

## Supporting Information

### Long-wavelength dual-state luminescent naphthalimide derivatives for bio-imaging

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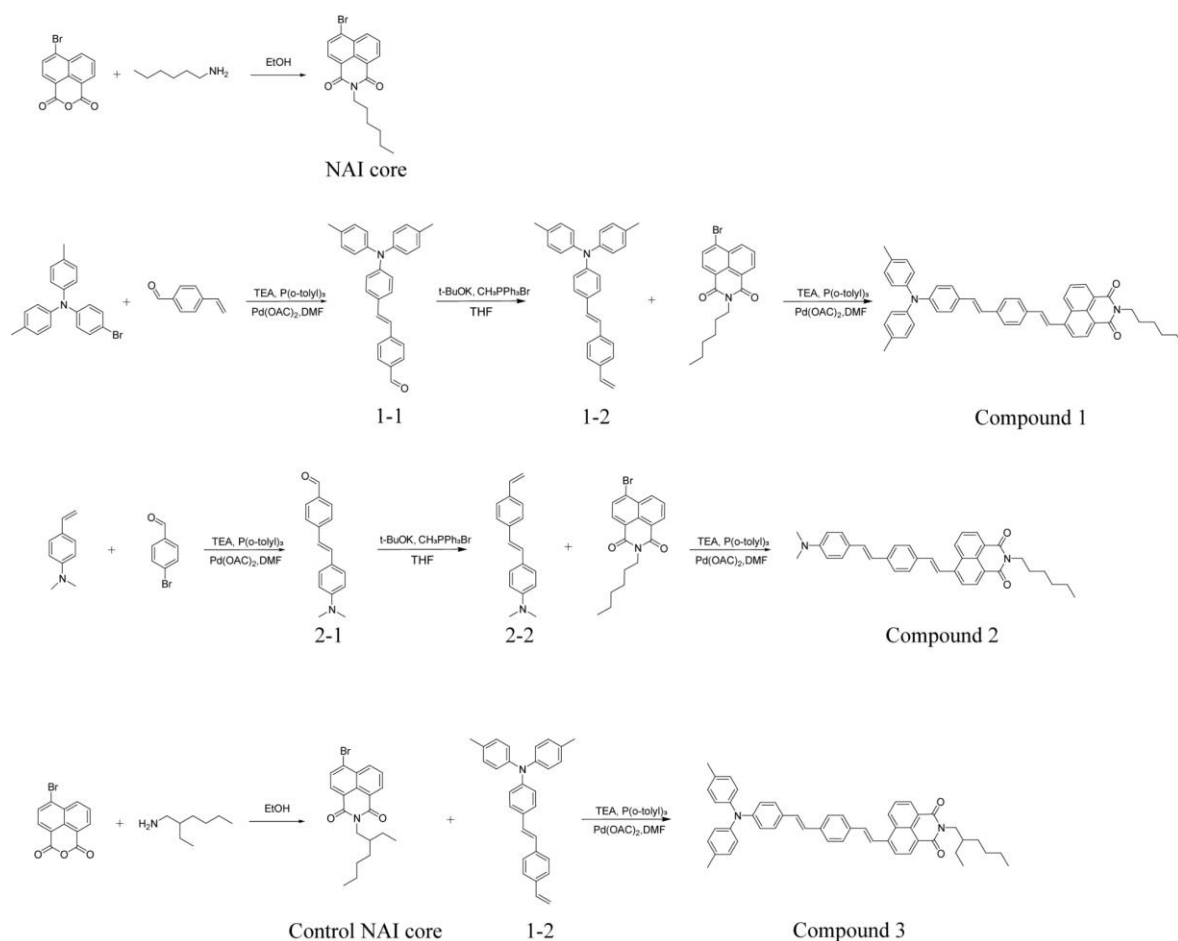
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## 1. Synthesis



**Scheme S1.** Synthetic routes to compounds **1-3**.

The NAI and control NAI cores were synthesized according to reported procedures.<sup>1, 2</sup>

Synthesis of compound **1-1**: A flask was charged with a mixture of 4-bromo-N,N-diphenylbenzylamine (1.47 g, 4.16 mmol), 4-vinylbenzaldehyde (0.50 g, 3.78 mmol), Pd(OAc)<sub>2</sub> (8.5 mg, 0.038 mmol), P(o-tolyl)<sub>3</sub> (52 mg, 0.19 mmol), DMF (10 mL), and triethylamine (3.0 mL). The reaction mixture was stirred at 100 °C for 24 h under nitrogen atmosphere. Upon cooling to room temperature, the solution was poured into water and extracted with DCM. The organic layer was dried with anhydrous sodium sulfate and concentrated by vacuum evaporation. The crude product was purified by silica-gel column chromatography using PE/DCM (1/1) as an eluent to obtain the desired compound as yellow solid (0.82 g) with a yield of 53.9%. **<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>, δ): 9.97 (s, 1H), 7.84 (d, J = 8.1 Hz, 2H), 7.61 (d, J = 8.1 Hz, 2H), 7.37 (d, J = 8.5 Hz, 2H), 7.20 (d, J = 16.3 Hz, 1H), 7.09 (d, J = 8.2 Hz, 4H), 7.05-6.95 (m, 7H), 2.33 (s, 6H); **<sup>13</sup>C NMR** (101 MHz, CDCl<sub>3</sub>, δ): 191.55, 148.69, 144.82, 144.04, 133.20, 131.93, 130.25, 130.00, 127.74, 126.54, 125.11, 124.81, 121.69, 20.85; **HRMS** (ESI) *m/z*: [M + H]<sup>+</sup> calcd for C<sub>29</sub>H<sub>26</sub>NO<sup>+</sup> 404.2009; found: 404.2009.

Synthesis of compound **1-2**: A mixture of 1-1 (0.70 g, 1.74 mmol), potassium tert-butyrate (0.58 g, 5.21 mmol), and  $\text{CH}_3\text{PPh}_3\text{Br}$  (1.55 g, 4.35 mmol) in dry THF (50 mL) was stirred at 0 °C for 4 h under nitrogen atmosphere. After vacuum distillation of the reaction mixture to remove part of THF, the solution was poured into water and extracted with DCM. The organic layer was dried with anhydrous sodium sulfate and concentrated by vacuum evaporation. The crude product was purified by silica-gel column chromatography using PE/DCM (4/1) as an eluent to obtain the desired compound as a yellow solid (0.43 g) with a yield of 63.5%.  **$^1\text{H}$  NMR** (400 MHz,  $\text{CDCl}_3$ ,  $\delta$ ): 7.44 (d,  $J = 8.2$  Hz, 2H), 7.38 (d,  $J = 8.2$  Hz, 2H), 7.34 (d,  $J = 8.6$  Hz, 2H), 7.07 (d,  $J = 8.2$  Hz, 4H), 7.04-6.91 (m, 7H), 6.71 (dd,  $J = 17.5, 10.8$  Hz, 1H), 5.75 (d,  $J = 17.4$  Hz, 1H), 5.23 (d,  $J = 11.0$  Hz, 1H), 2.32 (s, 6H);  **$^{13}\text{C}$  NMR** (101 MHz,  $\text{CDCl}_3$ ,  $\delta$ ): 136.52, 132.76, 131.08, 129.90, 128.26, 127.22, 126.52, 126.40, 124.80, 123.48, 122.35, 113.41, 20.81; **HRMS** (ESI)  $m/z$ :  $[\text{M}]$  calcd for  $\text{C}_{30}\text{H}_{27}\text{N}$  401.2143; found: 401.2144.

Synthesis of compound **1**: A flask was charged with a mixture of **1-2** (0.30 g, 0.77 mmol), NAI core (0.30 g, 0.85 mmol),  $\text{Pd}(\text{OAc})_2$  (1.8 mg, 0.008 mmol),  $\text{P}(\text{o-tolyl})_3$  (10 mg, 0.039 mmol), DMF (10 mL), and triethylamine (3.0 mL). The reaction mixture was stirred at 100 °C for 24 h under nitrogen atmosphere. Upon cooling to room temperature, the solution was poured into water and extracted with DCM. The organic layer was dried with anhydrous sodium sulfate and concentrated by vacuum evaporation. The crude product was purified by silica-gel column chromatography using PE/DCM (2/1) as an eluent to obtain the desired compound as an orange solid (0.21 g) with a yield of 40.1%.  **$^1\text{H}$  NMR** (400 MHz,  $\text{DMSO-}d_6$ ,  $\delta$ ): 9.04 (d,  $J = 9.1$  Hz, 1H), 8.56 (d,  $J = 7.1$  Hz, 1H), 8.50 (d,  $J = 7.6$  Hz, 1H), 8.31-8.21 (m, 2H), 7.93 (t,  $J = 8.2$  Hz, 1H), 7.87 (d,  $J = 8.6$  Hz, 2H), 7.67-7.61 (m, 3H), 7.49 (d,  $J = 8.3$  Hz, 2H), 7.29 (d,  $J = 16.7$  Hz, 1H), 7.14 (d,  $J = 8.1$  Hz, 5H), 6.95 (d,  $J = 8.4$  Hz, 4H), 6.89 (d,  $J = 8.2$  Hz, 2H), 4.09-4.02 (m, 2H), 2.28 (s, 6H), 1.70-1.58 (m, 2H), 1.37-1.27 (m, 6H), 0.87 (t,  $J = 6.3$  Hz, 3H);  **$^{13}\text{C}$  NMR** (101 MHz,  $\text{CDCl}_3$ ,  $\delta$ ) 164.29, 164.06, 148.12, 145.00, 141.46, 138.56, 135.37, 135.05, 133.81, 132.93, 131.17, 131.08, 130.18, 129.96, 129.59, 129.17, 128.77, 127.52, 127.39, 126.92, 126.74, 125.65, 124.91, 123.81, 123.22, 122.90, 122.12, 121.45, 40.52, 31.58, 28.10, 26.83, 22.58, 20.85, 14.07; **HRMS** (ESI)  $m/z$ :  $[\text{M} + \text{H}]^+$  calcd for  $\text{C}_{48}\text{H}_{45}\text{N}_2\text{O}_2^+$  681.3476; found: 681.3476.

Synthesis of compound **2-1**: A flask was charged with a mixture of *N,N*-dimethyl-4-vinylbenzenamine (0.50 g, 3.40 mmol), 4-bromobenzaldehyde (0.69 g, 3.75 mmol),  $\text{Pd}(\text{OAc})_2$  (7.5 mg, 0.034 mmol),  $\text{P}(\text{o-tolyl})_3$  (47 mg, 0.17 mmol), DMF (10 mL), and triethylamine (3.0 mL). The reaction mixture was stirred at 100 °C for 24 h under nitrogen atmosphere. Upon cooling to room temperature, the solution was poured into water and extracted with DCM. The

organic layer was dried with anhydrous sodium sulfate and concentrated by vacuum evaporation. The crude product was purified by silica-gel column chromatography using PE/DCM (2/1) as an eluent to obtain the desired compound as a yellow solid (0.45 g) with a yield of 58.6%. **<sup>1</sup>H NMR** (400 MHz, DMSO-*d*<sub>6</sub>, δ): 9.94 (s, 1H), 7.86 (d, J = 8.3 Hz, 2H), 7.74 (d, J = 8.3 Hz, 2H), 7.50 (d, J = 8.8 Hz, 2H), 7.37 (d, J = 16.4 Hz, 1H), 7.08 (d, J = 16.4 Hz, 1H), 6.75 (d, J = 8.9 Hz, 2H), 2.96 (s, 6H); **<sup>13</sup>C NMR** (101 MHz, CDCl<sub>3</sub>, δ): 191.59, 134.74, 132.18, 132.14, 132.04, 130.27, 128.51, 128.26, 126.41, 40.95; **HRMS** (ESI) *m/z*: [M + H]<sup>+</sup> calcd for C<sub>17</sub>H<sub>18</sub>NO<sup>+</sup> 252.1383; found: 252.1383.

Synthesis of compound **2-2**: A mixture of **2-1** (0.30 g, 1.19 mmol), potassium tert-butyrate (0.40 g, 3.58 mmol), and CH<sub>3</sub>PPh<sub>3</sub>Br (1.07 g, 2.98 mmol) in dry THF (50 mL) was stirred at 0 °C for 4 h under nitrogen atmosphere. After vacuum distillation of the reaction mixture to remove part of THF, the solution was poured into water and extracted with DCM. The organic layer was dried with anhydrous sodium sulfate and concentrated by vacuum evaporation. The crude product was purified by silica-gel column chromatography using PE/DCM (5/1) as an eluent to obtain the desired compound as a pale-yellow solid (0.25 g) with a yield of 83.7%. **<sup>1</sup>H NMR** (400 MHz, DMSO-*d*<sub>6</sub>, δ): 7.50 (d, J = 8.3 Hz, 2H), 7.43 (d, J = 9.1 Hz, 4H), 7.14 (d, J = 16.4 Hz, 1H), 6.96 (d, J = 16.4 Hz, 1H), 6.76-6.67 (m, 3H), 5.82 (d, J = 17.5 Hz, 1H), 5.23 (d, J = 11.3 Hz, 1H), 2.94 (s, 6H); **<sup>13</sup>C NMR** (101 MHz, CDCl<sub>3</sub>, δ): 137.75, 136.56, 135.95, 128.73, 127.57, 126.45, 126.10, 113.07, 112.48, 112.45, 40.47; **HRMS** (ESI) *m/z*: [M + H]<sup>+</sup> calcd for C<sub>18</sub>H<sub>20</sub>N<sup>+</sup> 250.1590; found: 250.1590.

