*Electronic Supplementary Information*

# From ACQ to AIE: the Suppression of the Strong π-π Interaction of Naphthalene Diimide Derivatives through the Adjustment of Their Flexible Alkyl Chains

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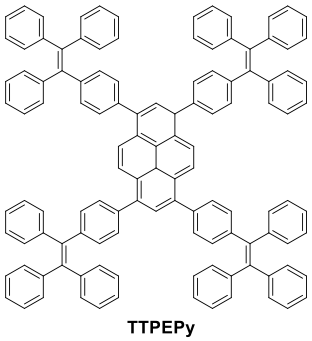



**Chart S1.** The structure of **TTPEPy** with pyrene as the core and TPE as the peripheral unit.[1]

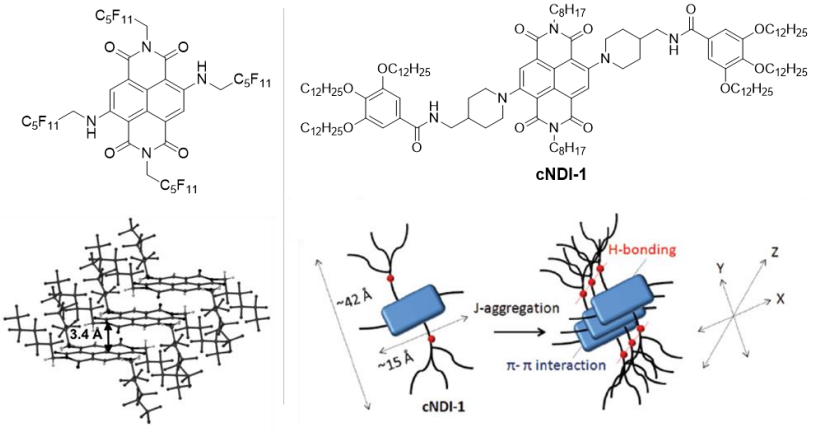



**Chart S2.** The structures and crystal packing/macroscopic assembly of cNDIs.[2]

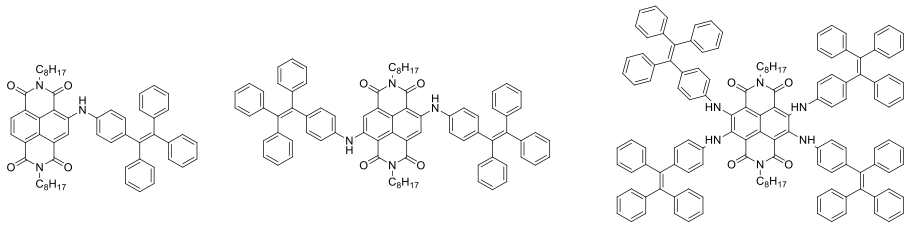
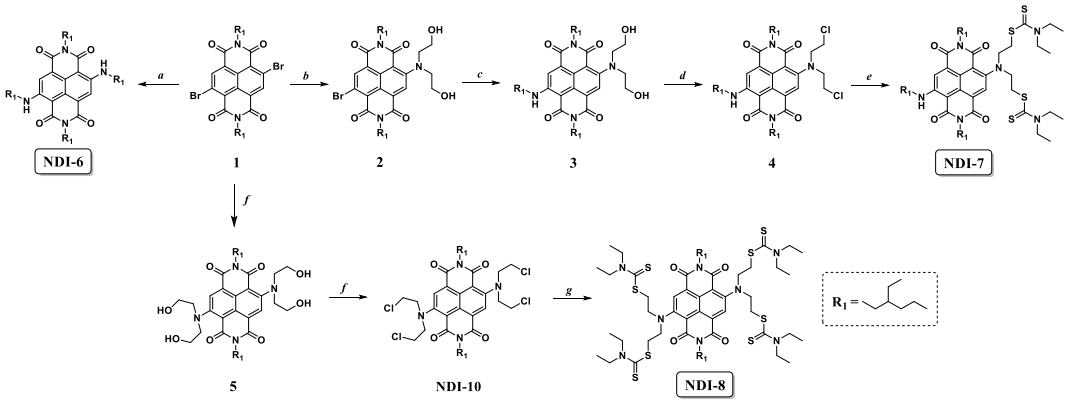


**Chart S3.** The structures of the AIEgens based on cNDIs with TPE as the peripheral unit.[3-5]




**Scheme S1.** The synthetic routs of compound **NDI-6**, **NDI-7** and **NDI-8**. (a) 2-ethyl-hexylamine, DMF, 100 $^{o}$C , 1h; (b) diethanolamine, DMF, 100 $^{o}$C, 18h; (c) 2-ethyl-hexylamine, DMF, 100 $^{o}$C, 2.5h; (d) $POCl_3$, 100 $^{o}$C, 3h; (e) sodium diethyldithiocarbamate, potassium carbonate, potassium iodide, ethyl alcohol, reflux, 12h; (f) $POCl_3$, 0 $^{o}$C, 20 min, then heated to100 $^{o}$C, 3h; (g) sodium diethyldithiocarbamate, potassium carbonate, potassium iodide, ethyl alcohol, reflux, 12h.

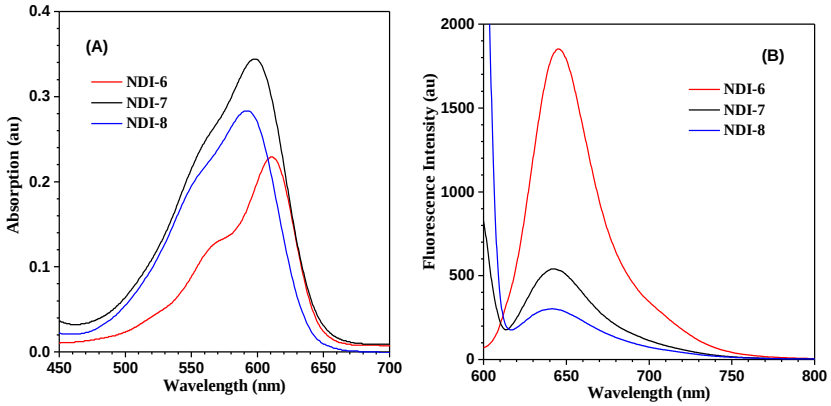



**Fig. S1** The UV-visible spectra (A) and the fluorescence spectra (B) of **NDI-6**, **NDI-7** and **NDI-8** ($2\times10^{-5}$ mol/L) in acetone.

