Supplementary information

Aqueous up-conversion organic phosphorescence and tunable dual emission in a single-molecular emitter

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Experimental section

Instrumentation and methods. All reagents and solvents were commercially available and used without further purification unless otherwise noted. ^{1}H NMR and ^{13}C NMR spectra were measured on a Bruker AV-400 spectrometer. The electronic spray ionization (ESI) high-resolution mass spectra were tested on a Waters LCT Premier XE spectrometer. The UV-Vis absorption spectra were obtained on a Shimadzu UV-2600 spectrophotometer. Fluorescence, phosphorescence, and lifetime of delayed emission spectra were recorded on an Agilent Cary Eclipse spectrophotometer. Phosphorescence mode; Delay time = 0.1 ms, Photoluminescence spectra were record on Shimadzu RF-6000 spectrometer. Fluorescence lifetimes were measured on Edinburgh Instruments Fluorescence Spectrometer (FLS1000). Absolute PL quantum yields were determined with a spectrometer C11347-11 (Hamamatsu, Japan). Leica TCS-SP8 fluorescence microscope equipped with an oil immersion objective (63×) was used for two-photon confocal imaging. The phosphorescence lifetime imaging microscope (PLIM) image setup was integrated with an Olympus IX81 laser scanning confocal microscope.

Theoretical Calculation. The Gaussian 09 software package was employed to perform Density Functional Theory (DFT) and Time-Dependent (TD) DFT calculations. The ground-state (S_0) geometries were optimized using the B3LYP functional and 6-311G* basis set. Subsequently, the energies in both singlet and triplet states were obtained by applying the time-dependent DFT method based on the optimized S_0 molecular structure. Our theoretical calculations were carried out in water phase. The optimized recursive convolution algorithm (ORCA) software was utilized to compute the SOC values. This method has been seamlessly integrated into our computational protocol, allowing for the convenient extraction of SOC values following Gaussian calculations.

Cell culture and cytotoxicity experiments. The HeLa cells were cultured in Gulbecco's modified Eagle medium (DMEM) supplemented with 10% fetal bovine serum (FBS) and 1% penicillin/streptomycin. The incubation of HeLa cells was performed using DMEM medium containing 10% FBS and 1% penicillin/streptomycin, under a humidified atmosphere with 5% CO_2 at 37°C. Subsequently, the cells were treated with different concentrations of guest and host-guest complexes **Y3** for a duration of 24 hours. The relative cellular viability was assessed using the MTT assay following the provided instructions.

PLIM cell imaging. The HeLa cells were cultured with **Y3** (50 μM) for 6 hours. Following incubation, the cells were washed three times with PBS (pH 7.4). Subsequently, phosphorescence cell images were acquired using PLIM through integration with an Olympus IX81 laser scanning confocal microscope. The confocal microscope system detected the phosphorescence signals, and data analysis was performed using professional software provided by PicoQuant Company. The PLIM data was processed in SymPhoTime 64 pro software (Pico Quant Company) and exported in ASCII format for line profiles or BMP format for images. Double exponential tailfit was applied to fit the PLIM data obtained from regions of interest sized at 256 × 256 pixels, with a binning factor of 1 in SymPhoTime 64 pro software.

Cellular imaging at different temperatures. The HeLa cells were meticulously washed with PBS and subsequently incubated with Y3 (0.5 mg mL^{-1}) at 37 °C for a duration of 30 minutes. Any extracellular Y3 molecules were gently eliminated through PBS washing. Subsequently, the HeLa cells subjected to various incubation temperatures were analyzed using confocal imaging techniques. The temperature settings for all experiments were accurately calibrated using an infrared camera (Fotric).

Calculation of the thermal sensitivity and uncertainty

Thermal relative sensitivity (S_r) of **Y3** is calculated by:

$$Sr = \frac{1dR}{RdT}$$

where R is the intensity or lifetime ratio value of fluorescence and phosphorescence and T is the temperature.

