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**장훈**

전체 청구항 수 : 총 8 항

(54) 발명의 명칭 **유기 전계 발광 화합물 및 이를 포함하는 유기 전계 발광 소자**

## (57) 요 약

본원은 유기 전계 발광 화합물 및 이를 포함하는 유기 전계 발광 소자에 관한 것으로, 본원에 따른 유기 전계 발광 화합물을 포함함으로써 낮은 구동전압, 높은 발광효율 및/또는 개선된 수명 특성을 갖는 유기 전계 발광 소자를 제공할 수 있다.

(52) CPC특허분류
*C09K 2211/1029* (2013.01)
*C09K 2211/1044* (2013.01)
*C09K 2211/1048* (2013.01)
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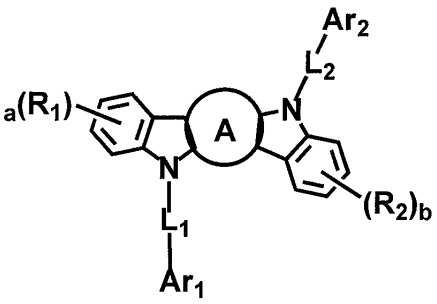
# 명 세 서

## 청구범위

### 청구항 1

하기 화학식 1로 표시되는 유기 전계 발광 화합물:



상기 화학식 1에서,

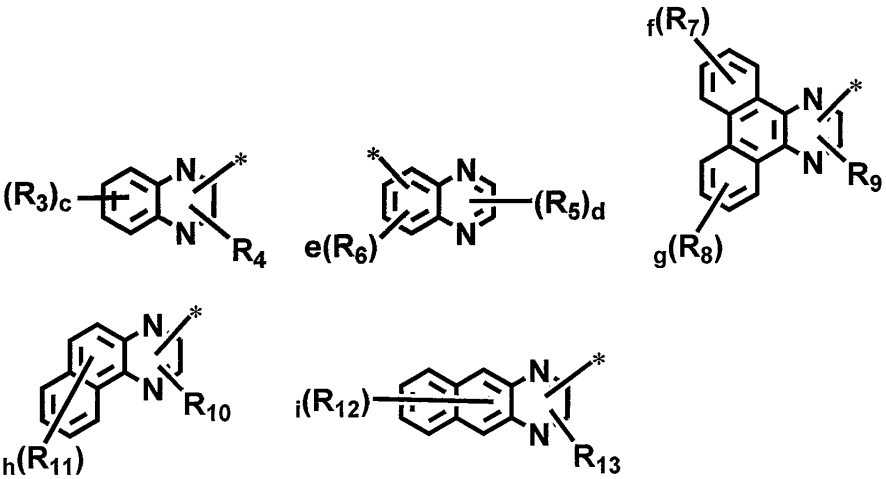
고리 A는 치환 또는 비치환된 나프탈렌이고,

$R_1$ 및 $R_2$은 각각 독립적으로 수소, 중수소, 할로겐, 시아노, 치환 또는 비치환된 (C1-C30)알킬, 치환 또는 비치환된 (C6-C30)아릴, 치환 또는 비치환된 (3-30원)헤테로아릴, 치환 또는 비치환된 (C3-C30)시클로알킬, 치환 또는 비치환된 (C1-C30)알콕시, 치환 또는 비치환된 트리(C1-C30)알킬실릴, 치환 또는 비치환된 디(C1-C30)알킬(C6-C30)아릴실릴, 치환 또는 비치환된 (C1-C30)알킬디(C6-C30)아릴실릴, 치환 또는 비치환된 트리(C6-C30)아릴실릴, 치환 또는 비치환된 모노- 또는 디- (C1-C30)알킬아미노, 치환 또는 비치환된 모노- 또는 디- (C6-C30)아릴아미노, 또는 치환 또는 비치환된 (C1-C30)알킬(C6-30)아릴아미노이거나, 둘 이상의 $R_1$은 서로 연결되어 고리를 형성하거나, 둘 이상의 $R_2$는 서로 연결되어 고리를 형성할 수 있고,

$L_1$ 및 $L_2$은 각각 독립적으로 단일결합, 치환 또는 비치환된 (C6-C30)아릴렌, 또는 치환 또는 비치환된 (3-30원)헤테로아릴렌이며,

$Ar_1$은 수소, 중수소, 할로겐, 시아노, 치환 또는 비치환된 (C1-C30)알킬, 치환 또는 비치환된 (C6-C30)아릴, 또는 치환 또는 비치환된 (3-30원)헤테로아릴이고,

$Ar_2$은 하기 화학식에서 선택되는 어느 하나이며,



상기 식에서,

$R_3$ 내지 $R_{13}$은 각각 독립적으로 수소, 중수소, 할로겐, 시아노, 치환 또는 비치환된 (C1-C30)알킬, 치환 또는 비

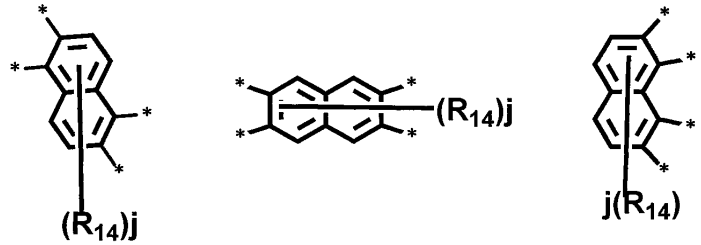
치환된 (C6-C30)아릴, 치환 또는 비치환된 (3-30원)헤테로아릴, 치환 또는 비치환된 (C3-C30)시클로알킬, 치환 또는 비치환된 (C1-C30)알콕시, 치환 또는 비치환된 트리(C1-C30)알킬실릴, 치환 또는 비치환된 디(C1-C30)알킬(C6-C30)아릴실릴, 치환 또는 비치환된 (C1-C30)알킬디(C6-C30)아릴실릴, 치환 또는 비치환된 트리(C6-C30)아릴실릴, 치환 또는 비치환된 모노- 또는 디- (C1-C30)알킬아미노, 치환 또는 비치환된 모노- 또는 디- (C6-C30)아릴아미노, 또는 치환 또는 비치환된 (C1-C30)알킬(C6-30)아릴아미노이며,

a, b, c, f 및 g는 4이고, d는 2이며, e는 3이고, h 및 i는 6이며, 각각의 $R_1$, 각각의 $R_2$, 각각의 $R_3$, 각각의 $R_5$, 각각의 $R_6$, 각각의 $R_7$, 각각의 $R_8$, 각각의 $R_{11}$, 및 각각의 $R_{12}$는 서로 동일하거나 상이할 수 있고,

*은 $L_2$와의 연결 부위를 나타낸다.

**청구항 2**

제1항에 있어서, 고리 A 는 하기 식 중 어느 하나로 표시되는 것인, 유기 전계 발광 화합물:




상기 식에서,

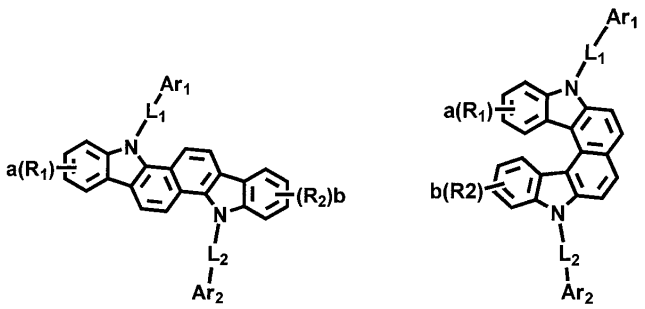
j는 4이고,

$R_{14}$는 각각 독립적으로 수소, 중수소, 할로겐, 시아노, 치환 또는 비치환된 (C1-C30)알킬, 치환 또는 비치환된 (C6-C30)아릴, 또는 치환 또는 비치환된 (3-30원)헤테로아릴이고, 각각의 $R_{14}$은 서로 동일하거나 상이할 수 있다.

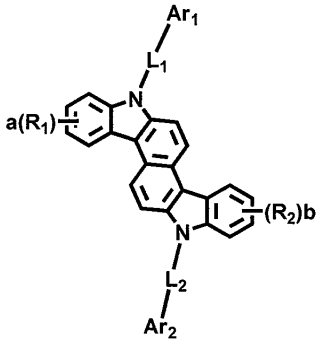
**청구항 3**

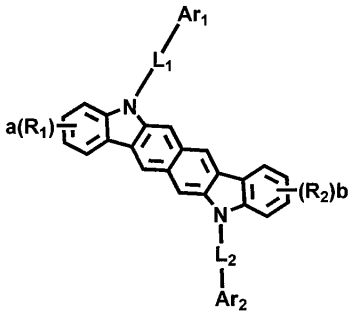
제1항에 있어서, 상기 화학식 1은 하기 화학식 2-1 내지 2-4 중 어느 하나로 표시되는 것인, 유기 전계 발광 화합물:

[화학식 2-1] [화학식 2-2]



[화학식 2-3] [화학식 2-4]



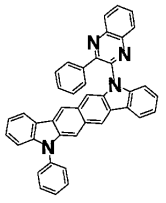

상기 화학식 2-1 내지 2-4에서, $L_1$, $L_2$, $Ar_1$, $Ar_2$, $R_1$, $R_2$, a 및 b는 청구항 1에서의 정의와 동일하다.

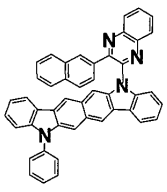
**청구항 4**

제1항에 있어서, 상기 고리 A, $L_1$, $L_2$, $Ar_1$, 및 $R_1$ 내지 $R_{13}$에서 치환된 나프탈렌, 치환된 (C1-C30)알킬, 치환된 (C6-C30)아릴(렌), 치환된 (3-30원)헤테로아릴(렌), 치환된 (C3-C30)시클로알킬, 치환된 (C1-C30)알콕시, 치환된 트리(C1-C30)알킬실릴, 치환된 디(C1-C30)알킬(C6-C30)아릴실릴, 치환된 (C1-C30)알킬디(C6-C30)아릴실릴, 치환된 트리(C6-C30)아릴실릴, 치환된 모노- 또는 디- (C1-C30)알킬아미노, 치환된 모노- 또는 디- (C6-C30)아릴아미노, 및 치환된 (C1-C30)알킬(C6-C30)아릴아미노의 치환기는 각각 독립적으로 중수소, 할로겐, 시아노, 카르복실, 니트로, 히드록시, (C1-C30)알킬, 할로(C1-C30)알킬, (C2-C30)알케닐, (C2-C30)알키닐, (C1-C30)알콕시, (C1-C30)알킬티오, (C3-C30)시클로알킬, (C3-C30)시클로알케닐, (3-7원)헤테로시클로알킬, (C6-C30)아릴옥시, (C6-C30)아릴티오, (C6-C30)아릴로 치환 또는 비치환된 (3-30 원)헤테로아릴, (3-30원)헤테로아릴로 치환 또는 비치환된 (C6-C30)아릴, 트리(C1-C30)알킬실릴, 트리(C6-C30)아릴실릴, 디(C1-C30)알킬(C6-C30)아릴실릴, (C1-C30)알킬디(C6-C30)아릴실릴, 아미노, 모노- 또는 디- (C1-C30)알킬아미노, (C1-C30)알킬로 치환 또는 비치환된 모노- 또는 디- (C6-C30)아릴아미노, (C1-C30)알킬(C6-C30)아릴아미노, (C1-C30)알킬카보닐, (C1-C30)알콕시카보닐, (C6-C30)아릴카보닐, 디(C6-C30)아릴보로닐, 디(C1-C30)알킬보로닐, (C1-C30)알킬(C6-C30)아릴보로닐, (C6-C30)아르(C1-C30)알킬, 및 (C1-C30)알킬(C6-C30)아릴로 이루어진 군으로부터 선택되는 하나 이상인, 유기 전계 발광 화합물.

**청구항 5**

제1항에 있어서, 상기 화학식 1로 표시되는 화합물은 하기 화합물들로부터 선택되는 어느 하나인, 유기 전계 발광 화합물.


H-1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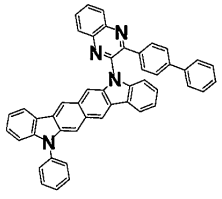
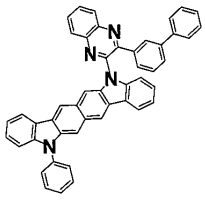
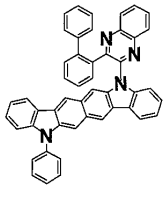
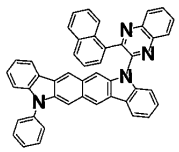
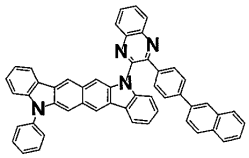
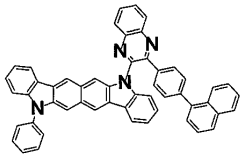

H-3

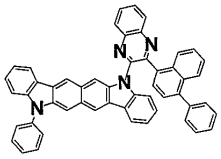

H-4

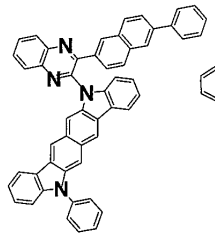

H-5


H-6

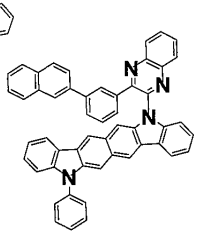

H-7


H-8

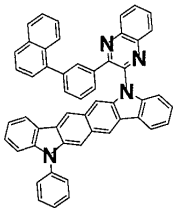

H-9



H-10



H-11



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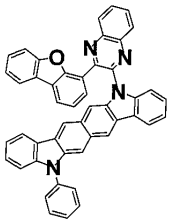

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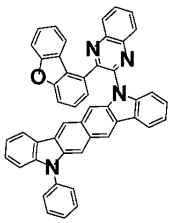
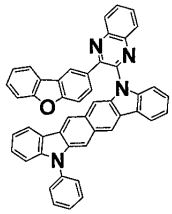
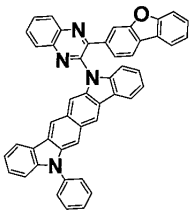


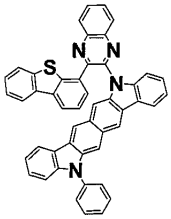
H-14



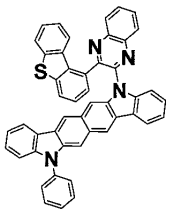
H-15



H-16



H-17



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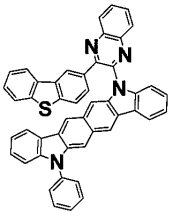

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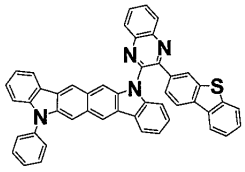

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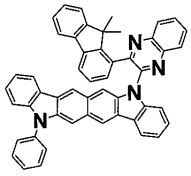

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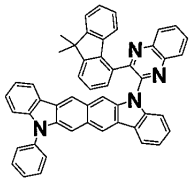

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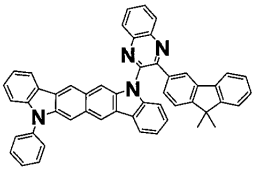

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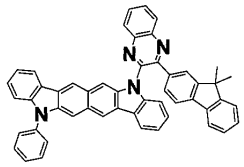

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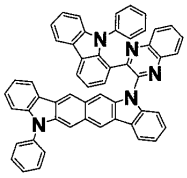

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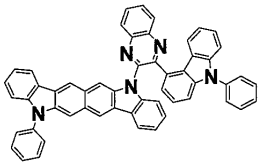

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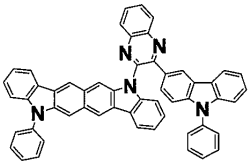

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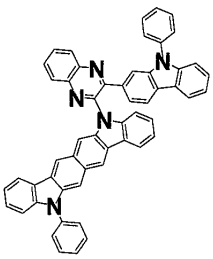

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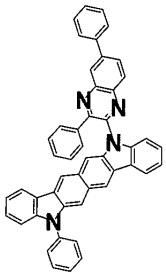

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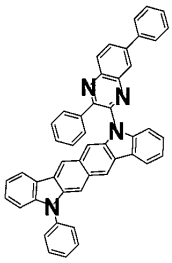

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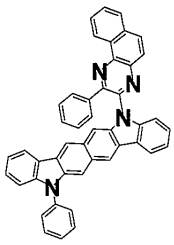

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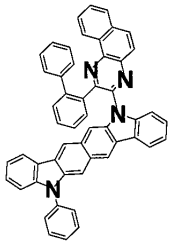

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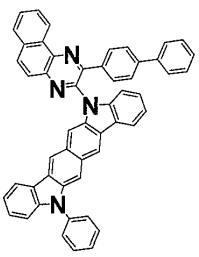

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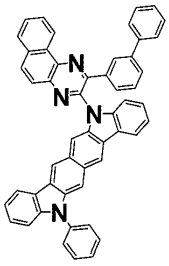

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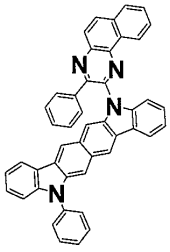

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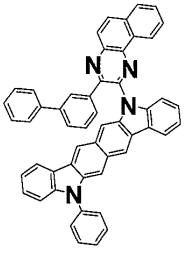

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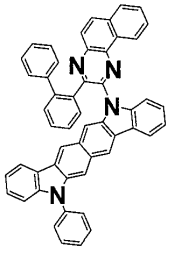

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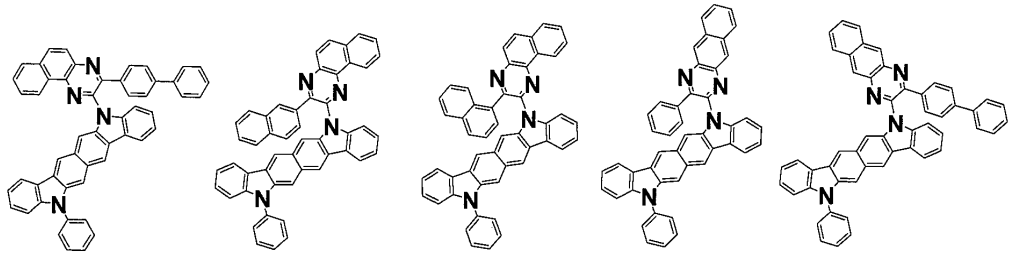

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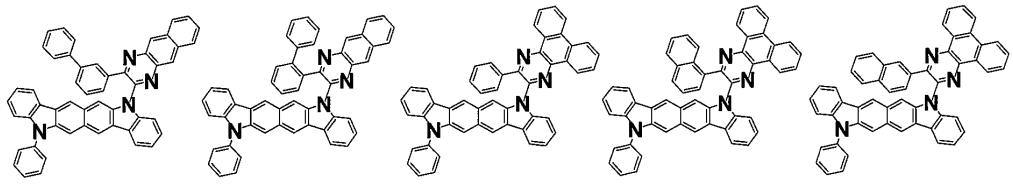

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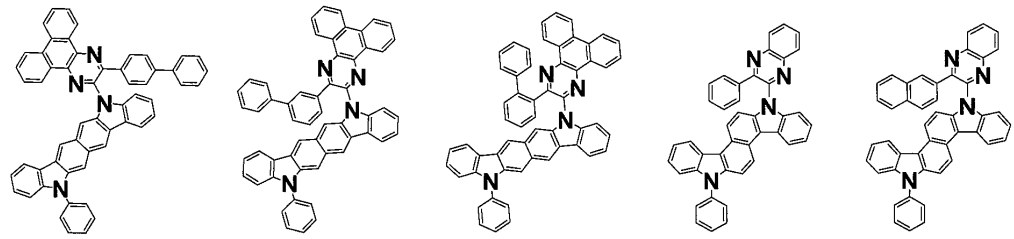

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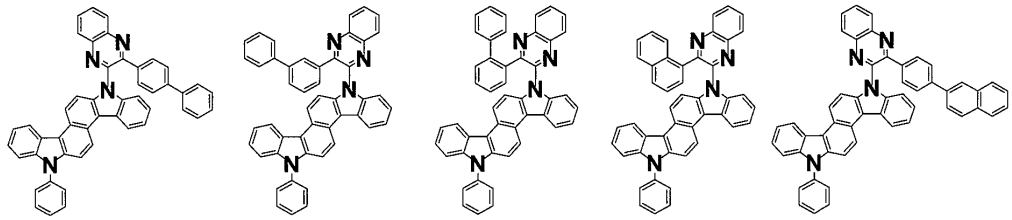

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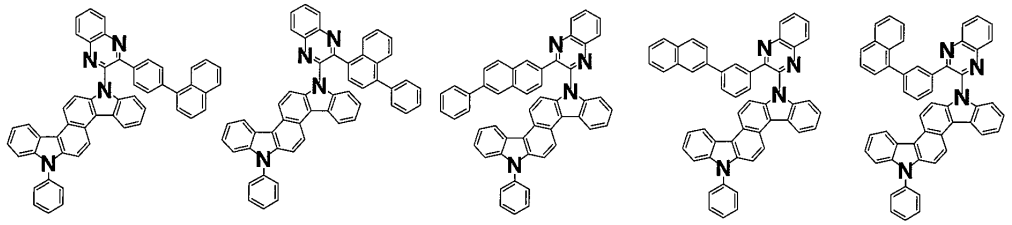

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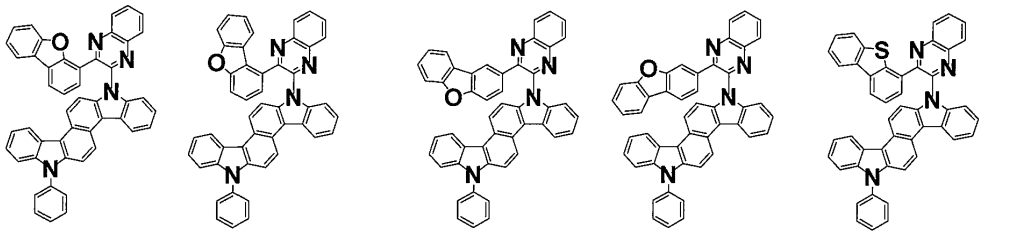

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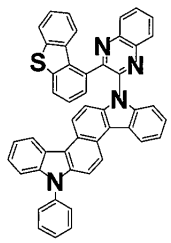
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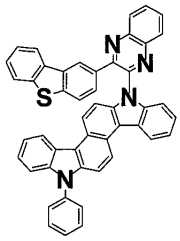
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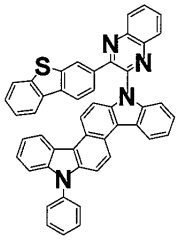
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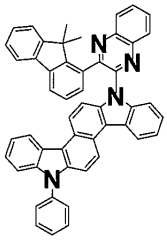
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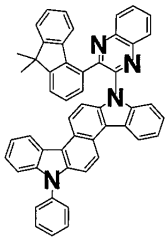
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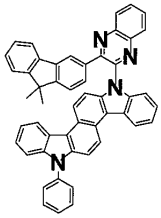
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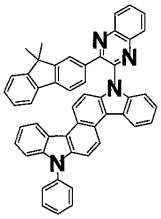
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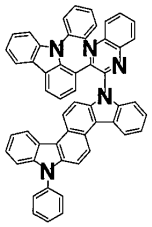
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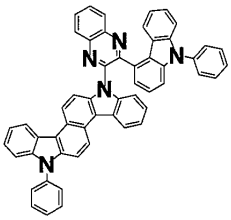
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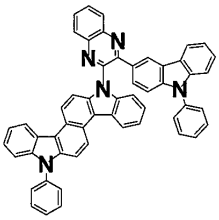
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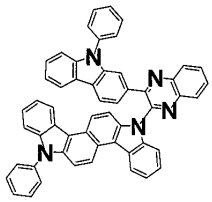
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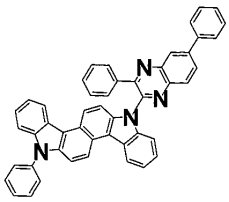
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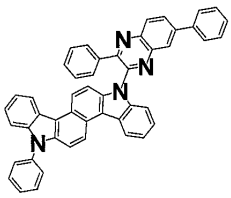
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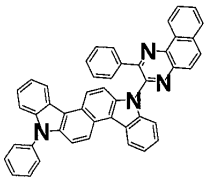
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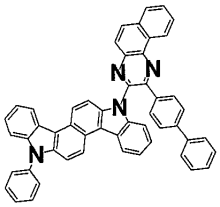
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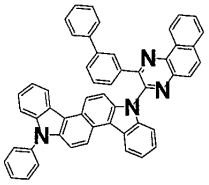
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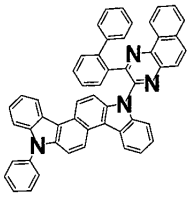
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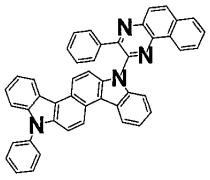
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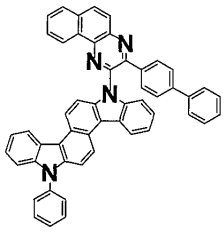
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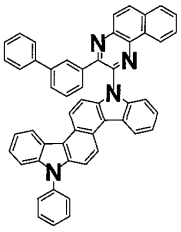
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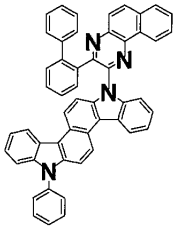
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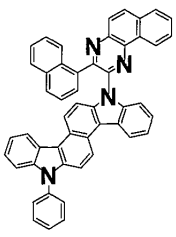
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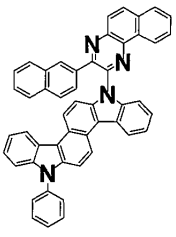
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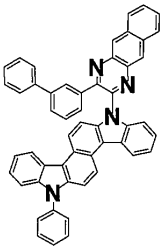
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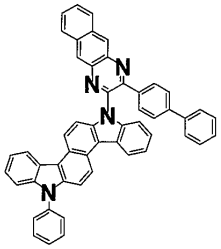
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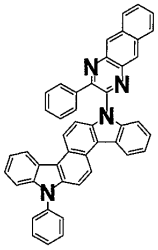
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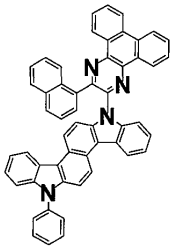
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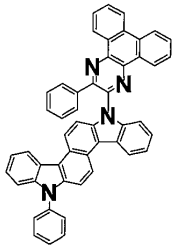
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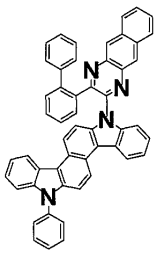
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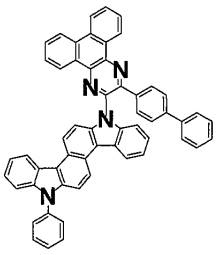
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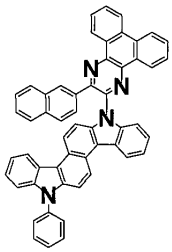
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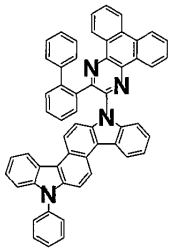
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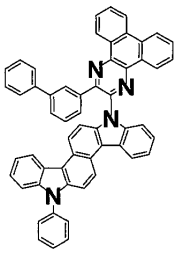
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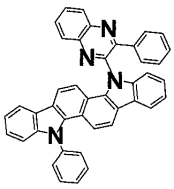
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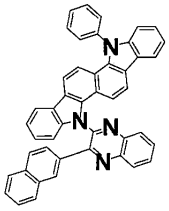
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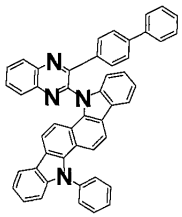
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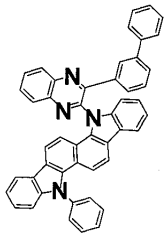
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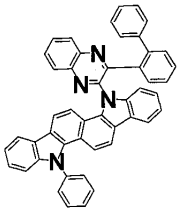
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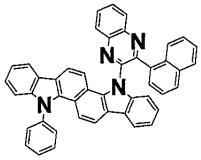
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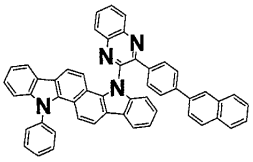
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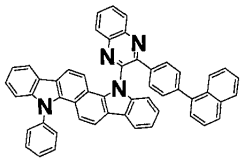
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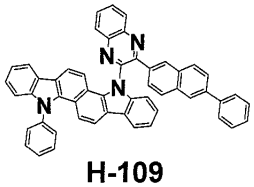
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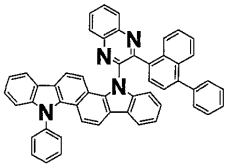
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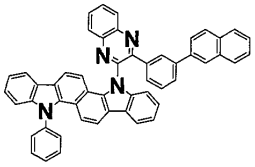
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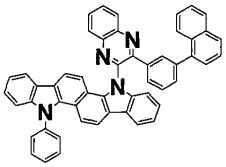
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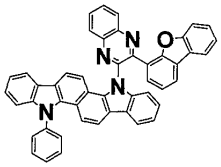
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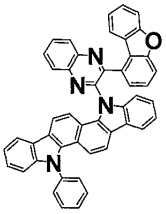
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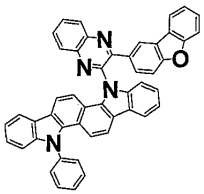
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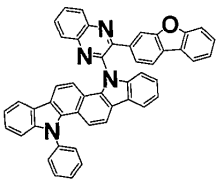
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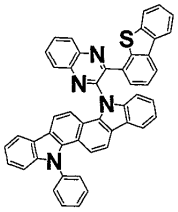
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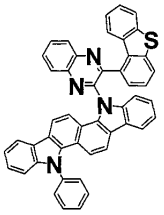
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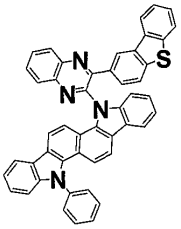
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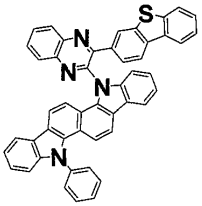
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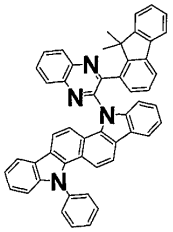
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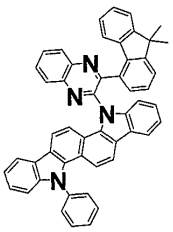
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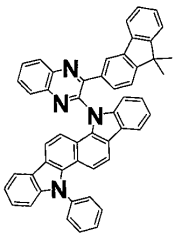
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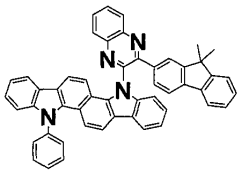

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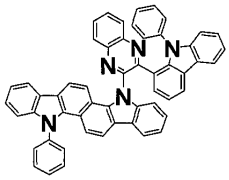

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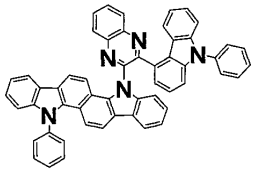

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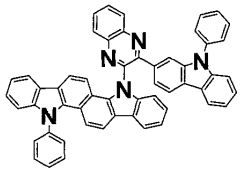

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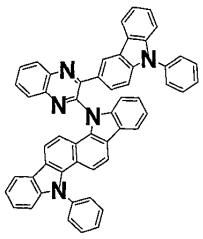

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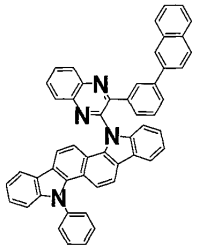

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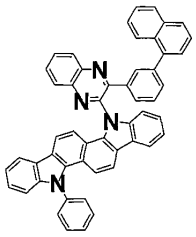

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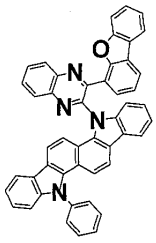

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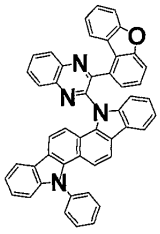

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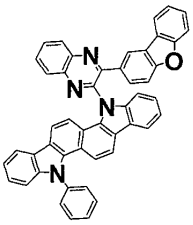

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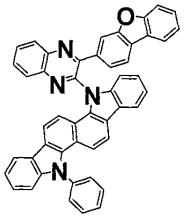

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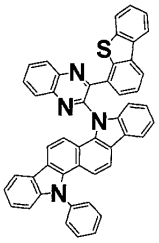

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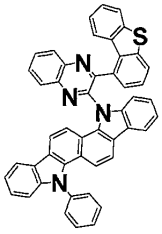

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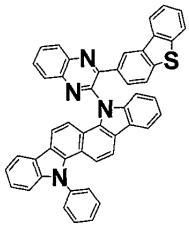

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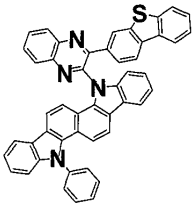

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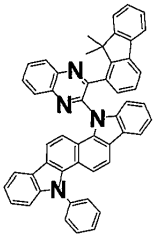

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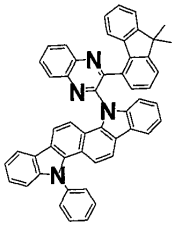

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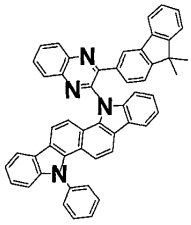

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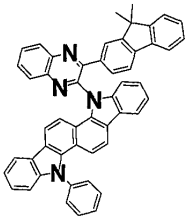

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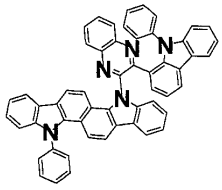

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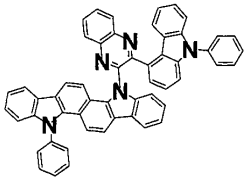

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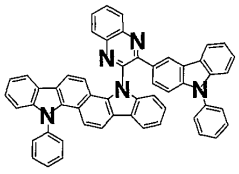

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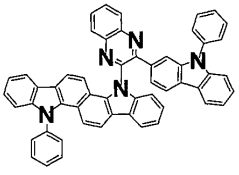

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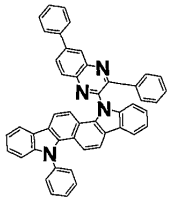

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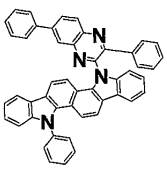

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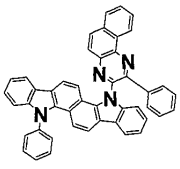

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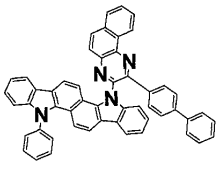

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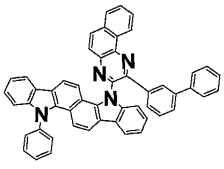

