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(54) Title: NOVEL ORGANIC DYES AND SOLAR CELLS CONTAINING THE SAME

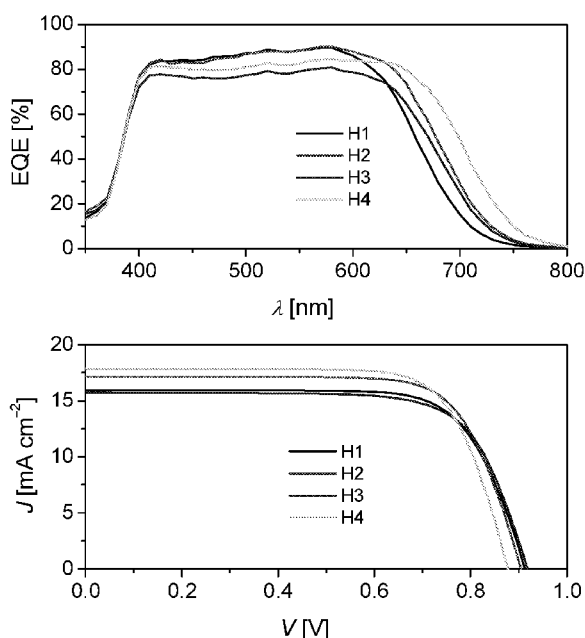


Figure 2

(57) Abstract: The present invention concerns novel organic compounds that can be used as dyes or sensitizers of optoelectronic devices, in particular dye-sensitized solar cells. The invention further concerns optoelectronic devices comprising the compounds.

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Novel Organic Dyes And Solar Cells Containing the Same

Technical Field

5 The present invention relates to novel compounds, to the use of the compounds as dyes and/or sensitizers, and to optoelectronic devices, preferably solar cells, comprising the dyes and/or sensitizers.

Background Art and Problems Solved by the Invention

10 The worlds increasing demand for energy and global warming alarming us to reduce the use of fossil fuels and find alternate renewable energy sources. In the field of solar energy conversion to electricity, the dye sensitized solar cells (DSCs) have attracted considerable attention in recent years due to its low cost and high efficiency. For example, DSCs based on
15 ruthenium sensitizers have reached overall power conversion efficiencies (PCE) of over 11% under standard Air Mass 1.5G illumination. With ruthenium being a relatively expensive earth metal, there have been efforts in replacing such dyes with organic dyes.

In recent years many efforts have been devoted to develop organic sensitizers for practical use
20 due to their high molar absorption coefficients, ease of synthesis and structural modifications and to avoid the use of costly metal having limited availability.

Thus, PCE of donor- π -acceptor (D- π -A) organic sensitizers are attractive candidates to be used as sensitizers for DSC, since they reach more than 10% power conversion efficiency (Ito
25 et al., Chem Commun., 2008, 5194).

It is a permanent objective to provide dyes that allow obtaining devices with a high power conversion efficiency. When it comes to produce dye-sensitized solar cells for practical applications, additional constraints have to be considered, such as manufacturing costs. It is
30 an objective of the present invention to provide a dye that can be produced at comparatively low costs and in high amounts. Preferably, the dye can be produced with starting materials that are readily available at comparatively low costs, few synthetic steps and comparatively high yields during each steps.

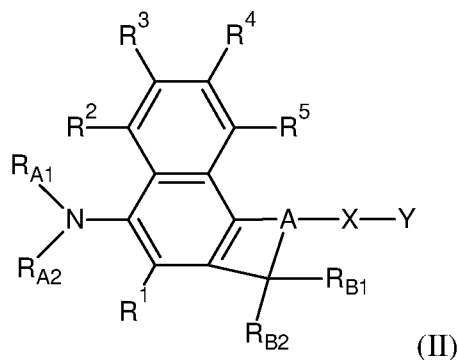
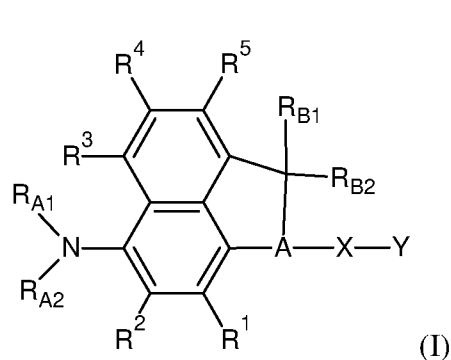
The present invention is further interested in the use of dye-sensitized solar cells as construction elements, for example in windows, glass-structures in buildings in general, and/or facings for buildings, for example. Glass and plastic are widely-used in construction, for example for increasing the use of natural and/or sunlight inside buildings and also for exploiting the sunlight's heating properties. When using construction elements comprising dye-sensitized solar cells, aesthetic factors, such as the color of the sensitizer also becomes relevant. Generally, certain brownish colors may be considered less decorative than bright and basic colors, such as green, blue, red, and yellow, for example. It is an objective of the present invention to provide sensitizing dyes having a red, red-like or red-related color, which when used in a dye-sensitized solar cell, provide devices with high stability and good power conversion efficiencies.

The present invention addresses the problems depicted above.

Summary of the Invention

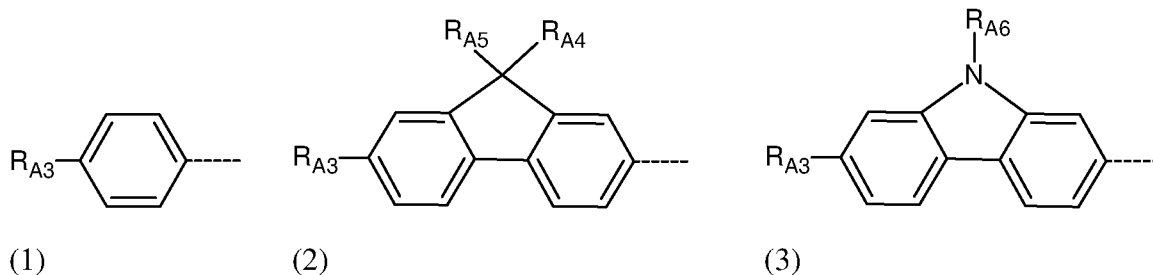
Remarkably, the present inventors provide novel compounds that are useful as sensitizers in dye-sensitized solar cells. The sensitizers have an interesting, characteristic red color, which renders the compounds suitable for dye-sensitized solar cells that are intended for use as construction elements, such solar cells thus fulfilling a functional purpose as construction element (window, cladding panel, facing tile, and ornamental element, for example), in addition to the benefit of producing electricity.

In an aspect, the invention provides a compound of formula (I) or (II):



wherein:

R_{A1} , R_{A2} , R_{B1} , and R_{B2} are independently selected from C1-C36 alkyl, and from the substituents (1) to (3) below:



and wherein:

R_{A3} , R_{A4} , R_{A5} , in as far as present, are selected independently from H, C1-C36 alkyl, C1-C36 alkoxy, C1-C36 thioalkyl, C1-C36 alkyl substituted phenyl, C1-C36 alkoxy substituted phenyl and C1-C36 thioalkyl substituted phenyl;

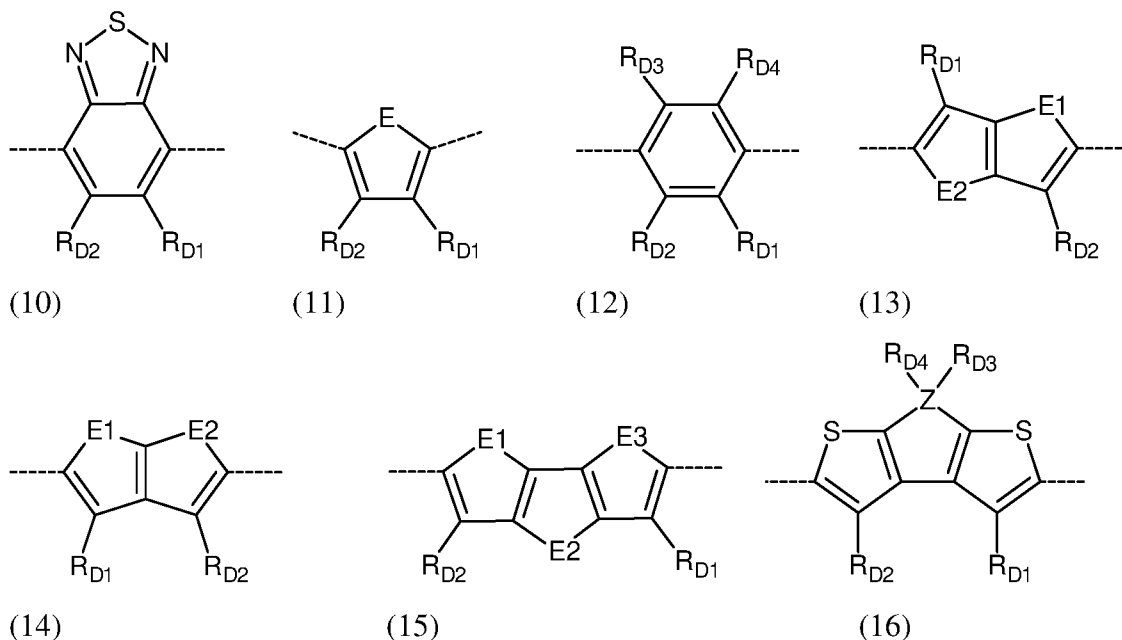
wherein R_{A6} is selected from H, C1-C36 alkyl, C1-C36 alkyl substituted phenyl, C1-C36 alkoxy substituted phenyl and C1-C36 thioalkyl substituted phenyl;

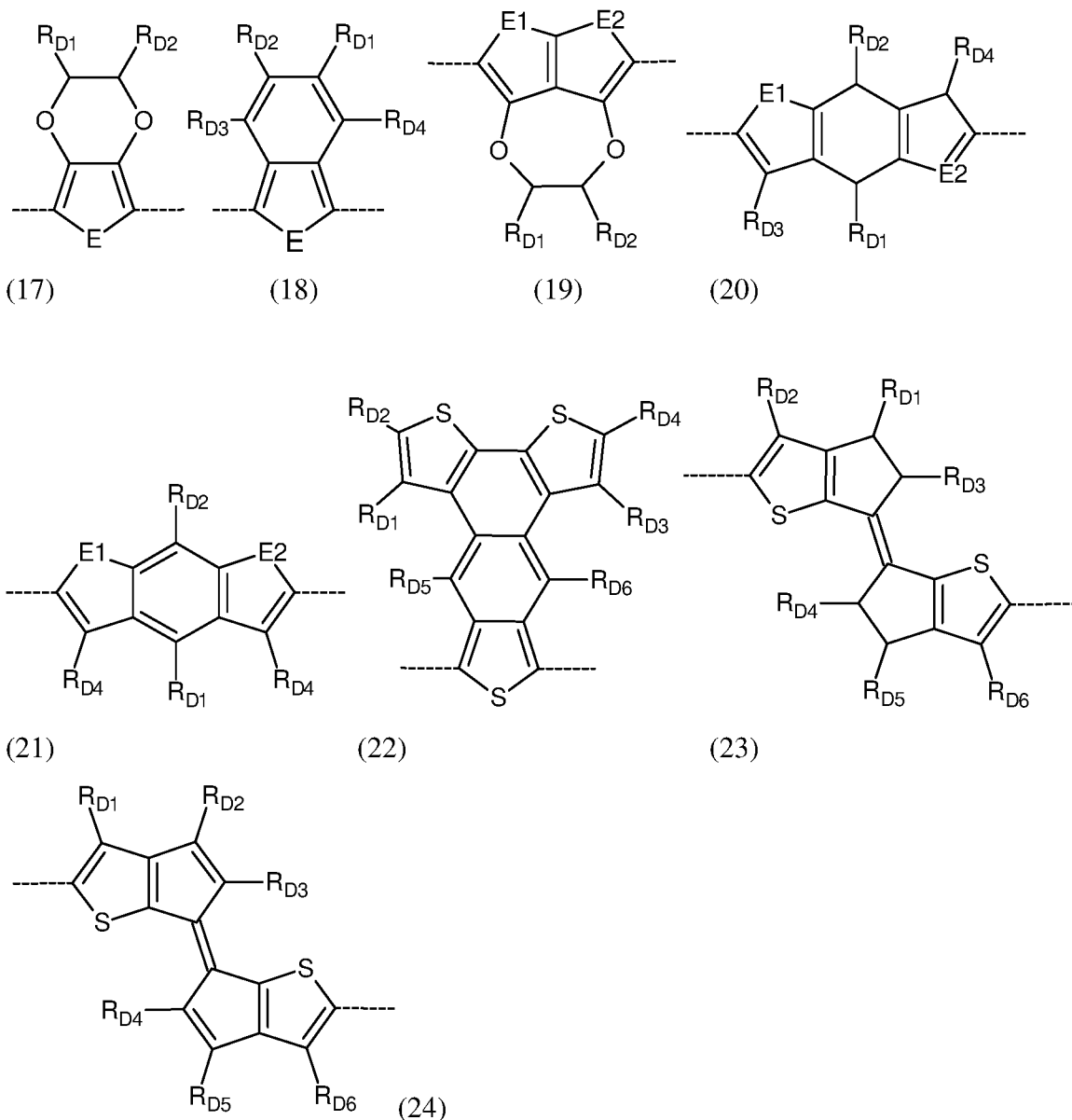
wherein R_{B1} and R_{B2} may further be selected independently from H, C1-C36 alkoxy, C1-C36 thioalkyl;

R^1 - R^5 , in as far as present, are selected independently from the substituents as specified for R_{A3} - R_{A5} ;

A is an optionally substituted cyclic moiety comprising from 3 to 10 carbons and 0 to 3 heteroatoms, or, methanetriyl, wherein optional substituents of said cyclic moiety are independently selected from C1-C36 alkyl, C1-C36 alkoxy, C1-C36 thioalkyl, C1-C36 alkyl substituted phenyl, C1-C36 alkoxy substituted phenyl and C1-C36 thioalkyl substituted phenyl;

X is a moiety selected from the moieties (10) to (24) below,



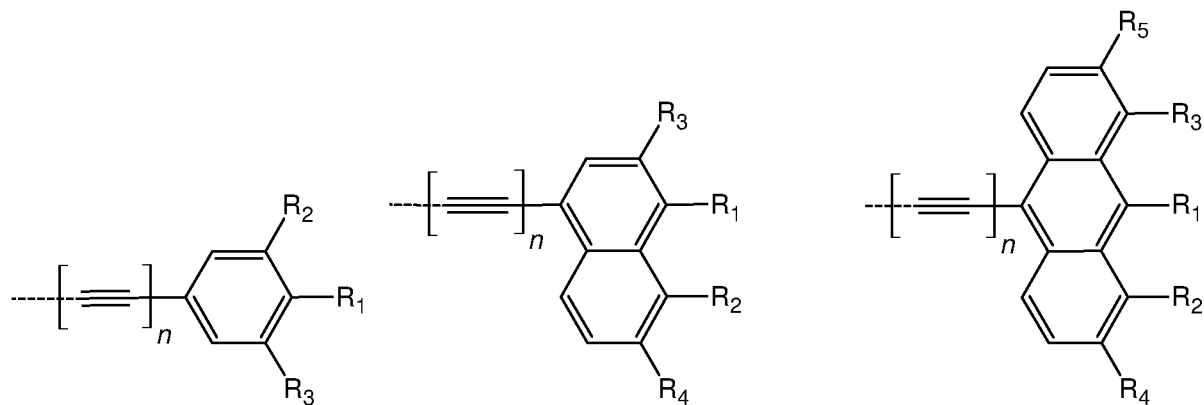


wherein:

in moieties (10)-(24), R_{D1}, R_{D2}, R_{D3}, R_{D4}, R_{D5}, and R_{D6}, in as far as present, are independently selected from H, C1-C36 alkyl, C1-C36 alkoxy, C1-C36 thioalkyl, C1-C36 alkyl substituted phenyl, C1-C36 alkoxy substituted phenyl and C1-C36 thioalkyl substituted phenyl, wherein, E, E1, E2, and E3, in as far as present, are independently selected from S, O, Se, and Te;

