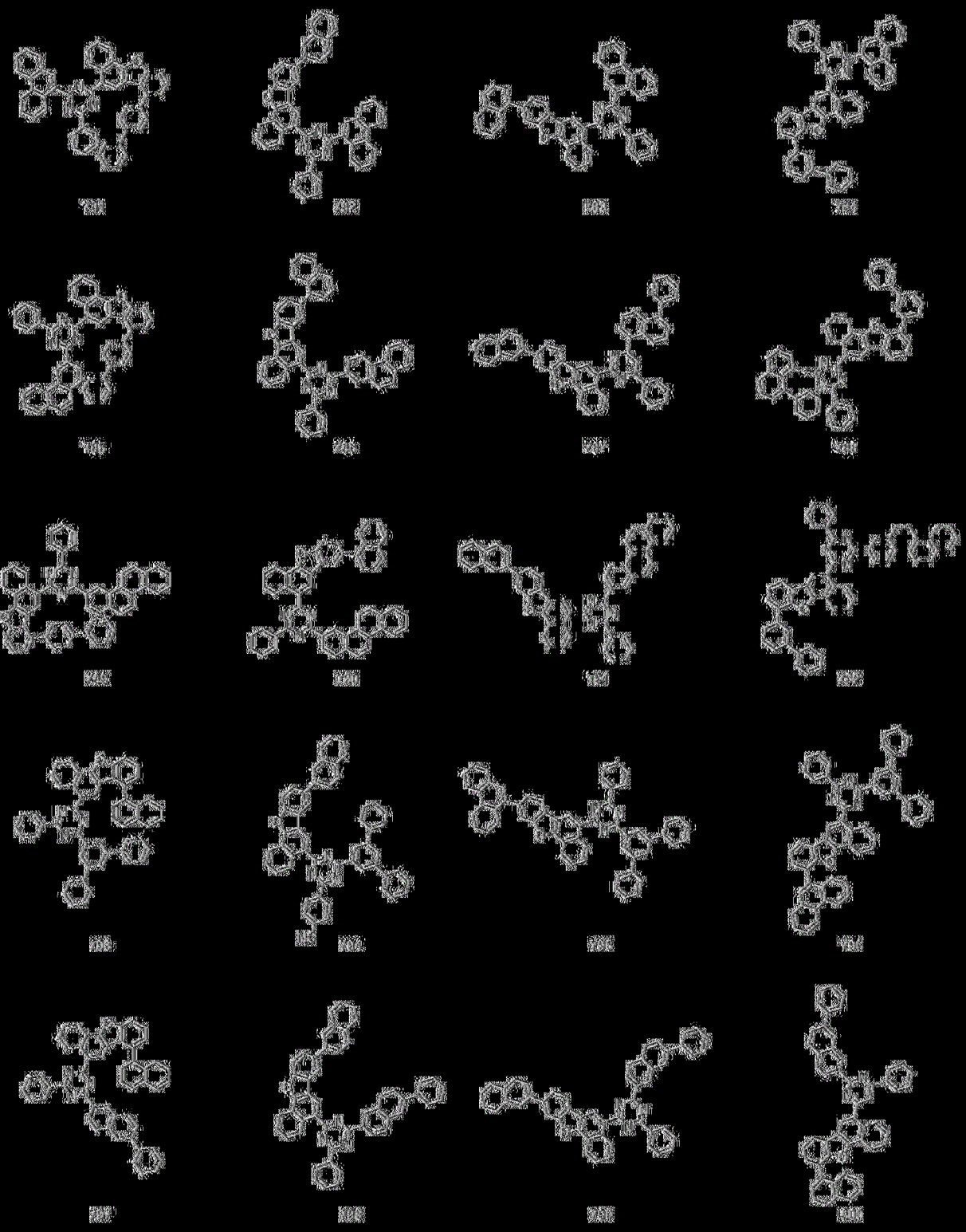


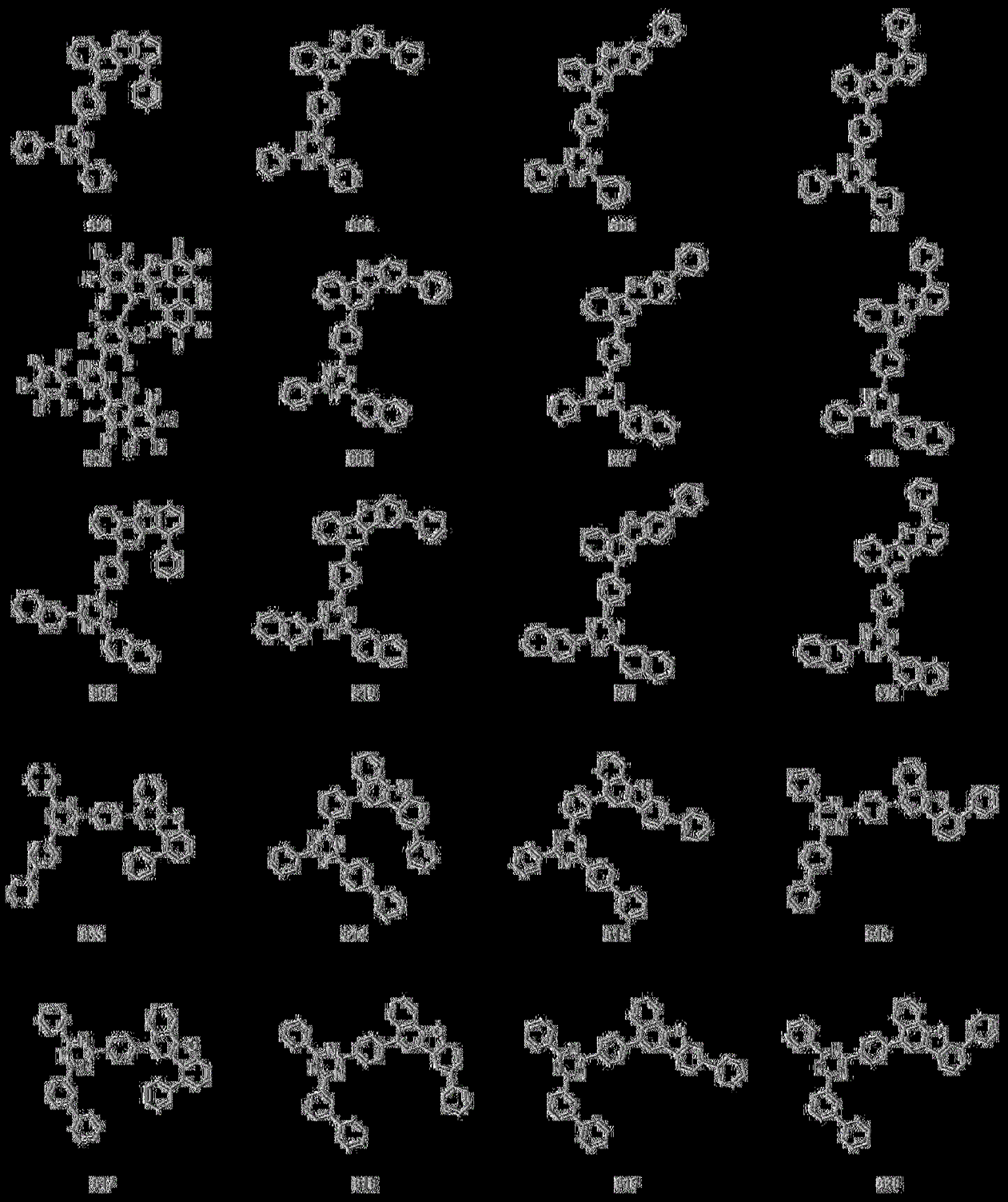


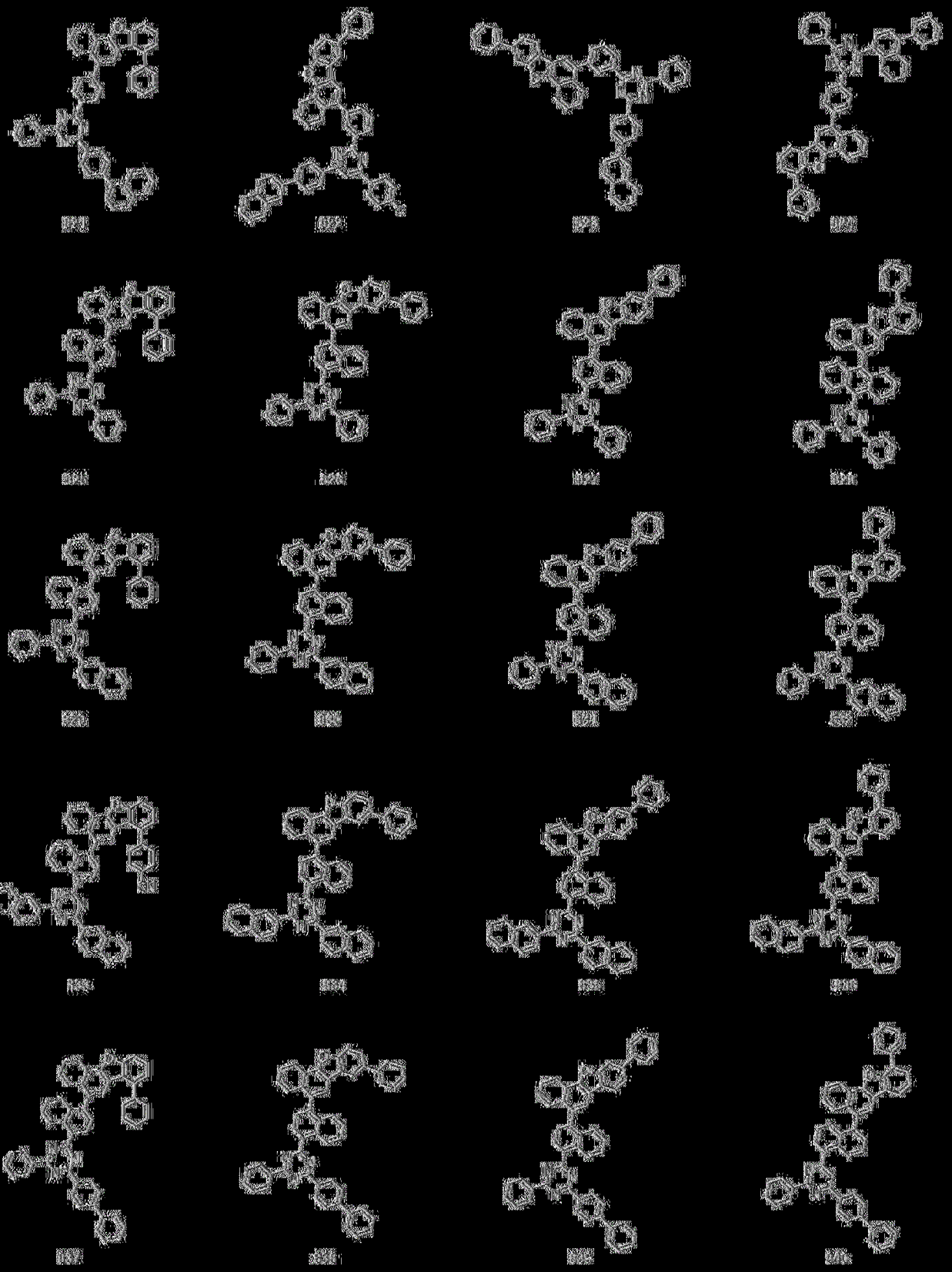


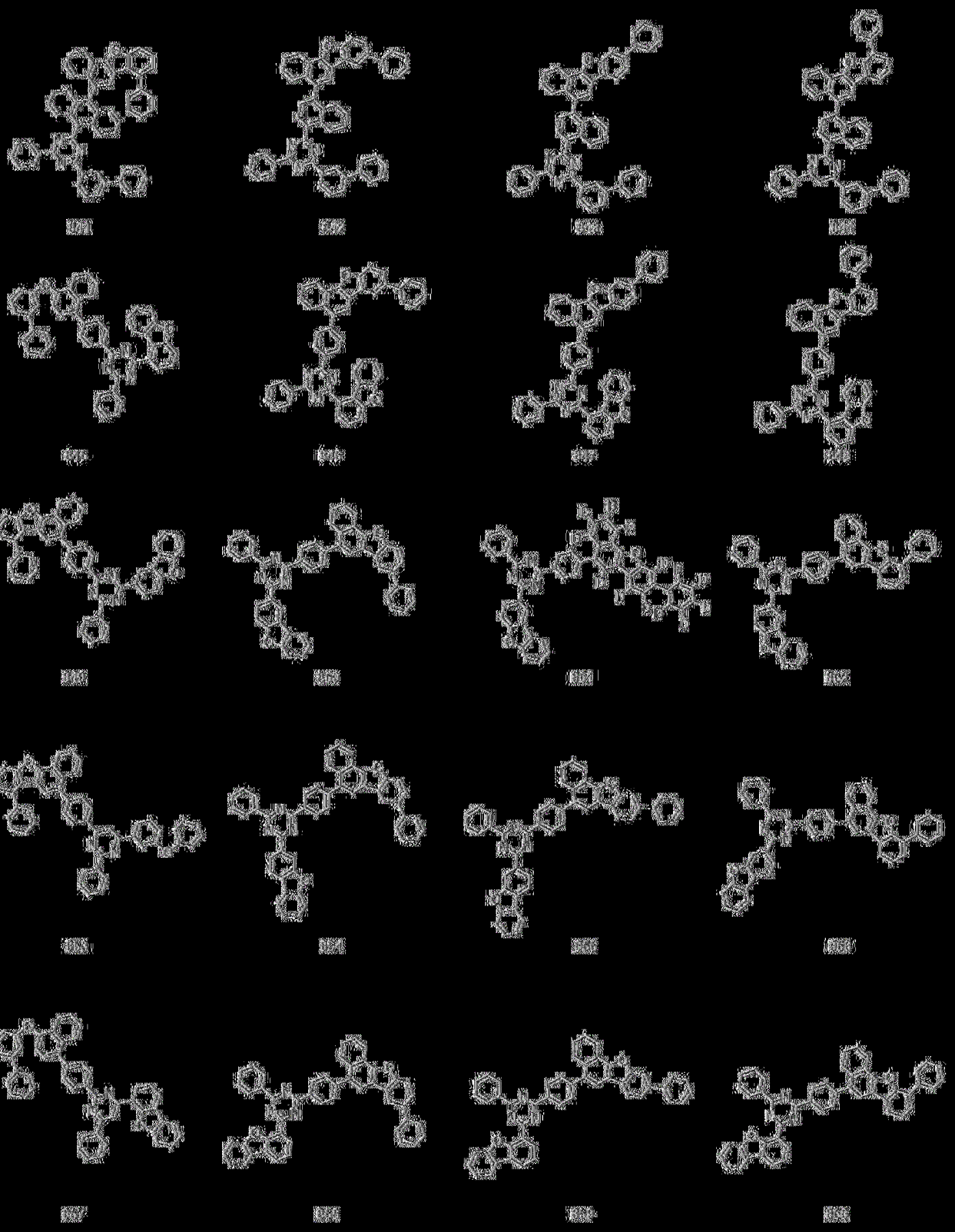


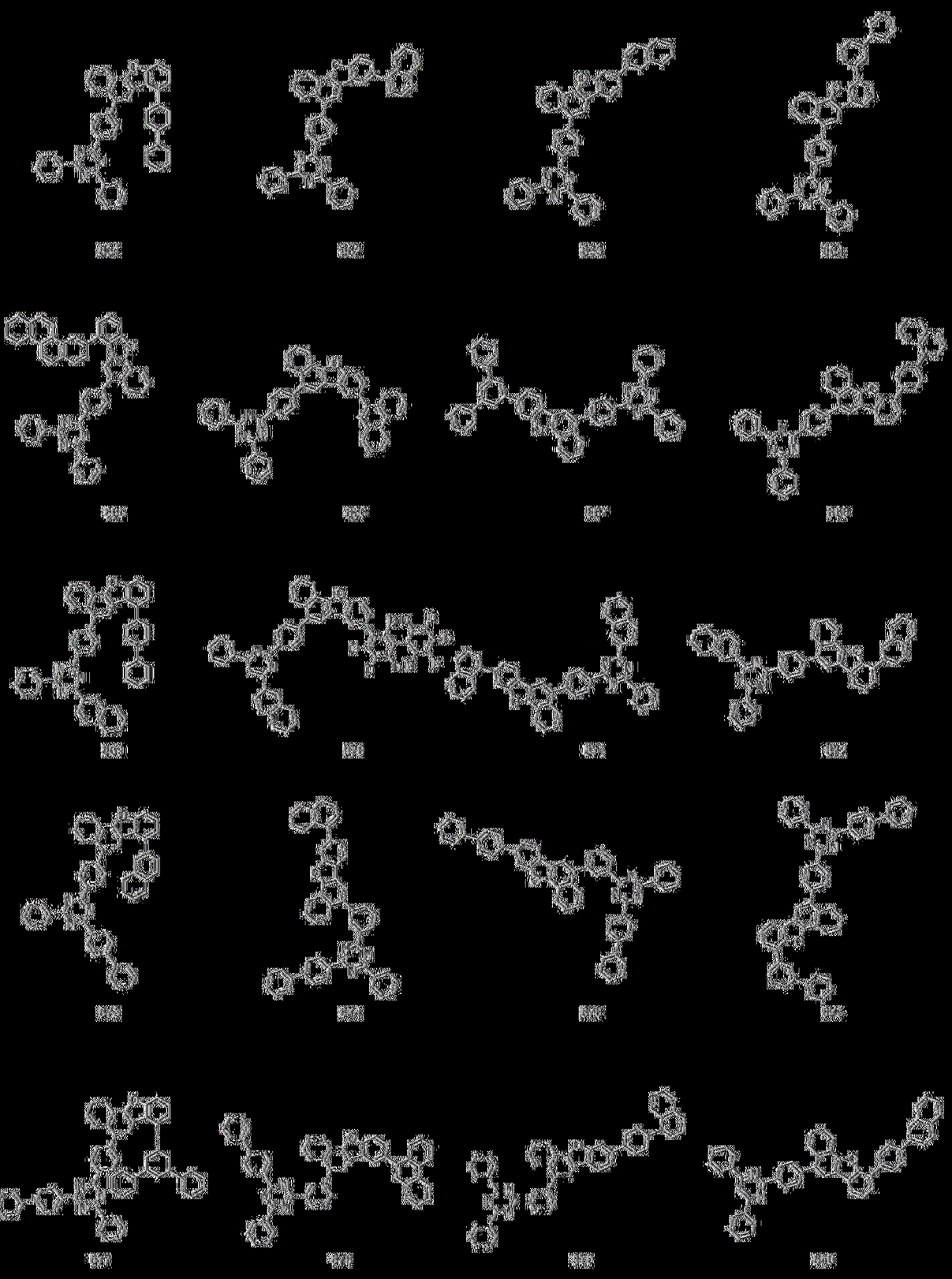


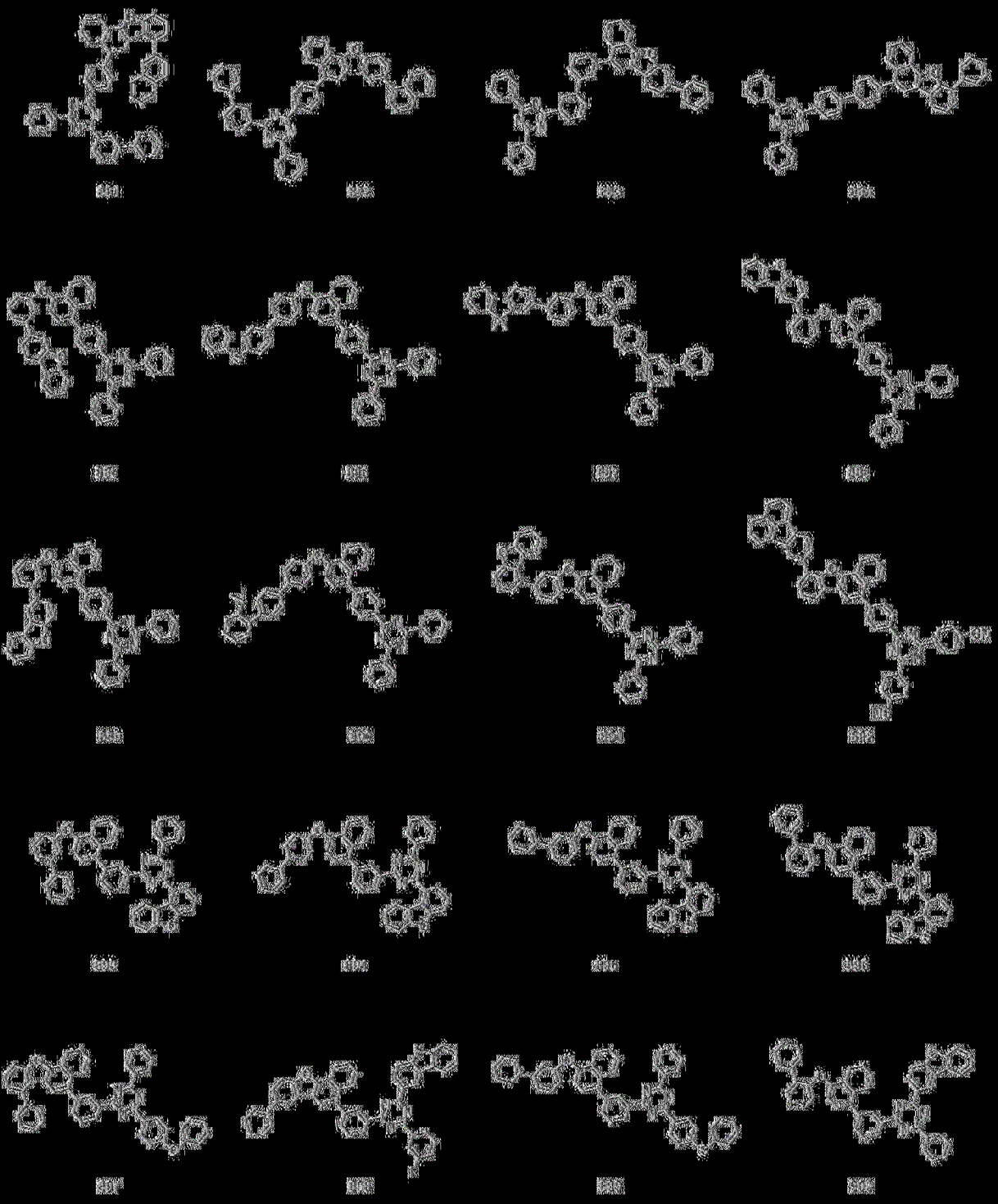


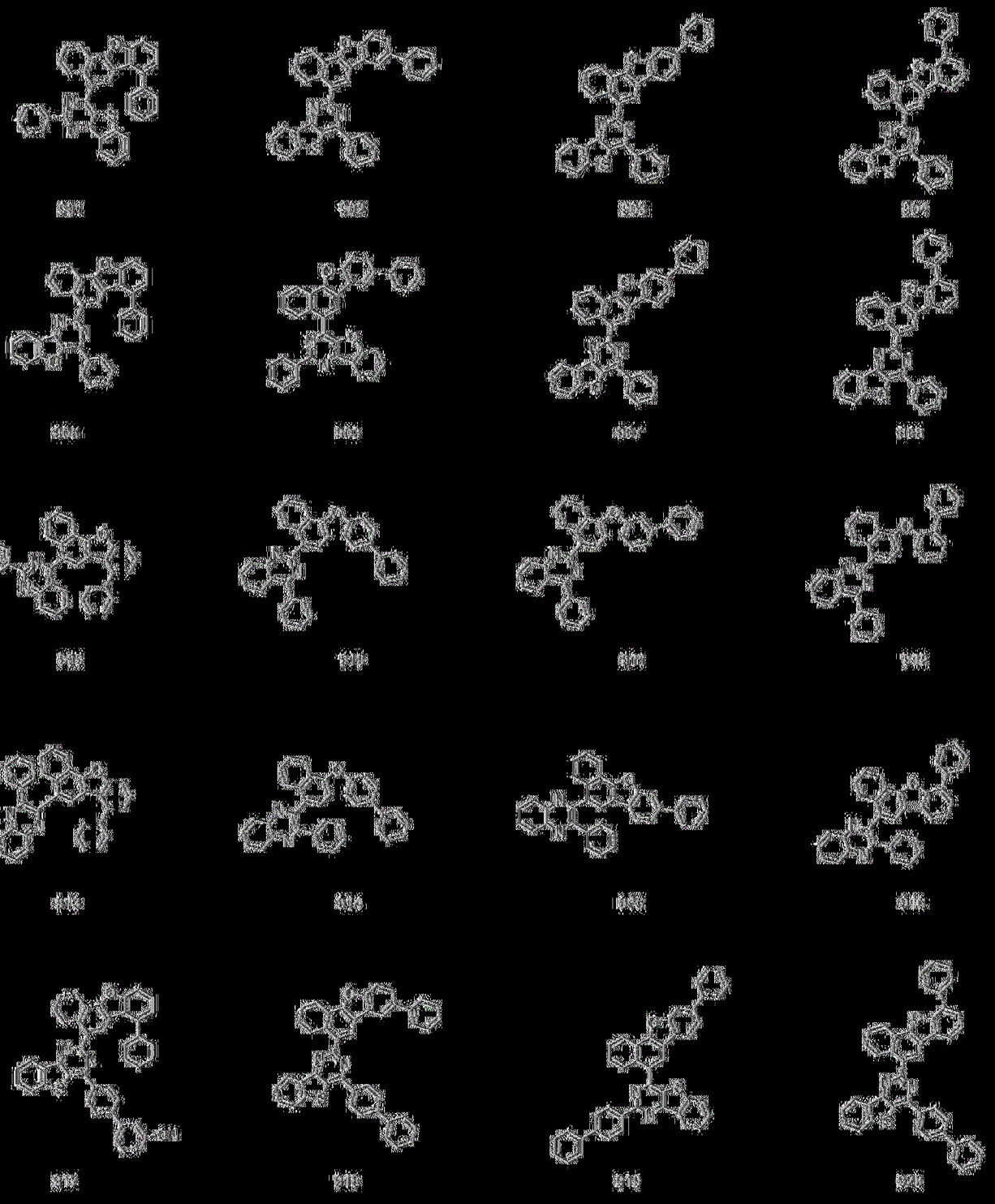


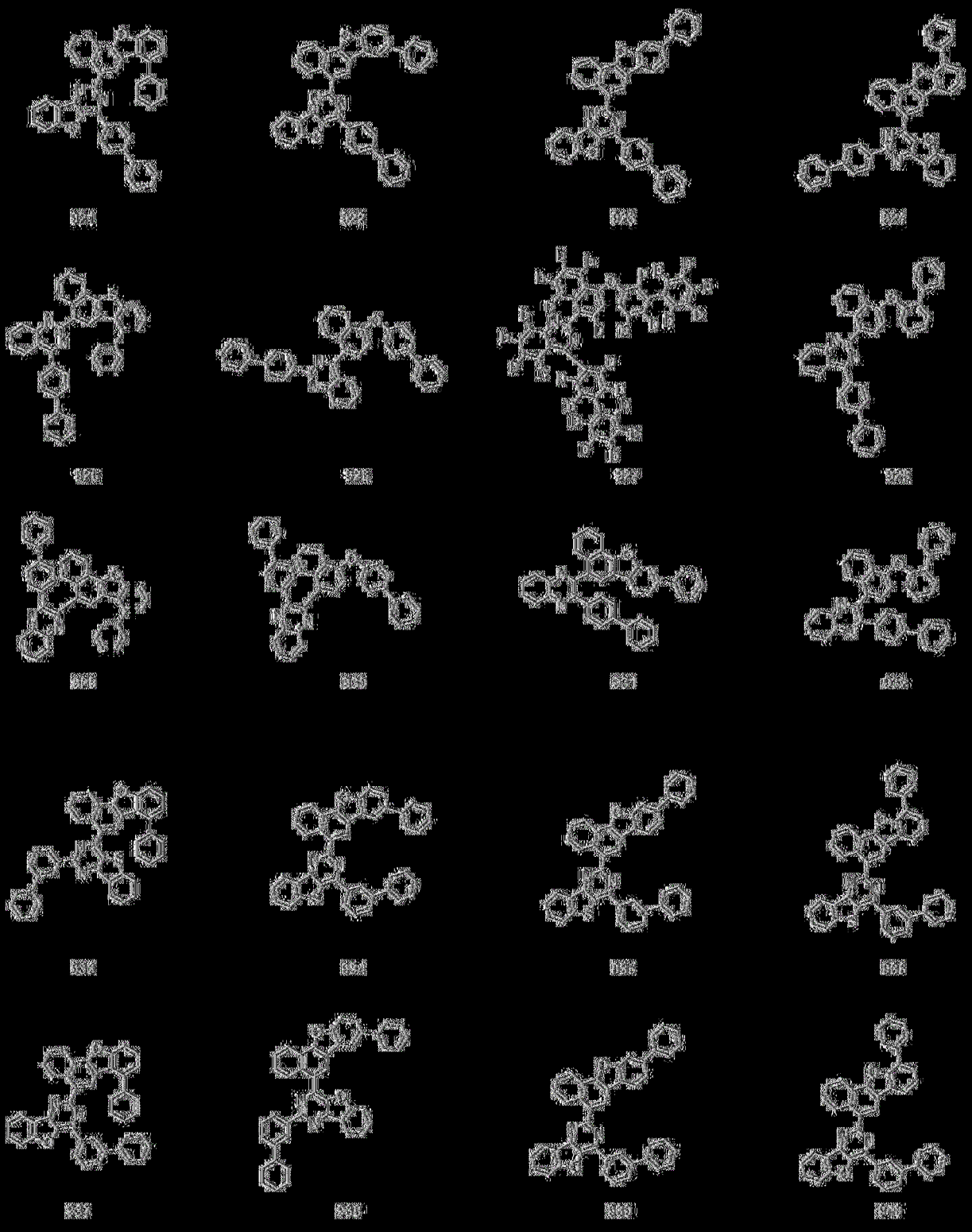


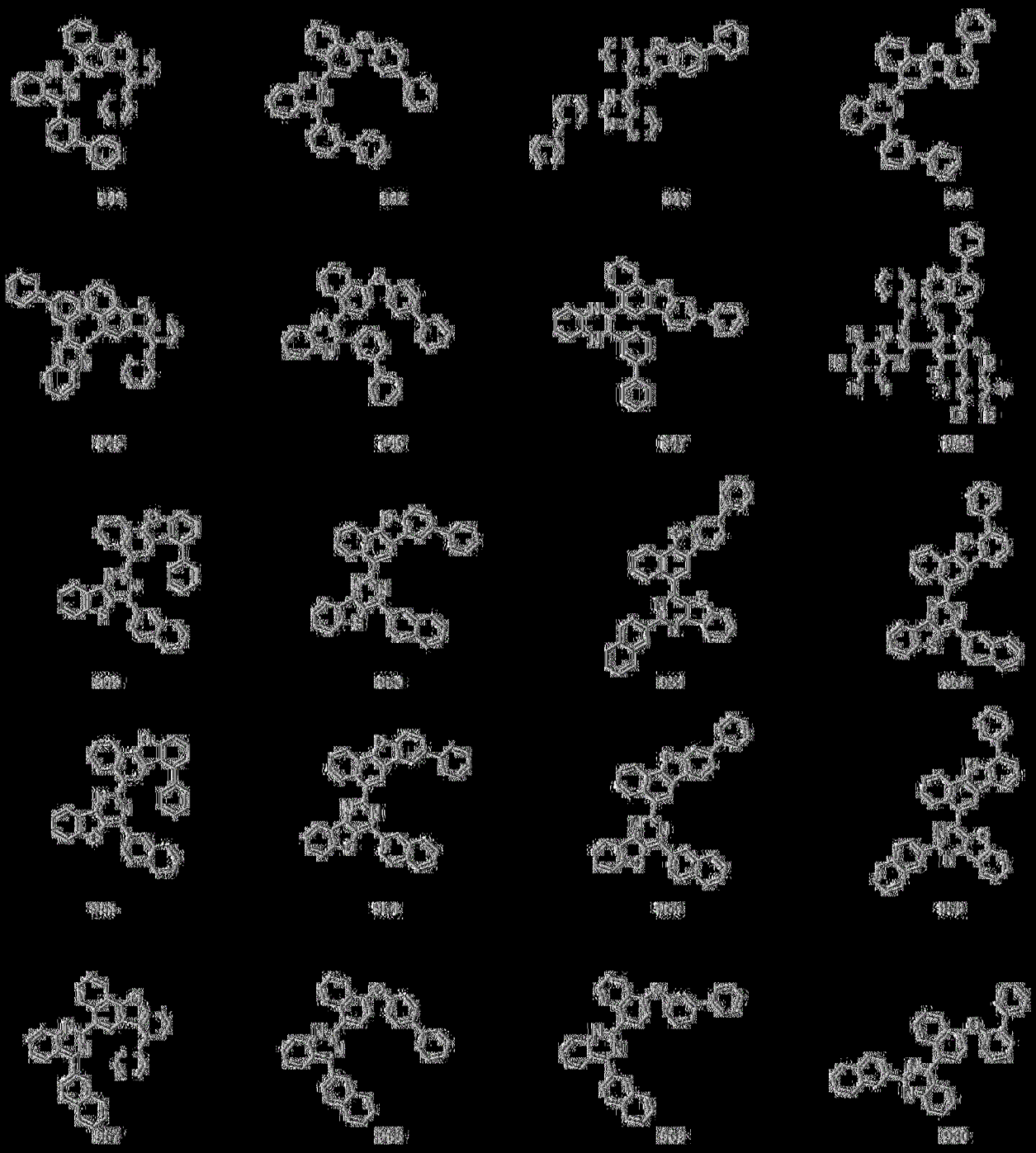


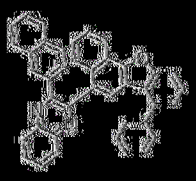


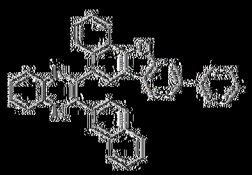


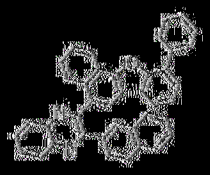


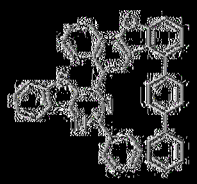


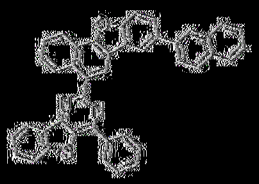


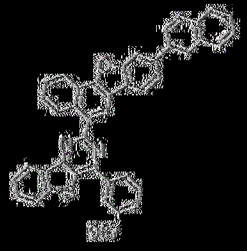


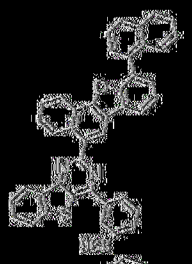


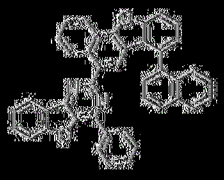


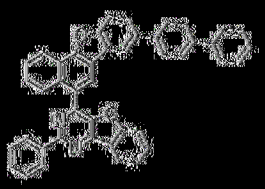


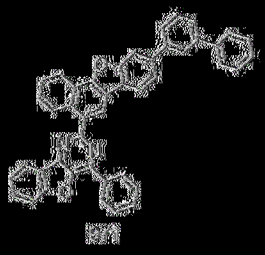


