Supporting Information for

Donor and Acceptor Engineering for BINOL based AIEgens with Enhanced Fluorescence Performance

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1. Experimental Section

1.1 General information

All chemicals and solvents were commercially available and were used without further purification. All commercially available reagents were used as received unless otherwise stated. $^1$H NMR, $^{13}$C NMR spectra were measured on a Agilent AV-400 NMR spectrometer. Proton Chemical shifts of NMR spectra were given in ppm relative to internals reference TMS (1H, 0.00 ppm). ESI-HRMS spectral data were recorded on a Finnigan LCQDECA mass spectrometer. Fluorescence emission spectra were obtained using Hitachi F-7000 spectrometer at 298 K. Absorption spectra were recorded on a Hitachi PharmaSpec UV-1900 UV-Visible Spectrophotometer. The absolute fluorescence quantum yield was measured using a Hamamatsu quantum yield spectrometer C11347 Quantaurus_QY. The fluorescence lifetime was measured using a Hamamatsu Compact Fluorescence Lifetime Spectrometer C11367. The particle size was measured using a MAL-DLS Zetasizer Nano-ZS90. Single crystals were grown from isopropanol/dichloroethane via solute solution diffusion method. Single crystal X-ray diffraction intensity data of 2b were collected on Agilent Technologies (Gemini), and the data of 1c were collected on Broker D8 venture with METAUET D2 X-ray source 153K, and the data of 2c were collected Bruker apex II DUO with microfocus Mo X-ray Source 153K. The ground-state geometries were optimized using the density function theory (DFT) method with B3LYP hybrid functional at the basis set level of 6-31G (d,p). All the calculations were performed using Gaussian 09 package. MTS method was used for testing the cell viability and described in the experimental section. HepG 2 cells were obtained from Shanghai Institute of Biochemistry and Cell Bioc emistry and Cell Biology, Chinese Academy of Science. Confocal lasing scanning microscopic (CLSM) images of single-photo were obtained using LSM 780 (Zeiss). Unless otherwise noted, materials were obtained from commercial suppliers and were used without further purification. All the solvents were dried according to the standard methods prior to use. All of the solvents were either HPLC or spectroscopic grade in the optical spectroscopic studies.
1.2 Reaction procedures

Synthesis of BIN-5, BIN-COM and BIN-COP

The synthesis methods of BIN-COM and BIN-COP can be found in our previous work. The synthesis methods of BIN-5 can be found in reference. All of them have been characterized by NMR and HRMS which are same as reference.

**Scheme S1. Synthesis of BIN-6**

Synthesis of BIN-6

Added 20 mL dioxane and 10 mL K$_2$CO$_3$ (2 M) in a flask. After solution was purged with argon, **BIN-5** (499.9 mg, 1 mmol), 4-methoxyphenylboronic acid (456 mg, 3 mmol), Pd (PPh$_3$)$_4$ (227 mg, 0.2 mmol), and PPh$_3$ (104.8 mg, 0.4 mmol) were added. The gas phase mutually was displaced for 3 times. Then the mixture was heated at 80°C for about 8 h. After cooling down to room temperature, filter the solid residue, collect the filtrate, added an equal volume of water, part the organic phase. The combined organic extracts were washed with brine and dried over Na$_2$SO$_4$. After removal of the solvent, the residue was purified by column chromatography on silica gel eluted with hexane/ethyl acetate (5:1). **BIN-6** was obtained as orange solids in 86% yield. H NMR (400 MHz, CDCl$_3$): δ (TMS, ppm) 10.62 (s, 2H), 10.22 (s, 2H), 8.40 (s, 2H), 8.14 (d, $J = 1.6$ Hz, 2H), 7.67 (dd, $J = 8.9, 1.9$ Hz, 2H), 7.60 (d, $J = 8.8$ Hz, 4H), 7.30 (d, $J = 8.8$ Hz, 2H), 7.02 (d, $J = 8.8$ Hz, 4H), 3.87 (s, 6H).
Scheme S2. Synthesis of 1c and 2c

**Synthesis of 1c**

After compound **BIN-6** (555 mg, 1 mmol) and ethyl acetoacetate (286.3 mg, 2.2 mmol) were added in toluene (10 mL), two drops piperidine were dropped to the stirred solution. Then the mixture was heated at reflux for about 4 h. After cooling down to room temperature, filter the solid residue, and the solid was washed with EtOH (5 mL× 3). The product was purified by recrystallized with methanol. 1c was obtained as yellow solid in 77.4% yield. $^1$H NMR (400 MHz, CDCl$_3$) δ (TMS, ppm) 8.77 (s, 2H), 8.47 (s, 2H), 8.23 (s, 2H), 7.69 (d, $J = 7.8$ Hz, 2H), 7.63 (d, $J = 8.8$ Hz, 4H), 7.28 (s, 2H), 7.04 (d, $J = 7.9$ Hz, 4H), 3.89 (s, 6H), 2.70 (s, 6H). $^{13}$C NMR (101 MHz, CDCl$_3$) δ(TMS, ppm) 195.4, 159.6, 158.8, 148.5, 147.6, 138.7, 134.1, 132.9, 132.1, 130.8, 129.8, 128.3, 126.1, 126.0, 125.1, 118.6, 116.3, 114.5, 55.4, 30.6.