Z in moiety (16) is selected from carbon and Si;

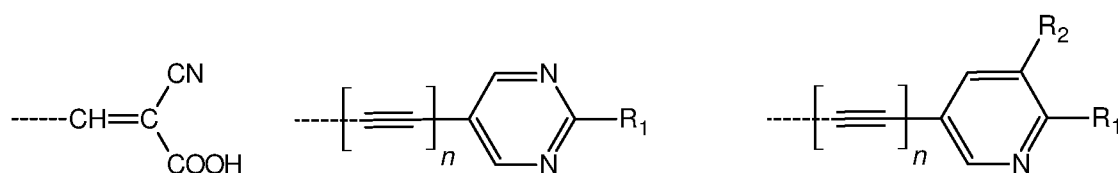
Y is selected from the substituents (30) to (43) below,



(30)

(31)

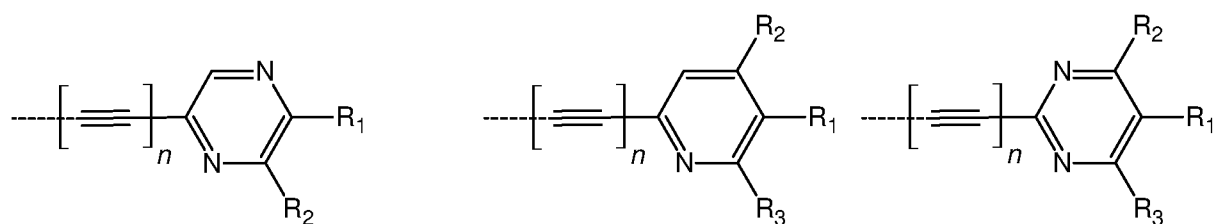
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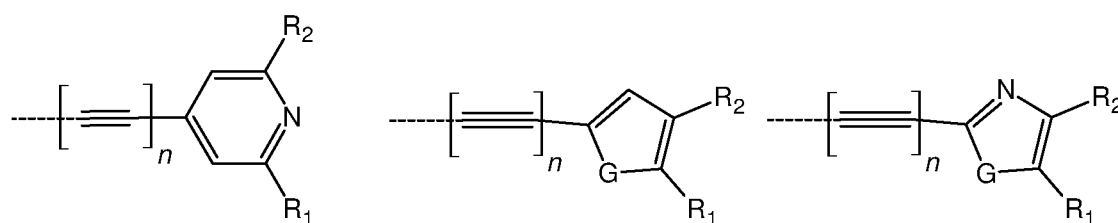
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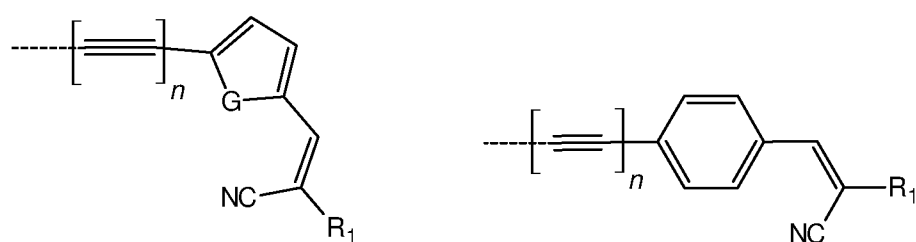
(38)



(39)

(40)

(41)



(42)

(43)

wherein,

R₁, R₂, R₃, R₄, and R₅, in as far as present, are selected independently from H and from anchoring groups selected from the group consisting of -COOH, -CONHOH, -PO₃H₂, -PO₄H₂, -P(R₈)O₂H, -SO₃H₂, -SO₄H₂, 1,2-hydroxybenzene, 1-hydroxy-2-carboxybenzene,

acetylacetonate, deprotonated forms of the aforementioned, organic and/or inorganic salts of said deprotonated forms, and chelating groups with π -conducting character, R_8 is selected from alkyl, alkenyl, alkynyl, aryl, alkylaryl, alkoxyaryl, and thioalkylaryl, with the proviso that each substituent Y comprises at least one of said anchoring groups; wherein G is selected from S and O;
n is 1 or 0.

In an aspect, the present invention provides an optoelectronic device comprising the compound of any one of the preceding claims, said optoelectronic device preferably being a dye-sensitized solar cell.

In an aspect, the present invention provides the use of the compounds of the invention as sensitizers, in particular as sensitizers of an optoelectronic device, in particular a dye-sensitized solar cell.

In an aspect, the present invention provides a dye-sensitized solar cell comprising a sensitizer, wherein said sensitizer is selected from the compounds of the present invention.

In an aspect, the present invention provides a construction element comprising the optoelectronic device of the invention, in particular the dye-sensitized solar cell of the invention.

Further aspects and preferred embodiments are described in the detailed description of preferred embodiments and the appended claims.

Brief Description of the Drawings

Figure 1 shows the reaction scheme for synthesizing compounds H1-H4 in accordance with preferred embodiments of the present invention.

Figure 2 shows the photocurrent action spectrum of a dye-sensitized solar cell sensitized with dyes H1-H4 shown in Figure 1 (top graph), and the current density-voltage characteristics of the solar cells under illumination of the AM 1.5G full sunlight (100mW cm^{-2}) (bottom graph).

Detailed Description of the Preferred Embodiments

For the purpose of the present specification, the expression "comprising", and its various grammatical forms, means "includes, amongst other". It is not intended to mean "consists only of".

In a preferred embodiment, said C1-C36 alkyl, C1-C36 alkoxy, C1-C36 thioalkyl, C1-C36 alkyl substituted phenyl, C1-C36 alkoxy substituted phenyl and C1-C36 thioalkyl substituted phenyl are C1-C20 alkyl, C1-C20 alkoxy, C1-C20 thioalkyl, C1-C10 alkyl substituted phenyl, C1-C20 alkoxy substituted phenyl and C1-C20 thioalkyl substituted phenyl, preferably C1-C10 alkyl, C1-C10 alkoxy, C1-C10 thioalkyl, C1-C10 alkyl substituted phenyl, C1-C10 alkoxy substituted phenyl and C1-C10 thioalkyl substituted phenyl and most preferably C2-C8 alkyl, C2-C8 alkoxy, C2-C8 thioalkyl, C2-C8 alkyl substituted phenyl, C2-C8 alkoxy substituted phenyl and C2-C8 thioalkyl substituted phenyl.

In a preferred embodiment of the compound of formulae (I) or (II), R_{A3} , R_{A4} , R_{A5} , in as far as present, are selected independently from H, C1-C20 alkyl, C1-C20 alkoxy, C1-C20 thioalkyl, C1-C20 alkyl substituted phenyl, C1-C20 alkoxy substituted phenyl and C1-C20 thioalkyl substituted phenyl, preferably from H, C1-C10 alkyl, C1-C10 alkoxy, C1-C10 thioalkyl, C1-C10 alkyl substituted phenyl, C1-C10 alkoxy substituted phenyl and C1-C10 thioalkyl substituted phenyl, most preferably from H, C2-C8 alkyl, C2-C8 alkoxy, C2-C8 thioalkyl.

In a preferred embodiment of the compound of formulae (I) or (II), R_{A6} is selected from H, C1-C20 alkyl, C1-C20 alkyl substituted phenyl, C1-C20 alkoxy substituted phenyl and C1-C20 thioalkyl substituted phenyl, more preferably from H, C1-C10 alkyl, C1-C10 alkyl substituted phenyl, C1-C10 alkoxy substituted phenyl and C1-C10 thioalkyl substituted phenyl, most preferably from H, C2-C8 alkyl, C2-C8 alkyl substituted phenyl, C2-C8 alkoxy substituted phenyl and C2-C8 thioalkyl substituted phenyl.

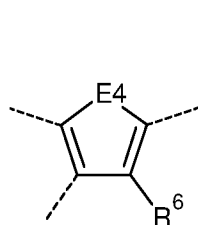
In a preferred embodiment of the compound of formulae (I) or (II), R_{A1} and R_{A2} are independently selected from substituents of the formula (1), and R_{A3} is selected from C1-C20 alkyl, C1-C20 alkoxy, C1-C20 thioalkyl, preferably C1-C10 alkyl, C1-C10 alkoxy, C1-C10 thioalkyl, more preferably C2-C8 alkyl, C2-C8 alkoxy and C2-C8 thioalkyl, most preferably C2-C8 alkoxy.

In a preferred embodiment of the compound of formulae (I) and (II), R^1 - R^5 , in as far as present, are selected independently from H and from the substituents as specified for R_{A3} - R_{A5} indicated above. Preferably, R^1 - R^5 are H.

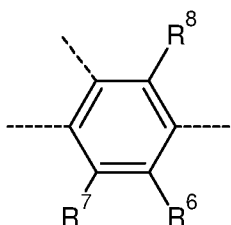
- 5 In a preferred embodiment of the compound of formulae (I) and (II), R_{B1} , and R_{B2} are independently selected from C1-C20 alkyl and from the substituents of formula (1) as defined above, preferably from substituents of formula (1), in which R_{A3} is selected from C1-C20 alkyl, C1-C20 alkoxy, C1-C20 thioalkyl, preferably R_{A3} is selected from C1-C10 alkyl, C1-C10 alkoxy, C1-C10 thioalkyl, more preferably C2-C8 alkyl.

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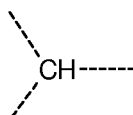
In a preferred embodiment of the compound of formulae (I) or (II), A is selected from any one of the moieties (50)-(52) below:



(50)



(51)



(52)

15 wherein,

the dotted line on the right side in the moieties (50) to (52) as shown above represents the single bond by which the moiety connects to X in formulae (I) or (II);

the dotted line towards the left side in the moieties (50) and (51) as shown above, on the carbon adjacent to E4 (moiety (50)) or adjacent to the carbon carrying R^8 (moiety (51)), respectively, represents the single bond by which the moiety connects to the carbon of the naphthalene moiety in formulae (I) and (II);

the dotted line towards the left side in the moieties (50) and (51) as shown above, on the carbon adjacent to the carbon carrying R^6 (moiety (50)) or adjacent to the carbon carrying R^7 (moiety (51)), represents the single bond by which the moiety connects carbon carrying substituents R_{B1} and R_{B2} in formulae (I) and (II);

R^6 , R^7 and R^8 , in as far as present, are independently selected from H, and from the same substituents as specified for R_{A3} - R_{A5} ;

E4 is selected from S, O, Se and Te. Preferably, E4 is S or O, more preferably S.

30 More preferably, A is selected from the moieties (50) and (51), and most preferably A is

moiety (50), wherein in moiety (50) E4 is preferably S or O, more preferably S. Preferably, R⁶, R⁷ and R⁸, in as far as present, are independently selected from H, C1-C10 alkyl, C1-C10 alkoxy and C1-C10 thioalkyl. Most preferably R⁶, R⁷ and R⁸, in as far as present, are H.

- 5 In a preferred embodiment of the compound of formulae (I) or (II), X is selected from moieties (10)-(15), preferably (12)-(12), more preferably X is moiety (10). E, E1, E2, and E3 are preferably independently selected from S and O. R_{D1}, R_{D2}, R_{D3}, and R_{D4}, in as far as present, are preferably independently selected from H, C1-C10 alkyl, C1-C10 alkoxy and C1-C10 thioalkyl, more preferably R_{D1}, R_{D2}, R_{D3}, and R_{D4}, in as far as present, are H.

10

In a preferred embodiment of the compound of formulae (I) or (II), Y is selected from the substituents of formulae (30)-(33). Preferably, R₂-R₄, in as far as present, are H. Preferably, R₁ is an anchoring group selected from the group consisting of -COOH, -CONHOH, -PO₃H₂, -PO₄H₂, -P(R₈)O₂H, -SO₃H₂, -SO₄H₂, 1,2-hydroxybenzene, 1-hydroxy-2-carboxybenzene, acetylacetonate, deprotonated forms of the aforementioned, organic and/or inorganic salts of said deprotonated forms. Most preferably, R₁ is selected from -COOH, the deprotonated form of the aforementioned, and organic and/or inorganic salts of said deprotonated form.

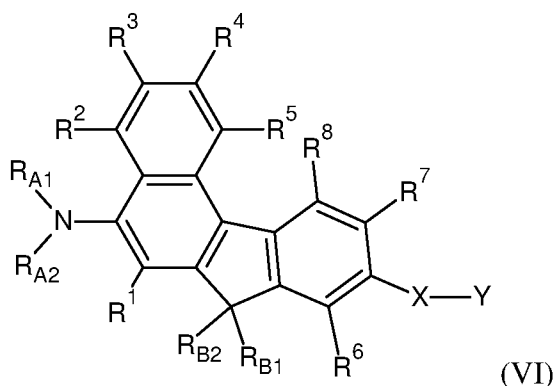
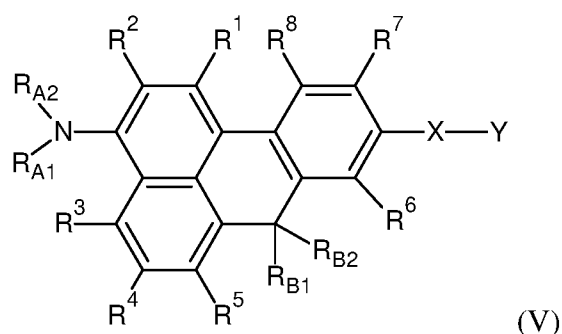
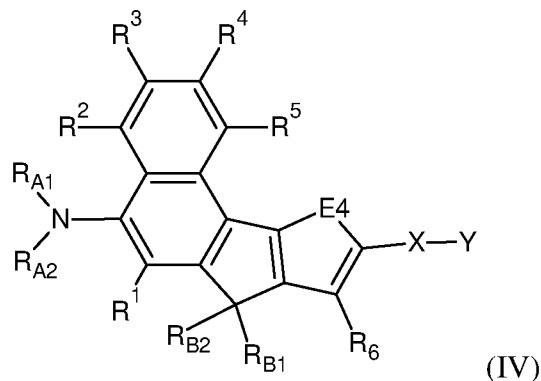
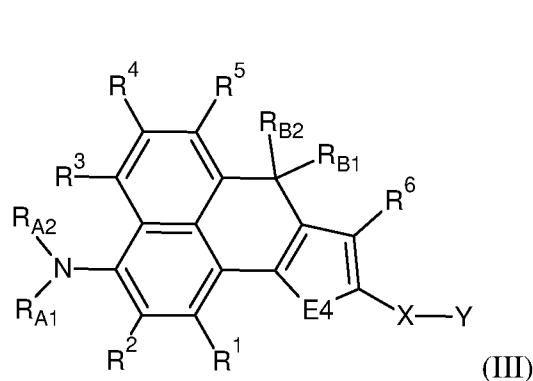
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- In a preferred embodiment, A is selected from moiety (50) and (51) as shown herein above, wherein E4 is selected from S, O, Se and Te, and R⁶, R⁷ and R⁸ are independently selected from H, C1-C36 alkyl, C1-C36 alkoxy, C1-C36 substituted phenyl, and C1-C36 alkoxy substituted phenyl; R¹ to R⁶, in as far as present, are all H; X is selected from moieties (10), (11) and (12) as shown herein above, wherein E in moiety (11) is selected S, O, Se, and Te, and R_{D1}-R_{D4}, in as far as present, are independently selected from H, from H, C1-C36 alkyl, C1-C36 alkoxy, C1-C36 alkyl substituted phenyl, and C1-C36 alkoxy substituted phenyl; Y is selected of the substituents (30), (31), (32) and (33), in which R₁ is -COOH, and R₂ to R₅, in as far as present, are all H.

25

- In an embodiment, the compound of the invention comprises the structure of any one of formulae (III), (IV), (V) or (VI) below:

30



wherein,

5 R_{A1} , R_{A2} , R_{B1} , R_{B2} , X, Y, and, in as far as present, R^1 , R^2 , R^3 , R^4 , and R^5 are independently as defined herein above with respect to the compounds of formulae (I) and (II) and preferred embodiments thereof.