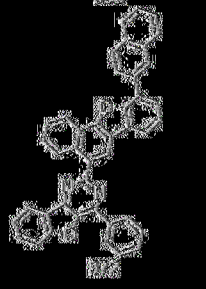


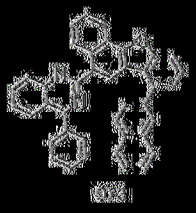


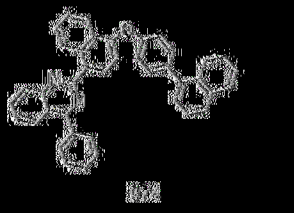


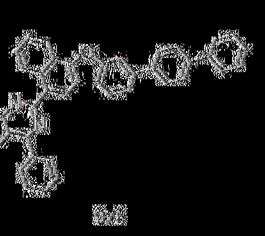


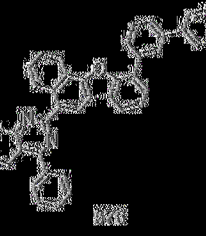


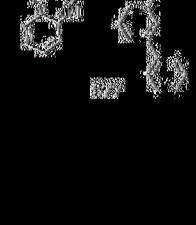


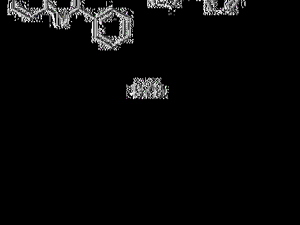


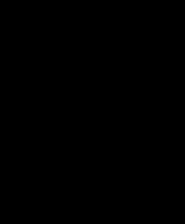


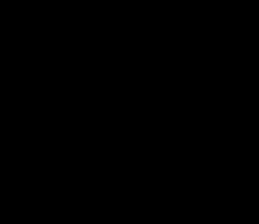


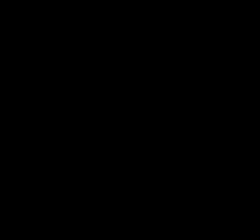


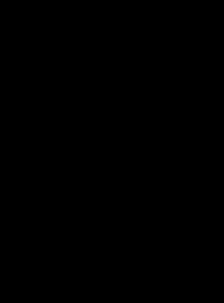


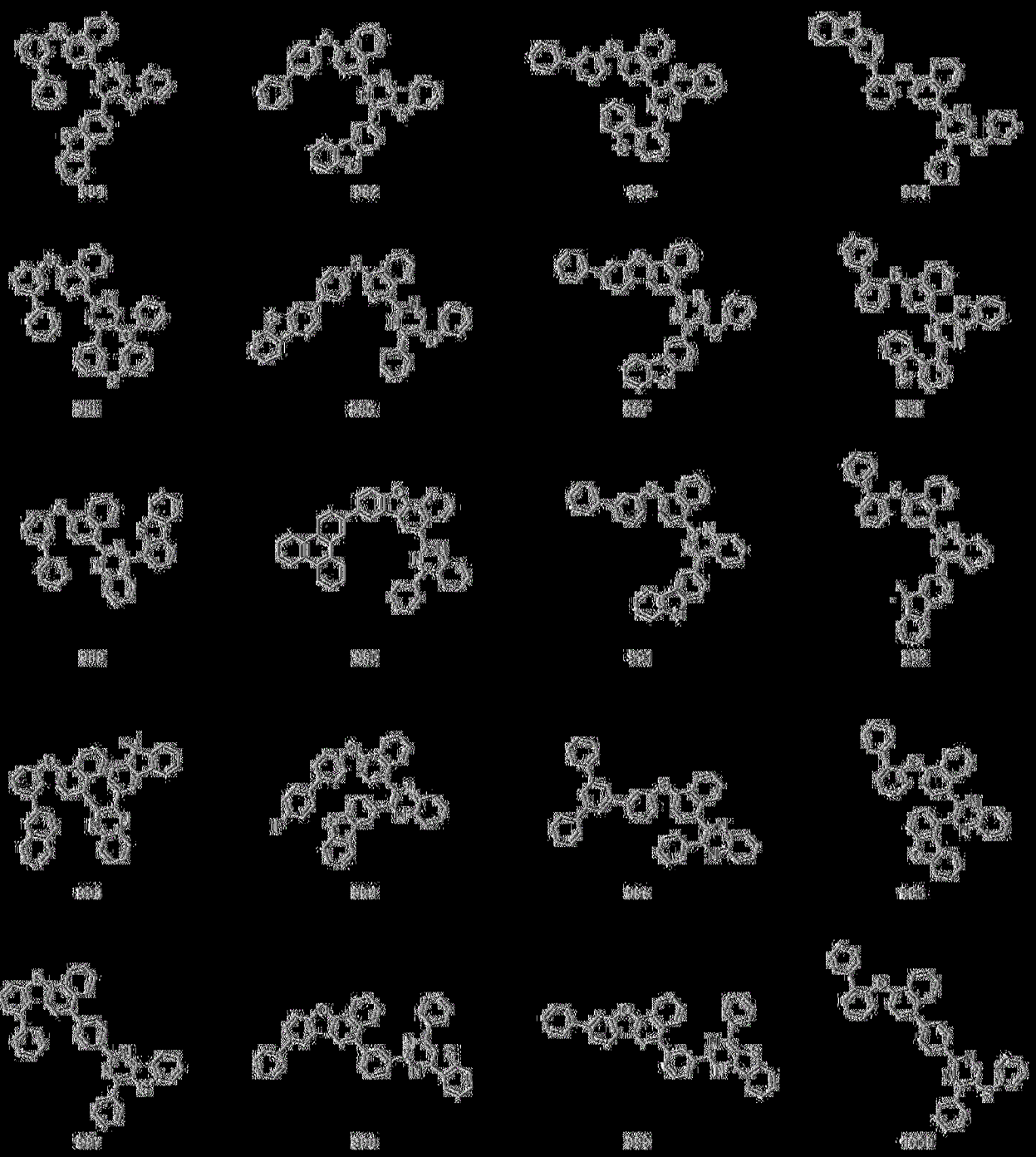












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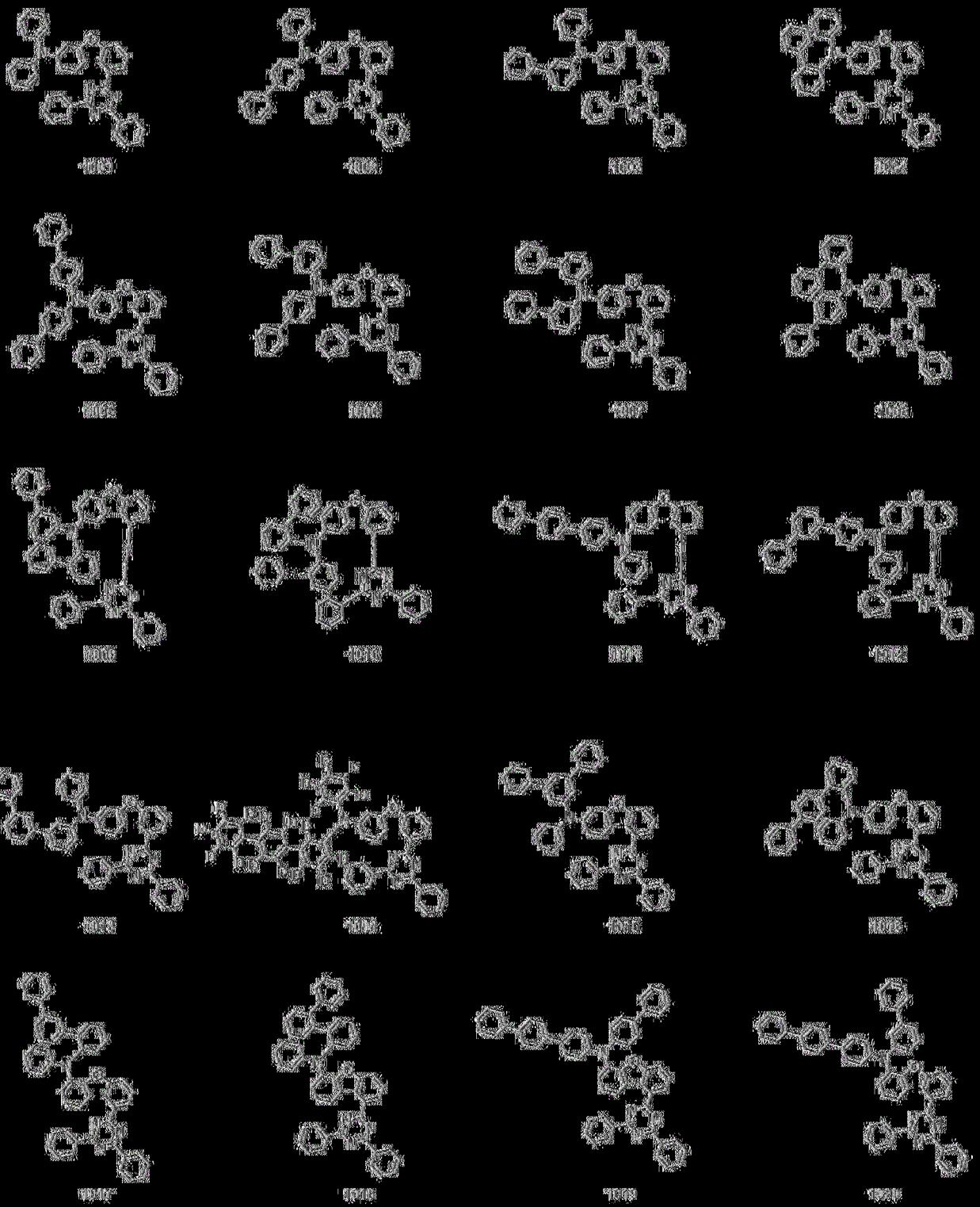
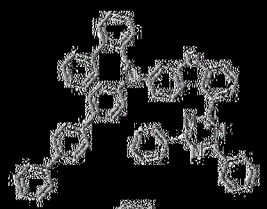
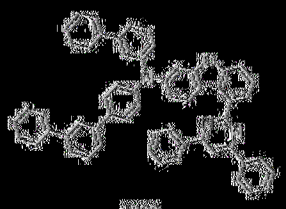
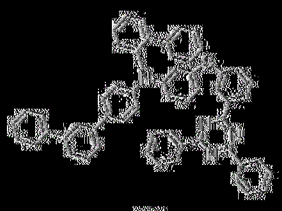
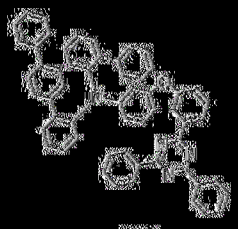
[請求項8] 如請求項1所述的有機發光裝置，其中化學式2為以下化合物中的任一個表示：

