Supporting Information

Anti-Solvatochromic and Highly Emissive Twisted D-A structure with Intramolecular Hydrogen Bond

Hong-Wen Liang,§ Tian Jia,§ Zhen-Zhen Wang,§ Jia-Qi Wang, Da-Yong Hou, Lei Wang, Xingfa Gao,* He-Lue Sun* and Hao Wang*

§ These authors contributed equally to this work.

Table of Contents

General method

Materials: All reactions dealing with air- and moisture-sensitive compounds were carried out in dry reaction vessels under a nitrogen atmosphere. The starting material 3-methylene-2-(quinolin-8-yl) isoindolin-1-one and corresponding compounds were prepared by the procedures described in the literatures. Unless otherwise noted, materials were purchased from commercial suppliers and were used as received. Anhydrous solvents were distilled over CaH_2 and stored under Ar. EJ cells were purchased from the cell culture center of the Institute of Basic Medical Sciences, Chinese Academy of Medical Science (Beijing, China). MTT and LysoTracker Red are purchased from Beyotime institute of Biotechnology.

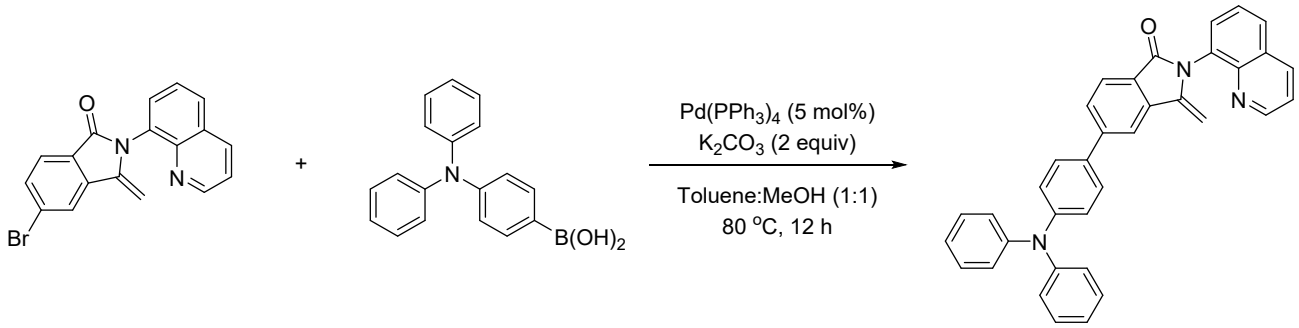
Instruments and Characterizations: ^1H and ^{13}C nuclear magnetic resonance (NMR) spectra were recorded on Bruker AVIII 400 MHz NMR spectrometer. ^1H and ^{13}C NMR spectra are reported in parts per million (ppm) downfield from an internal standard, tetramethylsilane (0 ppm) and $CHCl_3$ (77.0 ppm), respectively. ESI high-resolution mass spectra (HRMS) were recorded on a Waters SYNPAT G2. Melting points were determined using a capillary melting point apparatus and are uncorrected. Absorption spectra were recorded on SHIMADZU UV-2600 (1 cm quartz cell), and fluorescence spectra were recorded by HORIBA Fluoromax 4 and Varian Cary Eclipse. Fluorescence lifetimes and absolute quantum yield were measured on HORIBA Fluoromax 4 and Varian Cary Eclipse at room temperature. Powder X-Ray diffraction patterns were performed on an X'Pert PRO MPD diffractometer with Cu Kα radiation (λ = 1.5418 Å) at 25 °C (scan range: 3-40°). Transmission electron microscopy (TEM) micrographs were collected on a FEI Tecnai G2 F30 TEM. Photographs were taken with a digital camera (NIKON Coolpix 4500 Microsystem, 4.0 megapixels). The detail information of NMR spectra, absorption spectra, emission spectra, time-resolved fluorescence curves and TEM images are given in the Supporting Information. Fluorescence lifetimes and absolute quantum yield were measured on HORIBA Fluoromax 4 at room temperature and all data were expressed as mean ± standard deviation of the indicated number of parallel experiments. Statistical comparisons were made using Student's t-test. Differences with p-values < 0.05 were considered statistically significant.

Cell culture and Confocal images: EJ cells were seeded and grown in DMEM supplemented by 10% Fetal Bovine Serum (FBS) and 1% penicillin-streptomycin (PS) under ambient conditions of 5% CO_2 and humidity at 37 ^oC. At 80 % confluence, these cells were trypsinized and about 2 × 105 cells were added to each well of 96-well culture plate. After 12 h of growth, the medium was replaced and the cells were incubated with the prepared nanoparticles at different concentrations in culture medium under 37 ^oC for 6 h. After washing off the excess nanoparticles, and staining lysosomes with Lyso-Tracker Red, the cells were viewed under confocal microscope (Zeiss LSM710 CLSM) at the excitation of 405 and 550 nm.

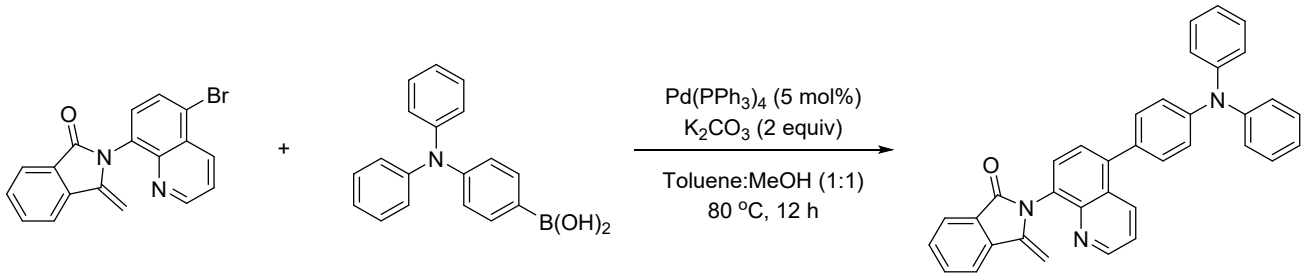
MTT assay for cytotoxicity evaluation: The cytotoxicity assay was performed by MTT assay against EJ cells. The EJ cells in 96-well plates were incubated with a series of concentrations of nanoparticles 1/F127 for 24 h. Then, 10 μL of MTT solutions (0.5 mg/mL) were added and further reacted for 4 h. The concentration of proliferating cells in each well was determined using a microplate reader at test wavelength 570 nm. Relative cell viability was obtained by the following equation:

$$\text{Cell viability (\%)} = (A_{samples}-A_0) / (A_{control}-A_0) \times 100\%$$

Synthesis



Scheme S1. Synthetic routes to 5-(4-(diphenylamino)phenyl)-3-methylene-2-(quinolin-8-yl)isoindolin-1-one (**1**).[1]

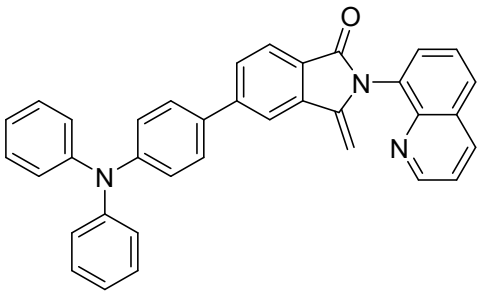


Scheme S2. Synthetic routes to 2-(5-(4-(diphenylamino)phenyl)quinolin-8-yl)-3-methyleneisoindolin-1-one (**2**). [1]

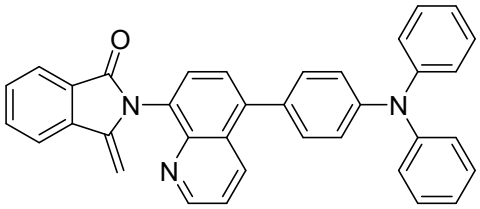
Synthesis of compound **1** and **2**

To a solution of 5-bromo-3-methylene-2-(quinolin-8-yl) isoindolin-1-one (5 mmol, 1 equiv), tetrakis (triphenylphosphine) palladium (0.25 mmol, 0.05 equiv), potassium carbonate (10 mmol, 2 equiv) and (4-(diphenylamino) phenyl) boronic acid (6 mmol, 1.2 equiv) under nitrogen. And, the Schlenk tube was quickly evacuated and refilled with nitrogen for three times, followed by addition of 1:1 mixture of MeOH/Toluene (50 mL). The Schlenk tube was sealed with a Teflon screwcap and the reaction mixture was stirred at 80 °C for 12 h. Upon cooling to room temperature, the reaction mixture was diluted with 10 mL of ethyl acetate, filtered through a pad of silica gel, followed by washing the pad of the silica gel with ethyl acetate (20 mL). Subsequently, the filtrate was concentrated under reduced pressure. The residue was purified by flash chromatography on silica gel using hexane/ethyl acetate mixture (1:1, v/v) as eluent to afford the 2.21 g (86%) of 5-(4-(diphenylamino) phenyl)-3-methylene-2-(quinolin-8-yl) isoindolin-1-one (1) as a yellow solid.

To a solution of 2-(5-bromoquinolin-8-yl)-3-methyleneisoindolin-1-one (5 mmol, 1 equiv), tetrakis (triphenylphosphine) palladium (0.25 mmol, 0.05 equiv), potassium carbonate (10 mmol, 2 equiv) and (4-(diphenylamino) phenyl) boronic acid (6 mmol, 1.2 equiv) under nitrogen. And, the Schlenk tube was quickly evacuated and refilled with nitrogen for three times, followed by addition of 1:1 mixture of MeOH/Toluene (50 mL). The Schlenk tube was sealed with a Teflon screwcap and the reaction mixture was stirred at 80 °C for 12 h. Upon cooling to room temperature, the reaction mixture was diluted with 10 mL of ethyl acetate, filtered through a pad of silica gel, followed by washing the pad of the silica gel with ethyl acetate (20 mL). Subsequently, the filtrate was concentrated under reduced pressure. The residue was purified by flash chromatography on silica gel using hexane/ethyl acetate mixture (1:1, v/v) as eluent to afford the 1.85 mg (72%) of 2-(5-(4-(diphenylamino) phenyl) quinolin-8-yl)-3-methyleneisoindolin-1-one (2) as a yellow solid.



5-(4-(diphenylamino)phenyl)-3-methylene-2-(quinolin-8-yl)isoindolin-1-one (**1**): Yellow solid; (86% yield, eluent = petroleum ether/EtOAc (3:1)); Mp = 201 - 202 °C; **^{1}H NMR** (400MHz, $CDCl_3$): δ 8.92 (d, *J* = 2.7 Hz, 1H), 8.24 (d, *J* = 8.0 Hz, 1H), 7.99 (dd, *J* = 21.5, 7.6 Hz, 3H), 7.79 (t, *J* = 9.0 Hz, 2H), 7.69 (t, *J* = 7.7 Hz, 1H), 7.56 (d, *J* = 8.3 Hz, 2H), 7.44 (dd, *J* = 8.0, 4.0 Hz, 1H), 7.31 (t, *J* = 7.6 Hz, 4H), 7.18 (d, *J* = 7.4 Hz, 6H), 7.08 (t, J = 7.2 Hz, 2H), 5.24 (s, 1H), 4.44 (s, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 166.31, 150.04, 146.99, 146.37, 143.98, 143.68, 143.09, 136.36, 135.26, 132.82, 131.59, 129.87, 128.46, 128.31, 128.25, 127.23, 127.09, 126.68, 125.23, 123.64, 123.01, 122.37, 122.24, 120.73, 117.26, 89.07; **HRMS** (ESI): Calculated for $C_{36}H_{25}N_3O$ $[M + H]^+$ 516.2067, found 516.2062.