R^6 , R^7 and R^7 are independently defined as R^1 - R^5 ;

10 E4 in moieties (III) and (IV), are as defined herein above with respect to the compounds of formulae (I) and (II) and preferred embodiments thereof.

In a preferred embodiment of the compound of formulae (III)-(VI), R_{A1} and R_{A2} are independently selected from H, C1-C20 alkyl and from substituents of the formula (1), wherein R_{A3} is selected from H, C1-C20 alkyl, C1-C20 alkoxy, C1-C20 thioalkyl, preferably
15 C1-C10 alkyl, C1-C10 alkoxy, C1-C10 thioalkyl, more preferably C2-C8 alkyl, C2-C8 alkoxy and C2-C8 thioalkyl, most preferably C2-C8 alkoxy.

In a preferred embodiment of the compound of formulae (III)-(VI), R_{B1} and R_{B2} , are independently selected from H, C1-C20 alkyl and from the substituents of formula (1) as
20 defined above, preferably from substituents of formula (1), in which R_{A3} is independently selected from H, C1-C20 alkyl, C1-C20 alkoxy, C1-C20 thioalkyl, preferably R_{A3} is selected

from C1-C10 alkyl, C1-C10 alkoxy, C1-C10 thioalkyl, more preferably C2-C8 alkyl.

In a preferred embodiment of the compound of formulae (III)-(IV), E4 is selected from S and O, more preferably E4 is S.

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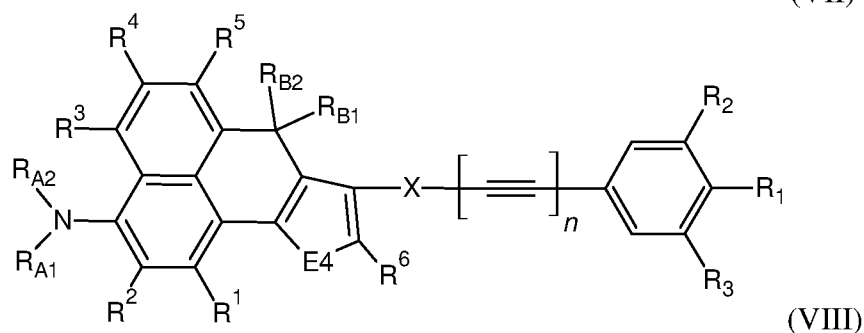
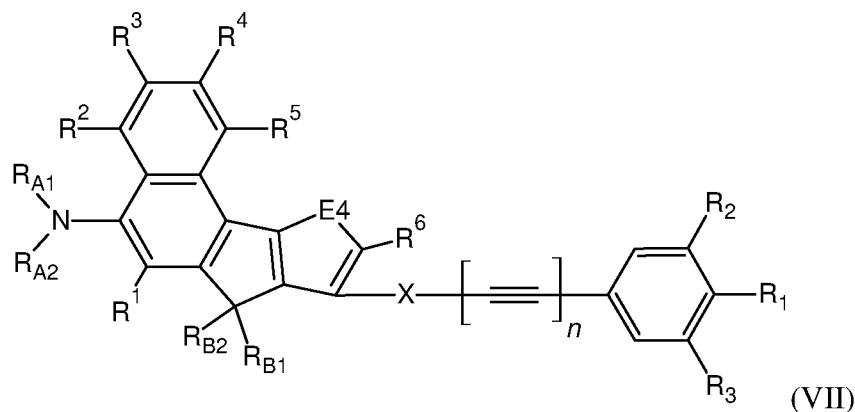
In a preferred embodiment of the compound of formulae (III)-(VI), X is selected from moieties (10)-(15), preferably moieties (10)-(12), more preferably X is moiety (10). E, E1, E2, and E3, in as far as present, are preferably selected independently from S, O, Se and Te, preferably from S and O. R_{D1}, R_{D2}, R_{D3}, and R_{D4}, in as far as present, are preferably selected
10 independently from H, C1-C10 alkyl, C1-C10 alkoxy and C1-C10 thioalkyl, more preferably R_{D1}, R_{D2}, R_{D3}, and R_{D4}, in as far as present, are H.

In a preferred embodiment of the compound of formulae (III)-(VI), Y is selected from the substituents of formulae (30)-(33). Preferably, R₂-R₄, in as far as present, are H. Preferably,
15 R₁ is an anchoring group selected from the group consisting of -COOH, -CONHOH, -PO₃H₂, -PO₄H₂, -P(R₈)O₂H, -SO₃H₂, -SO₄H₂, 1,2-hydroxybenzene, 1-hydroxy-2-carboxybenzene, acetylacetonate, deprotonated forms of the aforementioned, organic and/or inorganic salts of said deprotonated forms. Most preferably, R₁ is selected from -COOH, the deprotonated form of the aforementioned, and organic and/or inorganic salts of said deprotonated form.

20

In a preferred embodiment of the compound of formulae (III)-(VI), R¹, R², R³, R⁴, R⁵, R⁶, R⁷, and R⁸, in as far as present, are selected independently from H, C1-C20 alkyl, C1-C20 alkoxy, C1-C20 thioalkyl, preferably C1-C10 alkyl, C1-C10 alkoxy, C1-C10 thioalkyl, more preferably C2-C8 alkyl, C2-C8 alkoxy and C2-C8 thioalkyl, most preferably C2-C8 alkoxy.
25 More preferably, R¹-R⁸, in as far as present, are H.

In a preferred embodiment, the compound of the invention comprises the structure of any one of formulae (VII) and (VIII):

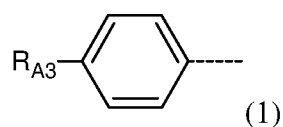


wherein,

- 5 n is = 0 or is 1;
 E4 is independently selected from S, O, Se, and Te;

 X is selected from any one of the moieties (10)-(12) as shown in claim 1, wherein, in moieties (10)-(12), R_{D1} - R_{D4} , in as far as present, are independently selected from H, C1-C15 alkyl, C1-C15 alkoxy, C1-C15 thioalkyl, C1-C10 alkyl substituted phenyl, C1-C15 alkoxy substituted phenyl and C1-C15 thioalkyl substituted phenyl, wherein, E, in as far as present, is
 10 independently selected from S and O;

R_{A1} , R_{A2} , R_{B1} , and R_{B2} are independently selected from C1-C36 alkyl and from substituents of formula (1):



- 15 wherein R_{A3} is selected from H, C1-C15 alkyl, C15-C15 alkoxy, C1-C15 thioalkyl, C1-C15 alkoxy substituted phenyl and C1-C15 thioalkyl substituted phenyl;

 wherein R_{B1} , and R_{B2} may further be selected, independently, from C1-C15 alkoxy, C1-C15 thioalkyl;

- R^1 - R^6 , in as far as present, are selected independently from the substituents as
 20 specified for R_{A3} ;

R_1 , R_2 , and R_3 , are selected independently from H and from anchoring groups selected

from the group consisting of -COOH, -CONHOH, -PO₃H₂, -PO₄H₂, -P(R₈)O₂H, -SO₃H₂, -SO₄H₂, 1,2-hydroxybenzene, 1-hydroxy-2-carboxybenzene, acetylacetonate, deprotonated forms of the aforementioned, organic and/or inorganic salts of said deprotonated forms, and chelating groups with π -conducting character, R₈ is selected from alkyl, alkenyl, alkynyl, aryl, alkylaryl, alkoxyaryl, and thioalkylaryl, with the proviso that at least one of said R₁, R₂, and R₃, is an anchoring group.

In a preferred embodiment of the compound of formulae (VII)-(VIII), E₄ is independently selected from S, O. Preferably E₄ is S.

In a preferred embodiment of the compound of formulae (VII)-(VIII), X is selected from the moieties (10)-(15), preferably (10)-(12), preferably moiety (10), wherein R_{D1}-R_{D4}, in as far as present, are independently selected from H, C1-C10 alkyl, C1-C10 alkoxy, C1-C10 thioalkyl, C1-C8 alkyl substituted phenyl, C1-C8 alkoxy substituted phenyl and C1-C8 thioalkyl substituted phenyl, wherein, E, E₁, E₂ and E₃, in as far as present, are independently selected from S and O, preferably S. Preferably, R_{D1}-R_{D4}, in as far as present, are H.

In a preferred embodiment of the compound of formulae (VII)-(VIII), R_{A1}, R_{A2}, R_{B1}, and R_{B2} are independently selected from C1-C20 alkyl and from substituents of formula (1), wherein R_{A3} is selected from H, C1-C15 alkyl, C1-C15 alkoxy, and C1-C15 thioalkyl, preferably R_{A3} is selected from C1-C10 alkyl, C1-C10 alkoxy, and C1-C10 thioalkyl, and more preferably R_{A3} is selected from C2-C8 alkyl, C2-C8 alkoxy, and C2-C8 thioalkyl. Preferably, R_{A1}, R_{A2}, R_{B1}, and R_{B2} are independently selected from substituents of formula (1).

In a preferred embodiment of the compound of formulae (VII)-(VIII), R₁, R₂, and R₃, are selected independently from H and from anchoring groups selected from the group consisting of -COOH, -CONHOH, -PO₃H₂, -PO₄H₂, -P(R₈)O₂H, -SO₃H₂, -SO₄H₂, 1,2-hydroxybenzene, 1-hydroxy-2-carboxybenzene, acetylacetonate, deprotonated forms of the aforementioned, and organic and/or inorganic salts of said deprotonated forms.

In a preferred embodiment of the compound of formulae (VII)-(VIII), R₂ and R₃ are H, and R₁ is selected from anchoring groups as defined in the present specification. A preferred anchoring group is -COOH, including the deprotonated form of the later and salts of said

deprotonated form.

In a preferred embodiment of the compound of formulae (I)-(VIII), X is selected from moieties (10)-(21), preferably moieties (10)-(18).

5

In a preferred embodiment of the compound of formulae (I)-(VIII), X is selected from moieties (10)-(15), preferably (10)-(12). Most preferably, X is selected from moieties of formula (10).

- 10 In a preferred embodiment of the compound of formulae (I)-(VIII), X, in as far as present, is selected from the moieties of formulae (10)-(12) as shown in claim 1, with E being selected from S and O, preferably S, and R_{D1} - R_{D4} , in as far as present, are independently selected from H, C1-C20 alkyl, C1-C20 alkoxy, C1-C20 thioalkyl, C1-C20 alkyl substituted phenyl, C1-C20 alkoxy substituted phenyl and C1-C20 thioalkyl substituted phenyl. Preferably R_{D1} - R_{D4} ,
15 in as far as present, are independently selected from H, C1-C10 alkyl, C1-C10 alkoxy, C1-C10 thioalkyl, more preferably from H, C1-C6 alkyl, C1-C6 alkoxy, C1-C6 thioalkyl. Most preferably, R_{D1} - R_{D4} are all H.

- In a preferred embodiment of the compound of formulae (I)-(VIII), R_{D1} , R_{D2} , R_{D3} , R_{D4} , R_{D5} ,
20 and R_{D6} , in as far as present, are independently selected from H, C1-C10 alkyl, C1-C10 alkoxy, C1-C10 thioalkyl, C1-C10 alkyl substituted phenyl, C1-C10 alkoxy substituted phenyl and C1-C10 thioalkyl substituted phenyl, and E, E1, E2, and E3, in as far as present, are independently selected from S and O.

- 25 In a preferred embodiment, R_{D1} , R_{D2} , R_{D3} , R_{D4} , R_{D5} , and R_{D6} , in as far as present, are independently selected from H, C1-C10 alkyl, C1-C10 alkoxy, C1-C10 thioalkyl.

In a preferred embodiment, R_{D1} , R_{D2} , R_{D3} , R_{D4} , R_{D5} , and R_{D6} , in as far as present, are H.

- 30 In a preferred embodiment, E, E1, E2, and E3, in as far as present, are independently selected from S and O, preferably are S.

In a preferred embodiment of the compound of formulae (I)-(VIII), R^1 , R^2 , R^3 , R^4 , R^5 and R^6 , in as far as present, are independently selected from H, C1-C15 alkyl, C1-C15 alkoxy, C1-

C15 thioalkyl, C1-C15 alkyl substituted phenyl, C1-C15 alkoxy substituted phenyl and C1-C15 thioalkyl substituted phenyl.

5 In a preferred embodiment of the compound of formulae (I)-(VIII), R^1 , R^2 , R^3 , R^4 , R^5 and R^6 , in as far as present, are independently selected from H, C1-C10 alkyl, C1-C10 alkoxy, C1-C10 thioalkyl, C1-C10 alkyl substituted phenyl, C1-C10 alkoxy substituted phenyl and C1-C10 thioalkyl substituted phenyl.

10 In a preferred embodiment of the compound of formulae (I)-(VIII), R^1 , R^2 , R^3 , R^4 , R^5 and R^6 , in as far as present, are independently selected from H, C1-C10 alkyl, C1-C10 alkoxy, and C1-C10 thioalkyl.

In a preferred embodiment of the compound of formulae (I)-(VIII), R^1 , R^2 , R^3 , R^4 , R^5 and R^6 , in as far as present, are H.

15 In a preferred embodiment of the compound of formulae (I)-(VIII), R_{A1} , R_{A2} , R_{B1} , and R_{B2} are independently selected from C1-C36 alkyl, C1-C20 alkyl substituted phenyl, C1-C20 alkoxy substituted phenyl and C1-C20 thioalkyl substituted phenyl, and wherein R_{B1} , and R_{B2} may further be independently selected from C1-C20 alkoxyl and C1-C20 thioalkyl.

20 In a preferred embodiment of the compound of formulae (I)-(VIII), R_{A1} , R_{A2} , R_{B1} , and R_{B2} are independently selected from C1-C20 alkyl, C1-C15 alkyl substituted phenyl, C1-C15 alkoxy substituted phenyl and C1-C15 thioalkyl substituted phenyl, and wherein R_{B1} , and R_{B2} may further be independently selected from C1-C15 alkoxyl and C1-C15 thioalkyl.

25 In a preferred embodiment, R_{A1} , R_{A2} , R_{B1} , and R_{B2} are independently selected from C1-C15 alkyl, C1-C10 alkyl substituted phenyl, C1-C10 alkoxy substituted phenyl and C1-C10 thioalkyl substituted phenyl, and wherein R_{B1} , and R_{B2} may further be independently selected from C1-C10 alkoxyl and C1-C10 thioalkyl.

30 In a preferred embodiment, R_{A1} , R_{A2} , R_{B1} , and R_{B2} are independently selected from C1-C10 alkyl substituted phenyl, C1-C10 alkoxy substituted phenyl and C1-C10 thioalkyl substituted phenyl.

In a preferred embodiment, R_{A1} , R_{A2} are independently selected from C1-C10 alkoxy substituted phenyl and C1-C10 thioalkyl substituted phenyl, and, R_{B1} , and R_{B2} are independently selected from C1-C10 alkyl substituted phenyl.