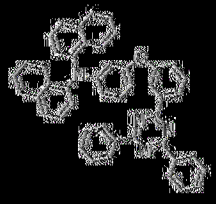


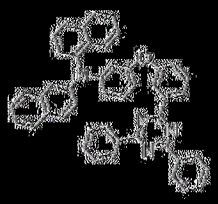


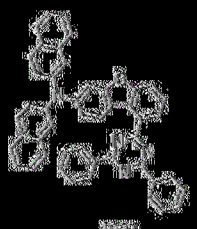


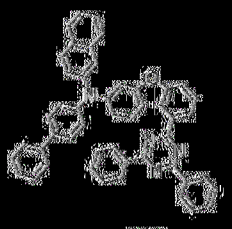


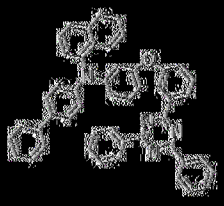


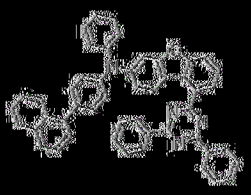


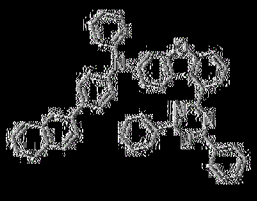


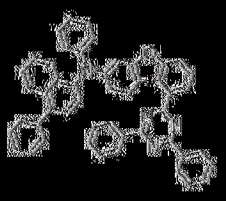


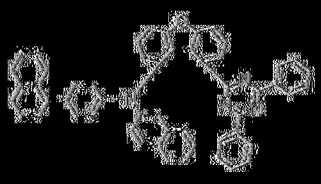


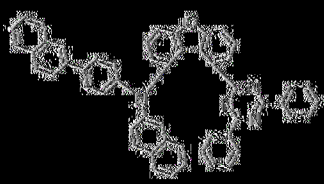


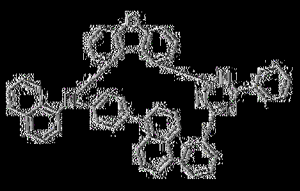


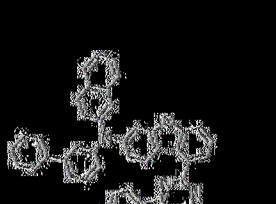


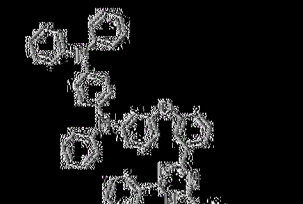


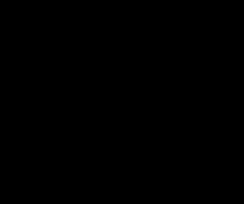


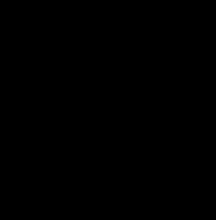


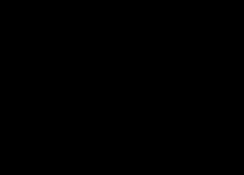


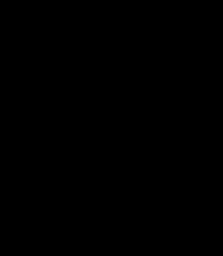


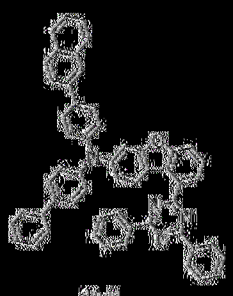


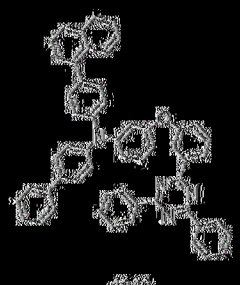


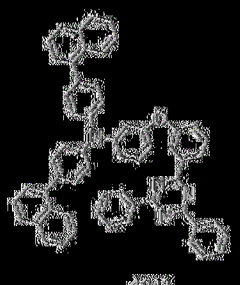


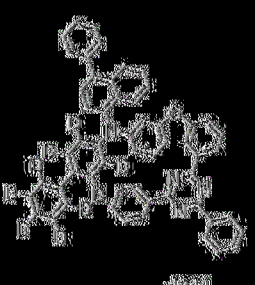


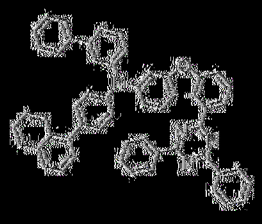


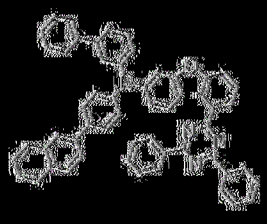


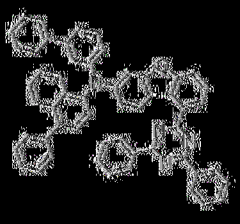


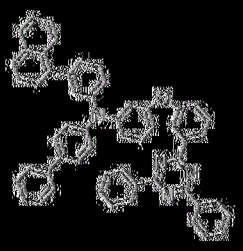


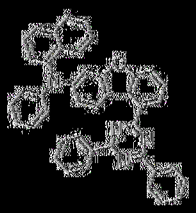


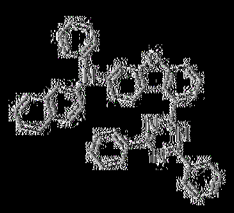


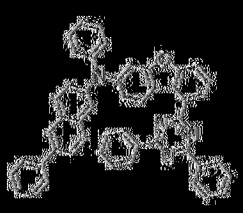


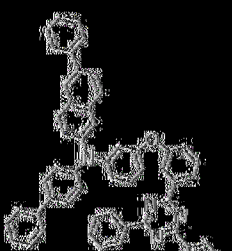


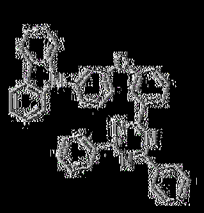


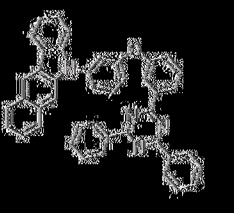


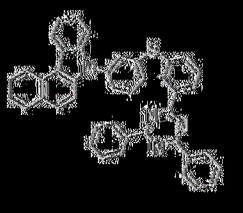


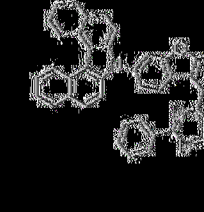


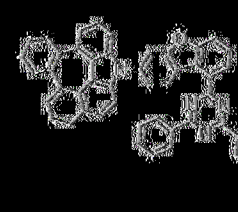


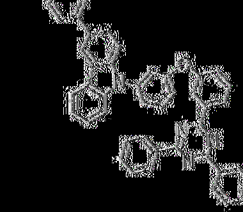


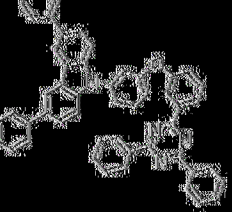


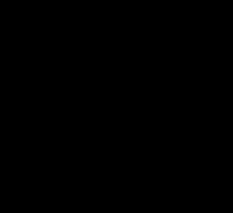


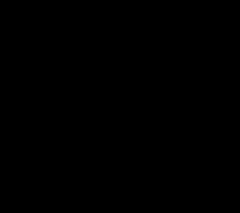


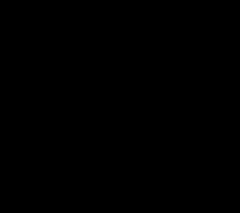


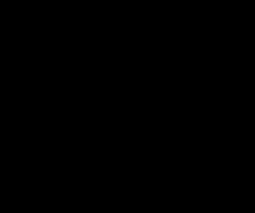


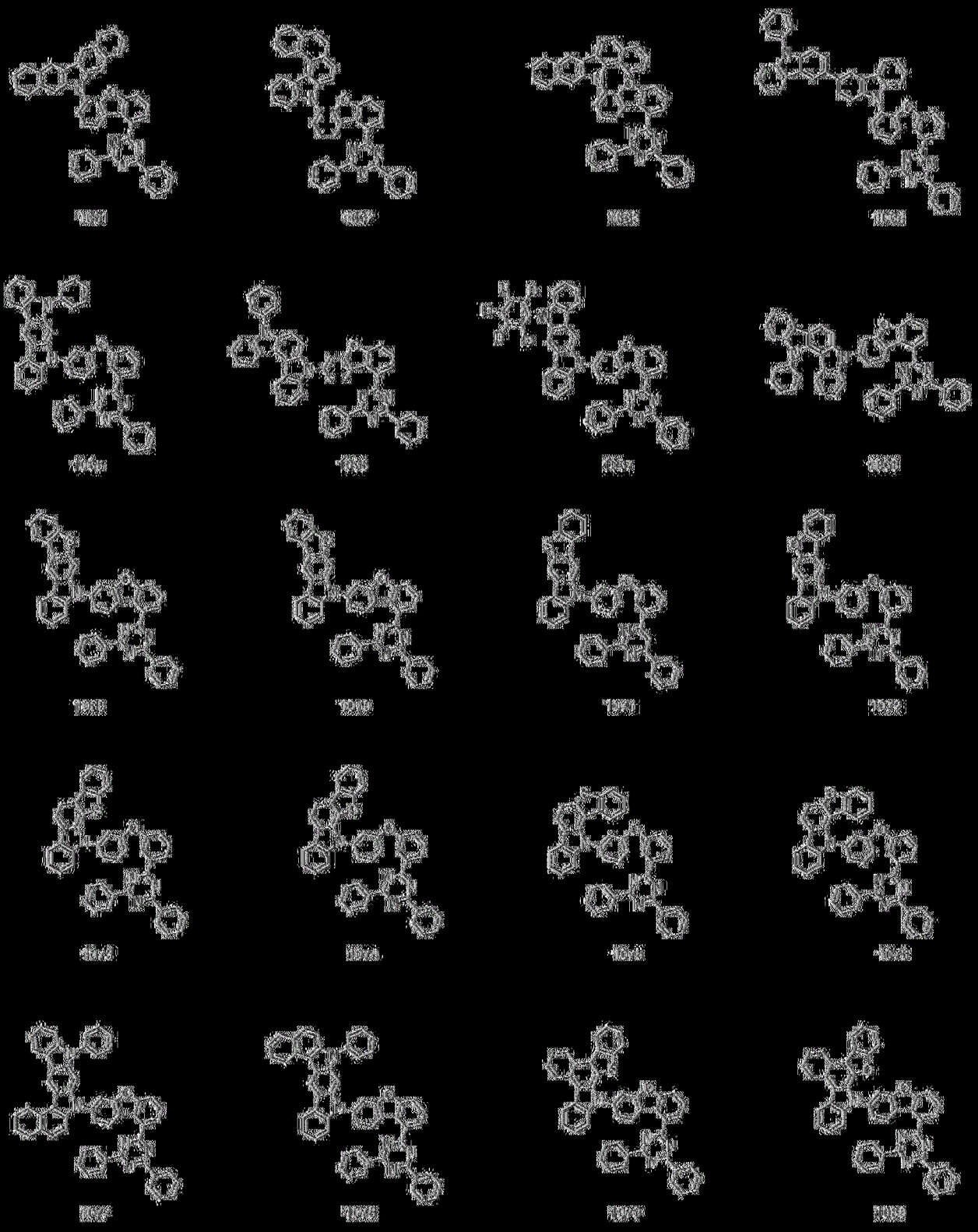


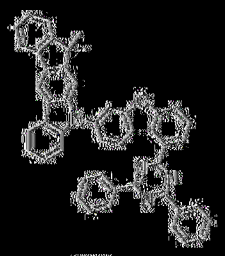


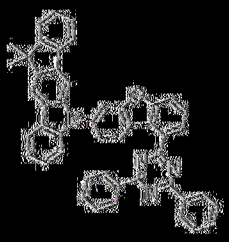


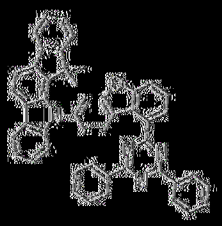


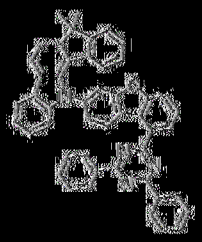


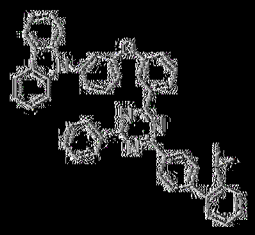


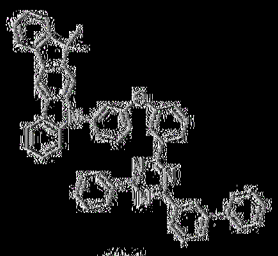


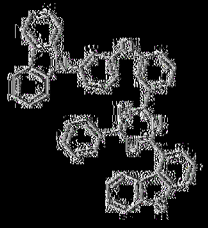


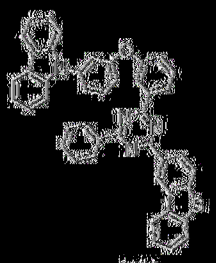


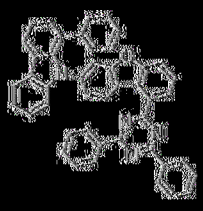


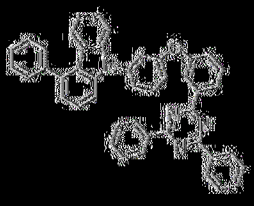


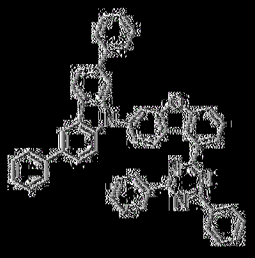


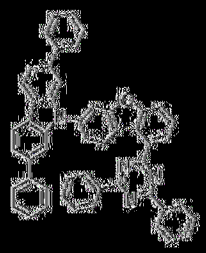


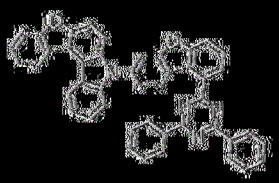


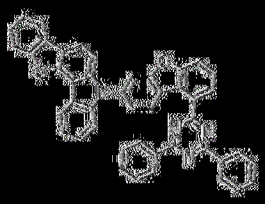


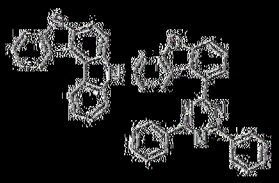


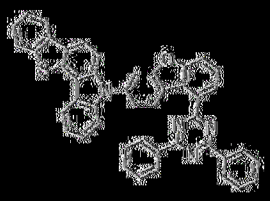


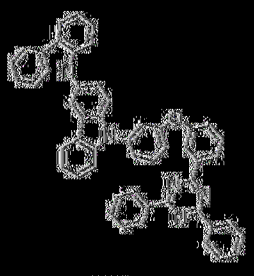


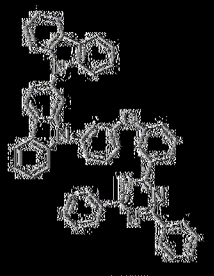


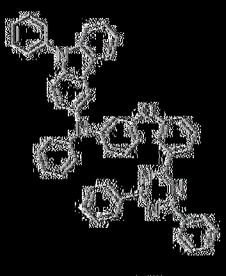


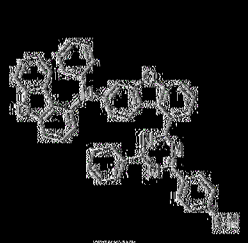


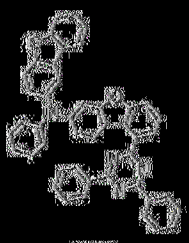


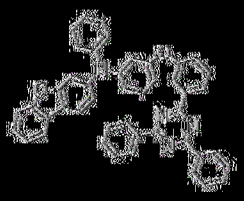


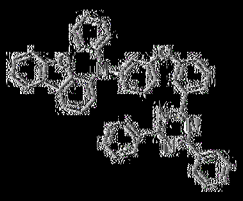


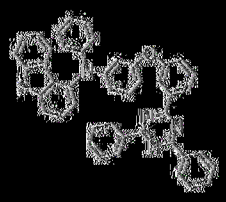


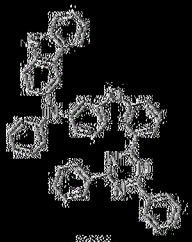


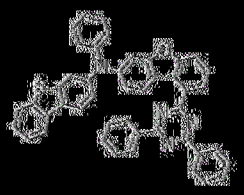


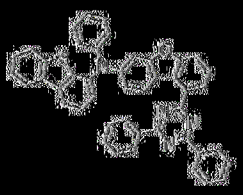