**Synthesis of 2c**

The synthesis steps are the same as 1c. 2c was obtained as orange-red solid in 52% yield. $^1$H NMR (400 MHz, CDCl$_3$) δ (TMS, ppm) 8.33 (d, $J = 18.2$ Hz, 4H), 8.19 (s, 2H), 7.96 (d, $J = 7.6$ Hz, 4H), 7.69 (d, $J = 9.3$ Hz, 2H), 7.62 (d, $J = 7.6$ Hz, 6H), 7.48 (t, $J = 7.4$ Hz, 4H), 7.30 (d, $J = 8.9$ Hz, 2H), 7.02 (d, $J = 8.4$ Hz, 4H), 3.86 (s, 6H). $^{13}$C NMR (101 MHz, CDCl$_3$) δ (TMS, ppm) 191.6, 159.6, 158.1, 148.4, 145.4, 138.7, 136.1, 133.9, 133.8, 132.2, 131.4, 130.9, 129.8, 129.5, 128.6, 128.3, 127.6, 126.1, 125.9, 118.5, 116.7, 114.4, 55.3.
Synthesis of \(1\mathbf{b}\), \(1\mathbf{d}\), \(2\mathbf{b}\) and \(2\mathbf{d}\).

**Synthesis of \(1\mathbf{b}\)**

BIN-COM (230 mg, 0.4 mmol) and malononitrile (158.4 mg, 2.4 mmol) was added in a round-bottomed flask. Add as little dichloroethane as possible to dissolve it. Then \(\text{NH}_4\text{AcO}\) (186 mg, 2.4 mmol) and AcOH (0.3 mL) was added. The mixture was heated at reflux for about 0.5 h. After cooling down to room temperature, added 20 mL DCM and 20 mL water, part the organic phase. The combined organic extracts were washed with brine and dried over \(\text{Na}_2\text{SO}_4\). After removal of the solvent, the residue was purified by column chromatography on silica gel. Elution with DCM. \(1\mathbf{b}\) was obtained as yellow solid in 87% yield. \(^1\text{H}\) NMR (400 MHz, \(\text{d}_6\)-DMSO) \(\delta\) (TMS, ppm) 8.81 (d, \(J = 5.2\) Hz, 4H), 8.35 (d, \(J = 8.3\) Hz, 2H), 7.67 (t, \(J = 7.6\) Hz, 2H), 7.56 (t, \(J = 7.2\) Hz, 2H), 7.20 (d, \(J = 8.5\) Hz, 2H), 2.59 (s, 6H). \(^{13}\text{C}\) NMR (101 MHz, \(\text{d}_6\)-DMSO) \(\delta\) (TMS, ppm) 176.8, 161.7, 152.7, 150.5, 139.3, 137.4, 135.4, 135.2, 135.0, 131.7, 130.3, 129.5, 123.0, 120.8 117.5, 117.4, 92.6, 28.2.

**Synthesis of \(1\mathbf{d}\)**

The synthesis steps of \(1\mathbf{d}\) were the same as \(1\mathbf{b}\). \(1\mathbf{d}\) was obtained as a red solid in 73% yield. \(^1\text{H}\) NMR (400 MHz, \(\text{CDCl}_3\)) \(\delta\) (TMS, ppm) 8.42 (s, 2H), 8.23 (s, 4H), 7.74 (dd, \(J = 8.9, 1.8\) Hz, 2H), 7.63 (d, \(J = 8.8\) Hz, 4H), 7.30 (d, \(J = 8.9\) Hz, 2H), 7.04 (d, \(J = 8.8\) Hz, 4H), 3.87 (s, 6H), 2.66 (s, 6H). \(^{13}\text{C}\) NMR (101 MHz, \(\text{CDCl}_3\)) \(\delta\) (TMS, ppm) 171.5, 159.7, 157.0, 147.7, 144.5, 139.2, 133.9, 131.9, 130.9, 130.2, 128.4, 126.2, 126.1, 124.5, 117.6, 116.6, 114.5, 111.7, 111.5, 88.6, 55.4, 22.8.