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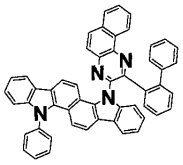
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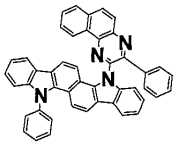
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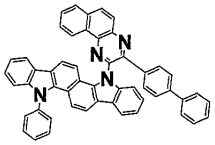
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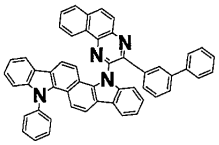
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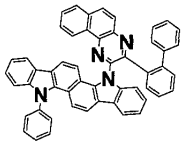
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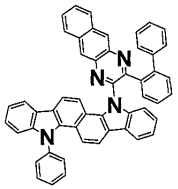
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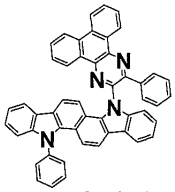
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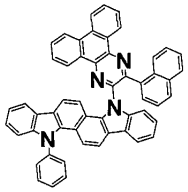
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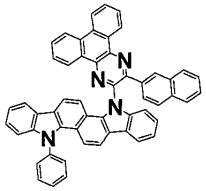
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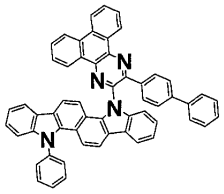
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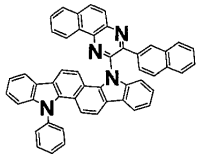
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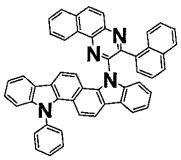
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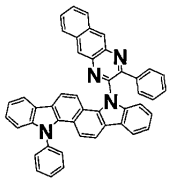
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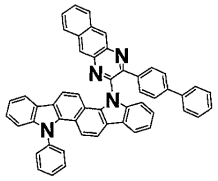
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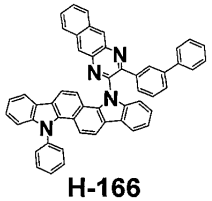
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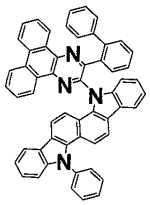
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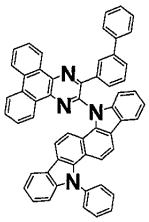
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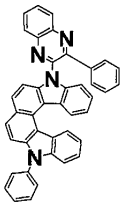
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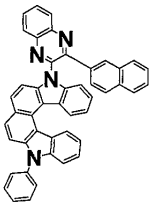
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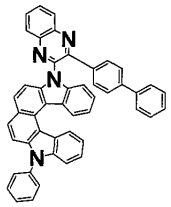
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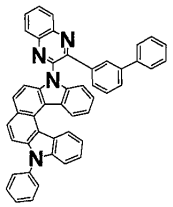
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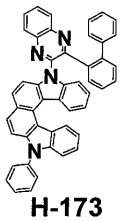
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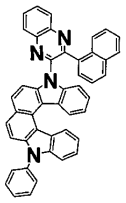
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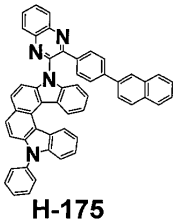
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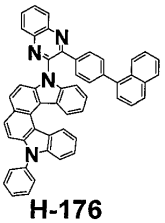
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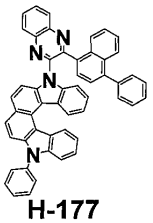
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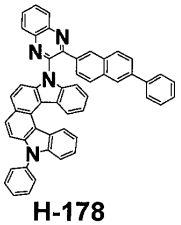
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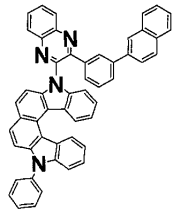
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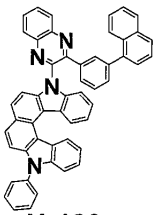
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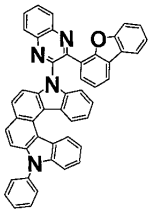
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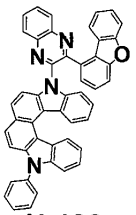
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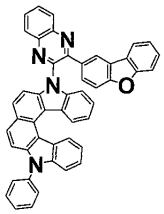
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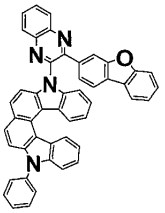
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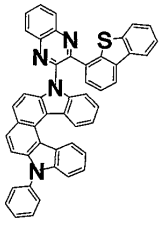
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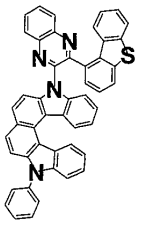
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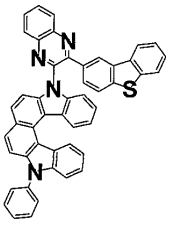
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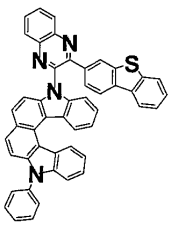
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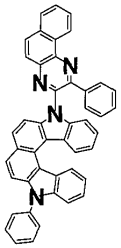
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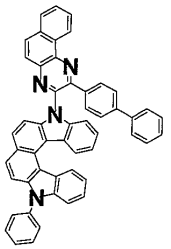
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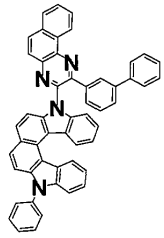
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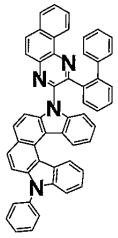
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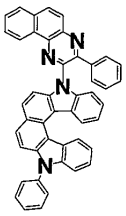
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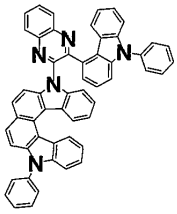
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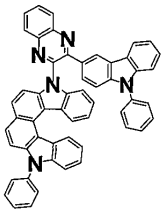
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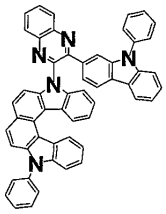
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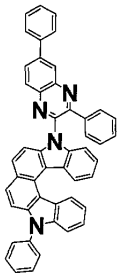
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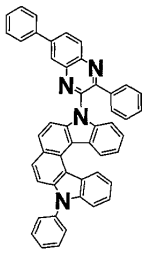
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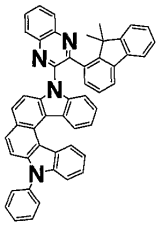
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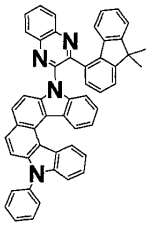
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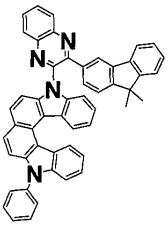
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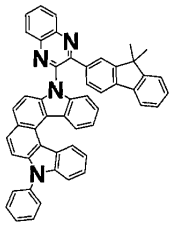
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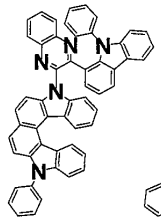
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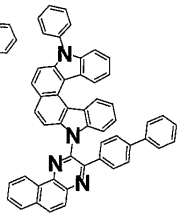
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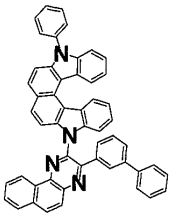
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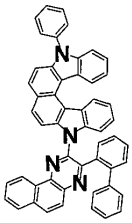
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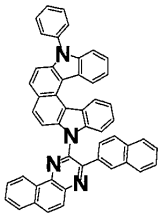
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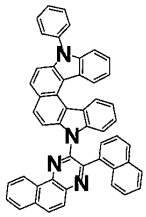
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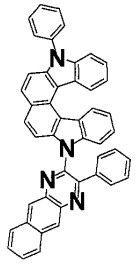
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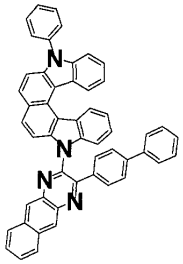
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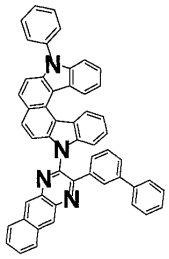
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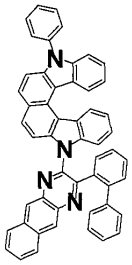
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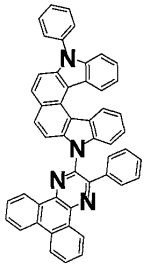
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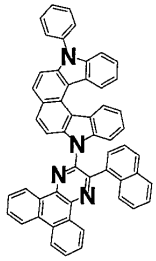
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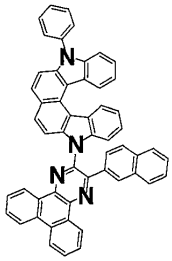
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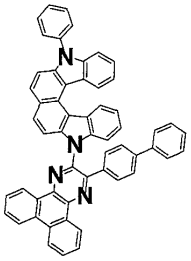
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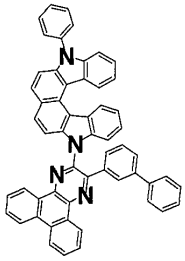
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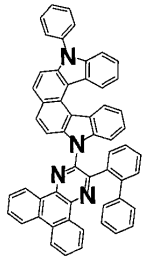
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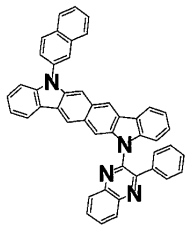
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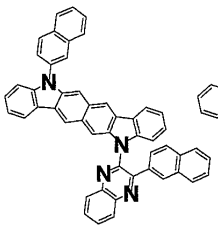
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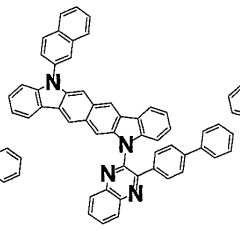
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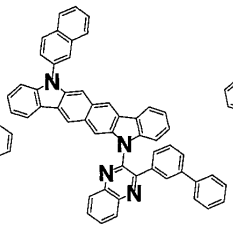
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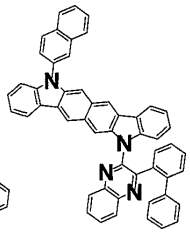
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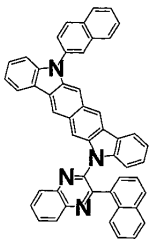

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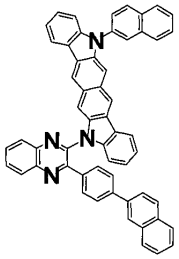

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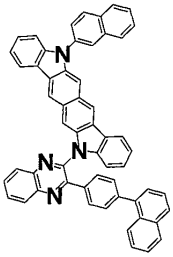

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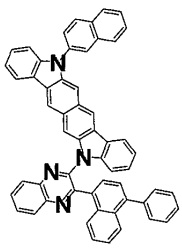

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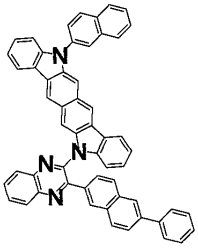

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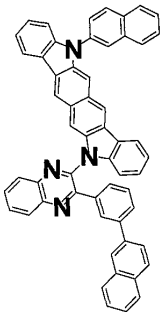

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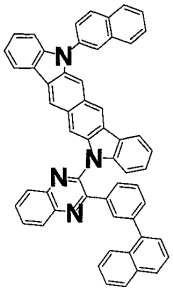

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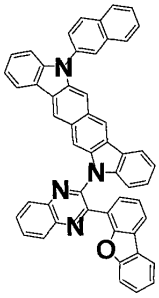

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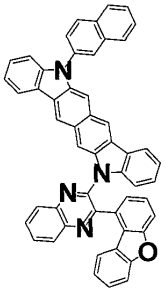

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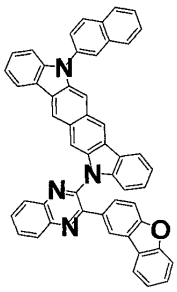

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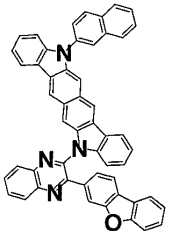

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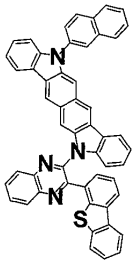

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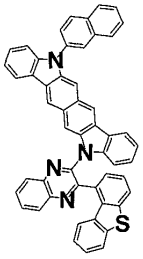

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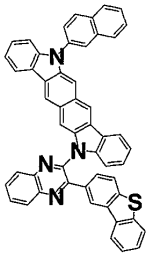

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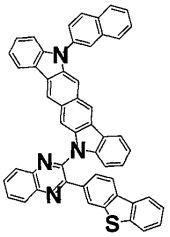

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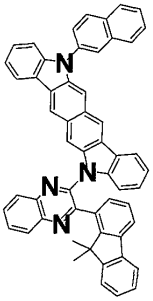

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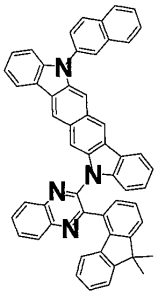

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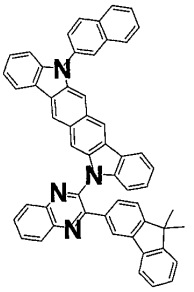

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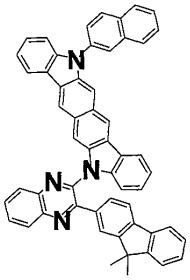

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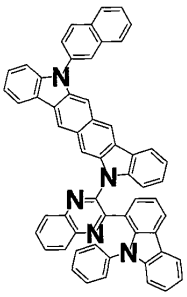

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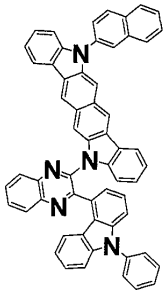

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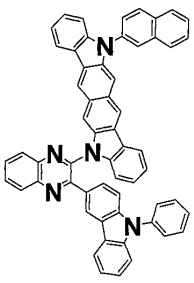

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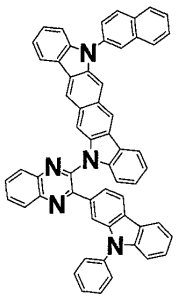

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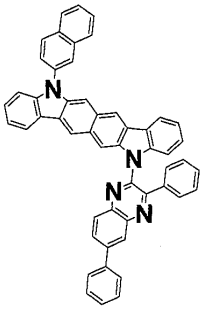

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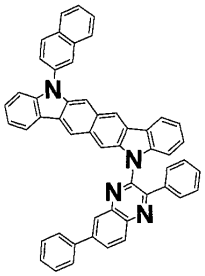

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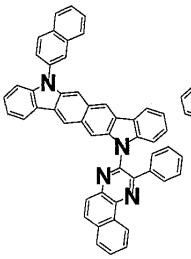
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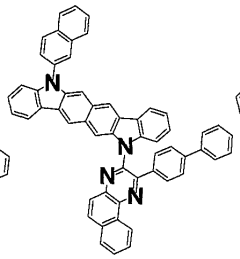
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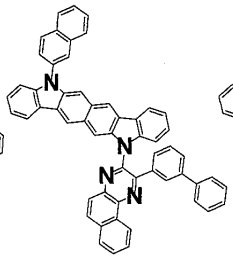
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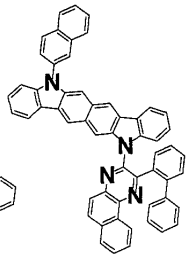
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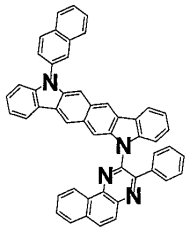
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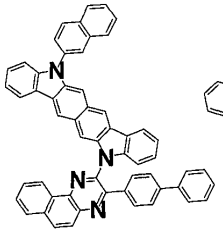
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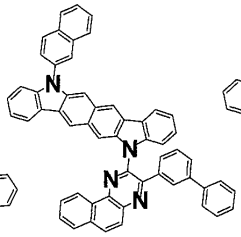
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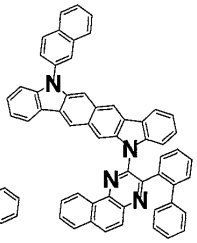
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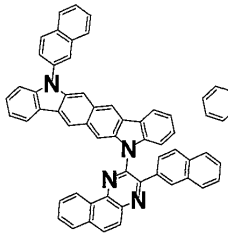
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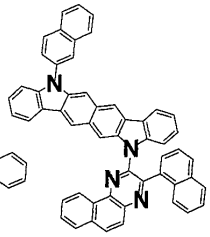
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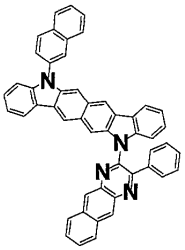
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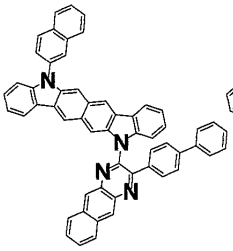
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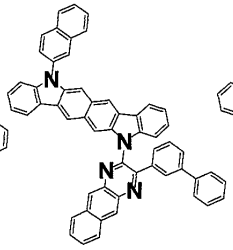
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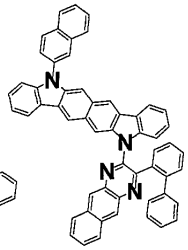
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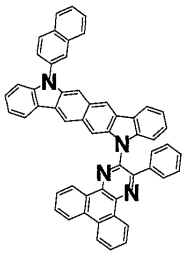
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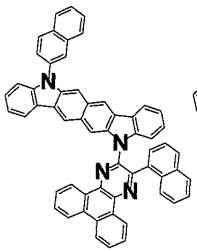
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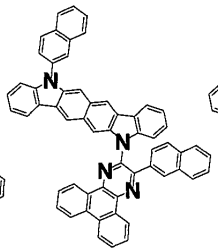
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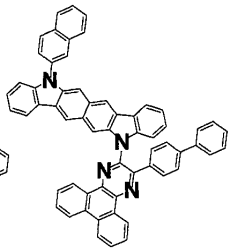
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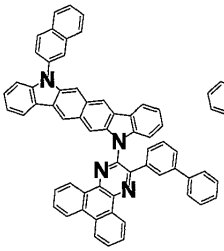
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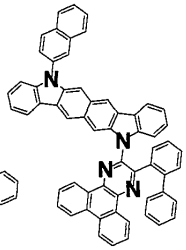
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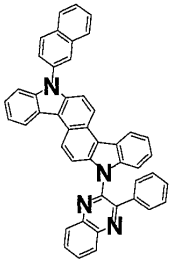
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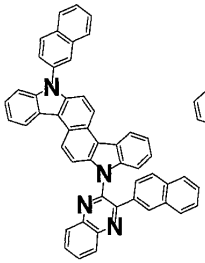
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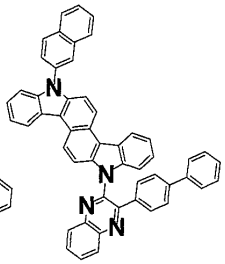
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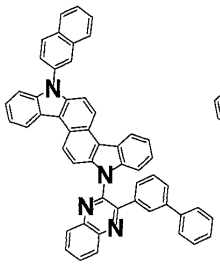
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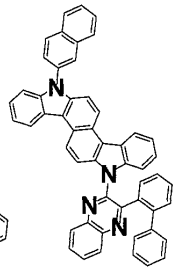
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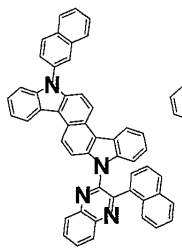
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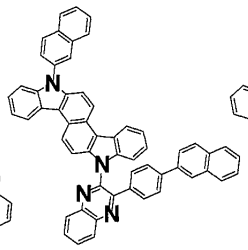
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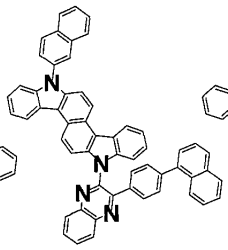
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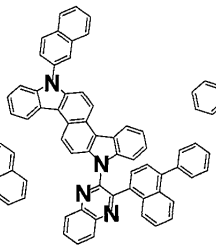
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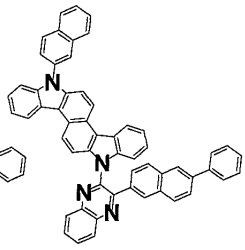
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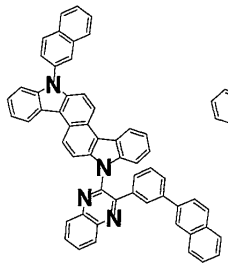
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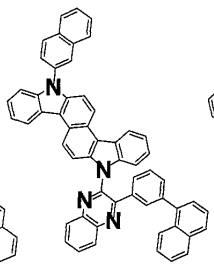
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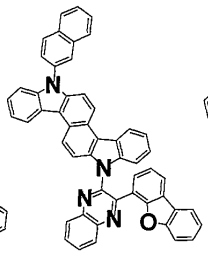
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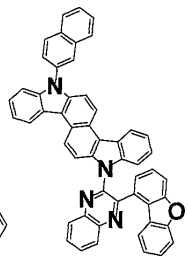
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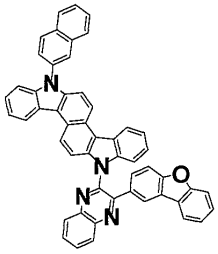
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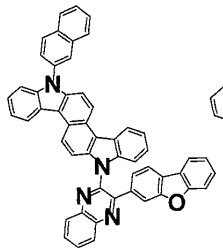
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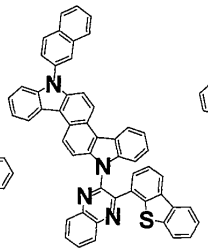
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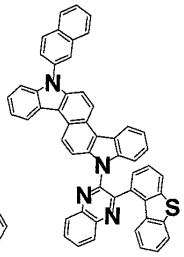
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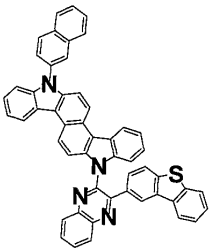
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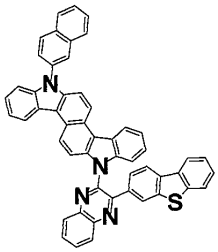
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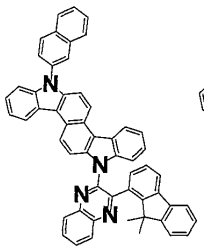
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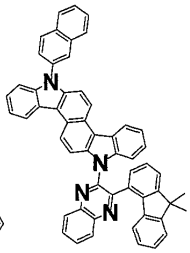
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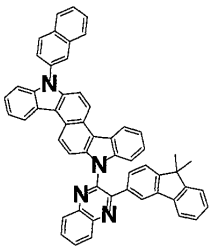
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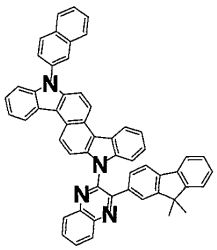
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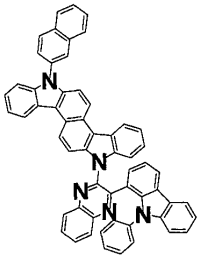
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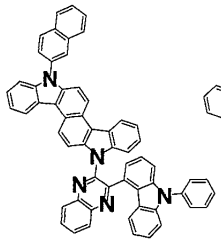
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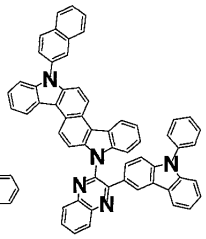
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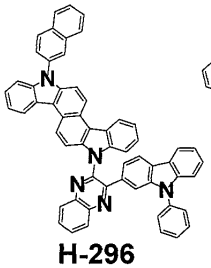
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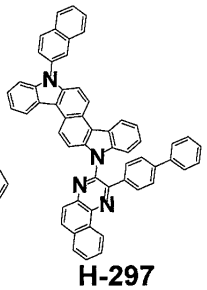
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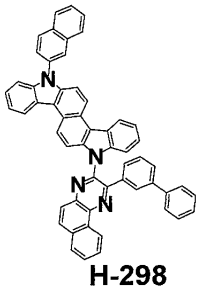
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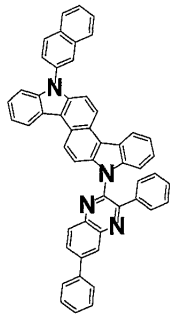

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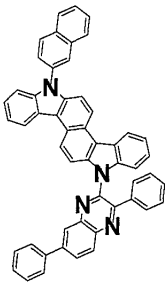

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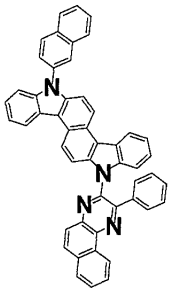

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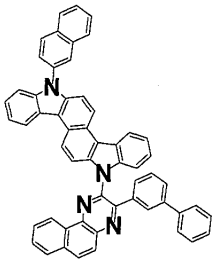

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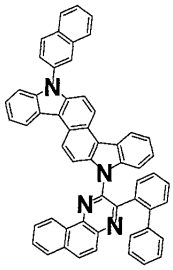

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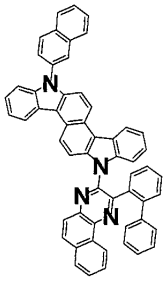

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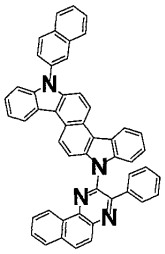

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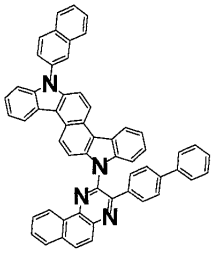

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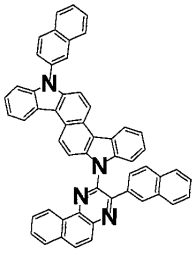

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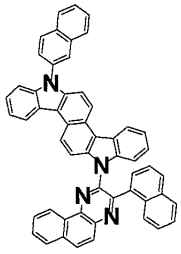

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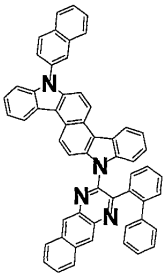

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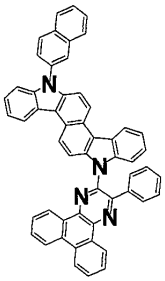

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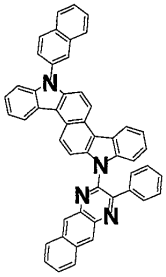

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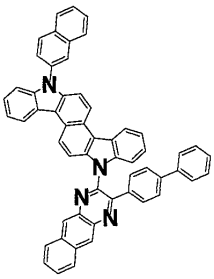

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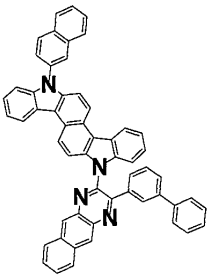

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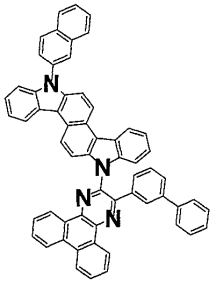

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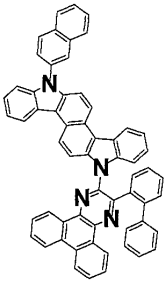

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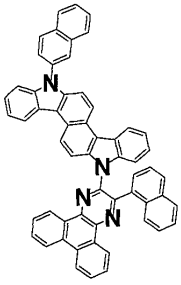

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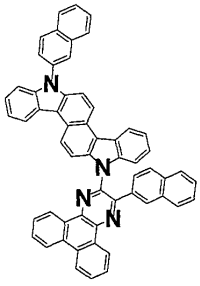

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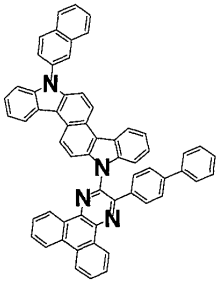

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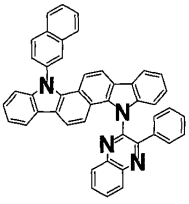

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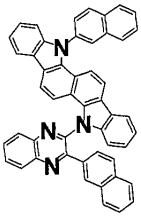

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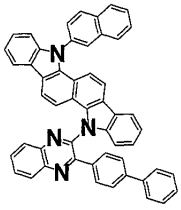

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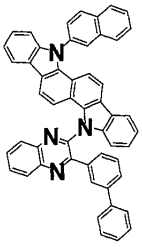

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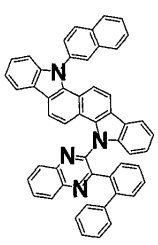

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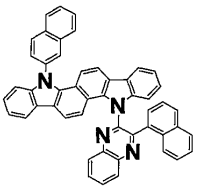
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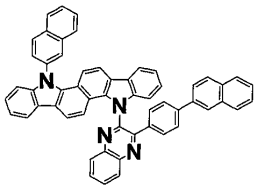
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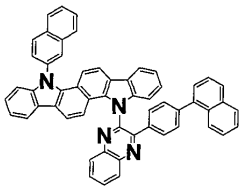
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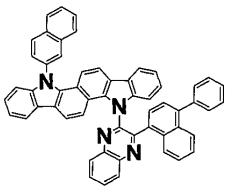
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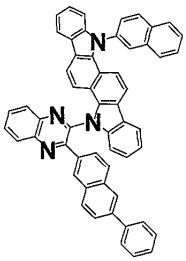
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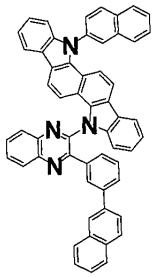
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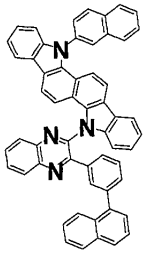
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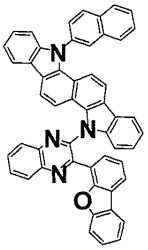
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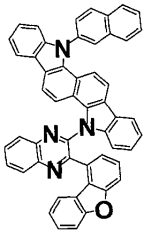
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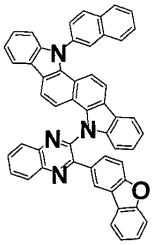
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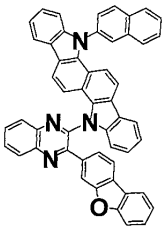
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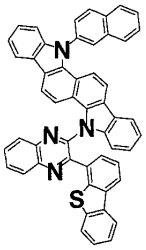
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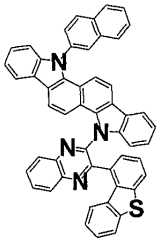
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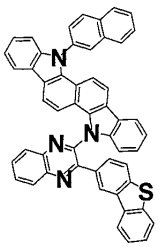
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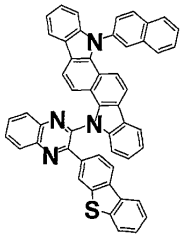
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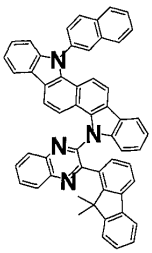
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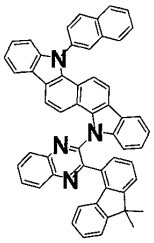
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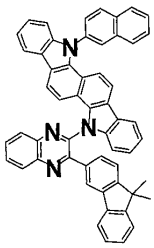
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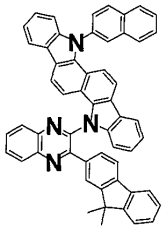
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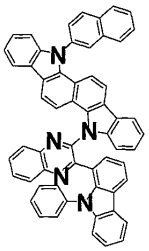
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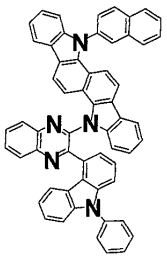
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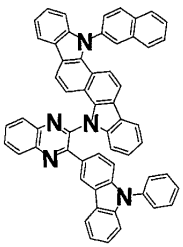
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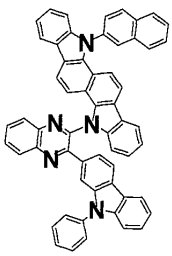
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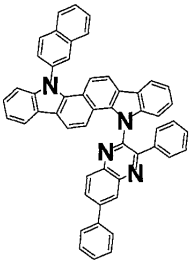
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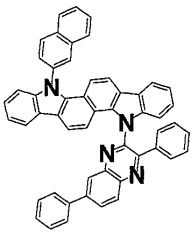
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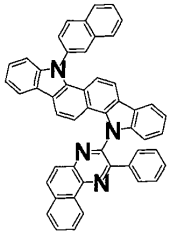
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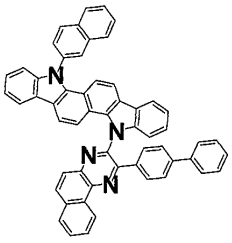
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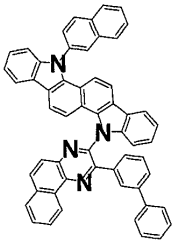
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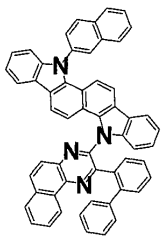
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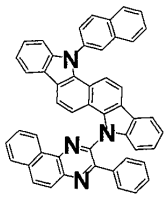

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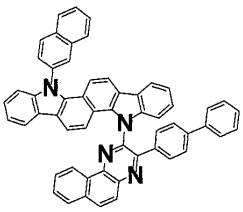

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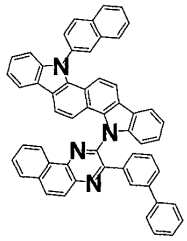

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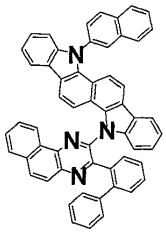

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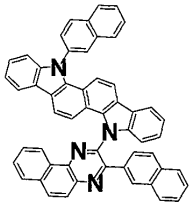

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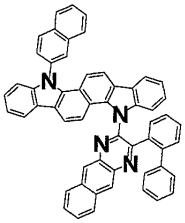

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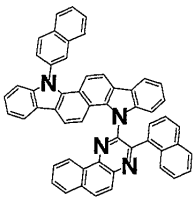

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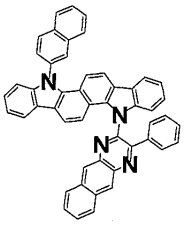

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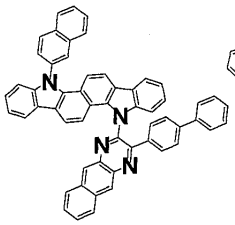

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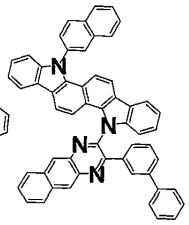

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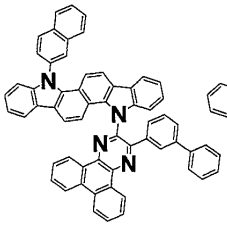

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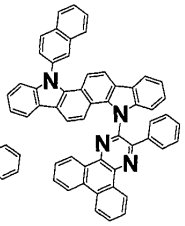

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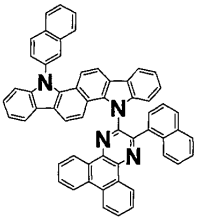

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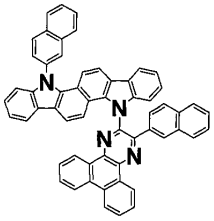

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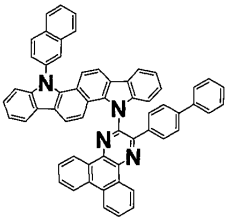

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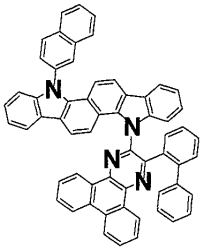

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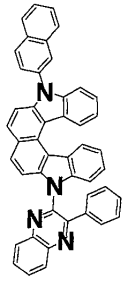

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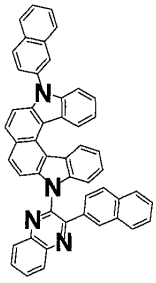

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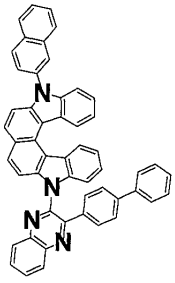