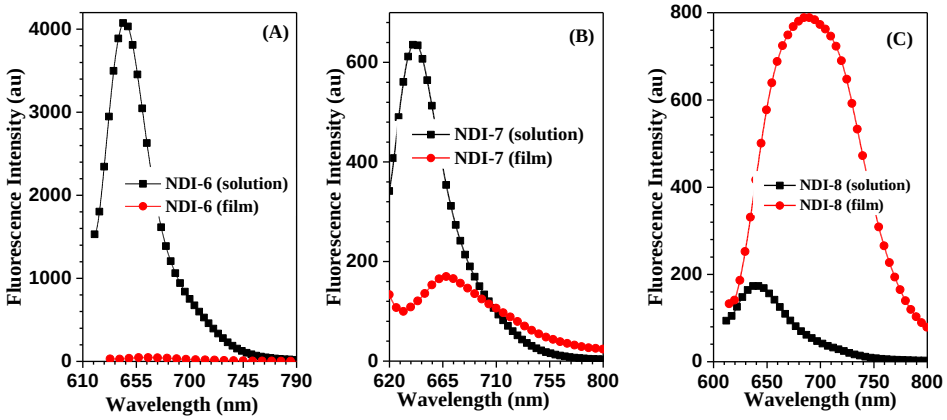


**Fig. S2** The fluorescence spectra of **NDI-6** (A), **NDI-7** (B) and **NDI-8** (C) in solution and thin film.

**Table S1.** Some parameters of the three molecules from TDDFT calculations and optical spectra.

| | $\lambda_{abs}$ (nm) | $\lambda_{em}$ (nm) | Stokes shift (nm) | | HOMO (eV) | LUMO (eV) | Length of *C-N* bond (Å) | |
|---|---|---|---|---|---|---|---|---|
| **NDI-6** | 611 | 645 | 34 | Ground state | -5.47 | -2.70 | 1.374 | 1.380 |
| | | | | Excited state | -5.32 | -2.82 | 1.371 | 1.376 |
| **NDI-7** | 598 | 642 | 44 | Ground state | -5.33 | -2.67 | 1.394 | 1.372 |
| | | | | Excited state | -4.81 | -3.36 | 1.451 | 1.393 |
| **NDI-8** | 594 | 642 | 48 | Ground state | -5.30 | -2.69 | 1.391 | 1.391 |
| | | | | Excited state | -4.78 | -3.30 | 1.451 | 1.403 |

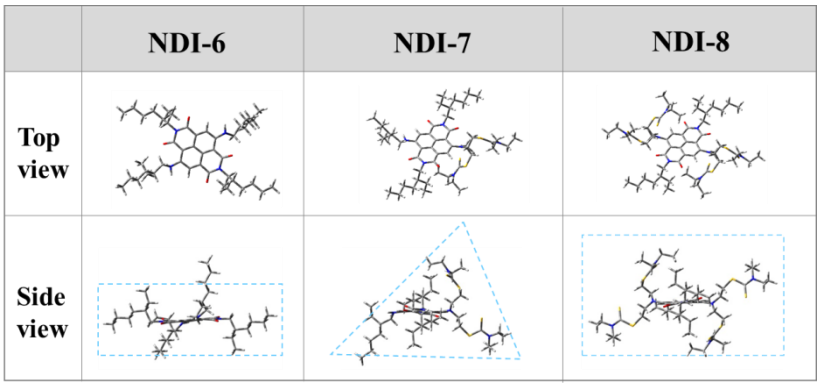



**Fig. S3** The optimized structures of **NDI-6**, **NDI-7** and **NDI-8** from different views, which were calculated by using TDDFT calculations with Gaussian 09 program.

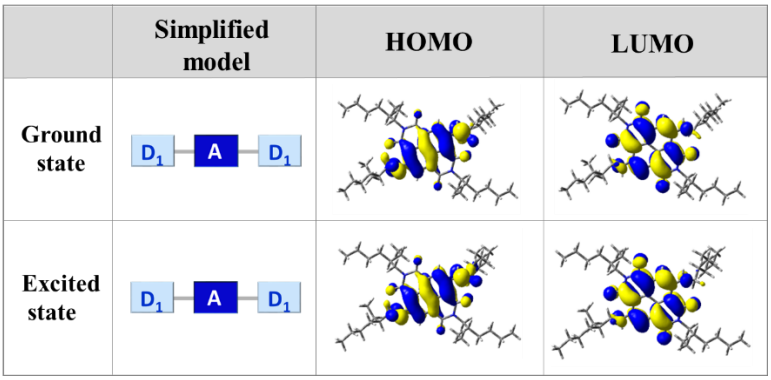



**Fig. S4** Simplified models, HOMO and LUMO of **NDI-6** in ground state and excited state, which were calculated by using TDDFT calculations with Gaussian 09 program.

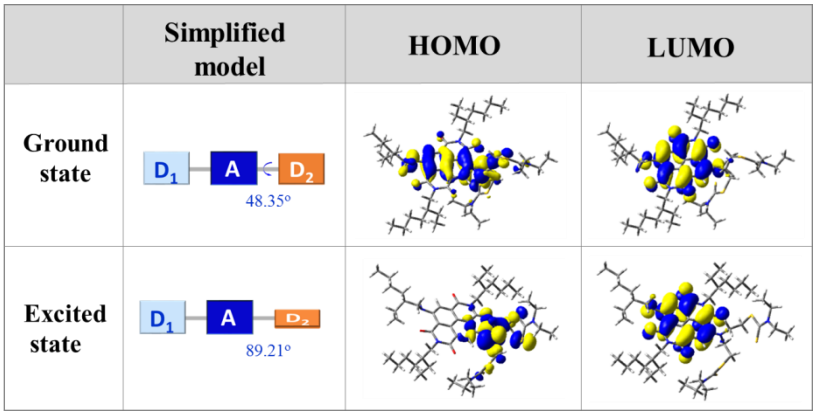


**Fig. S5** Simplified models, HOMO and LUMO of **NDI-7** in ground state and excited state, which were calculated by using TDDFT calculations with Gaussian 09 program.

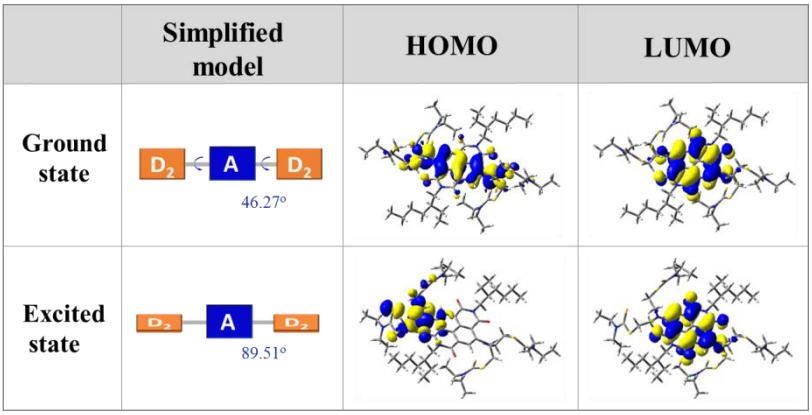



**Fig. S6** Schematic diagram of the formation of TICT state and HOMO, LUMO of **NDI-8** in ground state and excited state, which were calculated by using TDDFT calculations with Gaussian 09 program.