**Synthesis of \(2\mathbf{b}\)**
The synthesis steps of 2b were the same as 1b. 2b was obtained as an orange solid in 85% yield. $^1$H NMR (400 MHz, CDCl$_3$) δ (TMS, ppm) 8.37 (s, 2H), 8.21 (s, 2H), 8.09 (d, $J$ = 8.6 Hz, 2H), 7.62 (dd, $J$ = 4.8, 3.8 Hz, 4H), 7.60 – 7.54 (m, 4H), 7.50 (d, $J$ = 7.9 Hz, 6H), 7.27 (s, 1H), 7.25 (s, 1H). $^{13}$C NMR (101 MHz, CDCl$_3$) δ (TMS, ppm) 168.0, 156.8, 148.1, 147.1, 135.2, 134.0, 133.1, 132.2, 130.6, 129.6, 129.3, 129.3, 126.8, 125.7, 124.55 117.5, 116.7, 115.2, 112.9, 112.8, 85.6.

Synthesis of 2d

The synthesis steps of 2d were the same as 1b. 2d was obtained as red solid in 68% yield. $^1$H NMR (400 MHz, CDCl$_3$) δ (TMS, ppm) 8.39 (s, 2H), 8.21 (d, $J$ = 6.5 Hz, 4H), 7.75 (dd, $J$ = 8.9, 1.9 Hz, 2H), 7.65 – 7.62 (m, 8H), 7.57 (d, $J$ = 7.5 Hz, 2H), 7.50 (t, $J$ = 7.5 Hz, 4H), 7.35 (d, $J$ = 8.9 Hz, 2H), 7.05 – 7.02 (m, 4H), 3.87 (s, 6H). $^{13}$C NMR (101 MHz, CDCl$_3$) δ (TMS, ppm) 168.1, 159.7, 156.9, 147.9, 147.0, 139.2, 134.1, 134.0, 133.1, 132.1, 132.0, 130.8, 130.4, 129.3, 128.4, 126.2, 126.1, 124.5, 117.8, 114.5, 112.8, 112.8, 85.6, 55.4.

Scheme S4. Synthesis of 1a and 2a.

Synthesis of 1a

BIN-COM (230 mg, 0.4 mmol) and malononitrile (52.8 mg, 0.8 mmol) was added in a round-bottomed flask. Add as little dichloroethane as possible to dissolve it. Then NH$_4$AcO (62 mg, 0.8 mmol) and AcOH (0.1 mL) was added. The mixture was heated at reflux for about 0.5 h. After cooling down to room temperature, added 20 mL DCM and 20 mL water, part the organic phase. The combined organic extracts were washed with brine and dried over Na$_2$SO$_4$. After removal of the solvent, the residue was purified by column chromatography on silica gel. Elution with DCM. 1a was obtained as orange-red solid in 41% yield and 1b was obtained as yellow solid in 35% yield. $^1$H NMR (400 MHz, CDCl$_3$) of 1a. δ (TMS, ppm) 8.74 (s, 1H), 8.41 (d, $J$ = 16.9 Hz, 2H), 8.22 (s, 1H), 8.10 (d, $J$ = 8.2 Hz, 2H), 7.57 (dd, $J$ = 13.4, 6.7 Hz, 2H), 7.44 (dt, $J$ = 16.1, 7.4 Hz, 2H), 7.18 (d, $J$ = 7.6 Hz, 2H), 2.67 (s, 3H), 2.65 (s, 3H). $^{13}$C NMR (101 MHz, CDCl$_3$) δ (TMS, ppm) 195.2, 171.6, 158.8, 157.0, 148.6, 147.8, 147.6, 144.4, 135.2, 133.1, 131.9, 130.4, 130.3, 130.3, 129.6, 129.5, 126.7, 126.4, 125.6, 125.5, 125.1, 124.4, 121.3, 118.1, 117.3, 117.1, 115.9, 111.7, 111.5, 88.5, 30.6, 22.8.
Synthesis of 2a

The synthesis steps of 2a were the same as 1a. 2a was obtained as orange solid in 39% yield and 2b was obtained as orange solid in 36% yield. $^1$H NMR (400 MHz, CDCl$_3$) of 2a. $\delta$(TMS, ppm) 8.38 (s, 1H), 8.34 (s, 1H), 8.27 (s, 1H), 8.22 (s, 1H), 8.11 – 8.05 (m, 2H), 7.95 – 7.91 (m, 2H), 7.66 – 7.45 (m, 12H), 7.25 – 7.21 (m, 2H). $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ (TMS, ppm) 191.4, 168.1, 158.0, 156.9, 148.4, 148.1, 147.1, 145.3, 136.0, 135.4, 134.8, 134.0, 133.9, 133.1, 132.1, 131.5, 130.4, 130.4, 130.3, 130.0, 129.8, 129.6, 129.3, 129.3, 128.6, 127.5, 126.7, 126.4, 125.6, 125.6, 124.5, 118.0, 117.6, 117.2, 116.3, 112.9, 112.8, 85.8.