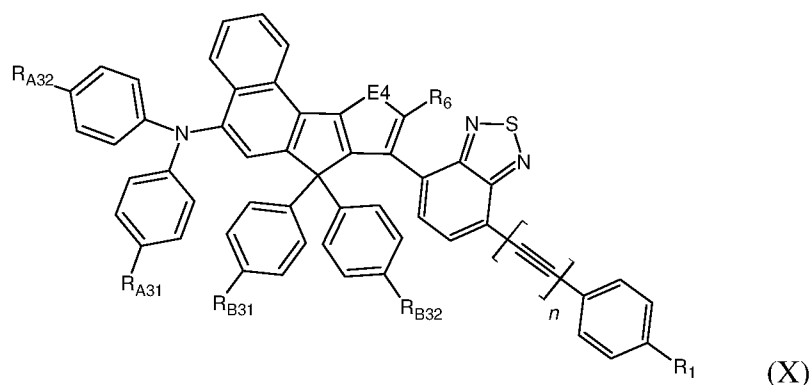
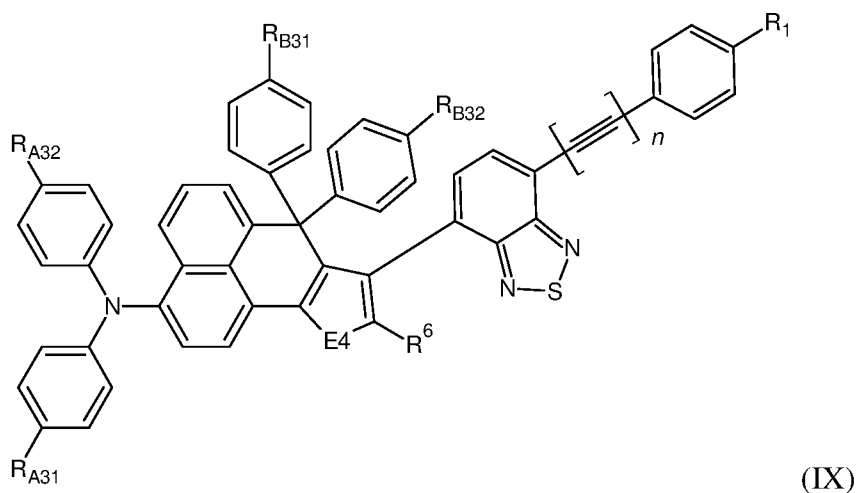
5 In a preferred embodiment of the compound of formulae (I)-(VIII), R_{A1} and R_{A2} , are identical.

In a preferred embodiment of the compound of formulae (I)-(VIII), R_{B1} and R_{B2} , are identical.

10 In a preferred embodiment of the compound of formulae (I)-(VIII), wherein R_1 is selected from said anchoring groups and R_2 to R_5 , in as far as present, are H.

In a preferred embodiment of the compound of formulae (I)-(VIII), said anchoring group is -COOH, the deprotonated form thereof or a salt of said deprotonated form.

15 In an embodiment, the compound of the invention comprises the structure of any one of formulae (IX) or (X):



wherein:

20 n is 0 or is 1;

E4 is S or O, preferably S;

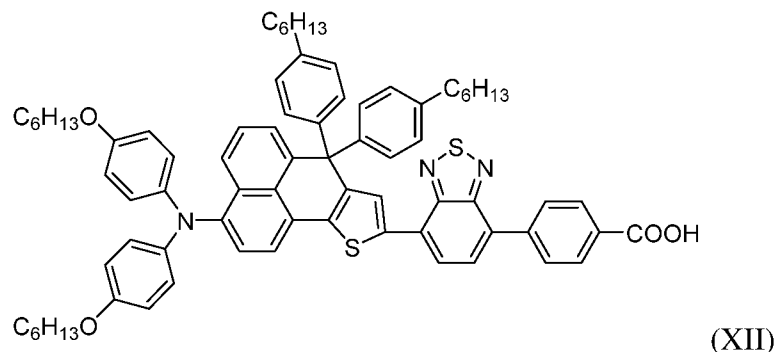
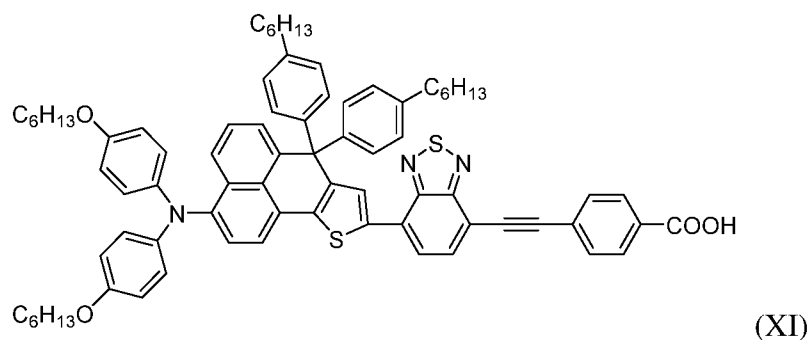
R_{A31} , R_{A32} , R_{B31} , R_{B32} , are independently selected from H, C1-C20 alkyl, C1-C20 alkoxy, C1-C20 thioalkyl, C1-C20 alkyl substituted phenyl, C1-C20 alkoxy substituted phenyl and C1-C20 thioalkyl substituted phenyl;

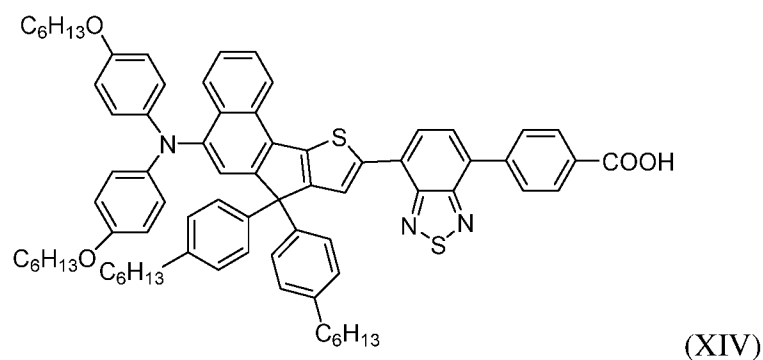
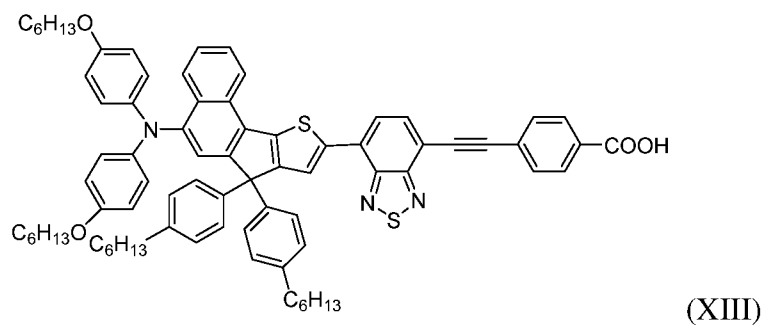
- 5 R_1 is an anchoring group selected from -COOH, -CONHOH, -PO₃H₂, -PO₄H₂, -P(R₈)O₂H, -SO₃H₂, -SO₄H₂, 1,2-hydroxybenzene, 1-hydroxy-2-carboxybenzene, acetylacetonate, deprotonated forms of the aforementioned, organic and/or inorganic salts of said deprotonated forms, and chelating groups with π -conducting character, R_8 is selected from alkyl, alkenyl, alkynyl, aryl, alkylaryl, alkoxyaryl, and thioalkylaryl, preferably R_1 is -COOH.

10 In an embodiment of the compound of formulae (IX) and (X), R_{A31} , R_{A32} , R_{B31} , R_{B32} , are independently selected from H, C1-C10 alkyl, C1-C10 alkoxy and C1-C10 thioalkyl.

15 In an embodiment of the compound of formulae (IX) and (X) R_{A31} , R_{A32} , are independently selected from C1-C10 alkyl, C1-C10 alkoxy and C1-C10 thioalkyl, preferably C2-C8 alkoxy and C2-C8 thioalkyl, and, R_{B1} , and R_{B2} are independently selected from C1-C10 alkyl, preferably C2-C8 alkyl.

20 In a preferred embodiment, the compound of the invention comprises the structure of any one of formulae (XI) to (XIV):





5

The compounds of the invention are useful as dyes and/or sensitizers. For example, they are useful in optoelectronic devices, in particular solar cells. In an embodiment, the optoelectronic device preferably is a dye-sensitized solar cell.

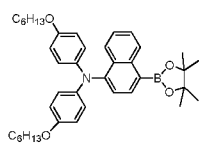
- 10 The following examples provide illustrative way of practicing the instant invention and are not intended to limit the scope of the invention in any way.

Examples

15 Examples 1-4: Synthesis of compounds H1-H4

The synthetic scheme in Figure 1 shows the synthesis of compounds H1-H4 and also the intermediate products 1-5.

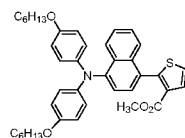
- 20 N,N-bis(4-(hexyloxy)phenyl)-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)naphthalen-1-amine (2)



intermediate 2

In a dried three-neck round-bottom were dissolved compound 1 in Fig. 1 (2.32 g, 4.04 mmol), bis(pinacolato)diboron (902mg, 4.85 mmol) and KOAc (1.19 g, 12.12 mmol) in toluene. Then Pd(dppf)Cl₂ (147mg, 0.20 mmol) was added to the reaction mixture under argon, which was refluxed 6 h. The mixture was extracted with dichloromethane before the organic phase was washed with water and dried over anhydrous sodium sulfate. After solvent removal under reduced pressure, the crude product 2 was purified by column chromatography (toluene/petroleum ether 60–90 °C, 2/1, v/v) on silica gel to yield a yellow solid as the desired product 2 (2.13g, 87% yield). ¹H NMR (400 MHz, CDCl₃) δ: 8.02-7.95 (m, 2H), 7.48-7.39 (m, 2H), 7.31-7.27 (m, 1H), 7.16 (d, *J* = 6.8 Hz, 1H), 6.88 (br, 4H), 6.74-6.72 (m, 4H), 3.89 (t, *J* = 5.8Hz, 4H), 1.77-1.71 (m, 4H), 1.48-1.42 (m, 16H), 1.33-1.27 (m, 8H), 0.92-0.88 (m, 6H). ¹³C NMR (100 MHz, CDCl₃) δ: 163.46, 154.57, 149.10, 145.89, 142.86, 134.37, 130.68, 130.51, 129.38, 128.64, 128.29, 126.50, 126.20, 125.99, 125.08, 124.95, 124.50, 123.99, 115.27, 68.42, 51.58, 31.79, 29.53, 25.95, 22.80, 14.24. HR-MS (MALDI-TOF) *m/z* calcd. for (C₄₀H₅₂BNO₄): 621.39894. Found: 621.40984. Anal. Calcd. for C₄₀H₅₂BNO₄: C, 77.28%; H, 8.43%; N, 2.25%. Found: C, 77.28%; H, 8.44%; N, 2.26%.

Methyl 2-(4-(bis(4-(hexyloxy)phenyl)amino)naphthalen-1-yl)thiophene-3-carboxylate (3)



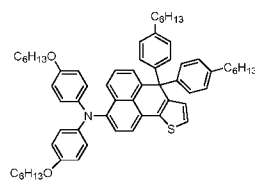
Intermediate 3

N,N-bis(4-(hexyloxy)phenyl)-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)naphthalen-1-amine (intermediate 2) (2.89 g, 4.64 mmol) with methyl 2-bromothiophene-3-carboxylate (1.1 g, 4.98 mmol) was performed by sing catalytic amount of Pd(OAc)₂ (47 mg, 0.21 mmol) and Sphos (86 mg, 0.21 mmol) in the presence of K₃PO₄ (4.4 g, 20.73 mmol) in dioxane/H₂O (5/1, v/v), then, the reaction mixture was refluxed 4h. The mixture was poured into water and extracted with dichloromethane after cooling. The organic phase was dried over anhydrous sodium sulfate and then the volatile was removed. The residue product was purified by column chromatography (toluene/petroleum ether 60–90 °C, 2/1, v/v) on silica gel to yield a yellow solid as the desired intermediate product 3 (2.58g, 88% yield). ¹H NMR (500 MHz, CDCl₃) δ: 8.02 (d, *J* = 8.0 Hz, 1H), 7.62-7.60 (m, 2H), 7.40 (d, *J* = 7.7 Hz, 1H), 7.35 (d, *J* = 5.5 Hz, 1H), 7.34-7.28 (m, 2H), 7.19 (d, *J* = 7.7 Hz, 1H), 6.95-6.93 (m, 4H), 6.77-6.74 (m, 4H), 3.89 (t, *J* = 6.6 Hz, 4H), 3.50 (s, 3H), 1.78-1.72 (m, 4H), 1.47-1.41 (m, 4H), 1.34-1.31 (m, 8H), 0.97-0.88 (m, 6H). ¹³C NMR (125 MHz, CDCl₃) δ: 163.46, 154.57, 149.10, 145.89, 142.86, 134.37, 130.68, 130.51, 129.38, 128.64, 128.29, 126.50, 126.20,

125.99, 125.08, 124.95, 124.50, 123.99, 115.27, 68.42, 51.58, 31.79, 29.53, 25.95, 22.80, 14.24. HR-MS (MALDI-TOF) m/z calcd. for (C₄₀H₄₅NO₄S): 635.30693. Found: 636.31603. Anal. Calcd. for C₄₀H₄₅NO₄S: C, 75.56%; H, 7.13%; N, 2.20%. Found: C, 77.54%; H, 7.14%; N, 2.21%.

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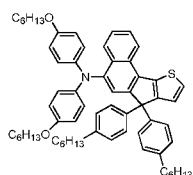
N,N-bis(4-(hexyloxy)phenyl)-7,7-bis(4-hexylphenyl)-7H-phenaleno[1,2-b]thiophen-3-amine
(4)



Intermediate 4

Intermediate 3 (1.27 g, 2.00 mmol), (4-hexylphenyl)magnesium bromide (8 mL, 2M in THF, 16.00 mmol), and THF (15 mL) were added to a three-neck flame-dried round-bottom flask. The resulting mixture was refluxed overnight under argon and then cooled to room temperature. Water was added to terminate the reaction, and the mixture was poured into cold 1 M hydrochloric acid aqueous solution. The resulting solution was extracted three times with dichloromethane before the organic phase was washed with water and dried over anhydrous sodium sulfate. After solvent removal under reduced pressure, the residue tertiary alcohol was used in the next reaction directly. The tertiary alcohol, Amberlyst 15 (0.75 g), and toluene (20 mL) were added to a three-neck round-bottom flask. The resulting mixture was refluxed overnight under argon and then cooled to room temperature. The solution was filtered and the filtrate was concentrated under reduced pressure. The residue was purified by column chromatography toluene/petroleum ether 60–90 °C, 1/3, *v/v*) on silica gel to yield a orange oil as the desired intermediate product 4 (819 mg, 45% yield). ¹H NMR (400 MHz, THF-*d*₈) δ : 7.89 (d, *J* = 9.2 Hz, 1H), 7.54 (d, *J* = 7.8 Hz, 1H), 7.33-7.27 (m, 1H), 7.23-7.17 (m, 2H), 7.13 (d, *J* = 7.8 Hz, 1H), 7.06-7.00 (m, 8H), 6.90-6.87 (m, 4H), 6.75-6.70 (m, 5H), 3.86 (t, *J* = 6.4 Hz, 4H), 2.53 (t, *J* = 7.7 Hz, 4H), 1.76-1.69 (m, 4H), 1.61-1.53 (m, 4H), 1.50-1.42 (m, 4H), 1.36-1.31 (m, 20H), 0.93-0.87 (m, 12H). ¹³C NMR (100 MHz, THF-*d*₈) δ : 155.70, 147.27, 145.54, 144.78, 143.83, 141.63, 135.83, 131.81, 131.14, 130.59, 130.50, 128.99, 128.74, 128.67, 126.83, 126.73, 126.66, 124.58, 124.23, 124.18, 120.43, 115.92, 68.84, 58.95, 36.54, 36.46, 32.86, 32.76, 32.70, 32.62, 30.52, 30.27, 30.20, 26.91, 23.70, 23.65, 14.60, 14.58. HR-MS (MALDI-TOF) m/z calcd. for (C₆₃H₇₅NO₂S): 909.55185. Found: 910.55912. Anal. Calcd. for C₆₃H₇₅NO₂S: C, 83.12%; H, 8.30%; N, 1.54%. Found: C, 83.10%; H, 8.31%; N, 1.55%.