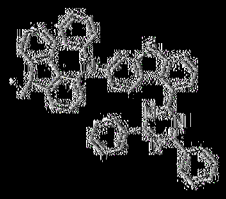


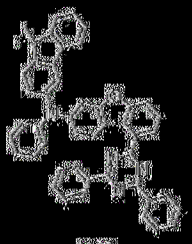


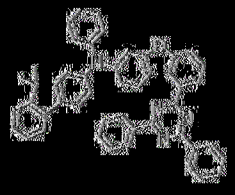


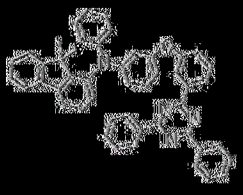


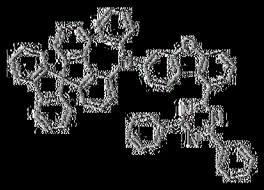


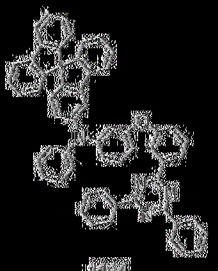


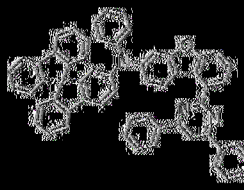


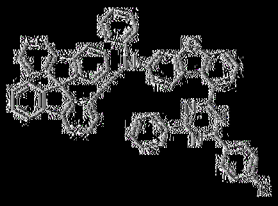


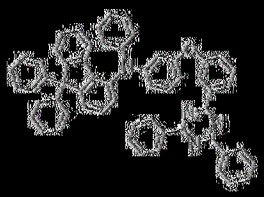


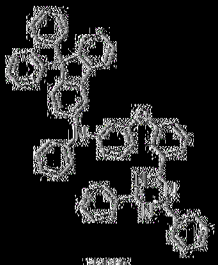


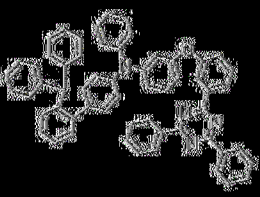


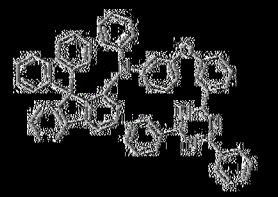


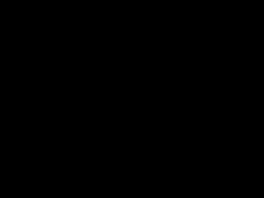


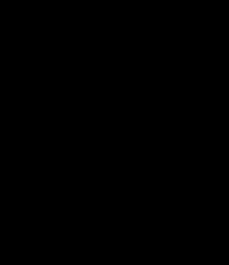


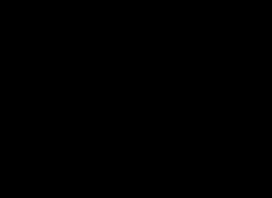


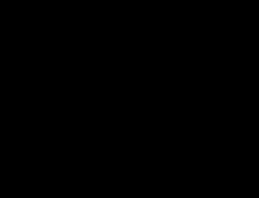


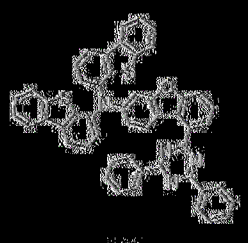


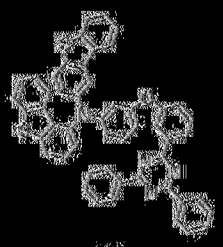


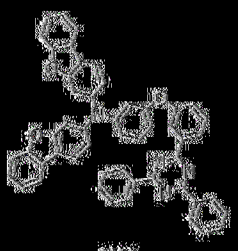


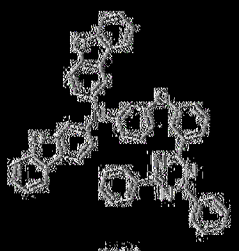


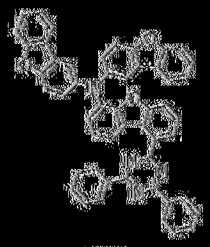


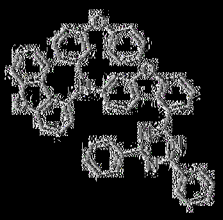


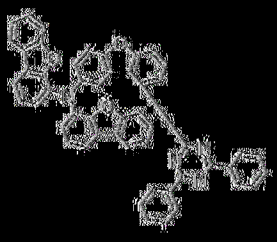


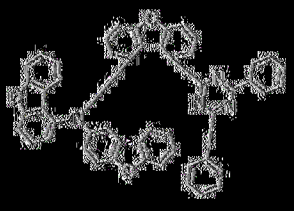


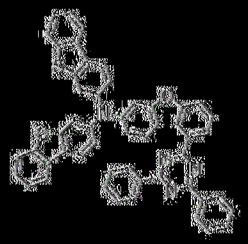


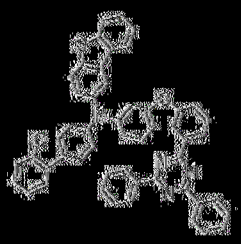


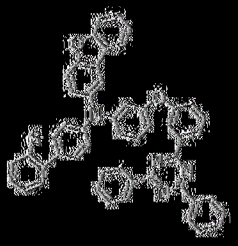


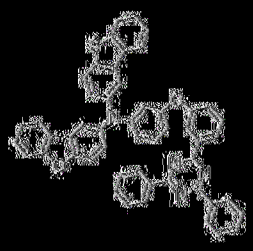


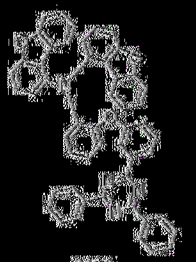


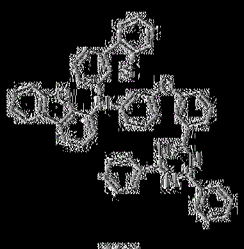


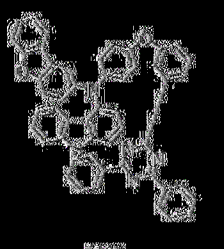


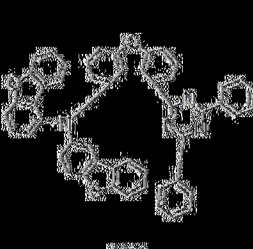


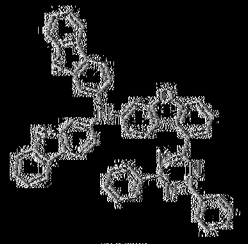


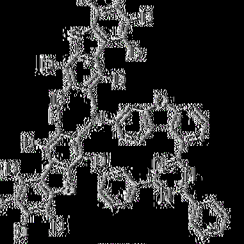


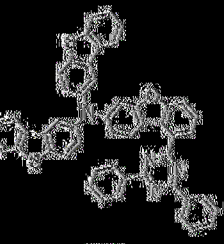


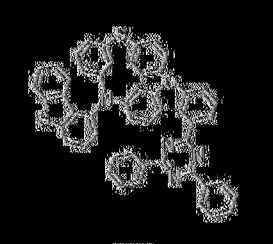


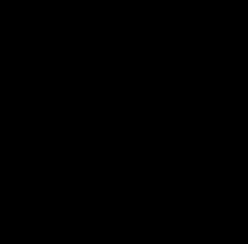


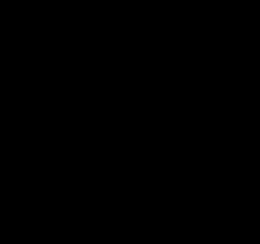


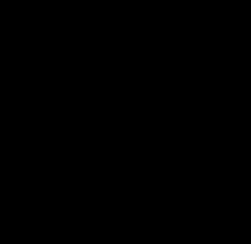


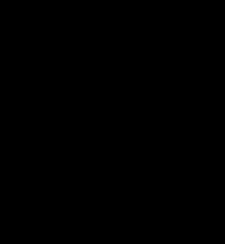


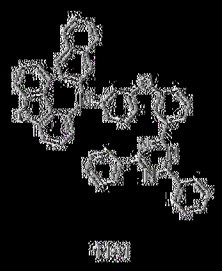


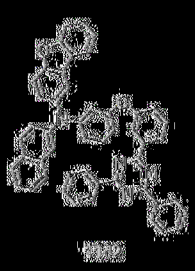


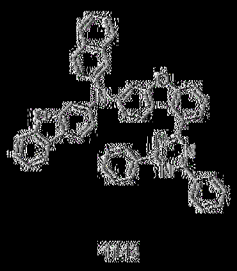


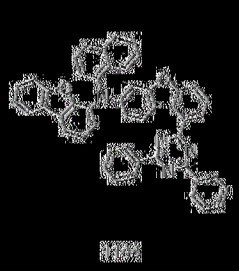


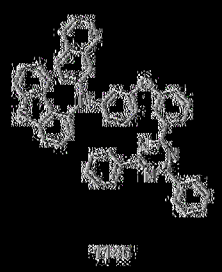


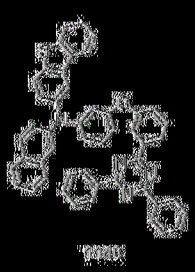


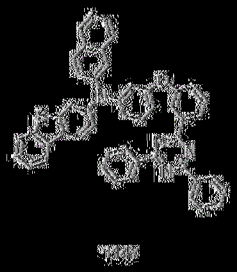


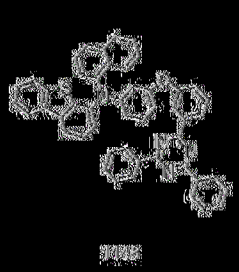


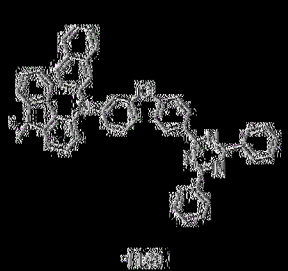


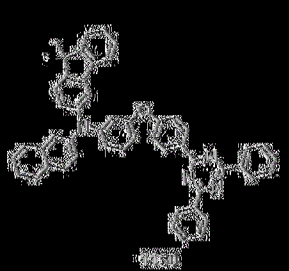


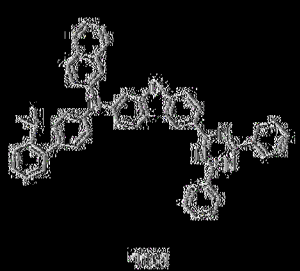


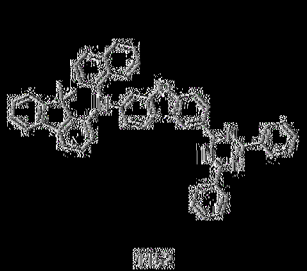


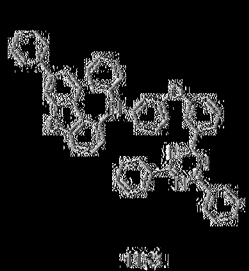


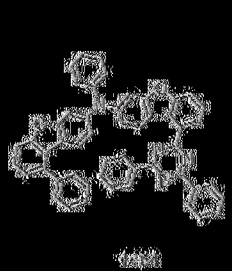


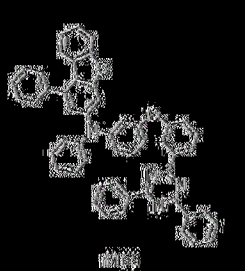


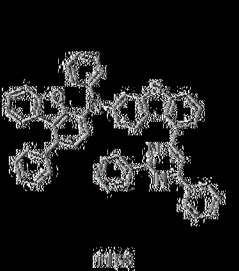


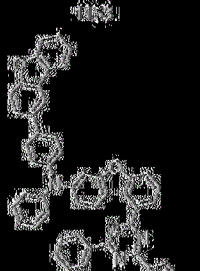


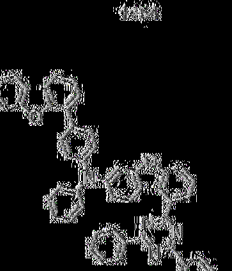


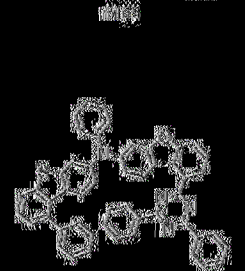


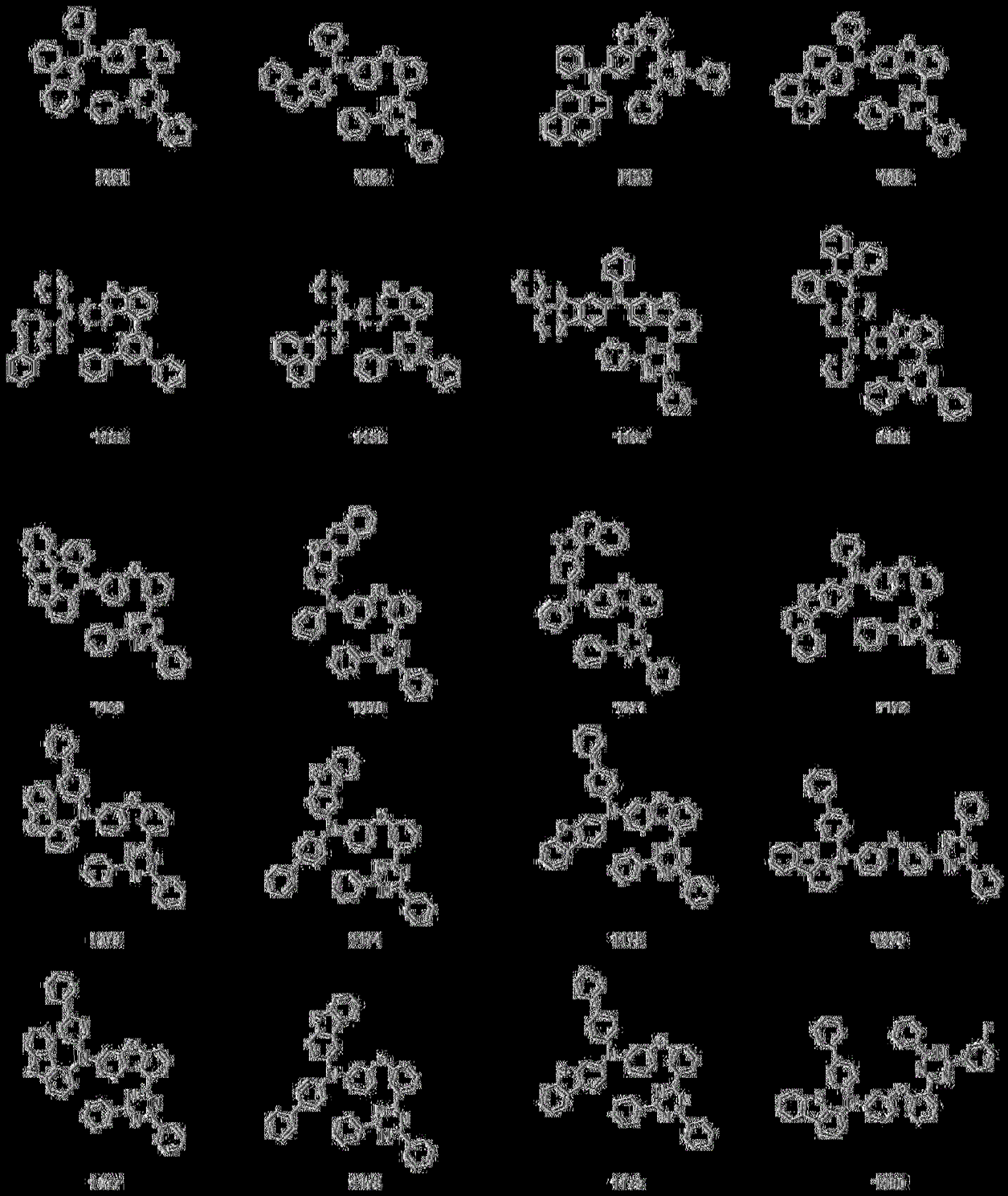












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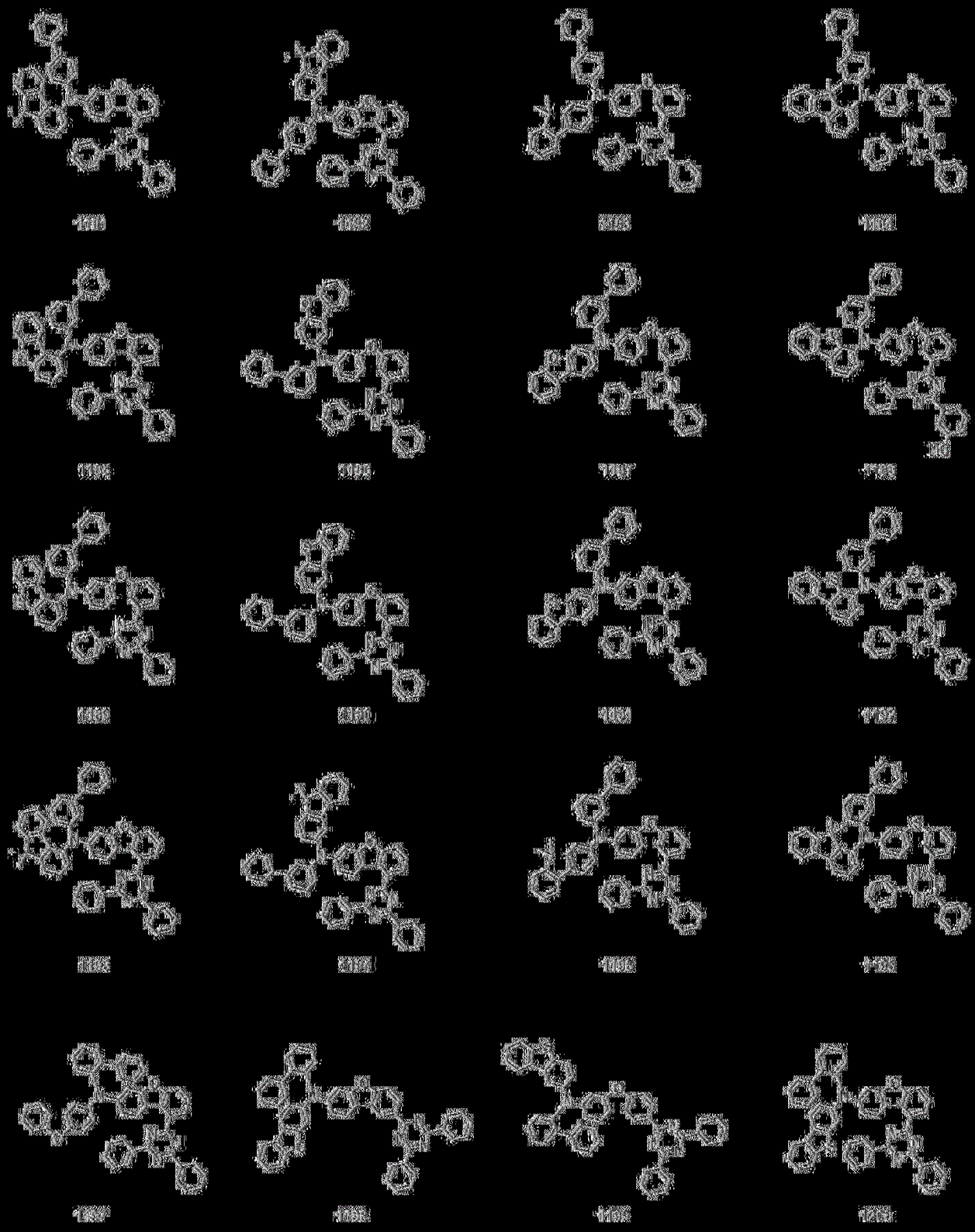
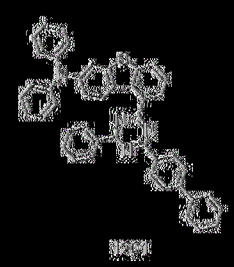
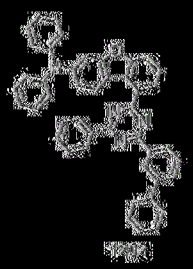
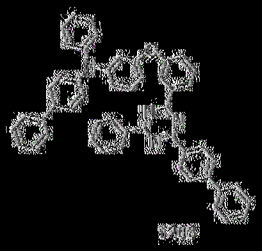
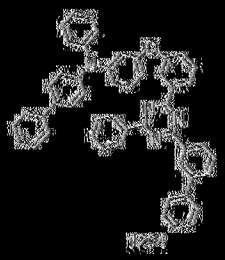
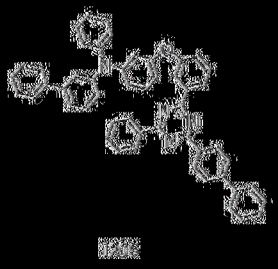