1.3 Cell culture and imaging

HepG 2 cells were cultured in Dulbecco’s modified Eagle medium (DMEM) containing 10% fetal bovine serum and 1% Antibiotic-antimycotic at 37°C in a 5% CO$_2$/95% air incubator. For fluorescence imaging, cells ($4 \times 10^3$/well) were passed on a 6-well plate and incubated for 24 h. For fluorescence imaging, cells ($4 \times 10^3$/well) were passed on a 6-well plate and incubated for 24 h. Before the staining experiment, cells were washed twice with physiological saline, incubated with 5 μM probe and 2 μl oleic acid for different times at 37°C. Then washed 3-6 times with physiological saline. The confocal fluorescent images were captured with an excitation light at 405 nm. For co-localization experiment, cells were incubated with 5 μM probe and 2μl oleic acid for 6h, then washed 3-6 times with physiological saline, then incubated with 1μm BODIPY 493/503 for 15 min. The excitation light of BODIPY 493/503 is 488 nm.

1.4 Cytotoxicity study

Toxicity toward HepG 2 cells was determined by MTS (3-(4, 5-dimethylthiazol-2-yl)-5-(3-carboxymethoxyphenyl)-2-(4-sulfophenyl)-2H-tetrazolium reduction assay following literature procedures. About 10000 cells per well were seeded in 96-well plates and cultured overnight for 70-80% cell confluence. The medium was replaced with 100 μL of fresh medium with different concentration of probes, to which 100 μL complexes at 200 μL. 24 hours later, 100 μL of 20% MTS solution in PBS was replaced with the old medium in each well for additional 0.5h incubation. The metabolic activity of the probes treated cells was expressed as a relative to untreated cell controls taken as 100% metabolic activity.
2. Views of the molecular stacking structures in single crystals

**Figure S1.** Views of crystal packing mode of 1c, 2b and 2c. Carbon, hydrogen, oxygen and nitrogen atoms are shown in gray, green, red and blue, respectively. The single-crestal data can be found on CCDC, the deposition number of 2b, 1c and 2c are 1907970, 1907963 and 1907968, respectively.
Table S1. The dihedral angle and the distance data of 1c, 2b, and 2c.

| Compounds | $\phi_{P-D}$ | $\phi_{P-A}$ | $\phi_{P,P}$ | $d_{D-D}$ | $d_{A,A}$ | $d_{A-P}$ | $d_{P,P}$ | $d_{P-P}$ |
|-----------|--------------|--------------|--------------|-----------|-----------|-----------|-----------|-----------|
| 1c        | 17.62        | 34.63        | 65.52        | 4.847     | 4.755     | -         | 3.851     | 3.944     |
|           |              |              |              | 4.207     |           | 4.013     | 4.156     |
| 2b        | -            | 67.32        | 102.04       | -         | -         | 4.207     | -         | -         |
| 2c        | 33.10        | 78.80        | 109.96       | 4.884     | 9.844     | -         | 4.013     | 4.156     |

a The dihedral angle of purine core and donor group ($\phi_{P-D}$) or acceptor group ($\phi_{P,A}$).
b The distance of adjacent molecule’s purine core (P), donor group (D), and acceptor group (A).
c The vertical distance of adjacent molecule’s purine core (P).

3. Crystallographic data of 1c, 2b, and 2c

Crystal data and structure refinements of 1c:

Deposition number of CCDC: 1907963

| Identification code | 1c |
|---------------------|----|
| Chemical formula    | $C_{44}H_{30}O_8$ |
| Formula weight      | 686.68 g/mol |
| Temperature         | 296(2) K |
| Wavelength          | 0.71073 Å |
| Crystal size        | 0.200 x 0.200 x 0.200 mm |
| Crystal system      | monoclinic |
| Space group         | C 1 2 1 |
| Unit cell dimensions| $a = 25.64(2)$ Å $\alpha = 90^\circ$ |
|                     | $b = 23.425(18)$ Å $\beta = 125.282(13)^\circ$ |
|                     | $c = 18.464(15)$ Å $\gamma = 90^\circ$ |
| Volume              | 9053.(12) Å³ |
| $Z$                 | 8 |

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Density (calculated) 1.008 g/cm³
Absorption coefficient 0.069 mm⁻¹
F(000) 2864
Theta range for data collection 1.42 to 25.23°
Reflections collected 8290
Independent reflections 8290 [R(int) = 0.0797]
Coverage of independent reflections 98.7%
Absorption correction Multi-Scan
Max. and min. transmission 0.9860 and 0.9860
Structure solution technique direct methods
Structure solution program SHELXT 2014/5 (Sheldrick, 2014)
Refinement method Full-matrix least-squares on F²
Refinement program SHELXL-2018/3 (Sheldrick, 2018)
Function minimized Σ w(F_o² - F_c²)²
Data / restraints / parameters 8290 / 718 / 945
Goodness-of-fit on F² 1.050
Δ/σ_max 0.025
Final R indices 5060data; I>2σ(I) R₁ = 0.0928, wR₂ = 0.2271
all data R₁ = 0.1310, wR₂ = 0.2419
Weighting scheme w = 1/[σ²(F_o²)+(0.0800P)²+35.0000P]
where P = (F_o²+2F_c²)/3
Absolute structure parameter -0.6(19)
Largest diff. peak and hole 0.338 and -0.305 eÅ⁻³
R.M.S. deviation from mean 0.068 eÅ⁻³
**Crystal data and structure refinements of 2b:**