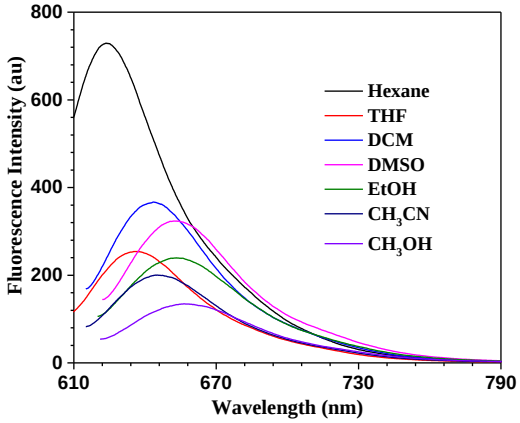



**Fig. S7** Fluorescence spectra of **NDI-8** in different solvents.

**Table S2.** Maximum wavelengths of absorption and fluorescence peaks, Stokes shifts of **NDI-8** in solvents with different polarity parameters ($\Delta f$).

| Solvent | $\lambda_{abs}$ (nm) | $\lambda_{em}$ (nm) | Stokes shift (nm) | $\varepsilon$ | $n$ | $\Delta f$ |
|---|---|---|---|---|---|---|
| Hexane | 586 | 624 | 38 | 1.9 | 1.388 | -0.0034 |
| THF | 588 | 635 | 47 | 7.58 | 1.407 | 0.2094 |
| DCM | 595 | 644 | 49 | 8.93 | 1.424 | 0.2171 |
| DMSO | 602 | 653 | 51 | 46.7 | 1.478 | 0.2634 |
| EtOH | 600 | 653 | 53 | 24.5 | 1.361 | 0.2887 |
| $CH_3CN$ | 595 | 645 | 50 | 37.5 | 1.344 | 0.3054 |
| $CH_3OH$ | 601 | 657 | 56 | 32.7 | 1.328 | 0.308 |

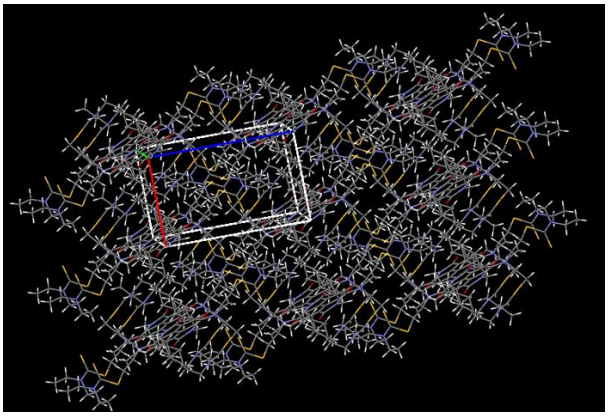


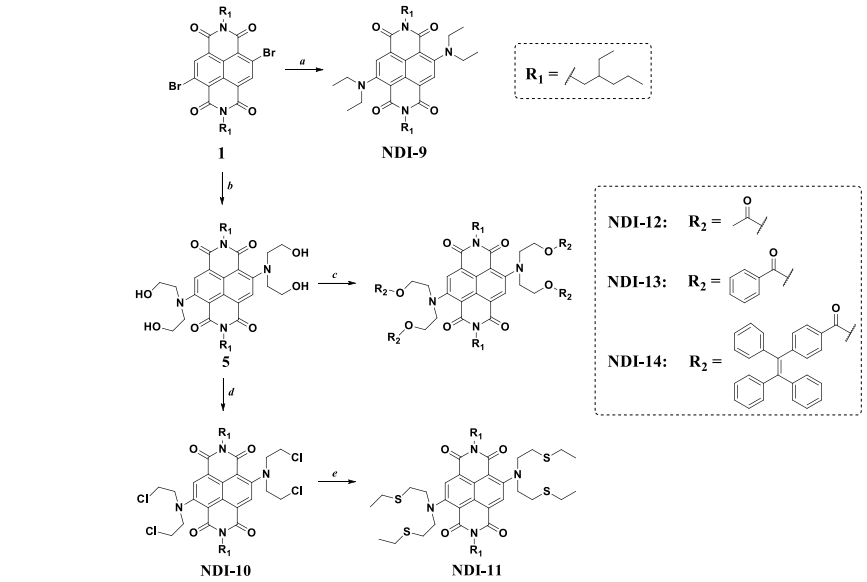
**Fig. S8** The packing state of **NDI-8** in crystal.

**Table S2.** X-ray data for the single crystal of **NDI-8.**

| Number | Bond | Bond length/Å | Band angel/$^{o}$ |
|---|---|---|---|
| **1** | C-H···O | 3.53 | 151.42 |
| **2** | C-H···O | 2.46 | 148.62 |
| **3** | C-H···O | 3.83 | 99.15 |
| **4** | C-H···π | 3.65 | 121.05 |

**Table S3.** Crystallographic data.

| Formula | $C_{29}H_{46}N_4O_2S_4$ |
|---|---|
| T (K) | 173 (2) |
| a (Å) | 8.580 (3) |
| b (Å) | 13.558 (5) |
| c (Å) | 13.879 (5) |
| a [deg] | 85.002 (3) |
| ß [deg] | 87.556 (3) |
| γ [deg] | 85.019 (3) |
| V [Å$^3$] | 1601.26 (10) |
| Z | 2 |
| Crystal size [mm$^3$] | 0.15x0.14x0.12 |
| F (000) | 656 |
| Reflections collected / unique ($R_{int}$) | 17886/6384(0.0501) |
| data / restraints/parameter | 6384/0/384 |
| Dc / mg m$^{-3}$ | 1.267 |
| goodness-of fit on $F^2$ | 1.091 |
| $R_1$,w$R_2$[I $\geqslant$ 2 σ (I)] | 0.0549, 0.1474 |
| $R_1$,w$R_2$(all data) | 0.0642, 0.1613 |




**Scheme S2.** The synthetic route to **NDI-9**-**NDI-14**. (a) diethylamine, DMF, 100 $^{o}$C, 1h; (b) dihydroxyethylamine, 2-methoxyethanol, reflux, 18h; (c) EDC, DMAP, anhydrous dichloromethane, room temperature, 24h; (d) phosphorus oxychloride, 0 $^{o}$C, 20 min, then reflux, 3h; (e) $C_2H_5SH$, room temperature, 20 min, then reflux, 24h.