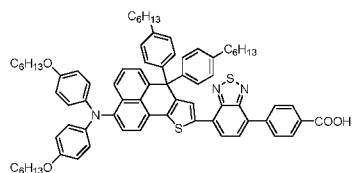
N,N-bis(4-(hexyloxy)phenyl)-7,7-bis(4-hexylphenyl)-7H-benzo[6,7]indeno[1,2-b]thiophen-5-amine (5)



Intermediate 5

Intermediate 3 (1.27 g, 2.00 mmol), (4-hexylphenyl)magnesium bromide (8 mL, 2M in THF, 16.00 mmol), and THF (15 mL) were added to a three-neck flame-dried round-bottom flask. The resulting mixture was refluxed overnight under argon and then cooled to room temperature. Water was added to terminate the reaction, and the mixture was poured into cold 1 M hydrochloric acid aqueous solution. The resulting solution was extracted three times with dichloromethane before the organic phase was washed with water and dried over anhydrous sodium sulfate. After solvent removal under reduced pressure, the residue tertiary alcohol was used in the next reaction directly. The tertiary alcohol, Amberlyst 15 (0.75 g), and toluene (20 mL) were added to a three-neck round-bottom flask. The resulting mixture was refluxed overnight under argon and then cooled to room temperature. The solution was filtered and the filtrate was concentrated under reduced pressure. The residue was purified by column chromatography toluene/petroleum ether 60–90 °C, 1/3, v/v) on silica gel to yield a orange oil as the desired intermediate product 5 (819 mg, 45% yield). ¹H NMR (400 MHz, THF-*d*₈) δ: 8.18 (d, *J* = 8.2 Hz, 1H), 8.01 (d, *J* = 8.6 Hz, 1H), 7.55-7.51 (m, 1H), 7.48 (d, *J* = 4.9 Hz, 1H), 7.36 (s, 1H), 7.33-7.29 (s, 1H), 7.15 (d, *J* = 4.9 Hz, 1H), 7.07-7.05 (m, 4H), 6.98-6.96 (m, 4H), 6.86-6.84 (m, 4H), 6.71-6.68 (m, 4H), 3.86 (t, *J* = 6.4 Hz, 4H), 2.55-2.50 (m, 4H), 1.76-1.70 (m, 4H), 1.57-1.52 (m, 4H), 1.48-1.43 (m, 4H), 1.36-1.31 (m, 20H), 0.93-0.86 (m, 12H). ¹³C NMR (100 MHz, THF-*d*₈) δ: 157.60, 155.52, 152.99, 144.16, 143.70, 142.46, 142.21, 140.63, 131.96, 131.35, 129.10, 129.15, 129.10, 128.83, 127.41, 126.64, 126.50, 125.97, 125.66, 124.20, 124.02, 115.84, 68.86, 64.53, 36.54, 32.86, 32.78, 32.69, 30.53, 30.24, 26.93, 23.71, 23.67, 14.63, 14.59. HR-MS (MALDI-TOF) *m/z* calcd. for (C₆₃H₇₅NO₂S): 909.55185. Found: 910.55912. Anal. Calcd. for C₆₃H₇₅NO₂S: C, 83.12%; H, 8.30%; N, 1.54%. Found: C, 83.11%; H, 8.32%; N, 1.54%.

4-(7-(3-(bis(4-(hexyloxy)phenyl)amino)-7,7-bis(4-hexylphenyl)-7H-phenaleno[1,2-b]thiophen-9-yl)benzo[c][1,2,5]thiadiazol-4-yl)benzoic acid (H1)



H1

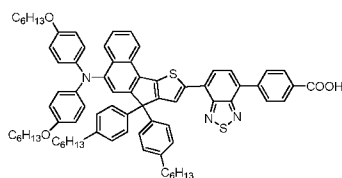
In a three-neck flame-dried round-bottom flask was dissolved intermediate 4 (273 mg, 0.30 mmol) in THF (10 mL) and cooled to $-78\text{ }^{\circ}\text{C}$ using a dry ice/acetone cold bath. Under argon, *n*-BuLi (0.37 mL, 1.6 M in hexanes, 0.60 mmol) was added dropwise to the reaction mixture, which was stirred for 0.5 h at $-78\text{ }^{\circ}\text{C}$. After trimethylstannyl chloride (120 mg, 0.60 mmol) was added in one portion *via* syringe, the mixture was slowly warmed up and stirred for 2 h at room temperature. Water was slowly added to terminate the reaction and the mixture was extracted three times with diethyl ether before the organic phase was washed with water and dried over anhydrous sodium sulfate. After solvent removal under reduced pressure, the crude product N,N-bis(4-(hexyloxy)phenyl)-4,4-bis(4-hexylphenyl)-2-(trimethylstannyl)-4H-benzo[1,10]phenanthro[4,3-b]thiophen-8-amine was used as a precursor to synthesize H1 without further purification.

In a dried Schlenk tube were dissolved N,N-bis(4-(hexyloxy)phenyl)-7,7-bis(4-hexylphenyl)-9-(trimethylstannyl)-7H-phenaleno[1,2-b]thiophen-3-amine and butyl 4-(7-bromobenzo[c][1,2,5]thiadiazol-4-yl)benzoate (138 mg, 0.36 mmol) in toluene (10 mL). Then $\text{Pd}(\text{PPh}_3)_2\text{Cl}_2$ (26 mg, 0.04 mmol) was added to the reaction mixture, which was refluxed for 6 h. Water was added to terminate the reaction and the mixture was extracted three times with chloroform before the organic phase was washed with water and dried over anhydrous sodium sulfate. After solvent removal under reduced pressure, the crude product was purified by column chromatography (toluene/petroleum ether $60\text{--}90\text{ }^{\circ}\text{C}$, 2/1, *v/v*) on silica gel to yield a black powder as the desired butyl ester.

In a three-neck round-bottom flask were dissolved butyl ester and KOH (152 mg, 2.70 mmol) in a solvent mixture of THF/ H_2O (8 mL, 3/1, *v/v*). The reaction mixture was refluxed overnight and then cooled to room temperature. Chloroform was added before the organic phase was washed with 0.1 M hydrochloric acid and deionized water in turn and then dried over anhydrous sodium sulfate. After solvent removal under reduced pressure, the crude product was purified by column chromatography (chloroform/methanol, 10/1, *v/v*) on silica gel to yield a black solid as the desired product H1 (283 mg, 81% yield). ^1H NMR (500 MHz, $\text{THF}-d_8$) δ : 8.14–8.10 (m, 4H), 7.99 (s, 1H), 7.93 (d, $J = 8.3\text{ Hz}$, 1H), 7.90 (d, $J = 7.3\text{ Hz}$, 1H),

7.77 (d, $J = 7.4$ Hz, 1H), 7.67 (d, $J = 7.7$ Hz, 1H), 7.32 (d, $J = 7.3$ Hz, 1H), 7.26 (t, $J = 8.0$ Hz, 1H), 7.18-7.16 (m, 5H), 7.06-7.04 (m, 4H), 6.92-6.90 (m, 4H), 6.74-6.72 (m, 4H), 3.87 (t, $J = 6.3$ Hz, 4H), 2.53 (t, $J = 7.7$ Hz, 4H), 1.75-1.70 (m, 4H), 1.59-1.53 (m, 4H), 1.49-1.43 (m, 4H), 1.36-1.28 (m, 20H), 0.92-0.85 (m, 6H). ^{13}C NMR (125 MHz, $\text{THF-}d_8$) δ : 167.58, 155.84, 154.69, 153.60, 147.27, 145.75, 143.82, 143.66, 142.28, 141.79, 137.94, 137.82, 132.08, 131.87, 131.70, 131.48, 130.71, 129.99, 129.53, 129.05, 128.66, 127.88, 126.93, 126.03, 124.81, 124.44, 121.08, 115.98, 68.86, 58.92, 36.48, 32.84, 32.77, 32.57, 30.89, 30.80, 30.71, 30.64, 30.43, 30.28, 26.92, 23.70, 23.64, 14.59. HR-MS (MALDI-TOF) m/z calcd. for $(\text{C}_{76}\text{H}_{81}\text{N}_3\text{O}_4\text{S}_2)$: 1163.56685. Found: 1164.57412. Anal. Calcd. for $\text{C}_{76}\text{H}_{81}\text{N}_3\text{O}_4\text{S}_2$: C, 78.38%; H, 7.01%; N, 3.61%. Found: C, 78.39%; H, 7.02%; N, 3.62%.

4-(7-(5-(bis(4-(hexyloxy)phenyl)amino)-7,7-bis(4-hexylphenyl)-7H-benzo[6,7]indeno[1,2-b]thiophen-9-yl)benzo[c][1,2,5]thiadiazol-4-yl)benzoic acid (H2)



H2

In a three-neck flame-dried round-bottom flask was dissolved 5 (273mg, 0.3 mmol) in THF (10 mL) and cooled to -78 °C using a dry ice/acetone cold bath. Under argon, *n*-BuLi (0.37 mL, 1.6 M in hexanes, 0.60 mmol) was added dropwise to the reaction mixture, which was stirred for 0.5 h at -78 °C. After trimethylstannyl chloride (120 mg, 0.60 mmol) was added in one portion *via* syringe, the mixture was slowly warmed up and stirred for 2 h at room temperature. Water was slowly added to terminate the reaction and the mixture was extracted three times with diethyl ether before the organic phase was washed with water and dried over anhydrous sodium sulfate. After solvent removal under reduced pressure, the crude product N,N-bis(4-(hexyloxy)phenyl)-7,7-bis(4-hexylphenyl)-9-(trimethylstannyl)-7H-benzo[6,7]indeno[1,2-b]thiophen-5-amine as a precursor to synthesize H2 without further purification.

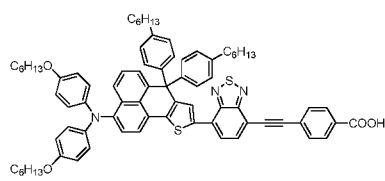
In a dried Schlenk tube were dissolved N,N-bis(4-(hexyloxy)phenyl)-7,7-bis(4-hexylphenyl)-9-(trimethylstannyl)-7H-phenaleno[1,2-b]thiophen-3-amine and butyl 4-(7-bromobenzo[c][1,2,5]thiadiazol-4-yl)benzoate (138 mg, 0.36 mmol) in toluene (10 mL). Then Pd(PPh₃)₂Cl₂ (26 mg, 0.04 mmol) was added to the reaction mixture, which was refluxed for 6 h. Water was added to terminate the reaction and the mixture was extracted three times with

chloroform before the organic phase was washed with water and dried over anhydrous sodium sulfate. After solvent removal under reduced pressure, the crude product was purified by column chromatography (toluene/petroleum ether 60–90 °C, 2/1, v/v) on silica gel to yield a black powder as the desired butyl ester.

5

In a three-neck round-bottom flask were dissolved butyl ester and KOH (152 mg, 2.70 mmol) in a solvent mixture of THF/H₂O (8 mL, 3/1, v/v). The reaction mixture was refluxed overnight and then cooled to room temperature. Chloroform was added before the organic phase was washed with 0.1 M hydrochloric acid and deionized water in turn and then dried over anhydrous sodium sulfate. After solvent removal under reduced pressure, the crude product was purified by column chromatography (chloroform/methanol, 10/1, v/v) on silica gel to yield a black solid as the desired product H2 (283 mg, 81% yield). ¹H NMR (500 MHz, THF-*d*₈) δ: 8.33 (s, 1H), 8.30 (d, *J* = 8.3 Hz, 1H), 8.18-8.13 (m, 4H), 8.09-8.03 (m, 2H), 7.88 (d, *J* = 7.6 Hz, 1H), 7.60-7.58 (m, 1H), 7.38-7.34 (m, 2H), 7.20-7.18 (m, 4H), 7.03-7.02 (m, 4H), 6.89-6.87 (m, 4H), 6.73-6.71 (m, 4H), 3.88 (t, *J* = 6.3 Hz, 4H), 2.55-2.52 (m, 4H), 1.77-1.74 (m, 4H), 1.58-1.53 (m, 4H), 1.49-1.47 (m, 4H), 1.36-1.28 (m, 20H), 0.93-0.85 (m, 12H). ¹³C NMR (125 MHz, THF-*d*₈) δ: 167.61, 158.12, 155.69, 154.79, 153.50, 153.44, 145.08, 143.69, 143.49, 143.11, 142.43, 142.31, 142.28, 131.70, 131.44, 131.38, 130.71, 129.98, 129.67, 129.26, 128.97, 128.71, 127.72, 126.86, 126.70, 126.27, 125.35, 125.33, 124.44, 124.36, 115.91, 68.89, 65.01, 36.57, 32.86, 32.78, 32.70, 30.89, 30.80, 30.72, 30.64, 30.53, 30.26, 26.94, 23.71, 23.66, 14.61, 14.58. HR-MS (MALDI-TOF) *m/z* calcd. for (C₇₆H₈₁N₃O₄S₂): 1163.56685. Found: 1164.57209. Anal. Calcd. for C₇₆H₈₁N₃O₄S₂: C, 78.38%; H, 7.01%; N, 3.61%. Found: C, 78.40%; H, 7.03%; N, 3.60%.

25 4-((7-(3-(bis(4-(hexyloxy)phenyl)amino)-7,7-bis(4-hexylphenyl)-7H-phenaleno[1,2-b]thiophen-9-yl)benzo[c][1,2,5]thiadiazol-4-yl)ethynyl)benzoic acid (H3)



In a three-neck flame-dried round-bottom flask was dissolved 4 (282 mg, 0.30 mmol) in THF (10 mL) and cooled to –78 °C using a dry ice/acetone cold bath. Under argon, *n*-BuLi (0.37 mL, 1.6 M in hexanes, 0.60 mmol) was added dropwise to the reaction mixture, which was stirred for 0.5 h at –78 °C. After trimethylstannyl chloride (120 mg, 0.60 mmol) was added in

30

one portion *via* syringe, the mixture was slowly warmed up and stirred for 2 h at room temperature. Water was slowly added to terminate the reaction and the mixture was extracted three times with diethyl ether before the organic phase was washed with water and dried over anhydrous sodium sulfate. After solvent removal under reduced pressure, the crude product

5 N,N-bis(4-(hexyloxy)phenyl)-4,4-bis(4-hexylphenyl)-2-(trimethylstannyl)-4H-benzo[1,10]phenanthro[4,3-b]thiophen-8-amine as a precursor to synthesize H3 without further purification.

In a dried Schlenk tube were dissolved N,N-bis(4-(hexyloxy)phenyl)-7,7-bis(4-hexylphenyl)-

10 9-(trimethylstannyl)-7H-phenaleno[1,2-b]thiophen-3-amine and butyl 4-((7-bromobenzo[*c*][1,2,5]thiadiazol-4-yl)ethynyl)benzoate (150 mg, 0.36 mmol) in toluene (10 mL). Then Pd(PPh₃)₂Cl₂ (26 mg, 0.04 mmol) was added to the reaction mixture, which was refluxed for 6 h. Water was added to terminate the reaction and the mixture was extracted three times with chloroform before the organic phase was washed with water and dried over

15 anhydrous sodium sulfate. After solvent removal under reduced pressure, the crude product was purified by column chromatography (toluene/petroleum ether 60–90 °C, 2/1, *v/v*) on silica gel to yield a black powder as the desired butyl ester.