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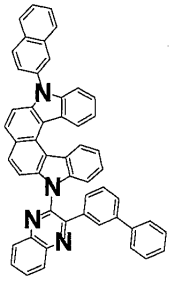

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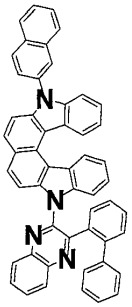

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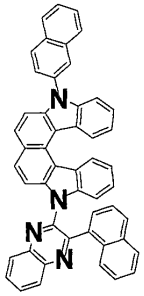

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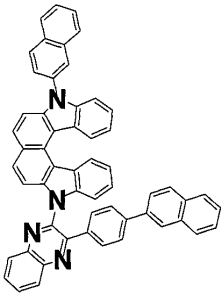

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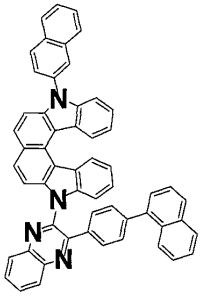

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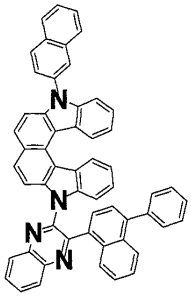

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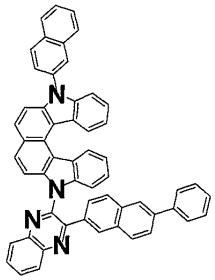

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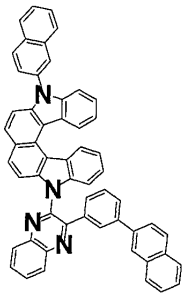

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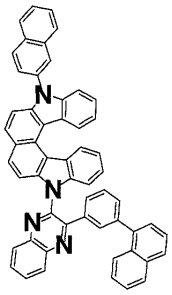

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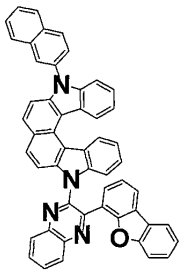

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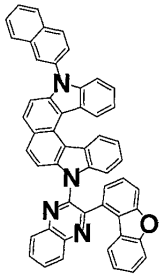

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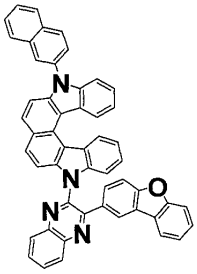

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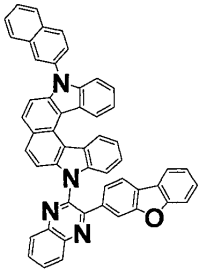

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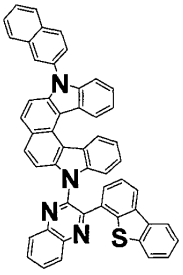

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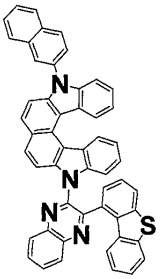

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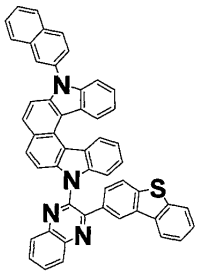

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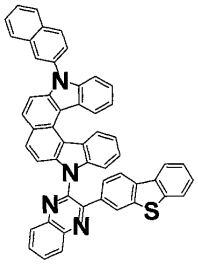

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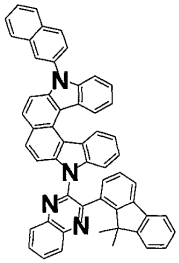

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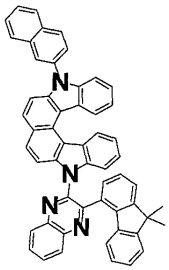

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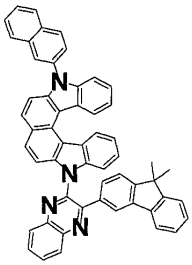

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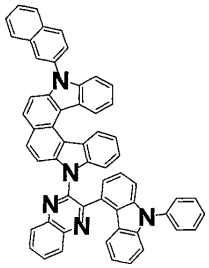

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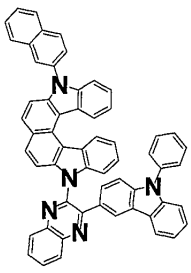

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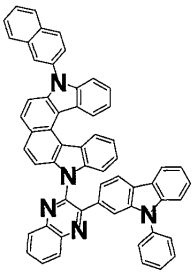

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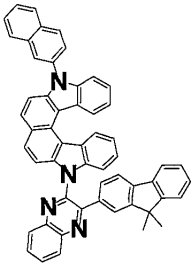

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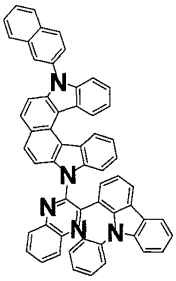

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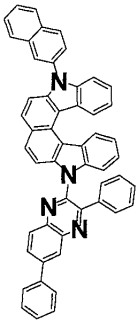

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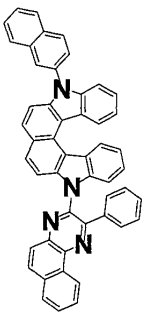

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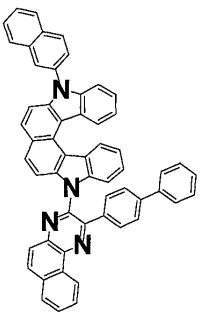

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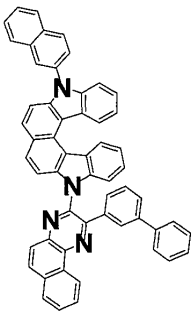

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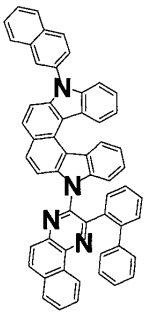

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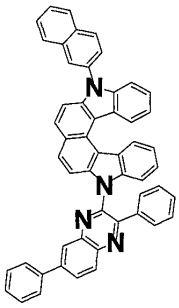

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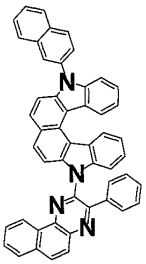

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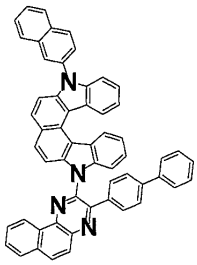

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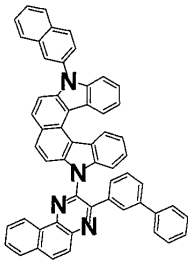

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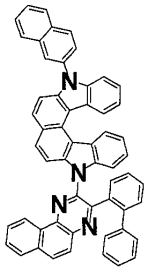

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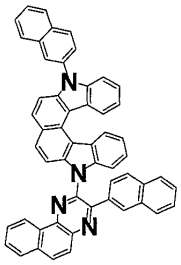

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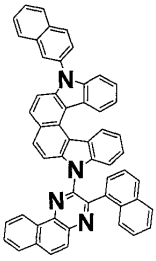

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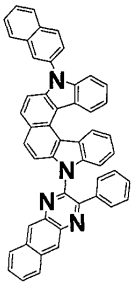

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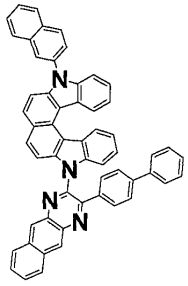

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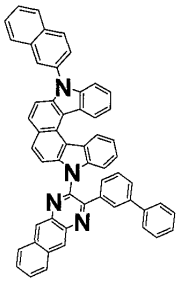

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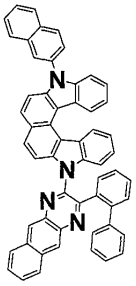

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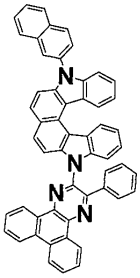

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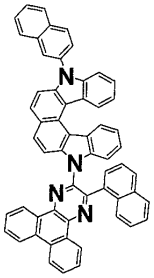

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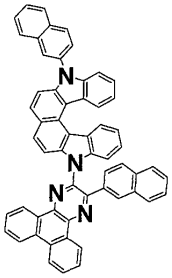

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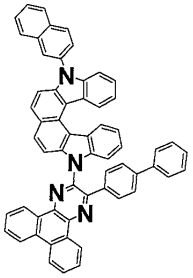

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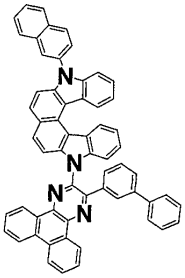

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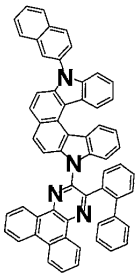

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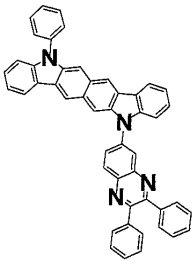

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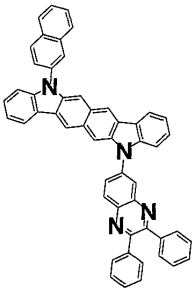

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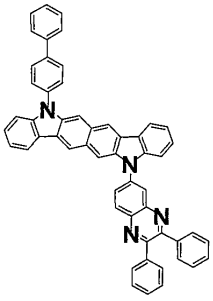

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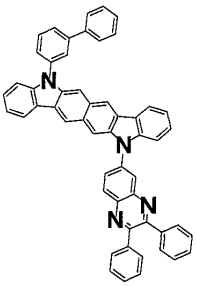

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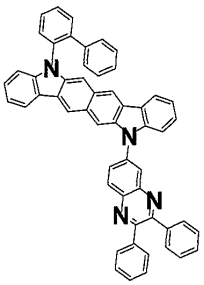

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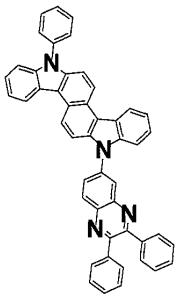

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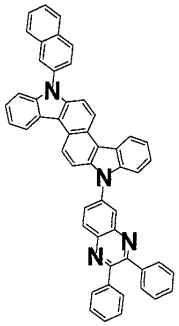

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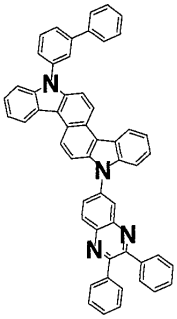

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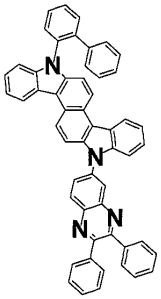

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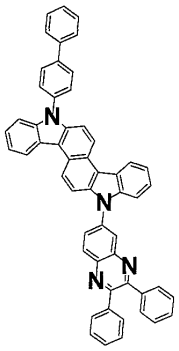

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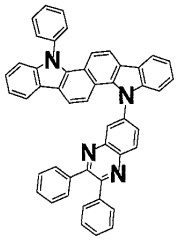

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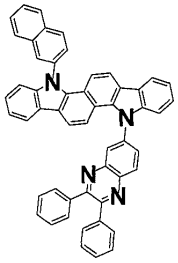

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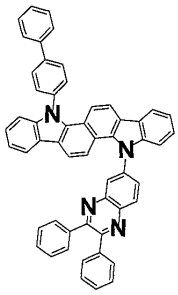

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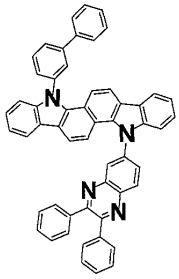

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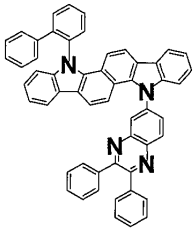

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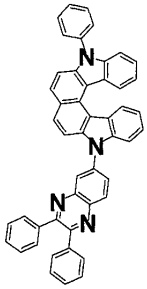

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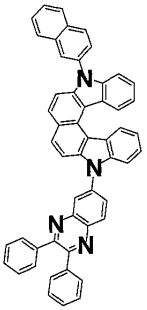

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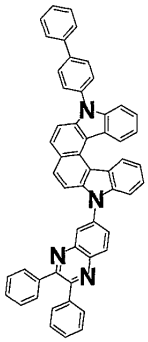

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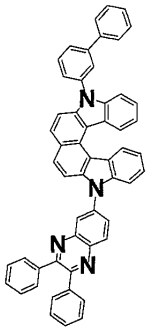

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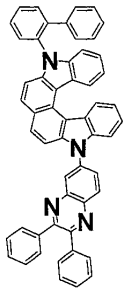

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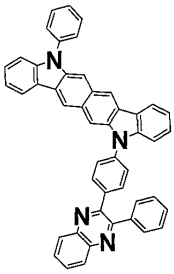

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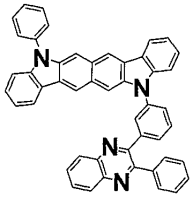

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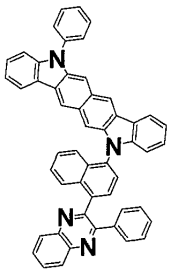

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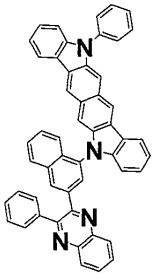

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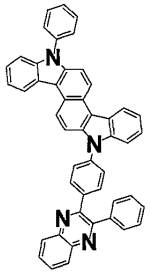

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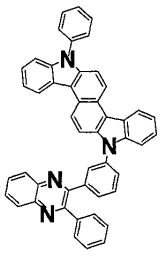

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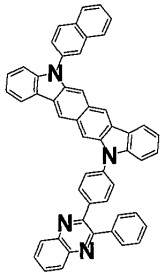

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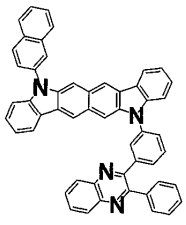

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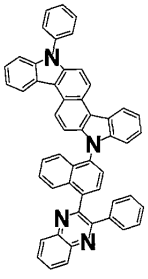

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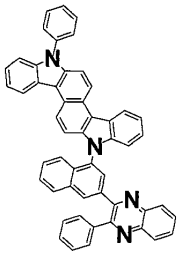
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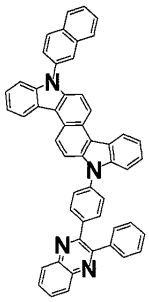
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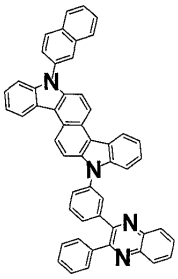
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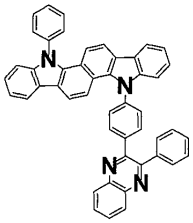
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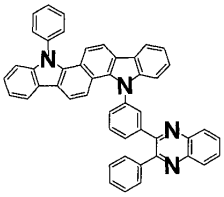
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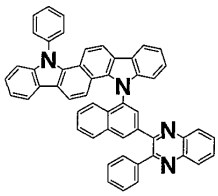
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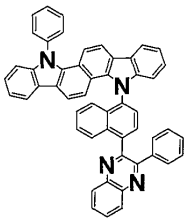
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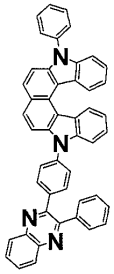
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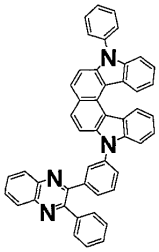
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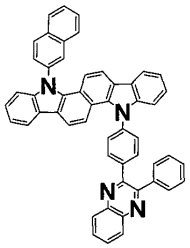
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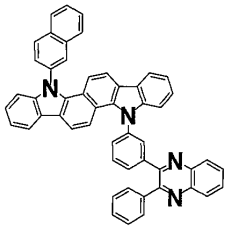
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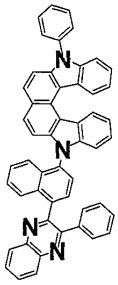
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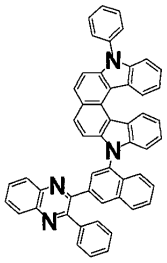
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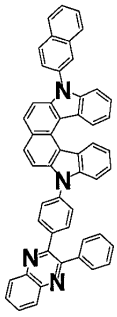
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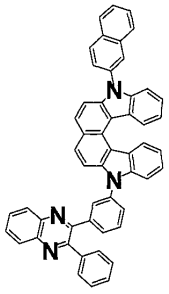
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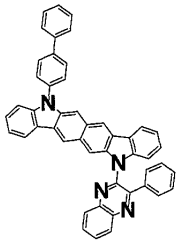
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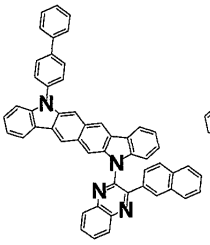
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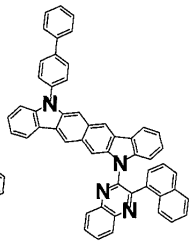
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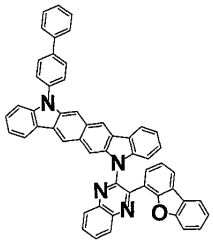
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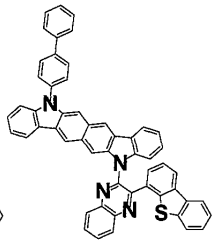
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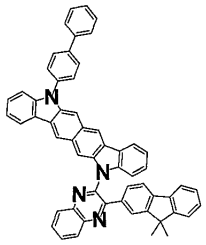
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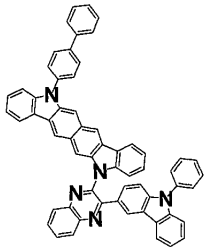
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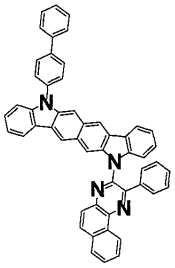
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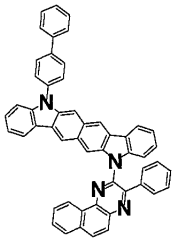
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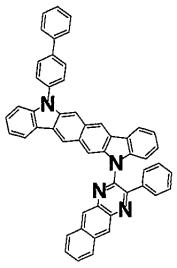
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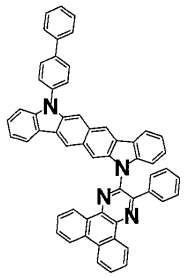

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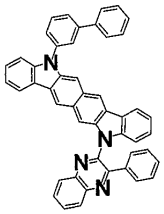

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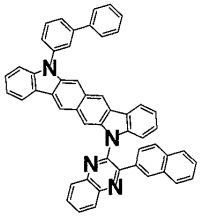

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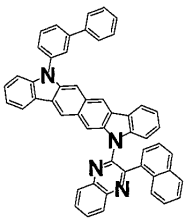

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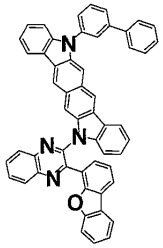

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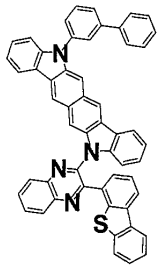

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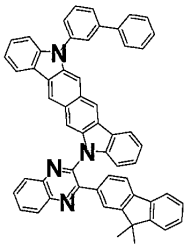

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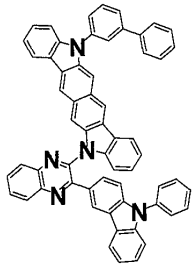

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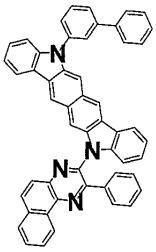

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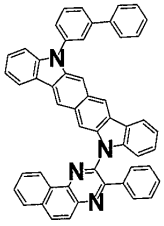

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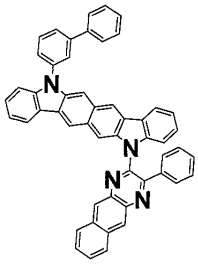

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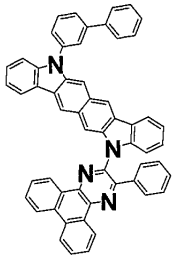

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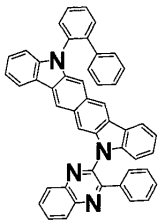

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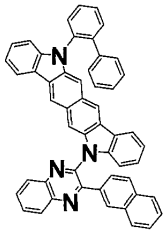

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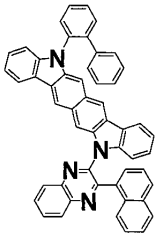

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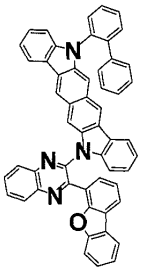

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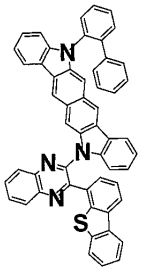

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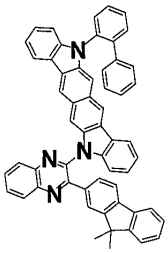

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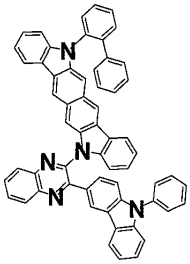

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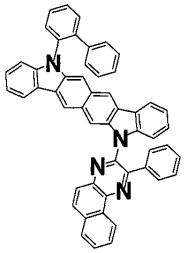

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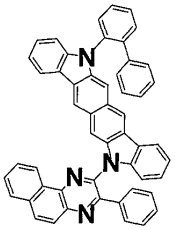

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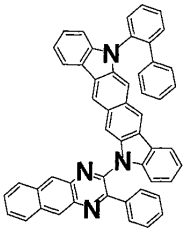

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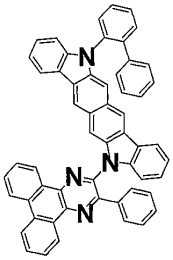

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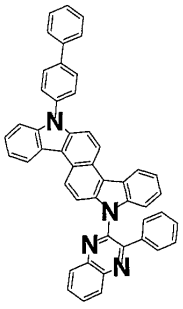

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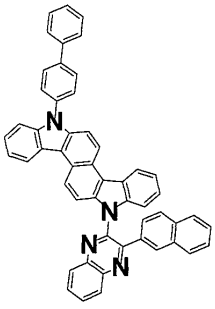

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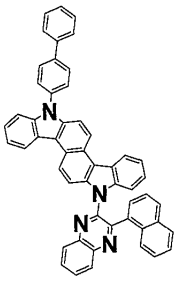

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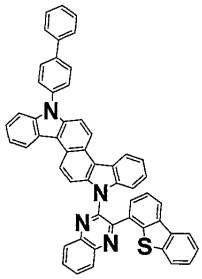

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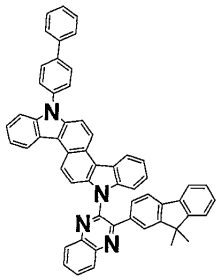

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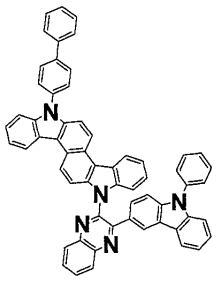

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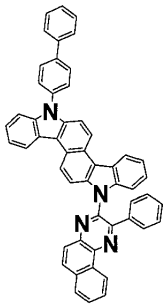

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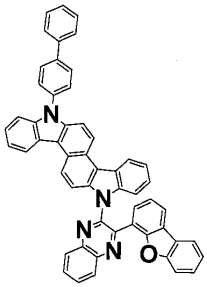

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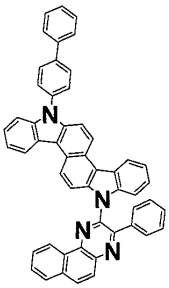

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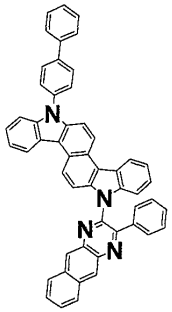

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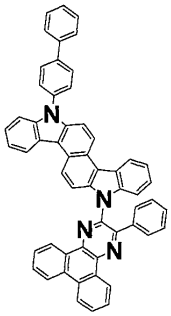

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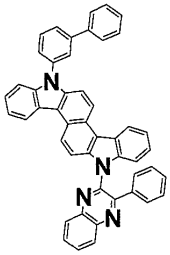

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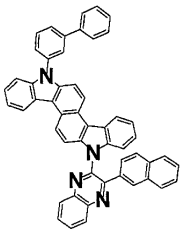

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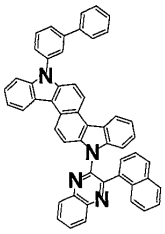

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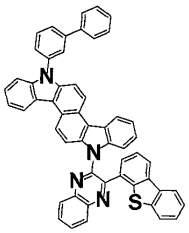

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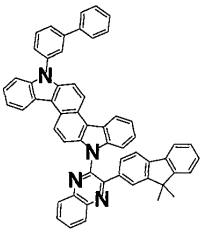

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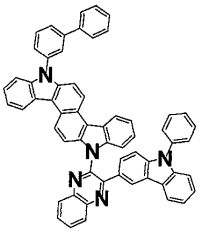

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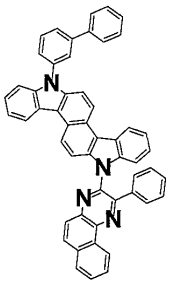

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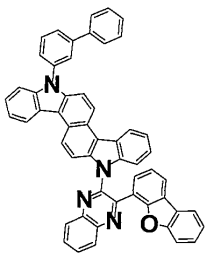

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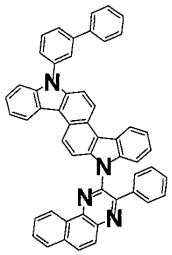

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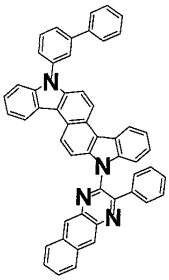

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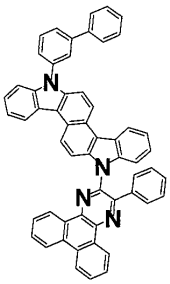

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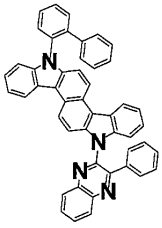

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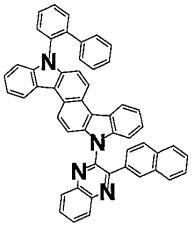

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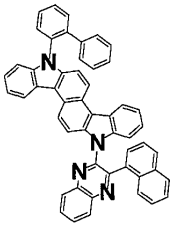

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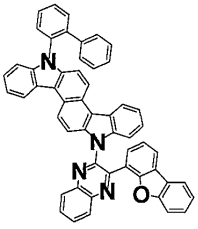

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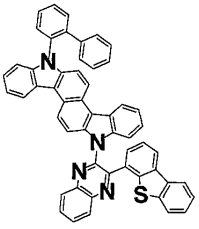

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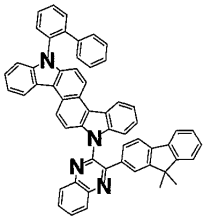
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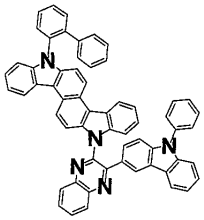
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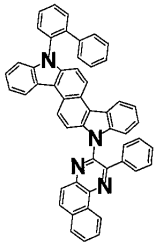
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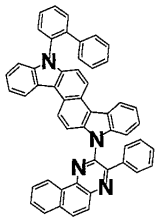
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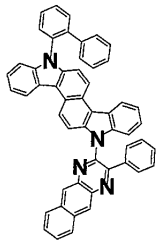
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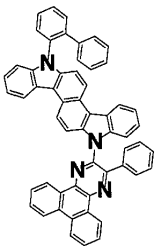
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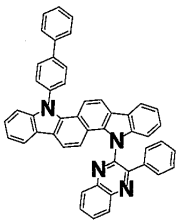
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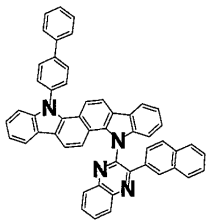
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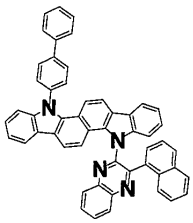
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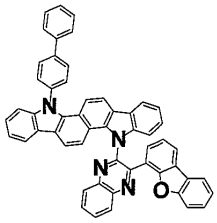
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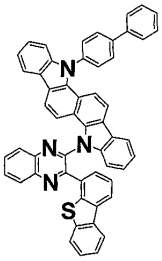
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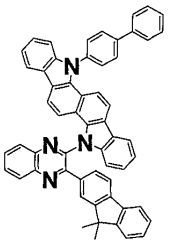
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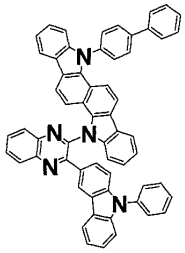
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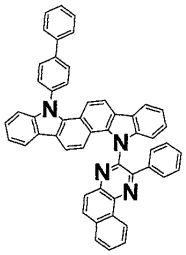
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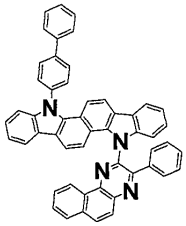
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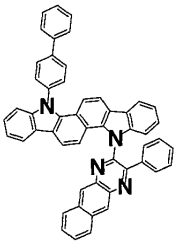
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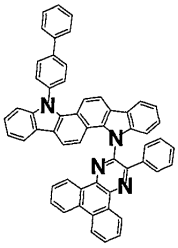
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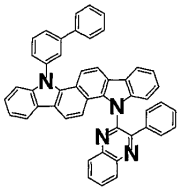
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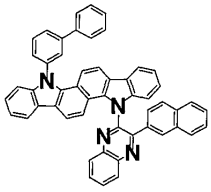
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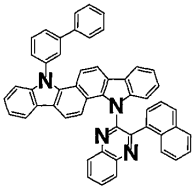
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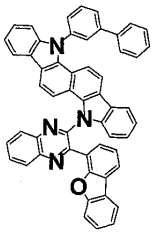
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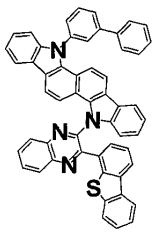
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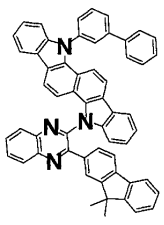
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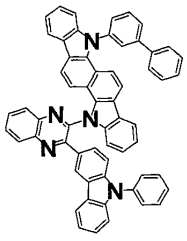
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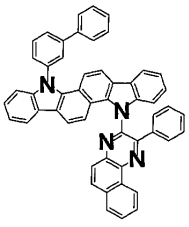
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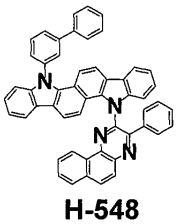
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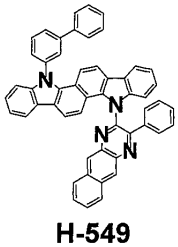
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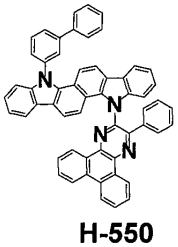
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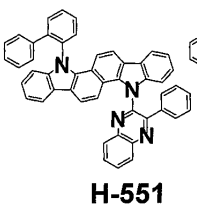
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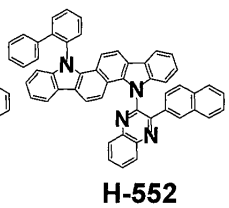
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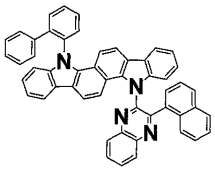

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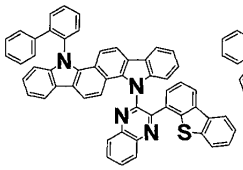

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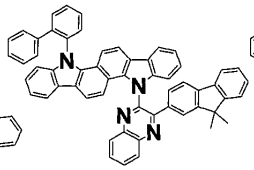

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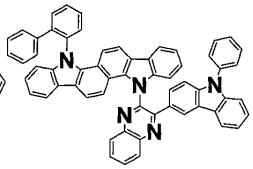

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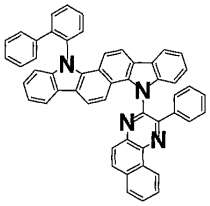

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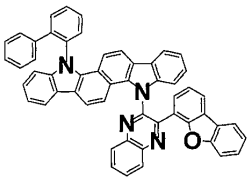

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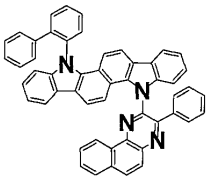

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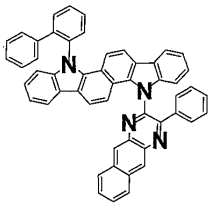

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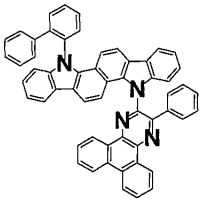

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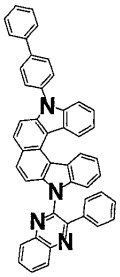

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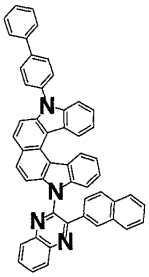

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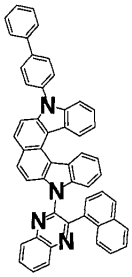

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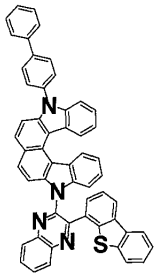

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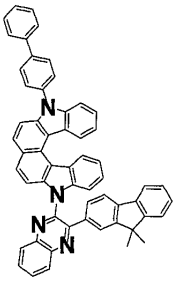

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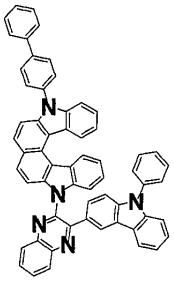

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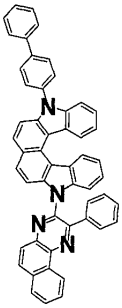

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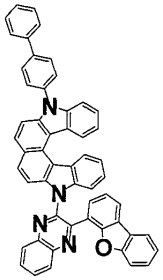

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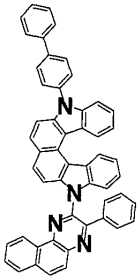

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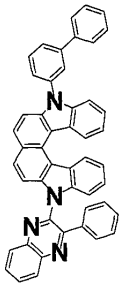

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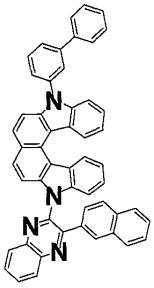
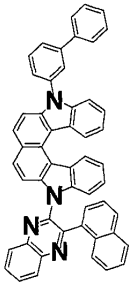
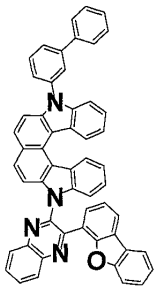


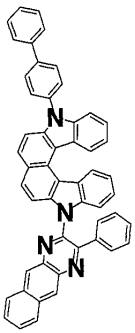
H-572



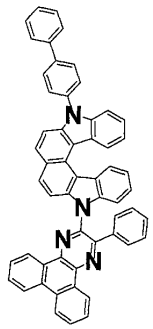
H-573



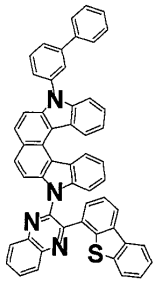
H-574



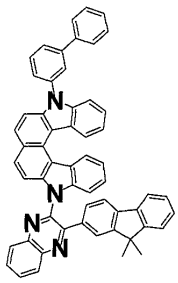
H-575



H-576



H-577



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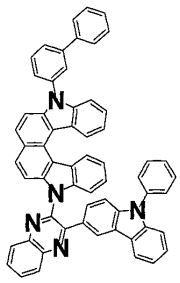

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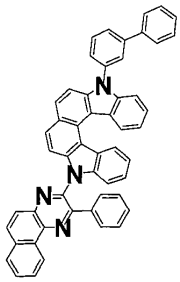

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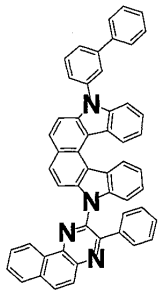

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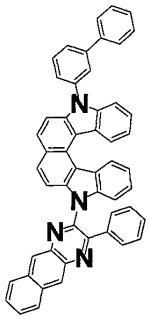

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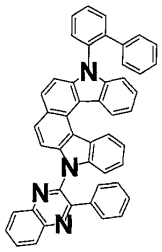
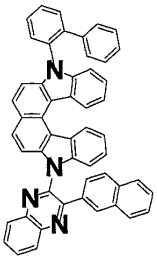


H-583



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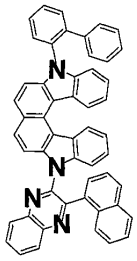
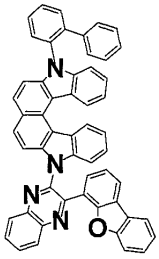
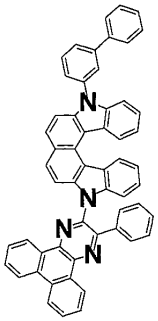


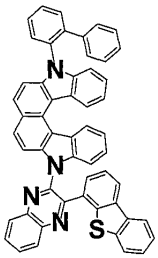
H-585



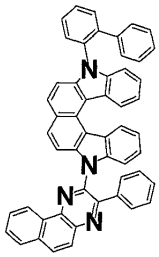
H-586



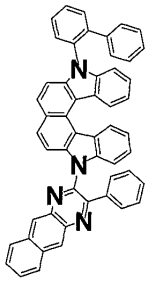
H-587



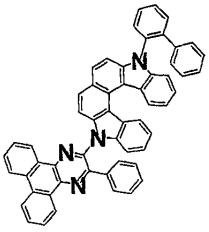
H-588



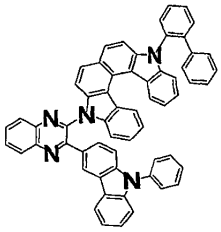
H-589



H-590



H-591



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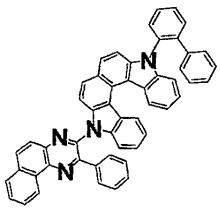
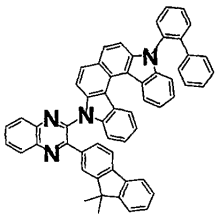


H-593



H-594

**청구항 6**

제1항에 기재된 유기 전계 발광 화합물을 포함하는, 유기 전계 발광 재료.