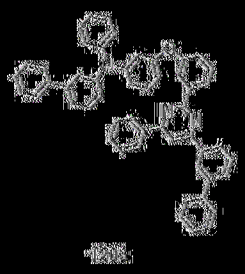


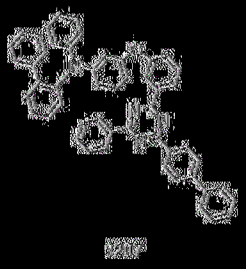


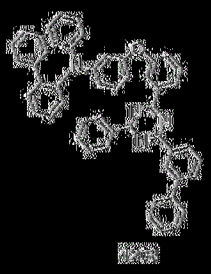


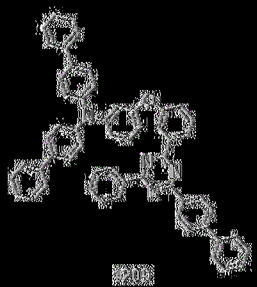


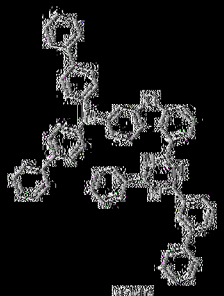


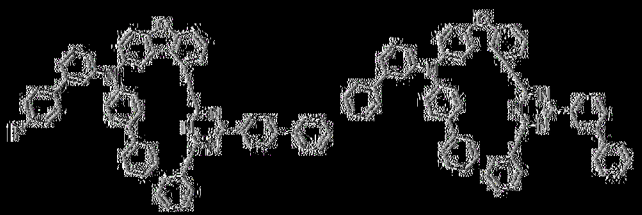


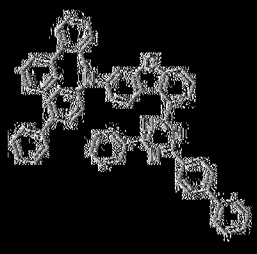


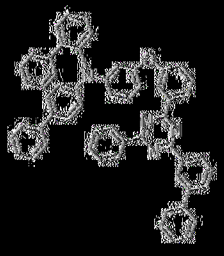


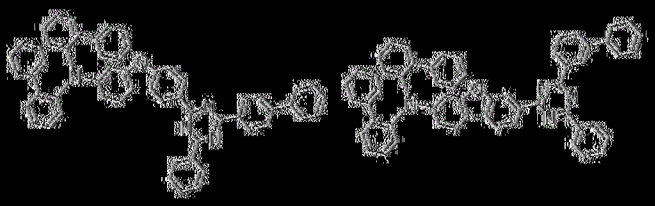


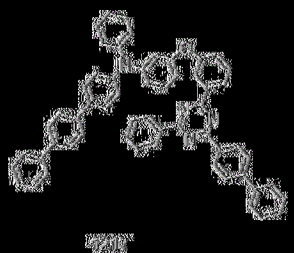


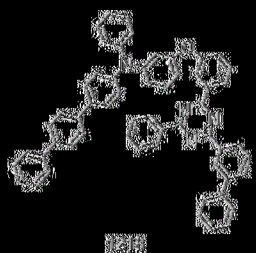


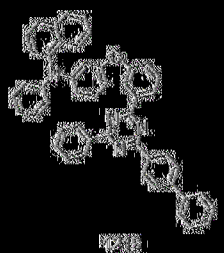


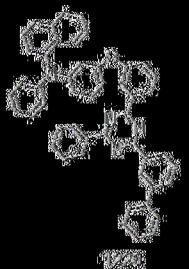


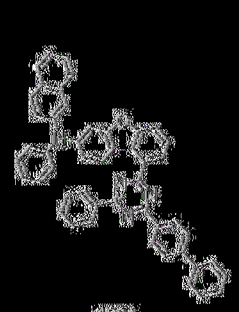


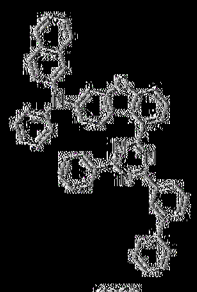


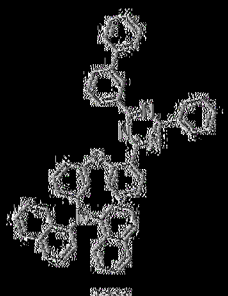


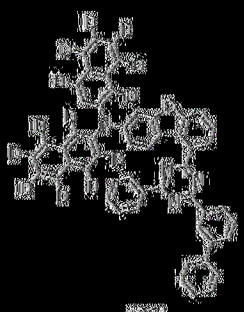


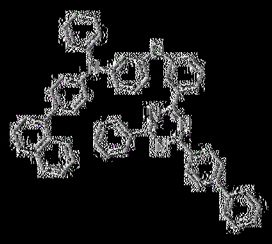


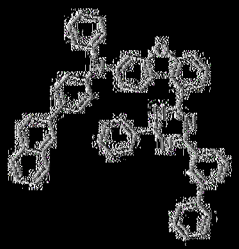


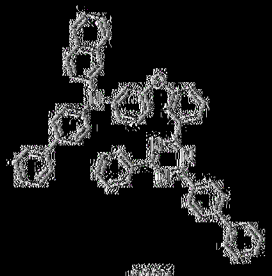


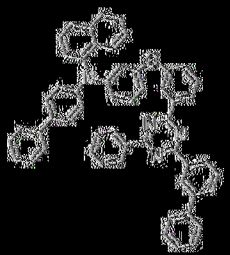


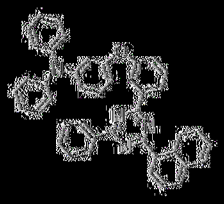


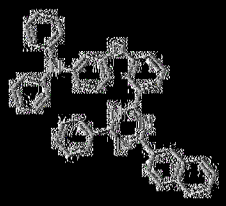


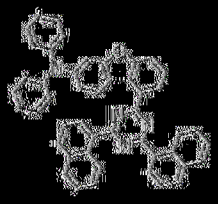


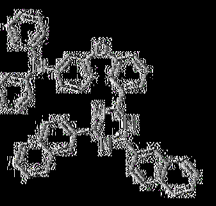


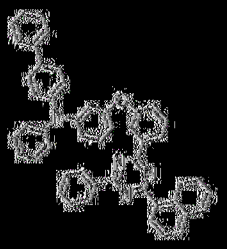


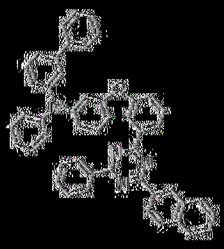


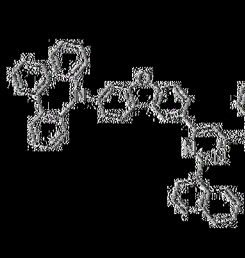


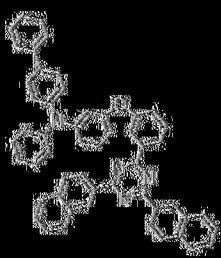


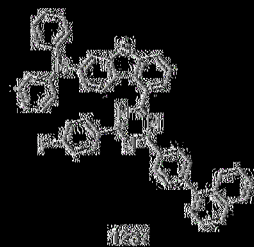


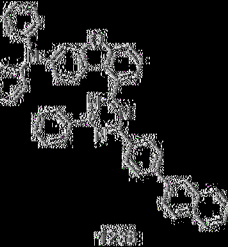


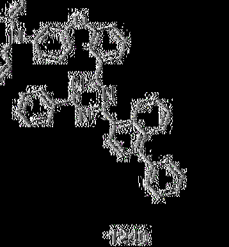


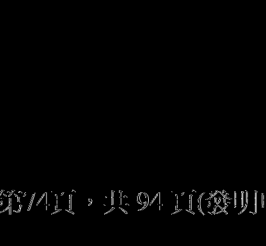


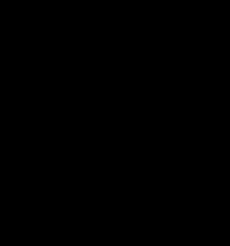


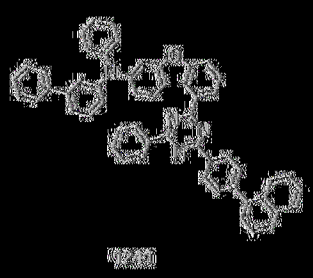


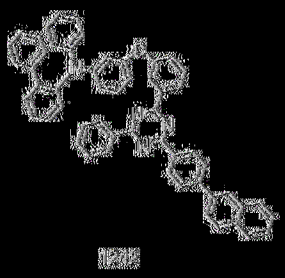


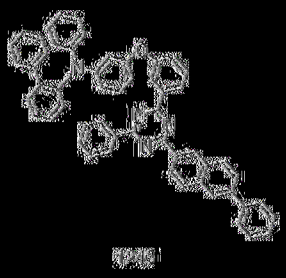


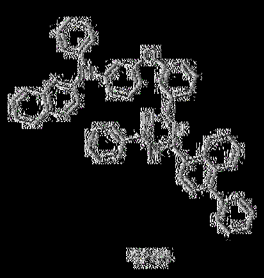


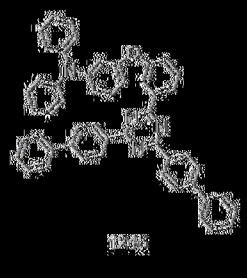


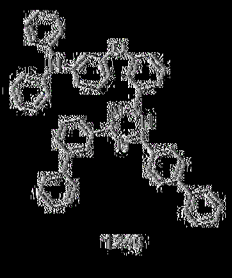


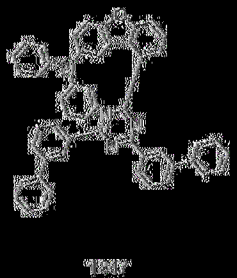


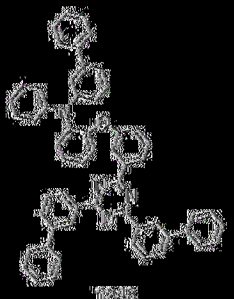


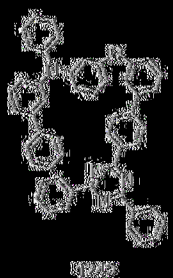


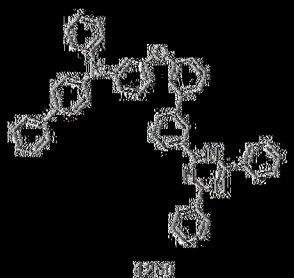


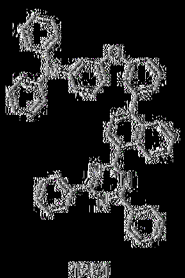


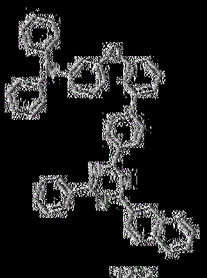


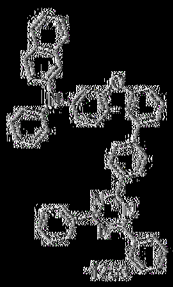


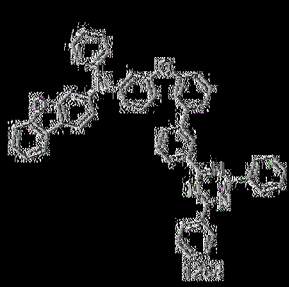


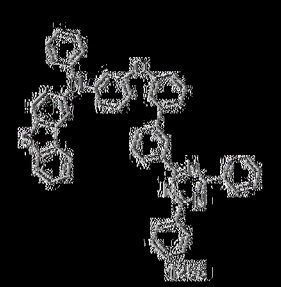


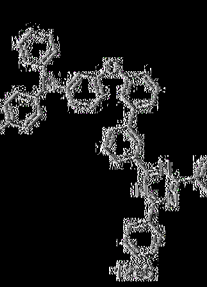


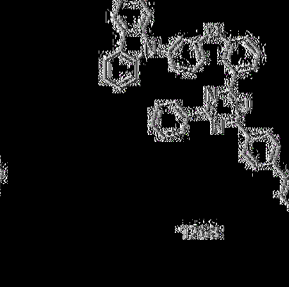


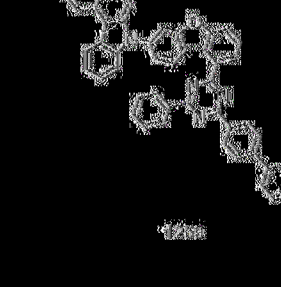


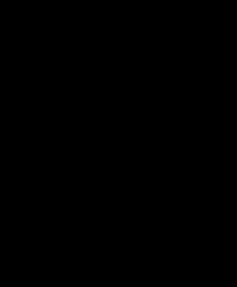


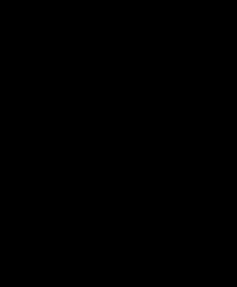


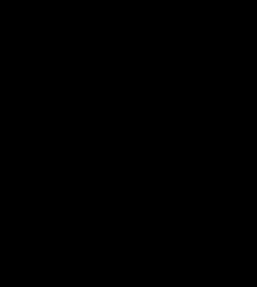


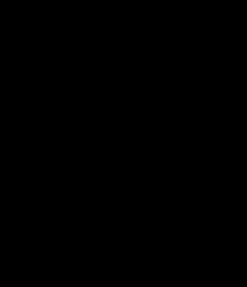


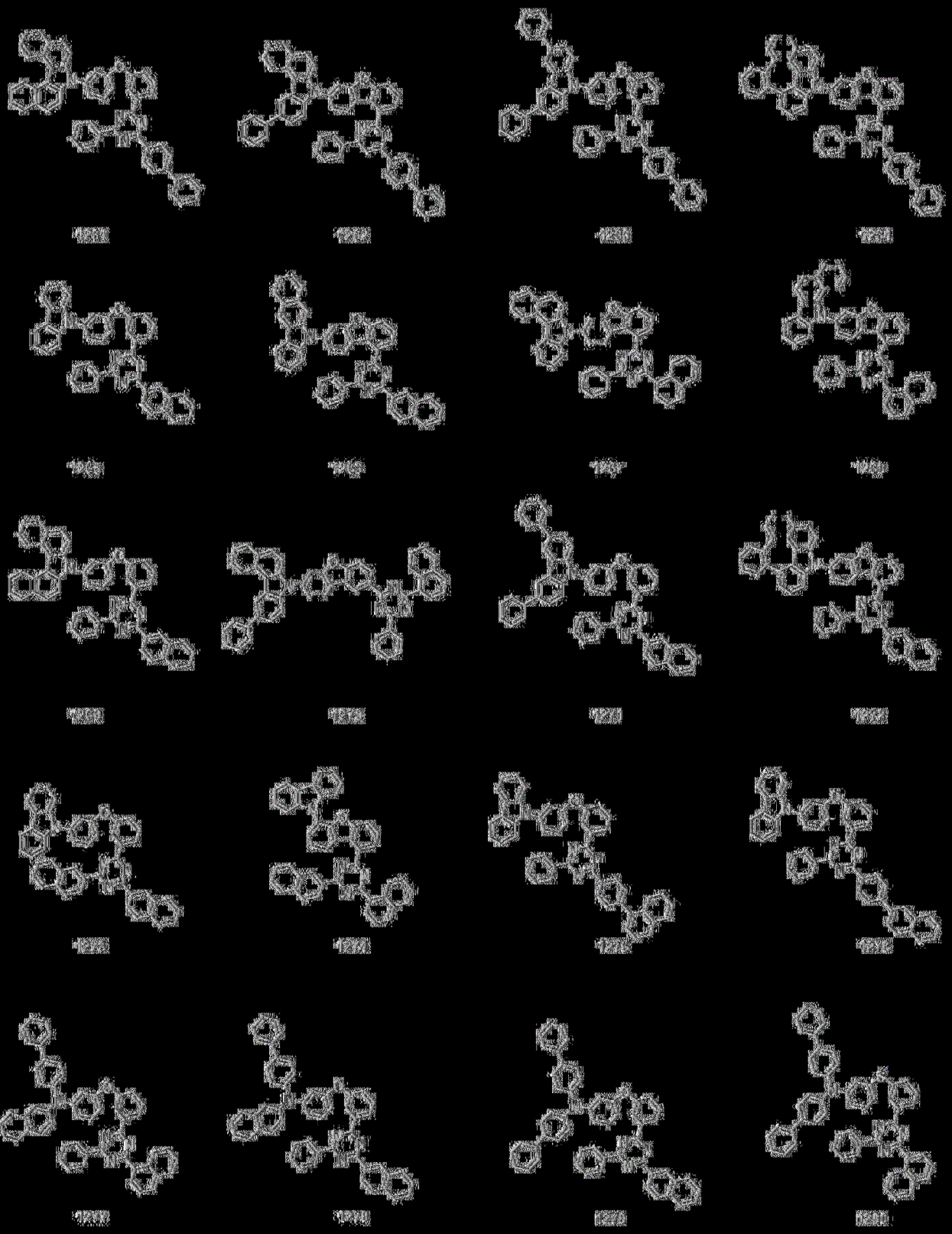


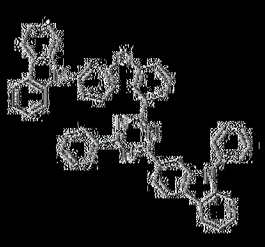


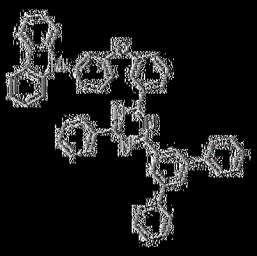


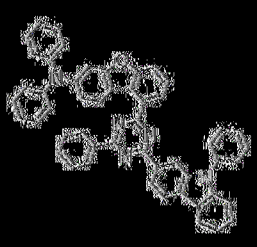


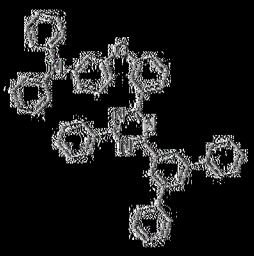


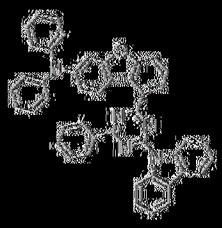


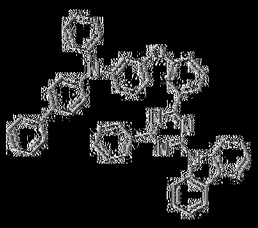


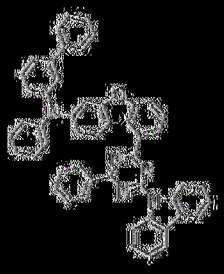


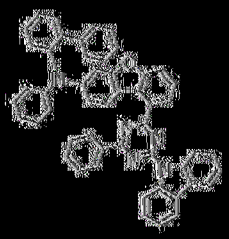


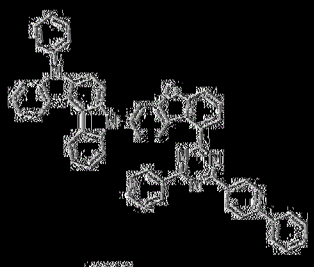


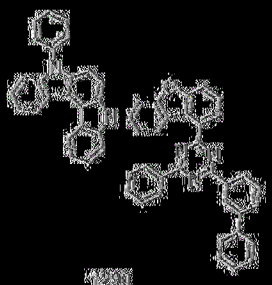


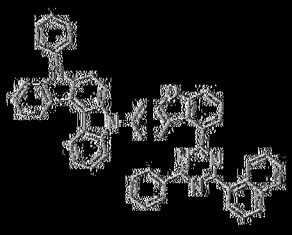


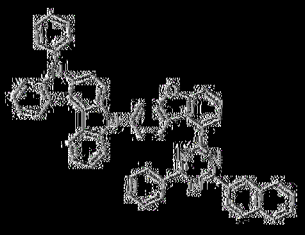


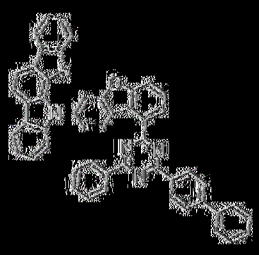


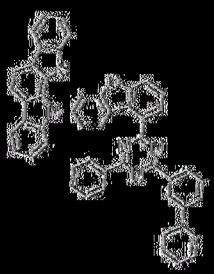


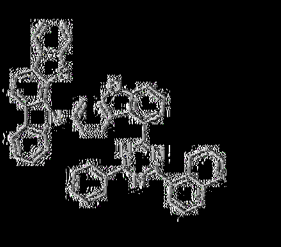


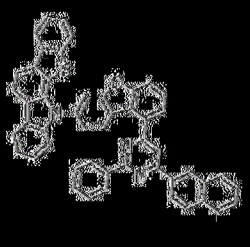


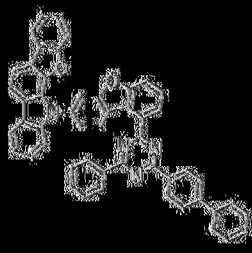


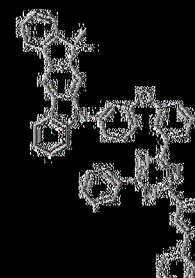


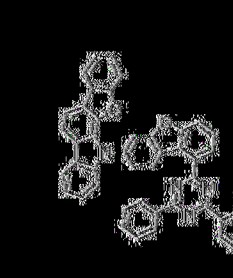


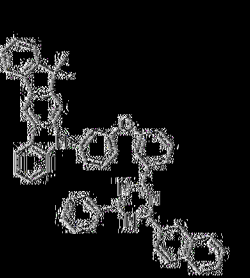


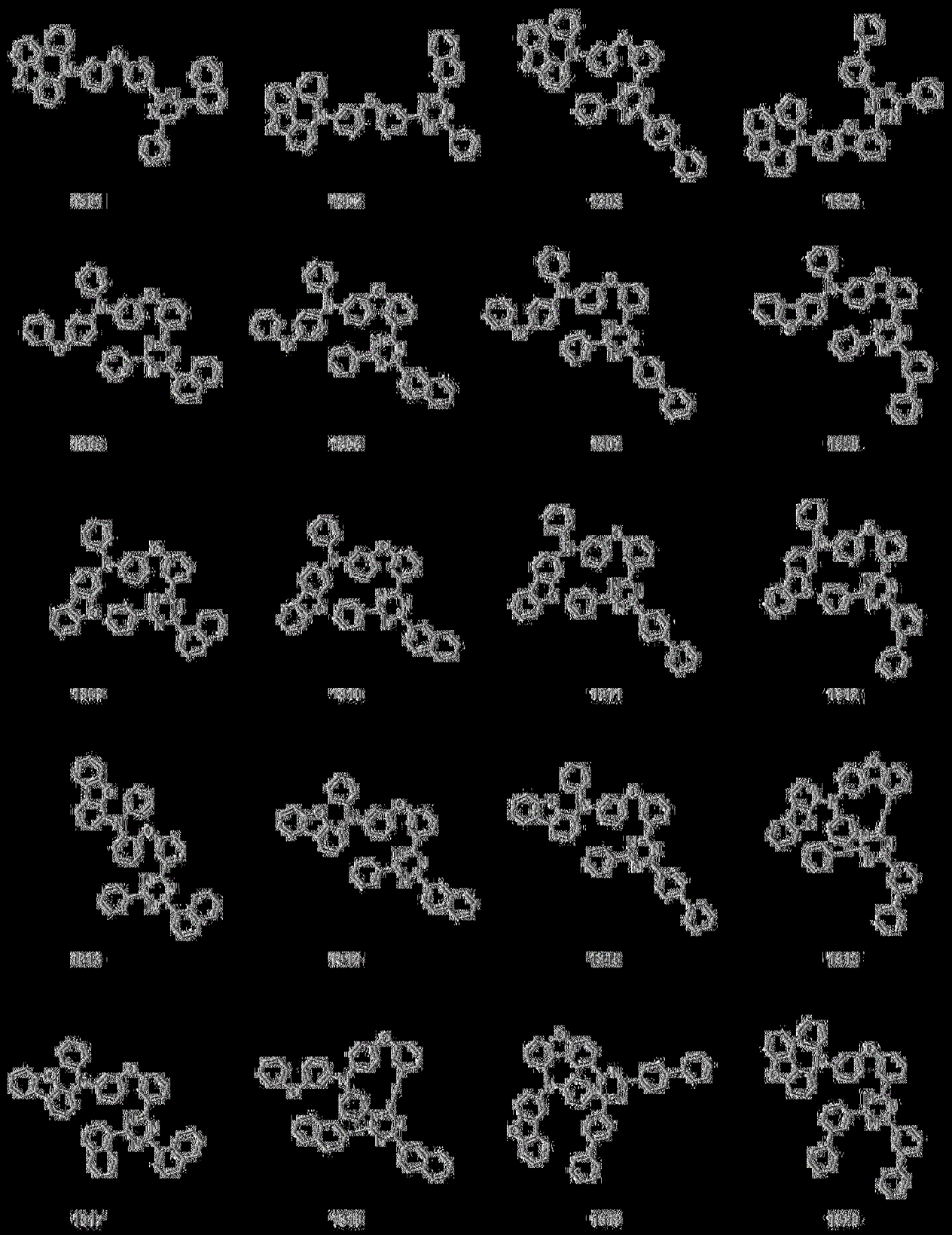


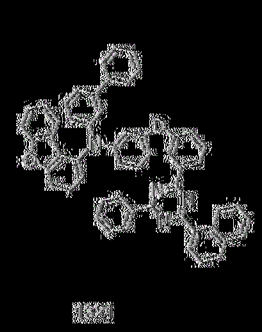


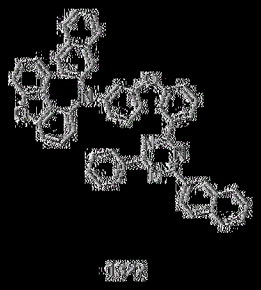


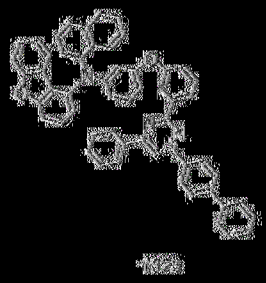