Deposition number of CCDC: 1907970

| Property                          | Value                                      |
|-----------------------------------|--------------------------------------------|
| Identification code               | 2b                                         |
| Chemical formula                  | C_{46}H_{22}N_{4}O_{4}                      |
| Formula weight                    | 694.67 g/mol                               |
| Temperature                       | 291.16(10) K                               |
| Crystal system                    | orthorhombic                               |
| Space group                       | P2_{1}2_{1}2_{1}                           |
| Unit cell dimensions              | a = 9.6696(3) Å, b = 13.5192(3) Å, c = 30.1865(8) Å, α = 90°, β = 90°, γ = 90° |
| Volume                            | 3946.13(17) Å^{3}                         |
| Z                                 | 4                                          |
| Density (calculated)              | 1.169 g/cm^{3}                             |
| Absorption coefficient            | 0.614 mm^{-1}                              |
| F(000)                            | 1432.0                                     |
| Crystal size/mm^{3}               | 0.7 × 0.4 × 0.2                            |
| Radiation                         | CuKα (λ = 1.54184)                         |
| Theta range for data collection   | 8.782 to 145.394°                         |
| Reflections collected             | 8290                                       |
| Independent reflections           | 7042 [R_{int} = 0.0276, R_{sigma} = 0.0355] |
| Data/restraints/parameters        | 7042/84/527                                |
| Goodness-of-fit on F^{2}          | 1.039                                      |
| Final R indexes [I>=2σ (I)]       | R_{1} = 0.0553, wR_{2} = 0.1545            |
| Final R indexes [all data] | $R_1 = 0.0594$, $wR_2 = 0.1603$ |
|---------------------------|----------------------------------|
| Largest diff. peak/hole / $e$ Å$^3$ | 0.38/-0.32 |
| Flack parameter | 0.87(14) |

**Crystal data and structure refinements of 2c:**

Deposition number of CCDC: 1907968

| Identification code | 2c |
|---------------------|----|
| Chemical formula    | $C_{54}H_{34}O_8$ |
| Formula weight      | 810.81 g/mol |
| Temperature         | 193(2) K |
| Wavelength          | 1.34139 Å |
| Crystal size        | 0.100 x 0.100 x 0.100 mm |
| Crystal system      | monoclinic |
| Space group         | $P 1 21 1$ |
| Unit cell dimensions| $a = 18.690(4)$ Å, $\alpha = 90^\circ$  $b = 23.158(6)$ Å, $\beta = 98.343(12)^\circ$  $c = 21.551(5)$ Å, $\gamma = 90^\circ$ |
| Volume              | 9229.(4) Å$^3$ |
| $Z$                 | 8 |
| Density (calculated) | 0.403 mm$^{-1}$ |
| Absorption coefficient | 0.069 mm$^{-1}$ |
| $F(000)$            | 3376 |
| Theta range for data collection | 1.80 to 51.60° |
| **Index ranges**    | -21$\leq$ $h$$\leq$ 18, -26$\leq$ $k$$\leq$ 25, -25$\leq$ $l$$\leq$ 24 |
| Reflections collected | 46510 |
|                     | s12 |
| Parameter                                      | Value                                           |
|-----------------------------------------------|-------------------------------------------------|
| Independent reflections                      | 25262 [R(int) = 0.1185]                         |
| Coverage of independent reflections          | 96.5%                                           |
| Absorption correction                        | Multi-Scan                                      |
| Max. and min. transmission                   | 0.9610 and 0.9610                               |
| Structure solution technique                 | direct methods                                  |
| Structure solution program                   | SHELXT 2014/5 (Sheldrick, 2014)                 |
| Refinement method                            | Full-matrix least-squares on F^2                |
| Refinement program                           | SHELXL-2018/3 (Sheldrick, 2018)                 |
| Function minimized                           | Σ w(F_o^2 - F_c^2)^2                            |
| Data / restraints / parameters               | 25262 / 1705 / 2096                            |
| Goodness-of-fit on F^2                       | 0.967                                           |
| Δ/σ_{max}                                    | 0.012                                           |
| Final R indices                              | 8764 data; I>2σ(I)                             |
|                                               | R_1 = 0.0928, wR_2 = 0.2271                    |
|                                               | all data                                       |
|                                               | R_1 = 0.1310, wR_2 = 0.2419                    |
| Weighting scheme                             | w=1/[(σ^2(F_o^2) + (0.0800P)^2 + 10.0000P)]    |
|                                               | where P = (F_o^2 + 2F_c^2)/3                    |
| Absolute structure parameter                 | -0.1(6)                                        |
| **Extinction coefficient**                   | 0.0012(1)                                      |
| Largest diff. peak and hole                  | 0.270 and -0.257 eÅ\(^{-3}\)                   |
| R.M.S. deviation from mean                   | 0.056 eÅ\(^{-3}\)                             |
4. Molar Extinction Coefficient of all compounds