Synthesis of compound **2**: A flask was charged with a mixture of **2-2** (0.20 g, 0.80 mmol), NAI core (0.32 g, 0.88 mmol), Pd(OAc)<sub>2</sub> (1.8 mg, 0.008 mmol), P(*o*-tolyl)<sub>3</sub> (11 mg, 0.04 mmol), DMF (10 mL), and triethylamine (3.0 mL). The reaction mixture was stirred at 100 °C for 24 h under nitrogen atmosphere. Upon cooling to room temperature, the solution was poured into water and extracted with DCM. The organic layer was dried with anhydrous sodium sulfate and concentrated by vacuum evaporation. The crude product was purified by silica-gel column chromatography using PE/DCM (1/1) as an eluent to obtain the desired compound as an orange solid (0.12 g) with a yield of 28.6%. **<sup>1</sup>H NMR** (400 MHz, DMSO-*d*<sub>6</sub>, δ): 9.04 (d, J = 8.4 Hz, 1H), 8.55 (d, J = 6.8 Hz, 1H), 8.49 (d, J = 7.8 Hz, 1H), 8.25 (dd, J = 18.4, 12.0 Hz, 2H), 7.95-7.88 (m, 1H), 7.85 (d, J = 8.3 Hz, 2H), 7.66-7.58 (m, 3H), 7.47 (d, J = 8.8 Hz, 2H), 7.25 (d, J = 16.4 Hz, 1H), 7.03 (d, J = 16.4 Hz, 1H), 6.74 (d, J = 8.9 Hz, 2H), 4.08-3.99 (m, 2H), 2.95 (s, 6H), 1.68-1.59 (m, 2H), 1.30 (d, J = 8.1 Hz, 6H), 0.87 (t, J = 6.9 Hz, 3H); **<sup>13</sup>C NMR** (101 MHz, CDCl<sub>3</sub>, δ): 164.27, 164.04, 144.56, 141.49, 138.93, 135.10, 134.89, 131.12, 131.05, 129.93, 129.59, 129.53, 128.73, 127.75, 127.47, 126.61, 126.46, 123.70, 123.14, 122.53, 121.31,

120.67, 118.39, 112.52, 40.56, 40.47, 31.54, 28.06, 26.79, 22.55, 14.04; **HRMS** (ESI)  $m/z$ :  $[M + H]^+$  calcd for  $C_{36}H_{37}N_2O_2^+$  529.2850; found: 529.2850.

**Synthesis of compound 3:** A flask was charged with a mixture of **1-2** (0.30 g, 0.77 mmol), Control NAI core (0.33 g, 0.85 mmol),  $Pd(OAc)_2$  (1.8 mg, 0.008 mmol),  $P(o\text{-tolyl})_3$  (10 mg, 0.039 mmol), DMF (10 mL), and triethylamine (3.0 mL). The reaction mixture was stirred at 100 °C for 24 h under nitrogen atmosphere. Upon cooling to room temperature, the solution was poured into water and extracted with DCM. The organic layer was dried with anhydrous sodium sulfate and concentrated by vacuum evaporation. The crude product was purified by silica-gel column chromatography using PE/DCM (2/1) as an eluent to obtain the desired compound as an orange solid (0.16 g) with a yield of 29.4%.  **$^1H$  NMR** (400 MHz,  $DMSO-d_6$ ,  $\delta$ ): 9.04 (d,  $J = 8.8$  Hz, 1H), 8.54 (dd,  $J = 22.9, 7.4$  Hz, 2H), 8.31-8.21 (m, 2H), 8.01-7.78 (m, 4H), 7.78-7.57 (m, 4H), 7.49 (d,  $J = 8.8$  Hz, 2H), 7.28 (d,  $J = 15.8$  Hz, 2H), 7.13 (t,  $J = 7.8$  Hz, 4H), 6.92 (dd,  $J = 25.8, 8.4$  Hz, 4H), 4.01 (t,  $J = 6.8$  Hz, 2H), 2.28 (s, 6H), 1.87 (s, 1H), 1.42-1.19 (m, 8H), 0.86 (dt,  $J = 13.8, 7.2$  Hz, 6H);  **$^{13}C$  NMR** (101 MHz,  $CDCl_3$ ,  $\delta$ ) 164.69, 164.46, 148.12, 145.00, 141.42, 138.56, 135.36, 135.03, 133.24, 132.93, 131.25, 131.16, 130.17, 129.96, 129.57, 129.17, 128.81, 127.52, 127.39, 127.06, 126.74, 125.65, 124.91, 123.82, 123.20, 122.87, 122.12, 121.43, 44.20, 37.97, 30.81, 28.75, 24.12, 23.10, 20.85, 14.11, 10.69; **HRMS** (ESI)  $m/z$ :  $[M + H]^+$  calcd for  $C_{50}H_{49}N_2O_2^+$  709.3789; found: 709.3789.

## 2. Experimental methods

### 2.1 Materials and instrumentations

4-Bromo-1,8-naphthalic anhydride, hexan-1-amine, methyltriphenylphosphonium bromide, 2-ethylhexan-1-amine, palladium diacetate, tri-*o*-tolylphosphine, potassium *tert*-butanolate, sodium *tert*-butanolate, *N,N*-dimethyl-4-vinylbenzenamine, triethylamine, 4-bromobenzaldehyde and 4-bromo-*N,N*-dip-tolylbenzenamine were all purchased from Adamas-beta®. All reagents were used as received without any further purification.

$^1H$  NMR and  $^{13}C$  NMR were measured on a Bruker 400 MHz spectrometer. High-resolution mass spectra (HRMS) were carried out on a Bruker Micro TOF II 10257 instrument with the electro-spray ionization (ESI) technique and direct injection method. Absorption spectra were recorded on a Shimadzu 1800 spectrophotometer, while the fluorescent spectra were taken with an Edinburgh FLS1000 spectrofluorometer. The fluorescent lifetimes were measured using an Edinburgh FLS1000 spectrofluorometer with a time-correlated single photon counting technique. The quantum yields of samples were measured on a Hamamatsu Photonics C11347-11 with a Quantaaurus-QY measurement system. TEM images were captured on a Hitachi

HT7700 Exa-lens using transmission electron microscopy with an acceleration voltage of 120 kV by dropping the solution onto a carbon-coated copper grid. Dynamic light scattering (DLS) experiments were carried out with a Nano-Zeta Potential Analyzer ZS-90. The confocal microscope was performed on a Lecia DMI8 fluorescence microscopy. The photos were taken by Canon EDS 90D camera or Huawei P20 Pro phone.

## **2.2 Preparation of coassembly films**

PMMA (5 g) was added to chloroform (100 mL), which was stirred at room temperature for 10 min. Small organic molecules with 1 mg/mL in THF were added to the prepared PMMA solution (10 mL). The obtained solutions were then ultrasonicated at room temperature for about 20 min for a full coassembly. Dropping the solutions (about 0.5 mL) on quartz glass and keeping them at 80 °C for 5 min resulted in the coassembly films.

## **2.3 Preparation of F-127 nanoparticles**

Compound **1** (0.1 mg) in THF (2 mL) and F-127 (10 mg) in deionized water (5 mL) were mixed in a flask followed by sonication for 30 minutes. THF was evaporated by reduced pressure. The solution was filtered through a 0.22 µm microfilter to obtain the NPs solution.

## **2.4 Cytotoxicity assay**

HeLa cells were seeded in a 96-well plate with culture media (DMEM). After growing for 24 h in the well, different concentrations of NPs were added and incubated for 24 h. The MTT assay was conducted using 0.5 mg/mL of MTT (sigma) media. MTT media was added to the cells for 4 h, and the formazan produced was dissolved in 0.1 mL of dimethylsulfoxide (DMSO). The absorbance at 570 nm was determined using a microplate reader (Bio Tek Instruments, Inc). The cell viability was calculated as the ratio of the average absorbance of samples to that of control.

## **2.5 Cell Culture and Staining**

HeLa cells were cultivated in the standard culture media at 37 °C for 24 h. Then the culture media was changed into standard culture media containing various concentration NPs, and cells were incubated for 4 h. After that, the cells were washed carefully with PBS for three times to remove free NPs suspended in the media and ready for fluorescence imaging. HeLa cells incubated with NPs, and HeLa cells pretreated with nystatin for 30 min and then stained with NPs for 4 hours at 37 °C. After that, the cells were washed carefully with PBS for three times to remove free NPs suspended in the media and ready for fluorescence lifetime imaging and fluorescence imaging. Fluorescence intensities were quantified from region of interests in the cells by an imaging J software.

### 3. Computational details

Ground state molecular structures of naphthalimide core-based materials were optimized in gas phase by using DFT/B3LYP/6-31G(d) level of theory.<sup>3,4</sup> Becke three-parameter hybrid functional (B3LYP) was found to be a well-performing method for charge transport and photophysical properties of naphthalimide derivatives.<sup>5-7</sup> The resulted minimized geometry is then considered as initial guess for the geometry optimization at the same level of theory within the polarizable continuum model (PCM). We used the time-dependent density functional theory (TD-DFT)<sup>8,9</sup> to calculate the  $S_0 \rightarrow S_1$  vertical absorption, and  $S_1 \rightarrow S_0$  vertical emission of compounds. Both calculations were investigated with the same solvation model as was used for optimized ground state  $S_0$  geometry. The same method B3LYP/6-31G(d) was employed for TD-DFT calculations. In addition, the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) distributions for the  $S_1$  and  $S_2$  excited states were investigated. All computational calculations were performed using the quantum chemistry package Gaussian 16 (Rev. B. 01).<sup>10</sup>



#### 4. Additional figures and images

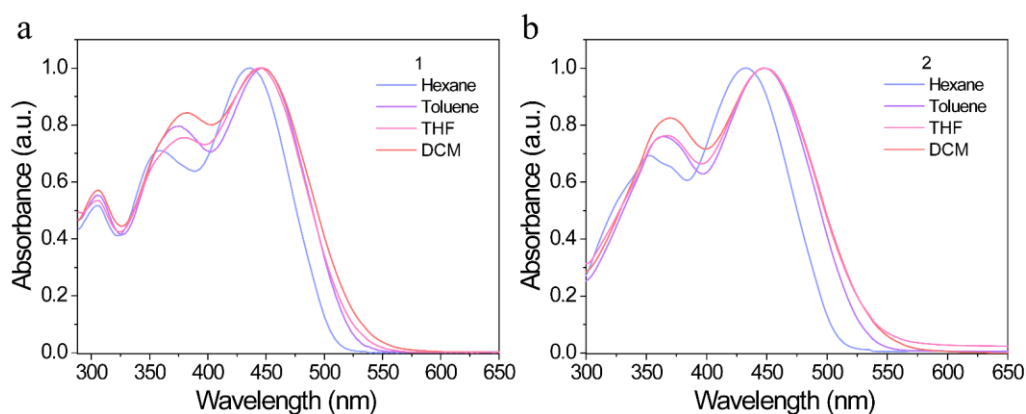


Figure S1. Normalized absorption spectra of (a) **1** and (b) **2** in different solvents. The concentration is 10  $\mu\text{M}$ .

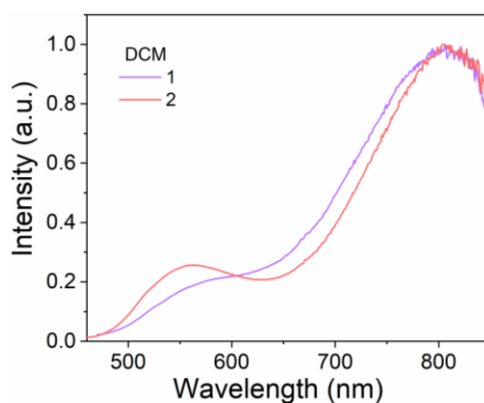


Figure S2. Normalized fluorescence spectra of **1** and **2** in DCM measured by PMT detector at room temperature. The excitation wavelength is 450 nm. The concentration is 10  $\mu\text{M}$ .

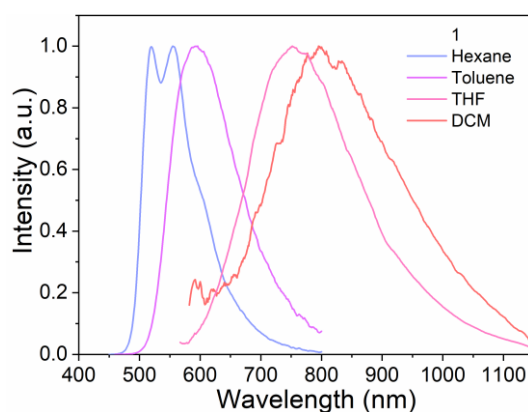


Figure S3. Normalized fluorescence spectra of **1** in different solvents at room temperature. The excitation wavelength is 380 nm. The concentration is 10  $\mu\text{M}$ . The emissions in hexane and toluene were measured by the PMT detector, and the emissions in DCM and THF were measured by NIR detector.