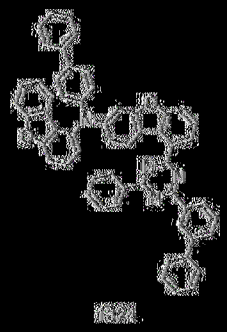


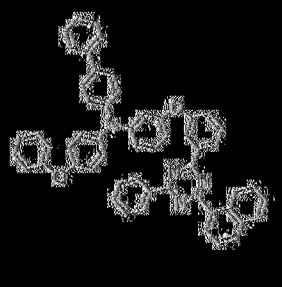


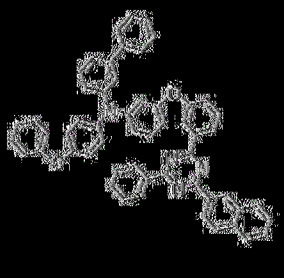


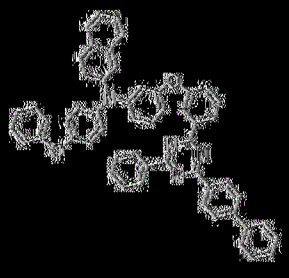


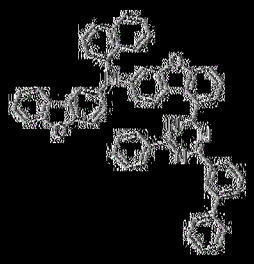


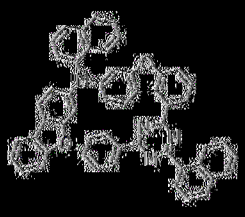


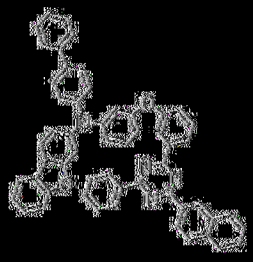


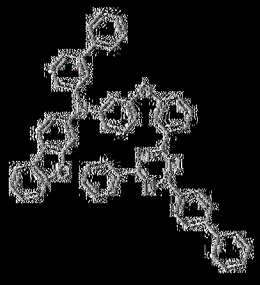


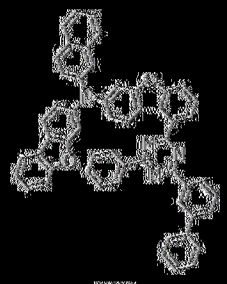


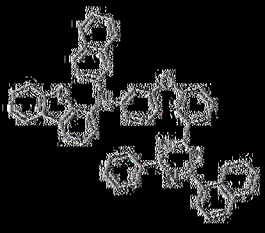


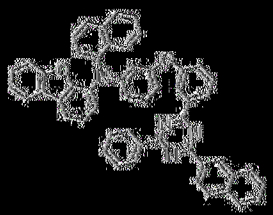


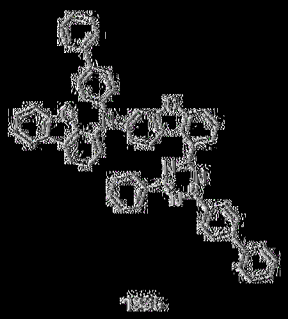


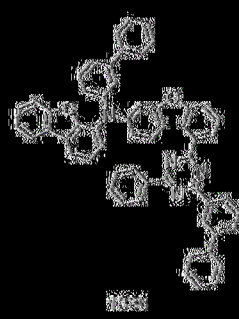


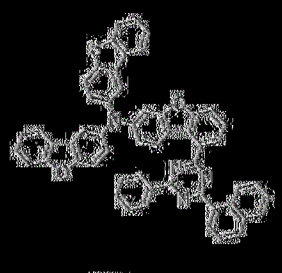


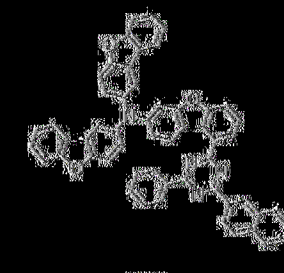


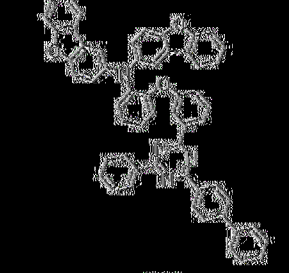


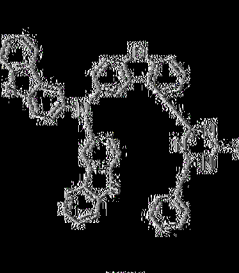


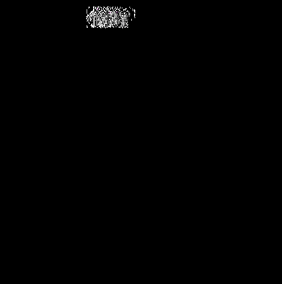


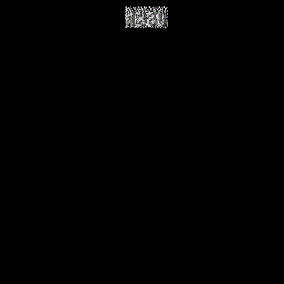


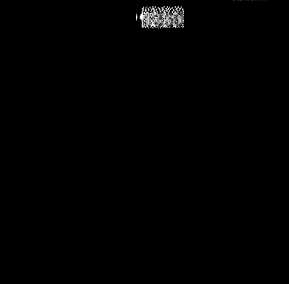


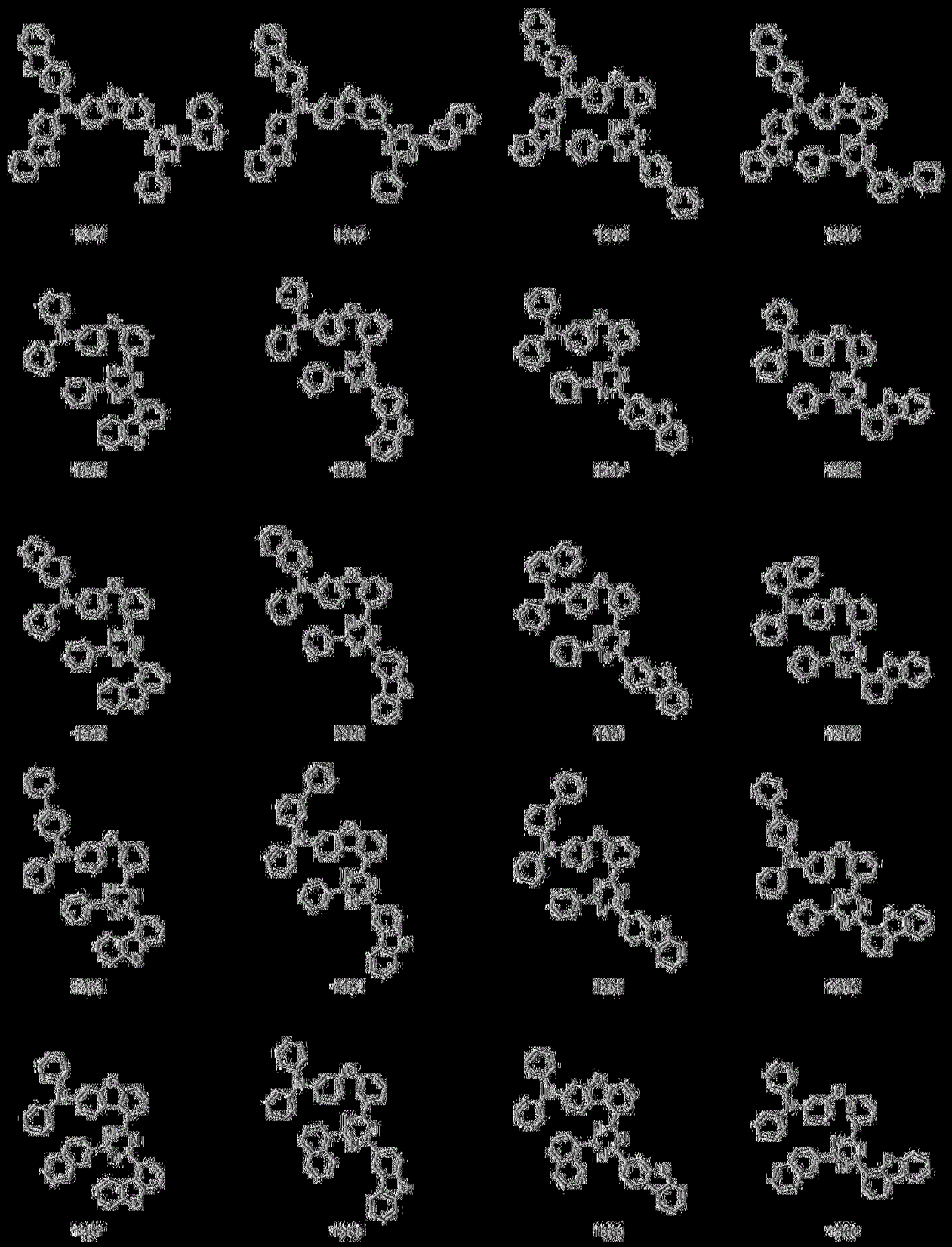


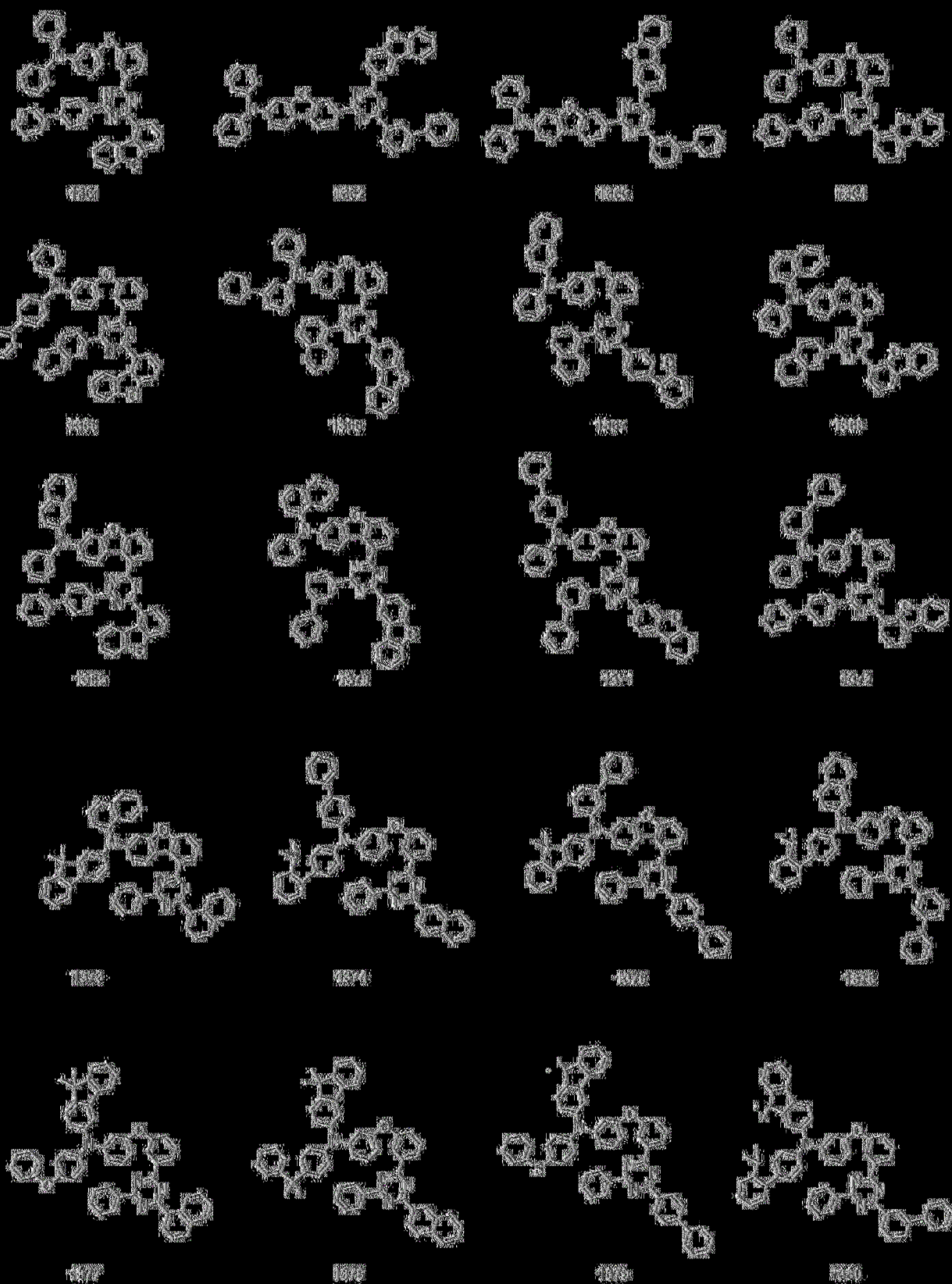


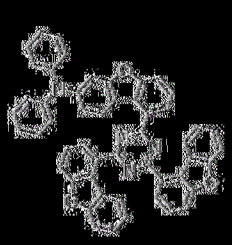


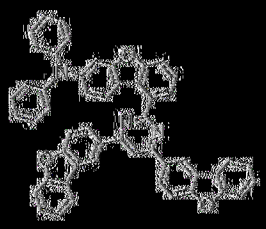


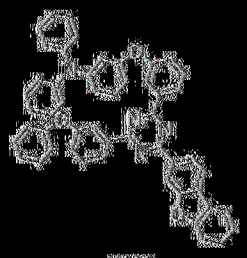


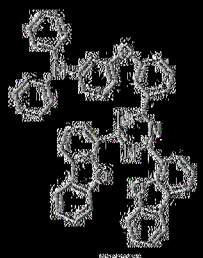


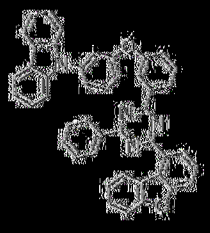


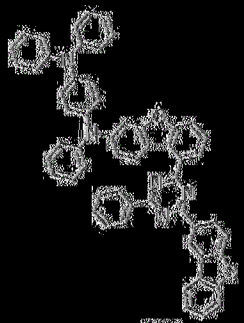


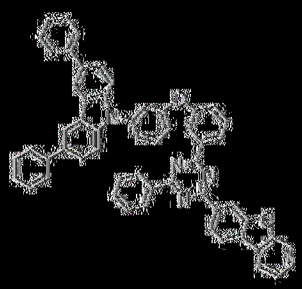


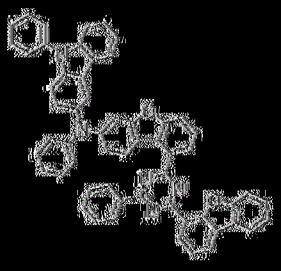


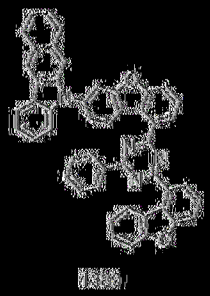


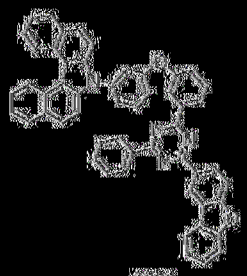


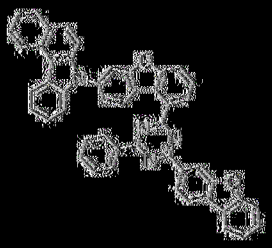


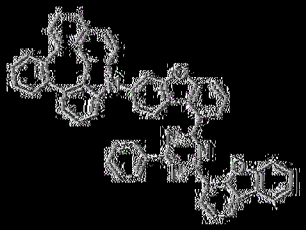


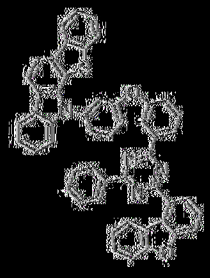


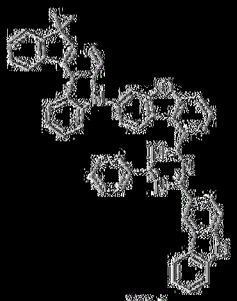


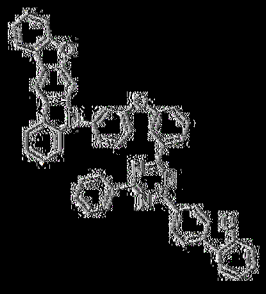


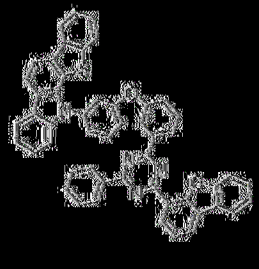


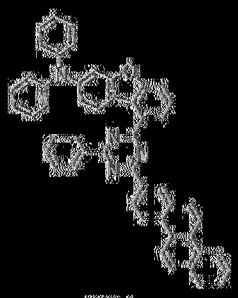


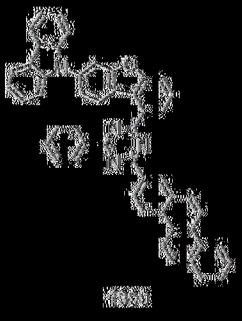


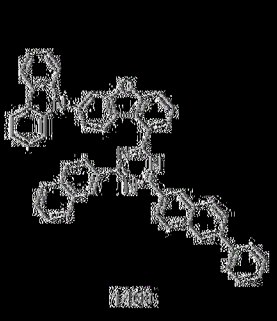


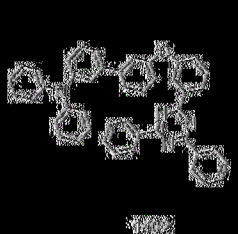


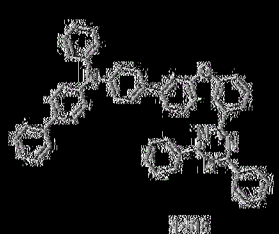


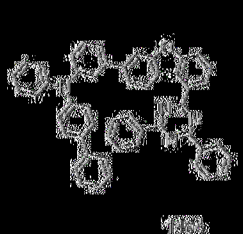


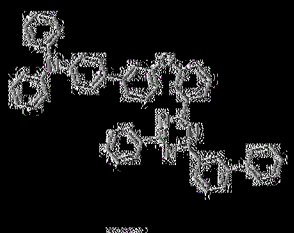


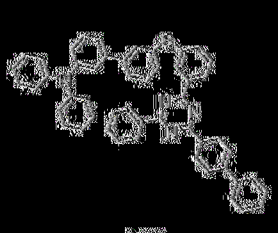


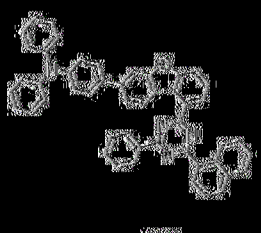


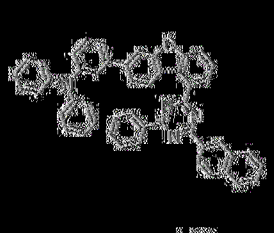


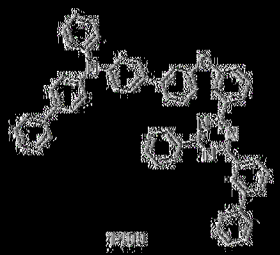


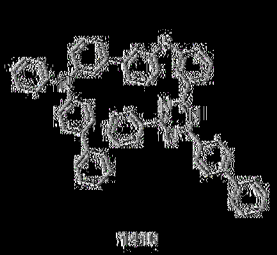


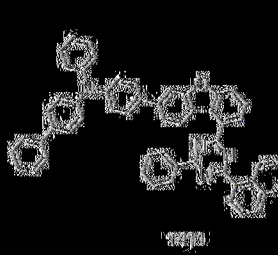


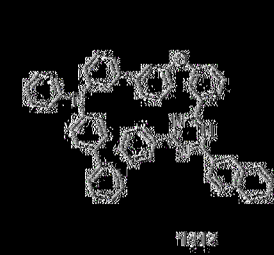


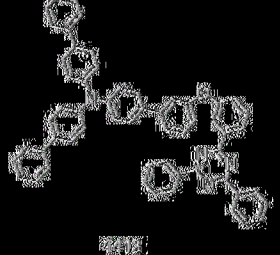


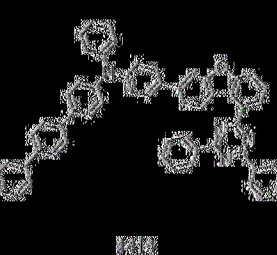


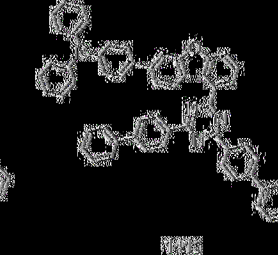


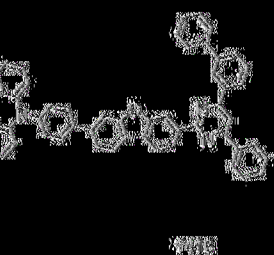


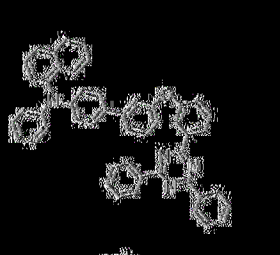


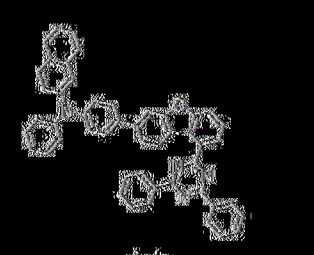


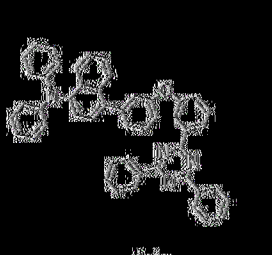


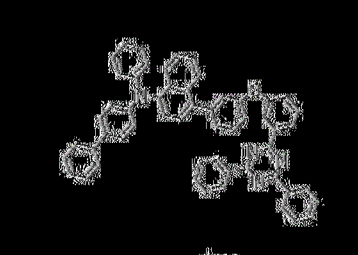


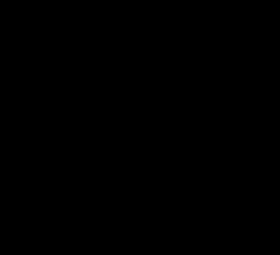


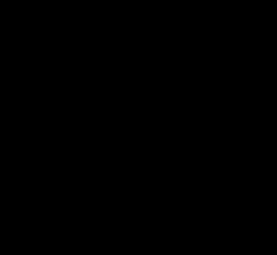


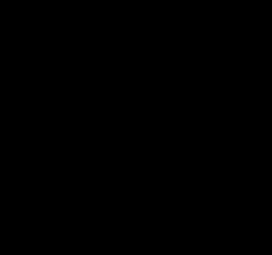


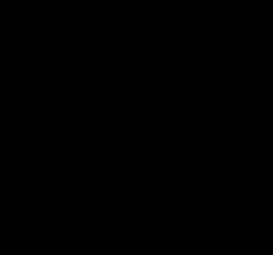


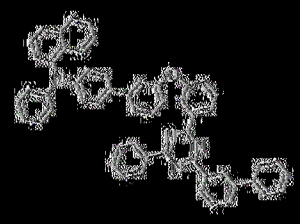


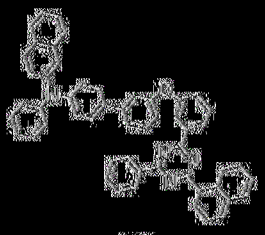


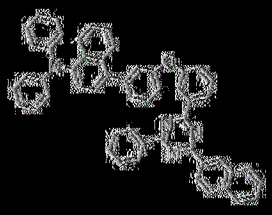


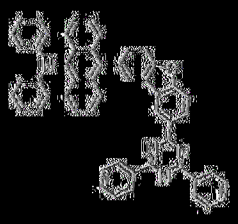


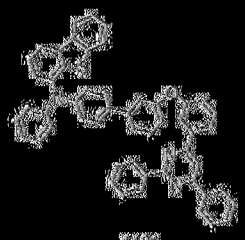


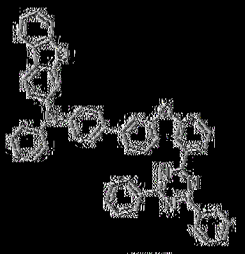


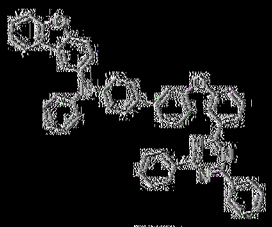


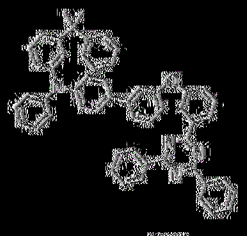


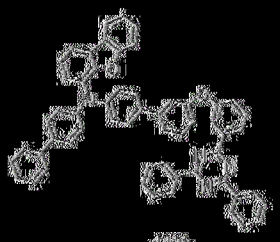


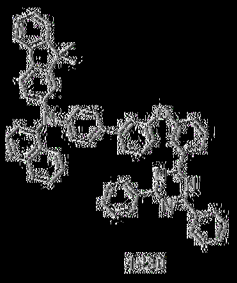


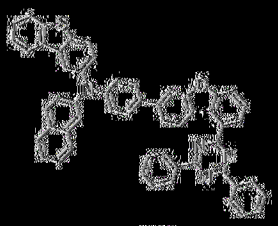


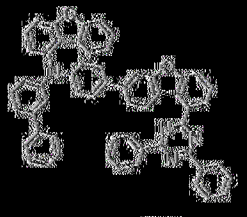


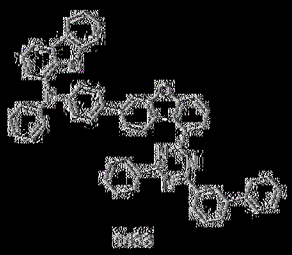


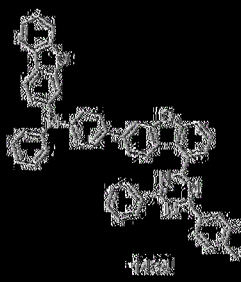


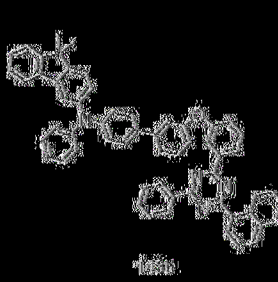


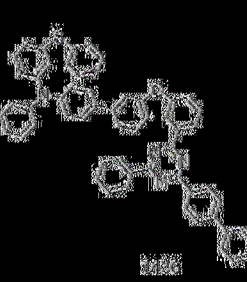


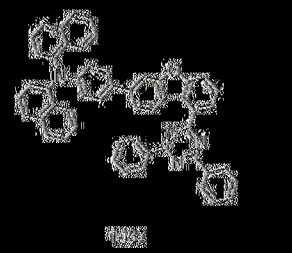


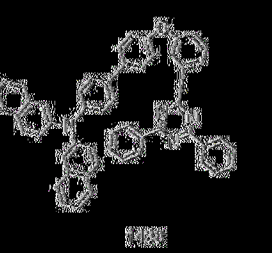