**A**

![Graph A](image)

**B**

![Graph B](image)

**C**

![Graph C](image)

**D**

![Graph D](image)

**E**

![Graph E](image)

**F**

![Graph F](image)

**G**

![Graph G](image)

**H**

![Graph H](image)
Figure S2. UV spectra and absorption-concentration curve of fluorophores 1a-2d at different concentrations (0.5, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10 μM) in DMSO. 1a: (A) and (B); 1b: (C) and (D); 1c: (E) and (F); 1d: (G) and (H); 2a: (I) and (J); 2b: (K) and (L); 2c: (M) and (N); 2d: (O) and (P).
Figure S3. UV spectra and absorption-concentration curve of fluorophores 1a-2d at different concentrations (0.5, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10 μM) in water. 1a: (A) and (B); 1b: (C) and (D); 1c: (E) and (F); 1d: (G) and (H); 2a: (I) and (J); 2b: (K) and (L); 2c: (M) and (N); 2d: (O) and (P).
Table S2. Summary of all the compounds’ molar extinction coefficient

| Compounds | DMSO | Water |
|-----------|------|-------|
|           | $\lambda_{\text{Abs}}$ (nm) | $\varepsilon$ (M$^{-1}$ cm$^{-1}$) | $\lambda_{\text{Abs}}$ (nm) | $\varepsilon$ (M$^{-1}$ cm$^{-1}$) |
| 1a        | 340  | $5.24 \times 10^4$ | 346 | $4.84 \times 10^4$ |
| 1b        | 346  | $4.21 \times 10^4$ | 350 | $3.21 \times 10^4$ |
| 1c        | 349  | $3.29 \times 10^4$ | 339 | $1.53 \times 10^4$ |
| 1d        | 379  | $1.35 \times 10^4$ | 347 | $1.50 \times 10^4$ |
| 2a        | 354  | $6.20 \times 10^4$ | 337 | $2.31 \times 10^4$ |
| 2b        | 354  | $6.22 \times 10^4$ | 346 | $4.90 \times 10^4$ |
| 2c        | 340  | $4.80 \times 10^4$ | 340 | $3.13 \times 10^4$ |
| 2d        | 353  | $5.14 \times 10^4$ | 357 | $3.92 \times 10^4$ |

5. Solvent effect of all compounds
Figure S4. Normalized absorption and fluorescence spectra of fluorophores in different solvents (Toluene, H$_2$O, MeCN, DMSO).
Figure S5. Fluorescence emission spectra of 1a-2d in different solvents (Toluene, H₂O, MeCN, DMSO). Concentration: 5 μM.

Table S3. Optical transitions of all the compounds in different solvents, Δλ = λₑm-λₐbs.

|      | toluene | water  | acetonitrile | DMSO   |
|------|---------|--------|--------------|--------|
|      | λₐbs   | λₑm   | Δλ           | λₐbs   | λₑm   | Δλ | λₐbs | λₑm   | Δλ | λₐbs | λₑm   | Δλ |
| 1a   | 345     | 523   | 178          | 346    | 544   | 198 | 340   | 555   | 215 | 340   | 562   | 222 |
| 1b   | 349     | 524   | 175          | 339    | 546   | 211 | 340   | 558   | 218 | 349   | 574   | 225 |
| 1c   | 349     | 532   | 183          | 350    | 588   | 238 | 339   | 593   | 254 | 346   | 605   | 259 |
6. Fluorescence spectra of all compounds in DMSO/PBS mixtures
Figure S6. Fluorescence spectra of all the compounds in DMSO/H₂O mixtures and dependence of the I/I₀ ratios of all the compounds on the solvent composition of the DMSO/H₂O mixture. 1a: (A) and (B), Ex = 353 nm; 1b: (C) and (D) Ex = 366 nm; 1c: (E) and (F) Ex = 370 nm; 2a: (G) and (H) Ex = 350 nm; 2b: (I) and (J) Ex = 372 nm; 2c: (K) and (L) Ex = 350 nm; 2d: (M) and (N) Ex = 372 nm, concentration: 5 μM. Insert: photographs of each compound in DMSO/H₂O mixtures with fᵢ values of 0 and 90% under irradiation with 365 nm UV light.
7. Particle size of all compounds in aggregation state