In a three-neck round-bottom flask were dissolved butyl ester and KOH (152 mg, 2.70 mmol)

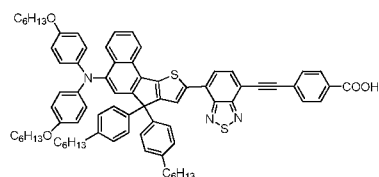
20 in a solvent mixture of THF/H₂O (8 mL, 3/1, *v/v*). The reaction mixture was refluxed overnight and then cooled to room temperature. Chloroform was added before the organic phase was washed with 0.1 M phosphoric acid and deionized water in turn and then dried over anhydrous sodium sulfate. After solvent removal under reduced pressure, the crude product was purified by column chromatography (chloroform/methanol, 10/1, *v/v*) on silica

25 gel to yield a black solid as the desired product H3 (292 mg, 82% yield). ¹H NMR (500 MHz, THF-*d*₈) δ: 8.06 (d, *J* = 8.1 Hz, 2H), 8.02 (s, 1H), 7.92 (d, *J* = 8.2 Hz, 1H), 7.88 (d, *J* = 7.6 Hz, 1H), 7.77 (d, *J* = 7.6 Hz, 1H), 7.70-7.67 (m, 3H), 7.31 (d, *J* = 7.3 Hz, 1H), 7.27-7.24 (m, 1H), 7.18 (s, 1H), 7.16-7.14 (m, 4H), 7.06-7.05 (m, 4H), 6.92-6.90 (m, 4H), 6.75-6.73 (m, 4H), 3.87 (t, *J* = 6.3 Hz, 4H), 2.54 (t, *J* = 7.7 Hz, 4H), 1.76-1.70 (m, 4H), 1.60-1.54 (m, 4H), 1.47-

30 1.45 (m, 4H), 1.35-1.28 (m, 20H), 0.92-0.87 (m, 12H). ¹³C NMR (125 MHz, THF-*d*₈) δ: 167.16, 156.21, 155.87, 152.65, 147.21, 146.44, 145.89, 143.81, 143.55, 141.82, 138.63, 137.54, 134.06, 132.50, 132.40, 132.02, 131.62, 130.81, 130.76, 130.69, 129.04, 128.91, 128.86, 128.30, 126.95, 126.61, 125.46, 125.35, 124.85, 124.47, 121.22, 115.98, 115.37, 96.24, 89.46, 68.86, 58.87, 36.47, 32.85, 32.76, 32.58, 30.52, 30.28, 26.92, 23.70, 23.64,

14.59, 14.57. HR-MS (MALDI-TOF) m/z calcd. for (C₇₈H₈₁N₃O₄S₂): 1187.56685. Found: 1188.57412. Anal. Calcd. for C₇₈H₈₁N₃O₄S₂: C, 78.82%; H, 6.87%; N, 3.54%. Found: C, 78.80%; H, 8.88%; N, 3.55%.

- 5 4-((7-(5-(bis(4-(hexyloxy)phenyl)amino)-7,7-bis(4-hexylphenyl)-7H-benzo[6,7]indeno[1,2-b]thiophen-9-yl)benzo[c][1,2,5]thiadiazol-4-yl)ethynyl)benzoic acid (H4)



(H4)

In a three-neck flame-dried round-bottom flask was dissolved 5 (273mg, 0.3 mmol) in THF (10 mL) and cooled to -78°C using a dry ice/acetone cold bath. Under argon, *n*-BuLi (0.37 mL, 1.6 M in hexanes, 0.60 mmol) was added dropwise to the reaction mixture, which was stirred for 0.5 h at -78°C . After trimethylstannyl chloride (120 mg, 0.60 mmol) was added in one portion *via* syringe, the mixture was slowly warmed up and stirred for 2 h at room temperature. Water was slowly added to terminate the reaction and the mixture was extracted three times with diethyl ether before the organic phase was washed with water and dried over anhydrous sodium sulfate. After solvent removal under reduced pressure, the crude product N,N-bis(4-(hexyloxy)phenyl)-7,7-bis(4-hexylphenyl)-9-(trimethylstannyl)-7H-benzo[6,7]indeno[1,2-b]thiophen-5-amine as a precursor to synthesize H4 without further purification.

In a dried Schlenk tube were dissolved N,N-bis(4-(hexyloxy)phenyl)-7,7-bis(4-hexylphenyl)-9-(trimethylstannyl)-7H-phenaleno[1,2-b]thiophen-3-amine and butyl 4-((7-bromobenzo[c][1,2,5]thiadiazol-4-yl)ethynyl)benzoate (150 mg, 0.36 mmol) in toluene (10 mL). Then Pd(PPh₃)₂Cl₂ (26 mg, 0.04 mmol) was added to the reaction mixture, which was refluxed for 6 h. Water was added to terminate the reaction and the mixture was extracted three times with chloroform before the organic phase was washed with water and dried over anhydrous sodium sulfate. After solvent removal under reduced pressure, the crude product was purified by column chromatography (toluene/petroleum ether 60–90 $^{\circ}\text{C}$, 2/1, *v/v*) on silica gel to yield a black powder as the desired butyl ester.

In a three-neck round-bottom flask were dissolved butyl ester and KOH (152 mg, 2.70 mmol) in a solvent mixture of THF/H₂O (8 mL, 3/1, *v/v*). The reaction mixture was refluxed

overnight and then cooled to room temperature. Chloroform was added before the organic phase was washed with 0.1 M phosphoric acid and deionized water in turn and then dried over anhydrous sodium sulfate. After solvent removal under reduced pressure, the crude product was purified by column chromatography (chloroform/methanol, 10/1, v/v) on silica gel to yield a black solid as the desired product H4 (292 mg, 82% yield). ¹H NMR (500 MHz, THF-*d*₈) δ : 8.34 (s, 1H), 8.29 (d, *J* = 8.3 Hz, 1H), 8.07 (d, *J* = 8.3 Hz, 2H), 8.04-8.01 (m, 2H), 7.82 (d, *J* = 7.6 Hz, 1H), 7.70 (d, *J* = 8.3 Hz, 2H), 7.61-7.58 (m, 1H), 7.37 (s, 1H), 7.35 (t, *J* = 8.0 Hz, 1H), 7.18-7.17 (m, 4H), 7.03-7.02 (m, 4H), 6.89-6.87 (m, 4H), 6.73-6.71 (m, 4H), 3.88 (t, *J* = 6.4 Hz, 4H), 2.55-2.52 (m, 4H), 1.76-1.74 (m, 4H), 1.59-1.53 (m, 4H), 1.50-1.44 (m, 4H), 1.36-1.28 (m, 20H), 0.93-0.85 (m, 12H). ¹³C NMR (125 MHz, THF-*d*₈) δ : 167.18, 158.23, 156.23, 156.28, 155.72, 153.63, 152.52, 145.34, 143.66, 142.83, 142.47, 142.17, 135.25, 132.48, 131.98, 131.54, 131.34, 130.77, 129.72, 129.27, 128.94, 128.37, 127.78, 126.88, 126.74, 126.23, 125.25, 124.85, 124.71, 124.50, 115.91, 114.92, 96.19, 89.59, 68.88, 64.99, 36.56, 32.86, 32.78, 32.70, 30.53, 30.26, 26.93, 23.71, 23.66, 14.61, 14.58. HR-MS (MALDI-TOF) *m/z* calcd. for (C₇₈H₈₁N₃O₄S₂): 1187.56685. Found: 1188.57940. Anal. Calcd. for C₇₈H₈₁N₃O₄S₂: C, 78.82%; H, 6.87%; N, 3.54%. Found: C, 78.81%; H, 8.89%; N, 3.56%.

Examples 5-8 preparation of dye-sensitized solar cells comprising sensitizers H1-H4

Dye-sensitized solar cells were prepared in accordance with a state of the art preparation protocol. A 4 μ m compact layer of TiO₂ was deposited on a transparent conductive ITO substrate (FTO glass). A mesoporous 4 μ m mesoporous TiO₂ layer was deposited on top the compact TiO₂ layer. The FTO glass comprising the TiO₂ layers was immersed in a solvent comprising the organic dyes H1-H4, respectively. Cells were sealed and solvent CF/EtOH 1/19 comprising a redox-shuttle based on 0.25M Cobpy(II), 0.15 M Cobpy(II), and additives 0.5M TBP, 0.1M LiTFSI.

The photovoltaic parameters of the cells were assessed. The results are shown in Figure 2 and Table 1 below:

Table 1: Photovoltaic parameters of dye-sensitized solar cells comprising sensitizers H1-H4

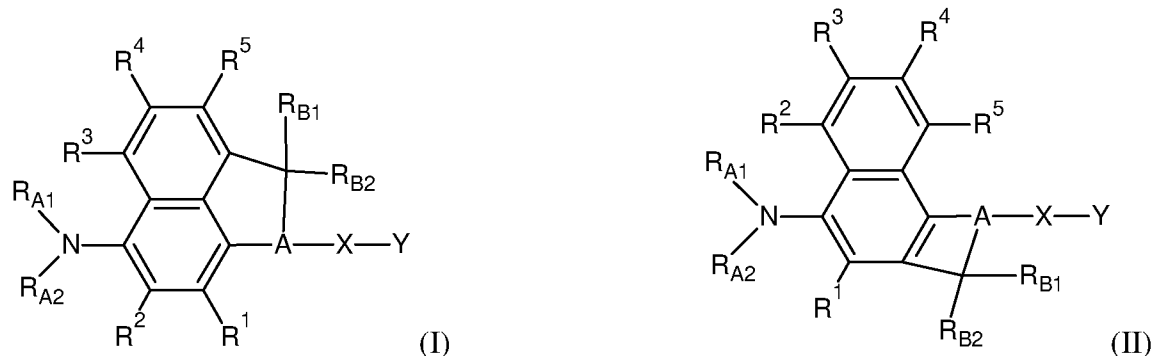
Dye	J_{SC}^{EQE} [mA cm ⁻²]	J_{SC} [mA cm ⁻²]	V_{OC} [mV]	FF [%]	PCE [%]
H1	15.59±0.06	16.17±0.09	937±6	73.9±0.3	11.2±0.1
H2	16.80±0.04	17.34±0.05	906±4	73.8±0.3	11.6±0.1
H3	15.06±0.06	15.73±0.09	919±6	72.2±0.3	10.4±0.1
H4	17.32±0.04	17.85±0.05	875±4	74.0±0.3	11.6±0.1

The results in Table 1 and Figure 2 show that the organic sensitizers H1-H4, which were prepared in accordance with the scheme of Figure 1, had impressive power conversion efficiencies of consistently above 10%. This renders the compounds H1-H4 suitable for use in solar cell applications

While certain of the preferred embodiments of the present invention have been described and specifically exemplified above, it is not intended that the invention be limited to such embodiments. Various modifications may be made thereto without departing from the scope and spirit of the present invention, as set forth in the following claims.

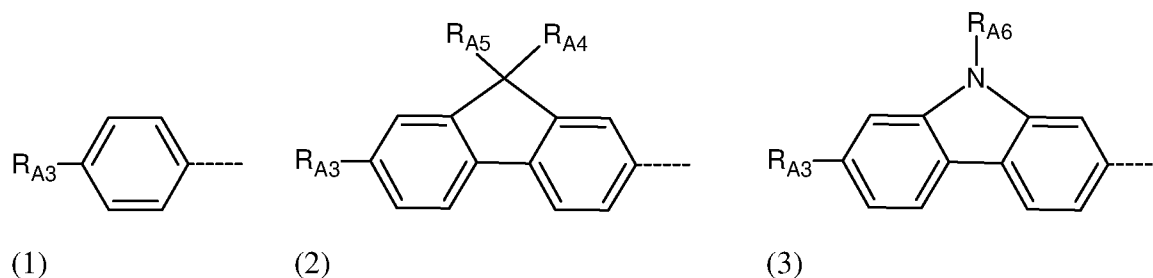
Claims

1. A compound comprising the structure of formula (I) or (II) below:



5 wherein

R_{A1} , R_{A2} , R_{B1} , and R_{B2} are independently selected from C1-C36 alkyl, and from the substituents (1) to (3) below:



10 and wherein

R_{A3} , R_{A4} , R_{A5} , in as far as present, are selected independently from H, C1-C36 alkyl, C1-C36 alkoxy, C1-C36 thioalkyl, C1-C36 alkyl substituted phenyl, C1-C36 alkoxy substituted phenyl and C1-C36 thioalkyl substituted phenyl;

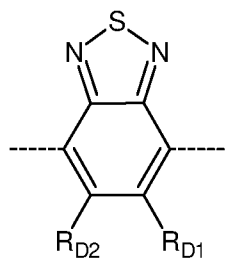
15 wherein R_{A6} is selected from H, C1-C36 alkyl, C1-C36 alkyl substituted phenyl, C1-C36 alkoxy substituted phenyl and C1-C36 thioalkyl substituted phenyl;

wherein R_{B1} and R_{B2} may further be selected independently from H, C1-C36 alkoxy, C1-C36 thioalkyl;

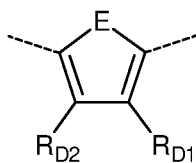
R^1 - R^5 , in as far as present, are selected independently from the substituents as specified for R_{A3} - R_{A5} ;

20 A is an optionally substituted cyclic moiety comprising from 3 to 10 carbons and 0 to 3 heteroatoms, or, methanetriyl, wherein optional substituents of said cyclic moiety are independently selected from C1-C36 alkyl, C1-C36 alkoxy, C1-C36 thioalkyl, C1-C36 alkyl substituted phenyl, C1-C36 alkoxy substituted phenyl and C1-C36 thioalkyl substituted phenyl;

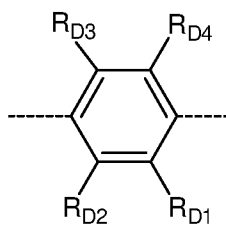
25 X is a moiety selected from the moieties (10) to (24) below,



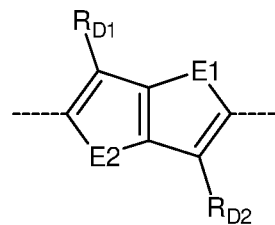
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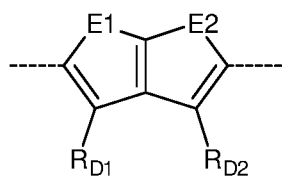
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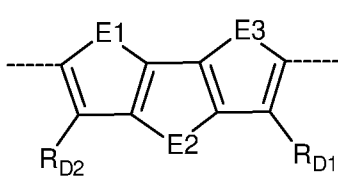
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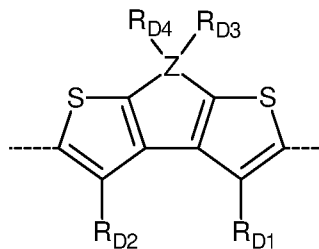
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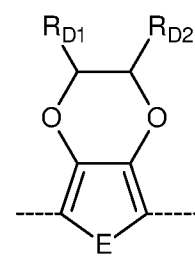
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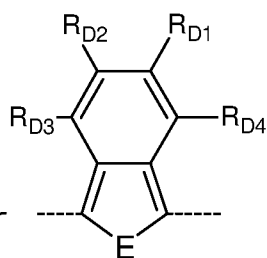
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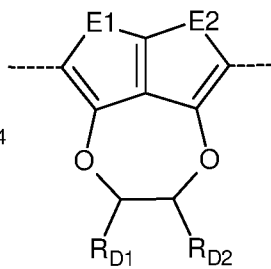
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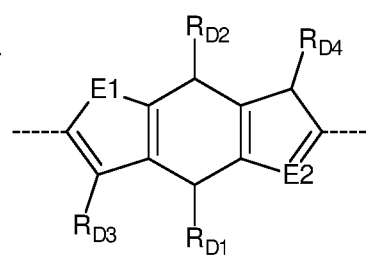
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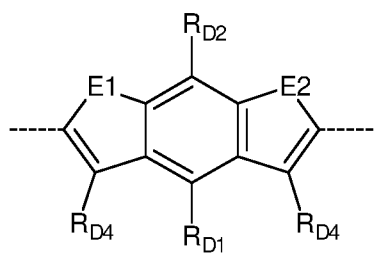
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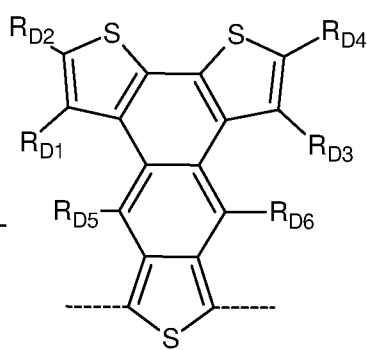
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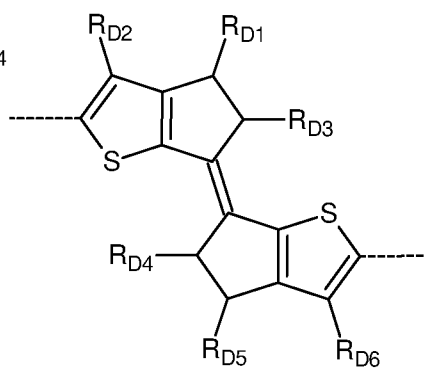
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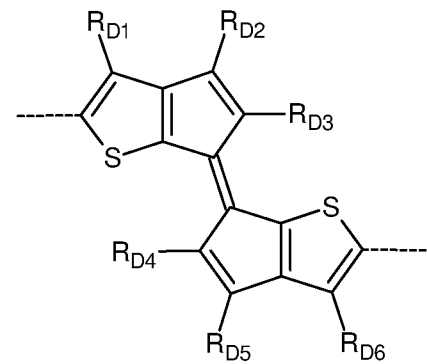
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(23)