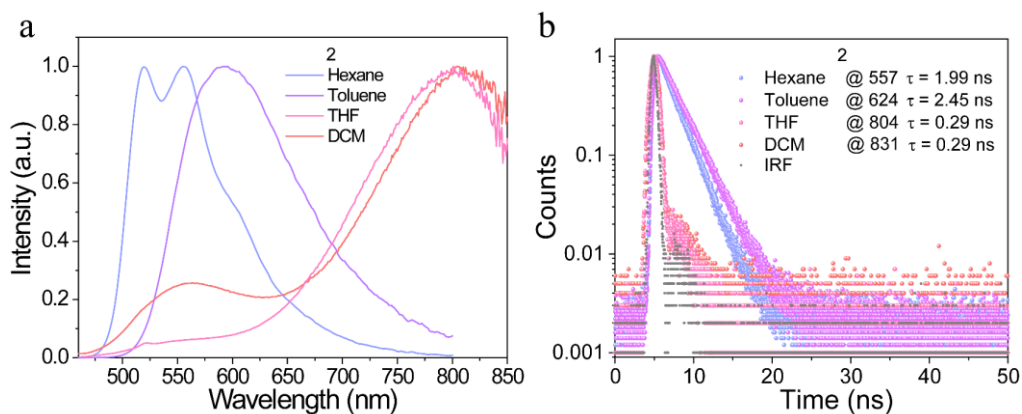


Figure S4. (a) Fluorescence (measured by PMT detector) spectra and (b) fluorescence decay of **2** in different solvents. The concentration is  $10 \mu\text{M}$ . The excitation wavelength is 380 nm.

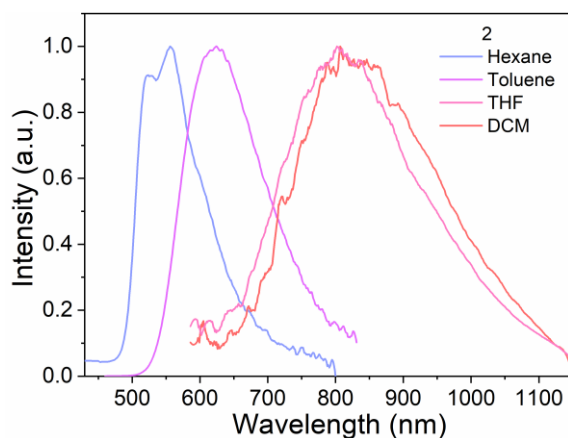


Figure S5. Normalized fluorescence spectra of **2** in different solvents at room temperature. The excitation wavelength is 380 nm. The concentration is  $10 \mu\text{M}$ . The emissions in hexane and toluene were measured by PMT detector, and the emissions in DCM and THF were measured by NIR detector.

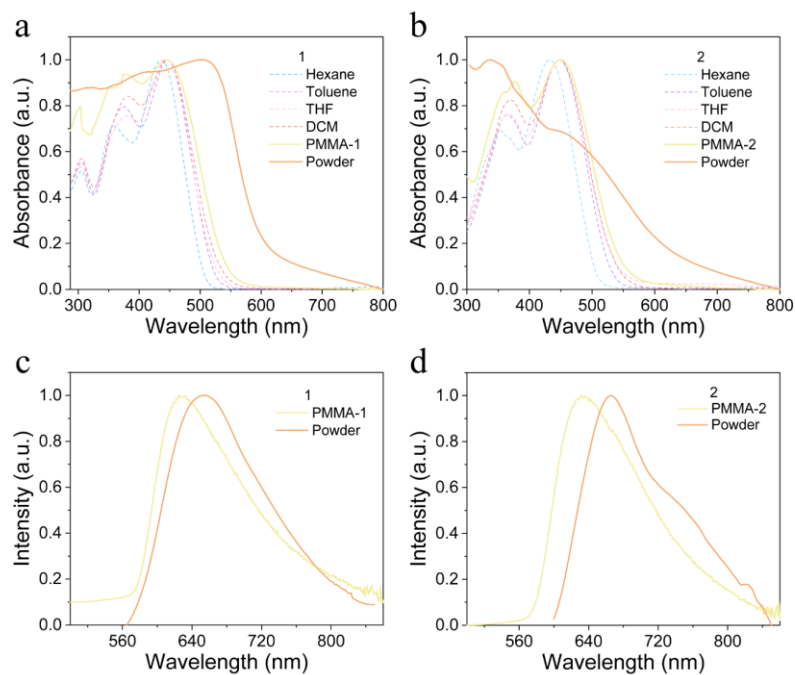


Figure S6. Normalized absorption spectra of **1** and **2** in different states (a and b). The concentration is  $10\ \mu\text{M}$ . Normalized fluorescence spectra of **1** and **2** in different states at room temperature (c and d). The excitation wavelength is  $450\ \text{nm}$ .

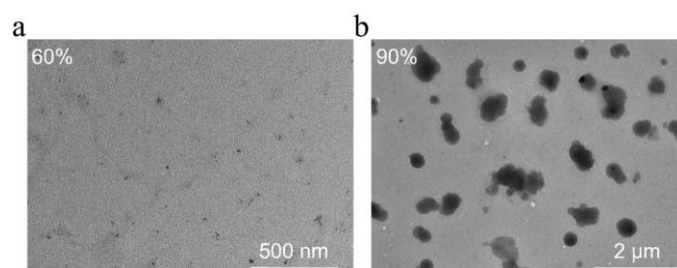


Figure S7. TEM images of compound **1** in THF/ $\text{H}_2\text{O}$  with 60% (a) and 90% (b) water fractions.

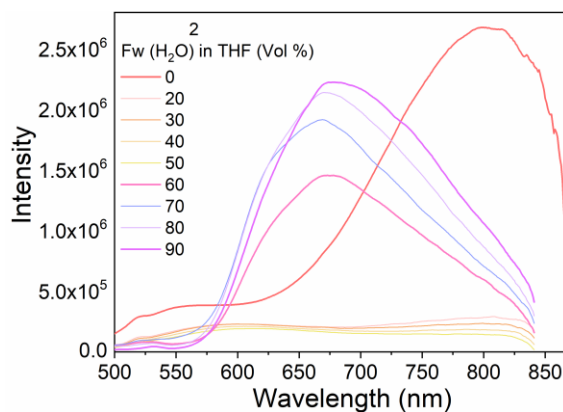


Figure S8. Fluorescence spectra of compound **2** ( $10\ \mu\text{M}$ ) in THF/ $\text{H}_2\text{O}$  with different water fractions. The excitation wavelength is  $450\ \text{nm}$ .

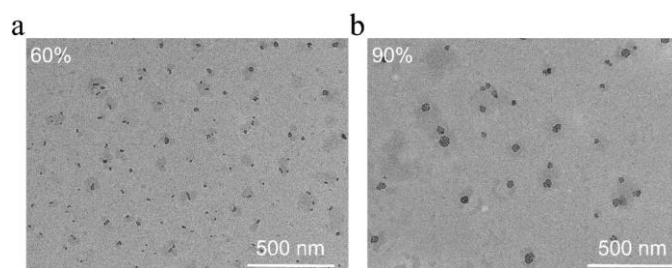


Figure S9. TEM images of compound **2** in THF/H<sub>2</sub>O with water fractions of 60% (a) and 90% (b).

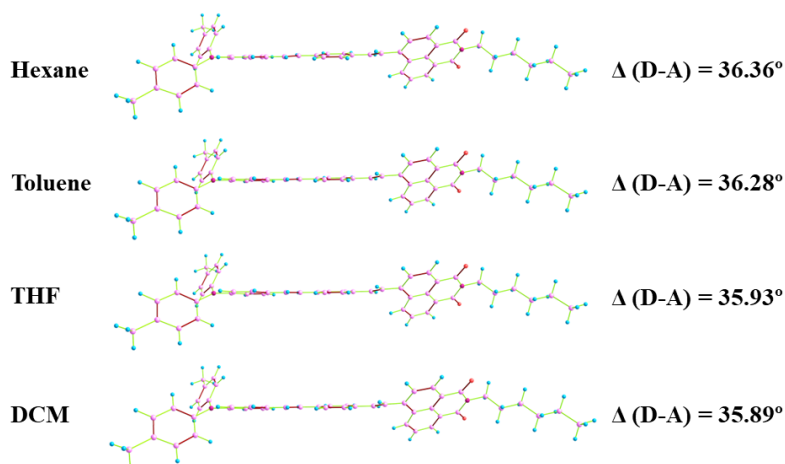


Figure S10. Ground state spatial configuration of **1** in different solvents with the dihedral angle,  $\Delta(\text{D-A})$ , between the donor (D) and the acceptor (A). Here, in DA structures, electronic donors are shown as planar layers.

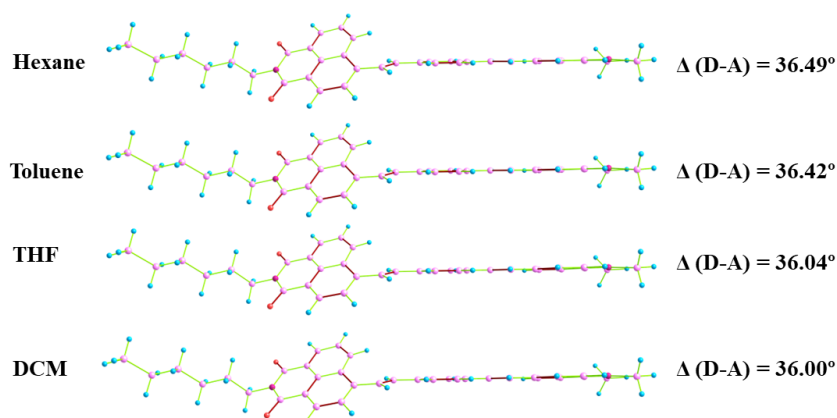


Figure S11. Ground state spatial configuration of **2** in different solvents with the dihedral angle,  $\Delta(\text{D-A})$ , between the donor (D) and the acceptor (A). Here, in DA structures, electronic donors are shown as planar layers.

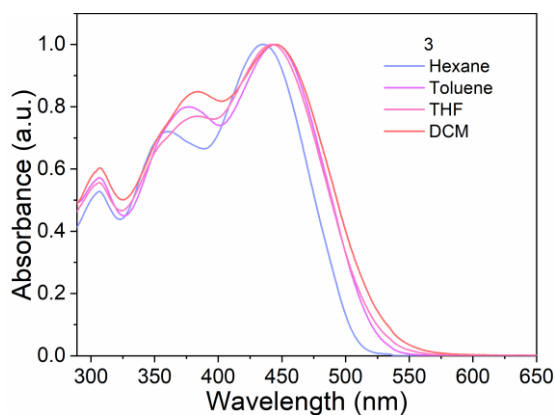


Figure S12. Normalized absorption spectra of **3** in different solvents. The concentration is 10  $\mu\text{M}$ .

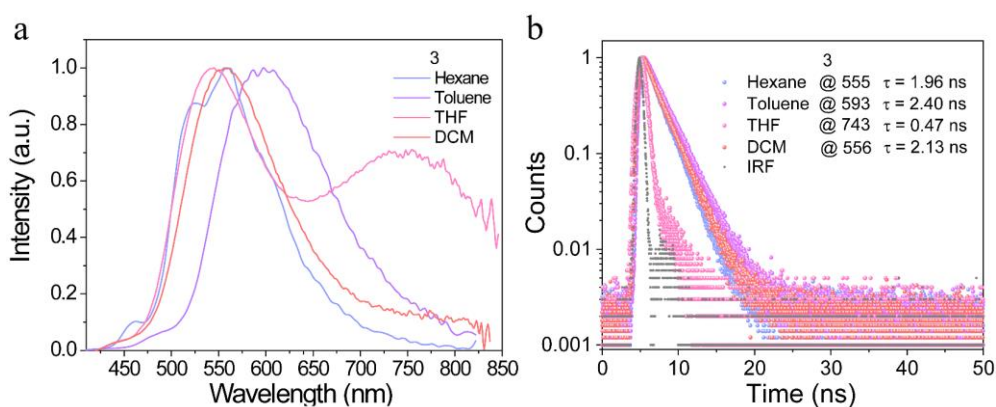


Figure S13. (a) Fluorescence (measured by PMT detector) spectra and (b) fluorescence decay of **3** in different solvents. The concentration is 10  $\mu\text{M}$ . The excitation wavelength is 380 nm.

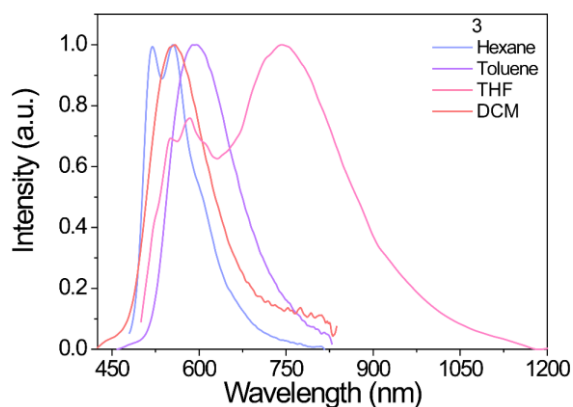


Figure S14. Normalized fluorescence spectra of **3** in different solvents at room temperature. The excitation wavelength is 380 nm. The concentration is 10  $\mu\text{M}$ . The emissions in hexane, toluene, and DCM were measured by PMT detector, and the emission of **3** in THF was measured by NIR detector.

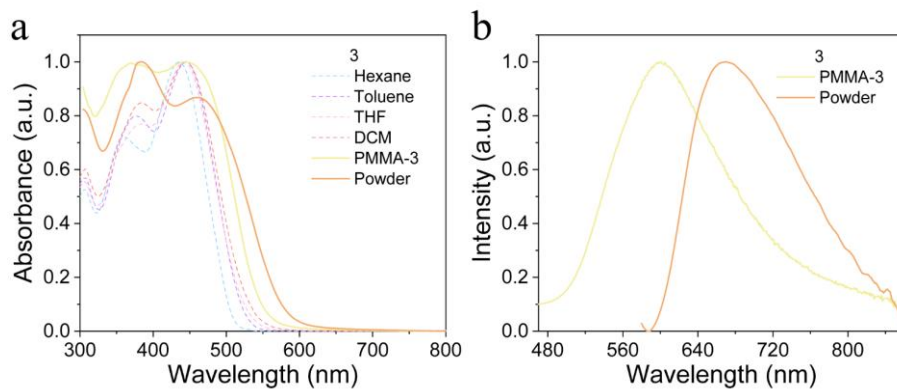


Figure S15. (a) Normalized absorption spectra of **3** in different states. The concentration is 10  $\mu\text{M}$ . (b) Normalized fluorescence spectra of **3** in different states at room temperature. The excitation wavelength is 450 nm.