Synthesis and compound characterization

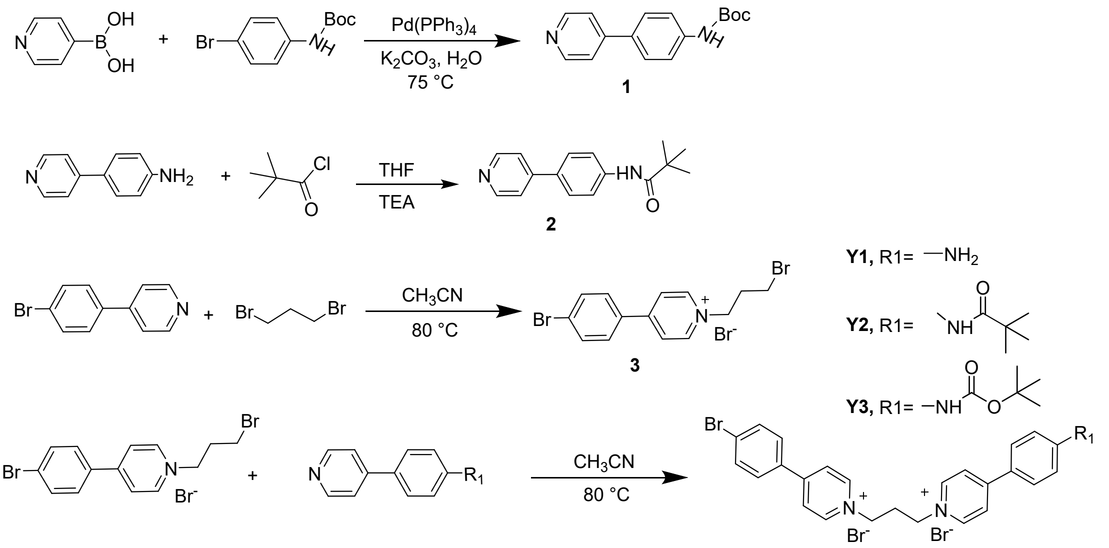


Figure S1. Synthetic routes of guest molecule **Yn** (n=1-3).

Synthesis of compound 1. The tert-butyl (4-bromophenyl)carbamate (0.81 g, 3 mmol), 4-pyridineboronic acid (0.41 g, 3.3 mmol), and K_2CO_3 (0.62 g, 4.5 mmol) were dissolved in anhydrous THF (30 mL) and degassed for 30 minutes prior to the addition of $Pd(PPh_3)_4$ (0.19 g, 0.16 mmol). After rapid addition of $Pd(PPh_3)_4$, the solution was further degassed for an additional 15 minutes before being heated at 75 °C under an argon atmosphere for a duration of 8 hours. Following the reaction, the crude product was transferred into water (50 mL) and subjected to three extractions with dichloromethane using portions of 20 mL each time. The organic layer was then dried over anhydrous Na_2SO_4, filtered, and concentrated by rotary evaporation. Finally, purification of the resulting residue was achieved through silica gel chromatography employing a dichloromethane: ethyl acetate eluent mixture in a ratio of 5:1 (v/v), yielding Compound **1** as a white solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.63 (d, *J* = 6.2 Hz, 2H), 7.60 (d, *J* = 8.7 Hz, 2H), 7.49 (m, 4H), 1.54 (s, 9H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 152.57, 150.22, 147.67, 139.49, 132.41, 127.61, 121.12, 118.80, 80.95, 28.34.