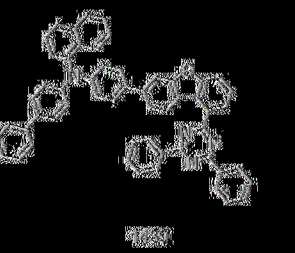


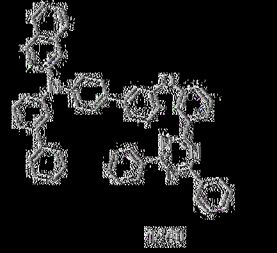


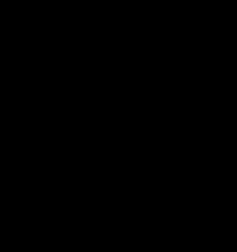


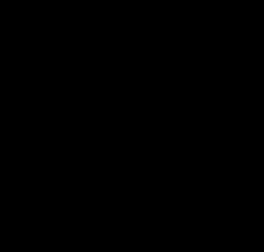


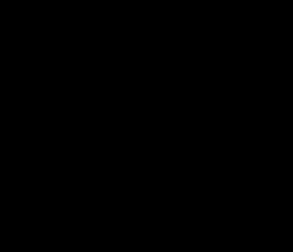


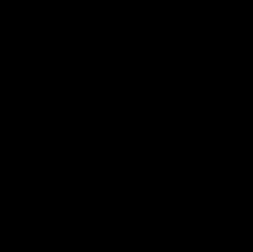


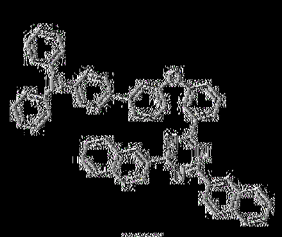


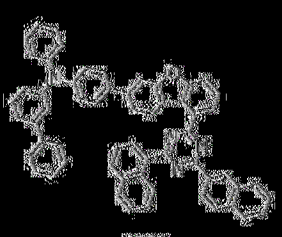


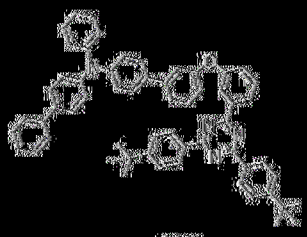


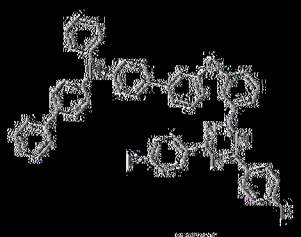


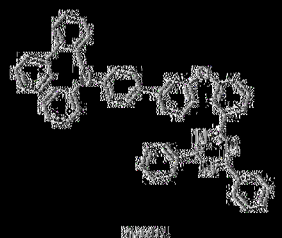


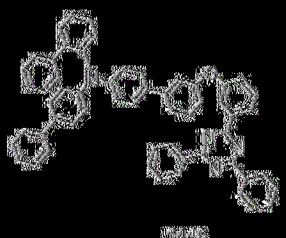


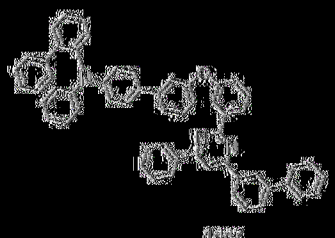


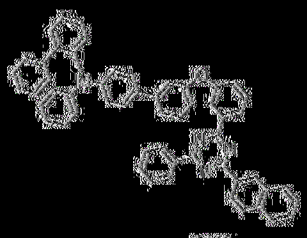


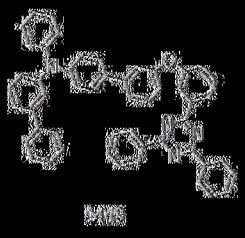


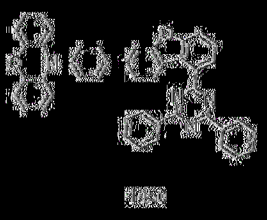


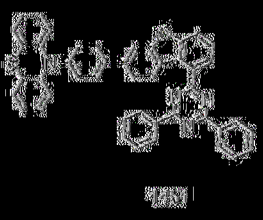


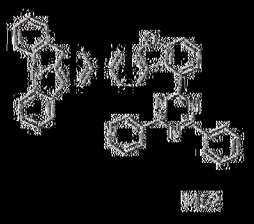


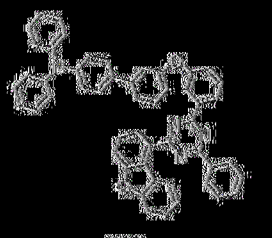


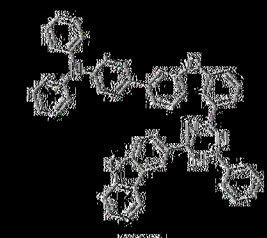


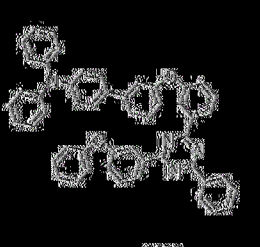


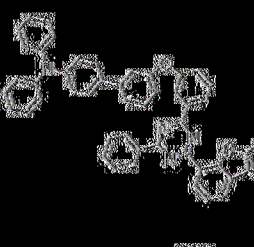


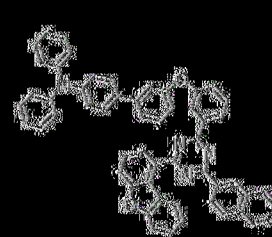


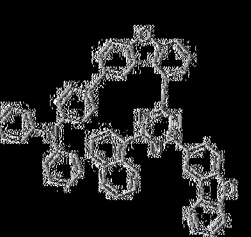


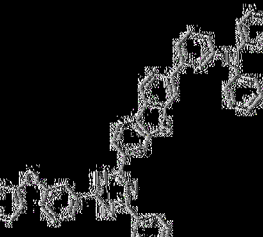


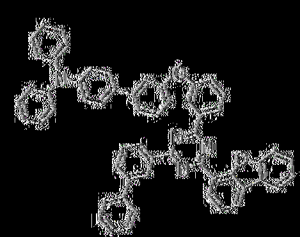


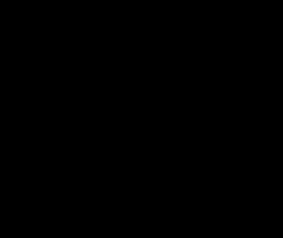


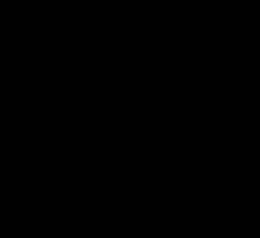


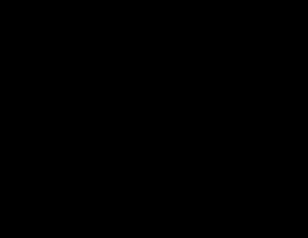


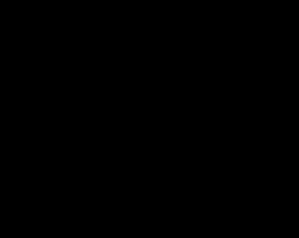


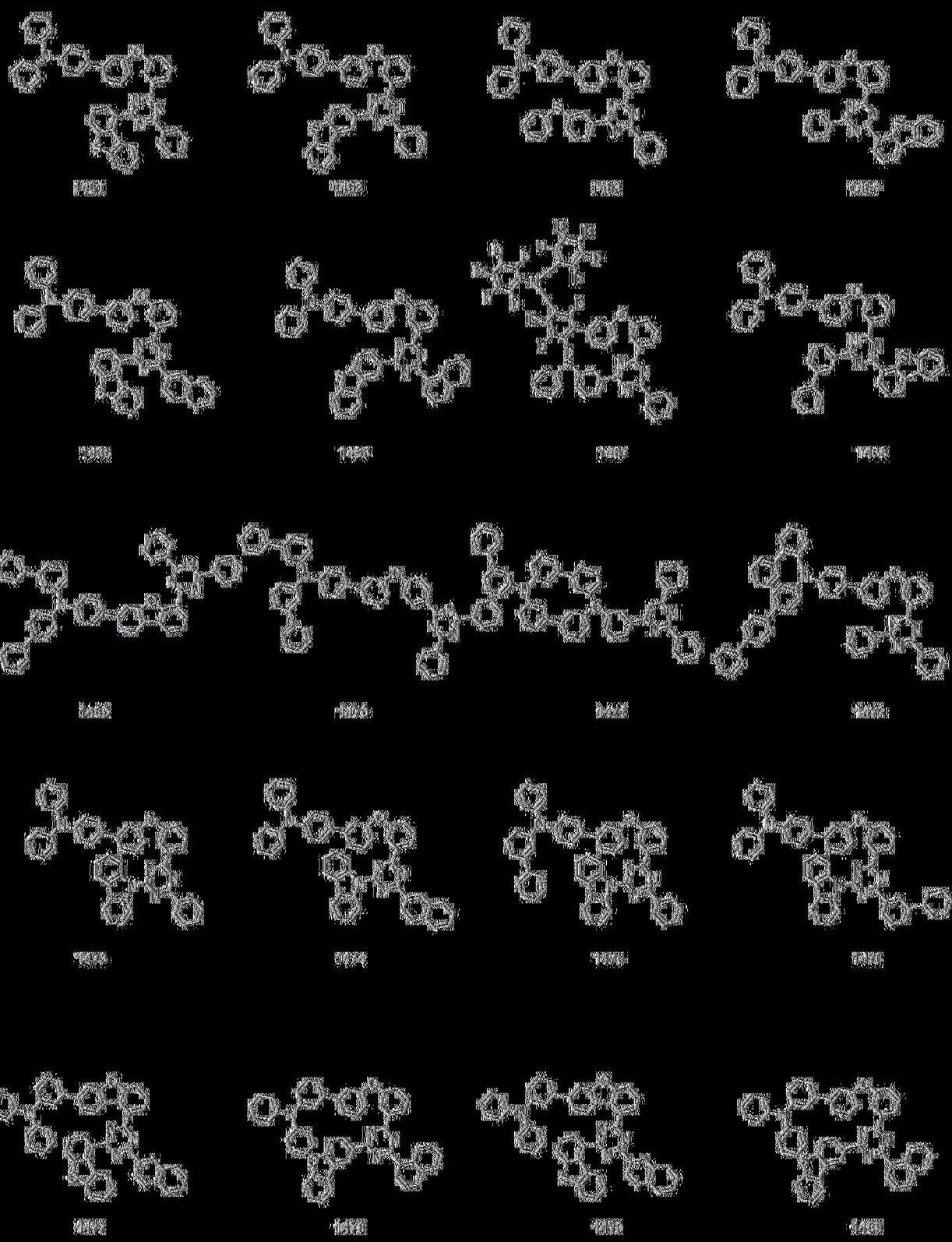


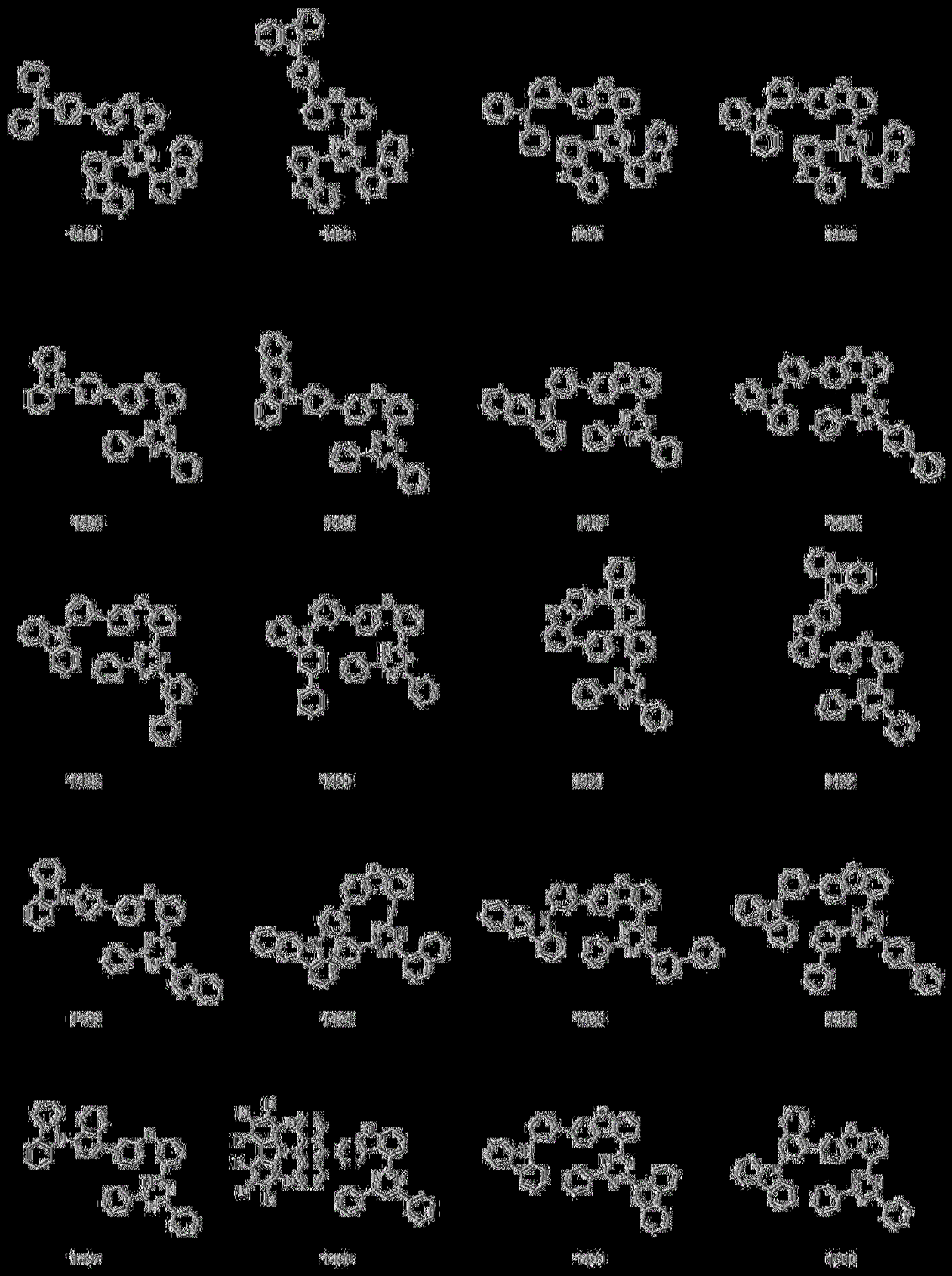


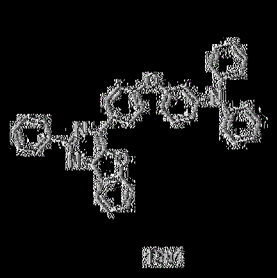


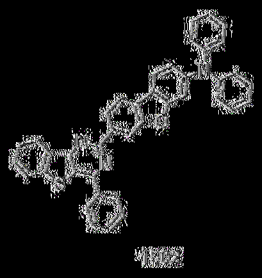


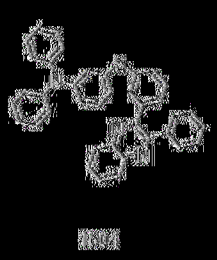


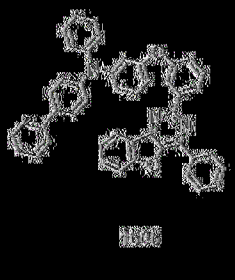


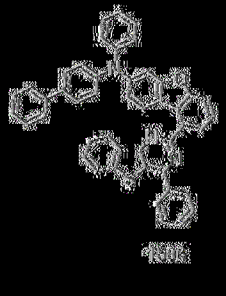


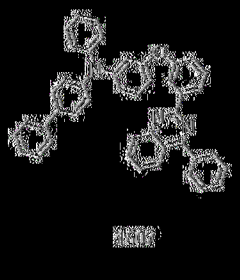


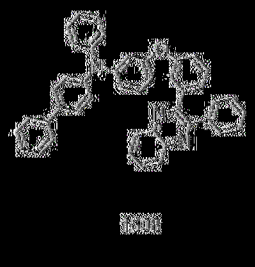


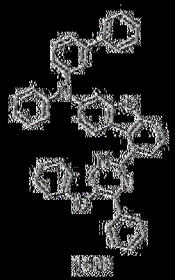


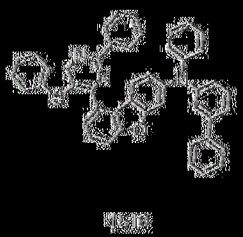


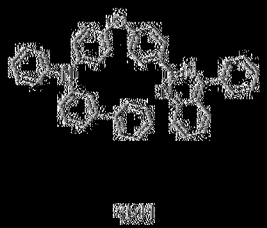


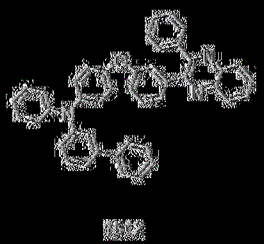


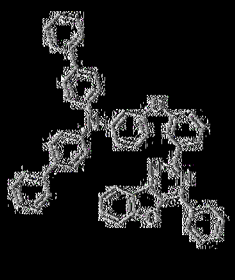


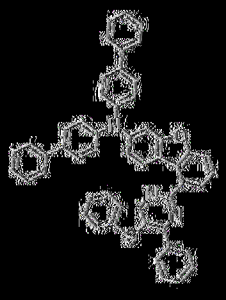


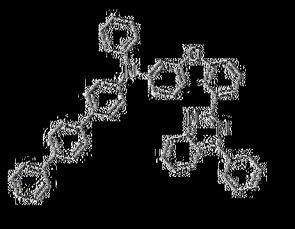


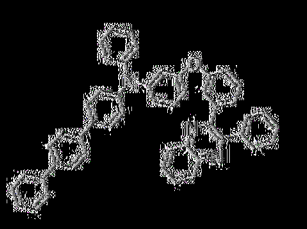


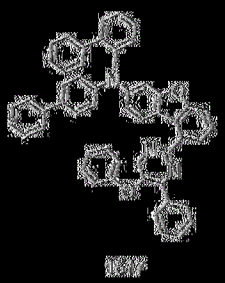


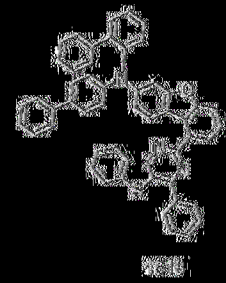


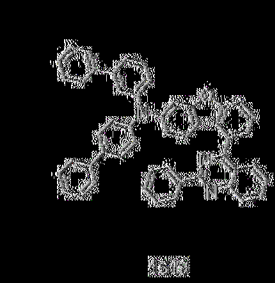


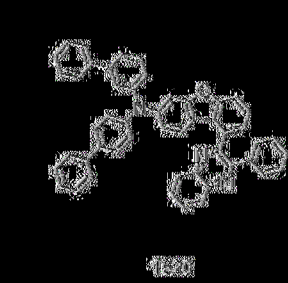


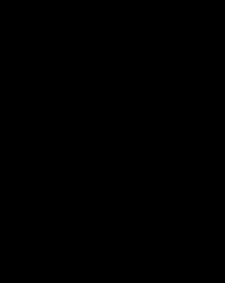


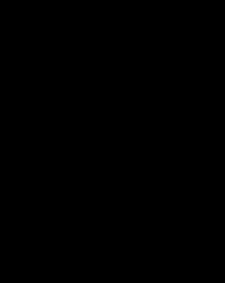


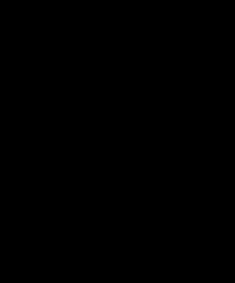


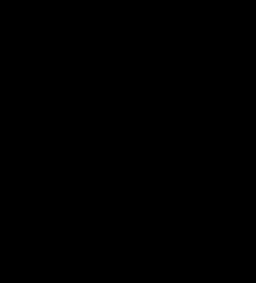


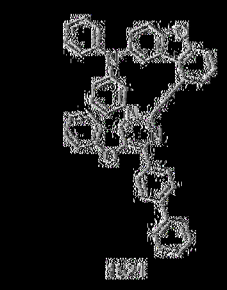


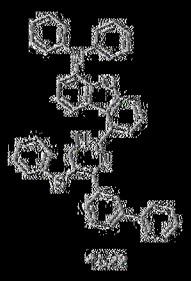


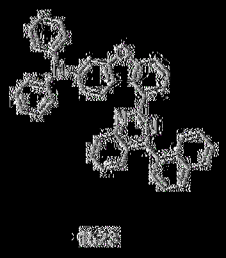


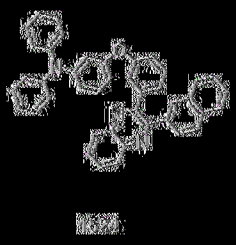


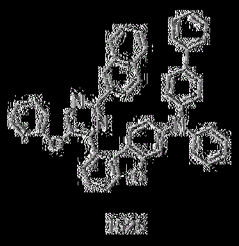


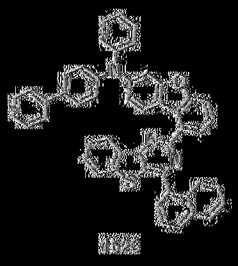


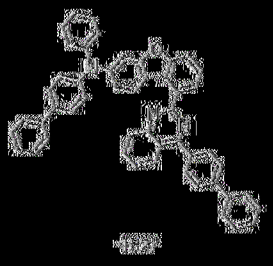


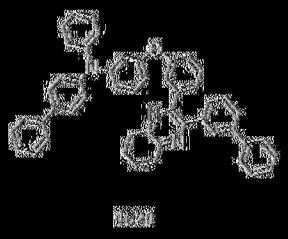


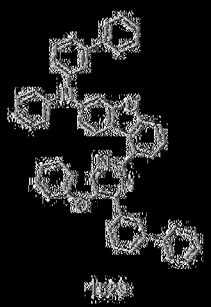


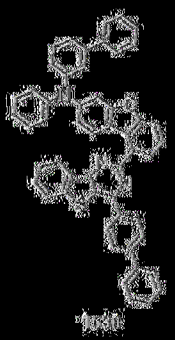


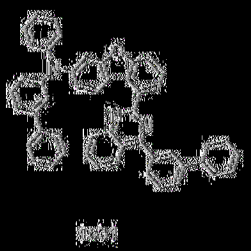


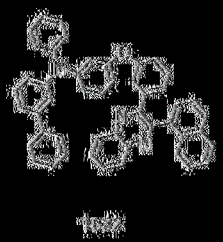


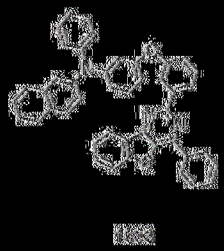


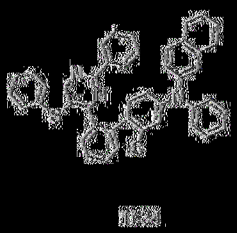


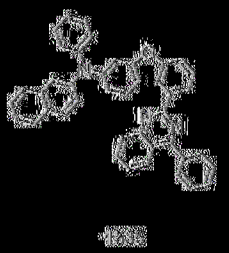


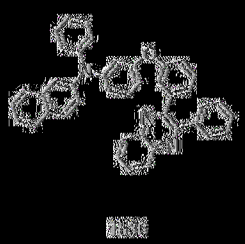


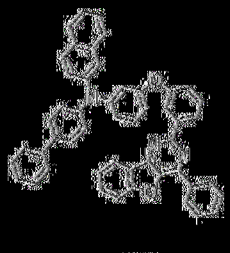


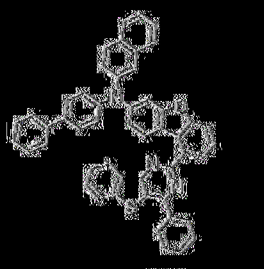


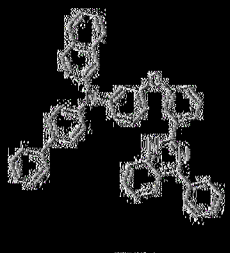


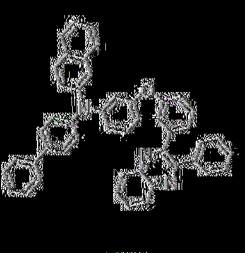


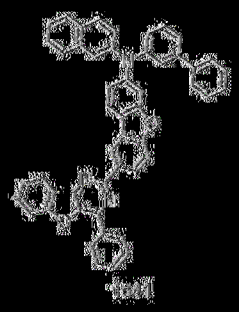


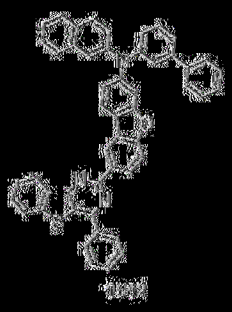


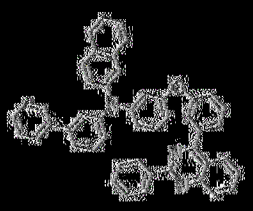


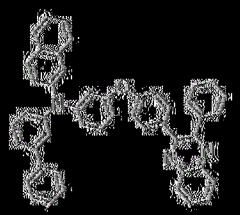


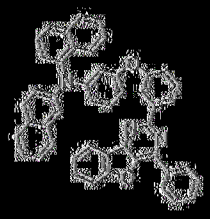


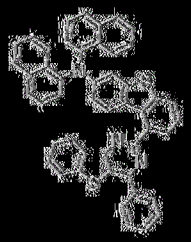