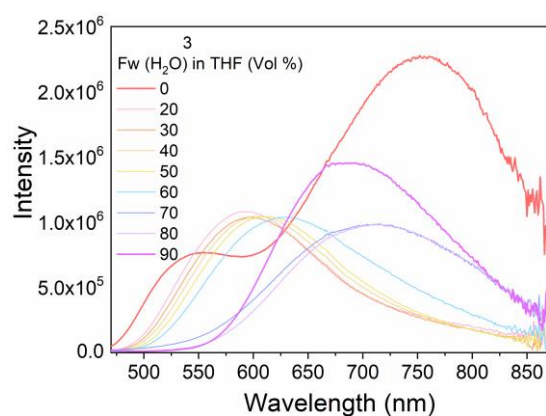


Figure S16. Fluorescence spectra of compound **2** (10  $\mu\text{M}$ ) in THF/ $\text{H}_2\text{O}$  with different water fractions. The excitation wavelength is 450 nm.

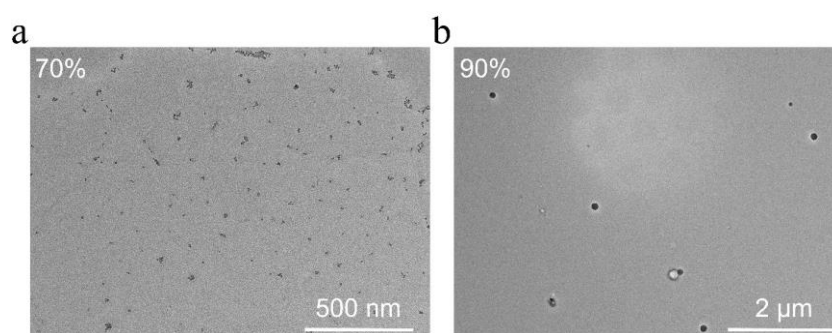


Figure S17. TEM images of compound **3** in THF/ $\text{H}_2\text{O}$  with water fractions of 70% (a) and 90% (b).

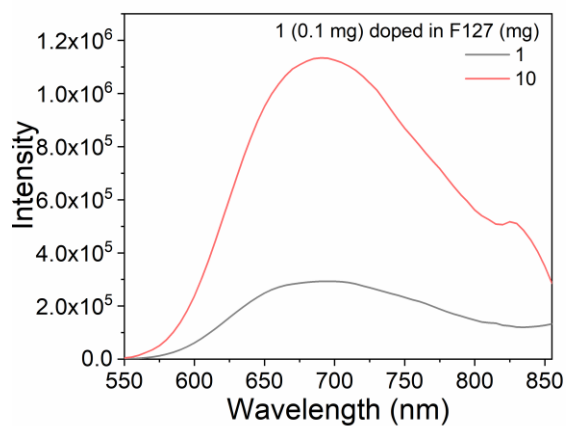


Figure S18. Fluorescence spectra of 0.1 mg compound **1** doping in different weight F127 upon 450 nm excitation at room temperature. The concentration is 10  $\mu$ M.

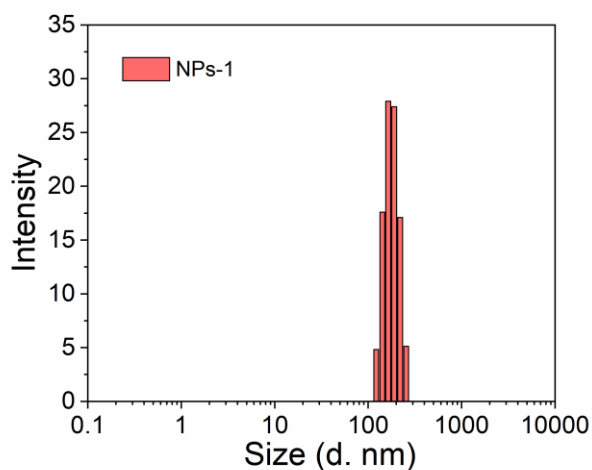


Figure S19. DLS of 0.1 mg compound **1** doping with 10 mg F127 in water. The concentration is 10  $\mu$ M.

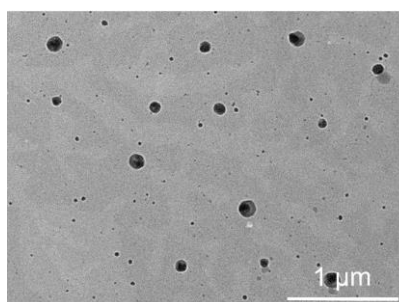


Figure S20. TEM image of 0.1 mg compound **1** doping with 10 mg F127 in water. The concentration is 10  $\mu$ M.

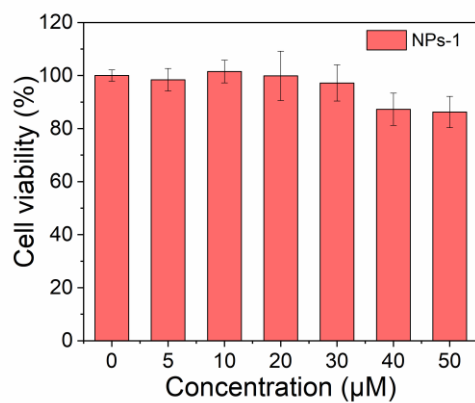


Figure S21. Cytotoxicity of NPs-1 to HeLa cells. Cellular internalization time is 24 hours at 37 °C.

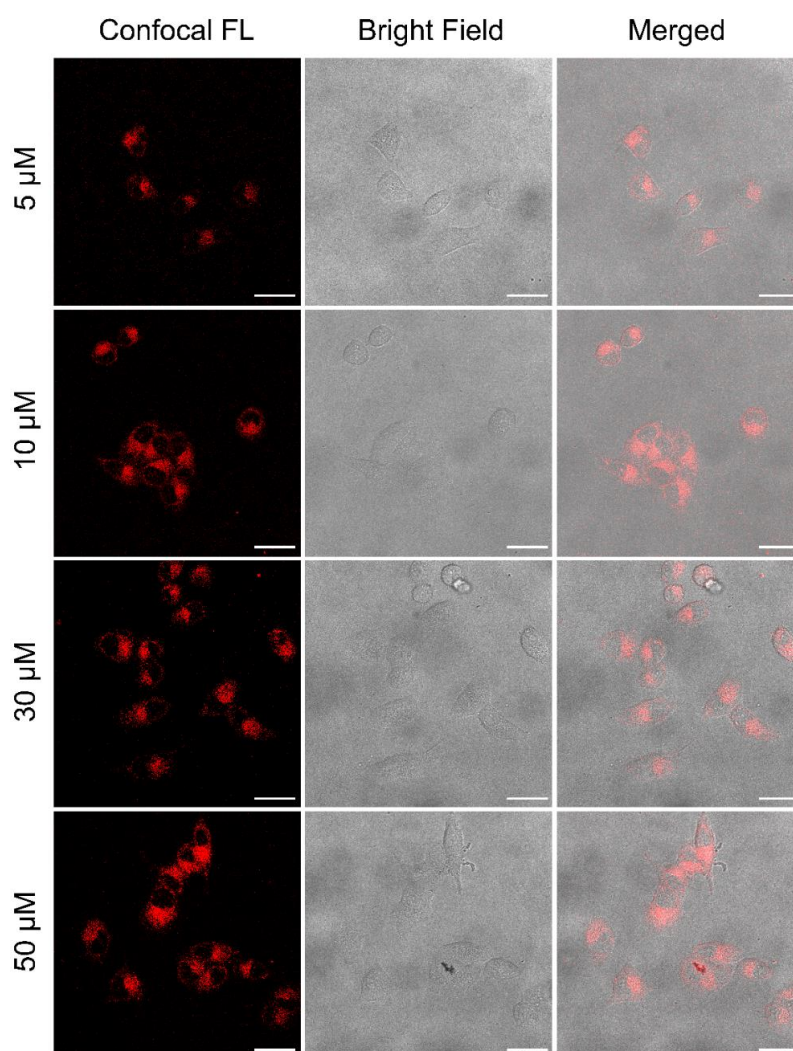


Figure S22. Confocal fluorescence images of HeLa cells incubated with NPs-1 in different concentrations for 4 hours at 37 °C obtained under 405 nm excitation. Scale bar = 30 µm.



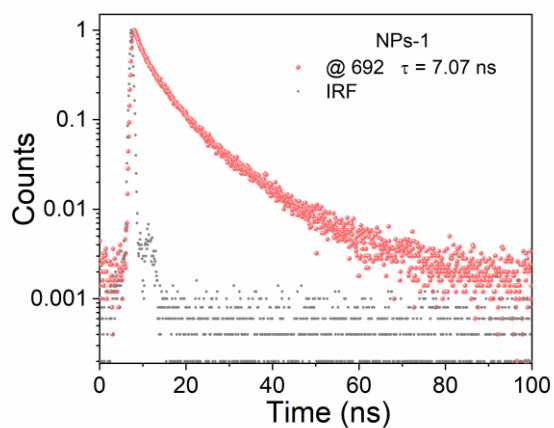


Figure S23. Fluorescence decay of NPs-1 in water at room temperature. The excitation wavelength is 405 nm. The concentration of the solution is 10  $\mu$ M.

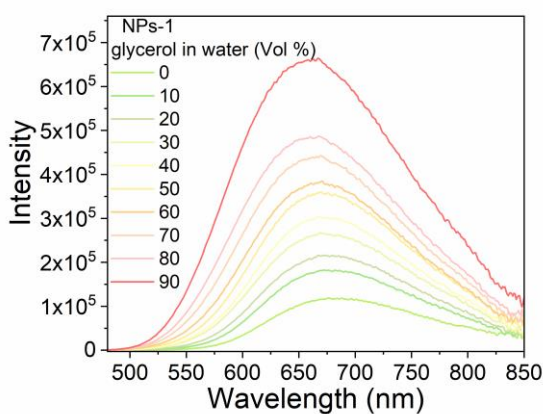


Figure S24. Fluorescence spectra of NPs-1 (10  $\mu$ M) in glycerol/H<sub>2</sub>O with different viscosities. The excitation wavelength is 405 nm.

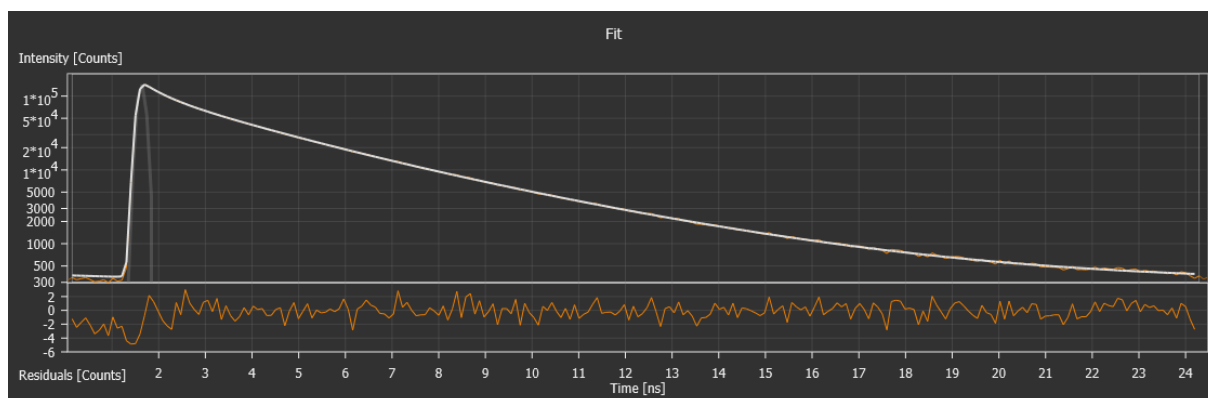


Figure S25. The fluorescence lifetime of HeLa cells incubated with NPs-1 for 4 h at 37°C obtained following 405 nm excitation.

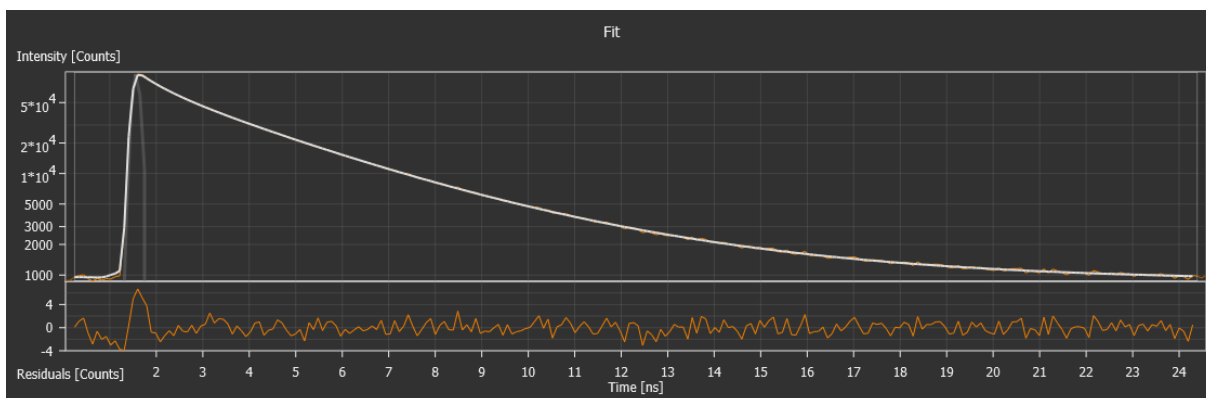


Figure S26. Fluorescence lifetime of HeLa cells pretreated with nystatin for 30 min and then stained with NPs-1 for 4 h at 37°C obtained following 405 nm excitation.