**청구항 7**

제1항에 기재된 유기 전계 발광 화합물을 포함하는, 유기 전계 발광 소자.

**청구항 8**

제7항에 있어서, 상기 유기 전계 발광 화합물을 발광층에 포함하는, 유기 전계 발광 소자.

## *발명의 설명*

## 기 술 분 야

[0001] 본원은 유기 전계 발광 화합물 및 이를 포함하는 유기 전계 발광 소자에 관한 것이다.

## 배 경 기 술

[0002] 이스트만 코닥 사의 Tang 등이 1987년에 발광층과 전하 전달층으로 이루어진 TPD/Alq3 이중층 저분자 녹색 유기 전계 발광 소자(OLED)를 처음으로 개발한 이후, 유기 전계 발광 소자에 대한 연구가 급속도로 빠르게 이루어져 현재 상용화에 이르렀다. 현재, 유기 전계 발광 소자는 패널 구현에 있어 발광 효율이 뛰어난 인광 물질을 주로 사용하고 있다. 그리고, 디스플레이의 장시간 사용과 높은 해상도를 위해서 낮은 구동 전압과 높은 발광 효율을 갖는 유기 전계 발광 소자가 지속적으로 요구되고 있다. 이에, 발광 효율, 구동 전압 또는 수명을 향상시키기 위해 유기 전계 발광 소자의 유기층에 사용되는 다양한 재료들이 개발되고 있다.

[0003] 한국 특허공개공보 제2010-0007780호, 제2014-0120090호, 제2011-0016033호 및 제2016-0007965호는 유기 전계 발광 소자에 포함되는 호스트 화합물로서 헤테로아릴 화합물을 개시하고 있으나, 퀴녹살린 유도체를 함유하는 24원 헤테로아릴 화합물에 대해 구체적으로 개시하고 있지 않다.

## 선행기술문헌

### 특허문헌

[0004] (특허문헌 0001) 한국 특허공개공보 제2010-0007780호 (2010. 1. 22. 공개)

(특허문헌 0002) 한국 특허공개공보 제2014-0120090호 (2014. 10. 13. 공개)

(특허문헌 0003) 한국 특허공개공보 제2011-0016033호 (2011. 2. 17. 공개)

(특허문헌 0004) 한국 특허공개공보 제2016-0007965호 (2016. 1. 21. 공개)

## 발명의 내용

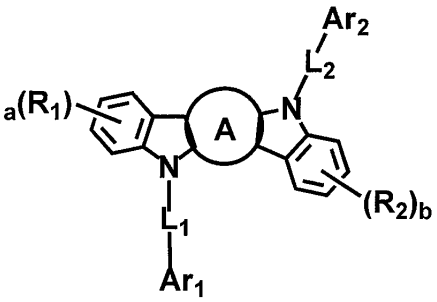
### 해결하려는 과제

[0005] 본원의 목적은, 낮은 구동전압, 높은 발광효율 및/또는 개선된 수명 특성을 갖는 유기 전계 발광 소자를 제공하는데 적합한 유기 전계 발광 화합물을 제공하는 것이다.

### 과제의 해결 수단

[0006] 본 발명자들은 하기 화학식 1로 표시되는 유기 전계 발광 화합물이 상술한 목적을 달성함을 발견하여 본 발명을 완성하였다.

[0007] [화학식 1]

[0008] 


[0009] 상기 화학식 1에서,

[0010] 고리 A는 치환 또는 비치환된 나프탈렌이고,

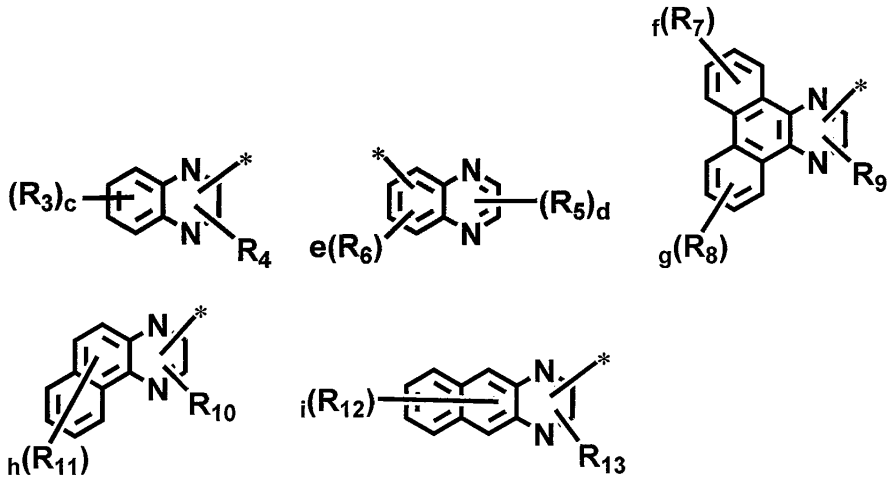
[0011] $R_1$ 및 $R_2$은 각각 독립적으로 수소, 중수소, 할로겐, 시아노, 치환 또는 비치환된 (C1-C30)알킬, 치환 또는 비치

환된 (C6-C30)아릴, 치환 또는 비치환된 (3-30원)헤테로아릴, 치환 또는 비치환된 (C3-C30)시클로알킬, 치환 또는 비치환된 (C1-C30)알콕시, 치환 또는 비치환된 트리(C1-C30)알킬실릴, 치환 또는 비치환된 디(C1-C30)알킬(C6-C30)아릴실릴, 치환 또는 비치환된 (C1-C30)알킬디(C6-C30)아릴실릴, 치환 또는 비치환된 트리(C6-C30)아릴실릴, 치환 또는 비치환된 모노- 또는 디- (C1-C30)알킬아미노, 치환 또는 비치환된 모노- 또는 디- (C6-C30)아릴아미노, 또는 치환 또는 비치환된 (C1-C30)알킬(C6-30)아릴아미노이거나, 둘 이상의 $R_1$은 서로 연결되어 고리를 형성하거나, 둘 이상의 $R_2$는 서로 연결되어 고리를 형성할 수 있고,

[0012] $L_1$ 및 $L_2$은 각각 독립적으로 단일결합, 치환 또는 비치환된 (C6-C30)아릴렌, 또는 치환 또는 비치환된 (3-30원)헤테로아릴렌이며,

[0013] $Ar_1$은 수소, 중수소, 할로겐, 시아노, 치환 또는 비치환된 (C1-C30)알킬, 치환 또는 비치환된 (C6-C30)아릴, 또는 치환 또는 비치환된 (3-30원)헤테로아릴이고,

[0014] $Ar_2$은 하기 화학식에서 선택되는 어느 하나이며,

[0015] 

[0016] 상기 식에서,

[0017] $R_3$ 내지 $R_{13}$은 각각 독립적으로 수소, 중수소, 할로겐, 시아노, 치환 또는 비치환된 (C1-C30)알킬, 치환 또는 비치환된 (C6-C30)아릴, 치환 또는 비치환된 (3-30원)헤테로아릴, 치환 또는 비치환된 (C3-C30)시클로알킬, 치환 또는 비치환된 (C1-C30)알콕시, 치환 또는 비치환된 트리(C1-C30)알킬실릴, 치환 또는 비치환된 디(C1-C30)알킬(C6-C30)아릴실릴, 치환 또는 비치환된 (C1-C30)알킬디(C6-C30)아릴실릴, 치환 또는 비치환된 트리(C6-C30)아릴실릴, 치환 또는 비치환된 모노- 또는 디- (C1-C30)알킬아미노, 치환 또는 비치환된 모노- 또는 디- (C6-C30)아릴아미노, 또는 치환 또는 비치환된 (C1-C30)알킬(C6-30)아릴아미노이며,

[0018] a, b, c, f 및 g는 4이고, d는 2이며, e는 3이고, h 및 i는 6이며, 각각의 $R_1$, 각각의 $R_2$, 각각의 $R_3$, 각각의 $R_5$, 각각의 $R_6$, 각각의 $R_7$, 각각의 $R_8$, 각각의 $R_{11}$, 및 각각의 $R_{12}$는 서로 동일하거나 상이할 수 있고,

[0019] *은 $L_2$와의 연결 부위를 나타낸다.

## 발명의 효과

[0020] 본원에 따른 유기 전계 발광 화합물은 낮은 구동 전압, 높은 발광 효율 및/또는 장 수명의 특성을 갖는 유기 전계 발광 소자를 제공할 수 있다.

## 발명을 실시하기 위한 구체적인 내용

[0021] 이하에서 본원을 더욱 상세히 설명하나, 이는 설명을 위한 것으로 본원의 범위를 제한하도록 해석되어서는 안된다.

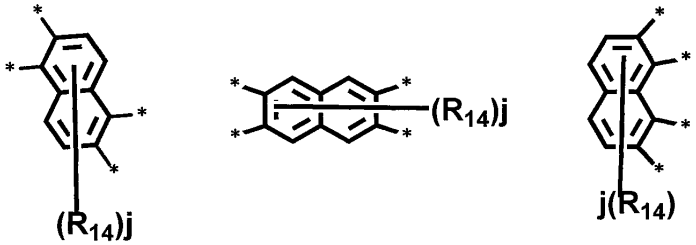
[0022] 본원에서 "유기 전계 발광 화합물"은 유기 전계 발광 소자에 사용될 수 있는 화합물을 의미하며, 필요에 따라 유기 전계 발광 소자를 구성하는 임의의 층에 포함될 수 있다.

[0023] 본원에서 "유기 전계 발광 재료"는 유기 전계 발광 소자에 사용될 수 있는 재료를 의미하고, 1종 이상의 화합물을 포함할 수 있으며, 필요에 따라 유기 전계 발광 소자를 구성하는 임의의 층에 포함될 수 있다. 예를 들면, 상기 유기 전계 발광 재료는 정공 주입 재료, 정공 전달 재료, 정공 보조 재료, 발광 보조 재료, 전자 차단 재료, 발광 재료, 전자 버퍼 재료, 정공 차단 재료, 전자 전달 재료, 전자 주입 재료 등 일 수 있다.

[0024] 본원의 유기 전계 발광 재료는 상기 화학식 1로 표시되는 1종 이상의 화합물을 포함할 수 있다. 이에 한정되는 것은 아니지만, 상기 화학식 1의 화합물은 발광층에 포함될 수 있으며, 발광층에 포함되는 경우 화학식 1의 화합물은 호스트로 포함될 수 있다.

[0025] 상기 화학식 1로 표시되는 화합물에 대해 보다 구체적으로 설명하면 다음과 같다.

[0026] 상기 화학식 1에서, 고리 A는 치환 또는 비치환된 나프탈렌이고, 본원의 일 양태에 따르면, 비치환된 나프탈렌이다. 또한, 고리 A 는 하기 식 중 어느 하나로 표시될 수 있다.

[0027] 

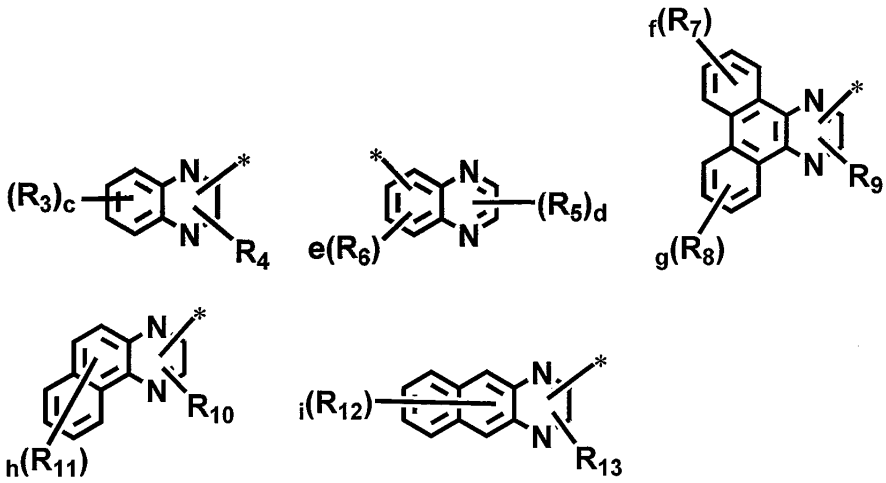

[0028] 상기 식에서, j는 4이고, $R_{14}$는 각각 독립적으로 수소, 중수소, 할로겐, 시아노, 치환 또는 비치환된 (C1-C30)알킬, 치환 또는 비치환된 (C6-C30)아릴, 치환 또는 비치환된 (3-30원)헤테로아릴이고, 각각의 $R_{14}$은 서로 동일하거나 상이할 수 있다. 본원의 일 양태에 따르면, $R_{14}$는 각각 독립적으로 수소, 중수소, 할로겐, 시아노, 비치환된 (C1-C10)알킬, 비치환된 (C6-C18)아릴, 또는 비치환된 (3-20원)헤테로아릴이다. 예를 들면, $R_{14}$는 수소이다.

[0029] 상기 화학식 1에서, $L_1$ 및 $L_2$은 각각 독립적으로 단일결합, 치환 또는 비치환된 (C6-C30)아릴렌, 또는 치환 또는 비치환된 (3-30원)헤테로아릴렌이고, 본원의 일 양태에 따르면, 단일결합, 또는 치환 또는 비치환된 (C6-C25)아릴렌이고, 본원의 다른 일 양태에 따르면, 단일결합, 또는 비치환된 (C6-C18)아릴렌이다. 예를 들면, $L_1$은 단일결합일 수 있고, $L_2$은 단일결합, 페닐렌, 또는 나프틸렌일 수 있다.

[0030] 상기 화학식 1에서, $Ar_1$은 수소, 중수소, 할로겐, 시아노, 치환 또는 비치환된 (C1-C30)알킬, 치환 또는 비치환된 (C6-C30)아릴, 또는 치환 또는 비치환된 (3-30원)헤테로아릴이고, 본원의 일 양태에 따르면, 치환 또는 비치환된 (C6-C25)아릴, 또는 치환 또는 비치환된 (5-25원)헤테로아릴이고, 본원의 다른 일 양태에 따르면, 치환 또는 비치환된 (C6-C18)아릴이다. 예를 들면, $Ar_1$은 페닐, 나프틸, 또는 비페닐일 수 있다.

[0031] 상기 화학식 1에서, $R_1$ 및 $R_2$은 각각 독립적으로 수소, 중수소, 할로겐, 시아노, 치환 또는 비치환된 (C1-C30)알킬, 치환 또는 비치환된 (C6-C30)아릴, 치환 또는 비치환된 (3-30원)헤테로아릴, 치환 또는 비치환된 (C3-C30)시클로알킬, 치환 또는 비치환된 (C1-C30)알콕시, 치환 또는 비치환된 트리(C1-C30)알킬실릴, 치환 또는 비치환된 디(C1-C30)알킬(C6-C30)아릴실릴, 치환 또는 비치환된 (C1-C30)알킬디(C6-C30)아릴실릴, 치환 또는 비치환된 트리(C6-C30)아릴실릴, 치환 또는 비치환된 모노- 또는 디- (C1-C30)알킬아미노, 치환 또는 비치환된 모노- 또는 디- (C6-C30)아릴아미노, 또는 치환 또는 비치환된 (C1-C30)알킬(C6-30)아릴아미노이거나, 둘 이상의 $R_1$은 서로 연결되어 고리를 형성하거나, 둘 이상의 $R_2$는 서로 연결되어 고리를 형성할 수 있고, 바람직하게는 수소, 중수소, 할로겐, 시아노, 치환 또는 비치환된 (C1-C20)알킬, 치환 또는 비치환된 (C6-C25)아릴, 또는 치환 또는 비치환된 (5-25원)헤테로아릴이고, 더욱 바람직하게는 수소, 비치환된 (C1-C10)알킬, 비치환된 (C6-C18)아릴, 또는 비치환된 (5-20원)헤테로아릴일 수 있다. 예를 들면, $R_1$ 및 $R_2$은 수소이다.

[0032] 상기 화학식 1에서, $Ar_2$은 하기 화학식에서 선택되는 어느 하나이다.

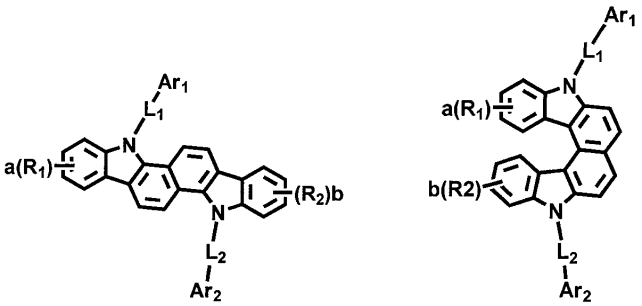
[0033] 

[0034] 상기 화학식에서, $R_3$ 내지 $R_{13}$은 각각 독립적으로 수소, 중수소, 할로겐, 시아노, 치환 또는 비치환된 (C1-C30)알킬, 치환 또는 비치환된 (C6-C30)아릴, 치환 또는 비치환된 (3-30원)헤테로아릴, 치환 또는 비치환된 (C3-C30)시클로알킬, 치환 또는 비치환된 (C1-C30)알콕시, 치환 또는 비치환된 트리(C1-C30)알킬실릴, 치환 또는 비치환된 디(C1-C30)알킬(C6-C30)아릴실릴, 치환 또는 비치환된 (C1-C30)알킬디(C6-C30)아릴실릴, 치환 또는 비치환된 트리(C6-C30)아릴실릴, 치환 또는 비치환된 모노- 또는 디- (C1-C30)알킬아미노, 치환 또는 비치환된 모노- 또는 디- (C6-C30)아릴아미노, 또는 치환 또는 비치환된 (C1-C30)알킬(C6-30)아릴아미노이며, 본원의 일 양태에 따르면, 수소, 치환 또는 비치환된 (C6-C25)아릴, 또는 치환 또는 비치환된 (3-30원)헤테로아릴이고, 본원의 다른 일 양태에 따르면, 수소, (C1-C10)알킬로 치환 또는 비치환된 (C6-C18)아릴, 또는 (C6-C18)아릴로 치환 또는 비치환된 (3-25원)헤테로아릴이다. 예를 들면, $R_3$은 각각 독립적으로 수소, 또는 비치환된 페닐이고, $R_4$는 페닐, 나프틸, 비페닐, 디메틸플루오레닐, 나프틸페닐, 페닐나프틸, 디벤조푸란일, 디벤조티오페닐, 또는 페닐카바졸릴이며, $R_5$는 각각 독립적으로 페닐이고, $R_6$ 내지 $R_{12}$는 수소이고, $R_9$, $R_{10}$ 및 $R_{13}$은 각각 독립적으로 페닐, 나프틸, 또는 비페닐이다.

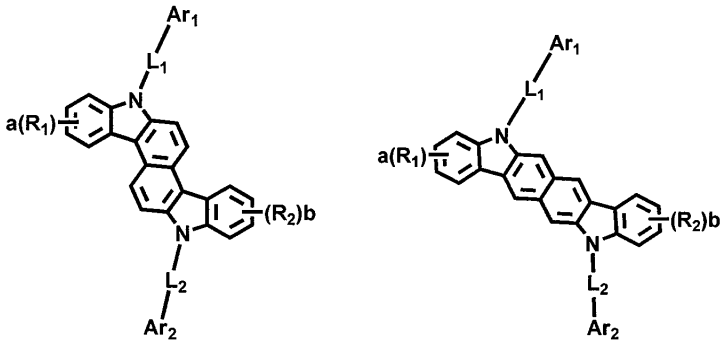
[0035] 상기 식에서, a, b, c, f 및 g는 4이고, d는 2이며, e는 3이고, h 및 i는 6이며, 각각의 $R_1$, 각각의 $R_2$, 각각의 $R_3$, 각각의 $R_5$, 각각의 $R_6$, 각각의 $R_7$, 각각의 $R_8$, 각각의 $R_{11}$, 및 각각의 $R_{12}$는 서로 동일하거나 상이할 수 있고, *은 $L_2$와의 연결 부위를 나타낸다.

[0036] 본원의 일 양태에 따르면, 상기 화학식 1의 화합물은 하기 화학식 2-1 내지 2-4 중 어느 하나로 표시되는 화합물일 수 있다.

[0037] [화학식 2-1] [화학식 2-2]

[0038] 

[0039] [화학식 2-3] [화학식 2-4]



[0040]

[0041] 상기 화학식 2-1 내지 2-4에서, $L_1$, $L_2$, $Ar_1$, $Ar_2$, $R_1$, $R_2$, a 및 b는 화학식 1에서의 정의와 동일하다.

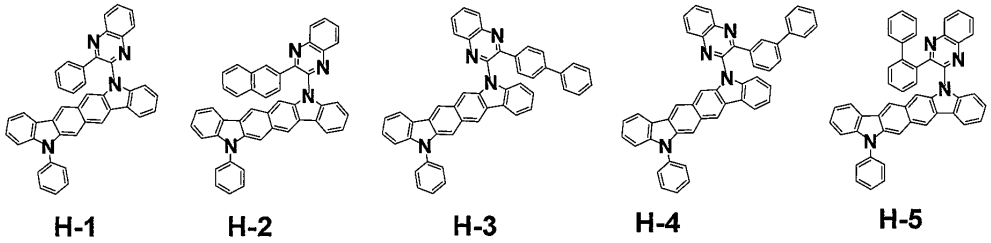
[0042] 본원에서 "(C1-C30)알킬"은 쇄를 구성하는 탄소수가 1 내지 30개인 직쇄 또는 분지쇄 알킬을 의미하고, 여기에서 탄소수는 바람직하게는 1 내지 20개, 더 바람직하게는 1 내지 10개이다. 상기 알킬의 구체적인 예로서, 메틸, 에틸, n-프로필, 이소프로필, n-부틸, 이소부틸 및 tert-부틸 등이 있다. 본원에서 "(C2-C30)알케닐"은 쇄를 구성하는 탄소수가 2 내지 30개인 직쇄 또는 분지쇄 알케닐을 의미하고, 여기에서 탄소수는 바람직하게는 2 내지 20개, 더 바람직하게는 2 내지 10개이다. 상기 알케닐의 구체적인 예로서, 비닐, 1-프로페닐, 2-프로페닐, 1-부테닐, 2-부테닐, 3-부테닐, 2-메틸부트-2-에닐 등이 있다. 본원에서 "(C2-C30)알키닐"은 쇄를 구성하는 탄소수가 2 내지 30개인 직쇄 또는 분지쇄 알키닐을 의미하고, 여기에서 탄소수는 바람직하게는 2 내지 20개, 더 바람직하게는 2 내지 10개이다. 상기 알키닐의 예로서, 에티닐, 1-프로피닐, 2-프로피닐, 1-부티닐, 2-부티닐, 3-부티닐, 1-메틸펜트-2-이닐 등이 있다. 본원에서 "(C3-C30)시클로알킬"은 환 골격 탄소수가 3 내지 30개인 단일환 또는 다환 탄화수소를 의미하고, 상기 탄소수는 바람직하게는 3 내지 20개, 더 바람직하게는 3 내지 7개이다. 상기 시클로알킬의 예로서, 시클로프로필, 시클로부틸, 시클로펜틸, 시클로헥실 등이 있다. 본원에서 "(3-7원)헤테로시클로알킬"은 환 골격 원자수가 3 내지 7개, 바람직하게는 5 내지 7개이고, B, N, O, S, Si 및 P로 이루어진 군, 바람직하게는 O, S 및 N로 이루어진 군에서 선택되는 하나 이상의 헤테로원자를 포함하는 시클로알킬을 의미하고, 예를 들어, 테트라하이드로푸란, 피롤리딘, 티올란, 테트라하이드로피란 등이 있다. 본원에서 "(C6-C30)아릴(렌)"은 환 골격 탄소수가 6 내지 30개인 방향족 탄화수소에서 유래된 단일환 또는 융합환계 라디칼을 의미하고, 부분적으로 포화될 수도 있다. 상기 환 골격 탄소수는 바람직하게는 6 내지 25개, 더 바람직하게는 6 내지 18개이다. 상기 아릴은 스피로 구조를 가진 것을 포함한다. 상기 아릴의 예로서, 페닐, 비페닐, 터페닐, 나프틸, 비나프틸, 페닐나프틸, 나프틸페닐, 페닐터페닐, 플루오레닐, 페닐플루오레닐, 벤조플루오레닐, 디벤조플루오레닐, 페난트레닐, 페닐페난트레닐, 안트라세닐, 인데닐, 트리페닐레닐, 피레닐, 테트라세닐, 페릴레닐, 크라이세닐, 나프타세닐, 플루오란테닐, 스피로비플루오레닐 등이 있다. 본원에서 "(3-30원)헤테로아릴(렌)"은 환 골격 원자수가 3 내지 30개이고, B, N, O, S, Si 및 P로 이루어진 군에서 선택된 하나 이상의 헤테로원자를 포함하는 아릴기를 의미한다. 헤테로원자수는 바람직하게는 1 내지 4개이고, 단일 환계이거나 하나 이상의 벤젠환과 축합된 융합환계일 수 있으며, 부분적으로 포화될 수도 있다. 또한, 본원에서 상기 헤테로아릴(렌)은 하나 이상의 헤테로아릴 또는 아릴기가 단일 결합에 의해 헤테로아릴기와 연결된 형태도 포함하며, 스피로 구조를 가진 것도 포함한다. 상기 헤테로아릴의 예로서, 푸릴, 티오펜일, 피롤릴, 이미다졸릴, 피라졸릴, 티아졸릴, 티아디아졸릴, 이소티아졸릴, 이속사졸릴, 옥사졸릴, 옥사디아졸릴, 트리아진일, 테트라진일, 트리아졸릴, 테트라졸릴, 푸라잔일, 피리딜, 피라진일, 피리미딘일, 피리다진일 등의 단일 환계 헤테로아릴, 벤조푸란일, 벤조티오펜일, 이소벤조푸란일, 디벤조푸란일, 디벤조티오펜일, 벤조이미다졸릴, 벤조티아졸릴, 벤조이소티아졸릴, 벤조이속사졸릴, 벤조옥사졸릴, 이소인돌릴, 인돌릴, 벤조인돌릴, 인다졸릴, 벤조티아디아졸릴, 퀴놀릴, 이소퀴놀릴, 신놀리닐, 퀴나졸리닐, 벤조퀴나졸리닐, 퀴녹살리닐, 벤조퀴녹살리닐, 나프티리디닐, 카바졸릴, 벤조카바졸릴, 디벤조카바졸릴, 페녹사진일, 페노티아진일, 페난트리딘일, 벤조디옥솔릴, 디하이드로아크리디닐 등의 융합 환계 헤테로아릴 등이 있다. 본원에서 "할로겐"은 F, Cl, Br 및 I 원자를 포함한다.

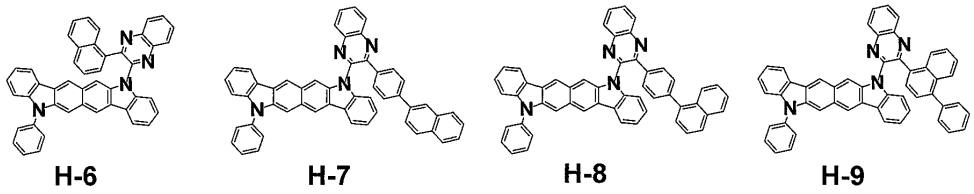
[0043] 또한, 본원에 기재되어 있는 "치환 또는 비치환" 이라는 기재에서 “치환”은 어떤 작용기에서 수소 원자가 다른 원자 또는 다른 작용기 (즉, 치환기)로 대체되는 것을 뜻한다. 본원의 화학식의 상기 고리 A, $L_1$, $L_2$, $Ar_1$, 및 $R_1$ 내지 $R_{14}$에서 치환된 나프탈렌, 치환된 (C1-C30)알킬, 치환된 (C6-C30)아릴(렌), 치환된 (3-30원)헤테로아

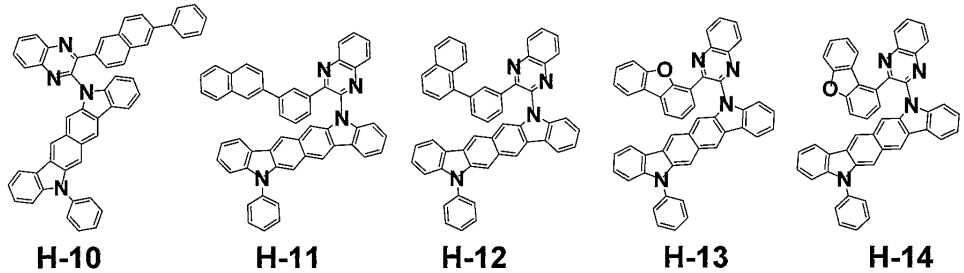
릴(렌), 치환된 (C3-C30)시클로알킬, 치환된 (C1-C30)알콕시, 치환된 트리(C1-C30)알킬실릴, 치환된 디(C1-C30)알킬(C6-C30)아릴실릴, 치환된 (C1-C30)알킬디(C6-C30)아릴실릴, 치환된 트리(C6-C30)아릴실릴, 치환된 모노- 또는 디- (C1-C30)알킬아미노, 치환된 모노- 또는 디- (C6-C30)아릴아미노, 및 치환된 (C1-C30)알킬(C6-C30)아릴아미노의 치환기는 각각 독립적으로 중수소, 할로겐, 시아노, 카르복실, 니트로, 히드록시, (C1-C30)알킬, 할로(C1-C30)알킬, (C2-C30)알케닐, (C2-C30)알키닐, (C1-C30)알콕시, (C1-C30)알킬티오, (C3-C30)시클로알킬, (C3-C30)시클로알케닐, (3-7원)헤테로시클로알킬, (C6-C30)아릴옥시, (C6-C30)아릴티오, (C6-C30)아릴로 치환 또는 비치환된 (3-30 원)헤테로아릴, (3-30원)헤테로아릴로 치환 또는 비치환된 (C6-C30)아릴, 트리(C1-C30)알킬실릴, 트리(C6-C30)아릴실릴, 디(C1-C30)알킬(C6-C30)아릴실릴, (C1-C30)알킬디(C6-C30)아릴실릴, 아미노, 모노- 또는 디- (C1-C30)알킬아미노, (C1-C30)알킬로 치환 또는 비치환된 모노- 또는 디- (C6-C30)아릴아미노, (C1-C30)알킬(C6-C30)아릴아미노, (C1-C30)알킬카보닐, (C1-C30)알콕시카보닐, (C6-C30)아릴카보닐, 디(C6-C30)아릴보로닐, 디(C1-C30)알킬보로닐, (C1-C30)알킬(C6-C30)아릴보로닐, (C6-C30)아르(C1-C30)알킬, 및 (C1-C30)알킬(C6-C30)아릴로 이루어진 군으로부터 선택되는 하나 이상일 수 있다. 상기 치환기는, 바람직하게는 (C1-C20)알킬, (C6-C25)아릴, 및 (5-25원)헤테로아릴로 이루어진 군으로부터 선택되는 하나 이상일 수 있고, 더욱 바람직하게는 (C1-C10)알킬 및 (C6-C18)아릴로 이루어진 군으로부터 선택되는 하나 이상일 수 있고, 예를 들면, 메틸, 페닐 및 나프틸로 이루어진 군으로부터 선택되는 하나 이상일 수 있다.

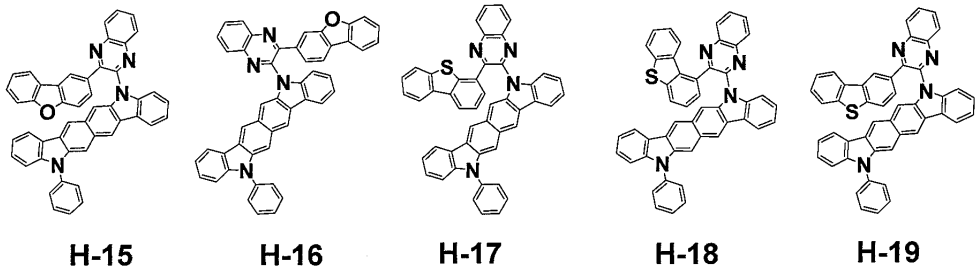
[0044] 본원 화학식에서, 인접한 치환기끼리 서로 연결되어 고리를 형성하는 경우, 상기 고리는 치환 또는 비치환된 (3-30원)의 단일환 또는 다환의 지환족, 방향족 또는 이들의 조합의 고리일 수 있다. 또한, 형성된 고리는 질소, 산소 및 황으로부터 선택되는 하나 이상의 헤테로원자를 포함할 수 있다.

[0045] 상기 화학식 1로 표시되는 화합물은 보다 구체적으로 하기의 화합물로서 예시될 수 있으나, 이들에 한정되는 것은 아니다.