Synthesis of compound 2. The dehydrated solution of pivaloyl chloride (0.31 g, 2.6

mmol) in THF (20 mL) was slowly added to a mixture of 4-(pyridin-4-yl)aniline (0.51 g, 3 mmol) and triethylamine (2.0 mL) in THF (20 mL), under an ice bath, followed by stirring at room temperature for 5 hours. Upon completion of the reaction, the THF solvent was evaporated and dichloromethane (300 mL) was added to the residue, which was then washed with water and saturated brine before being dried with Na_2SO_4 and concentrated. The resulting crude product was purified using silica gel column chromatography with dichloromethane/ethyl acetate (5/1) as the eluent to yield a white solid product (0.46 g, 60%). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.64 (m, 2H), 7.68 (d, *J* = 8.8 Hz, 2H), 7.62 (d, *J* = 8.7 Hz, 2H), 7.49 (m, 2H), 1.35 (s, 9H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 176.77, 150.25, 147.57, 139.06, 133.62, 127.56, 121.23, 120.33, 39.76, 27.63.

Synthesis of compound 3. The synthesis of Compound **3** was conducted according to the procedure outlined in the referenced literature[1]. A solution containing 4-(4-bromophenyl)pyridine (100 mg, 0.43 mmol) and 1,3-dibromopropane (0.35 g, 1.74 mmol) in CH_3CN (25 mL) was subjected to heating at a temperature of 60 °C for a duration of 12 hours. Upon cooling to room temperature, the resulting reaction mixture was dispersed in diethyl ether (200 mL). Subsequently, the mixture underwent filtration and the solid product obtained was washed with acetone. Finally, a white solid product with a yield of 108 mg (60%) was obtained.

Synthesis of compound Y1. The synthesis of compound **Y1** yielded a yellow powder with 33% efficiency (39 mg), utilizing 4-(pyridin-4-yl)aniline (34 mg, 0.2 mmol) and compound **3** (95 mg, 0.22 mmol) as starting materials. ^{1}H NMR (400 MHz, Deuterium Oxide) δ 8.65 (d, *J* = 6.8 Hz, 2H), 8.38 (d, *J* = 6.9 Hz, 2H), 8.06 (d, *J* = 6.8 Hz, 2H), 7.85 (d, *J* = 7.0 Hz, 2H), 7.56 (d, *J* = 8.7 Hz, 2H), 7.50 (m, 4H), 6.64 (d, *J* = 8.7 Hz, 2H), 4.63 (t, *J* = 6.6 Hz, 4H), 2.77 (t, *J* = 6.5 Hz, 2H). ^{13}C NMR (151 MHz, CD_3OD) δ 157.09, 155.86, 144.91, 144.88, 144.84, 144.68, 144.62, 133.77, 132.86, 132.82, 132.22, 132.20, 129.66, 129.61, 129.59, 129.55, 129.53, 129.51, 127.86, 127.04, 124.97, 124.93, 124.90, 124.88, 124.85, 57.22, 57.10, 32.05. HRMS (ESI) m/z for $C_{25}H_{24}BrN_3$ calcd. $[M-2Br]^{2+}$ 222.5579, found: 222.5571.

Synthesis of compound Y2. The synthesis of compound **Y2** yielded a white powder with 34% efficiency (47 mg), utilizing compound **2** (50.8 mg, 0.2 mmol) and compound **3** (95 mg, 0.22 mmol) as starting materials. ^{1}H NMR (400 MHz, Deuterium Oxide) δ 8.65 (d, *J* = 6.8 Hz, 2H), 8.60 (d, *J* = 6.7 Hz, 2H), 8.03 (dd, *J* = 9.3, 6.9 Hz, 4H), 7.60 (d, *J* = 8.7 Hz, 2H), 7.47 (d, *J* = 1.3 Hz, 4H), 7.42 (d, *J* = 8.8 Hz, 2H), 4.76 (s, 4H), 2.81 (m, 2H), 1.19 (s, 9H). ^{13}C NMR (151 MHz, CD_3OD) δ 178.75, 155.85, 144.83, 144.38, 143.34, 132.81, 129.58, 129.55, 128.59, 128.24, 127.05, 124.92, 123.92, 123.89, 121.05, 57.27, 56.88, 39.51, 31.97, 26.22. HRMS (ESI) m/z for $C_{30}H_{32}BrN_3O$ calcd. $[M-2Br]^{2+}$ 242.5866, found: 264.5859.