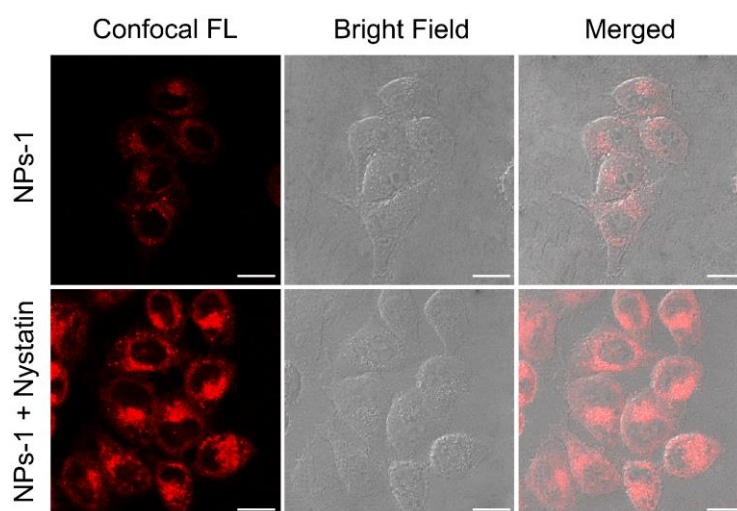


Figure S27. Confocal fluorescence images of HeLa cells incubated with NPs-1 and HeLa cells pretreated with nystatin for 30 min and then stained with NPs-1 for 4 hours at 37 °C obtained under 405 nm excitation. Scale bar = 15  $\mu$ m.

## 5. Additional tables

**Table S1.** Photophysical data of compounds **1-3** in solution state.

Compounds	Solvents	$\lambda_{\text{abs, max}}$ (nm)	$\lambda_{\text{em, max}}$ (nm)	Stokes shift (nm)	Fluorescence lifetime (ns)	Quantum yield (%)
<b>1</b>	Hexane	436	555	119	1.95	80.3
	Toluene	444	593	149	2.41	60.6
	THF	444	757	313	0.57	8.2
	DCM	446	811	365	0.31	1.9
<b>2</b>	Hexane	432	557	125	1.99	89.1
	Toluene	448	624	176	2.45	36.9
	THF	448	804	356	0.29	1.8
	DCM	448	831	383	0.29	2.2
<b>3</b>	Hexane	435	555	120	1.96	81.2
	Toluene	443	593	150	2.40	53.8
	THF	443	743	300	0.27	9.6
	DCM	445	556	111	2.13	3.2

**Table S2.** Photophysical data of compounds **1-3** in powder state.

Powder	$\lambda_{\text{em, max}}$ (nm)	Fluorescence lifetime (ns)	Quantum yield (%)
<b>1</b>	654	7.28	10.7
<b>2</b>	666	3.44	1.4
<b>3</b>	670	3.36	2.3

**Table S3.** Computed vertical excitations of **1** in different solvent media within the PCM solvent model using the TDDFT/B3LYP/6-31G(d) theoretical level. Absorption wavelengths, energies and their corresponding oscillator strength values of each vertical excitations (S<sub>1</sub>-S<sub>5</sub>) in different solvents are listed and compared with the experimental results.

Solvents	Excitation states	Wavelength (nm)	Energy (eV)	Oscillator strength	Experiment (nm)
Hexane ( $\epsilon=1.8819$ )	S <sub>1</sub>	598	2.07	0.8273	436
	S <sub>2</sub>	446	2.78	1.3921	
	S <sub>3</sub>	432	2.87	0.1527	358
	S <sub>4</sub>	361	3.43	0.0913	305
	S <sub>5</sub>	342	3.63	0.2253	
Toluene ( $\epsilon=2.3741$ )	S <sub>1</sub>	604	2.05	0.8440	444
	S <sub>2</sub>	449	2.76	1.3560	
	S <sub>3</sub>	434	2.86	0.1962	374
	S <sub>4</sub>	362	3.42	0.0900	305
	S <sub>5</sub>	343	3.62	0.2366	
THF ( $\epsilon=7.4257$ )	S <sub>1</sub>	611	2.03	0.8004	444
	S <sub>2</sub>	453	2.74	1.2592	
	S <sub>3</sub>	435	2.85	0.3117	378
	S <sub>4</sub>	364	3.41	0.0942	305
	S <sub>5</sub>	343	3.61	0.2339	
DCM ( $\epsilon=8.93$ )	S <sub>1</sub>	612	2.02	0.8042	446
	S <sub>2</sub>	453	2.74	1.2472	
	S <sub>3</sub>	435	2.85	0.3248	381
	S <sub>4</sub>	364	3.41	0.0933	305
	S <sub>5</sub>	343	3.61	0.2360	

**Table S4.** Computed vertical excitations of **2** in different solvent media within the PCM solvent model using the TDDFT/B3LYP/6-31G(d) theoretical level. Absorption wavelengths, energies and their corresponding oscillator strength values of each vertical excitations (S<sub>1</sub>-S<sub>4</sub>) in different solvents are listed and compared with the experimental results.

Solvents	Excitation states	Wavelength (nm)	Energy (eV)	Oscillator strength	Experiment (nm)
Hexane ( $\epsilon=1.8819$ )	S <sub>1</sub>	585	2.12	0.8695	432
	S <sub>2</sub>	421	2.95	1.2981	
	S <sub>3</sub>	403	3.07	0.1712	351
	S <sub>4</sub>	342	3.63	0.0194	
Toluene ( $\epsilon=2.3741$ )	S <sub>1</sub>	594	2.09	0.8851	448
	S <sub>2</sub>	424	2.92	1.3054	
	S <sub>3</sub>	407	3.05	0.1677	364
	S <sub>4</sub>	343	3.62	0.0235	
THF ( $\epsilon=7.4257$ )	S <sub>1</sub>	611	2.03	0.8232	448
	S <sub>2</sub>	430	2.88	1.2916	
	S <sub>3</sub>	411	3.02	0.2073	365
	S <sub>4</sub>	345	3.59	0.0354	
DCM ( $\epsilon=8.93$ )	S <sub>1</sub>	613	2.02	0.8257	448
	S <sub>2</sub>	431	2.88	1.2907	
	S <sub>3</sub>	412	3.01	0.2093	369
	S <sub>4</sub>	346	3.59	0.0363	

**Table S5.** Vertical (de)excitation  $S_1 \rightarrow S_0$  calculation of studied compounds at TD-DFT/B3LYP/6-31G(d) theoretical level.

Compounds	Solvents	Wavelength (nm)	Energy (eV)	Oscillator strength	Experiment (nm)
<b>1</b>	Hexane ( $\epsilon=1.8819$ )	686	1.81	0.9709	555
	Toluene ( $\epsilon=2.3741$ )	697	1.78	1.0557	593
	THF ( $\epsilon=7.4257$ )	737	1.68	1.3232	757
	DCM ( $\epsilon=8.93$ )	741	1.67	1.3496	811
<b>2</b>	Hexane ( $\epsilon=1.8819$ )	665	1.86	1.0038	557
	Toluene ( $\epsilon=2.3741$ )	680	1.82	1.0735	624
	THF ( $\epsilon=7.4257$ )	733	1.69	1.3142	804
	DCM ( $\epsilon=8.93$ )	739	1.68	1.3386	831
<b>3</b>	Hexane ( $\epsilon=1.8819$ )	691	1.79	0.9561	555
	Toluene ( $\epsilon=2.3741$ )	700	1.77	1.0441	593
	THF ( $\epsilon=7.4257$ )	738	1.68	1.3112	743
	DCM ( $\epsilon=8.93$ )	742	1.67	1.3369	556

**Table S6.** Representation of  $S_1 \rightarrow S_0$  charge transfer (CT) emission of **2** at TDDFT/B3LYP/6-31G(d) level.

Solvents	HOMO	LUMO
Hexane		
Toluene		
THF		
DCM		

**Table S7.** The dipole moments (Debye) in ground state and different excited state.

Compounds	Energy level state	Hexane	Toluene	THF	DCM
1	S <sub>0</sub>	9.1787	9.3988	10.0339	10.0914
	S <sub>1</sub>	11.9057	12.5377	14.3974	14.5812
	S <sub>2</sub>	11.9613	12.0816	13.0183	13.0790
2	S <sub>0</sub>	11.4415	11.7660	12.7461	12.8333
	S <sub>1</sub>	11.9172	12.4609	14.3157	14.5017
	S <sub>2</sub>	8.0728	7.9935	7.5804	7.5293
3	S <sub>0</sub>	9.3584	9.4977	10.0793	10.1286
	S <sub>1</sub>	11.8557	12.4723	14.3427	14.5240
	S <sub>2</sub>	11.8535	12.0370	12.7976	12.8667

**Table S8.** Vertical (de)excitation  $S_2 \rightarrow S_0$  calculation of studied compounds at TDDFT/B3LYP/6-31G(d) theoretical level. Here,  $S_2$  emission corresponds to HOMO-1 to LUMO transition.

Compounds	Solvents	Wavelength (nm)	Energy (eV)	Oscillator strength	Experiment (nm)
<b>1</b>	Hexane ( $\epsilon=1.8819$ )	531	2.34	1.2676	
	Toluene ( $\epsilon=2.3741$ )	540	2.29	1.2701	
	THF ( $\epsilon=7.4257$ )	581	2.14	1.3723	503
	DCM ( $\epsilon=8.93$ )	585	2.12	1.3759	568
<b>2</b>	Hexane ( $\epsilon=1.8819$ )	465	2.67	0.6596	
	Toluene ( $\epsilon=2.3741$ )	470	2.64	0.6388	
	THF ( $\epsilon=7.4257$ )	490	2.53	0.5517	558
	DCM ( $\epsilon=8.93$ )	492	2.52	0.5422	560
<b>3</b>	Hexane ( $\epsilon=1.8819$ )	531	2.34	1.2450	461
	Toluene ( $\epsilon=2.3741$ )	541	2.29	1.2594	483
	THF ( $\epsilon=7.4257$ )	579	2.14	1.3306	542
	DCM ( $\epsilon=8.93$ )	583	2.13	1.3361	556



**Table S9.** Representation of  $S_2 \rightarrow S_0$  charge transfer (CT+LE) emission of **1** at TDDFT/B3LYP/6-31G(d) level.

Solvents	HOMO-1	LUMO
Hexane		
Toluene		
THF		
DCM		

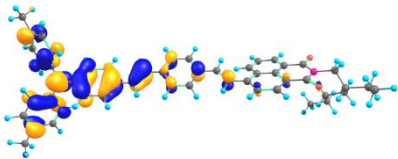
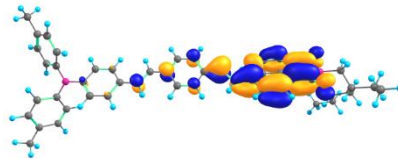
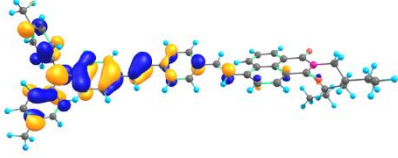
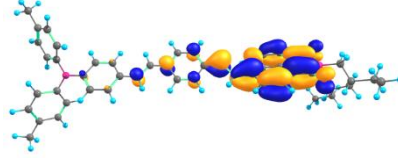
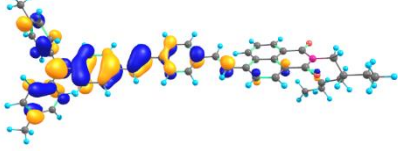
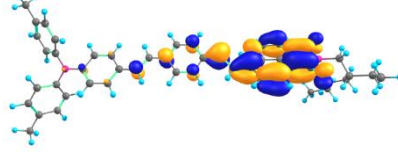
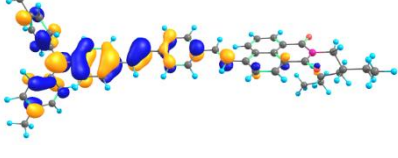
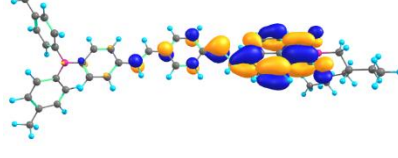
**Table S10.** Representation of  $S_2 \rightarrow S_0$  charge transfer (CT+LE) emission of **2** at TDDFT/B3LYP/6-31G(d) level.

Solvents	HOMO-1	LUMO
Hexane		
Toluene		
THF		
DCM		

**Table S11.** Computed vertical excitations of **3** in different solvent media within the PCM solvent model using the TDDFT/B3LYP/6-31G(d) theoretical level. Absorption wavelengths, energies and their corresponding oscillator strength values of each vertical excitations (S<sub>1</sub>-S<sub>5</sub>) in different solvents are listed and compared with the experimental results.