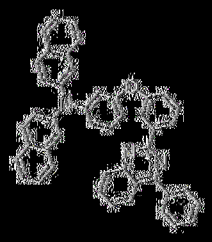


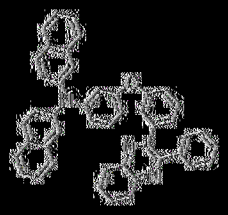


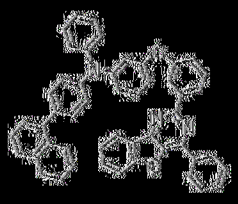


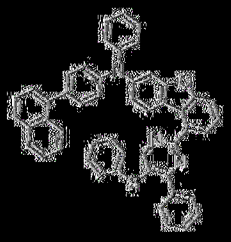


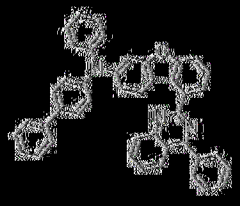


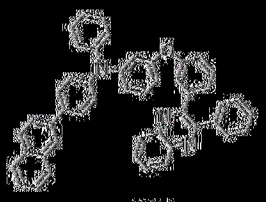


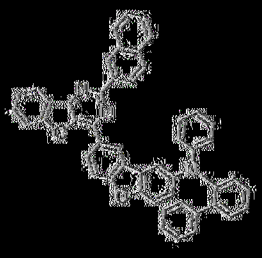


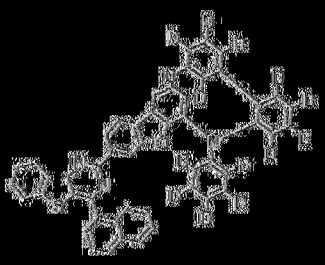


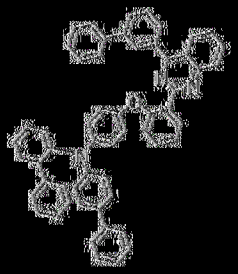


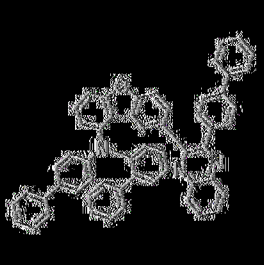


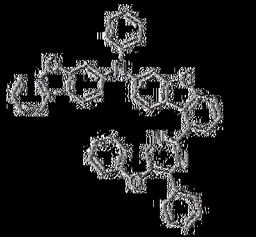


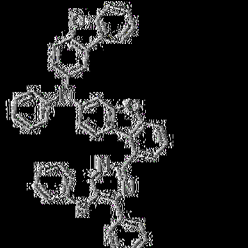


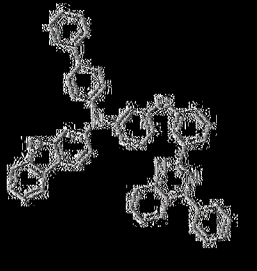


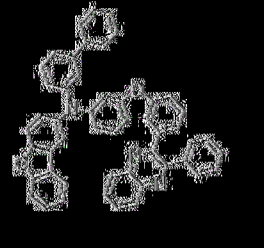


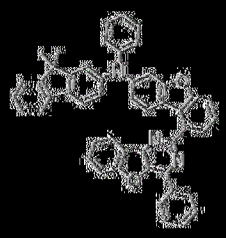


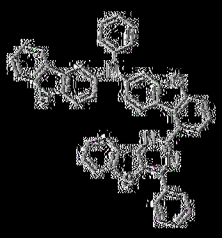


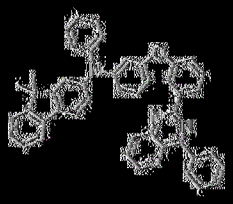


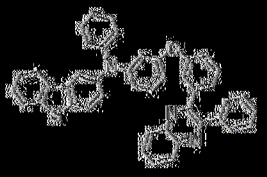


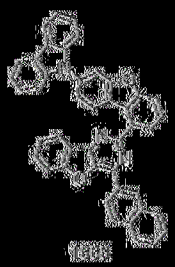


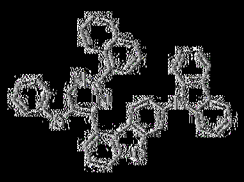


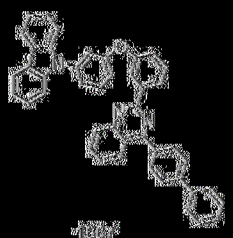


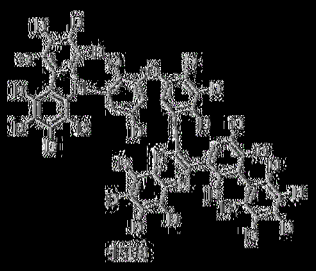


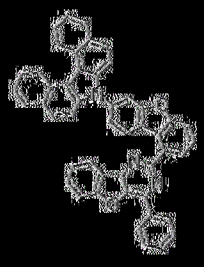


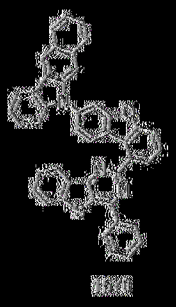


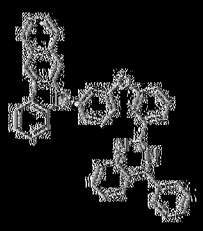


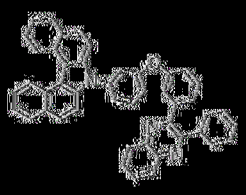


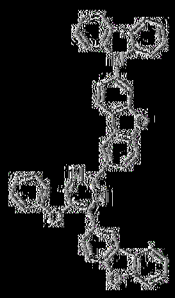


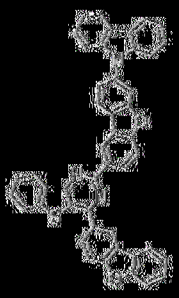


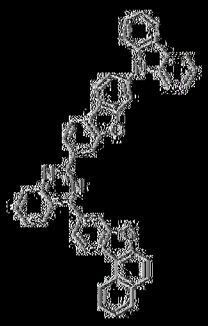


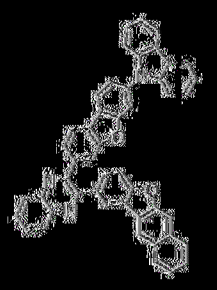


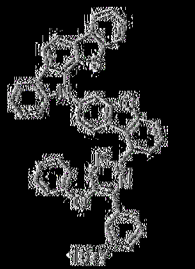


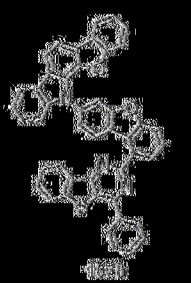


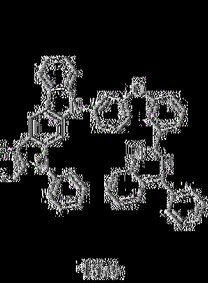


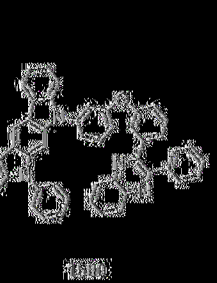


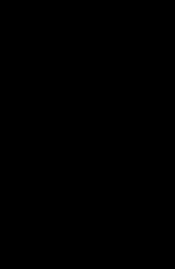


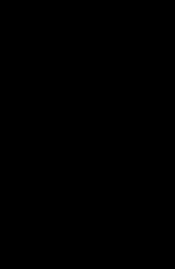


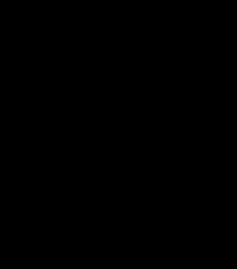


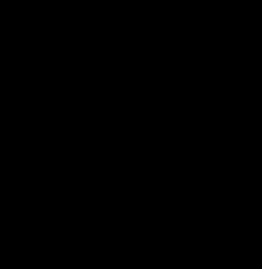


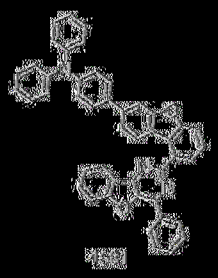


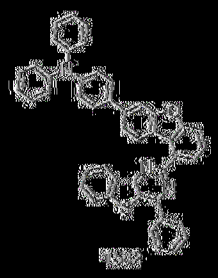


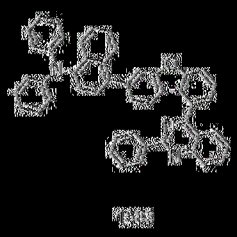


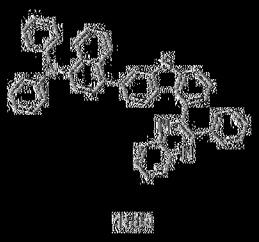


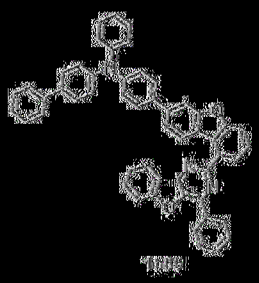


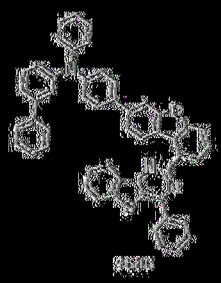


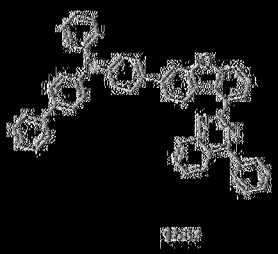


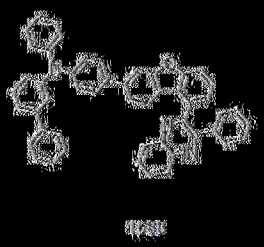


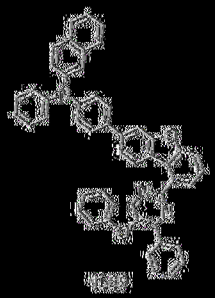


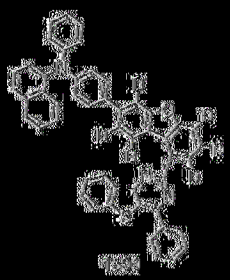


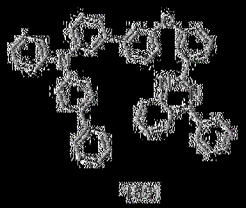


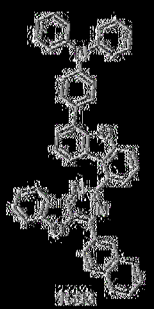


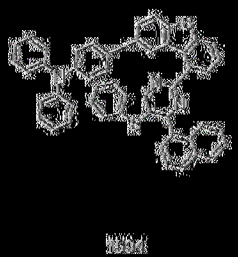


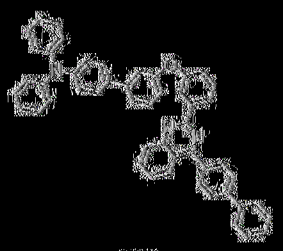


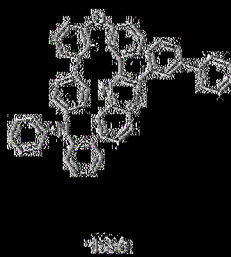


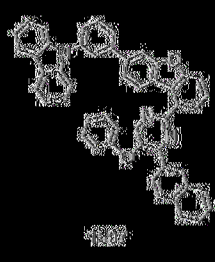


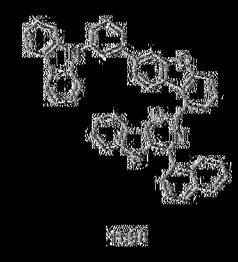


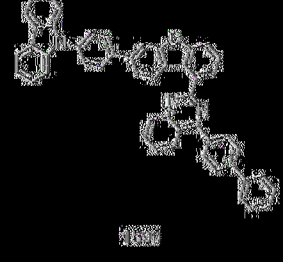


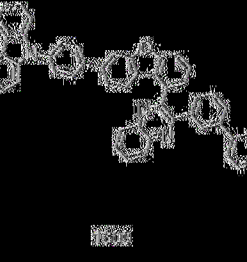


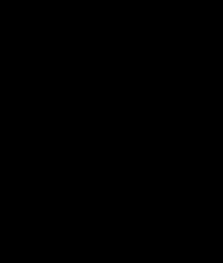


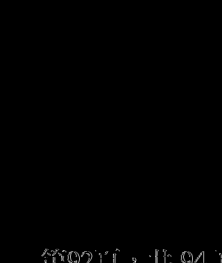


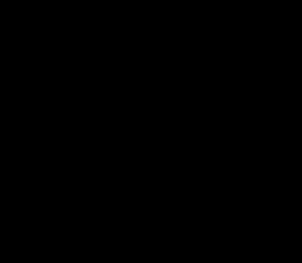












【請求項9】 如請求項1所述的有機發光裝置，其中，所述有機材料層包括發光層，且所述發光層包括由化學式1表示的雜環化合物和由化學式2表示的雜環化合物。

【請求項10】 如請求項9所述的有機發光裝置，其中，所述發光層可選地包括主體材料，且所述主體材料包括由化學式1表示的雜環化合物和由化學式2表示的雜環化合物。

【請求項11】 如請求項10所述的有機發光裝置，其中，所述主體材料可選地包括兩種或多於兩種主體材料，且在所述兩種或多於兩種主體材料中，由化學式1表示的雜環化合物為N型主體材料，而由化學式2表示的雜環化合物為P型主體材料。

【請求項12】 如請求項10所述的有機發光裝置，其中，所述主體材料可選地包括兩種或多於兩種主體材料，且所述兩種或多於兩種主體材料預先混合使用。

【請求項13】 一種用於如請求項1所述的有機發光裝置的有機材料層的組合物，其包含由化學式1表示的雜環化合物和由化學式2表示的化合物。

【請求項14】 如請求項13所述的組合物，其中在所述組合物中，由化學式1表示的雜環化合物與由化學式2表示的化合物的重量比為1:10至10:1。

【請求項15】 一種有機發光裝置的製造方法，包括：

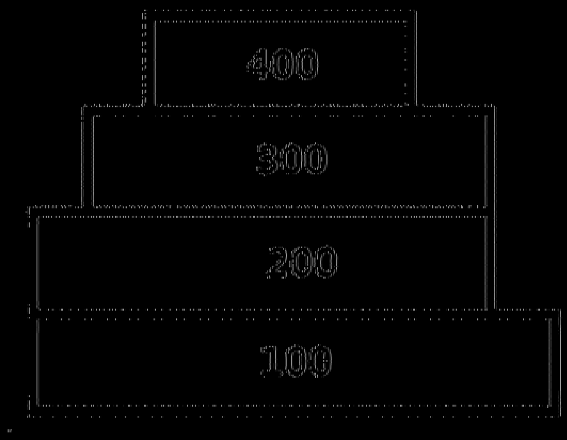
在基板上形成第一電極；

在所述第一電極上形成具有一層或多層的有機材料層；以及

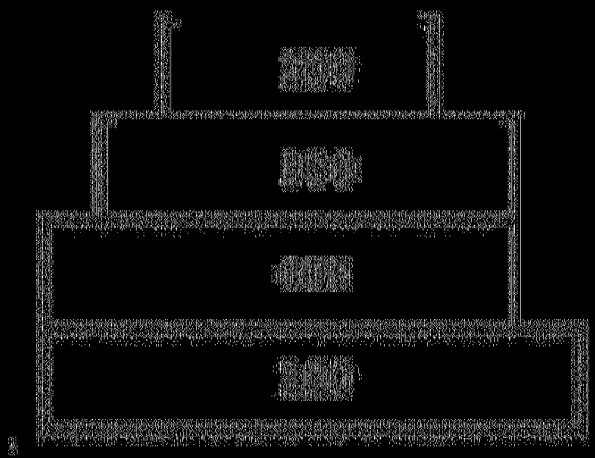
在所述有機材料層上形成第二電極，

其中形成所述有機材料層包括通過使用如請求項 13 所述的組合物形成具有一層或多層的有機材料層。

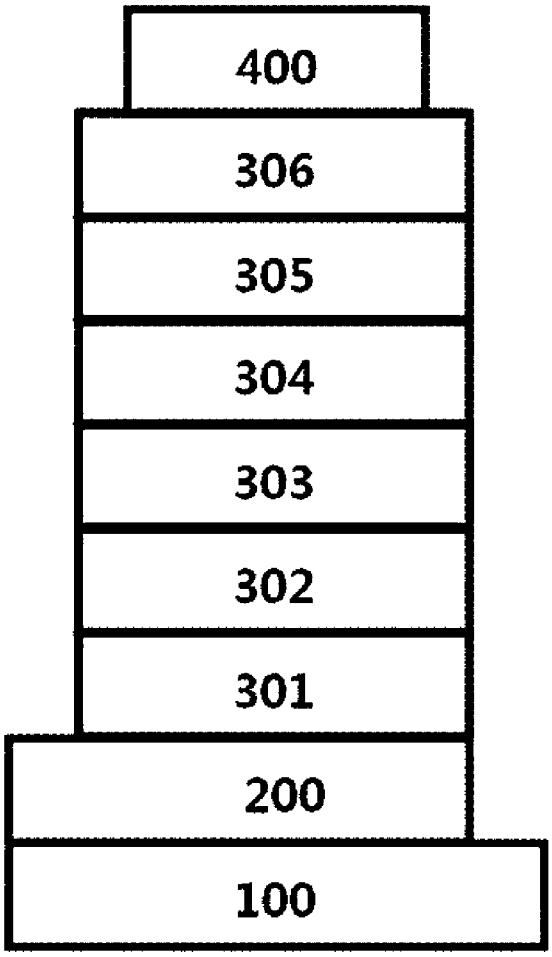
【發明圖式】



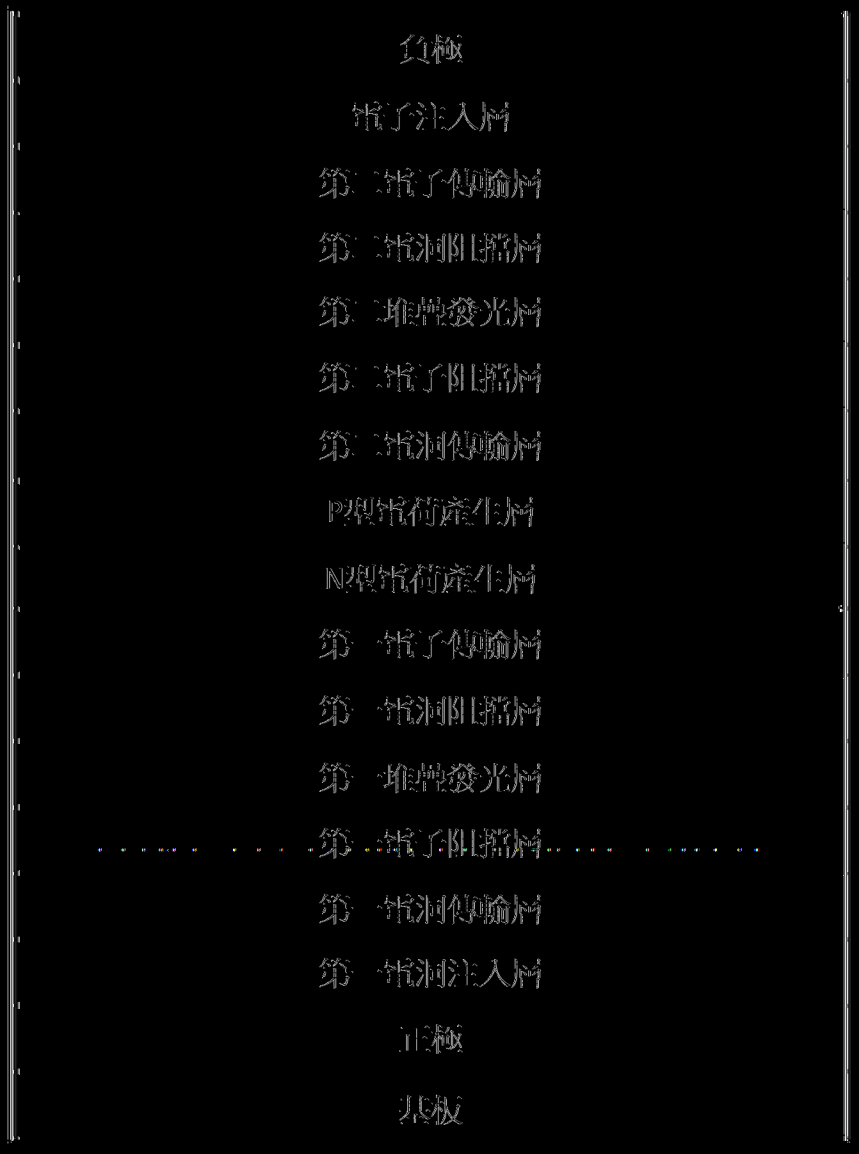
【圖1】



【圖2】



【圖3】


負極
電子注入層
第二電子傳輸層
第二電洞阻擋層
第二雙發光層
第二電子阻擋層
第二電洞傳輸層
P型電荷產生層
N型電荷產生層
第一電子傳輸層
第一電洞阻擋層
第一雙發光層
第一電子阻擋層
第一電洞傳輸層
第一電洞注入層
正極
基板

圖(4)