2-(5-(4-(diphenylamino)phenyl)quinolin-8-yl)-3-methyleneisoindolin-1-one (**2**): Yellow solid; (72% yield, eluent = petroleum ether/EtOAc (4:1)); Mp = 210 - 211 °C; **^{1}H NMR** (400MHz, $CDCl_3$): δ 8.90 (d, *J* = 2.7 Hz, 1H), 8.43 (d, *J* = 8.5 Hz, 1H), 8.00 (d, *J* = 7.5 Hz, 1H), 7.81 (t, *J* = 7.0 Hz, 2H), 7.70 – 7.63 (m, 2H), 7.59 (t, *J* = 7.4 Hz, 1H), 7.40 – 7.29 (m, 7H), 7.22 (d, *J* = 6.8 Hz, 6H), 7.09 (t, J = 7.2 Hz, 2H), 5.23 (d, *J* = 1.7 Hz, 1H), 4.52 (d, *J* = 1.6 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 166.18, 149.38, 146.40, 146.11, 143.56, 142.71, 140.34, 135.38, 133.57, 130.88, 130.76, 130.06, 129.41, 128.96, 128.20, 128.12, 128.03, 126.57, 125.39, 123.45, 122.35, 121.98, 121.46, 120.15, 118.93, 88.94; **HRMS** (ESI): Calculated for $C_{36}H_{25}N_3O$ $[M + H]^+$ 516.2067, found 516.2065.

Characterization

The maximum absorption and emission wavelength of compound **2** is 365 nm and 440 nm in toluene, respectively. They also exhibit similar absorption bands in different solvents, range from 440 to 530 nm (Fig. S1). Their emission band starts to redshifts with the increase of the solvent polarity and Fig. S2 shows bright emission in different solvents under the 365 nm light and color changes from sky-blue to orange-yellow. Moreover, compound **2** exhibits high emission efficiency up to 82.9 ± 0.1% in toluene, lower than compound **1**. Similar to compound **1**, compound **2** presents high quantum yield in different solvents that exhibits the remarkable anti-solvatochromic effect (82.9 ± 0.1% in toluene, 79.9 ± 0.1% in THF, 77.8 ± 0.1% in DCM, 75.8 ± 0.2% in DMF, 74.6 ± 0.1% in DMSO). The fluorescence lifetime (FLT) exhibits solvatochromic effect with the increase of the solvent polarity (2.2 ns in toluene, 4.4 ns in THF, 6.5 ns in DCM, 7.9 ns in DMF, 9.5 ns in DMSO) (Fig. S3).

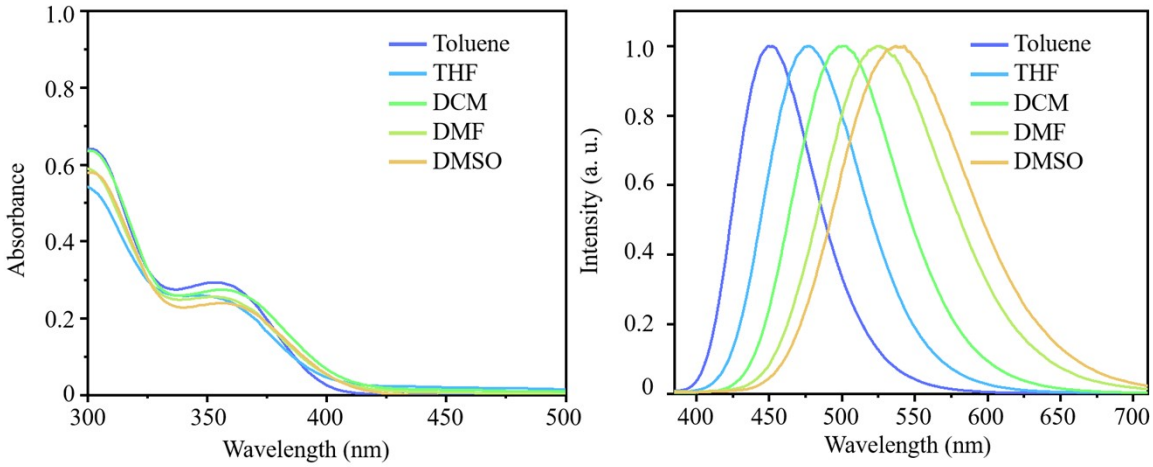


Fig. S1. The UV-vis absorbance (left) and fluorescence emission (right) spectra of compound **2** in different solvents. λ_{ex} = 365 nm. (Concentration: 10 μM)

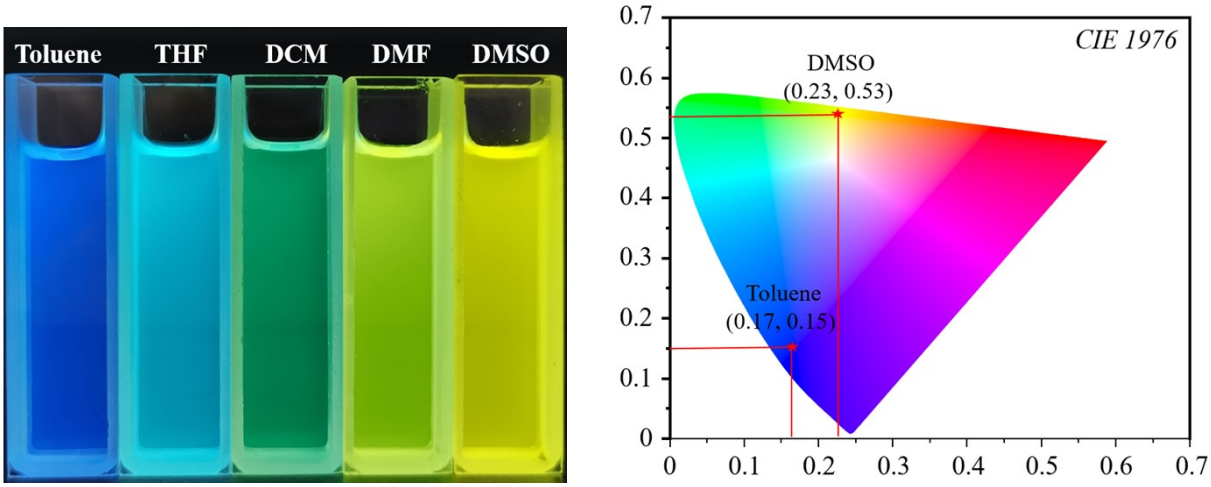


Fig. S2. Photographs of compound **2** in different solvents under 365 nm UV light (Left). CIE 1976 chromaticity diagram shows the luminescent color coordinates for compound **2** in toluene (0.17, 0.15) and DMSO (0.23, 0.53) (Right). (Concentration: 10 μM)

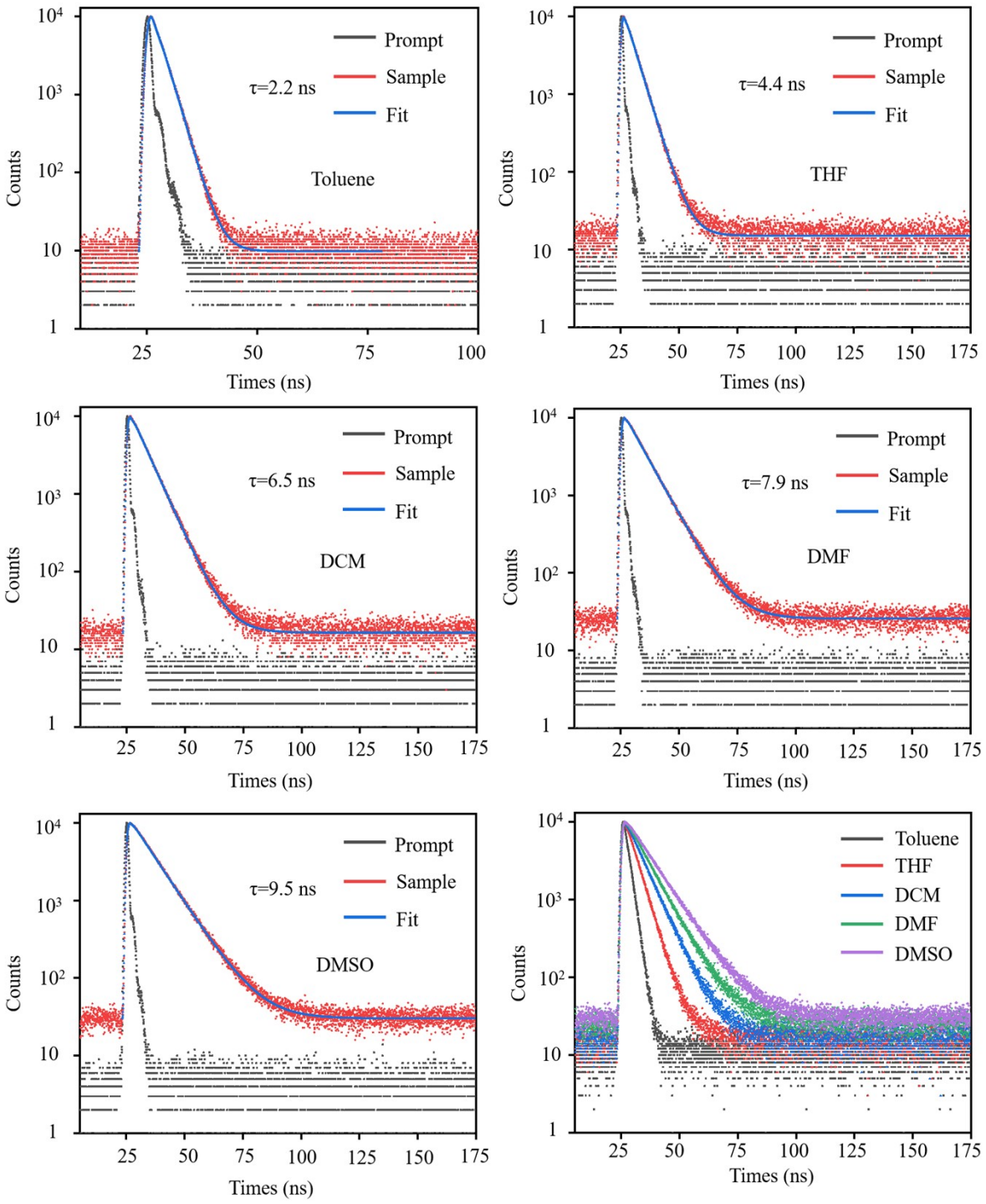


Fig. S3. Time-resolved fluorescence curves of compound **2** in different solvents.

The decay curve of **2** in toluene, THF, DCM, DMF and DMSO are fitted by 1-exponential method using the software supplied with the instrument, and then the fluorescence lifetime (τ) is calculated (2.2, 4.4, 6.5, 7.9, 9.5 ns, respectively). The quality of the fit is evaluated by analysis of goodness-of-fit parameter (χ2) (1.14, 1.17, 1.18, 1.05 and 1.04, respectively). (Concentration: 10 μM)

Photophyscial properties of compound **2** in the aggregated state, we monitored the emission behaviors in DMSO and DMSO/water mixture with varying water fractions. Compound **2** has the similar photophysical properties as compound **1**, Compound **2** shows red-shifts emission behavior with gradual decrease of emission intensity when the water content

changes from 0% to 40%, the maximum emission wavelength ranges from 525 to 570 nm. However, the emission behavior begins to blue-shift when the water fraction up to 50%, emission intensity increases first and then decrease with a small variation range. Correspondingly, photographs of compound **2** in DMSO/H_2O different water fractions under 365 nm UV light are also clearly distinguished (Fig. S4).