Solvents	Excitation states	Wavelength (nm)	Energy (eV)	Oscillator strength	Experiment (nm)
Hexane ( $\epsilon=1.8819$ )	S <sub>1</sub>	601	2.06	0.8181	434
	S <sub>2</sub>	448	2.77	1.3939	
	S <sub>3</sub>	433	2.86	0.1627	358
	S <sub>4</sub>	362	3.43	0.0941	306
	S <sub>5</sub>	343	3.62	0.2250	
Toluene ( $\epsilon=2.3741$ )	S <sub>1</sub>	606	2.05	0.8340	445
	S <sub>2</sub>	450	2.75	1.3652	
	S <sub>3</sub>	435	2.85	0.1942	376
	S <sub>4</sub>	363	3.42	0.0939	306
	S <sub>5</sub>	343	3.61	0.2364	
THF ( $\epsilon=7.4257$ )	S <sub>1</sub>	612	2.03	0.7977	443
	S <sub>2</sub>	453	2.74	1.2637	
	S <sub>3</sub>	435	2.85	0.3163	381
	S <sub>4</sub>	364	3.41	0.0954	306
	S <sub>5</sub>	344	3.61	0.2229	
DCM ( $\epsilon=8.93$ )	S <sub>1</sub>	613	2.02	0.8013	443
	S <sub>2</sub>	453	2.73	1.2521	
	S <sub>3</sub>	435	2.85	0.3290	381
	S <sub>4</sub>	364	3.41	0.0946	306
	S <sub>5</sub>	344	3.61	0.2252	

**Table S12.** Representation of  $S_1 \rightarrow S_0$  charge transfer (CT) emission of **3** at TDDFT/B3LYP/6-31G(d) level.

Solvents	HOMO	LUMO
Hexane		
Toluene		
THF		
DCM		

**Table S13.** Representation of  $S_2 \rightarrow S_0$  charge transfer (CT+LE) emission of **3** at TDDFT/B3LYP/6-31G(d) level.

Solvents	HOMO-1	LUMO
Hexane		
Toluene		
THF		
DCM		

## 6. NMR and HRMS spectra

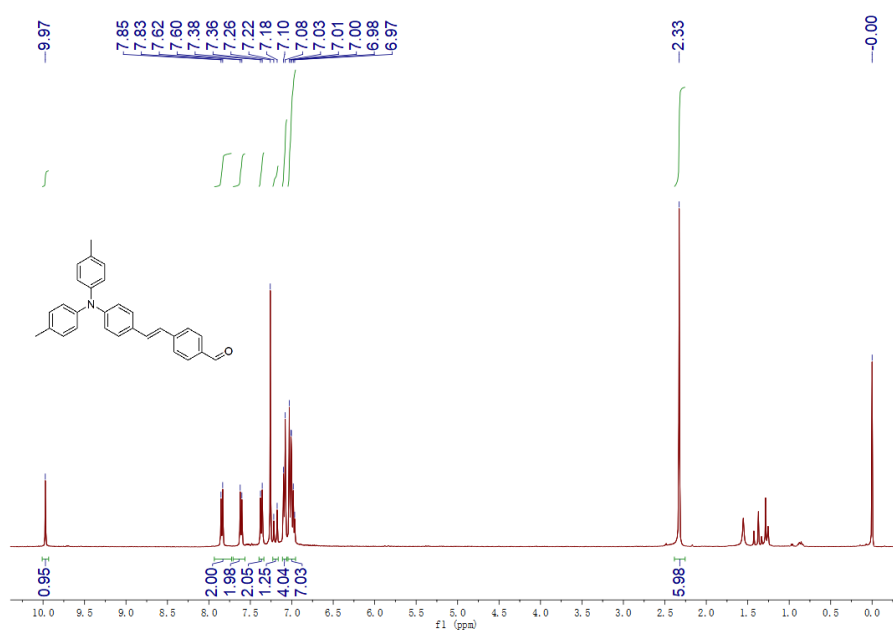


Figure S28.  $^1\text{H}$  NMR Spectrum of **1-1** in  $\text{CDCl}_3$ .

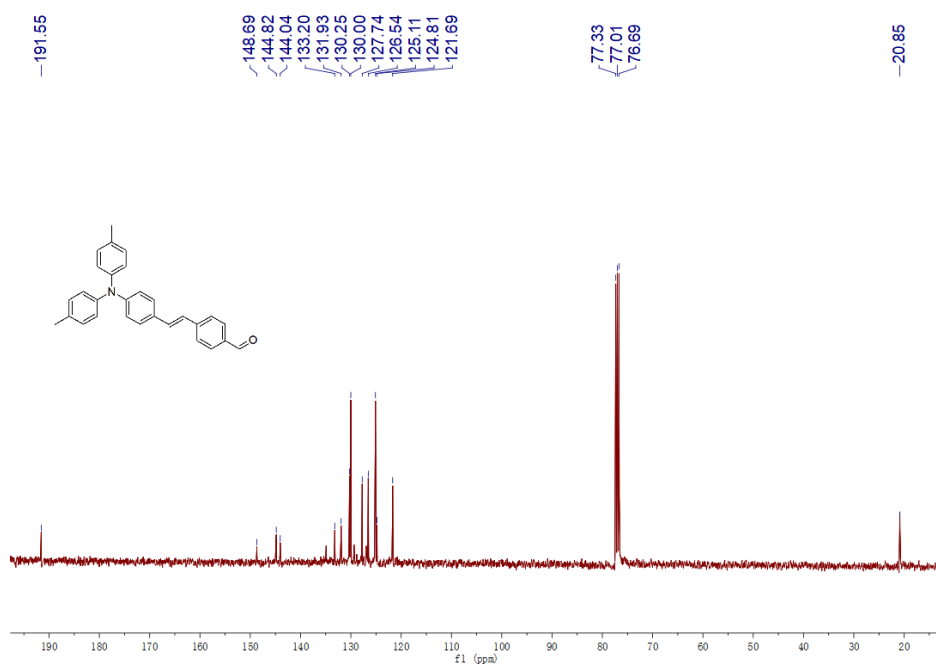


Figure S29.  $^{13}\text{C}$  NMR Spectrum of **1-1** in  $\text{CDCl}_3$ .

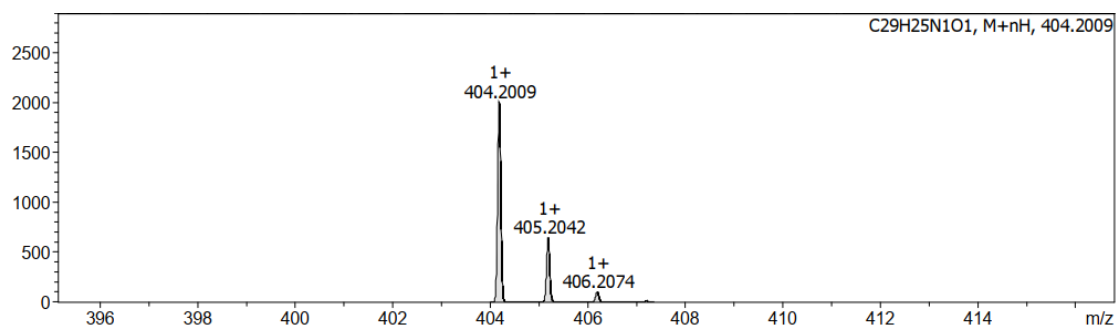


Figure S30. HRMS Spectrum of **1-1**.

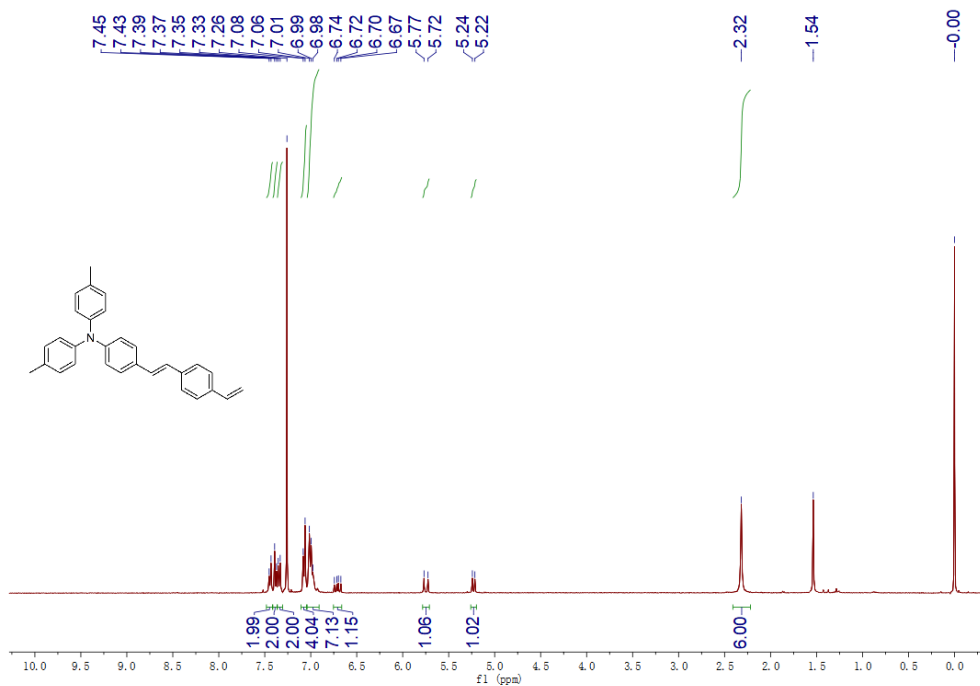


Figure S31.  $^1\text{H}$  NMR Spectrum of **1-2** in  $\text{CDCl}_3$ .

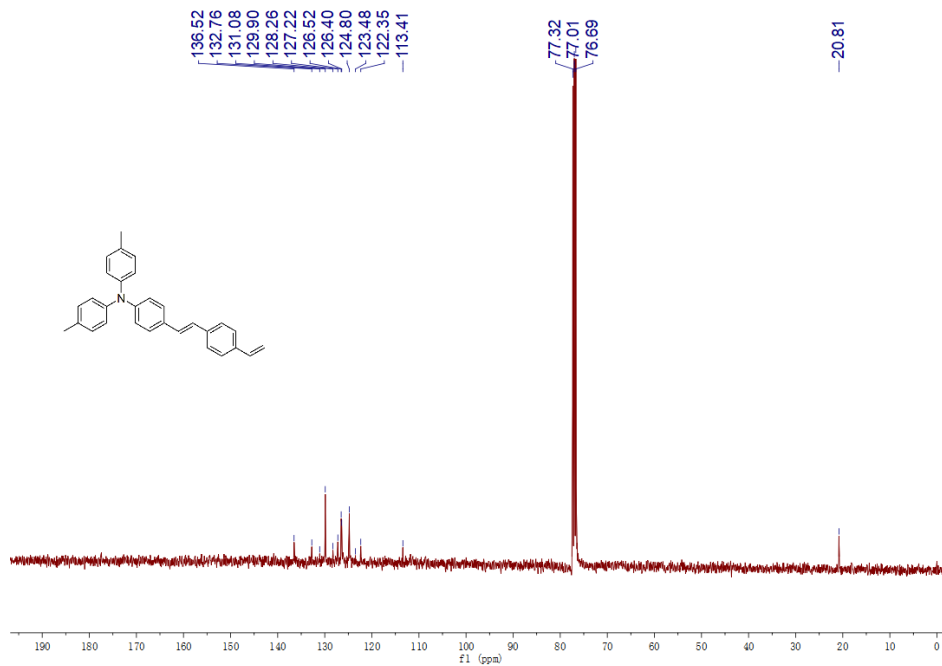


Figure S32.  $^{13}\text{C}$  NMR Spectrum of **1-2** in  $\text{CDCl}_3$ .

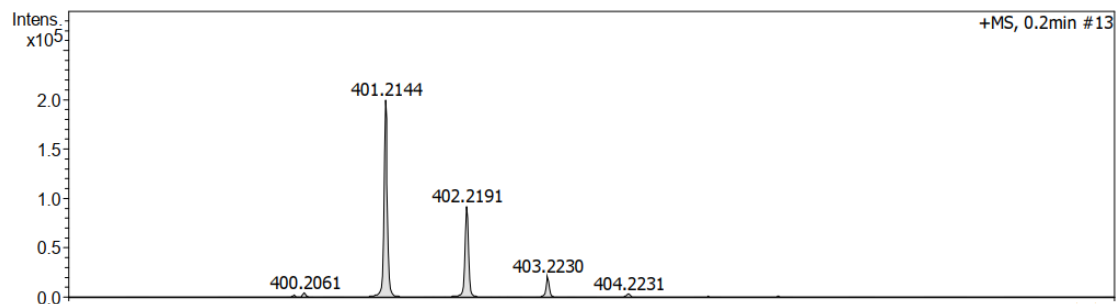


Figure S33. HRMS Spectrum of **1-2**.