[0046] 
H-1 H-2 H-3 H-4 H-5

[0047] 
H-6 H-7 H-8 H-9

[0048] 
H-10 H-11 H-12 H-13 H-14

[0049] 
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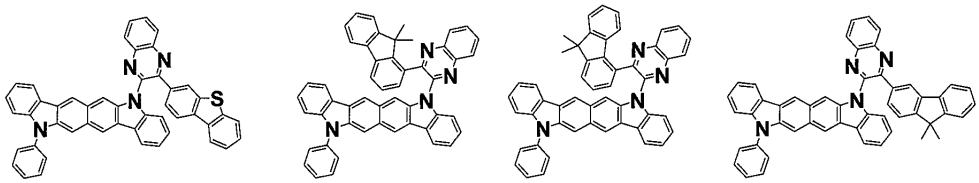
[0050] 
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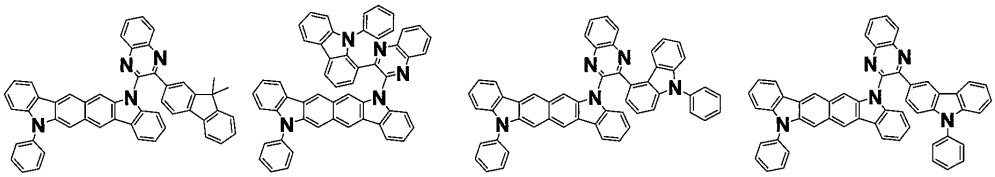
[0051] 
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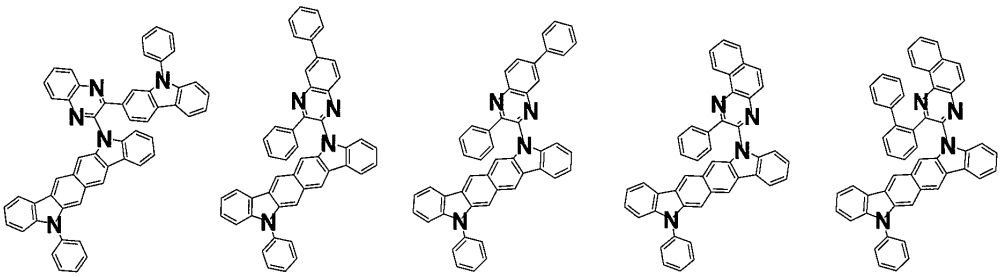
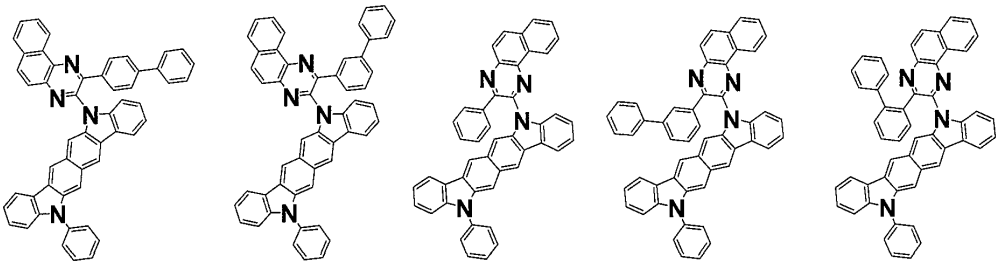
[0052] 
H-28 H-29 H-30 H-31 H-32

[0053] 
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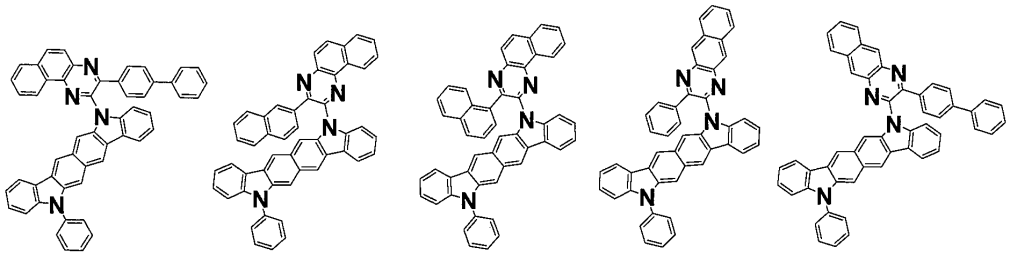
[0054] 
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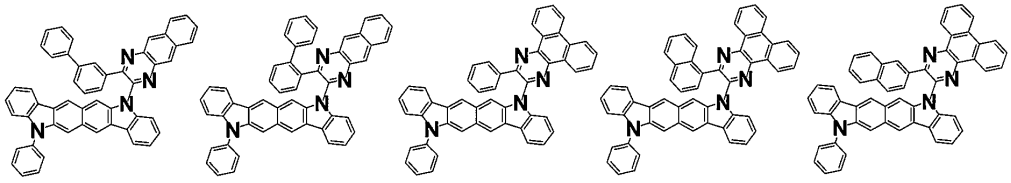
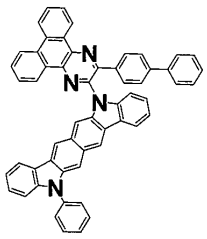
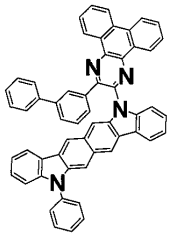
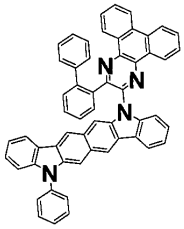
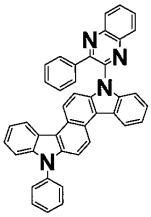
[0055] 
H-43 H-44 H-45 H-46 H-47

[0056]


H-48


H-49


H-50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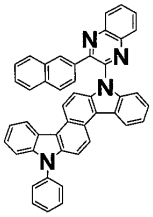
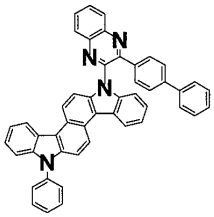
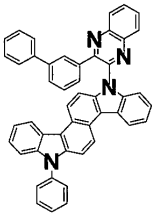
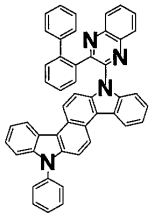
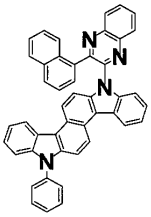

H-52

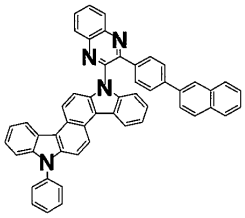
[0057]


H-53

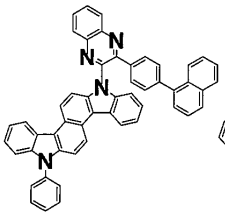

H-54


H-55


H-56


H-57

[0058]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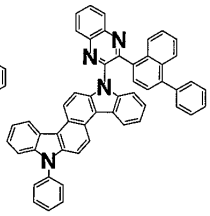
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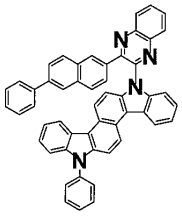
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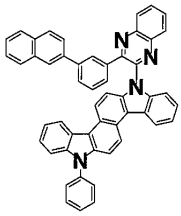
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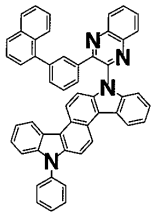
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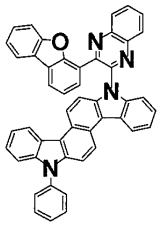
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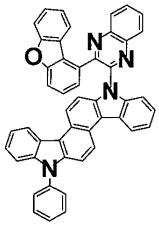
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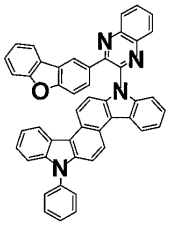
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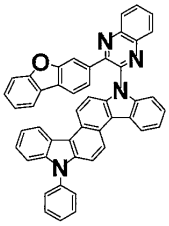
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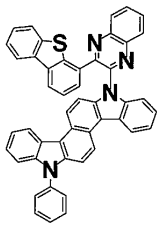
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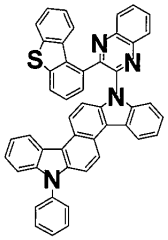
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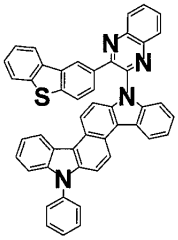
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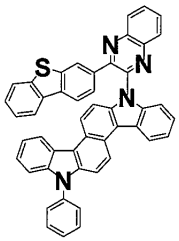
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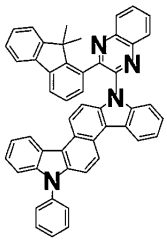
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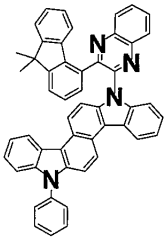
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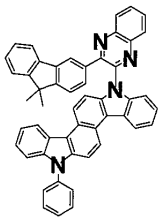
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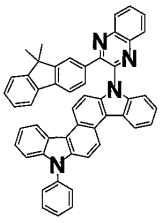
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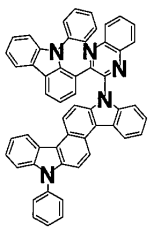
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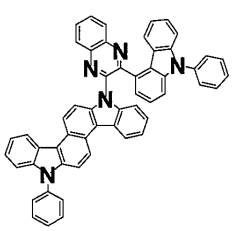
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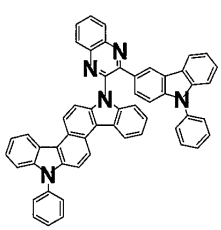
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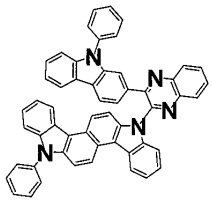

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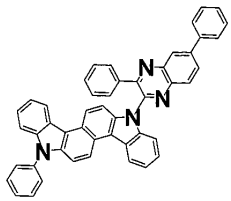

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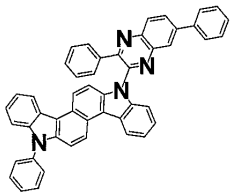

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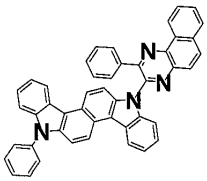

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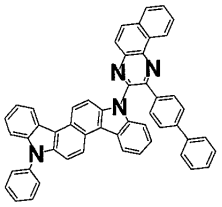

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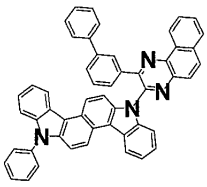

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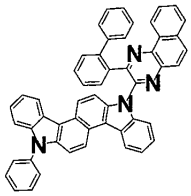

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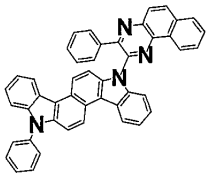

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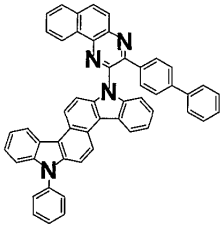

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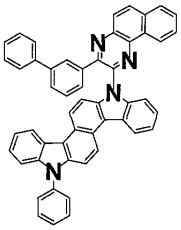

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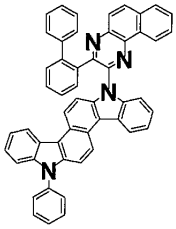

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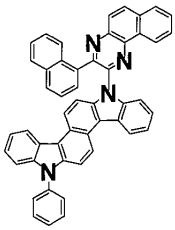

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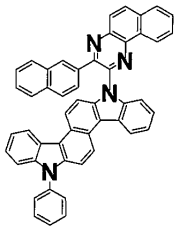

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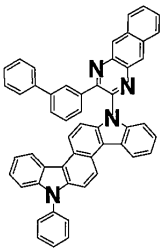

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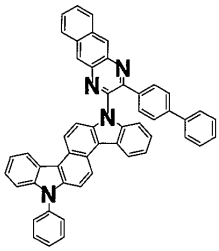

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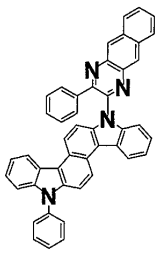

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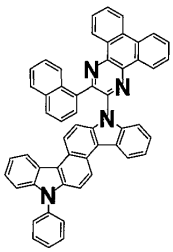

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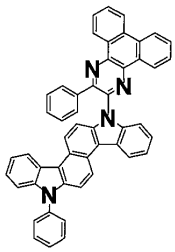

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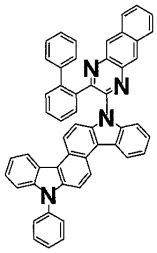

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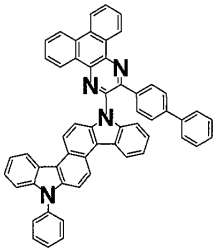

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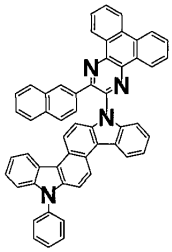

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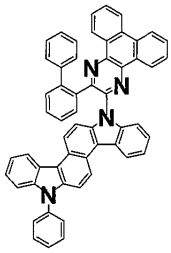

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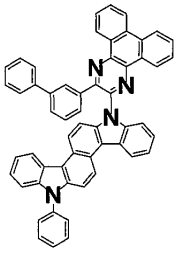

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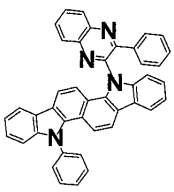

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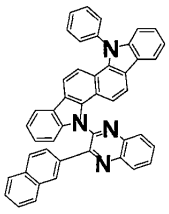

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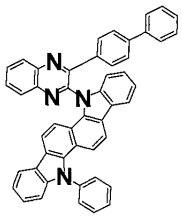

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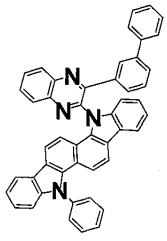

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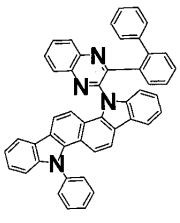

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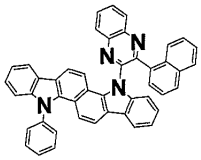
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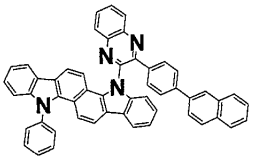
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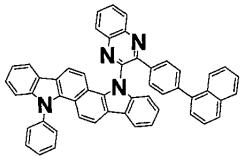
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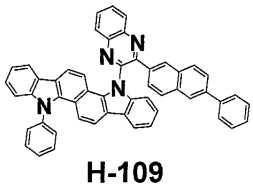
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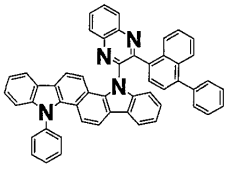
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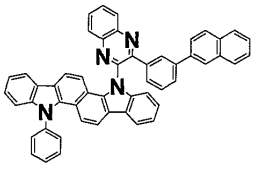
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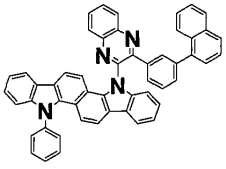
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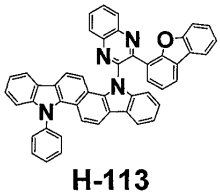
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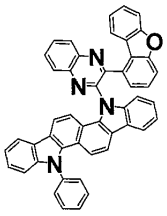
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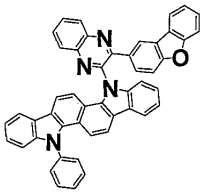
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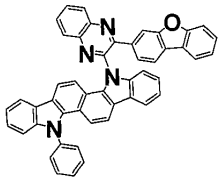
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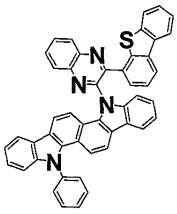
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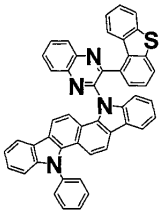
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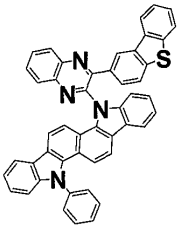
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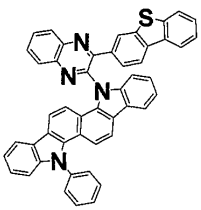
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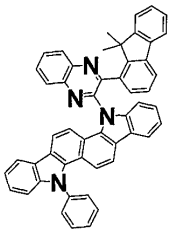
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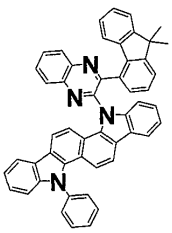
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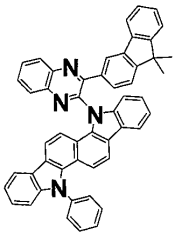
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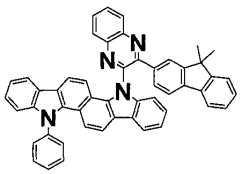
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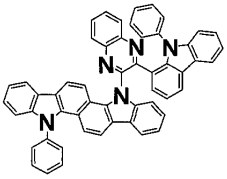
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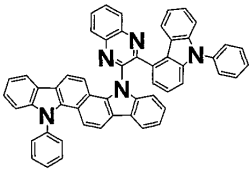
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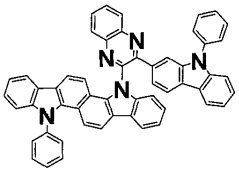
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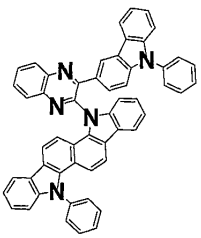
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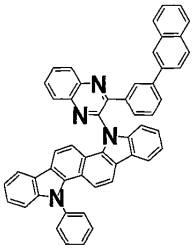
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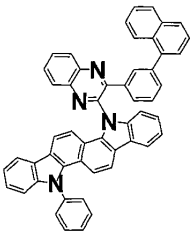
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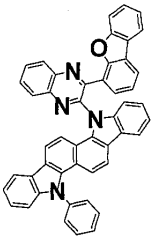
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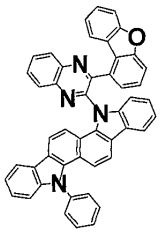
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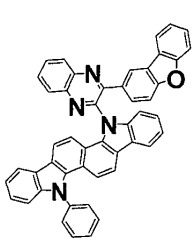
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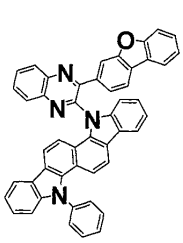
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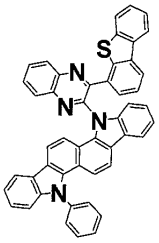
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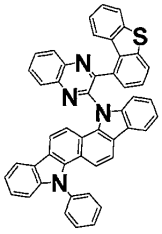
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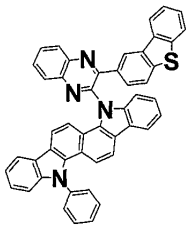
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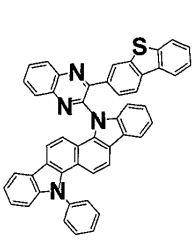
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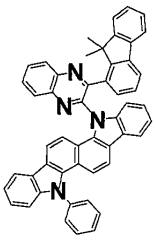
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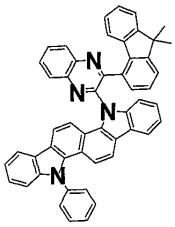
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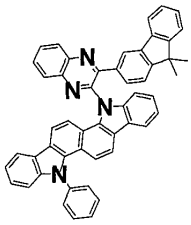
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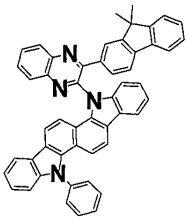
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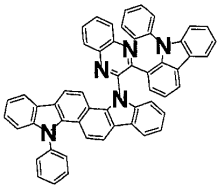
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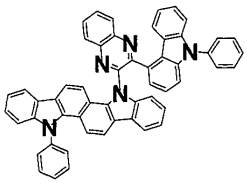
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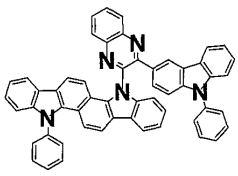
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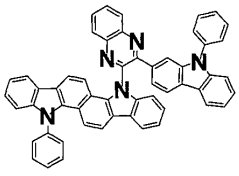
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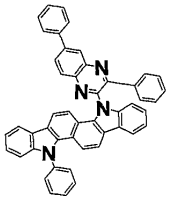
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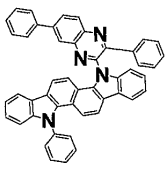
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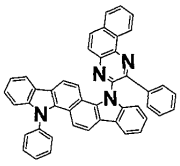
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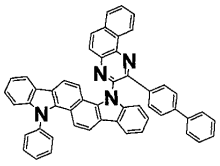
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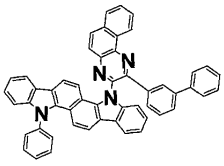
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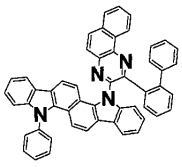
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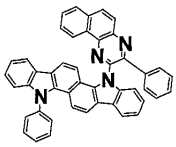
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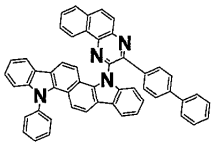
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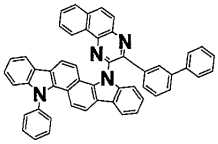
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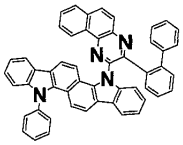
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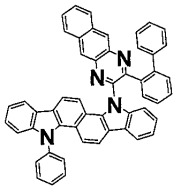
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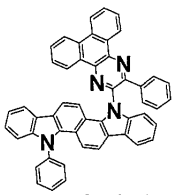
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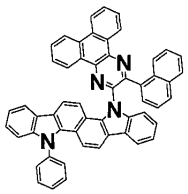
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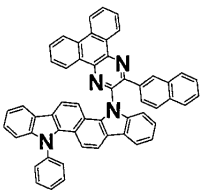
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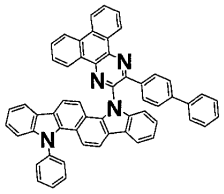
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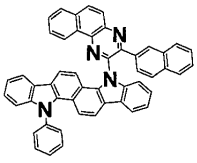
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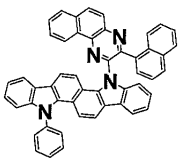
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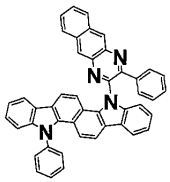
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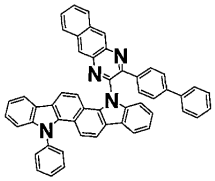
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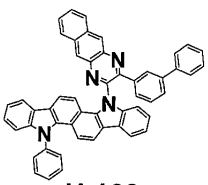
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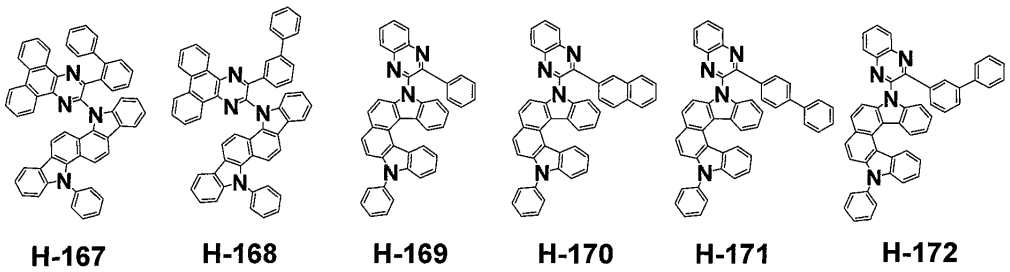
[0081] 
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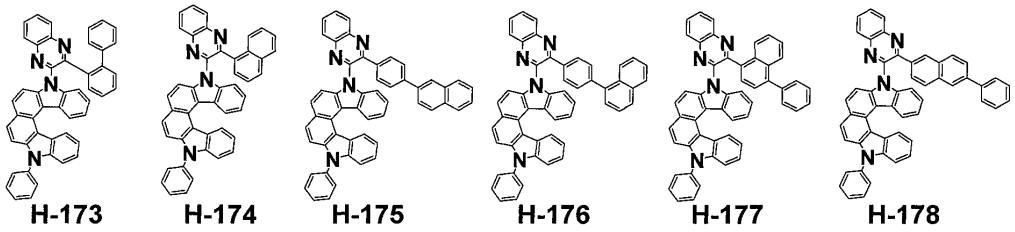
[0082] 
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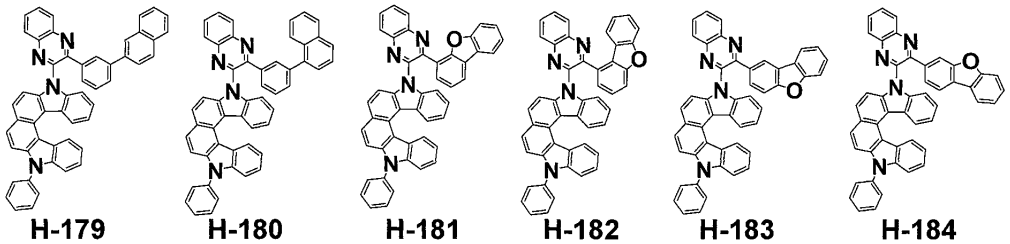
[0083] 
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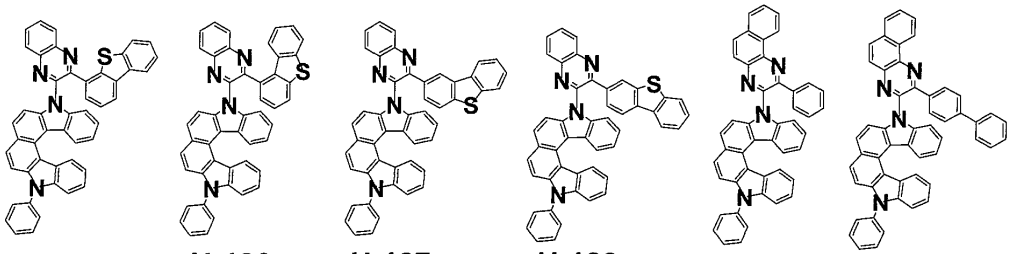
[0084] 
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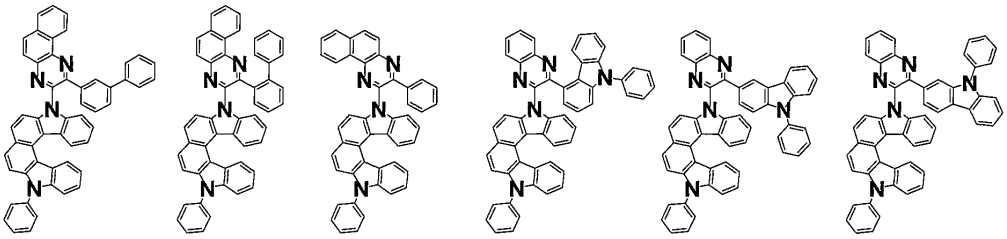
[0085] 
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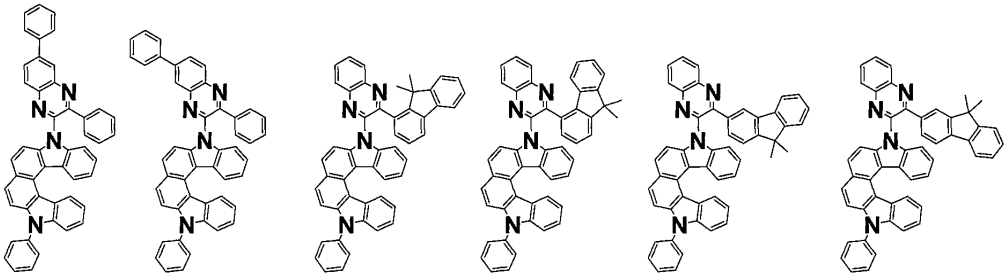
[0086] 
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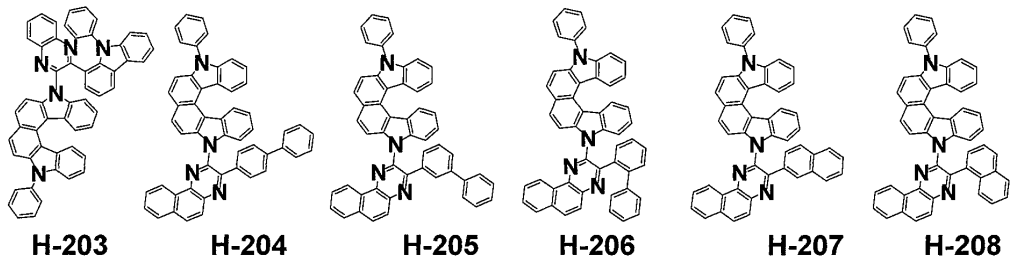
[0087] 
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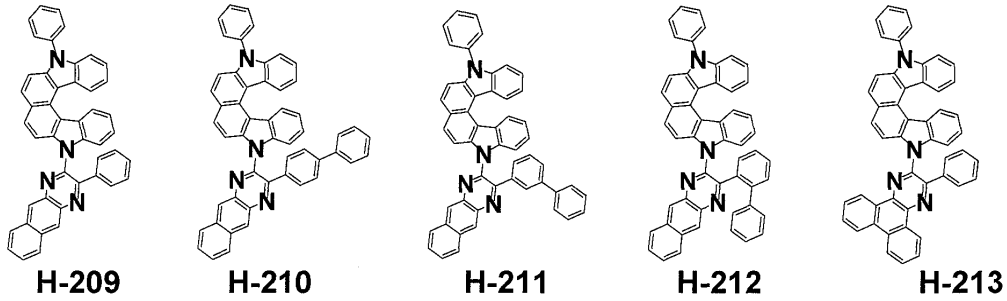
[0088] 
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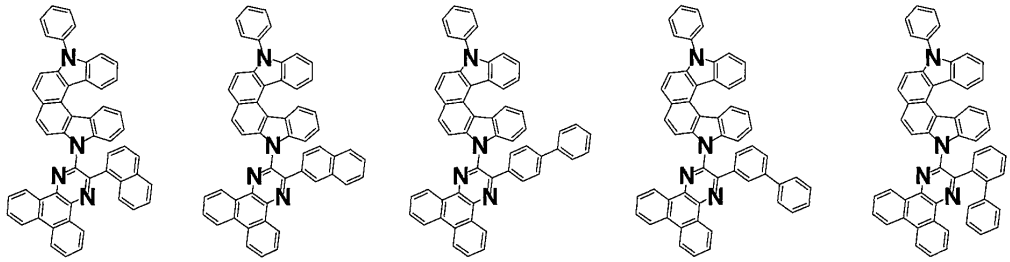
[0089] 
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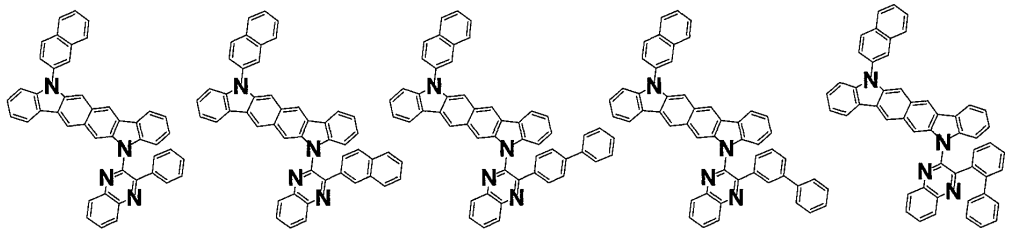
[0090] 
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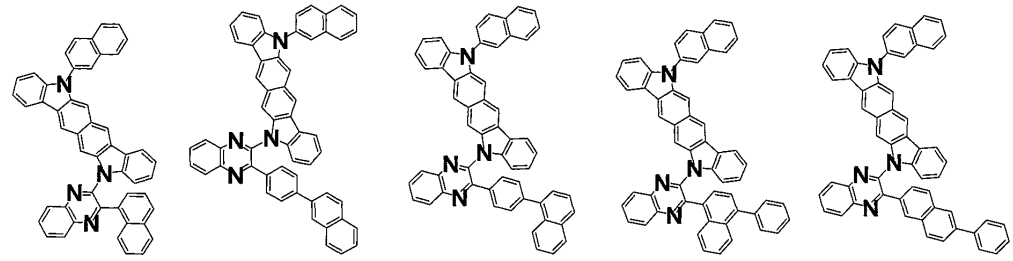
[0091] 
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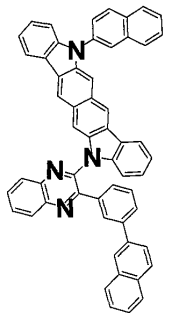
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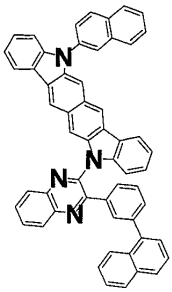
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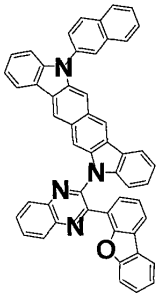
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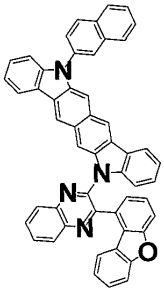
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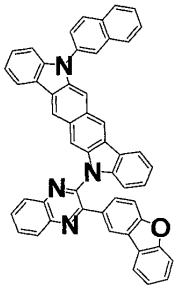
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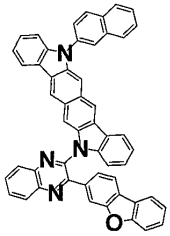
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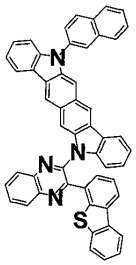
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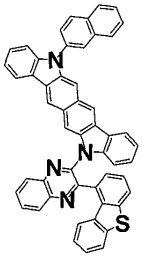
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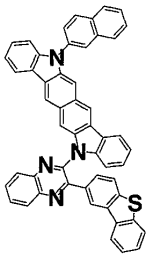
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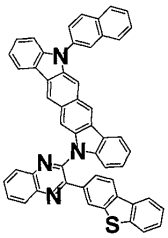
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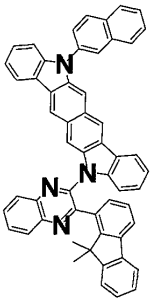
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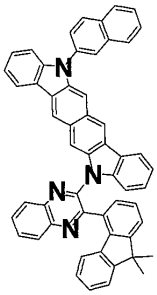
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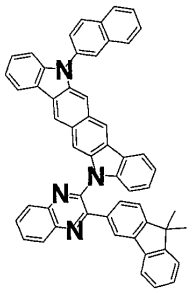
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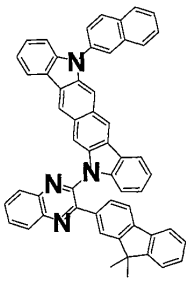
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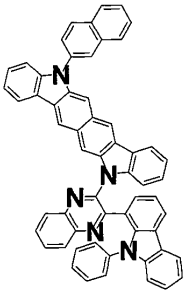
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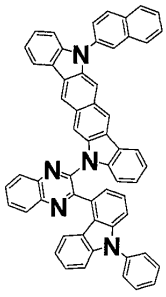
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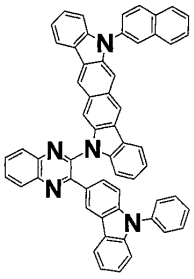
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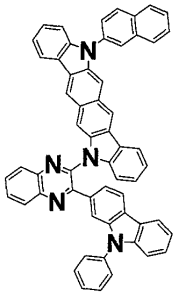
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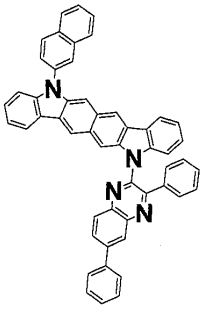
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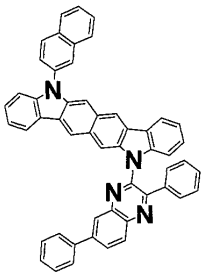
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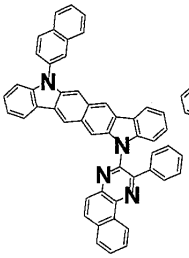
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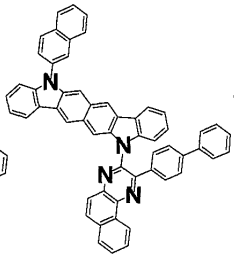
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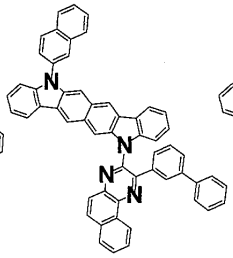
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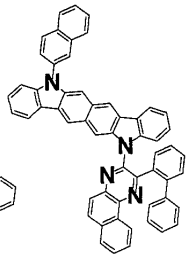
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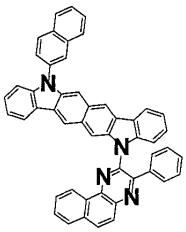
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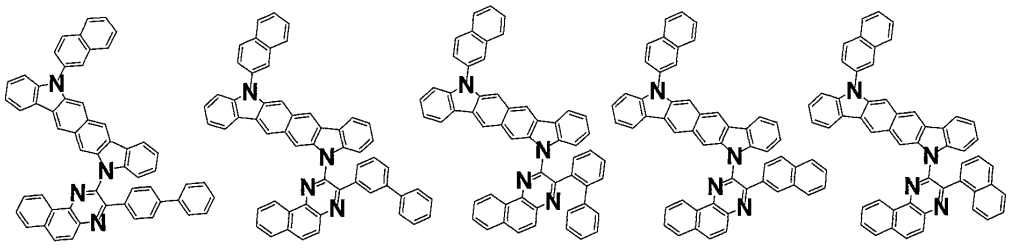