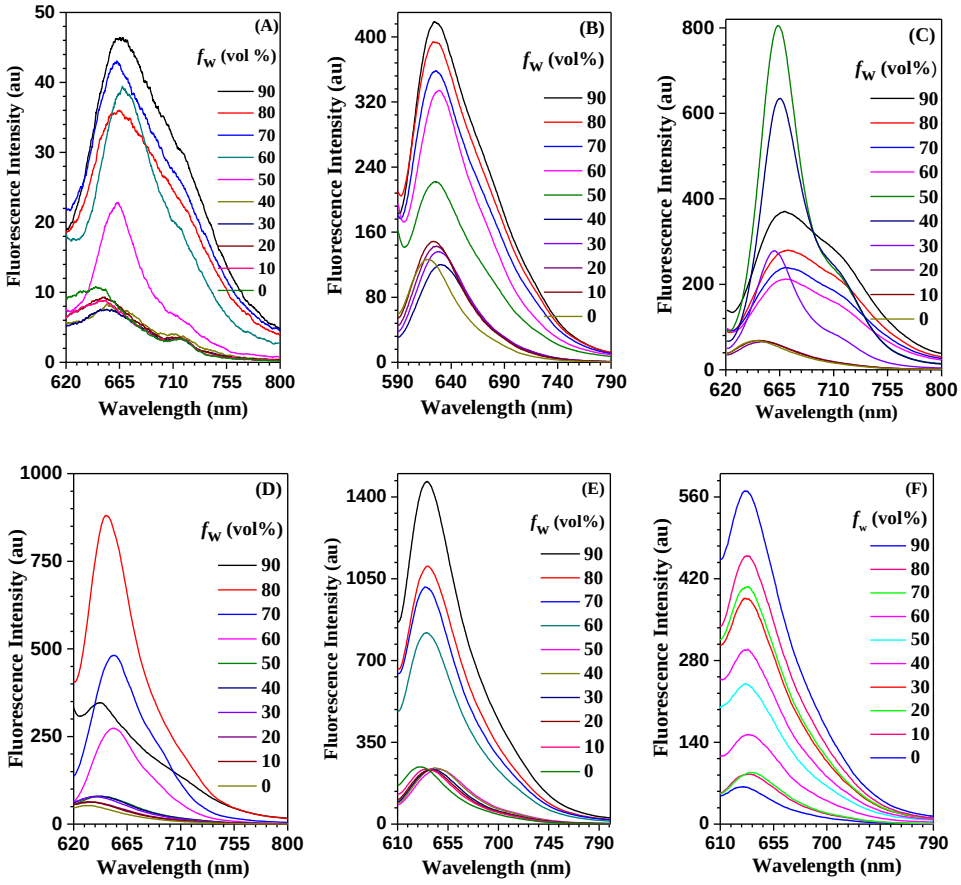



**Fig. S9** The fluorescence spectra of **NDI-9** (A), **NDI-10** (B), **NDI-11** (C), **NDI-12** (D), **NDI-13** (E), **NDI-14** (F) in acetone/water mixtures with different water fractions ($f_w$).

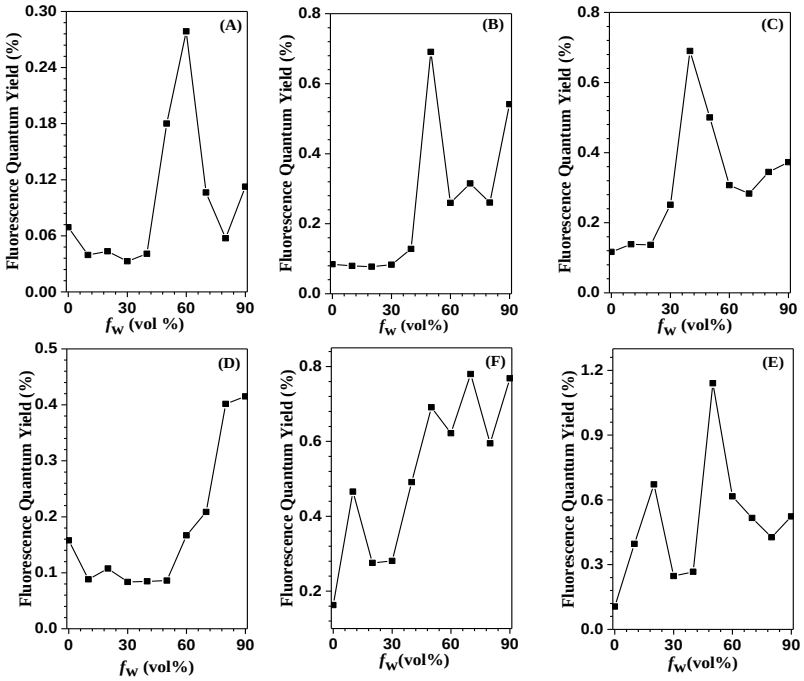



**Fig. S10** Plots of fluorescence quantum yields of **NDI-9** (A), **NDI-10** (B), **NDI-11** (C), **NDI-12** (D), **NDI-13** (E), **NDI-14** (F) in acetone/water mixtures with different water fractions ($f_w$).

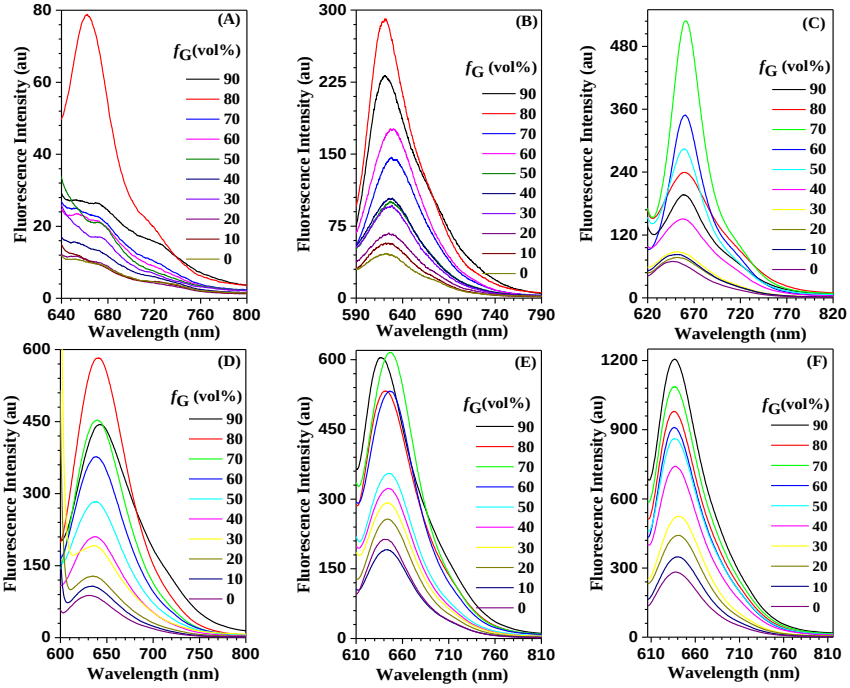



**Fig. S11** The fluorescence spectra of **NDI-9** (A), **NDI-10** (B), **NDI-11** (C), **NDI-12** (D) , **NDI-13** (E), **NDI-14** (F) in ethanol/glycerol mixtures with different glycerol fractions ($f_G$).