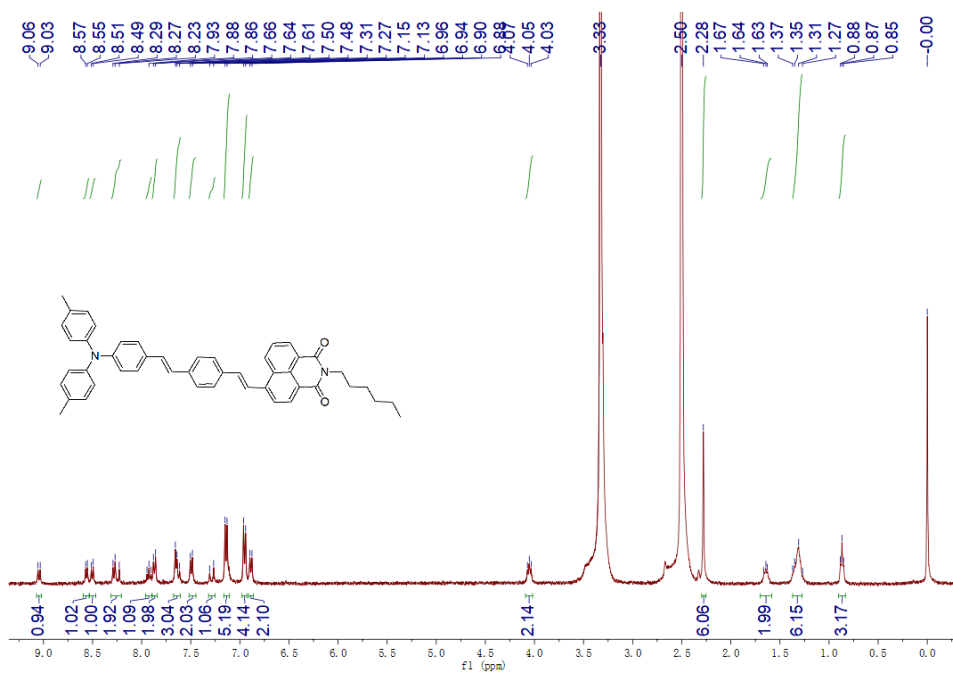


Figure S34.  $^1\text{H}$  NMR Spectrum of 1 in DMSO- $d_6$ .

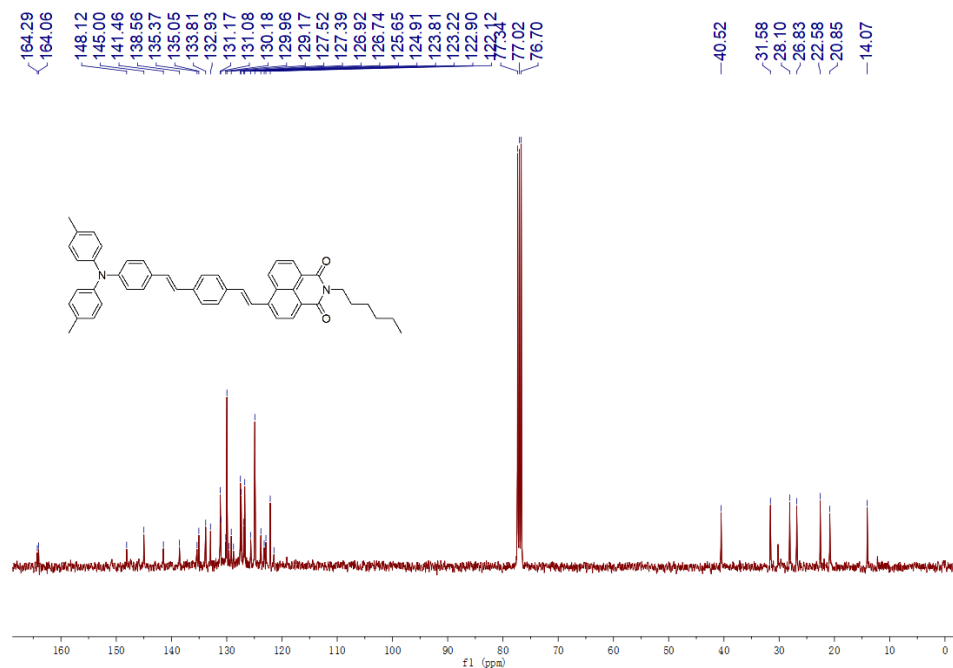


Figure S35.  $^{13}\text{C}$  NMR Spectrum of 1 in  $\text{CDCl}_3$ .

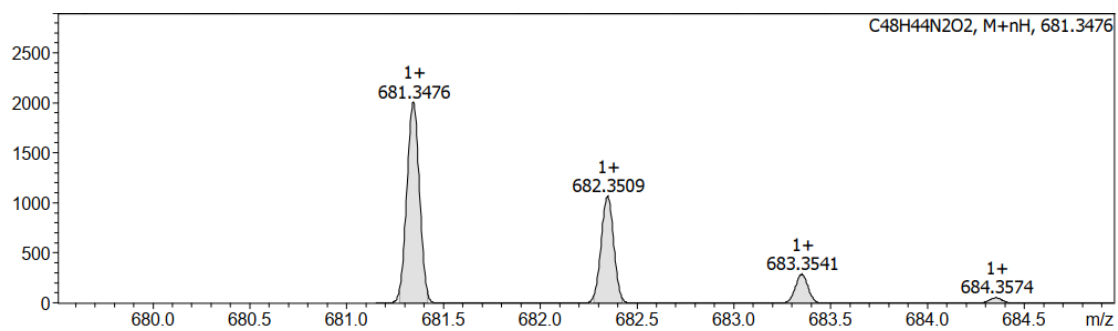


Figure S36. HRMS Spectrum of 1.

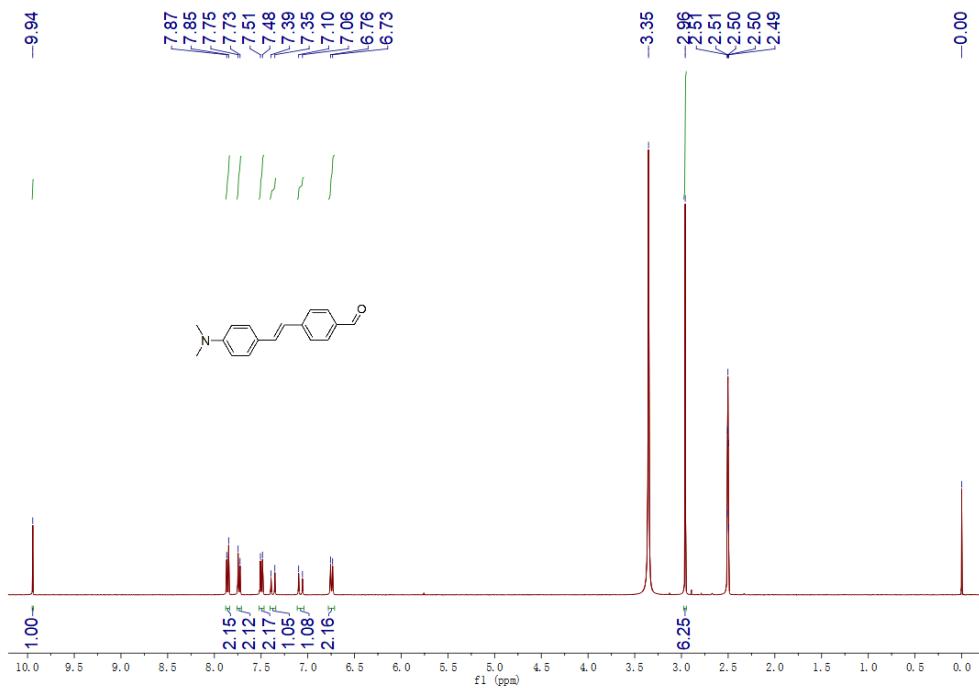


Figure S37. <sup>1</sup>H NMR Spectrum of 2-1 in DMSO-d<sub>6</sub>.

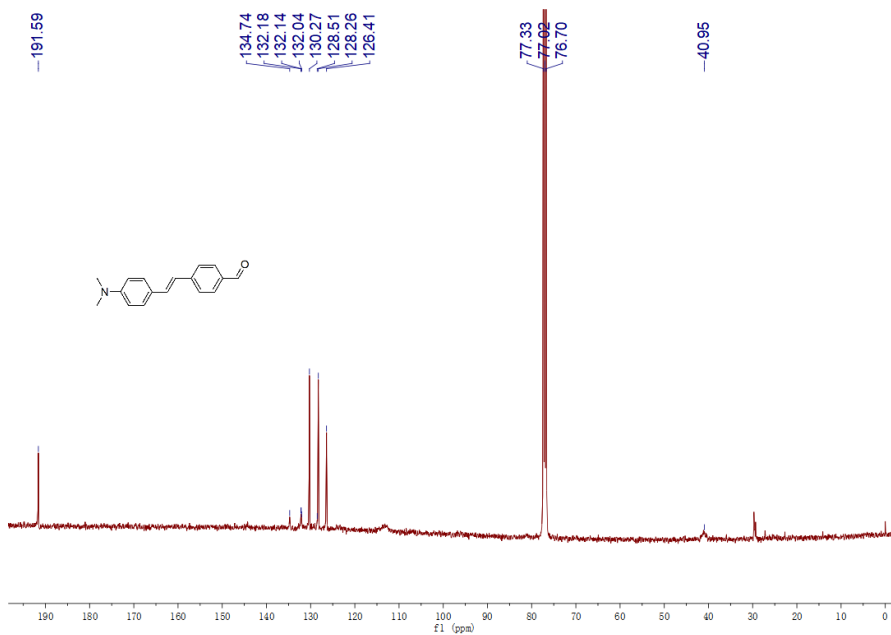


Figure S38. <sup>13</sup>C NMR Spectrum of 2-1 in CDCl<sub>3</sub>.

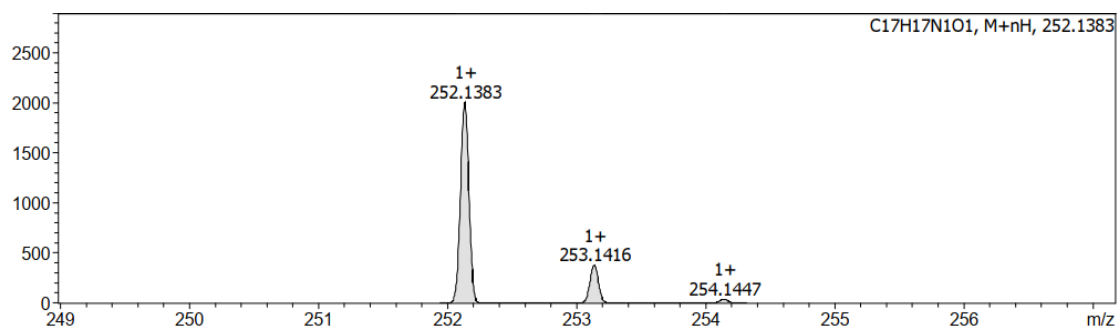


Figure S39. HRMS Spectrum of 2-1.



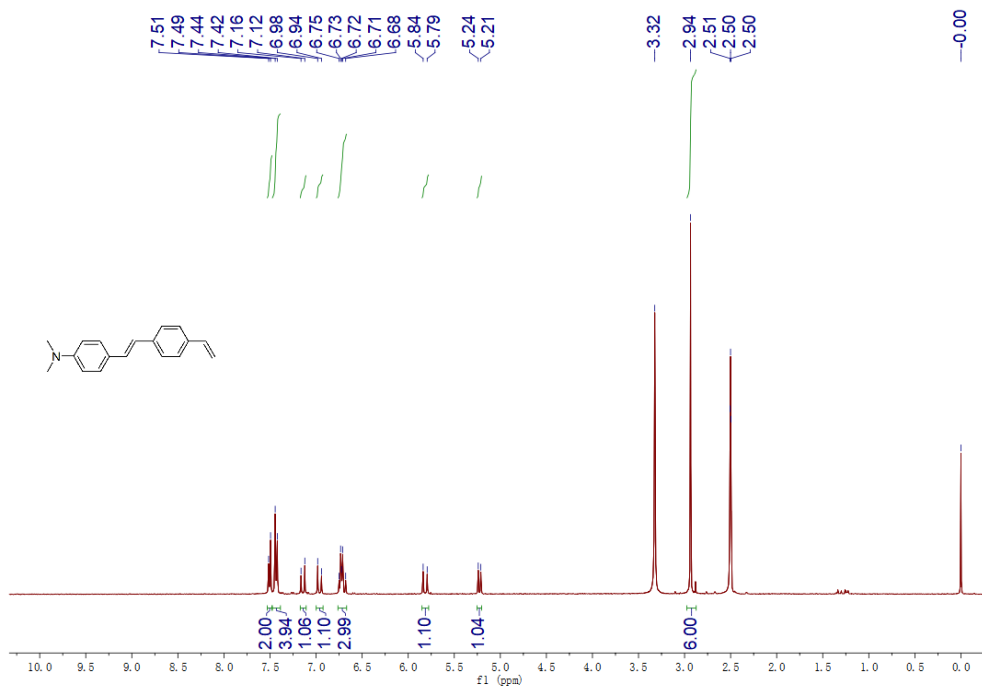


Figure S40.  $^1\text{H}$  NMR Spectrum of **2-2** in  $\text{DMSO-d}_6$ .