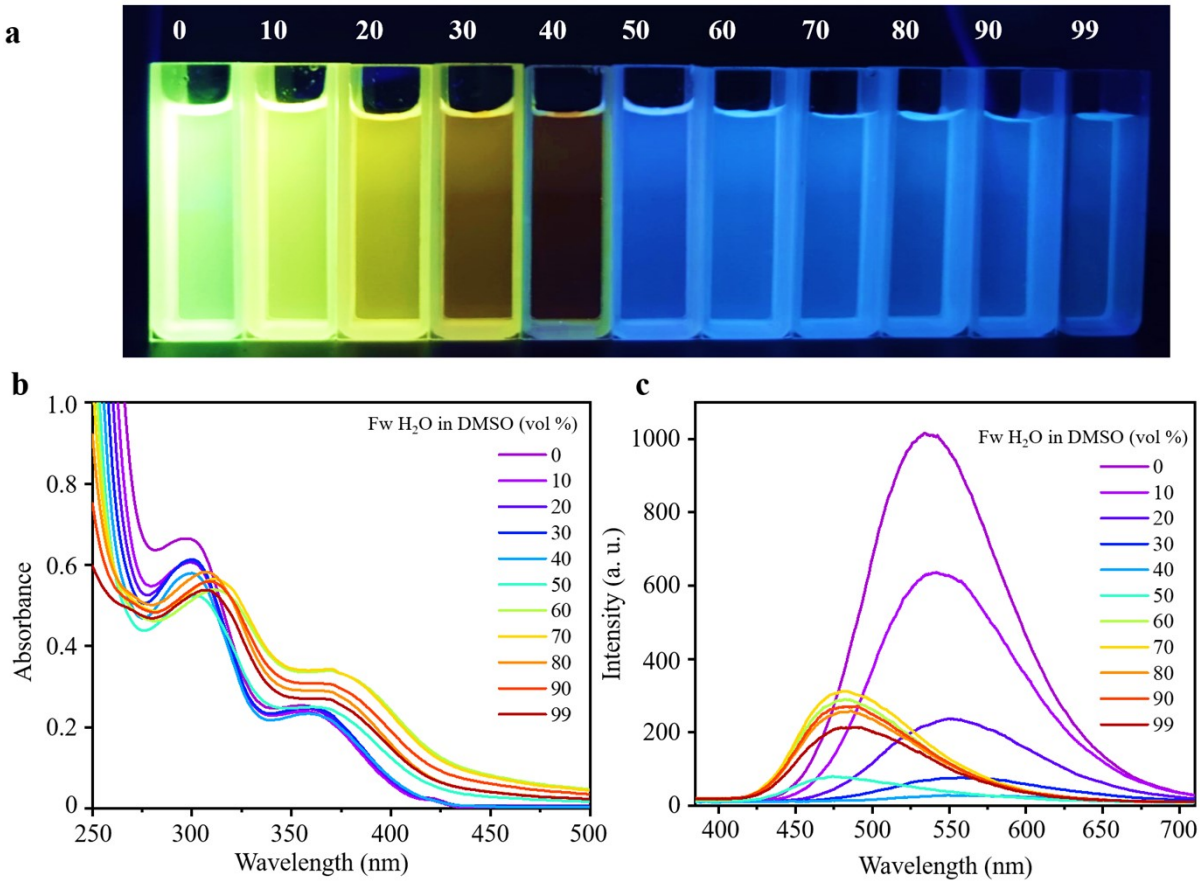


Fig. S4. (a) Photographs of compound **2** in DMSO/H_2O different water fractions under 365 nm UV light. (b) The changes of fluorescence spectra characteristics of compound **2** self-assembly process to form nanoparticles in different volume-ratio H_2O-DMSO solutions (V:V, 10 μM); (c) The fluorescence emission spectra of compound **2** in DMSO/H_2O different water fractions under 365 nm excitation (V:V, 10 μM).

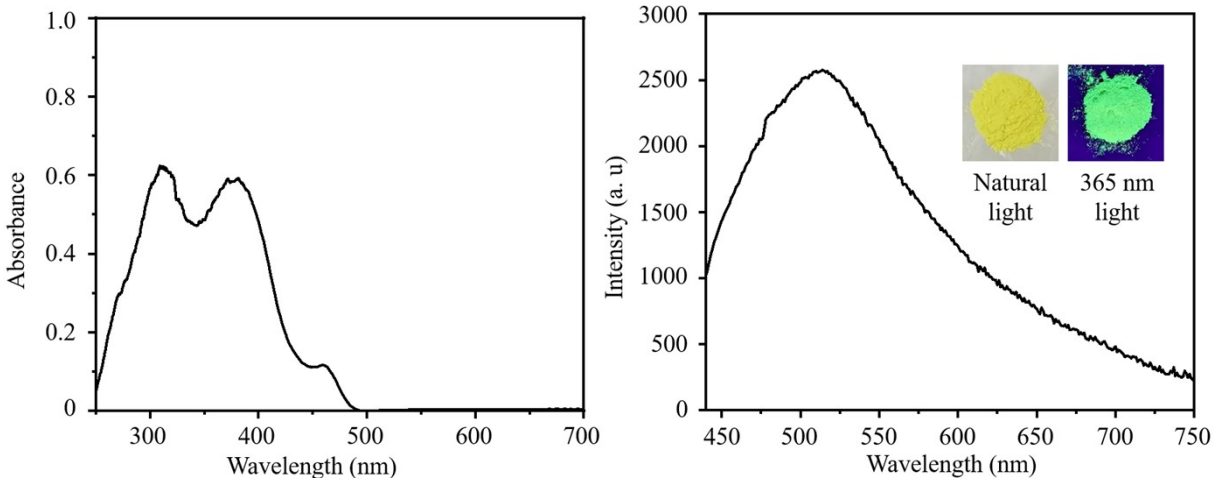


Fig. S5. The UV-vis absorbance (left) and fluorescence emission (right) spectra of the powders **2**. $\lambda_{max,\ abs}$ = 390 nm, $\lambda_{max,\ em}$ = 515 nm. Inset: Photos taken under natural light and 365 nm UV irradiation.

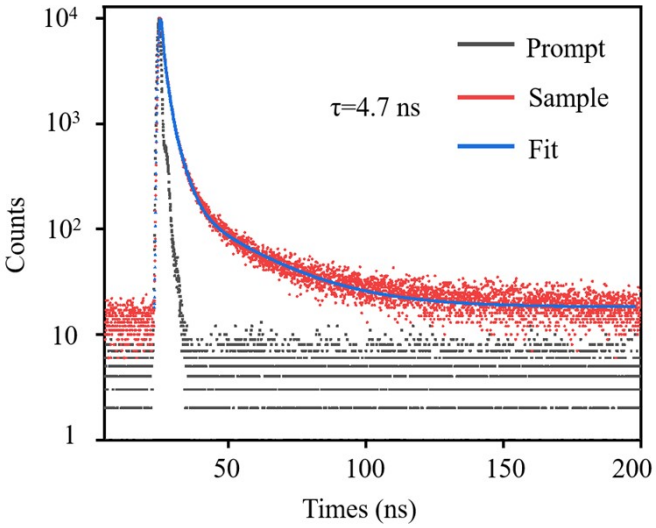


Fig. S6. Time-resolved fluorescence curves of the powders **2**.

The decay curve of **2** in solid state is fitted by 2-exponential method using the software supplied with the instrument, and then the average fluorescence lifetime (τ) is calculated. The quality of the fit is evaluated by analysis of goodness-of-fit parameter (χ2) (1.10).

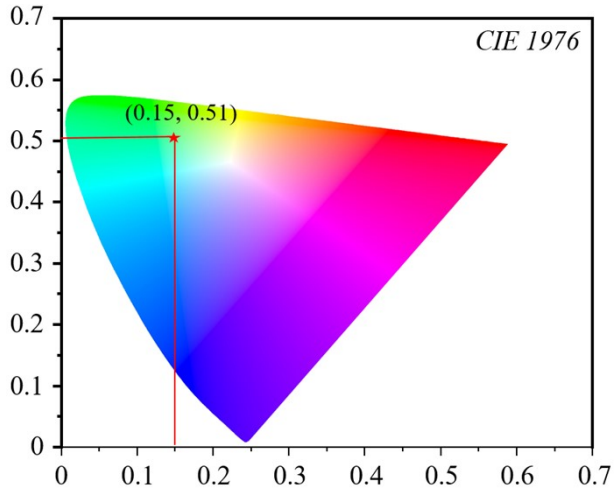


Fig. S7. CIE 1976 chromaticity diagram showing the luminescent color coordinates for the powders **2** (0.15, 0.51).

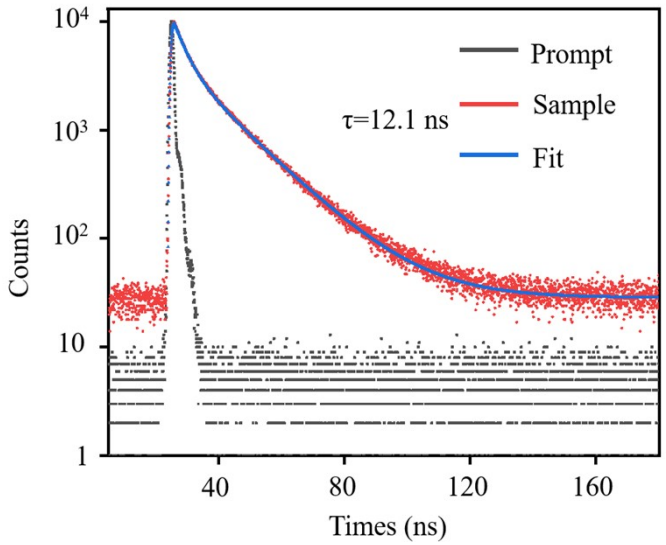


Fig. S8. Time-resolved fluorescence curves of TPA in toluene.

The decay curve of TPA in toluene is fitted by 2-exponential method using the software supplied with the instrument, and then the average fluorescence lifetime (τ) is calculated. The quality of the fit is evaluated by analysis of goodness-of-fit parameter (χ2) (1.15). (Concentration: 10 μM)

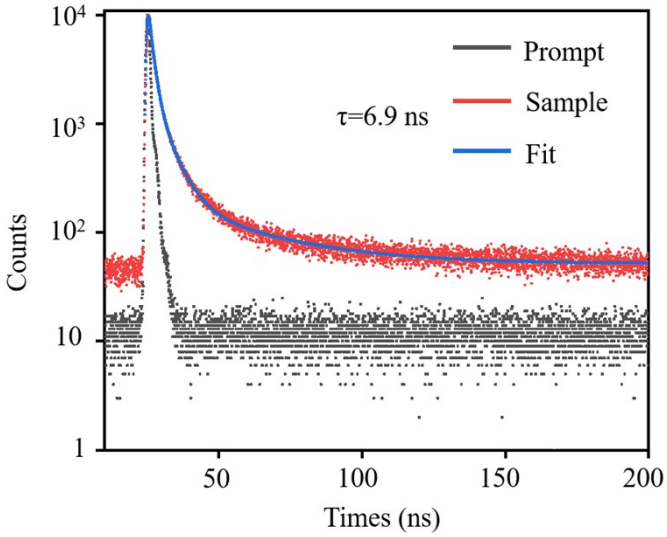


Fig. S9. Time-resolved fluorescence curves of MQIO in toluene.