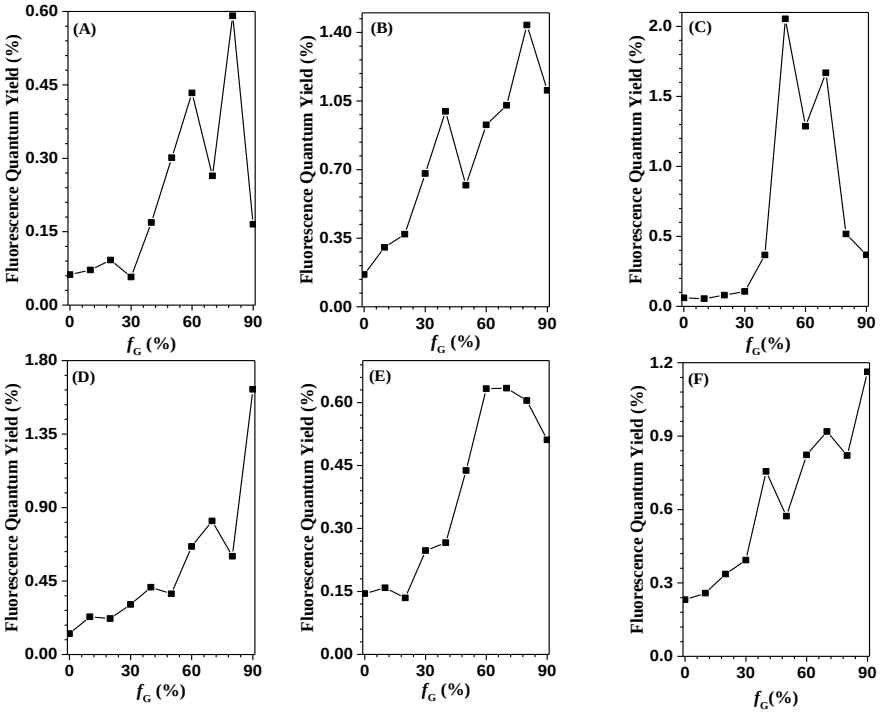



**Fig. S12** Plots of fluorescence quantum yields of **NDI-9** (A), **NDI-10** (B), **NDI-11** (C), **NDI-12** (D), **NDI-13** (E), **NDI-14** (F) in ethanol/glycerol mixtures with different glycerol fractions ($f_G$).

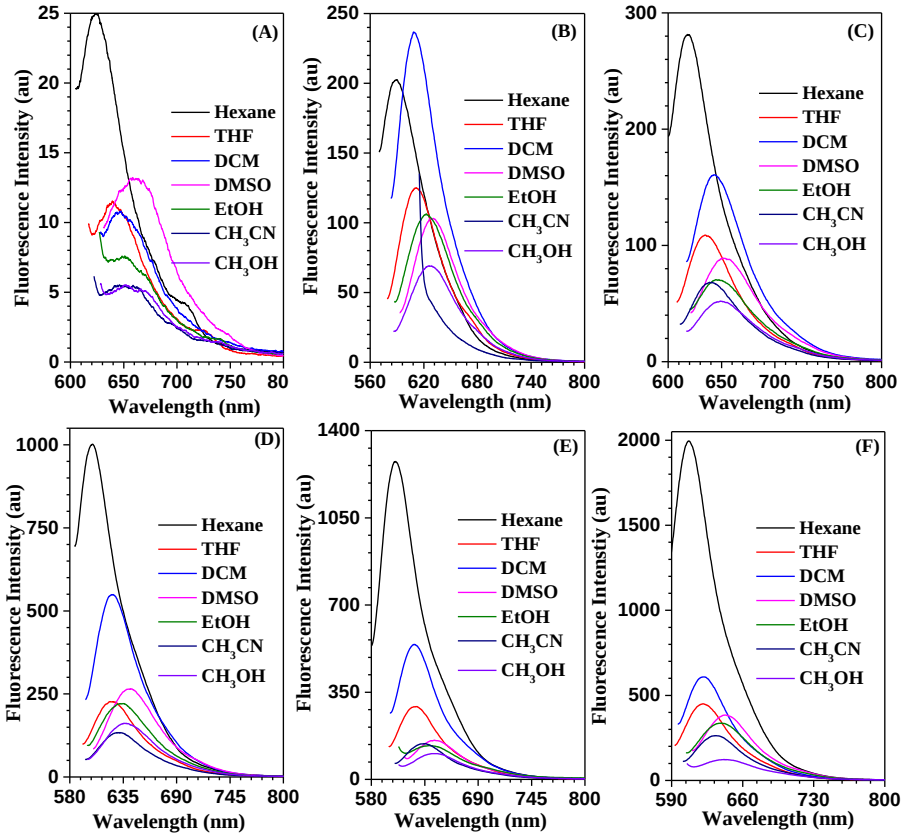



**Fig. S13.** The fluorescence spectra of **NDI-9** (A), **NDI-10** (B), **NDI-11** (C), **NDI-12** (D), **NDI-13** (E), **NDI-14** (F) in the solvent with different polarities

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**Table S4.** Maximum wavelengths of absorption and fluorescence peaks, Stokes shifts of **NDI-9**–**NDI-14** in different solvents

| | Solvent | $\lambda_{abs}$ (nm) | $\lambda_{em}$ (nm) | Stokes shift (nm) |
|---|---|---|---|---|
| **NDI-9** | Hexane | 585 | 625.4 | 40.4 |
| | THF | 613 | 656 | 43 |
| | DCM | 597 | 639.4 | 42.4 |
| | DMSO | 601 | 638.8 | 37.8 |
| | EtOH | 602 | 646.2 | 44.2 |
| | $CH_3CN$ | 607 | 653.6 | 46.6 |
| | $CH_3OH$ | 611 | 658.4 | 47.4 |
| **NDI-10** | Hexane | 550 | 589.6 | 39.6 |
| | THF | 559 | 610.8 | 51.8 |
| | DCM | 563 | 609.2 | 46.2 |
| | DMSO | 573 | 630.6 | 57.6 |
| | EtOH | 567 | 623 | 56 |
| | $CH_3CN$ | 564 | 619.2 | 55.2 |
| | $CH_3OH$ | 566 | 628 | 62 |
| **NDI-11** | Hexane | 581 | 618 | 37 |
| | THF | 588 | 635.2 | 47.2 |
| | DCM | 597 | 644 | 47 |
| | DMSO | 601 | 651.8 | 50.8 |
| | EtOH | 600 | 644.8 | 44.8 |
| | $CH_3CN$ | 591 | 640.6 | 49.6 |
| | $CH_3OH$ | 597 | 652.2 | 55.2 |
| **NDI-12** | Hexane | 565 | 603.6 | 38.6 |
| | THF | 573 | 622.4 | 49.4 |
| | DCM | 576 | 624.4 | 48.4 |
| | DMSO | 584 | 644 | 60 |
| | EtOH | 578 | 635 | 57 |
| | $CH_3CN$ | 576 | 633 | 57 |
| | $CH_3OH$ | 578 | 637.8 | 59.8 |
| **NDI-13** | Hexane | 569.4 | 603.8 | 34.4 |
| | THF | 577.6 | 625.4 | 47.8 |
| | DCM | 576 | 623.8 | 47.8 |
| | DMSO | 590 | 645.8 | 55.8 |
| | EtOH | 583.6 | 635.8 | 52.2 |
| | $CH_3CN$ | 583.8 | 642.4 | 58.6 |
| | $CH_3OH$ | 584.6 | 640.4 | 55.8 |
| **NDI-14** | Hexane | 567.2 | 607.2 | 40 |
| | THF | 573 | 620.8 | 47.8 |
| | DCM | 576 | 622 | 46 |
| | DMSO | 590 | 642.4 | 52.4 |
| | EtOH | 583.6 | 639.2 | 55.6 |
| | $CH_3CN$ | 581 | 633.8 | 52.8 |
| | $CH_3OH$ | 584.6 | 641.2 | 56.6 |

## Experimental section

### Materials

Tetrahydrofuran (THF) was distilled under normal pressure from sodium benzophenone ketyl under an atmosphere of dry argon immediately prior to use. Dichloromethane (DCM) was stirred with $CaH_2$ at room temperature for overnight and then distilled to obtain anhydrous DCM. **NDI-6** has been reported in the literature.[6] Other chemicals were used as received without further purification.