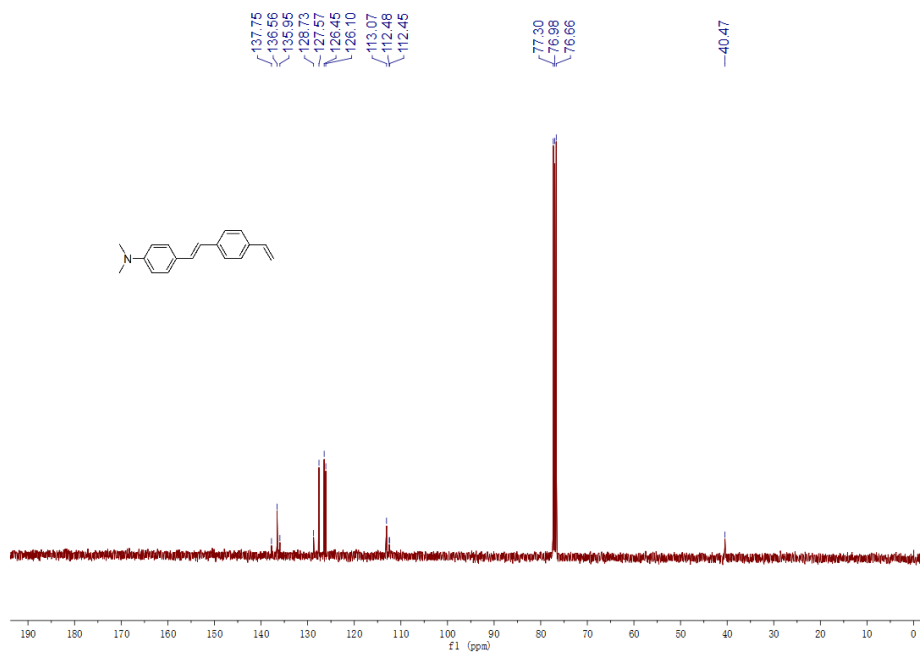


Figure S41.  $^{13}\text{C}$  NMR Spectrum of **2-2** in  $\text{CDCl}_3$ .

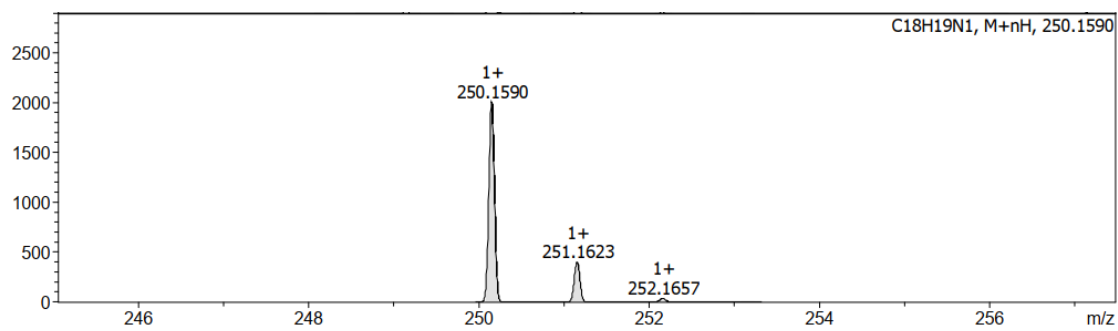


Figure S42. HRMS Spectrum of **2-2**.

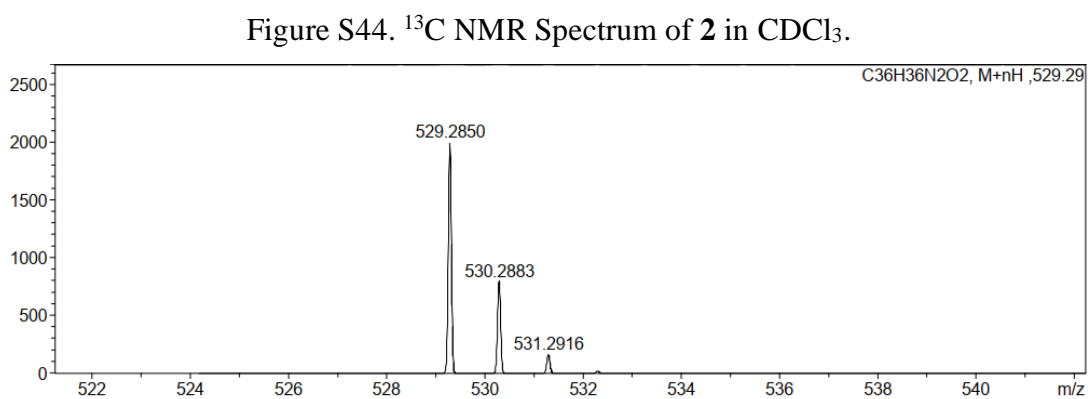
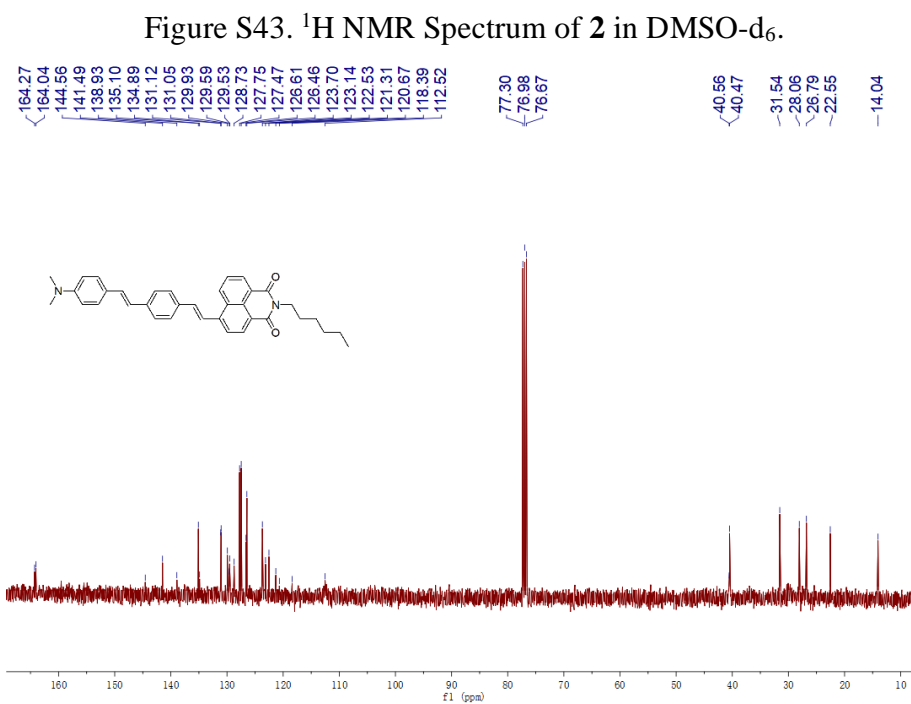
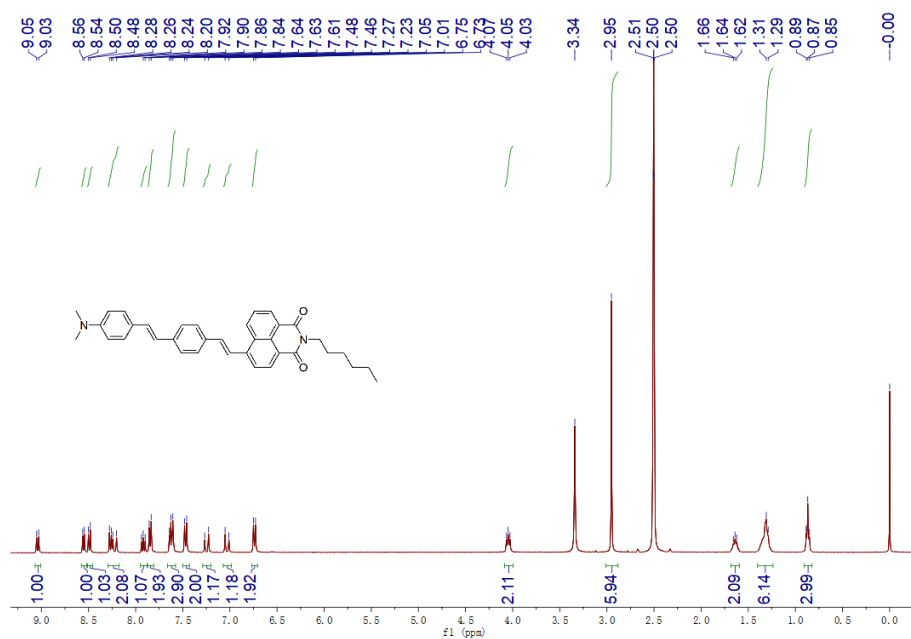


Figure S45. HRMS Spectrum of 2.

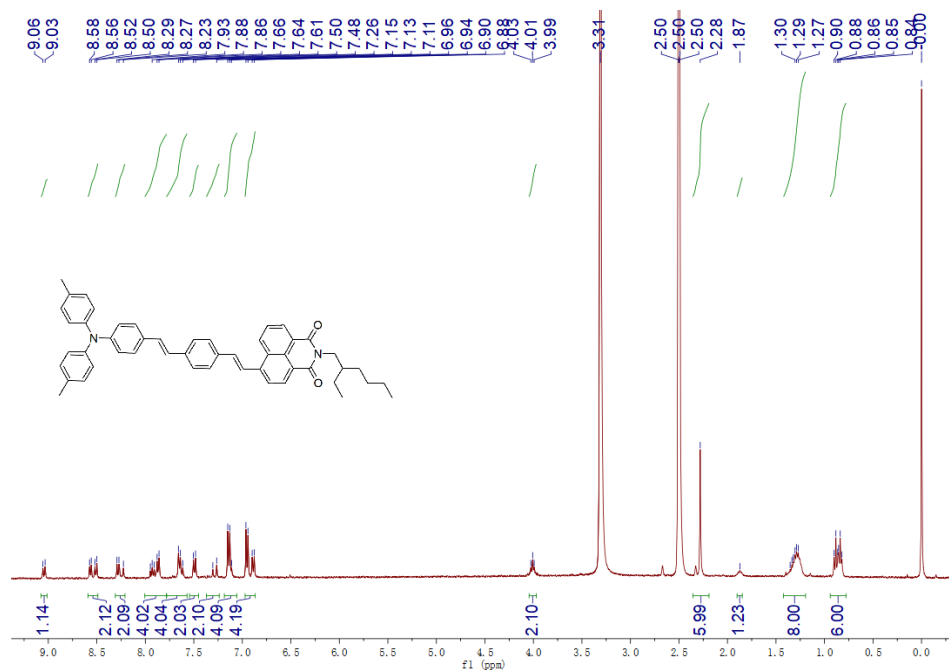


Figure S46. <sup>1</sup>H NMR Spectrum of **3** in DMSO-d<sub>6</sub>.

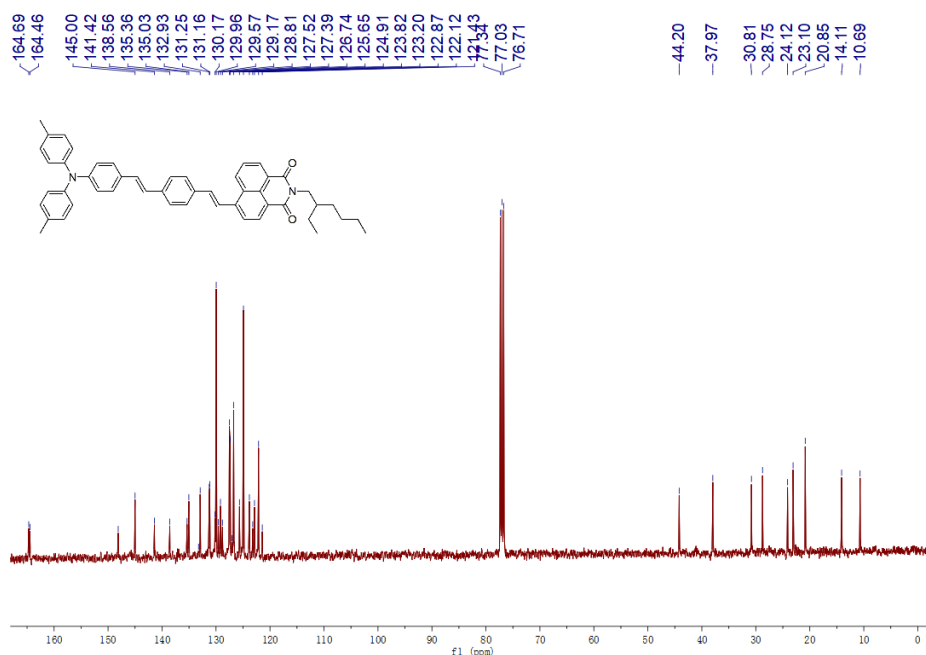


Figure S47. <sup>13</sup>C NMR Spectrum of **3** in CDCl<sub>3</sub>.

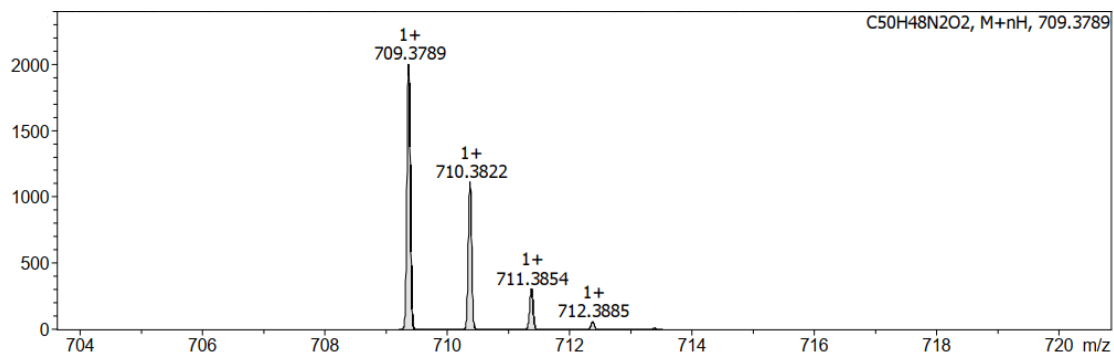


Figure S48. HRMS Spectrum of **3**.

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