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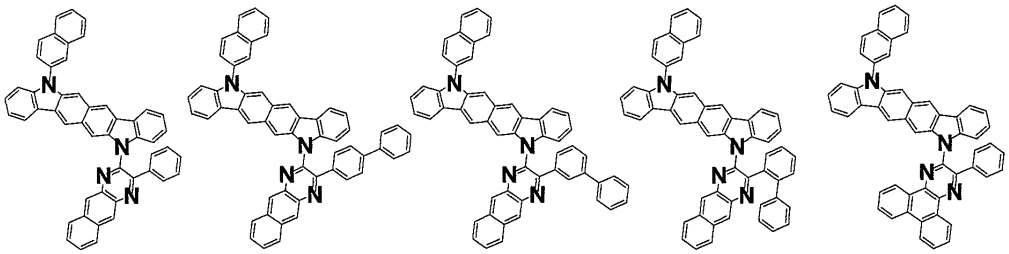

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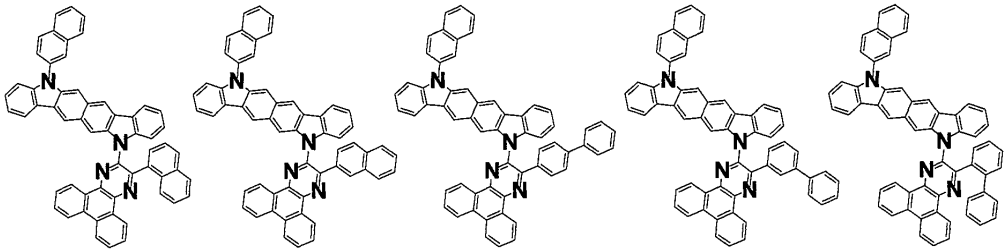

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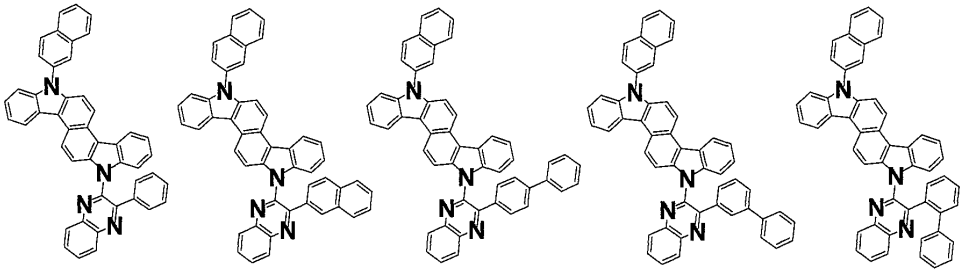

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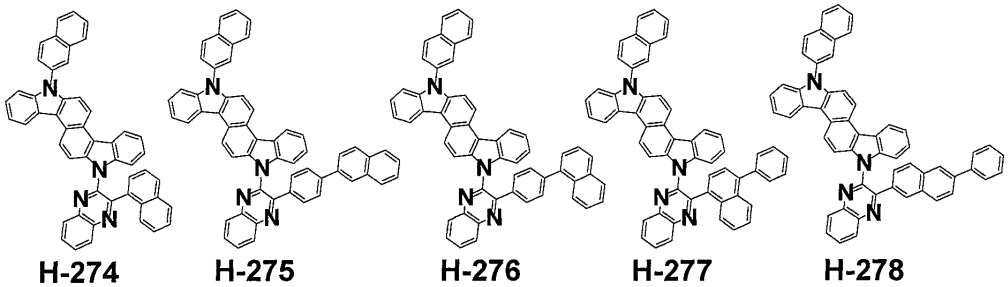

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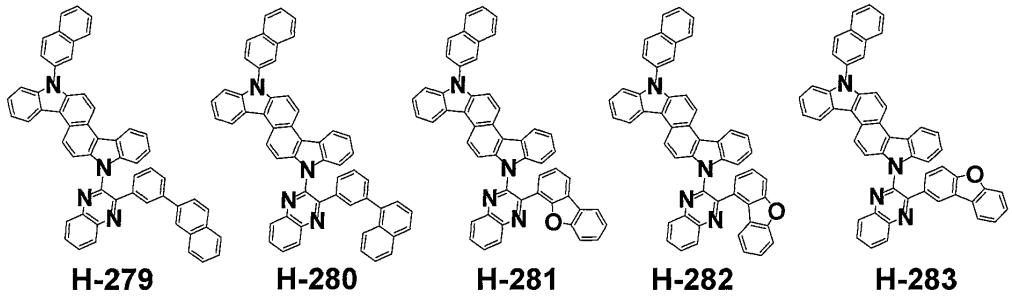
[0102] 
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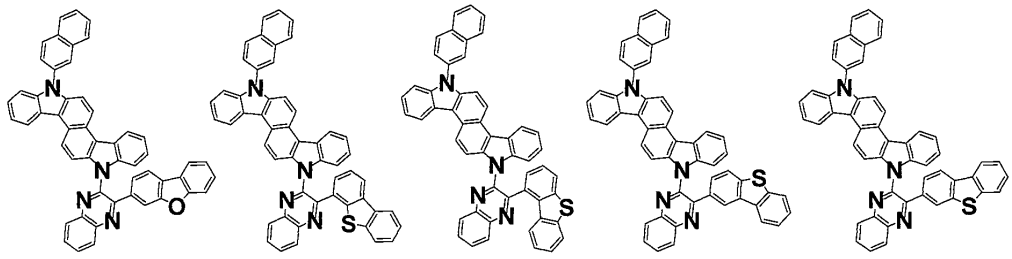
[0103] 
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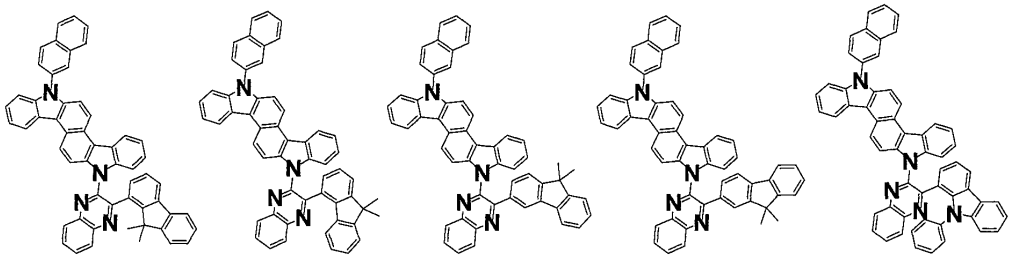
[0104] 
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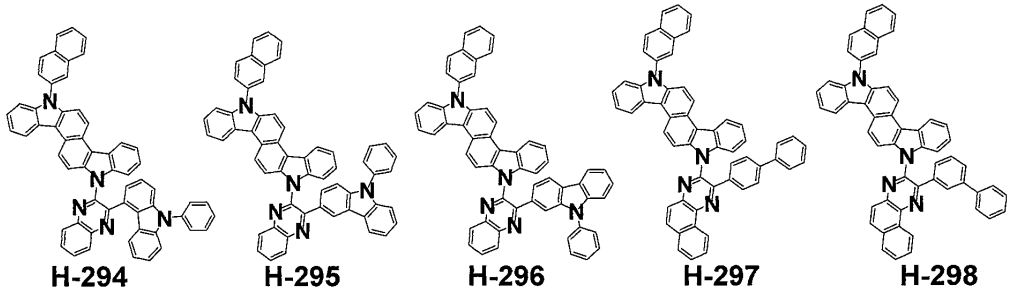
[0105] 
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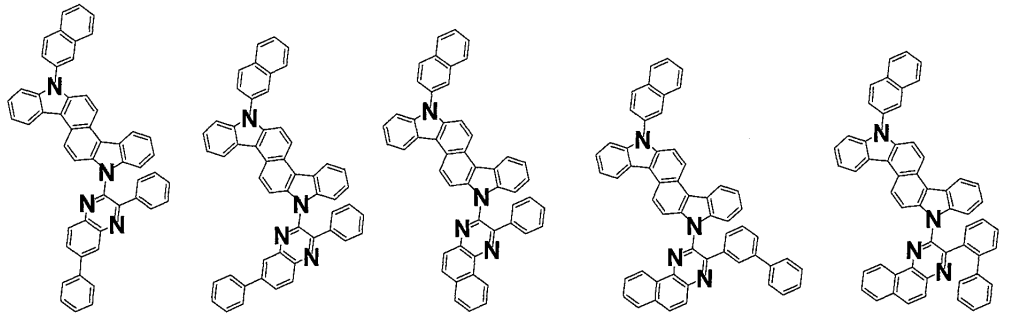
[0106] 
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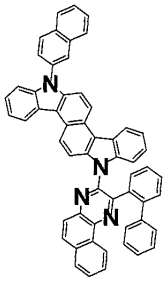
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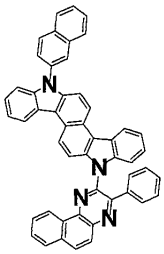
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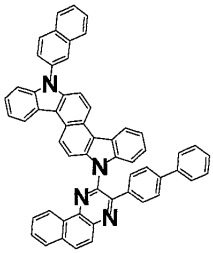
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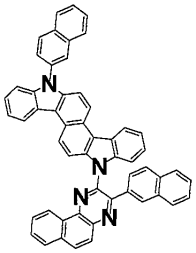
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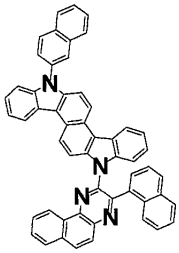
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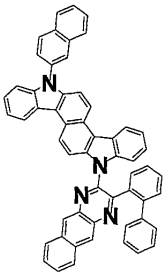
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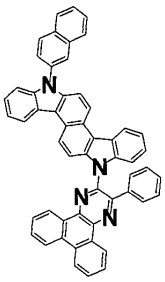
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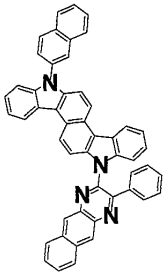
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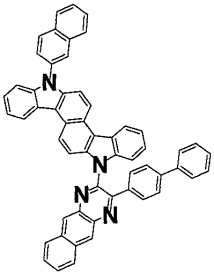
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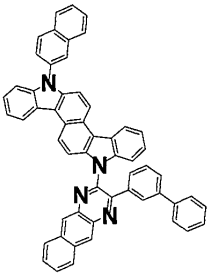
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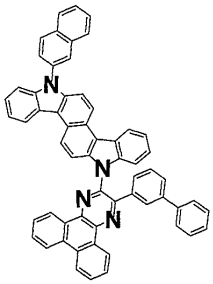
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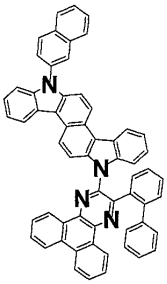
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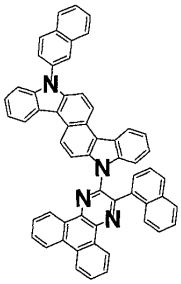
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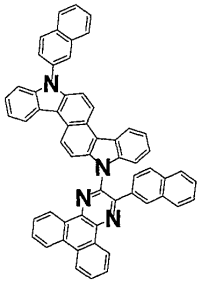
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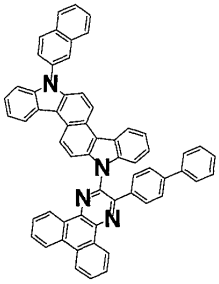
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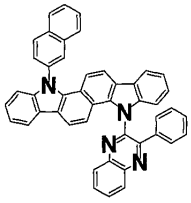
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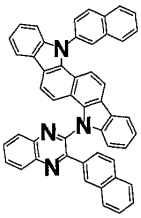
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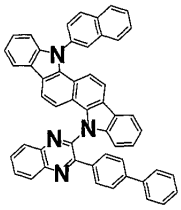
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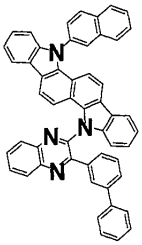
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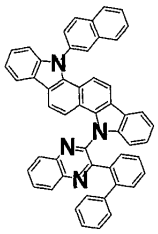
H-323

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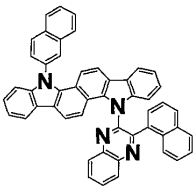
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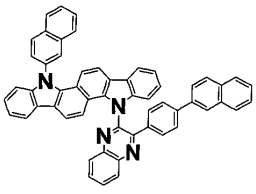
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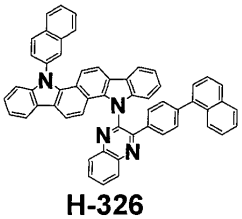
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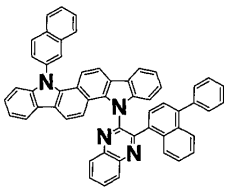
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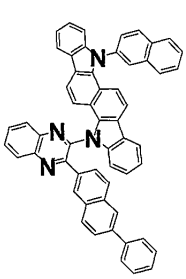
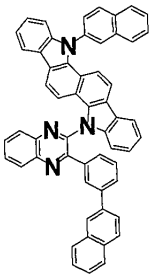
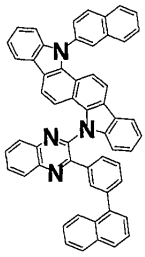
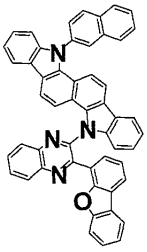
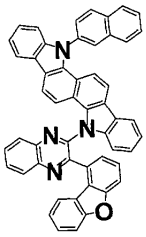
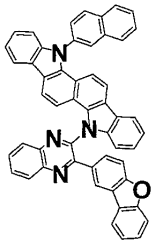
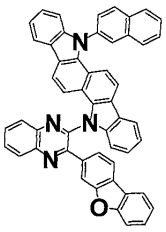
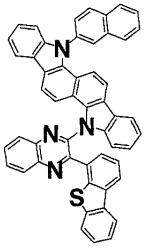
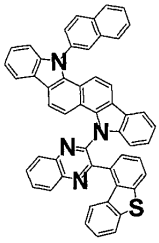
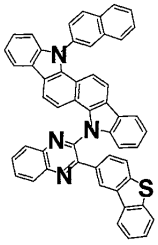
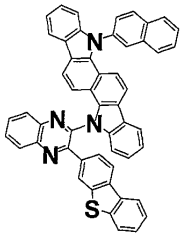
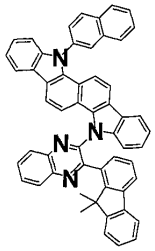
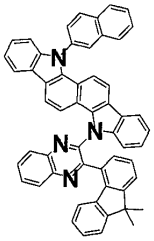
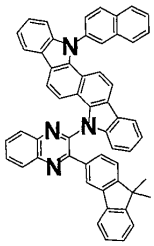
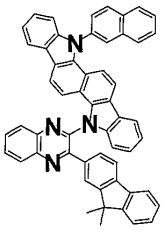
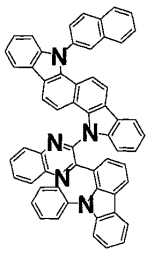
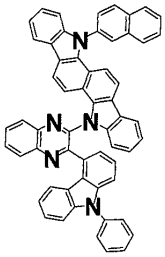
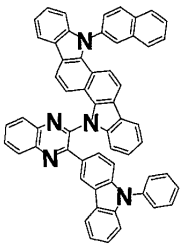
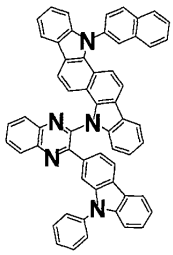
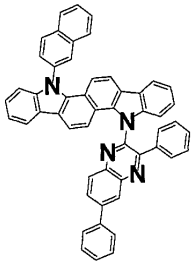
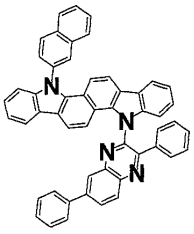
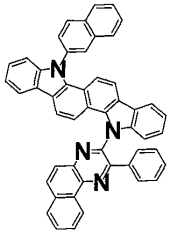
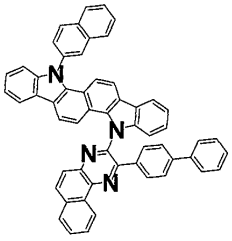
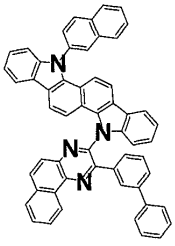
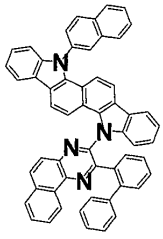
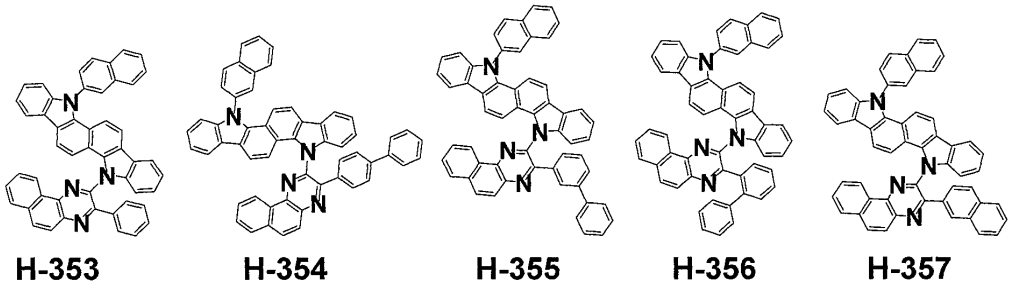
[0112]  H-328  H-329  H-330  H-331  H-332

[0113]  H-333  H-334  H-335  H-336  H-337

[0114]  H-338  H-339  H-340  H-341  H-342

[0115]  H-343  H-344  H-345  H-346  H-347

[0116]  H-348  H-349  H-350  H-351  H-352

[0117] 
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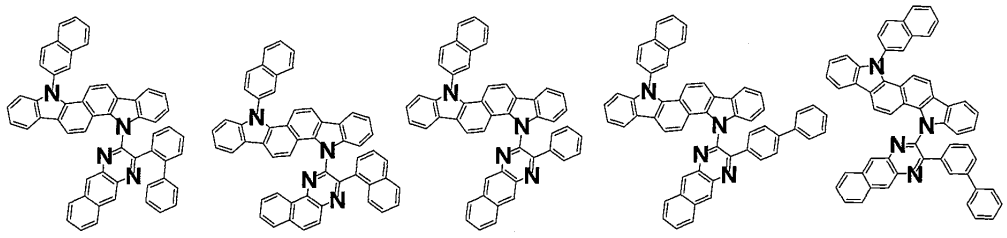
[0118] 
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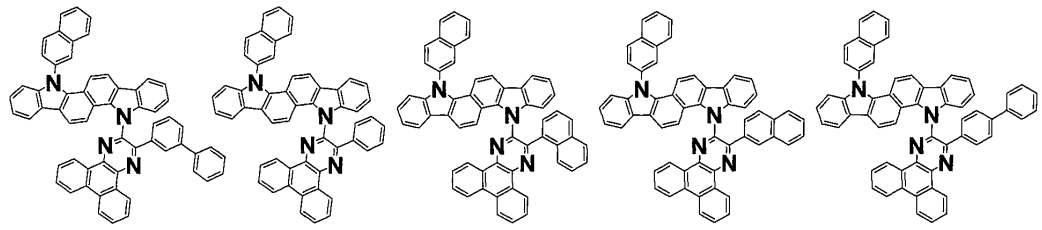
[0119] 
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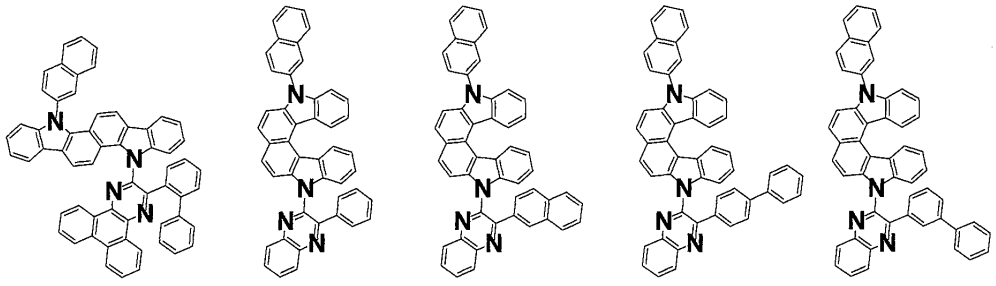
[0120] 
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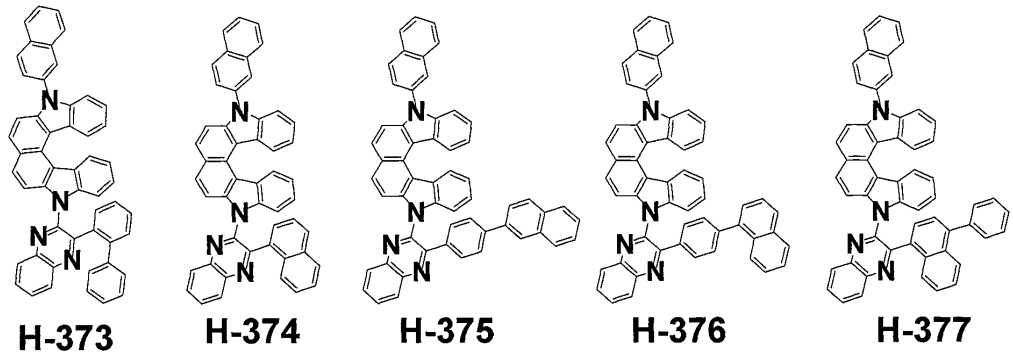
[0121] 
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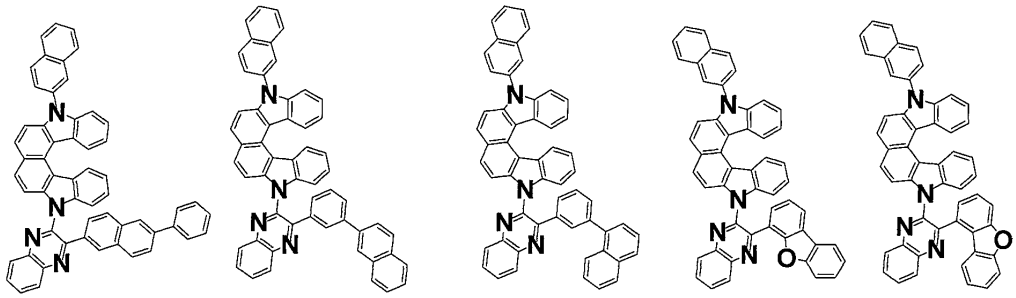


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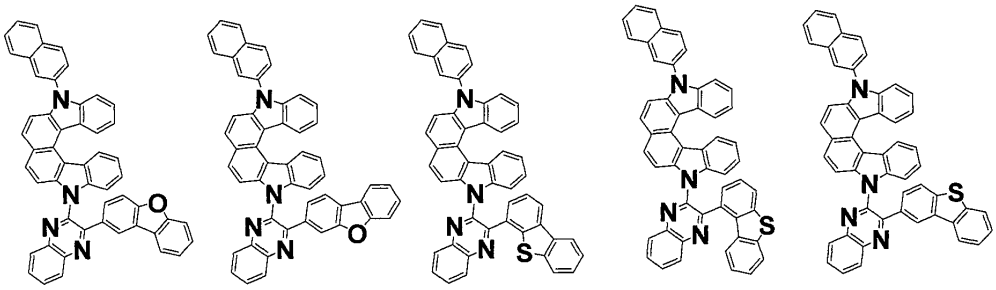


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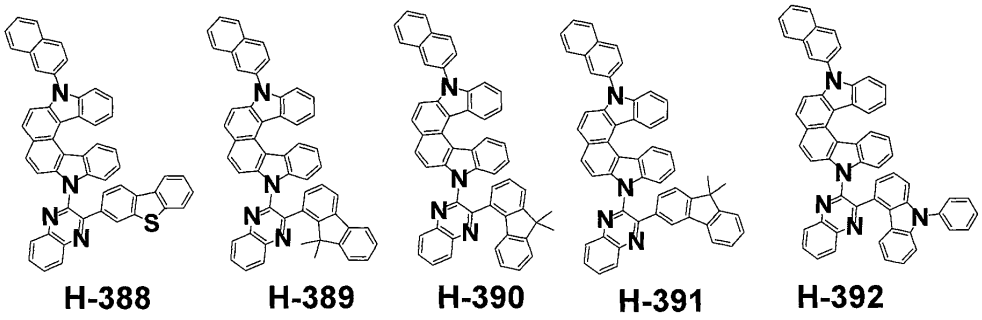


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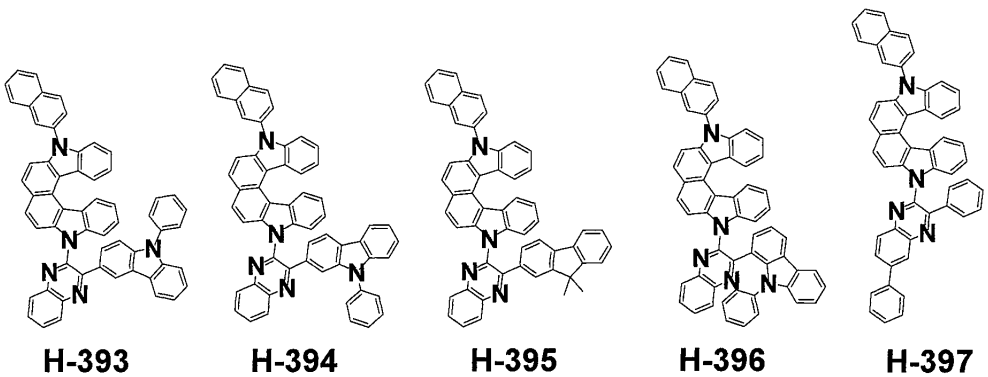


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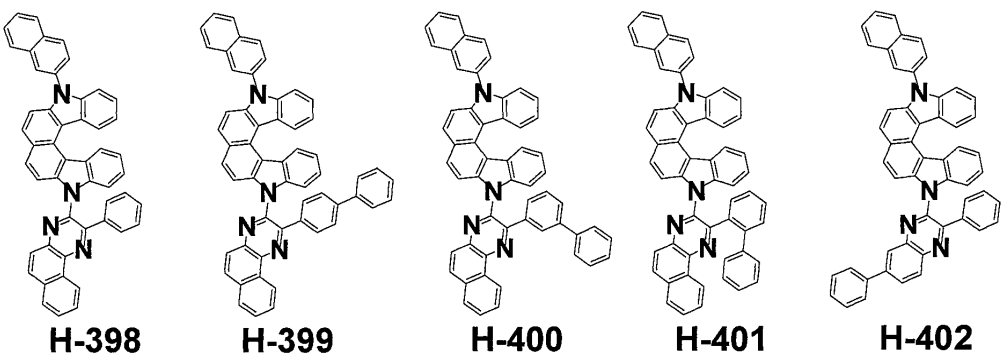
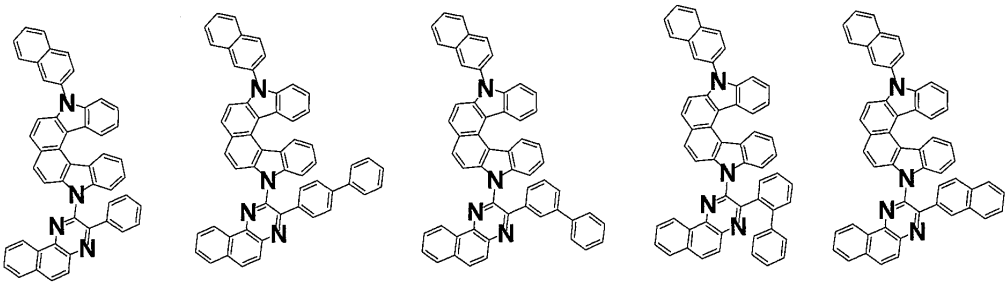


[0127] 
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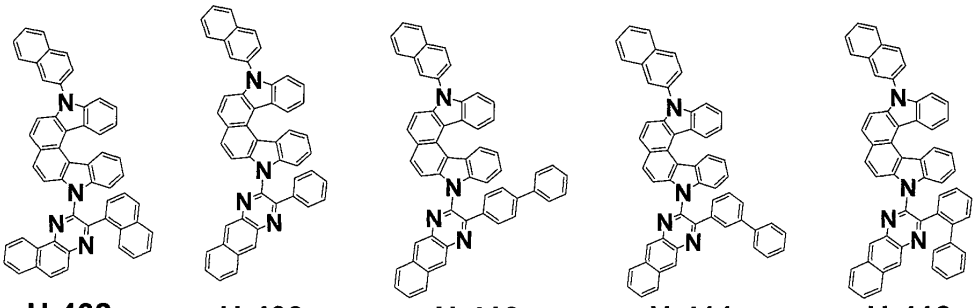
[0128] 
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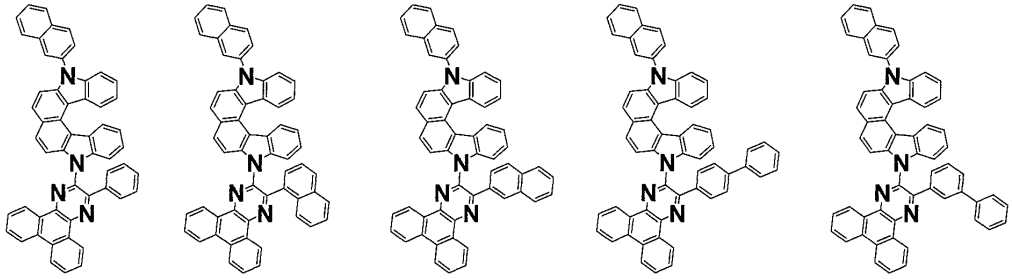
[0129] 
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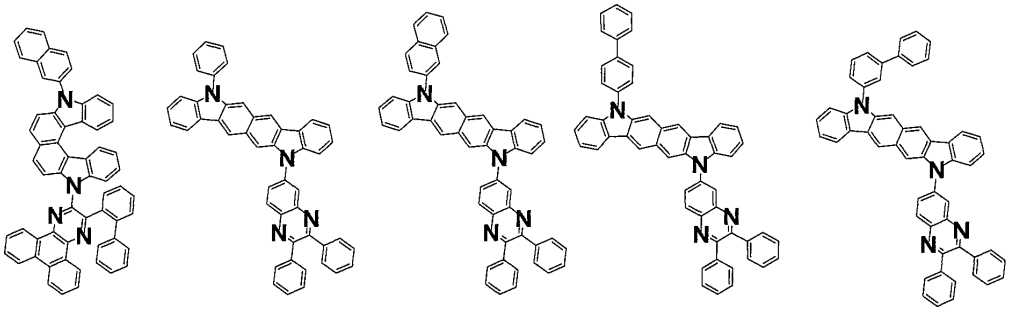
[0130] 
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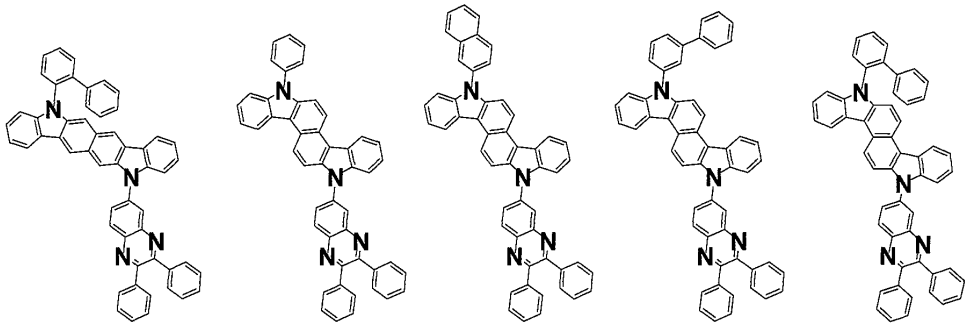
[0131] 
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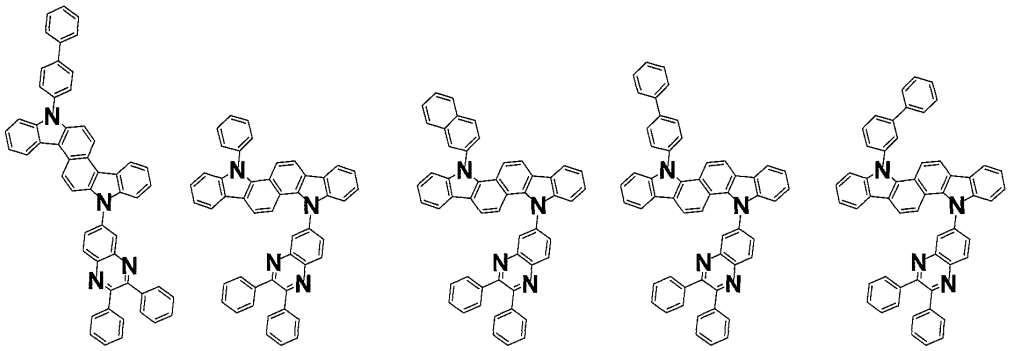
[0132] 
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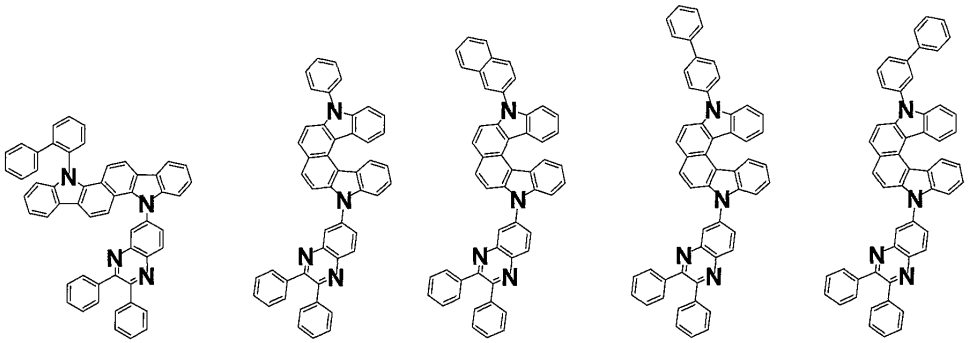
[0133] 
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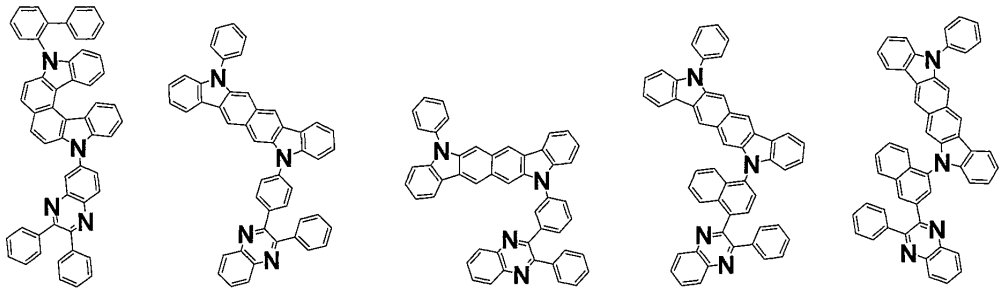
[0134] 
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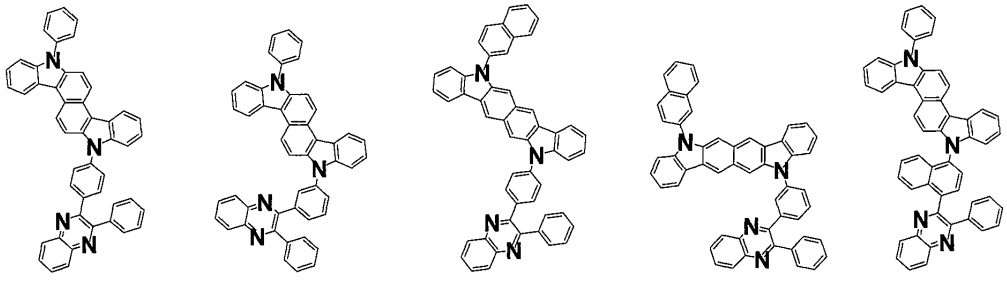
[0135] 
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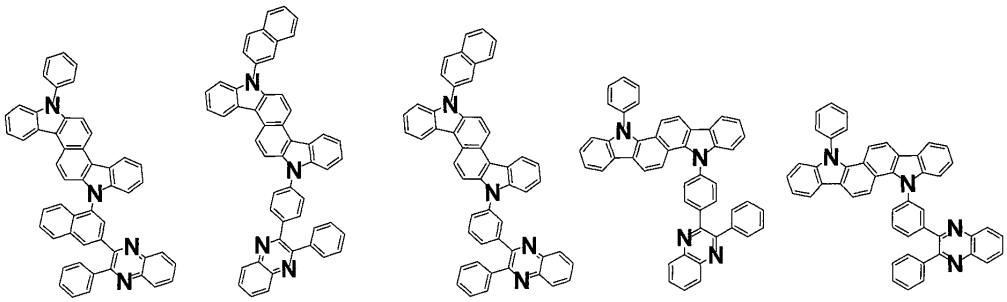