The decay curve of MQIO in toluene is fitted by 2-exponential method using the software supplied with the instrument, and then the average fluorescence lifetime (τ) is calculated. The quality of the fit is evaluated by analysis of goodness-of-fit parameter (χ2) (1.18). (Concentration: 10 μM)

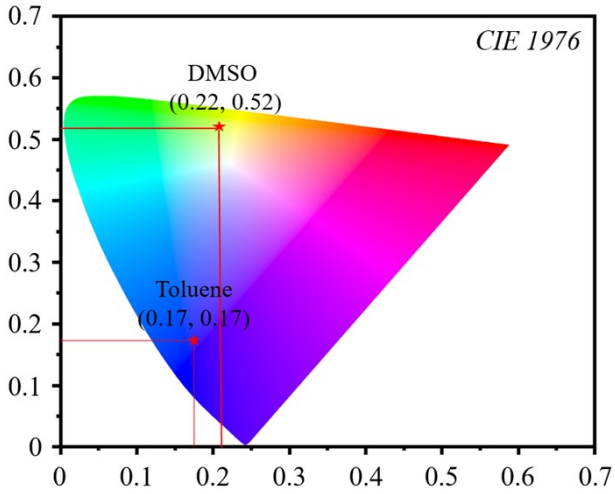


Fig. S10. CIE 1976 chromaticity diagram showing the luminescent color coordinates for compound **1** in toluene (0.17, 0.17) and DMSO (0.22, 0.52).

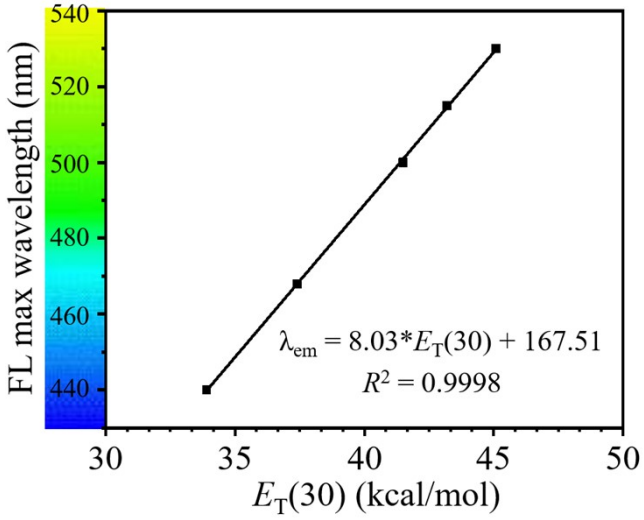


Fig. S11. Plot of the emission maximum of compound **1** in different solvents versus $E_T(30)$, where E_T (30) is the empirical parameter for solvent polarity;[2] λ_{ex} = 365 nm. All of the measurements are performed at room temperature (Concentration: 10 μM).

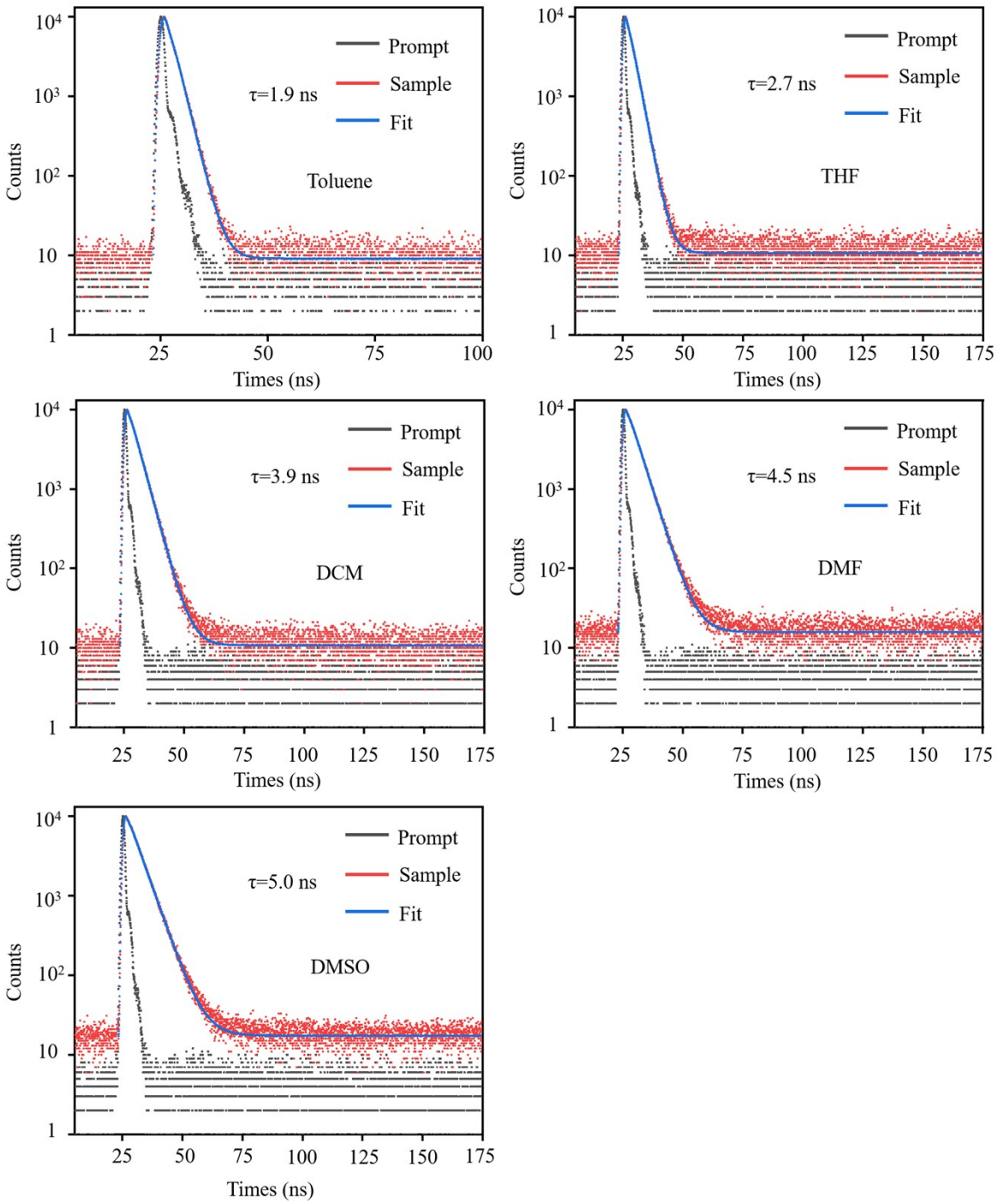


Fig. S12. Time-resolved fluorescence curves of compound **1** in different solvents.

The decay curve of **1** in toluene, THF, DCM, DMF and DMSO are fitted by 1-exponential method using the software supplied with the instrument, and then the fluorescence lifetime (τ) is calculated. The quality of the fit is evaluated by analysis of goodness-of-fit parameter (χ2) (1.28, 1.21, 1.14, 1.15 and 1.12, respectively). (Concentration: 10 μM)

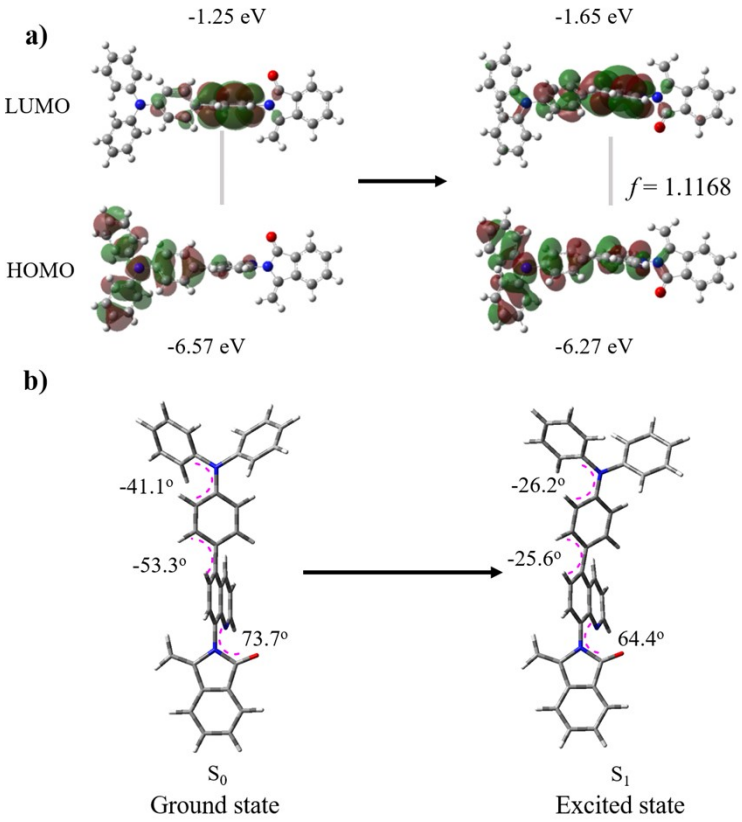


Fig. S13. a) HOMO and LUMO distribution, and photoexcitation properties of compounds **2**. b) Geometrical conformation of compound **2** in ground and excited states.

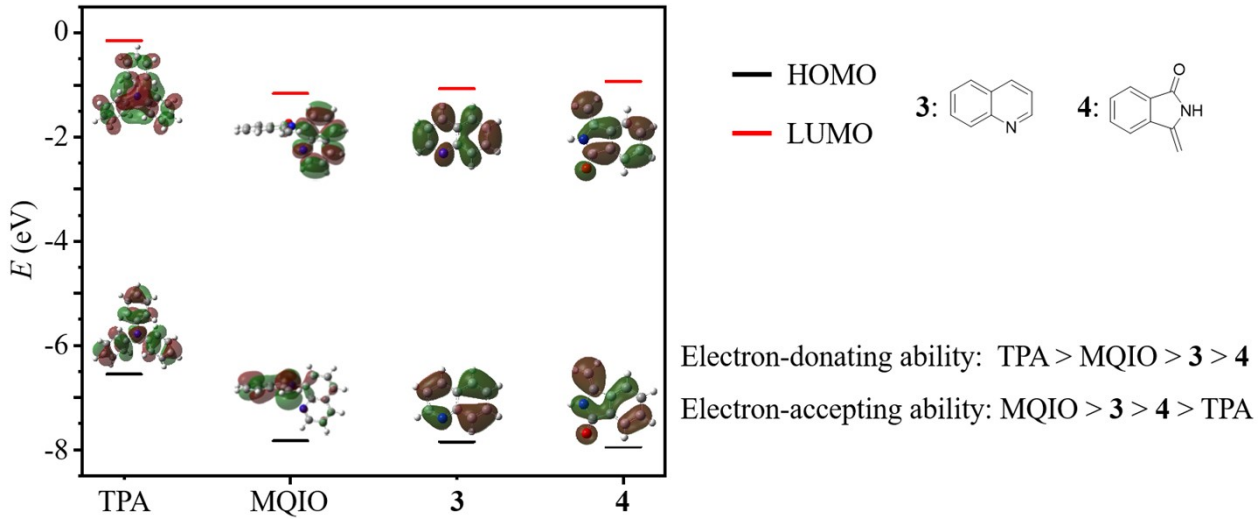


Fig. S14. Spatial distribution of HOMO−LUMO amplitudes and natural transition orbitals calculated for the first excited state in TPA, MQIO, **3** and **4**.