### Instrumentation

$^1H$ and $^{13}C$ NMR spectroscopy study were conducted with a Varian Mercury 300 spectrometer using tetramethylsilane (TMS; $\delta$ = 0 ppm) as internal standard. UV-visible spectra were obtained using a Shimadzu UV-2550 spectrometer. Fluorescence spectra were recorded with Hitachi F-4600 fluorescence spectrophotometer. Elemental analyses were performed by a CARLOERBA-1106 microelemental analyzer. GC–MS spectra were performed by Thermo DSQ II. The diffraction data of **NDI-8** was collected in an Agilent Supernova CCD diffractometer. The melting point was measured by SGW X-4B digital melting point tester.

### Synthesis of compound 2

Under the atmosphere of nitrogen, compound **1** (454 mg, 0.70 mmol) and dihydroxyethylamine (50 μL) were dissolved in DMF (10 mL), and the mixture was heated to 100 $^oC$ and stirred for 18 h. After being cooled to room temperature, it was poured into water, and filtered to yield a blue solid, which was washed with water for three times. The crude product was purified by column chromatography on silica gel (dichloromethane/ethyl acetate = 4/1) to give compound **2** as a blue solid (403 mg, 85.6%). $^1H$ NMR (300 MHz, $CDCl_3$) $\delta$ (ppm): 8.87 (s, 1H, ArH), 8.66 (s, 1H, ArH), 4.13 (m, 4H, -$CH_2$-), 3.82 (m, 4H, -$CH_2$-), 3.76 (m, 4H, -$CH_2$-), 1.91 (m, 2H, -CH-), 1.31 (m, 16H, -$CH_2$-), 0.91 (m, 12H, -$CH_3$).

**Synthesis of compound 3**

Under the atomosphere of nitrogen, compound **2** (214 mg, 0.32 mmol) was dissolved in 2-ethyl-hexylamine (2.5 mL) and stirred at 100 $^{o}$C for 2.5 h. After being cooled to room temperature, the mixture was pured into HCl (1 mol/L) and filtered. The crude product was purified by column chromatography on silica gel (chloroform/ ethyl acetate = 3/1) to give compound **3** as a blue solid (70 mg, 45.5%). $^{1}$H NMR (300 MHz, $CDCl_3$) $\delta$ (ppm): 9.83 (s, 1H, -NH), 8.59 (s, 1H, ArH), 8.21 (s, 1H, ArH), 4.13 (t, $J$ = 7.8 Hz, 4H, -$CH_2$-), 3.69 (m, 4H, -$CH_2$-), 3.58 (m, 4H, -$CH_2$-), 3.46 (t, $J$ = 6.0 Hz, 2H, -$CH_2$-), 1.92 (m, 2H, -CH-), 1.78 (m, 1H, -CH-), 1.45-1.31 (br, 24H, -$CH_2$-), 1.03-0.88 (br, 18H, -$CH_3$).

**Synthesis of compound 4**

Compound **4** was prepared according to the similar procedure as described for compound **NDI-10** (100 mg, 70.4%). $^{1}$H NMR (300 MHz, $CDCl_3$) $\delta$ (ppm): 9.84 (s, 1H, -NH), 8.55 (s, 1H, ArH), 8.22 (s, 1H, ArH), 4.13 (m, 4H, -$CH_2$-), 3.76 (m, 4H, -$CH_2$-), 3.63 (m, 4H, -$CH_2$-), 3.46 (m, 2H, -$CH_2$-),1.92 (m, 2H, -CH-), 1.78 (m, 1H, -CH-). 1.34 (m, 24H, -$CH_2$-), 0.93 (br, 18H, -$CH_3$).

**Synthesis of compound 5**

Under the atomosphere of nitrogen, compound **1** (712 mg, 1.10 mmol) and dihydroxyethylamine (6.5 mL, 67.8 mmol) were dissolved in 2-methoxyethanol (26 mL) and refluxed for 18 h. After being cooled to room temperature, the mixture was poured into water (165 mL) and filtered to yield a blue solid, which was washed with water for three times. The crude product was purified by column chromatography on silica gel (dichloromethane/ethyl acetate = 2/1) to give compound **5** as a blue solid (470 mg, 76.5%). $^{1}$H NMR (300 MHz, $CDCl_3$) $\delta$ (ppm): 8.58 (s, 2H, ArH), 4.13 (t, 4H, $J$ = 7.2 Hz, -$CH_2$-), 3.75 (m, 8H, -$CH_2$-), 3.67 (m, 8H, -$CH_2$-), 1.90 (m, 2H, -CH-), 1.36-1.28 (br, 16H, -$CH_2$-), 0.95-0.89 (br, 18H, -$CH_3$).

**Synthesis of compound NDI-7**

**NDI-7** was prepared according to the similar procedure as described for **NDI-8** (57 mg, 43.8%). m.p. = 98-99 $^{o}$C. $^{1}$H NMR (300 MHz, $CDCl_3$) $\delta$ (ppm): 9.65 (s, 1H, -NH), 8.56 (s, 1H, ArH), 8.11(s, 1H, ArH), 4.02 (m, 4H, -$CH_2$-), 3.88 (m,4H, -$CH_2$-), 3.74 (m, 4H, -$CH_2$-), 3.58-3.49 (br, 8H, -$CH_2$-), 3.38 (m, 2H, -$CH_2$-), 1.87 (m, 2H, -CH-), 1.71 (m, 1H, -CH-), 1.27 (m, 24H, -$CH_2$-), 1.14-1.07 (br, 12H, -$CH_3$), 0.93-0.82 (br, 18H, -$CH_3$). $^{13}$C NMR ($CDCl_3$) $\delta$ (ppm): 194.60, 166.59, 163.46, 161.85, 105.49, 149.27, 128.35, 127.21, 124.36, 123.72, 121.50, 118.50, 113.33, 100.72, 51.73, 49.39, 46.52, 46.22, 44.25, 43.79, 39.16, 37.74, 34.70, 31.08, 30.63, 28.60, 24.45, 23.93, 23.86, 23.01, 22.89, 13.98, 12.33, 11.41, 10.83, 10.53. Anal. calcd. for $C_{51}H_{80}N_6O_4S_4$, C 63.50, H 8.40, N 8.55, S 13.04, found C 63.45, H 8.47, N 8.55, S 12.99. Anal.calcd. for: $C_{51}H_{80}N_6O_4S_4$, 63.50, H 8.40, N 8.55, S 13.04, found C 63.45, H 8.47, N 8.55, S 12.99. MS-TOF m/z Anal.calcd. for $C_{51}H_{80}N_6O_4S_4$, 983.5353, found: 983.5361.