H-448 H-449 H-450 H-451 H-452

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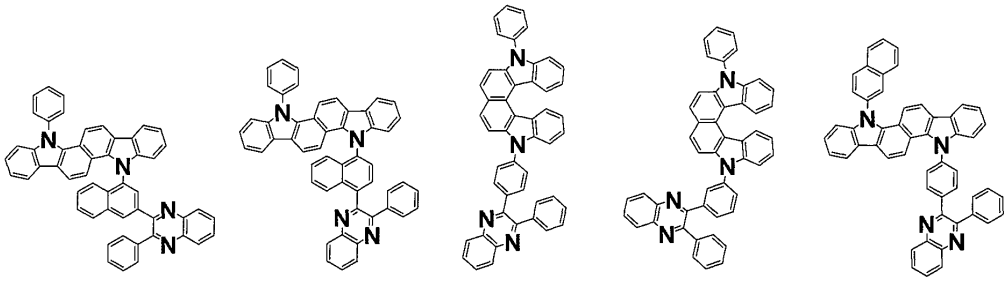

H-453 H-454 H-455 H-456 H-457

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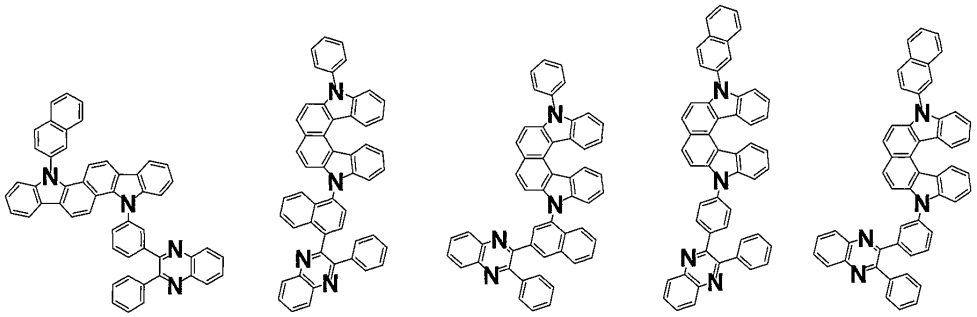

H-458 H-459 H-460 H-461 H-462

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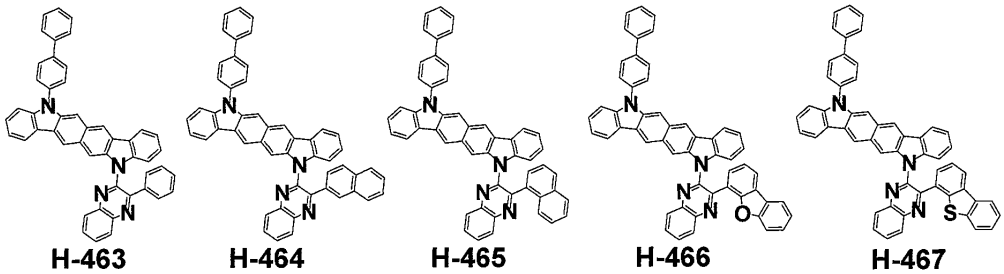

H-463 H-464 H-465 H-466 H-467

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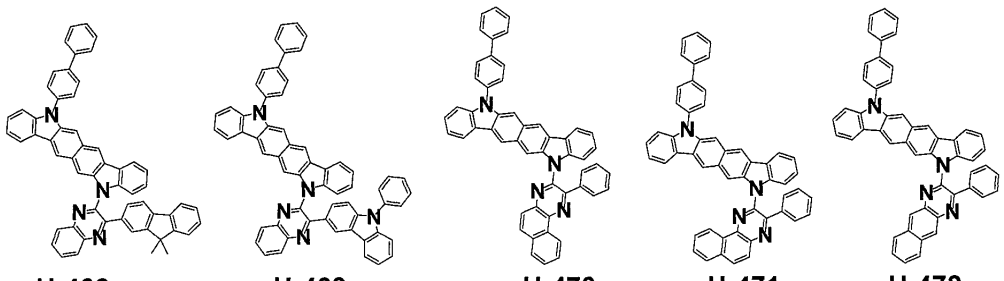
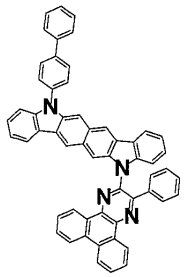
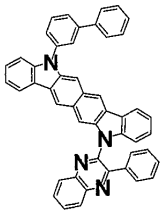
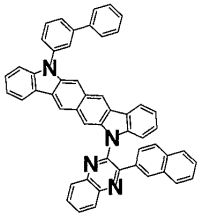
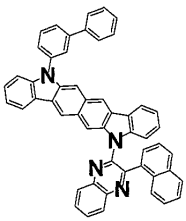
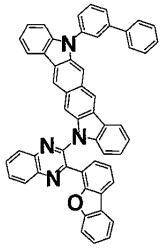
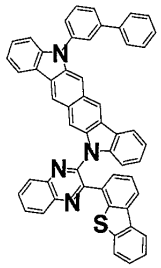
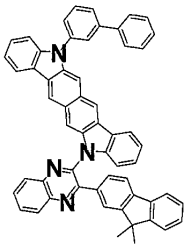
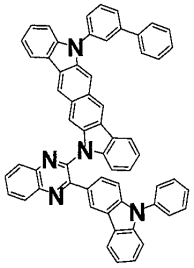
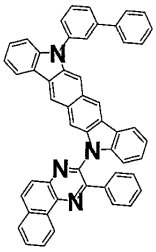
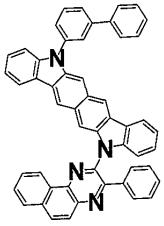
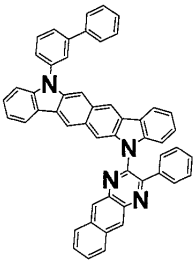
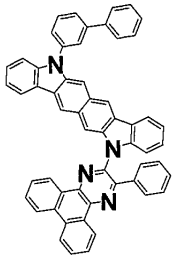
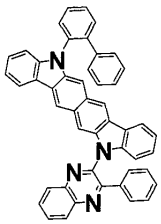
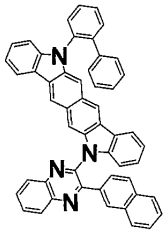
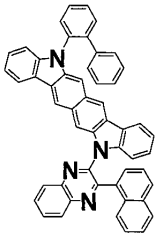
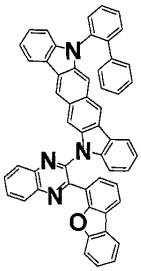
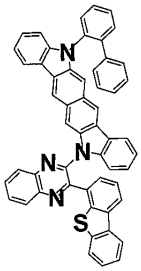
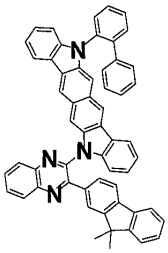
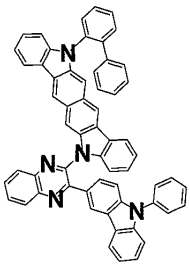
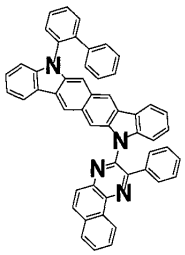


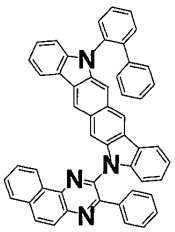
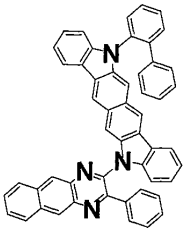
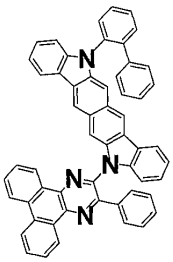
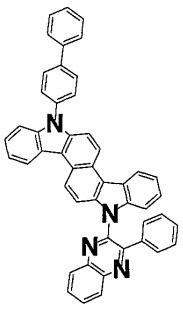
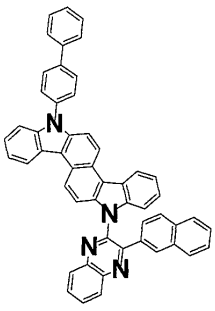
H-468 H-469 H-470 H-471 H-472

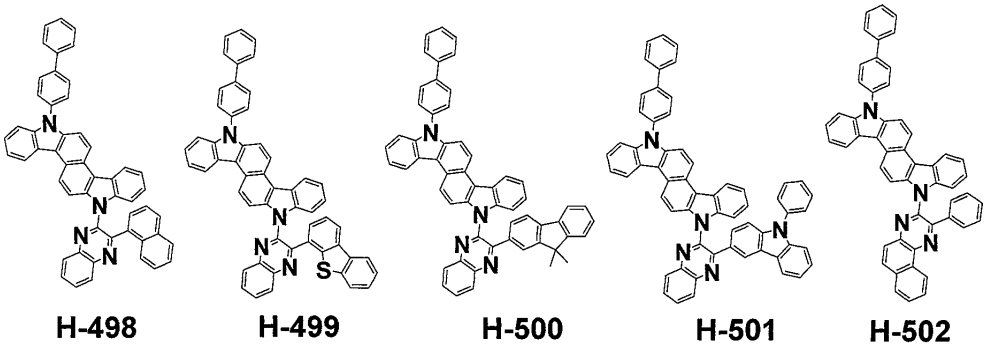
[0141]  H-473  H-474  H-475  H-476  H-477

[0142]  H-478  H-479  H-480  H-481  H-482

[0143]  H-483  H-484  H-485  H-486  H-487

[0144]  H-488  H-489  H-490  H-491  H-492

[0145]  H-493  H-494  H-495  H-496  H-497

[0146] 
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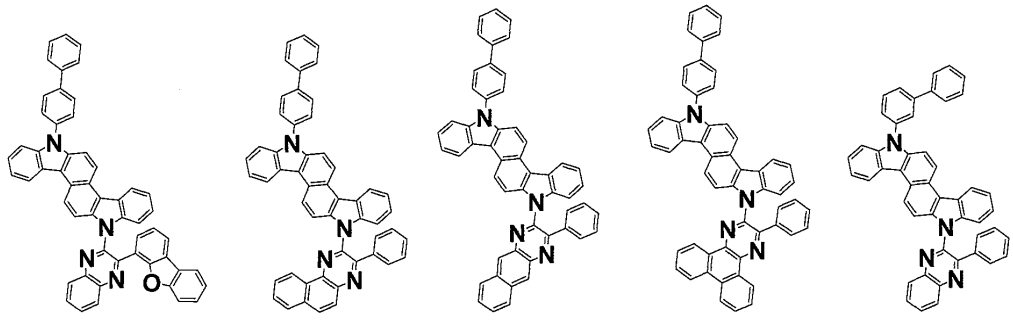
[0147] 
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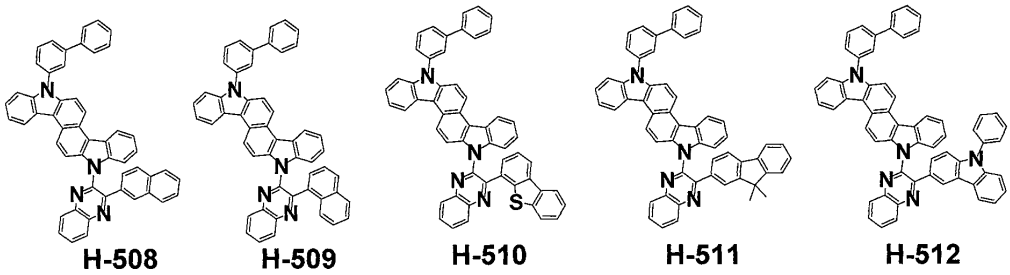
[0148] 
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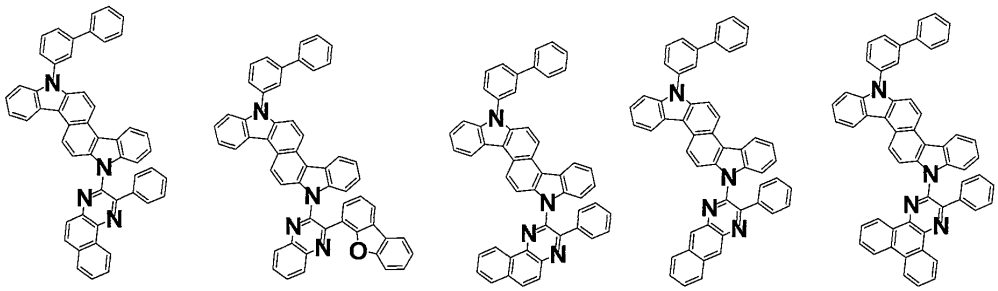
[0149] 
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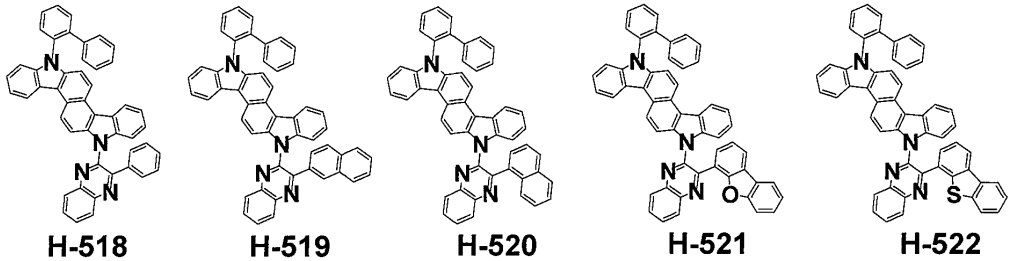
[0150] 
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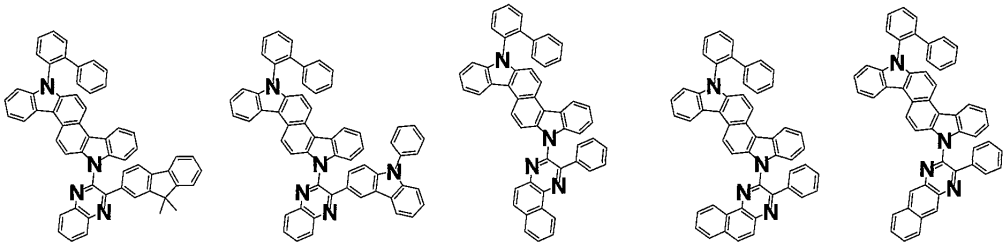

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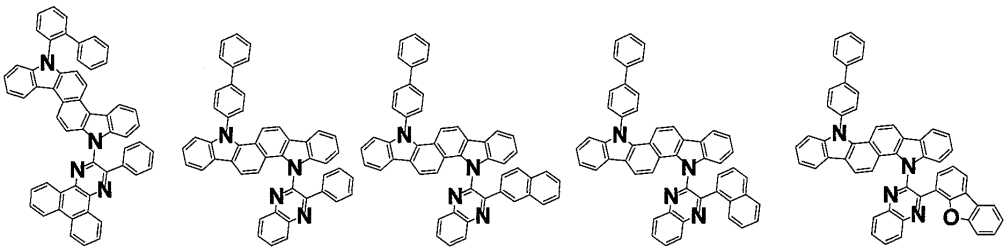

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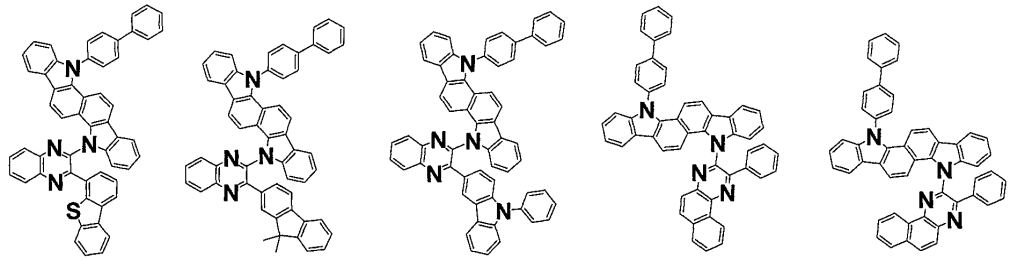

H-533 H-534 H-535 H-536 H-537

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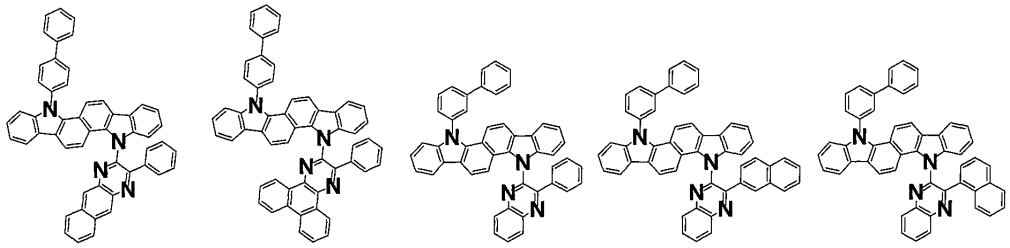

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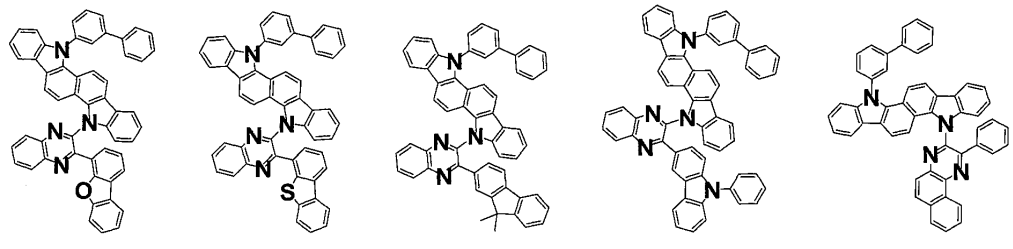
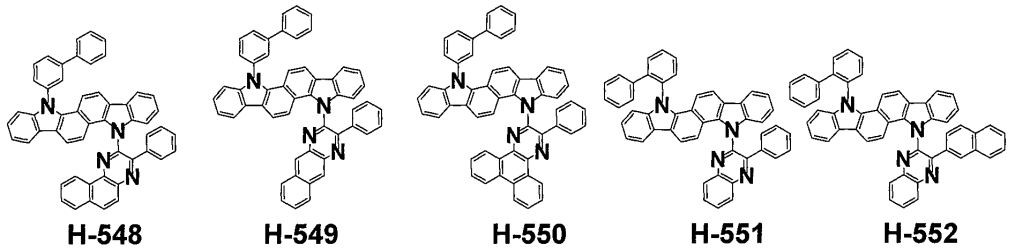


H-543 H-544 H-545 H-546 H-547

[0156]



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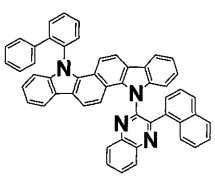
[0157]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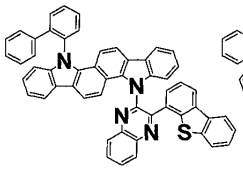
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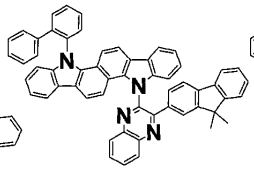
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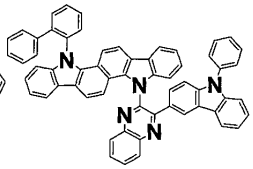
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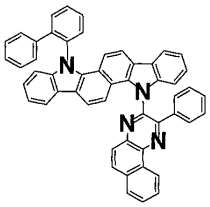
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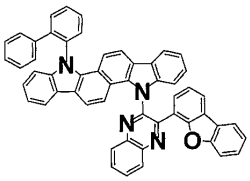
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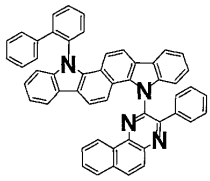
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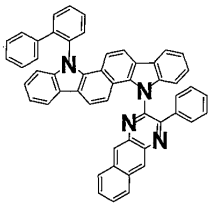
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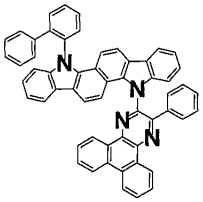
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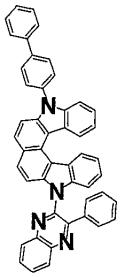
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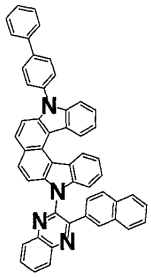
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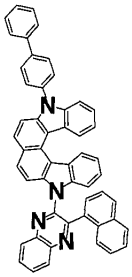
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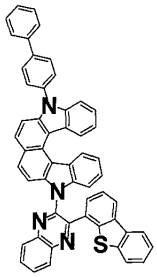
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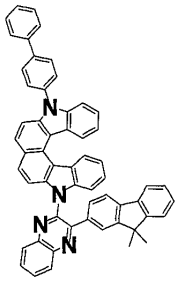
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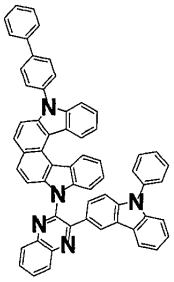
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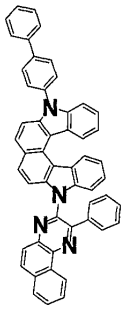
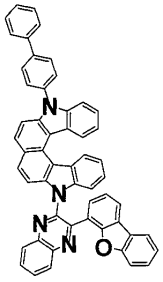

H-568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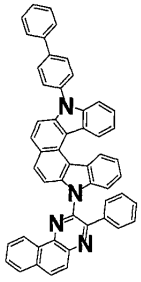
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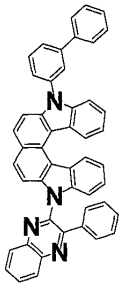
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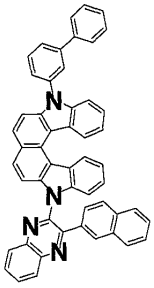
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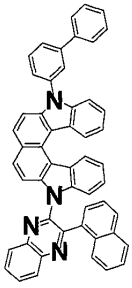
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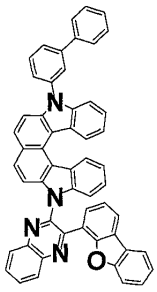
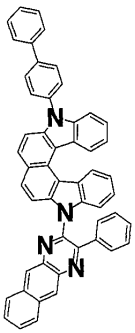
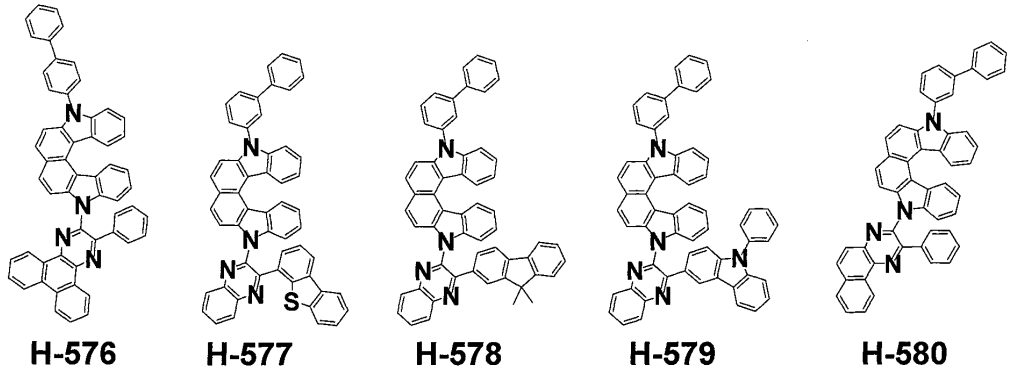
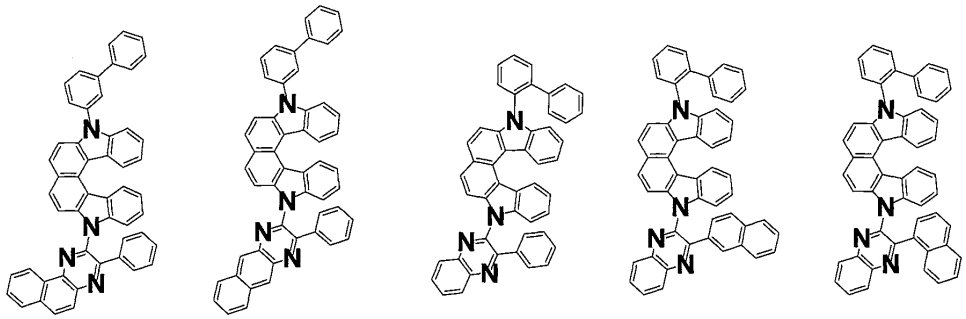
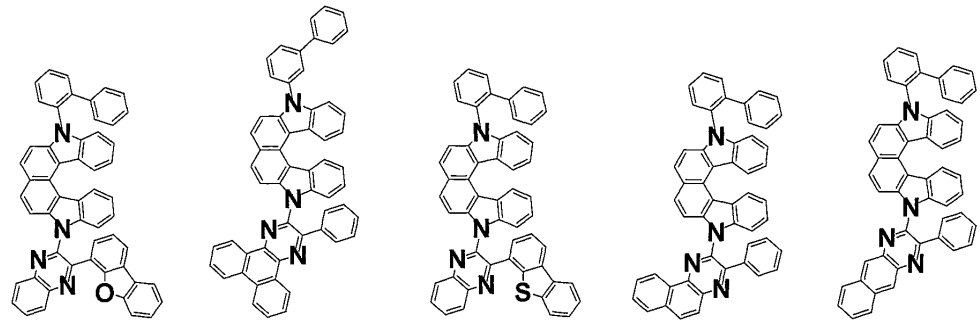
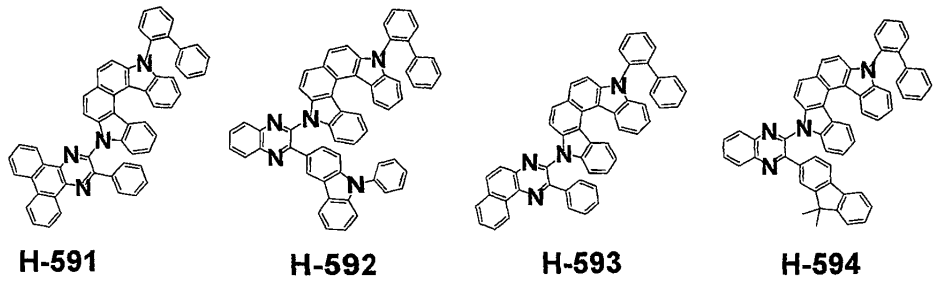

H-574


H-575

[0162] 
H-576 H-577 H-578 H-579 H-580

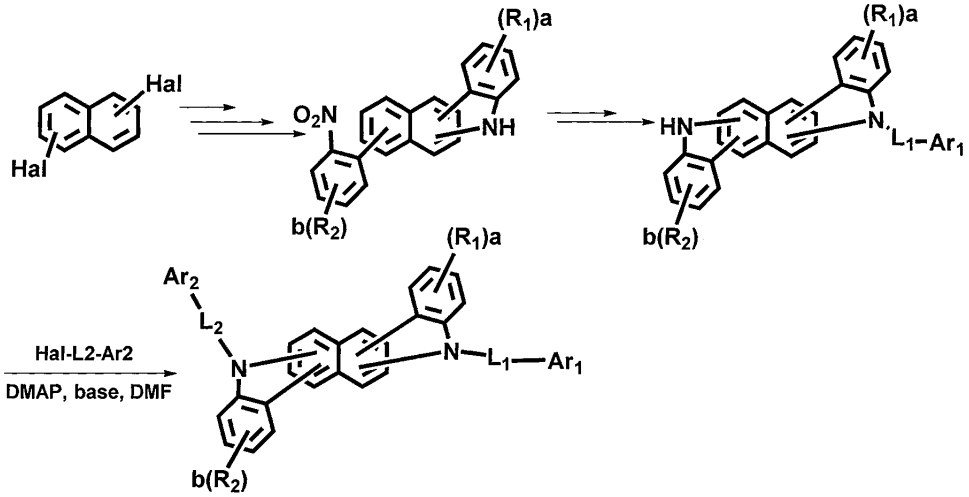
[0163] 
H-581 H-582 H-583 H-584 H-585

[0164] 
H-586 H-587 H-588 H-589 H-590

[0165] 
H-591 H-592 H-593 H-594

[0166] 본원에 따른 화학식 1의 화합물은 당업자에게 공지된 합성 방법으로 제조할 수 있으며, 예를 들면 하기 반응식 1에 나타난 바와 같이 제조할 수 있으나, 이에 한정되지는 않는다.

[0167] [반응식 1]




[0168]

[0169] 상기 반응식 1에서, $L_1$, $L_2$, $Ar_1$, $Ar_2$, $R_1$, $R_2$, a 및 b는 화학식 1에서의 정의와 동일하고, Hal는 할로겐원자이다.

[0170] 또한, 본원은 화학식 1의 유기 전계 발광 화합물을 포함하는 유기 전계 발광 재료, 및 상기 유기 전계 발광 재료를 포함하는 유기 전계 발광 소자를 제공할 수 있다. 상기 유기 전계 발광 재료는 본원의 유기 전계 발광 화합물 단독으로 이루어질 수 있고, 유기 전계 발광 재료에 포함되는 통상의 물질들을 추가로 포함할 수도 있다.

[0171] 한편, 본원에 따른 유기 전계 발광 소자는 제1 전극; 제2 전극; 및 상기 제1 전극 및 제2 전극 사이에 개재되는 1층 이상의 유기물층을 포함한다. 상기 유기물층은 상기 화학식 1의 유기 전계 발광 화합물을 하나 이상 포함할 수 있다. 또한, 상기 유기물층은 아릴아민계 화합물 및 스티릴아릴아민계 화합물로 이루어진 군으로부터 선택된 하나 이상의 화합물을 추가로 포함할 수 있다. 또한, 상기 유기물층은 1족, 2족, 4주기 전이금속, 5주기 전이금속, 란탄계열금속 및 d-전이원소의 유기금속으로 이루어진 군으로부터 선택되는 하나 이상의 금속, 또는 이러한 금속을 포함하는 하나 이상의 착체화합물을 추가로 포함할 수도 있다.

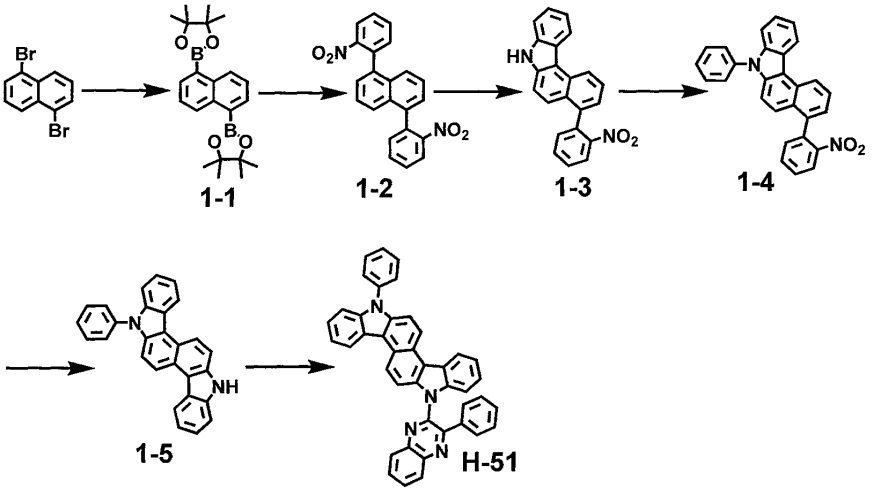
[0172] 상기 제1 전극과 제2 전극 중 하나는 양극(애노드)이고, 다른 하나는 음극(캐소드)일 수 있다. 상기 유기물층은 발광층을 포함하고, 정공 주입층, 정공 전달층, 정공 보조층, 발광 보조층, 전자 전달층, 전자 주입층, 계면층(interlayer), 정공 차단층, 전자 차단층, 및 전자 버퍼층에서 선택되는 1층 이상을 더 포함할 수 있다.