**Figure S7.** Particle size distribution of compounds 1a-1d: 1-4; 2a-2d: 5-8 in DMSO/H₂O mixture with an fₚ value of 99%. Concentration: 10 μM
8. Wavelength of solid fluorescence and their CIE diagram

Table S4. Coordinates of compounds 1a-1d and 2a-2d on CIE diagram.

| Compound | \( \lambda_{em} \) (nm) | Coordinate (X) | Coordinate (Y) |
|----------|------------------------|----------------|----------------|
| 1a       | 534                    | 0.352          | 0.5753         |
| 1b       | 538                    | 0.3536         | 0.563          |
| 1c       | 570                    | 0.4753         | 0.5168         |
| 1d       | 601                    | 0.5298         | 0.4621         |
| 2a       | 538                    | 0.3676         | 0.5808         |
| 2b       | 541                    | 0.3619         | 0.581          |
| 2c       | 560                    | 0.4304         | 0.538          |
| 2d       | 609                    | 0.5743         | 0.4236         |

9. Fluorescent lifetime and quantum yield of all compounds in solution, aggregation and solid state

Table S5. Fluorescent lifetime of all compounds in DMSO, water and solid state.

| Compd | Lifetime in solution (s) | Lifetime in aggregation (s) | Lifetime in solid state (s) |
|--------|--------------------------|------------------------------|----------------------------|
| 1a     | \( \tau_1=2.69 \times 10^{-9} \) (17%) | \( \tau_1=1.23 \times 10^{-9} \) (83%) | \( \tau_1=5.35 \times 10^{-9} \) (10%) |
|        | \( \tau_2=7.15 \times 10^{-10} \) (82%) | \( \tau_2=4.61 \times 10^{-9} \) (17%) | \( \tau_2=1.58 \times 10^{-7} \) (1%) |
|        | \( \tau_3=1.16 \times 10^{-8} \) (1%) | \( \tau_3=1.81 \times 10^{-9} \) | \( \tau_3=9.52 \times 10^{-10} \) (89%) |
|        | \( \tau_{avg}=1.18 \times 10^{-9} \) | | \( \tau_{avg}=1.66 \times 10^{-9} \) |
| 1b     | \( \tau_1=7.61 \times 10^{-10} \) (98%) | \( \tau_1=1.34 \times 10^{-9} \) (82%) | \( \tau_1=5.33 \times 10^{-9} \) (3%) |
|        | \( \tau_2=5.57 \times 10^{-9} \) (2%) | \( \tau_2=4.72 \times 10^{-9} \) (18%) | \( \tau_2=8.04 \times 10^{-10} \) (97%) |
|        | \( \tau_{avg}=8.52 \times 10^{-10} \) | | \( \tau_{avg}=1.10 \times 10^{-9} \) |
| 1c     | \( \tau_1=4.78 \times 10^{-10} \) (99%) | \( \tau_1=1.14 \times 10^{-9} \) (81%) | \( \tau_1=8.62 \times 10^{-9} \) (40%) |
|        | \( \tau_2=5.95 \times 10^{-9} \) (1%) | \( \tau_2=4.78 \times 10^{-9} \) (19%) | \( \tau_2=1.90 \times 10^{-7} \) (1%) |
|        | \( \tau_{avg}=5.19 \times 10^{-10} \) | \( \tau_{avg}=1.83 \times 10^{-9} \) | \( \tau_{avg}=1.76 \times 10^{-9} \) (59%) |
|        | | | \( \tau_{avg}=5.21 \times 10^{-9} \) |
## Table S6. Quantum yield of all compounds in DMSO, water and solid state.

| Compd. | Quantum yield in solution (%) | Quantum yield in aggregation (%) | Quantum yield in solid state (%) |
|--------|-------------------------------|---------------------------------|---------------------------------|
| 1a     | ~0.1                          | 0.58                            | 3.1                             |
| 1b     | ~0.1                          | 3.23                            | 2.55                            |
| 1c     | 0                             | 0.3                             | 2.93                            |
| 1d     | 0                             | ~0.1                            | 0.16                            |
| 2a     | ~0.1                          | 3.58                            | 4.43                            |
| 2b     | ~0.1                          | 5.41                            | 6.3                             |
| 2c     | 0                             | 3.46                            | 6.3                             |
| 2d     | 0                             | ~0.1                            | 0.15                            |
Table S7. The rate constants for radiative ($k_r$) and non-radiative decay ($k_{nr}$) were calculated from the $\Phi$ and $\tau$ values according to the formulae $k_r = \Phi / \tau$ and $k_{nr} = (1-\Phi) / \tau$.