**Synthesis of compound NDI-8**

Under the atomosphere of nitrogen, **NDI-10** (132 mg, 0.17mmol), sodium diethyldithiocarbamate (193 mg, 0.86 mmol), potassium carbonate (28 mg, 0.20 mmol) and potassium iodide (23 mg, 0.14 mmol) were dissolved in ethyl alcohol (4 mL) and refluxed for 12 h. After being cooled to room temperature, the solvent was evaporated under pressure. The crude product was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 6/1) to give compound **NDI-8** as a blue solid (125 mg, 59.8%). m.p. = 88-89 $^{o}$C. $^{1}$H NMR (300 MHz, $CDCl_3$) $\delta$ (ppm): 8.63 (s, 2H, ArH), 4.12 (m, 8H, -$CH_2$-), 3.95-3.59 (br, 16H, -$CH_2$-), 3.64-3.56 (br, 12H, -$CH_2$-), 1.93 (m, 2H, -CH-), 1.35 (m, 16H, -$CH_2$-), 1.19-1.16 (br, 24H, -$CH_3$), 0.93 (t, $J$ = 7.2 Hz, 12H, -$CH_3$). $^{13}$C NMR ($CDCl_3$) $\delta$ (ppm): 194.68, 163.70, 162.26, 150.98, 127.83, 125.52, 124.73, 111.62, 52.03, 49.75, 46.91, 44.52, 38.13, 34.95, 30.96, 28.93, 24.12, 23.39, 14.41, 12.64, 11.71, 10.87. Anal. calcd. for $C_{58}H_{92}S_8O_4N_4$, C 57.01, H 7.59, N 9.17, S 20.99, found C 57.06, H 7.44, N 9.18, S 20.88. MS-TOF m/z Anal.calcd. for $C_{58}H_{92}S_8O_4N_4$, 1221.5080, found: 1221.5088.

**Synthesis of compound NDI-9**

Under the atmosphere of nitrogen, compound **1** (97 mg, 0.15 mmol) and diethylamine (0.6 mL, 5.8 mmol) were dissolved in DMF (10 mL) and stirred at 100 $^{o}$C for 1 h. After being cooled to room temperature, the mixture was poured into water (100 mL) and filtered to afford a blue solid, which was washed with water for three times. The crude product was purified on silica chromatograph gel (dichloromethane) to give **NDI-9** as a blue solid (72 mg, 76%). $^{1}$H NMR (300 MHz, $CDCl_3$) $\delta$ (ppm): 8.44 (s, 2H, ArH), 4.14 (d, $J$ = 6.0 Hz, 4H, -$CH_2$-), 3.55 (m, 8H, -$CH_2$-), 1.93 (m, 2H, -CH-), 1.43-1.20 (br, 28H,-$CH_2$-), 0.96-0.86 (br, 12H, -$CH_3$). $^{13}$C NMR ($CDCl_3$) $\delta$ (ppm): 163.79, 161.97, 150.23, 125.81, 124.83, 109.67, 46.94, 44.23, 37.88, 30.69, 28.65, 23.93, 22.99, 13.98, 13.32, 13.32, 10.58. Anal.calcd. for: $C_{38}H_{56}N_4O_4$, C 72.12, H 8.92, N 8.85, found: C 72.03, H 9.04, N 8.84. MS-TOF m/z Anal. calcd. for $C_{38}H_{56}N_4O_4$,633.4374, found: 633.4380.

**Synthesis of compound NDI-10**

Under the atomosphere of nitrogen, compound **5** (359 mg, 0.52 mmol) was dissolved in phosphorus oxychloride (21.9 mL) and stirred at 0 $^{o}$C for 20 mins, then at 100 $^{o}$C for 3 h. After being cooled to room temperature, water was added slowly to the solution, and the mixture was extracted with chloroform (100 mL) for three times. The organic layer was dried over $Na_2SO_4$. The crude product was purified by column chromatography on silica gel (petroluem ether/ethyl acetate = 12/1) to give compound **NDI-10** as a red solid (397 mg, 93.2%). m.p. = 98-99 $^{o}$C. $^{1}$H NMR (300 MHz, $CDCl_3$) $\delta$ (ppm): 8.53 (s, 2H, ArH), 4.12 (m, 4H, -$CH_2$-), 3.82 (t, 8H, $J$ = 6.6 Hz, -$CH_2$-), 3.67 (t, 8H, $J$ = 6.6 Hz, -$CH_2$-), 1.93 (m, 2H, -CH-), 1.39-1.31 (br, 16H, -$CH_2$-), 0.97-0.92 (br, 12H, -$CH_3$). $^{13}$C NMR ($CDCl_3$) $\delta$ (ppm): 163.02, 161.72, 150.73, 128.36, 125.79, 124.93, 112.80, 54.70, 44.33, 41.54, 37.84, 30.66, 28.57, 23.92, 22.99, 14.01, 10.55. Anal. calcd. for: $C_{38}H_{52}N_4O_4Cl_4$, C 59.22, H 6.80, N 7.27, found C 59.36, H 6.82, N 7.21. MS-TOF m/z Anal. calcd. for: $C_{38}H_{52}N_4O_4Cl_4$, 769.2815, found 769.2809.

**Synthesis of compound NDI-11**

Under the atomosphere of nitrogen, to a solution of NaH (90 mg, 3.75 mmol) and $C_2H_5SH$ (1.8 mL) in dry THF (15 mL), **NDI-10** (115 mg, 0.12 mmol) in dry THF (15 mL) was added slowly. The mixture was stirred for 20 min at room temperature, then refluxed for 24 h. After being cooled to room temperature, the solvent was evaporated under reduced pressure and the crude products were purified by column chromatography on silica gel (petroluem ether/ethyl acetate = 12/1) to give **NDI-11** as a blue solid (112 mg, 85.5%). m.p. = 95-97 $^{o}$C. $^{1}$H NMR (300 MHz, THF-$d_8$) $\delta$ (ppm): 8.50 (s, 2H, ArH), 4.10 (t, $J$ = 8.1 Hz, 4H, -$CH_2$-), 3.68(t, $J$ = 7.2 Hz, 8H, -$CH_2$-), 2.77(t, $J$ = 7.5 Hz, 8H, -$CH_2$-), 2.53-2.42 (br, 8H, -$CH_2$-), 1.94 (m, 2H, -CH-), 1.34 (m, 16H,-$CH_2$-), 1.16(t, $J$ = 7.5 Hz,12H, -$CH_3$), 0.96-0.89 (br, 12H, -$CH_3$). $^{13}$C NMR ($CDCl_3$) $\delta$ (ppm):163.35, 161.78, 150.46, 126.87, 125.24, 124.46, 111.06, 52.97, 44.27, 37.80, 30.60, 30.03, 28.57, 26.10, 23.87, 23.00, 14.72, 14.02, 10.54. Anal.calcd. for: $C_46H_{72}O_4N_4S_4$, C 63.26, H 8.31, N 6.42, S 14.68, found C 63.30, H 8.30, N 6.50, S 14.75. MS-TOF m/z Anal. calcd. for $C_{46}H_{72}O_4N_4S_4$, 873.4509, found: 873.4517.