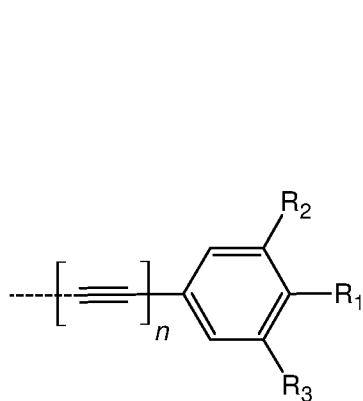
(24)

wherein,

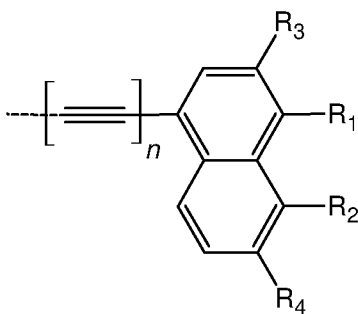
in moieties (10)-(24), R_{D1} , R_{D2} , R_{D3} , R_{D4} , R_{D5} , and R_{D6} , in as far as present, are independently selected from H, C1-C36 alkyl, C1-C36 alkoxy, C1-C36 thioalkyl, C1-C36 alkyl substituted phenyl, C1-C36 alkoxy substituted phenyl and C1-C36 thioalkyl substituted phenyl, wherein, E, E1, E2, and E3, in as far as present, are independently selected from S, O, Se, and Te;

Z in moiety (16) is selected from carbon and Si;

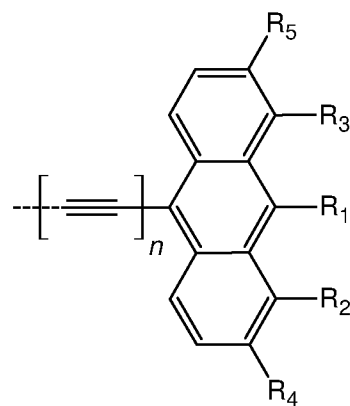
Y is selected from the substituents (30) to (43) below,



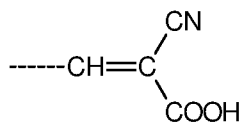
10 (30)



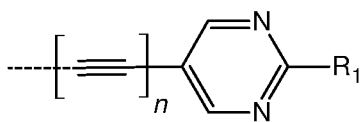
(31)



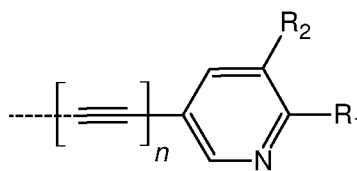
(32)



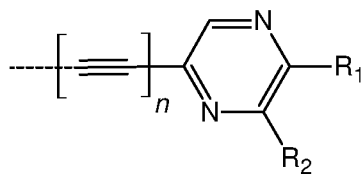
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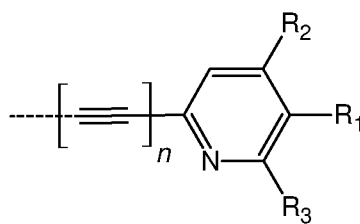
(34)



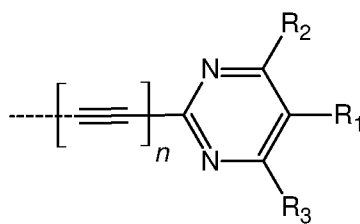
(35)



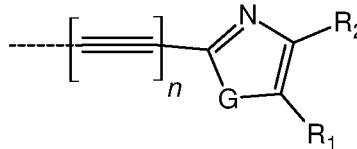
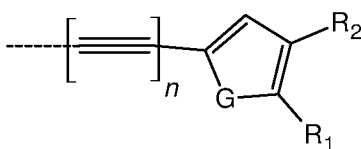
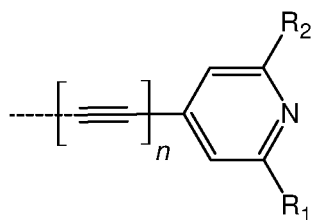
15 (36)



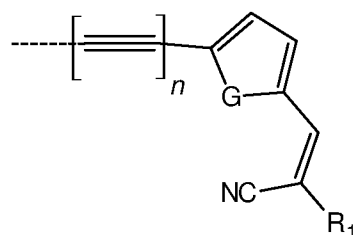
(37)



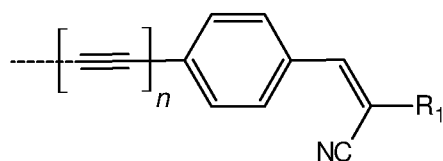
(38)



(39)



(40)



(41)

(42)

(43)

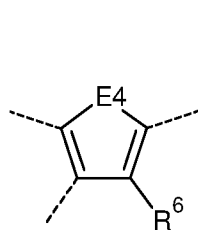
5 wherein,

R_1 , R_2 , R_3 , R_4 , and R_5 , in as far as present, are selected independently from H and from anchoring groups independently selected from the group consisting of -COOH, -CONHOH, - PO_3H_2 , - PO_4H_2 , - $P(R_8)O_2H$, - SO_3H_2 , - SO_4H_2 , 1,2-hydroxybenzene, 1-hydroxy-2-carboxybenzene, acetylacetonate, deprotonated forms of the aforementioned, organic and/or inorganic salts of said deprotonated forms, and chelating groups with π -conducting character, R_8 is selected from alkyl, alkenyl, alkynyl, aryl, alkylaryl, alkoxyaryl, and thioalkylaryl, with the proviso that each substituent Y comprises at least one of said anchoring groups; wherein G is selected from S and O;

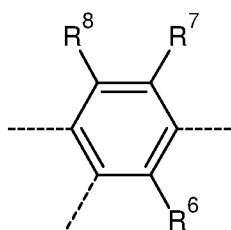
n is 1 or 0.

15

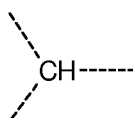
2. The compound of formula (I) or (II), wherein A is selected from any one of the moieties (50)-(52) below:



(50)



(51)



(52)

20 wherein,

the dotted line on the right side in the moieties (50) to (53) as shown above represents the single bond by which the moiety connects to X in formulae (I) or (II);

the dotted line towards the left side in the moieties (50) and (51) as shown above, on the carbon adjacent to E4 (moiety (50)) or adjacent to the carbon carrying R^8 (moiety (51)), respectively, represents the single bond by which the moiety connects to the carbon of the naphthalene moiety in formulae (I) and (II);

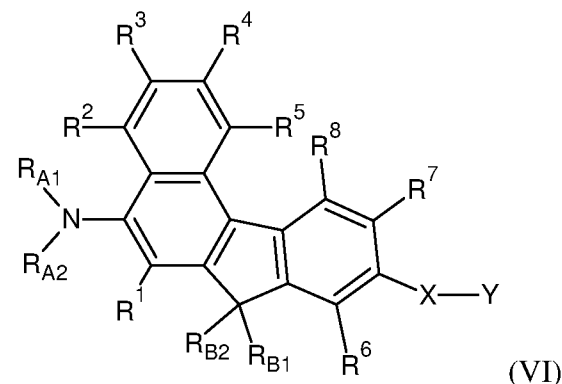
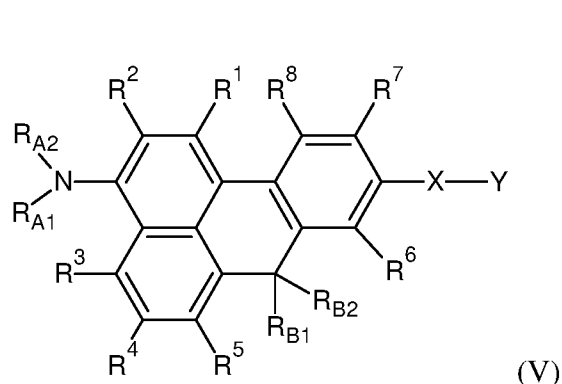
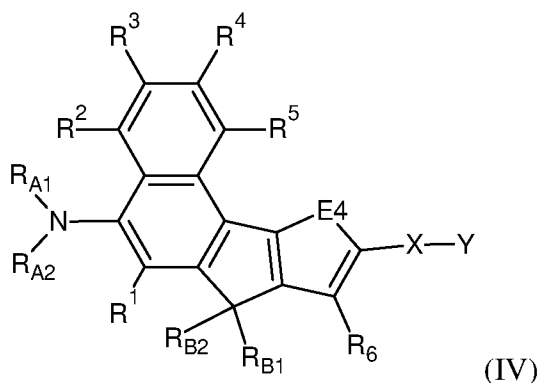
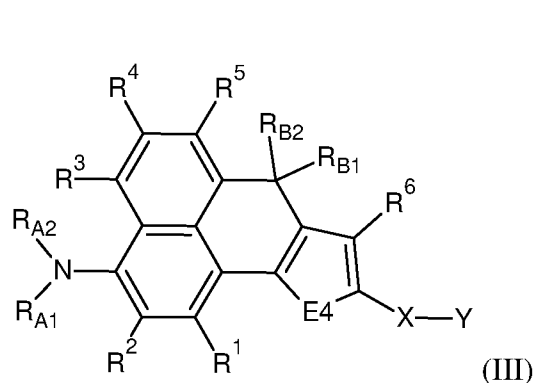
25

the dotted line towards the left side in the moieties (50) and (51) as shown above, on the carbon adjacent to the carbon carrying R^6 (moieties (50) and (51)), represents the single bond by which the moiety connects to the carbon carrying substituents R_{B1} and R_{B2} in formulae (I) and (II);

- 5 R^6 , R^7 and R^8 , in as far as present, are independently selected from H, and from the same substituents as specified for R_{A3} - R_{A5} ;

E4 is selected from S, O, Se and Te.

3. The compound of any one of claims 1 or 2, which comprises the structure of any one
10 of formulae (III), (IV), (V) or (VI) below:



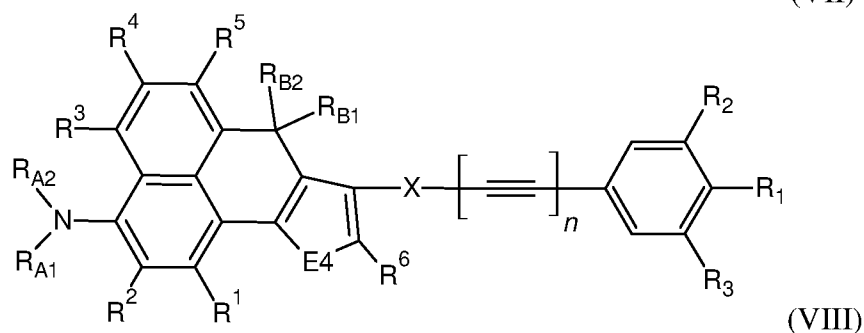
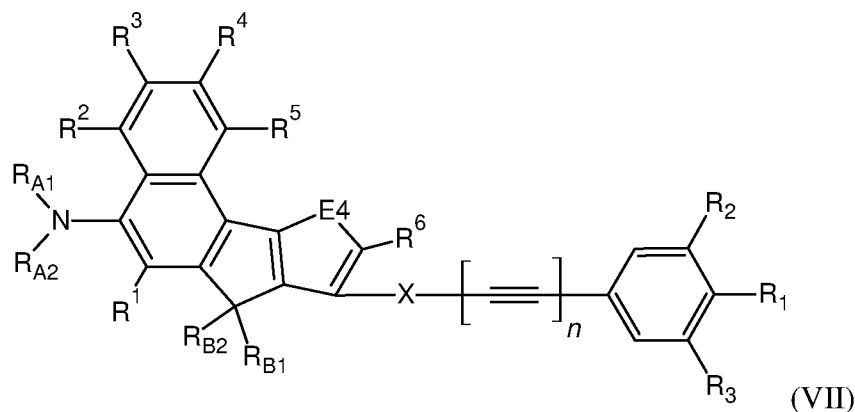
wherein,

- 15 R_{A1} , R_{A2} , R_{B1} , R_{B2} , X, Y, and, in as far as present, R^1 , R^2 , R^3 , R^4 , and R^5 are independently as defined in claim 1

R^6 , R^7 and R^8 are independently defined as R^1 - R^5 ;

E4 in moieties (III) and (IV), are as defined in claim 2.

- 20 4. The compound of any one of the preceding claims, which comprises the structure of any one of formulae (VII) and (VIII):

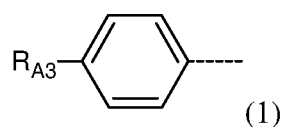


wherein,

- 5 n is = 0 or is 1;
 E4 is independently selected from S, O, Se, and Te;

 X is selected from any one of the moieties (10)-(12) as shown in claim 1, wherein, in moieties (10)-(12), R_{D1} - R_{D4} , in as far as present, are independently selected from H, C1-C15 alkyl, C1-C15 alkoxy, C1-C15 thioalkyl, C1-C10 alkyl substituted phenyl, C1-C15 alkoxy substituted phenyl and C1-C15 thioalkyl substituted phenyl, wherein, E, in as far as present, is
 10 independently selected from S and O;

R_{A1} , R_{A2} , R_{B1} , and R_{B2} are independently selected from C1-C36 alkyl and from substituents of formula (1):



- 15 wherein R_{A3} is selected from H, C1-C15 alkyl, C1-C15 alkoxy, C1-C15 thioalkyl, C1-C15 alkoxy substituted phenyl and C1-C15 thioalkyl substituted phenyl;

 wherein R_{B1} , and R_{B2} may further be selected, independently, from C1-C15 alkoxy, C1-C15 thioalkyl;

- R^1 - R^6 , in as far as present, are selected independently from the substituents as
 20 specified for R_{A3} ;

R₁, R₂, and R₃, are selected independently from H and from anchoring groups selected from the group consisting of -COOH, -CONHOH, -PO₃H₂, -PO₄H₂, -P(R₈)O₂H, -SO₃H₂, -SO₄H₂, 1,2-hydroxybenzene, 1-hydroxy-2-carboxybenzene, acetylacetonate, deprotonated forms of the aforementioned, organic and/or inorganic salts of said deprotonated forms, and chelating groups with π -conducting character, R₈ is selected from alkyl, alkenyl, alkynyl, aryl, alkylaryl, alkoxyaryl, and thioalkylaryl, with the proviso that at least one of said R₁, R₂, and R₃, is an anchoring group.

5. The compound of any one of the preceding claims, wherein X is selected from moieties (10)-(21), preferably moieties (10)-(18), more preferably from moieties (10)-(15) and most preferably from moieties (10)-(12).

6. The compound of any one of the preceding claims, wherein

R_{D1}, R_{D2}, R_{D3}, R_{D4}, R_{D5}, and R_{D6}, in as far as present, are independently selected from H, C1-C10 alkyl, C1-C10 alkoxy, C1-C10 thioalkyl.

7. The compound of any one of the preceding claims, wherein R_{D1} to R_{D6}, in far as present, are H.

8. The compound of any one of the preceding claims, wherein E, E1, E2, and E3, in as far as present, are independently selected from S and O, preferably are S.