| Compound | Solution $K_r$ (s$^{-1}$) | Solution $K_{nr}$ (s$^{-1}$) | Aggregation $K_r$ (s$^{-1}$) | Aggregation $K_{nr}$ (s$^{-1}$) | Solid state $K_r$ (s$^{-1}$) | Solid state $K_{nr}$ (s$^{-1}$) |
|----------|---------------------------|-----------------------------|-----------------------------|-----------------------------|---------------------------|-----------------------------|
| 1a       | 8.47 x 10$^5$             | 8.47 x 10$^8$               | 3.20 x 10$^6$               | 5.49 x 10$^8$               | 4.78 x 10$^7$             | 8.14 x 10$^8$               |
| 1b       | 1.17 x 10$^6$             | 1.17 x 10$^9$               | 1.65 x 10$^7$               | 4.94 x 10$^8$               | 2.32 x 10$^7$             | 8.86 x 10$^8$               |
| 1c       | 0                         | 1.93 x 10$^9$               | 1.64 x 10$^6$               | 5.45 x 10$^8$               | 5.62 x 10$^6$             | 1.86 x 10$^8$               |
| 1d       | 0                         | 2.00 x 10$^9$               | 1.03 x 10$^6$               | 1.03 x 10$^9$               | 1.04 x 10$^6$             | 6.48 x 10$^8$               |
| 2a       | 1.16 x 10$^6$             | 1.15 x 10$^9$               | 1.61 x 10$^7$               | 4.32 x 10$^8$               | 0.00E+00                  | 3.55 x 10$^8$               |
| 2b       | 1.44 x 10$^6$             | 1.44 x 10$^9$               | 1.47 x 10$^7$               | 2.58 x 10$^8$               | 2.53 x 10$^7$             | 3.76 x 10$^8$               |
| 2c       | 0                         | 1.39 x 10$^9$               | 1.12 x 10$^7$               | 3.11 x 10$^8$               | 2.50 x 10$^7$             | 3.72 x 10$^8$               |
| 2d       | 0                         | 1.04 x 10$^9$               | 7.63 x 10$^5$               | 7.63 x 10$^8$               | 8.45 x 10$^5$             | 7.03 x 10$^8$               |
Figure S8. Emission decay of compounds 1a-1d: 1-4; 2a-2d: 5-8 in DMSO, H₂O, and solid.

10. Particle size and fluorescence study of oleic acid, 2b and OA-2b in PBS

Figure S9. (A) Particle size distribution of oleic acid (OA), 2b and OA-2b in PBS, concentration: 10 μM; (B) Fluorescence spectra of 2b and OA-2b in PBS, Ex = 372 nm. concentration: 5 μM.
11. Single-photo CLSM images of HepG 2 incubated with OA-2b

**Figure S10.** Live HepG 2 cells incubated with OA-2b for different times and the process of expanding LDs: (P-T) enlarged LDs imaging of inset (the area of ellipse red line).

**Figure S11.** Live HepG 2 cells incubated with OA-2b for 0.5 h, 3 h and 5 h.
12. Cytotoxicity of 2b in HepG 2 cells evaluated by MTS assay

![Bar chart showing cell viability (%) for different concentrations of compound 2b (1.25, 2.5, 5, 10, 20 μM) for 24 h.]

**Figure S12.** Cell viabilities of HepG 2 cells after incubation with different concentrations of compound 2b (1.25, 2.5, 5, 10, 20 μM) for 24 h.

13. NMR Data

![NMR spectra of Compound BIN-6 in CDCl₃]

**Figure S13.** $^1$H NMR of Compound BIN-6 in CDCl₃
Figure S1. $^1$H NMR of Compound 1a in CDCl₃

Figure S14. $^1$H NMR of Compound 1a in CDCl₃

Figure S15. $^{13}$C NMR of Compound 1a in CDCl₃
Figure S16. $^1$H NMR of Compound 1b in d$_6$-DMSO

Figure S17. $^{13}$C NMR of Compound 1b in d$_6$-DMSO
Figure S18. $^1$H NMR of Compound 1c in CDCl$_3$

Figure S19. $^{13}$C NMR of Compound 1c in CDCl$_3$
Figure S20. $^1$H NMR of Compound 1d in CDCl$_3$

Figure S21. $^{13}$C NMR of Compound 1d in CDCl$_3$
Figure S22. $^1$H NMR of Compound 2a in CDCl$_3$

Figure S23. $^{13}$C NMR of Compound 2a in CDCl$_3$
Figure S24. $^1$H NMR of Compound 2b in CDCl$_3$

Figure S25. $^{13}$C NMR of Compound 2b in CDCl$_3$
Figure S26. $^1$H NMR of Compound 2c in CDCl$_3$

Figure S27. $^{13}$C NMR of Compound 2c in CDCl$_3$
Figure S28. $^1$H NMR of Compound 2d in CDCl$_3$

Figure S29. $^{13}$C NMR of Compound 2d in CDCl$_3$
14. ESI-MS Data
Figure S30. MS spectra of 1a-1d and 2a-2d.

15. References

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