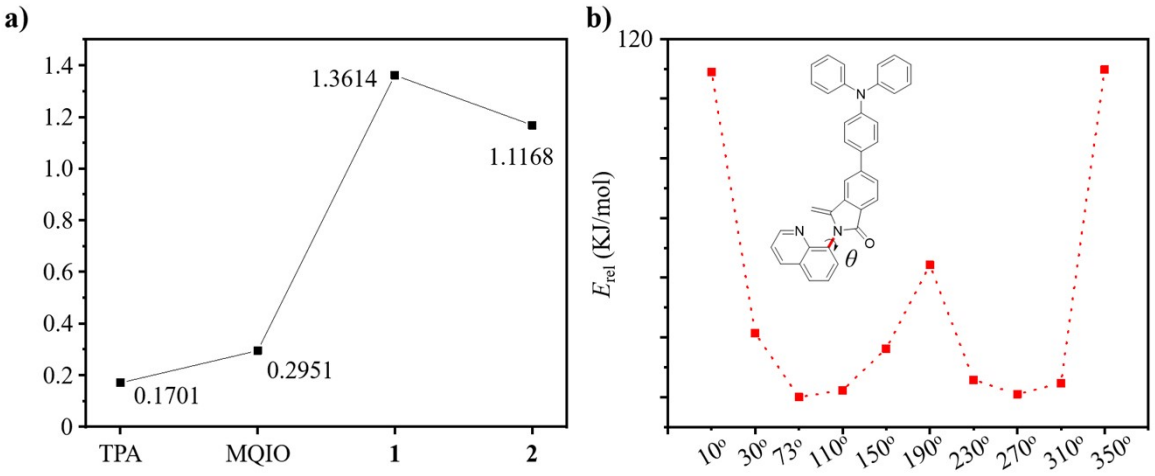


Fig. S15. (a) Photoexcitation to the S_1 state involves the transition from HOMO to LUMO with oscillator strength of values,respectively. (b) PES scan of the S_1 state around dihedral angle θ of C-N bond in MQIO molecules computed at the TDDFT/M062X/6-31+g(d)/PCM level.

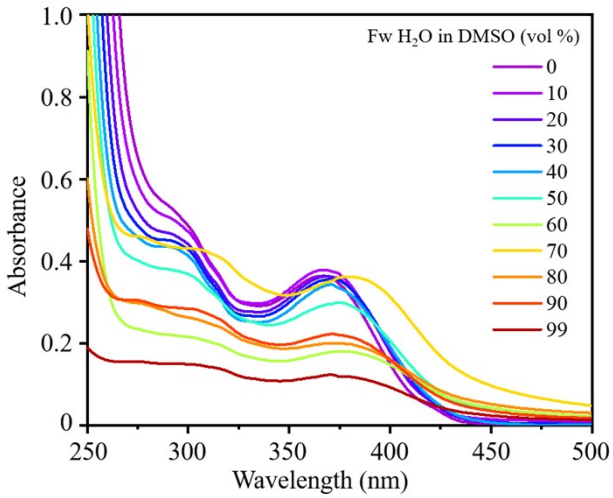


Fig. S16. The changes of fluorescence spectrum characteristics of compound **1** self-assembly process to form nanoparticles in different volume-ratio H_2O-DMSO solutions (V:V, 10 μM).

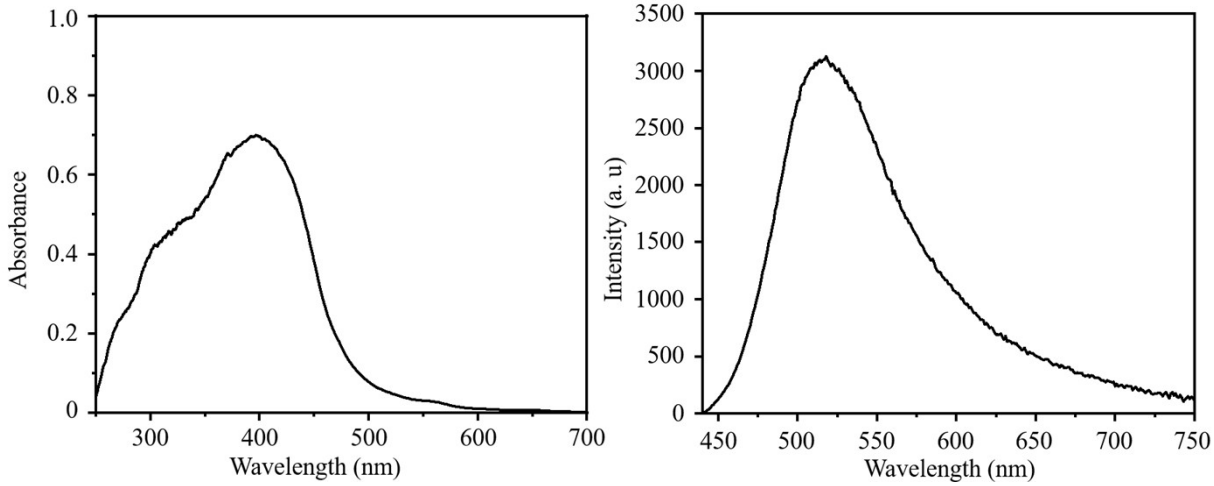


Fig. S17. The UV-vis absorbance (left) and fluorescence emission (right) spectrum of the powders **1**. $\lambda_{max,\ abs}$ = 400 nm, $\lambda_{max,\ em}$ = 520 nm.

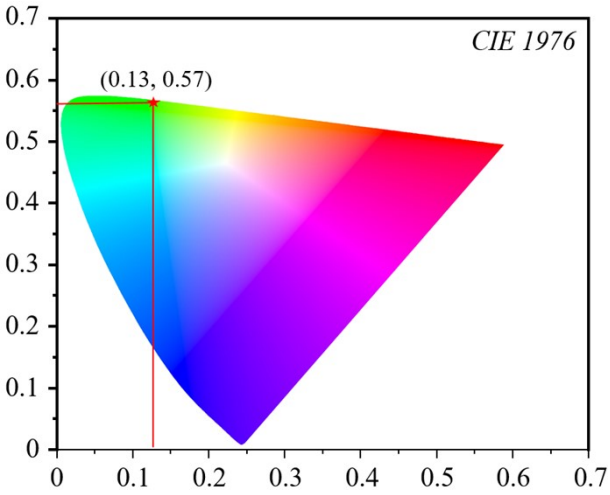


Fig. S18. CIE 1976 chromaticity diagram showing the luminescent color coordinates for the powders **1** (0.13, 0.57).

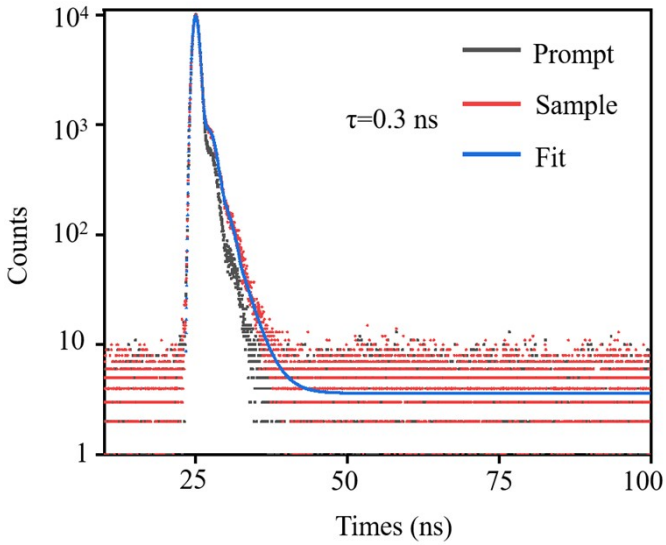


Fig. S19. Time-resolved fluorescence curves of the powders TPA.

The decay curve of the powders TPA is fitted by 2-exponential method using the software supplied with the instrument, and then the average fluorescence lifetime (τ) is calculated. The quality of the fit is evaluated by analysis of goodness-of-fit parameter (χ2) (1.29).

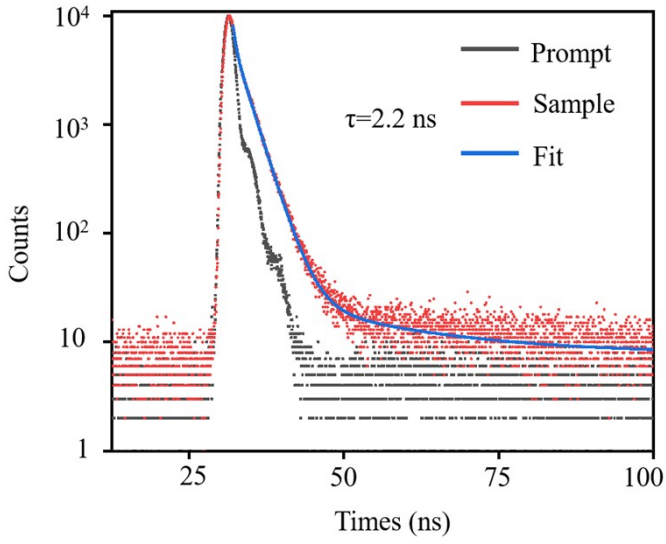


Fig. S20. Time-resolved fluorescence curves of the powders MQIO.

The decay curve of the powders MQIO is fitted by 2-exponential method using the software supplied with the instrument, and then the average fluorescence lifetime (τ) is calculated. The quality of the fit is evaluated by analysis of goodness-of-fit parameter (χ2) (1.21).

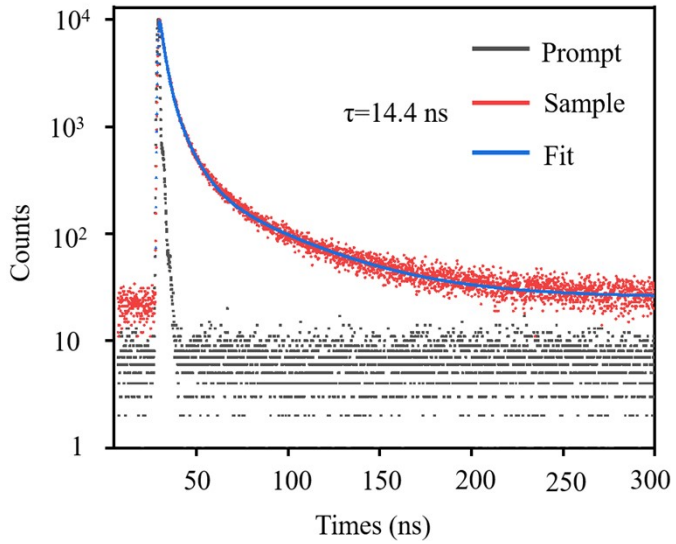


Fig. S21. Time-resolved fluorescence curves of the powders **1**.