9. The compound of any one of the preceding claims, wherein R¹, R², R³, R⁴, R⁵ and R⁶, in as far as present, are independently selected from H, C1-C10 alkyl, C1-C10 alkoxy, C1-C10 thioalkyl, C1-C10 alkyl substituted phenyl, C1-C10 alkoxy substituted phenyl and C1-C10 thioalkyl substituted phenyl.

10. The compound of any one of the preceding claims, wherein R¹, R², R³, R⁴, R⁵ and R⁶, in as far as present, are independently selected from H, C1-C10 alkyl, C1-C10 alkoxy, and C1-C10 thioalkyl.

11. The compound of any one of the preceding claims, wherein:

A is selected from moiety (50) and (51) as shown in claim 2, wherein E4 is selected from S, O, Se and Te, and R⁶, R⁷ and R⁸ are selected independently from H, C1-C36 alkyl, C1-C36 alkoxy, C1-C36 substituted phenyl, and C1-C36 alkoxy substituted phenyl;

R¹ to R⁶, in as far as present, are all H;

X is selected from moieties (10), (11) and (12) as shown in claim 1, wherein E in moiety (11) is selected S, O, Se, and Te, and R_{D1}-R_{D4}, in as far as present, are independently selected from H, from H, C1-C36 alkyl, C1-C36 alkoxy, C1-C36 alkyl substituted phenyl, and
5 C1-C36 alkoxy substituted phenyl;

Y is selected of the substituents (30), (31), (32) and (33), in which R₁ is -COOH, and R₂ to R₅, in as far as present, are all H.

12. The compound of any one of the preceding claims, wherein R_{A1}, R_{A2}, R_{B1}, and R_{B2} are
10 independently selected from C1-C36 alkyl, C1-C20 alkyl substituted phenyl, C1-C20 alkoxy substituted phenyl and C1-C20 thioalkyl substituted phenyl, and wherein R_{B1}, and R_{B2} may further be selected from C1-C20 alkoxyl and C1-C20 thioalkyl.

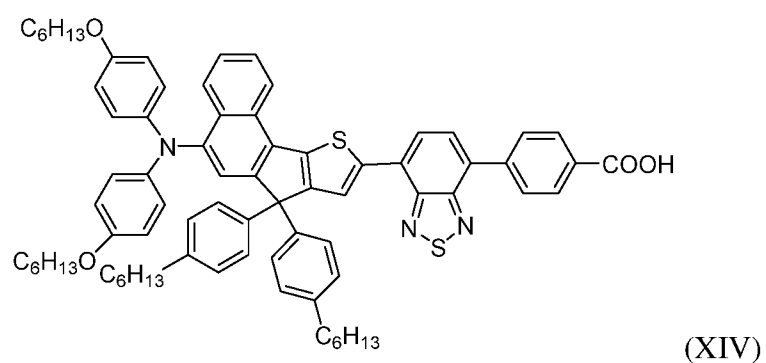
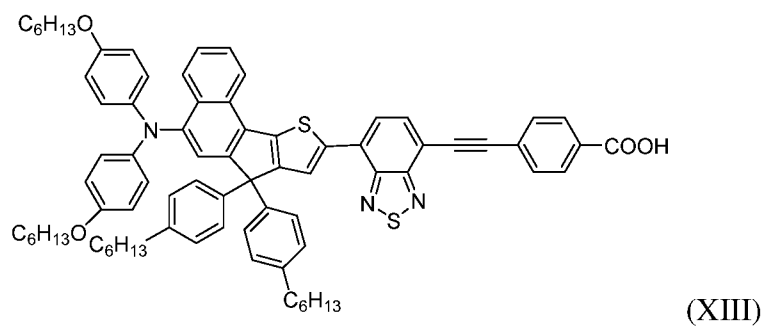
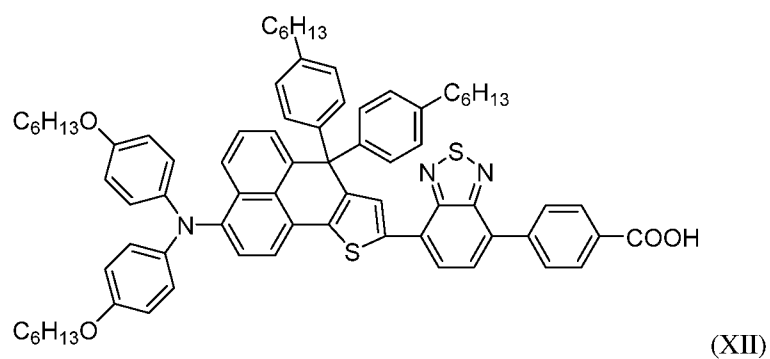
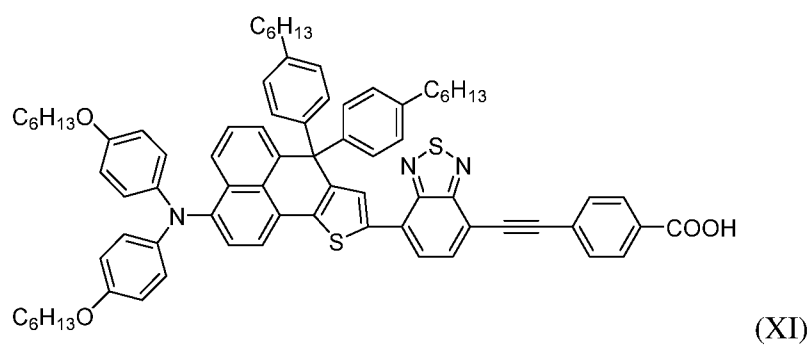
13. The compound of any one of the preceding claims, wherein R_{A1}, R_{A2}, R_{B1}, and R_{B2} are
15 independently selected from C1-C20 alkyl, C1-C15 alkyl substituted phenyl, C1-C15 alkoxy substituted phenyl and C1-C15 thioalkyl substituted phenyl, and wherein R_{B1}, and R_{B2} may further be selected from C1-C15 alkoxyl and C1-C15 thioalkyl.

14. The compound of any one of the preceding claims, wherein
20 R_{A1}, R_{A2} are independently selected from C1-C10 alkoxy substituted phenyl and C1-C10 thioalkyl substituted phenyl, and,
R_{B1}, and R_{B2} are independently selected from C1-C10 alkyl substituted phenyl.

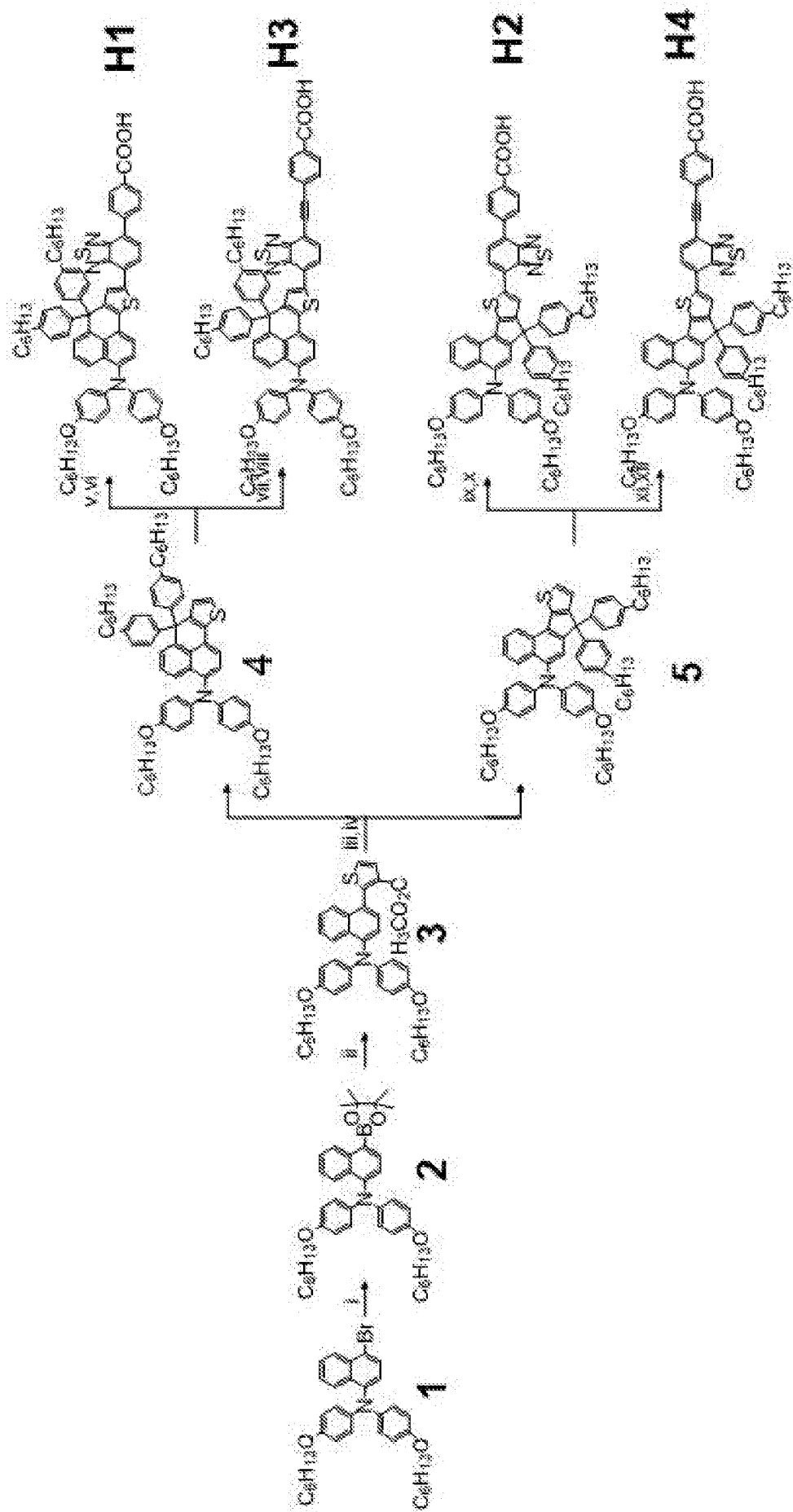
15. The compound of any one of the preceding claims, wherein R₁ is selected from said
25 anchoring groups and R₂ to R₅, in as far as present, are H.

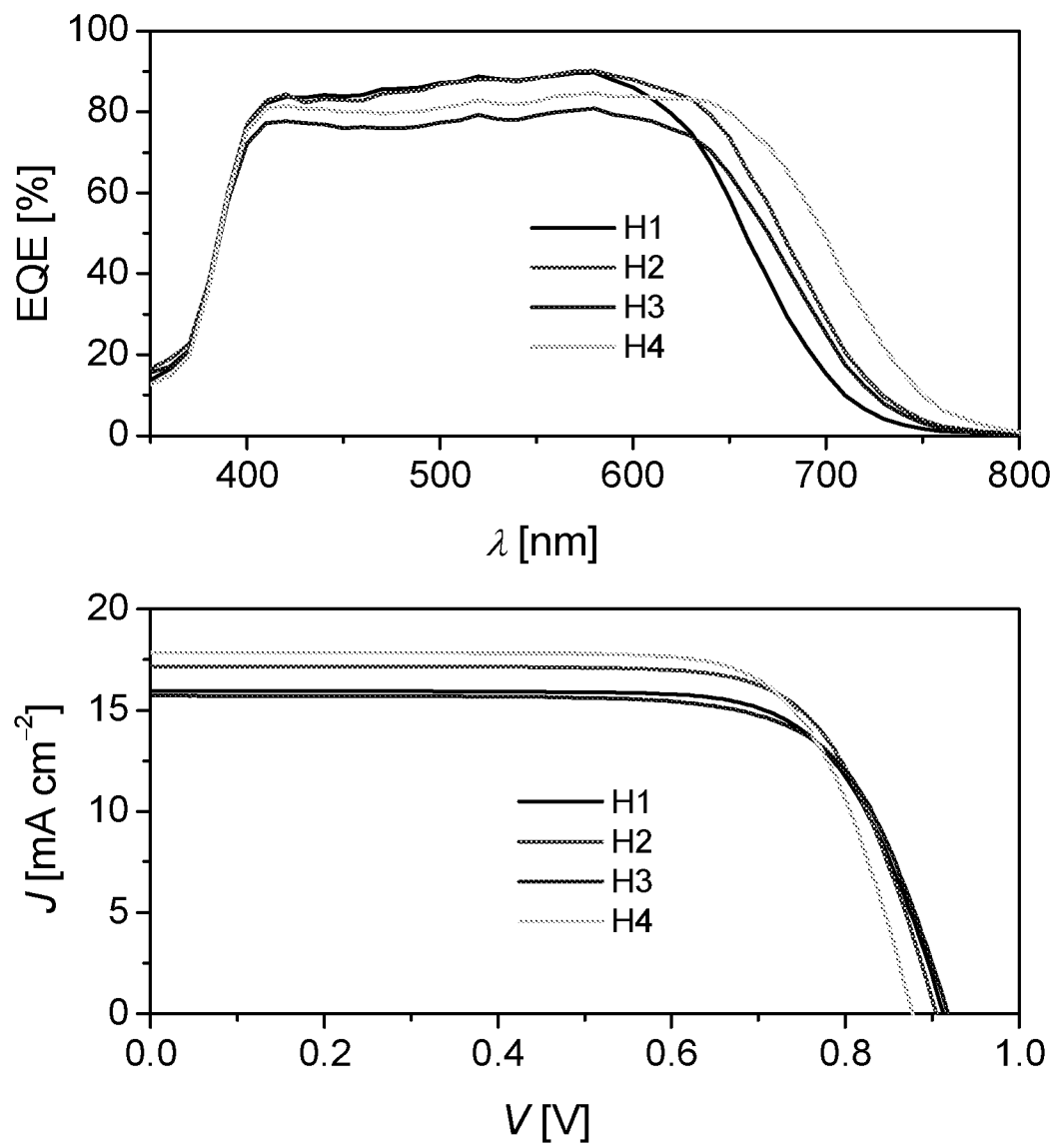
16. The compound of any one of the preceding claims, wherein said anchoring group is selected from -COOH, the deprotonated form thereof and/or a salt of said deprotonated form.

30 17. The compound of any one of the preceding claims, which comprises the structure of any one of formulae (XI) to (XIV):



18. An optoelectronic device comprising the compound of any one of the preceding
10 claims, said optoelectronic device preferably being a dye-sensitized solar cell.



**Figure 2**

INTERNATIONAL SEARCH REPORT

International application No.

PCT/IB2018/057816

A. CLASSIFICATION OF SUBJECT MATTER

C09B 5/00(2006.01)i; H01G 9/20(2006.01)i

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

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)

C07D, C09B

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

Electronic data base consulted during the international search (name of data base and, where practicable, search terms used)

CNABS, CNTXT, CNKI, VEN, CA Caplus: dye, dyestuff, colorant, sensitizer, sensitized, solar cell, DSC, power conversion efficiency, PCE

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
A	JP 6307298 B2 (HODOGAYA CHEM IND CO LTD) 04 April 2018 (2018-04-04) see claims 1-8; description; paragraphs 63-85	1-18
A	CN 101928469 A (PLASMAG TECHNOLOGY INC) 29 December 2010 (2010-12-29) see the whole document	1-18
A	CN 107541093 A (UNIV ZHEJIANG) 05 January 2018 (2018-01-05) see the whole document	1-18

☐ Further documents are listed in the continuation of Box C.☒ See patent family annex.

* Special categories of cited documents:

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

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

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

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

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

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

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

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

“&” document member of the same patent family

Date of the actual completion of the international search

16 May 2019

Date of mailing of the international search report

05 June 2019

Name and mailing address of the ISA/CN

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Facsimile No. (86-10)62019451

Telephone No. 62084595

INTERNATIONAL SEARCH REPORT
Information on patent family members

International application No.

PCT/IB2018/057816

Patent document cited in search report			Publication date (day/month/year)	Patent family member(s)			Publication date (day/month/year)
JP	6307298	B2	04 April 2018	JP	2015151505	A	24 August 2015
CN	101928469	A	29 December 2010	None			
CN	107541093	A	05 January 2018	None			