[0173] 본원의 화학식 1의 유기 전계 발광 화합물은 유기 전계 발광 소자의 발광층에 포함될 수 있다. 발광층에 사용될 경우, 본원의 화학식 1의 유기 전계 발광 화합물은 호스트 재료로서 포함될 수 있다. 바람직하게는, 상기 발광층은 하나 이상의 도판트를 추가로 더 포함할 수 있으며, 필요한 경우, 본원의 화학식 1의 유기 전계 발광 화합물 (제1 호스트 재료) 이외의 다른 화합물을 제2 호스트 재료로 추가로 포함할 수 있다. 이 때, 제1 호스트 재료와 제2 호스트 재료의 중량비는 1:99 내지 99:1 범위이다. 상기 제2 호스트 재료는 공지된 인광 호스트라면 어느 것이든 사용 가능하나, 이에 한정되는 것은 아니다.

[0174] 또한, 본원의 유기 전계 발광 화합물을 이용하여 표시 장치 또는 조명 장치를 제조하는 것이 가능하다. 구체적으로, 본원의 유기 전계 발광 소자를 포함하는 유기 전계 발광 소자를 이용하여 디스플레이 장치, 예를 들면, 스마트폰, 태블릿, 노트북, PC, TV 또는 차량용의 디스플레이 장치, 또는 조명 장치, 예를 들면, 옥외 또는 옥내용 조명 장치를 제조하는 것이 가능하다.

[0175] 이하에서, 본원의 상세한 이해를 위하여 본원의 대표 화합물을 들어 본원에 따른 화합물의 제조방법 및 이의 물성을 나타내었다. 그러나, 본원은 하기의 예들에 한정되는 것은 아니다.

[0176] **[실시예 1] 화합물 H-51의 제조**




[0177]

[0178] 화합물 1-1의 제조

[0179] 플라스크에 1,5-디브로모나프탈렌 (40 g, 140 mmol), 비스(피나코레이트)디보론 (78.14 g, 308 mmol), 비스(트리페닐포스핀)팔라듐(II) 디클로라이드 (3.9 g, 6 mmol), 포타슘 아세테이트 (60 g, 615 mmol), 및 1,4-디옥산 900 mL 를 넣고 녹인 후 120℃에서 3시간 동안 환류시켰다. 반응이 끝나면 에틸 아세테이트로 유기층을 분리하고 마그네슘 설페이트로 잔여수분을 건조시킨 후 컬럼 크로마토그래피로 분리하여 화합물 **1-1** (38 g, 71%) 를 얻었다.

[0180] 화합물 1-2의 제조

[0181] 플라스크에 화합물 **1-1** (38 g, 100 mmol), 1-브로모-2-니트로벤젠 (60.6 g, 300 mmol), 테트라키스트리페닐포스핀 팔라듐 (0) (23.1 g, 20 mmol), 탄산나트륨 (53 g, 500 mmol), 톨루엔 500 mL, 에탄올 250 mL, 물 250 mL 을 넣어 녹인 후 120℃에서 3시간 동안 환류시켰다. 반응이 끝나면 에틸아세테이트로 유기층을 분리하고 마그네슘 설페이트로 잔여수분을 건조시킨 후 컬럼 크로마토그래피로 분리하여 화합물 **1-2** (29.6 g, 79.9%) 를 얻었다.

[0182] 화합물 1-3의 제조

[0183] 플라스크에 화합물 **1-2** (30 g, 81 mmol), 트리페닐포스핀 (42.49 g, 162 mmol), 디클로로벤젠 405 mL 를 넣어 녹인 후 200℃에서 24시간 동안 환류시켰다. 반응이 끝나면 감압증류로 용매를 제거 한 후 컬럼 크로마토그래피로 분리하여 화합물 **1-3** (13.6 g, 49%) 를 얻었다.

[0184] 화합물 1-4의 제조

[0185] 플라스크에 화합물 **1-3** (13.6 g, 40 mmol), 아이오도벤젠 (12.3 g, 60 mmol), 쿠퍼아이오다이드 (5.3 g, 28 mmol), 1,2-디아미노시클로헥산 (6.8 g, 60 mmol), 세슘카보네이트 (39.3 g, 121 mmol), 및 자일렌 200 mL를 넣어 녹인 후 180℃에서 3시간 동안 환류시켰다. 반응이 끝나면 에틸 아세테이트로 유기층을 분리하고 마그세슘 설페이트로 잔여수분을 제거하고 건조시킨 후 컬럼 크로마토그래피로 분리하여 화합물 **1-4** (12 g, 75%)를 얻었다.

[0186] 화합물 1-5의 제조

[0187] 플라스크에 화합물 **1-4** (12 g, 48 mmol), 트리페닐포스핀 (30.38 g, 116 mmol), 및 디클로로벤젠 240 mL 를 넣어 녹인 후 200℃에서 24시간 동안 환류시켰다. 반응이 끝나면 감압증류로 용매를 제거한 후 컬럼 크로마토그래피로 분리하여 화합물 **1-5** (9 g, 82%)를 얻었다.

[0188] 화합물 H-51의 제조

[0189] 플라스크에 화합물 **1-5** (5 g, 13 mmol), 2-클로로-3-페닐퀴녹살린 (3.4 g, 14 mmol), 탄산칼륨 (5.4 g, 39 mmol), 디메틸아미노피리딘 (80 mg, 0.654 mmol), 및 디메틸포름아마이드 65 mL 를 넣어 녹인 후 180℃에서 24시간 동안 환류시켰다. 반응이 끝나면 에틸 아세테이트로 유기층을 추출하고 마그네슘 설페이트를 이용하여 잔

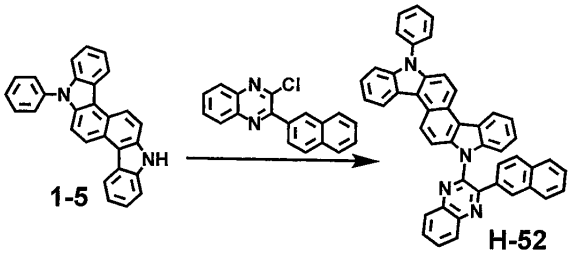
여 수분을 제거한 뒤 건조시키고 컬럼 크로마토그래피로 분리하여 화합물 **H-51** (4.2g, 54%) 를 얻었다.

[0190] $^1$H NMR (600MHz,CDCl3, δ) 8.935-8.915 (d, J=9Hz, 1H), 8.826-8.811 (d, J=9Hz, 1H), 8.648-8.635 (d, J=7.8Hz, 2H), 8.377-8.361 (d, J=7.8Hz, 1H), 8.251-8.236 (d, J=7.8Hz, 1H), 7.929-7.896 (m, 2H), 7.831-7.816 (d, J=9H, 1H), 7.695-7.640 (m, 5H), 7.555-7.524 (m, 2H), 7.465-7.403 (m, 6H), 7.361-7.349 (m, 1H), 7.110-7.065 (m, 3H)

[0191]

| 화합물 | MW | Tg | M.P. |
|---|---|---|---|
| H-51 | 586.70 | 158.2 | 310 |

[0192] **[실시예 2] 화합물 H-52의 제조**

[0193] 

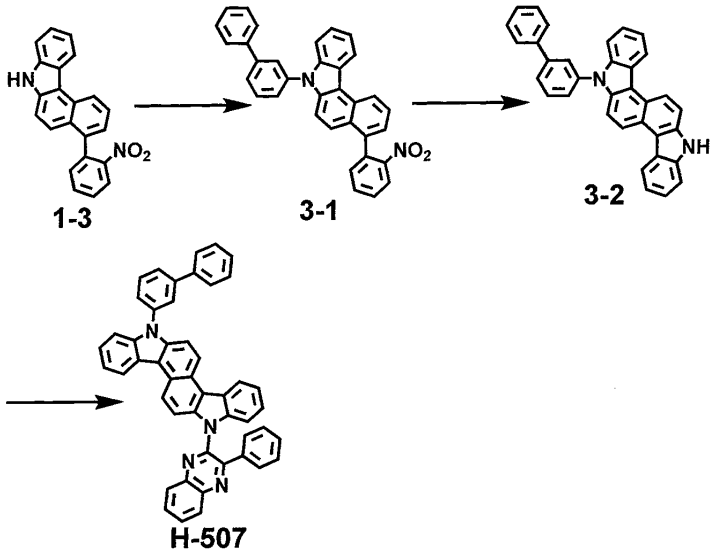

[0194] 플라스크에 화합물 **1-5** (3.8 g, 10 mmol), 2-클로로-3-나프틸퀴녹살린 (3.178 g, 11 mmol), 탄산칼륨 (4.1 g, 30 mmol), 디메틸 아미노 피리딘 (61 mg, 0.497 mmol), 및 디메틸포름아마이드 50 mL 를 넣어 녹인 후, 180℃에서 24시간 동안 환류시켰다. 반응이 끝나면 에틸 아세테이트로 유기층을 추출하고 마그네슘 설페이트를 이용하여 잔여 수분을 제거한 뒤 건조시키고 컬럼 크로마토그래피로 분리하여 화합물 **H-52** (1.5 g, 23.7%) 를 얻었다.

[0195] $^1$H NMR (600MHz,$CDCl_3$, δ) 8.905-8.890 (d, J=9Hz, 1H), 8.795-8.779 (d, J=9.6Hz, 1H), 8.615-8.580 (m, 2H), 8.396-8.382 (d, J=8.4Hz, 1H), 8.248-8.234 (d, J=8.4Hz, 1H), 8.121 (s, 1H), 7.928-7.887 (m, 2H), 7.801-7.786 (d, J=9Hz, 1H), 7.751-7.736 (d, J=9Hz, 1H), 7.669-7.612 (m, 4H), 7.574-7.489 (m, 4H), 7.448-7.415 (m, 4H),7.339-7.284 (m, 5H)

[0196]

| 화합물 | MW | Tg | M.P. |
|---|---|---|---|
| H-52 | 636.76 | 162.87 | 292 |

[0197] **[실시예 3] 화합물 H-507의 제조**




[0198]

[0199] 화합물 3-1의 제조

[0200] 플라스크에 화합물 **1-3** (11 g, 33 mmol), 아이오도바이페닐 (13.6 g, 49 mmol), 쿠퍼아이오다이드 (4.3 g, 23 mmol), 1,2-디아미노시클로헥산 (5.8 mL, 49 mmol), 세슘카보네이트 (31.7 g, 99 mmol), 및 자일렌 162 mL를 넣어 녹인 후, 180℃에서 3시간 동안 환류시켰다. 반응이 끝나면 에틸 아세테이트로 유기층을 분리하고 마그세슘 설페이트로 잔여수분을 제거하고 건조시킨 후 컬럼 크로마토그래피로 분리하여 화합물 **3-1** (15 g, 94%)를 얻었다.

[0201] 화합물 3-2의 제조

[0202] 플라스크에 화합물 **3-1** (15 g, 31 mmol), 트리페닐포스핀 (19.2 g, 73 mmol), 디클로로벤젠 152 mL를 넣어 녹인 후, 200℃에서 24시간 동안 환류시켰다. 반응이 끝나면 감압증류로 용매를 제거한 후 컬럼 크로마토그래피로 분리하여 화합물 **3-2** (11 g, 78%)를 얻었다.

[0203] 화합물 H-507의 제조

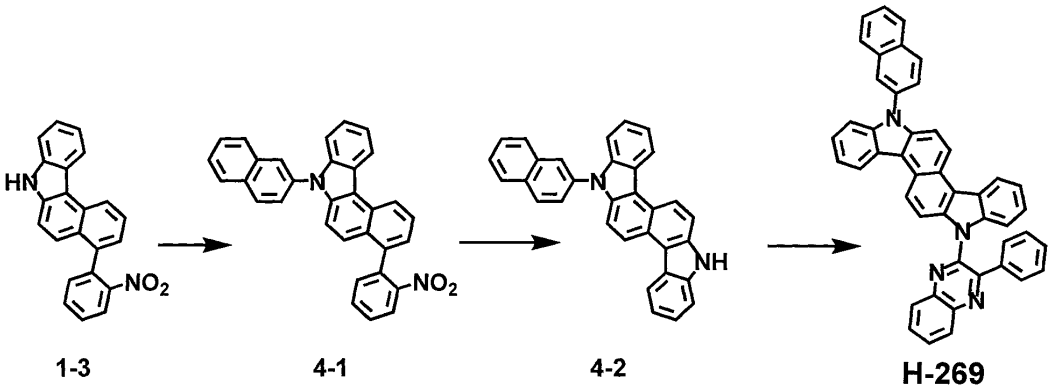
[0204] 플라스크에 화합물 **3-2** (6 g, 13 mmol), 2-클로로-3-페닐퀴녹살린 (3.4 g, 14 mmol), 탄산칼륨 (5.4 g, 39 mmol), 디메틸아미노피리딘 (799 mg, 7 mmol), 디메틸포름아마이드 64 mL 를 넣어 녹인 후, 180℃에서 24시간 동안 환류시켰다. 반응이 끝나면 에틸 아세테이트로 유기층을 추출하고 마그네슘 설페이트를 이용하여 잔여 수분을 제거한 뒤 건조시키고 컬럼 크로마토그래피로 분리하여 화합물 **H-507** (1.3 g, 15%) 를 얻었다.

[0205] $^1$H NMR (600MHz,CDCl3, δ) 8.935-8.920 (d, J=9Hz, 1H), 8.822-8.807 (d, J= 9Hz, 1H), 8.650-8.624 (t, J=7.8Hz, 2H), 8.365-8.350 (d, J=8.4Hz, 1H), 8.240-8.227 (d, J=7.8Hz, 1H), 7.916-7.873 (m, 4H), 7.767-7.735 (m, 2H) 7.694-7.673 (m, 3H), 7.629-7.584 (m, 2H), 7.493-7.389 (m, 9H), 7.348-7.336 (t, J=7.2Hz, 1H), 7.097-7.053 (m, 3H)

[0206]

| 화합물 | MW | Tg | M.P. |
|---|---|---|---|
| H-507 | 662.8 | 158.68 | 278 |

[0207] **[실시예 4] 화합물 H-269의 제조**

[0208] 


1-3 4-1 4-2 H-269

[0209] 화합물 4-1의 제조

[0210] 플라스크에 화합물 **1-3** (49 g, 144.8 mmol), 2-브로모 나프탈렌 (55.1 g, 217 mmol), 쿠퍼아이오다이드 (27.5 g, 101.3 mmol), 1,2-디아미노시클로헥산 (26 mL, 217.2 mmol) 세슘카보네이트 (141 g, 424 mmol), 및 자일렌 724 mL을 넣어 녹인 후, 180℃ 에서 3시간 동안 환류시켰다. 반응이 끝나면 에틸 아세테이트로 유기층을 분리하고 마그세슘 설페이트로 잔여수분을 제거하고 건조시킨 후 컬럼 크로마토그래피로 분리하여 화합물 **4-1** (44.7 g, 66.7%) 을 얻었다.

[0211] 화합물 4-2의 제조

[0212] 플라스크에 화합물 **4-1** (44.7 g, 96.2 mmol), 트리페닐포스핀 (60.5 g, 230 mmol) 및 디클로로벤젠 481 mL 를 넣어 녹인 후 200℃ 에서 24시간 동안 환류시켰다. 반응이 끝나면 감압증류로 용매를 제거한 후 컬럼 크로마토그래피로 분리하여 화합물 **4-2** (25 g, 61%) 를 얻었다.

[0213] 화합물 H-269의 제조

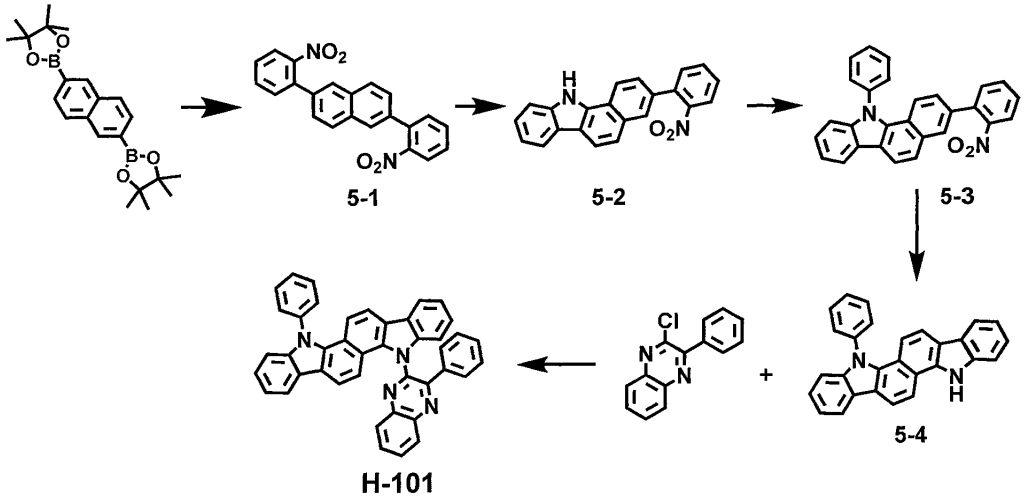
[0214] 플라스크에 화합물 **4-2** (25 g, 57.8 mmol), 2-클로로-3-페닐퀴녹살린 (16.6 g, 69.4 mmol), 탄산칼륨 (24 g, 173 mmol), 디메틸아미노피리딘 (353 mg, 2.89 mmol) 및 디메틸포름아마이드 385 mL 를 넣어 녹인 후 180℃ 에서 24시간 동안 환류시켰다. 반응이 끝나면 에틸 아세테이트로 유기층을 추출하고 마그네슘 설페이트를 이용하여 잔여 수분을 제거한 뒤 건조시키고 컬럼 크로마토그래피로 분리하여 화합물 **H-269** (16 g, 43%)를 얻었다.

[0215] $^1$H NMR (600MHz,DMSO,δ) 9.031-9.016 (d, J= 9 Hz, 1H), 8.915-8.900 (d, J=9Hz, 1H), 8.779-8.766 (d, J= 7.8Hz, 1H), 8.748-8.734 (d, J= 8.4Hz, 1H), 8.413-8.397 (d, J=8.4Hz, 1H), 8.352 (s, 1H), 8.314-8.300 (d, J= 8.4Hz, 1H), 8.259-8.245 (d, J=6.6Hz, 1H), 8.192-8.121 (m, 2H), 8.073-8.032 (m, 2H), 7.902-7.855(m, 3H), 7.702-7.687 (m, 2H), 7.591-7.577 (d, J=8.4Hz, 1H), 7.511-7.497 (t, J= 8.4Hz, 2H), 7.460-7.446 (m, 3H), 7.408-7.372 (m, 2H), 7.168-7.134 (m, 3H)

[0216]

| 화합물 | MW | Tg | M.P. |
|---|---|---|---|
| H-269 | 636.76 | 173.2 | 301 |

[0217] **[실시예 5] 화합물 H-101의 제조**




[0218]

[0219] 화합물 5-1의 제조

[0220] 플라스크에 2,6-비스(4,4,5,5-테트라메틸-1,3,2-디옥사보로란-2-일)나프탈렌 (51.6 g, 135.7 mmol), 1-브로모-2-니트로벤젠(82.2 g, 407.2 mmol), 테트라키스트리페닐포스핀 팔라듐(0) (31.4 g, 27.1 mmol), 탄산칼륨 (93.8 g, 678.5 mmol), 톨루엔 400 mL, 에탄올 340 mL, 및 물 340 mL을 넣어 녹인 후 120℃에서 환류시켰다. 반응이 끝나면 에틸아세테이트로 유기층을 분리하고 마그네슘 설페이트로 잔여수분을 건조 시킨 후 컬럼 크로마토그래피로 분리하여 화합물 **5-1** (42.6 g, 84%) 을 얻었다.

[0221] 화합물 5-2의 제조

[0222] 플라스크에 화합물 **5-1** (42.6 g, 115 mmol), 트리페닐포스핀 (60.3 g, 230 mmol), 디클로로벤젠 575 mL를 넣어 녹인 후 200℃ 에서 24시간 동안 환류시켰다. 반응이 끝나면 감압증류로 용매를 제거한 후 컬럼 크로마토그래피로 분리하여 화합물 **5-2** (20 g, 51%) 를 얻었다.

[0223] 화합물 5-3의 제조

[0224] 플라스크에 화합물 **5-2** (8.4 g, 24.8 mmol), 아이오도벤젠 (5.5 mL, 49.6 mmol), 트리스(디벤질리덴아세톤)디팔라듐(0) (1.1 g, 1.24 mmol), 트리-tert-부틸포스핀 (1.2 mL, 2.48 mmol), 나트륨-tert-부톡시드 (7.15 g, 74.4 mmol), 및 자일렌 124 mL를 넣어 녹인 후 180℃에서 3시간 동안 환류시켰다. 반응이 끝나면 에틸아세테이트로 유기층을 분리하고 마그네슘 설페이트로 잔여수분을 제거하고 건조시킨 후 컬럼 크로마토그래피로 분리하여 화합물 **5-3** (7.2 g, 70.5%) 를 얻었다.

[0225] 화합물 5-4의 제조

[0226] 플라스크에 화합물 **5-3** (7.2 g, 17.3 mmol), 트리페닐포스핀 (10.9 g, 41.6 mmol) 및 디클로로벤젠 87 mL를 넣어 녹인 후 200℃ 에서 24시간 동안 환류시켰다. 반응이 끝나면 감압증류로 용매를 제거한 후 컬럼 크로마토그래피로 분리하여 화합물 **5-4** (4.5 g, 66%) 를 얻었다.

[0227] 화합물 H-101의 제조

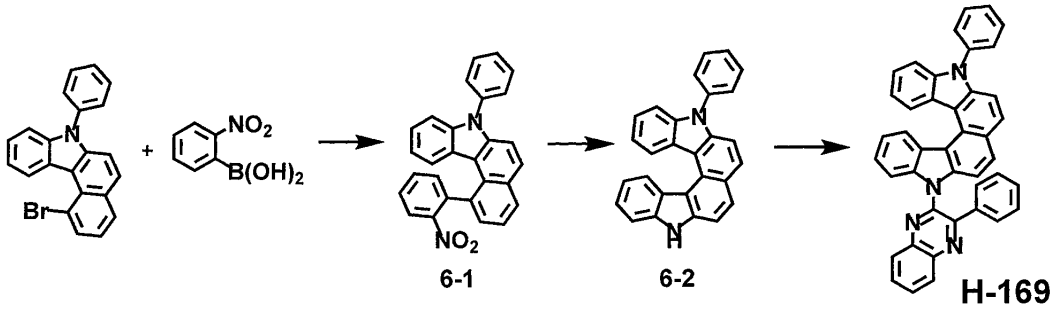
[0228] 플라스크에 화합물 **5-4** (4.5 g, 11.7 mmol), 2-클로로-3-페닐퀴녹살린 (16 g, 35.3 mmol), 세슘카보네이트 (40.4 g, 140.4 mmol), 디메틸아미노피리딘 (3 g, 23.4 mmol), 및 디메틸포름아마이드 110 mL를 넣어 녹인 후 230℃ 에서 24시간 동안 환류시켰다. 반응이 끝나면 에틸아세테이트로 유기층을 추출하고 마그네슘설페이트를 이용하여 잔여수분을 제거한 뒤 건조시키고 컬럼 크로마토그래피로 분리하여 화합물 **H-101** (1 g, 14%) 를 얻었다.

[0229] $^1$H NMR (600MHz,DMSO,δ) 8.445-8.432 (d, J=7.8Hz, 1H), 8.186-8.071 (m, 6H), 8.018-8.006(t, J=7.2Hz, 1H), 7.774-7.727 (m, 3H), 7.608-7.569 (m, 2H), 7.385-7.354 (m, 3H), 7.292-7.260(m, 4H), 7.228-7.212(m, 1H), 7.148-7.123(t, J= 7.8Hz, 1H), 7.086-7.073(d, J=7.8Hz, 1H), 7.046-7.020(t, J=7.8Hz, 2H), 6.936-6.921 (d, J=9Hz, 1H)

[0230]

| 화합물 | MW | Tg | M.P. |
|---|---|---|---|
| H-101 | 586.7 | 152.06 | 317 |

[0231] **[실시예 6] 화합물 H-169의 제조**

[0232] 


[0233] 화합물 6-1의 제조

[0234] 플라스크에 1-브로모-7-페닐-7H 벤조[c]카바졸 (7.5 g , 20 mmol), 니트로페닐보로닉에시드 (10 g, 60 mmol), 테트라키스트리페닐포스핀 팔라듐(0) (2.32 g, 2 mmol), 탄산칼륨 (8.3 g, 60 mmol), 테트라하이드로푸란 80 mL, 및 물 20 mL 을 넣어 녹인 후 120℃ 에서 24시간 동안 환류시켰다. 반응이 끝나면 에틸아세테이트로 유기층을 분리하고 마그네슘설페이트로 잔여수분을 제거한 후 컬럼 크로마*그래피로 분리하여 화합물 **6-1** (3 g, 36%)를 얻었다.

[0235] 화합물 6-2의 제조

[0236] 플라스크에 화합물 **6-1** (5.5 g, 13 mmol), 트리페닐포스핀 (8.7 g, 33 mmol), 및 디클로로벤젠 70 mL를 넣고 180℃ 에서 환류시켰다. 반응이 끝나면 감압증류로 용매를 제거한 후 컬럼 크로마토그래피로 분리하여 화합물 **6-2** (2 g, 40%) 를 얻었다.

[0237] 화합물 H-169의 제조

[0238] 플라스크에 화합물 **6-2** (2 g, 5.23 mmol), 2-클로로-3-페닐퀴녹살린 (1.38 g, 5.75 mmol), 세슘카보네이트 (1.7 g, 5.23 mmol), 디메틸아미노피리딘 (320 mg, 2.62 mmol) 및 디메틸포름아마이드 20 mL를 넣어 녹인 후 180℃ 에서 24시간 동안 환류시켰다. 반응이 끝나면 에틸 아세테이트로 유기층을 추출하고 마그네슘 설페이트를 이용하여 잔여수분을 제거한 뒤 건조시키고 컬럼 크로마토그래피로 분리하여 화합물 **H-169** (1.1 g, 35.8%) 를 얻었다.

[0239] $^1$H NMR (600MHz,DMSO,δ) 8.416-8.394 (m, 1H), 8.251-8.236 (d, J=8.4 Hz, 1H), 8.104-8.012 (m, 3H), 7.969-7.955 (m, 1H ) , 7.787-7.741 (m, 6H), 7.673-7.593 (m, 3H), 7.579- 7.478 (m, 4H), 7.414-7.390 (m, 1H), 7.306-7.299 (m, 1H), 7.289- 7.238 (m, 1H), 7.218- 7.194 (m, 3H), 7.006- 6.980 (t, J= 7.8Hz, 1H)

| 화합물 | MW | Tg | M.P. |
|---|---|---|---|
| H-169 | 586.7 | 162.74 | 184.8 |

[0240]

[0241] 이하에서, 본 발명의 상세한 이해를 위하여 본 발명의 화합물을 포함하는 유기 전계 발광 소자의 특성을 설명한다.

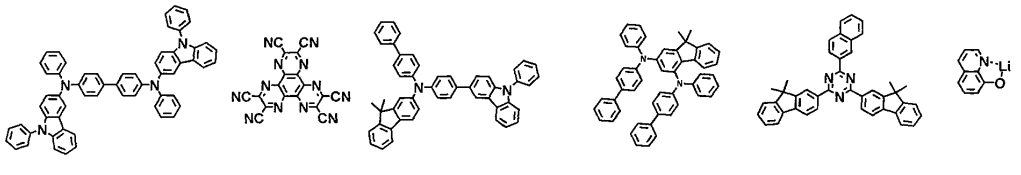
[0242] **[소자 제조예 1 내지 4] 본원에 따른 화합물을 호스트로 포함하는 OLED 소자 제조**

[0243] 본원에 따른 화합물을 포함하는 OLED 소자를 제조하였다. 우선, OLED용 글래스(지오마텍사 제조)로부터 얻어진 투명전극 ITO 박막(10Ω/□)을 아세톤, 에탄올 및 증류수를 순차적으로 사용하여 초음파 세척을 실시한 후, 이소프로판올에 넣어 보관한 후 사용하였다. 다음으로 진공 증착 장비의 기판 홀더에 ITO 기판을 장착한 후, 진공 증착 장비 내의 셀에 화합물 **HI-1**을 넣고 챔버 내의 진공도가 $10^{-6}$ torr에 도달할 때까지 배기시킨 후, 셀에 전류를 인가하여 증발시켜 ITO 기판 위에 80 nm 두께의 제1 정공 주입층을 증착하였다. 이어서, 진공 증착 장비 내의 다른 셀에 화합물 **HI-2**를 넣고, 셀에 전류를 인가하여 증발시켜 제1 정공 주입층 위에 5 nm 두께의 제2 정공 주입층을 증착하였다. 이어서, 진공 증착 장비 내의 셀에 화합물 **HT-1**을 넣고, 셀에 전류를 인가하여 증발시켜 제2 정공 주입층 위에 10 nm 두께의 제1 정공 전달층을 증착하였다. 진공 증착 장비 내의 다른 셀에 화합물 **HT-2**를 넣고, 셀에 전류를 인가하여 증발시켜 제1 정공 전달층 위에 60 nm 두께의 제2 정공 전달층을 증착하였다. 정공 주입층과 정공 전달층을 형성시킨 후, 그 위에 발광층을 다음과 같이 증착시켰다. 진공 증착 장비 내의 셀에 호스트로서 화합물은 하기 표 1의 호스트 물질을 넣고, 또 다른 셀에는 도판트로서 화합물 **D-1**을 넣은 후, 두 물질을 다른 속도로 증발시켜 각각 3 중량%의 양으로 도핑함으로써 상기 제2 정공 전달층 위에 40 nm 두께의 발광층을 증착하였다. 이어서, 또 다른 셀 두 군데에 화합물 **ET-1** 과 화합물 **EI-1**을 1:1의 속도로 증발시켜 발광층 위에 35 nm 두께의 전자 전달층을 증착하였다. 이어서, 전자 주입층으로 화합물 **EI-1**을 상기 전자 전달층 위에 2 nm 두께로 증착한 후, 다른 진공 증착 장비를 이용하여 Al 음극을 상기 전자 주입층 위에 80 nm의 두께로 증착하여 OLED 소자를 제조하였다.

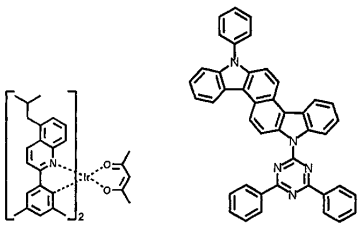
[0244] **[비교예 1] 호스트로서 비교 화합물을 포함하는 OLED 소자 제조**

[0245] 발광층의 호스트로서 하기의 화합물 **A**를 사용한 것 외에는 소자 제조예 1과 동일한 방법으로 OLED 소자를 제조하였다.

[0246] 상기 소자 제조예들 및 비교예에 사용된 화합물은 다음과 같다.



HI-1 HI-2 HT-1 HT-2 ET-1 EI-1



D-1 A

[0247]

[0248] 상기 소자 제조예들 및 비교예에서 제조한 OLED 소자의, 1,000 nits 에서의 구동전압과 발광 효율, 및 수명(5,000 nits의 휘도에서의 전류 값을 일정하게 가했을 때, 처음 나오는 빛의 세기를 100%로 보고 그 세기가 90%가 되는데 걸리는 시간으로 측정)을 하기 표 1에 기재하였다.

[0249] **[표 1]**

| | 호스트 물질 | 구동전압 (V) | 발광 효율 (cd/A) | 수명 (hr) |
|---|---|---|---|---|
| 소자 제조예 1 | H-51 | 3.1 | 29.0 | 323 |
| 소자 제조예 2 | H-507 | 3.2 | 27.7 | 179 |
| 소자 제조예 3 | H-52 | 3.1 | 23.7 | 406 |
| 소자 제조예 4 | H-269 | 3.1 | 28.0 | 525 |
| 비교예 1 | A | 4.1 | 22.4 | 88 |

[0250]

[0251] 상기 소자 제조예들 및 비교예에 사용된 호스트 물질의 물성은 하기 표 2와 같다.

[0252] [표 2]

| 호스트 물질 | LUMO 에너지 값 | HOMO 에너지 값 | 삼중항 에너지 값 |
|---|---|---|---|
| H-51 | -2.090 | -4.964 | 2.298 |
| H-52 | -2.101 | -4.967 | 2.290 |
| H-507 | -2.085 | -4.956 | 2.296 |
| H-269 | -2.089 | -4.959 | 2.297 |
| H-101 | -2.064 | -4.946 | 2.285 |
| H-169 | -2.082 | -5.024 | 2.361 |
| A | -1.896 | -5.081 | 2.404 |

[0253]

[0254] 상기 소자 실시예들 및 비교예로부터, 본원의 유기 전계 발광 화합물들을 포함하는 OLED 소자는 기존의 화합물을 포함하는 OLED 소자에 비해 낮은 구동전압, 높은 발광 효율 및/또는 장 수명의 특성을 갖는 것을 확인할 수 있다.

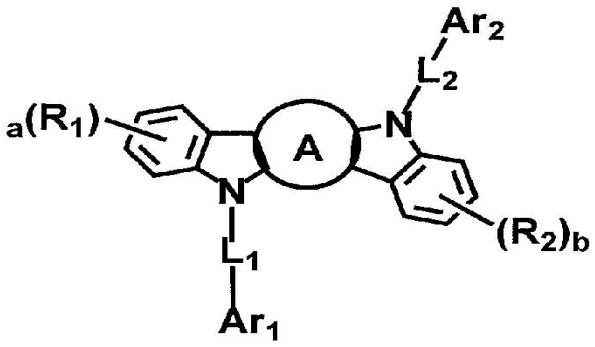
[0255] 구체적으로, 표 2에서 본원에 따른 호스트 물질로 기재된 화합물들은 나프탈렌으로 인해 HOMO 값이 높은데, 통상 HOMO 값이 높을수록 정공 이동도가 증가하는 경향이 있고, 이는 소자의 구동 전압을 낮추는데 기여한다. 이러한 HOMO 잔기에 트리아진 대신 퀴녹살린을 치환시키면, 퀴녹살린이 트리아진에 비해 LUMO 에너지 값 및 삼중항 에너지가 낮기 때문에, 삼중항의 밴드 갭이 낮아지는 것으로 이해된다. 이로 인해, 본원의 화합물은 적색 호스트에 대해 보다 적합한 에너지 값을 가지며, 이로 인해 전자 이동도, 전하 밸런스를 향상시킬 수 있다.

| | | | |
|---|---|---|---|
| 专利名称(译) | 有机电致发光化合物和包括该化合物的有机电致发光器件 | | |
| 公开(公告)号 | KR1020190115412A | 公开(公告)日 | 2019-10-11 |
| 申请号 | KR1020190033691 | 申请日 | 2019-03-25 |
| [标]申请(专利权)人(译) | 罗门哈斯电子材料有限公司 | | |
| 申请(专利权)人(译) | 롬엔드하스전자재료코리아유한회사 | | |
| [标]发明人 | 이효정<br>강현주<br>조상희<br>박효순 | | |
| 发明人 | 이효정<br>강현주<br>조상희<br>박효순 | | |
| IPC分类号 | C09K11/06 H01L51/50 | | |
| CPC分类号 | C09K11/06 H01L51/50 C09K2211/1029 C09K2211/1044 C09K2211/1048 C09K2211/1051 | | |
| 代理人(译) | 张本勋 | | |
| 优先权 | 1020180038319 2018-04-02 KR | | |
| 外部链接 | Espacenet | | |


摘要(译)

有机电致发光化合物和包括该有机电致发光器件的有机电致发光器件技术领域本发明涉及有机电致发光化合物和包括该有机电致发光化合物的有机电致发光器件。 通过包含根据本申请的有机电致发光化合物，可以提供具有低驱动电压，高发光效率和/或改善的使用寿命特性的有机电致发光器件。


하기 화학식 1로 표시되는 유기 전계 발




상기 화학식 1에서,