The decay curve of the powders **1** is fitted by 3-exponential method using the software supplied with the instrument, and then the average fluorescence lifetime (τ) is calculated. The quality of the fit is evaluated by analysis of goodness-of-fit parameter (χ2) (1.16).

Preparation of 1/F127 nanoparticles: Compound **1** and F127 (5 mg) were dissolved in THF followed by sonication for three minutes. THF was evaporated by reduced pressure. Then, the solid was dissolved in water and sonicated for five minutes. The solution was filtered through 0.22 μm microfilter to obtain the 1/F127 nanoparticles solution.

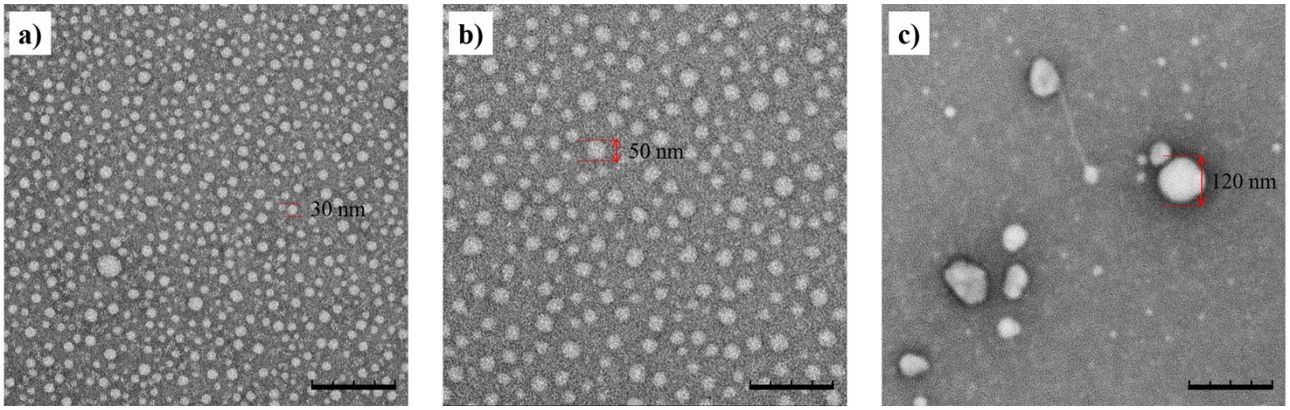


Fig. S22. TEM images of 1/F127 nanoparticles prepared from different concentrations. The scale bar is 200 nm. (a) 2 μM, (b) 20 μM, (c) 200 μM.

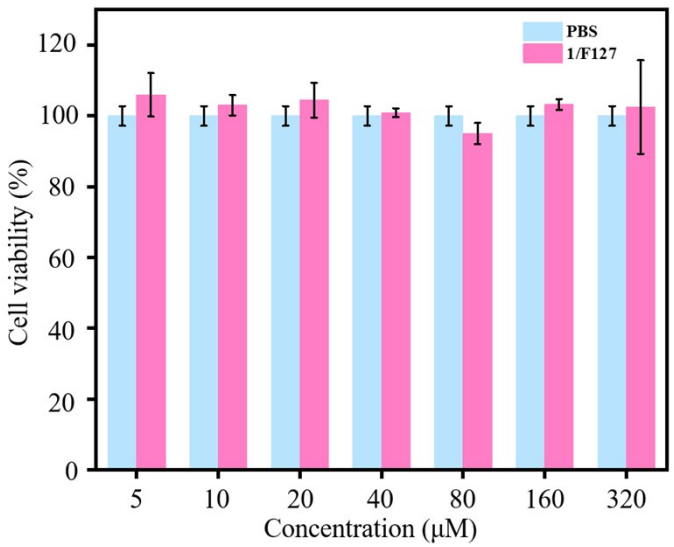


Fig. S23. Cytotoxicity of **1**/F127 nanoparticles to EJ cells. Cellular internalization time is 24 hours at 37 °C.

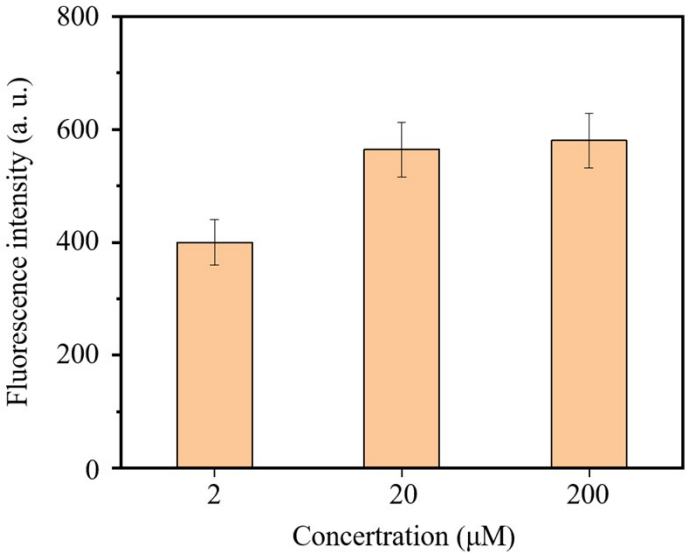


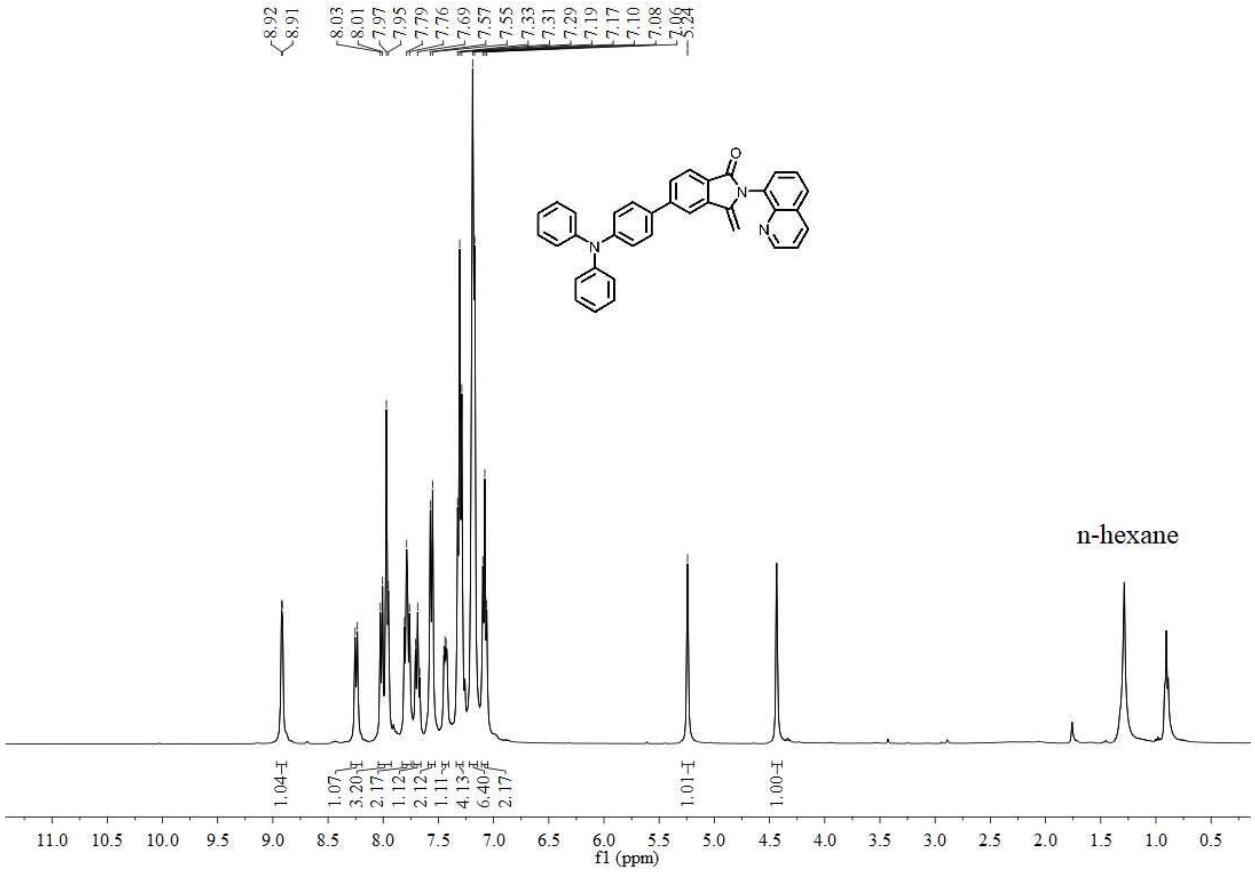
Fig. S24. Plot of fluorescence intensity of EJ cells with increasing concertration. Cellular internalization time is 24 hours at 37 °C.

References

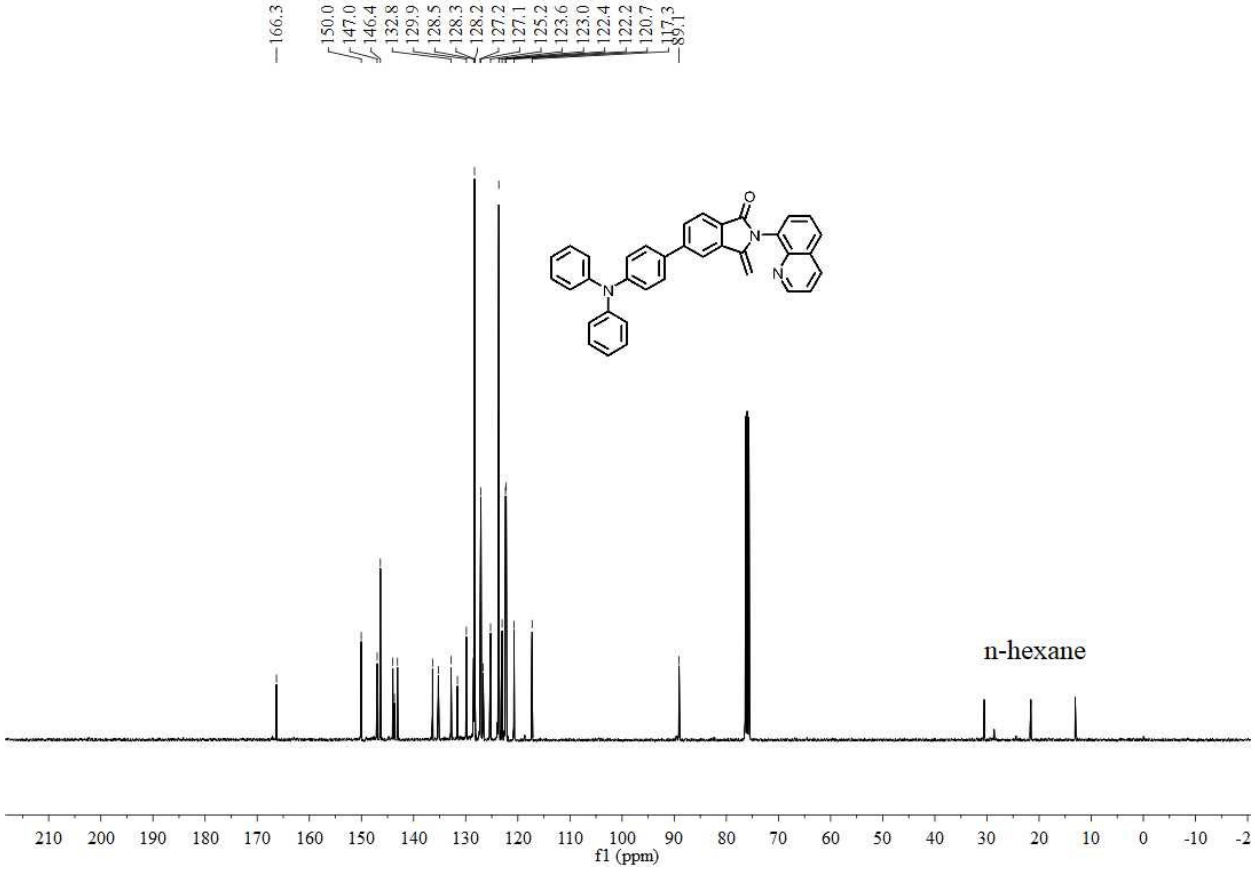
1. H. W. Liang, K. Jiang, W. Ding, Y. Yuan, L. Shuai, Y. C. Chen, Y. Wei, Redox-neutral palladium-catalyzed C-H functionalization to form isoindolinones with carboxylic acids or anhydrides as readily available starting materials. *Org. Lett.* **2015**, *17*, 2764-2767.
2. G. Chen, W. Li, T. Zhou, Q. Peng, D. Zhai, H. Li, W. Z. Yuan, Y. Zhang, B. Z. Tang, Conjugation-induced Rigidity in twisting molecules: Filling the gap between aggregation-caused quenching and aggregation-induced emission. *Adv. Mater.* **2015**, *27*, 4496-4501.