Synthesis of compound Y3. The mixture of Compound **1** (54 mg, 0.2 mmol) and Compound **3** (95 mg, 0.22 mmol) was dissolved in 5 mL of CH_3CN and subjected to heating at a temperature of 80 °C for a duration of 12 hours. Subsequently, the resulting residue was cooled to room temperature and evaporated to remove the solvent. The crude product underwent recrystallization using a combination of CH_3CN and ethyl acetate, resulting in the formation of a white powder with an overall yield of 38% (51 mg). ^{1}H NMR (400 MHz, Deuterium Oxide) δ 8.64 (d, *J* = 6.8 Hz, 2H), 8.55 (d, *J* = 6.7 Hz, 2H), 8.00 (d, *J* = 6.6 Hz, 2H), 7.94 (d, *J* = 6.7 Hz, 2H), 7.54 (d, *J* = 8.8 Hz, 2H), 7.43 (q, *J* = 8.7 Hz, 4H), 7.24 (d, *J* = 8.7 Hz, 2H), 4.77 (m, 4H), 2.84 (m, 2H), 1.42 (s, 9H). ^{13}C NMR (151 MHz, CD_3OD) δ 156.14, 155.81, 153.19, 144.89, 144.84, 144.32, 144.23, 132.88, 132.80, 129.59, 129.56, 129.54, 128.85, 128.81, 127.02, 126.54, 124.92, 124.82, 123.50, 123.47, 118.53, 118.49, 80.24, 57.28, 56.76, 31.97, 27.20. HRMS (ESI) m/z for $C_{30}H_{32}Br_3N_3O_2$ calcd. $[M-2Br]^{2+}$ 272.5838, found: 272.5828.