**Synthesis of compound NDI-12**

Under the atomosphere of nitrogen, to a solution of compound **5** (139 mg, 0.2 mmol), 1-(3-dimethylaminopropyl)-3-ethylcarbodiimide hydrochloride (95 mg, 0.5 mmol) and 4-dimethyl aminopyridine (4.9 mg, 0.4 μmol) in dry THF (15 mL) was added acetic anhydride (0.2 mL). The mixture was stirred at room temperature for 1 h. Then the solvent was evaporated under reduced pressure and the crude product was purified by column chromatography on silica gel (petroluem ether/ethyl acetate = 2/1) to give compound **NDI-12** as a purple-red solid (166 mg, 95.9%). m.p. = 81-82 $^{o}$C. $^{1}$H NMR (300 MHz, $CDCl_3$) $\delta$ (ppm): 8.55 (s, 2H, ArH), 4.27 (t, $J$ = 5.7 Hz, 8H,-$CH_2$-), 4.11 (t, $J$ = 7.2 Hz, 4H, -$CH_2$-), 3.77 (t, $J$ = 5.4 Hz, 8H, -$CH_2$-), 1.96 (s, 12H, -$CH_3$), 1.89 (m, 2H, -$CH_3$), 1.35-1.30 (br, 16H, -$CH_2$-), 0.95-0.86 (br, 12H, -$CH_3$). $^{13}$C NMR ($CDCl_3$) $\delta$ (ppm): 170.97, 163.50, 161.89, 127.69, 125.71, 124.94, 112.21, 61.89, 52.09, 44.62, 38.16, 30.97, 28.93, 24.16,

23.30, 21.03, 14.36, 10.89. Anal.calcd. for $C_{46}H_{64}O_{12}N_4$: C 63.87, H 7.46, N 6.48, found: C 64.05, H 7.41, N 6.65. MS-TOF m/z Anal. calcd. for $C_{46}H_{64}O_{12}N_4$, 865.4593, found:865.4595.

**Synthesis of compound NDI-13**

Under the atomosphere of nitrogen, compound **5** (94 mg, 0.25 mmol), benzoic acidand (132 mg, 100 mmol), EDC (1-(3-Dimethylaminopropyl)-3-ethylcarbodiimide hydrochloride) (250 mg, 1.3 mmol) and DMAP (4-dimethylaminopyridine) (25 mg, 0.2 mmol) were dissolved in anhydrous dichloromethane (20 mL) and stirred at room temperature for 18 h. Then the solvent was vaporated under reduced pressure, and the crude product was purified by column chromatography on silica gel (dichloromethane) to give **NDI-13** as a blue solid (104 mg, 37.4%). m.p. = 114-115 $^{o}$C. $^{1}$H NMR (300 MHz, $CDCl_3$) $\delta$ (ppm): 8.49 (s, 2H, ArH), 7.77 (d, $J$ = 7.2 Hz, 8H, ArH), 7.41 (t, $J$ = 7.2 Hz, 4H, ArH), 7.24-7.19 (br, 8H, ArH), 4.57 (m, 8H, -$CH_2$-), 4.01 (t, $J$ = 8.7 Hz, 12H, -$CH_2$-), 1.83 (m, 2H, -CH-), 1.29 (m, 16H, -$CH_2$-), 0.90 (t, $J$ = 7.2 Hz, 12H, -$CH_3$). $^{13}$C NMR ($CDCl_3$) $\delta$ (ppm):166.00, 162.80, 161.44, 151.28, 132.82, 129.45, 127.99, 127.38, 125.29, 124.48, 112.03, 62.36, 52.04, 44.44, 37.80, 30.65, 28.52, 23.80, 23.00, 14.01, 10.46. Anal.calcd. for: $C_{66}H_{72}O_{12}N_4$, C 71.02, H 6.42, N 5.03, found C 71.20, H 6.63, N 5.30. MS-TOF m/z Anal. calcd. for $C_{66}H_{72}O_{12}N_4$, 1113.5225, found: 1113.5211.

**Synthesis of compound NDI-14**

Under the atomosphere of nitrogen, compound **5** (70 mg, 0.1 mmol), 4-(1,2,2-triphenylvinyl)benzoic acid (240 mg, 0.6 mmol), EDC (1-(3-Dimethylaminopropyl)-3-ethylcarbodiimide hydrochloride) (250 mg, 1.3 mmol) and DMAP (4-dimethylaminopyridine) (25 mg, 0.2 mmol) were dissolved in anhydrous dichloromethane (20 mL) and stirred at room temperature for 36 h. Then the solvent was vaporated under reduced pressure and the crude product was purified by column chromatography on silica gel (ethyl acetate/petroluem ester = 1/5) to give **NDI-14** as a red-purple solid (70 mg, 32.7%). m.p. = 82-84 $^{o}$C. $^{1}$H NMR (300 MHz, $CDCl_3$) $\delta$ (ppm): 8.57 (s, 2H, ArH), 7.65 (d, $J$ = 8.7 Hz, 8H,

ArH), 7.07 (m, 42H, ArH), 6.98 (m, 24H, ArH), 4.47 (m, 8H, -$CH_2$-), 4.02 (m, 4H, -$CH_2$-), 3.88 (m, 8H, -$CH_2$-), 1.86 (m, 2H, -CH-), 1.26 (m, 16H, -$CH_2$-), 0.85 (t, $J$ = 3.6 Hz, 12H, -$CH_3$). $^{13}$C NMR ($CDCl_3$) $\delta$ (ppm): 166.02, 162.98, 161.56, 151.03, 148.91, 143.13, 142.96, 139.76, 131.16, 128.96, 127.76, 127.34, 126.80, 126.67, 125.58, 124.80, 112.12, 62.31, 52.14, 44.28, 37.82, 30.73, 29.61, 28.57, 23.86, 23.01, 14.06, 10.56. Anal. calcd. for: $C_{146}H_{128}O_{12}N_4$, C 82.30, H 6.06, N 2.63, found: C 82.19, H 5.95, N 2.62. MS-TOF m/z Anal.calcd. for: $C_{146}H_{128}O_{12}N_4$, 2129.9602, found: 2129.9270.

**Notes and reference**


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