^{1}H and ^{13}C NMR Spectra

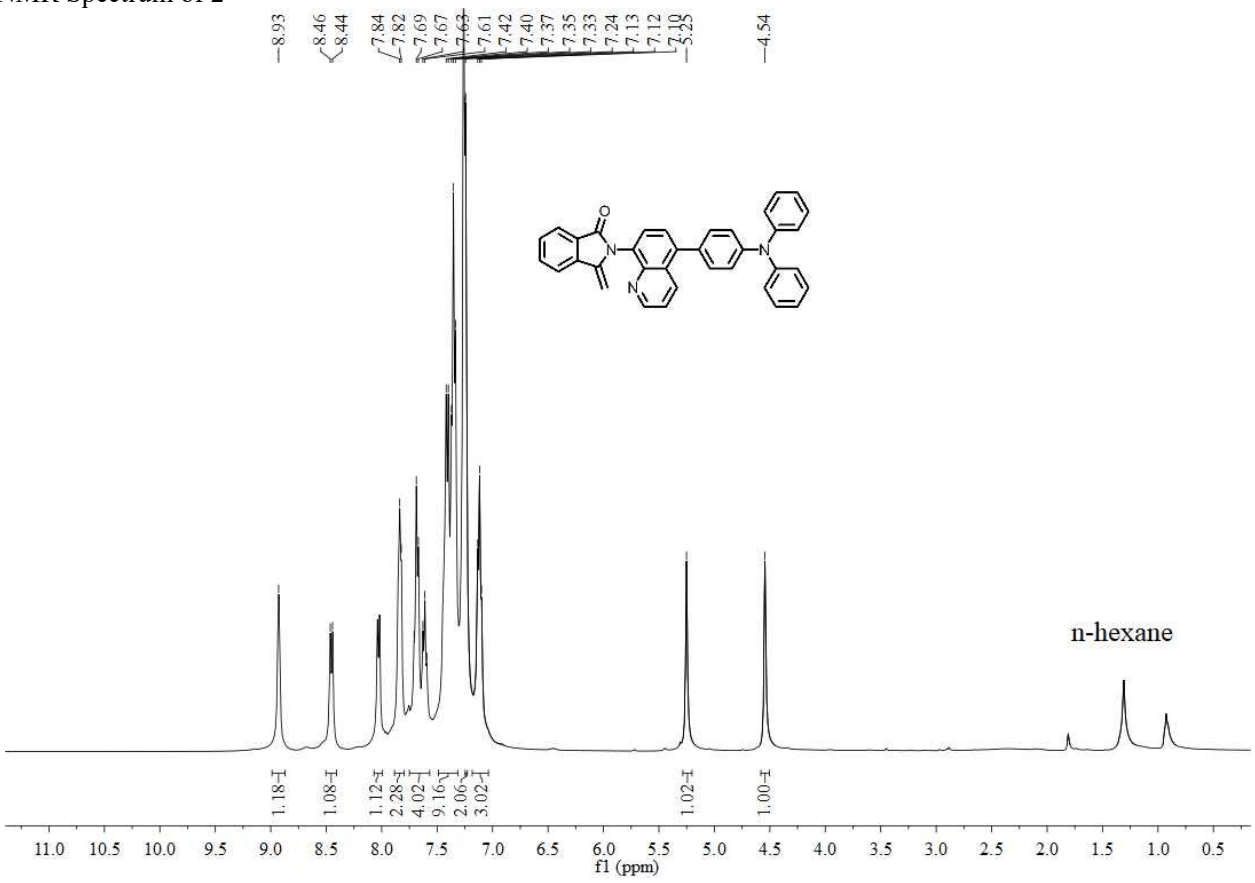
^{1}H NMR Spectrum of **1**



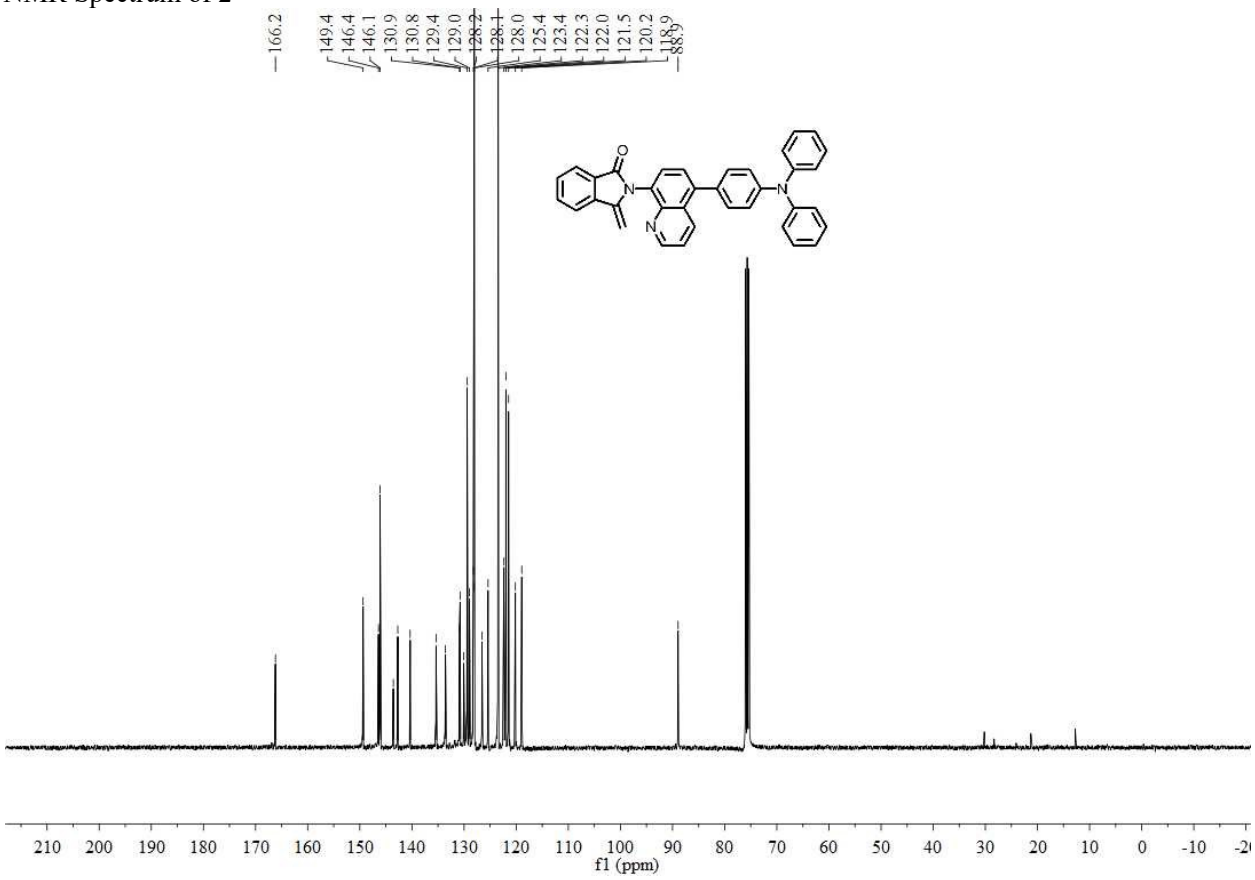
^{13}C NMR Spectrum of **1**



^{1}H NMR Spectrum of **2**



^{13}C NMR Spectrum of **2**



The ground and excited state coordinate of compound 1 and 2

The ground state coordinate of compound **1**

C	7.72986100	-3.40285800	-0.65647200
C	7.98394600	-2.27051900	-1.43153400
C	7.22373200	-1.11504600	-1.26901200
C	6.20391300	-1.07277500	-0.30990800
C	5.95742500	-2.20549100	0.47670900
C	6.70970400	-3.36273300	0.29469400
N	5.42887400	0.10042900	-0.13454600
C	4.04200800	-0.00084300	0.12180600
C	6.04207000	1.37691700	-0.20005400
C	7.29651300	1.59401200	0.38372900
C	7.89612300	2.84878000	0.30763100
C	7.24914200	3.90641300	-0.33319000
C	5.99498300	3.69232700	-0.90677300
C	5.39671300	2.43629700	-0.85057300
C	3.25730800	-0.94127600	-0.55804500
C	1.89663800	-1.04479900	-0.29390600
C	1.27455800	-0.21153900	0.64533400
C	2.06575500	0.73319100	1.31279000
C	3.42851000	0.83744300	1.06125500
C	-0.17796300	-0.32485100	0.92819800
C	-1.08663200	-0.55836300	-0.11454400
C	-2.43902900	-0.64815300	0.18969900
C	-2.88581300	-0.51653800	1.50399300
C	-2.00428300	-0.28910000	2.55276900
C	-0.64920000	-0.19476500	2.25041400
C	-3.61528000	-0.85973100	-0.67792700
N	-4.72447300	-0.90199700	0.19917000
C	-4.36307800	-0.64588100	1.51345500
O	-5.13506800	-0.56116200	2.45492700
C	-3.66970800	-0.97786100	-2.00739200
C	-6.07246100	-0.84621800	-0.24416600
C	-6.68818200	0.43419200	-0.38489000
C	-8.03664000	0.48888300	-0.82884100
C	-8.72825600	-0.71474900	-1.13044500
C	-8.10354600	-1.92919500	-0.99352800
C	-6.76169600	-1.99461500	-0.54193400

N	-5.96154000	1.54767300	-0.08820900
C	-6.55336700	2.71429300	-0.21911800
C	-7.89459000	2.88434200	-0.64857400
C	-8.63243000	1.77070500	-0.95329800
H	8.31913900	-4.30464800	-0.79184700
H	8.77222400	-2.28779400	-2.17903500
H	7.41854300	-0.24014200	-1.88297900
H	5.17301100	-2.17456000	1.22798200
H	6.50274700	-4.23329100	0.91065700
H	7.79831100	0.77660100	0.89396500
H	8.87019200	3.00123600	0.76366000
H	7.71656900	4.88490000	-0.38618600
H	5.48171300	4.50413800	-1.41414500
H	4.42541600	2.27106000	-1.30863900
H	3.71974700	-1.59897500	-1.28844200
H	1.31333200	-1.79600600	-0.82026000
H	1.61111500	1.40639800	2.03483600
H	4.02362900	1.57594400	1.59077800
H	-0.73421200	-0.63869300	-1.13952400
H	-2.36178300	-0.19457800	3.57396300
H	0.06706500	-0.03816200	3.05171000
H	-4.61033200	-1.12315300	-2.52824700
H	-2.75971100	-0.92696100	-2.59423700
H	-9.75863000	-0.65520900	-1.47151800
H	-8.63250500	-2.84799200	-1.22504500
H	-6.26663700	-2.95447600	-0.42640900
H	-5.95454300	3.58970100	0.02375800
H	-8.31104300	3.88247800	-0.73014900
H	-9.66332100	1.84939100	-1.28908400

The excited state coordinate of compound **1**

C	7.27273200	-3.74164300	-0.71500700
C	7.59228700	-2.65792800	-1.53839800
C	6.97496700	-1.42730800	-1.35340700
C	6.02846500	-1.27558700	-0.32834800
C	5.70391200	-2.36033300	0.50063500
C	6.32845600	-3.58629800	0.30190300
N	5.38418000	-0.02969800	-0.13559600

C	4.03948600	0.01927300	0.17275200
C	6.12803800	1.16802600	-0.27172200
C	7.43610400	1.24677000	0.23036000
C	8.14928500	2.43131500	0.09674500
C	7.57166800	3.54016700	-0.52871000
C	6.26940800	3.45684100	-1.02579700
C	5.54388500	2.27803800	-0.90066000
C	3.12841900	-0.93757000	-0.36879400
C	1.79344600	-0.86805200	-0.08246200
C	1.24197000	0.14307900	0.78366500
C	2.18889700	1.07941100	1.33429800
C	3.52258600	1.03086200	1.03522600
C	-0.15328000	0.22187600	1.06833900
C	-1.10974900	-0.57539100	0.35206000
C	-2.44846100	-0.44368300	0.62366200
C	-2.92579500	0.44959900	1.61397300
C	-2.01430300	1.23142900	2.34890500
C	-0.67063300	1.12153300	2.07841500
C	-3.61741700	-1.10372100	0.00872000
N	-4.72898100	-0.61607400	0.72110200
C	-4.36933000	0.37327800	1.65850000
O	-5.18835900	0.98980800	2.34452200
C	-3.66220300	-1.96887700	-1.01682700
C	-6.06244200	-0.77697400	0.26846200
C	-6.60042800	0.19057200	-0.63552400
C	-7.93482100	0.02089100	-1.09307600
C	-8.69382800	-1.09778900	-0.65666700
C	-8.14638100	-2.01389200	0.20627500
C	-6.81866300	-1.84811200	0.67428800
N	-5.81430800	1.23357000	-1.02446500
C	-6.33216400	2.11206900	-1.85426700
C	-7.65247100	2.04212800	-2.36835800
C	-8.45022300	0.99548300	-1.98624200
H	7.75717100	-4.70123400	-0.86553300
H	8.31992800	-2.77560500	-2.33527300
H	7.20708100	-0.58752500	-2.00139900
H	4.98476200	-2.22663800	1.30328500
H	6.08379700	-4.42101900	0.95138400

H	7.87519800	0.38825600	0.72968500
H	9.15821300	2.49404800	0.49249100
H	8.13424600	4.46321400	-0.62783300
H	5.81867500	4.30995000	-1.52330300
H	4.53968200	2.19838100	-1.30604900
H	3.50122500	-1.70209600	-1.04352400
H	1.14322800	-1.60970300	-0.53113200
H	1.85126700	1.86259400	2.00220700
H	4.20570000	1.74878400	1.47911100
H	-0.78898000	-1.25509000	-0.43008800
H	-2.36695500	1.91033700	3.12091000
H	0.01659000	1.71542400	2.66919100
H	-4.60041300	-2.37370300	-1.38126500
H	-2.74550600	-2.27695300	-1.50670500
H	-9.71159900	-1.21332600	-1.02024100
H	-8.72572100	-2.86963100	0.53803700
H	-6.38460700	-2.56937000	1.36071600
H	-5.68617100	2.93605200	-2.15122400
H	-8.00656900	2.80852100	-3.04939300
H	-9.46813000	0.89638600	-2.35499500

The ground state coordinate of compound **2**

C	-7.24536300	-3.63089800	-0.07563600
C	-7.59372700	-2.55749700	0.74460100
C	-6.87870400	-1.36329900	0.68851600
C	-5.81044300	-1.22455300	-0.20565900
C	-5.46706800	-2.29845400	-1.03634700
C	-6.17603500	-3.49466600	-0.96239100
N	-5.08107000	-0.00981900	-0.27243500
C	-3.66921300	-0.02951900	-0.31256400
C	-5.76495400	1.22582100	-0.13233600
C	-6.96186800	1.44843300	-0.82409900
C	-7.64245400	2.65404500	-0.67385000
C	-7.13267800	3.65777000	0.15127800
C	-5.93626700	3.43828300	0.83489500
C	-5.25924400	2.22836800	0.70380700
C	-2.94026800	-1.01065300	0.37345000

C	-1.55038200	-1.00154100	0.34562600
C	-0.84518000	-0.01361200	-0.35372800
C	-1.58133300	0.95406800	-1.04873000
C	-2.97114300	0.94659900	-1.03613700
C	9.43519400	0.63653400	-0.28414700
C	8.26364900	1.36191300	-0.50497800
C	7.05900900	0.66509300	-0.50406000
C	7.03927000	-0.71419200	-0.29423300
C	8.19979400	-1.44496700	-0.07515500
C	9.40808800	-0.74906000	-0.07109700
C	5.66839200	1.12214600	-0.69699400
N	4.87798500	-0.04984000	-0.64219400
C	5.62886200	-1.17604600	-0.34850600
O	5.18338100	-2.30083200	-0.18687900
C	5.20718400	2.36280500	-0.87759700
C	3.46091600	-0.03394000	-0.56657500
C	2.84540300	-0.02006800	0.72086000
C	1.42466400	0.00543400	0.80335900
C	0.64046200	-0.00348400	-0.39805700
C	1.28654900	0.00793800	-1.61650000
C	2.69709300	-0.00742900	-1.70407400
N	3.65477400	-0.01195300	1.81685700
C	3.08637000	0.03821700	3.00051500
C	1.68622900	0.10266000	3.20072100
C	0.86208600	0.08892000	2.10539100
H	-7.80069600	-4.56244600	-0.02547200
H	-8.41990500	-2.65071400	1.44370000
H	-7.14615800	-0.53308900	1.33617500
H	-4.64283700	-2.19060400	-1.73614300
H	-5.89773000	-4.32025900	-1.61112900
H	-7.35496100	0.67193000	-1.47473500
H	-8.57092400	2.81305300	-1.21489900
H	-7.66150900	4.59963700	0.26047300
H	-5.53116500	4.20680400	1.48700900
H	-4.33491100	2.05579100	1.24808400
H	-3.46516900	-1.78168800	0.92961700
H	-1.00564000	-1.77805300	0.87733100
H	-1.05771200	1.72856500	-1.60349300

H	-3.52303000	1.70869400	-1.57868700
H	8.29997500	2.43471200	-0.66987200
H	8.16146000	-2.51806000	0.08766800
H	10.33892800	-1.28127600	0.09819600
H	4.14843400	2.56469100	-1.00227400
H	5.89586800	3.19948900	-0.89951700
H	0.70041800	0.00063300	-2.53104800
H	3.18571700	-0.01159900	-2.67424100
H	3.75434000	0.04133600	3.85942300
H	1.28672000	0.17109100	4.20676900
H	-0.21443800	0.15612000	2.22623800
H	10.38871900	1.15615400	-0.27714800

The excited state coordinate of compound **2**

C	-6.89902800	-3.63618800	-0.94370700
C	-7.41710900	-2.76939600	0.02150400
C	-6.79430500	-1.55366700	0.28027200
C	-5.64324600	-1.20005800	-0.43441100
C	-5.12060600	-2.06274100	-1.40532800
C	-5.75125700	-3.27848500	-1.65320000
N	-5.01944100	0.05275300	-0.17747900
C	-3.65229400	0.15448100	-0.05860500
C	-5.85580600	1.19952000	-0.07832900
C	-6.88293000	1.38012200	-1.01269900
C	-7.71272600	2.49135800	-0.91628400
C	-7.52405000	3.42550200	0.10465400
C	-6.49815600	3.24050900	1.03366300
C	-5.66272700	2.13059400	0.94926200
C	-2.87017000	-0.95643900	0.37733000
C	-1.51280300	-0.84696400	0.51118300
C	-0.80419200	0.36380600	0.20205500
C	-1.61285800	1.45556000	-0.27083000
C	-2.97484400	1.36453200	-0.37972500
C	9.42023200	0.67010300	-0.77992900
C	8.32815800	1.43688400	-0.36895800
C	7.06947700	0.84620600	-0.40744200
C	6.91609600	-0.46905900	-0.84508200
C	7.99528600	-1.23827800	-1.26076100

C	9.25979200	-0.65062600	-1.22094000
C	5.73768600	1.36667300	-0.03920100
N	4.82678200	0.31998400	-0.32170700
C	5.47233800	-0.81440600	-0.79984300
O	4.92976000	-1.85160000	-1.14319200
C	5.42722900	2.55639800	0.48596100
C	3.43833900	0.38664200	-0.08435600
C	2.86116600	-0.43735300	0.92044900
C	1.44139100	-0.35906200	1.14520100
C	0.61640400	0.46991100	0.27018300
C	1.29390600	1.38492500	-0.60281400
C	2.65694300	1.32341300	-0.78598600
N	3.68255200	-1.21345300	1.67217500
C	3.15227400	-1.88698800	2.69351400
C	1.81086600	-1.80841000	3.05852200
C	0.95604200	-1.02183600	2.28042400
H	-7.38844500	-4.58450400	-1.14245900
H	-8.30591500	-3.04389400	0.58110500
H	-7.18774400	-0.87748700	1.03365500
H	-4.23935500	-1.76954800	-1.96884100
H	-5.35008500	-3.94300000	-2.41221800
H	-7.01892100	0.65322500	-1.80800800
H	-8.50385700	2.63210900	-1.64616200
H	-8.17381900	4.29210200	0.17632900
H	-6.35352700	3.95768100	1.83574300
H	-4.87580900	1.97080300	1.68094600
H	-3.36070200	-1.89496600	0.61333600
H	-0.95427100	-1.72526700	0.81479600
H	-1.14248200	2.40021700	-0.52079000
H	-3.54499600	2.21712000	-0.73425500
H	8.46600800	2.46018600	-0.03195500
H	7.85408000	-2.25951100	-1.60258900
H	10.13026700	-1.21869400	-1.53412300
H	4.40657400	2.82190400	0.73913200
H	6.20956000	3.28357200	0.67178900
H	0.71905900	2.05702500	-1.22918700
H	3.14061800	1.97050800	-1.51288600
H	3.84073200	-2.50652800	3.26544100

H	1.44399300	-2.34066000	3.92981300
H	-0.08003500	-0.90373300	2.57986200
H	10.41462600	1.10605600	-0.75835400