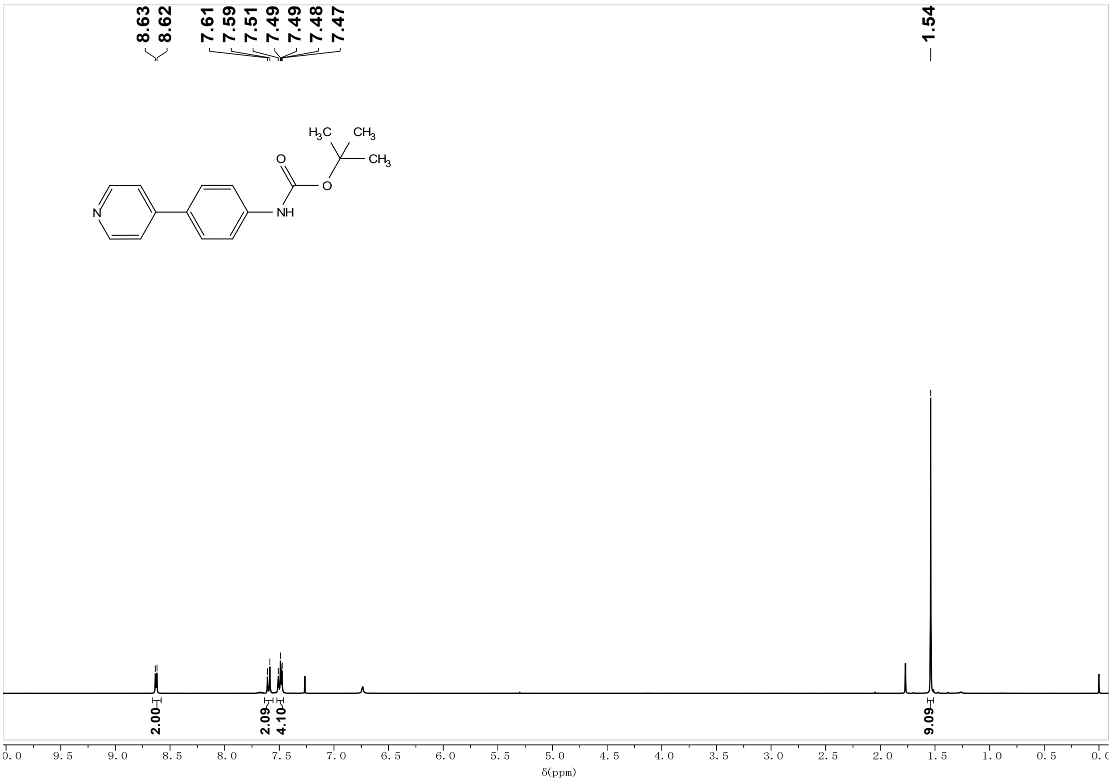


Figure S2. ^{1}H NMR spectrum of compound **1** in $CDCl_3$.

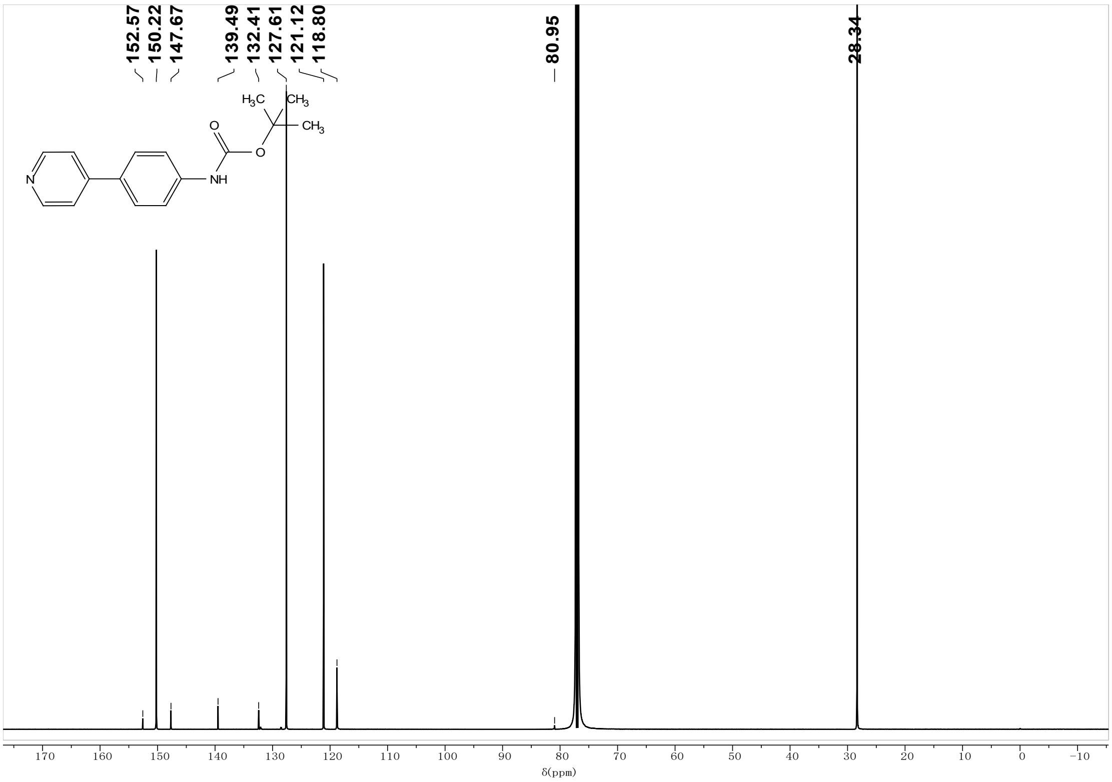


Figure S3. ^{13}C NMR spectrum of compound **1** in $CDCl_3$.

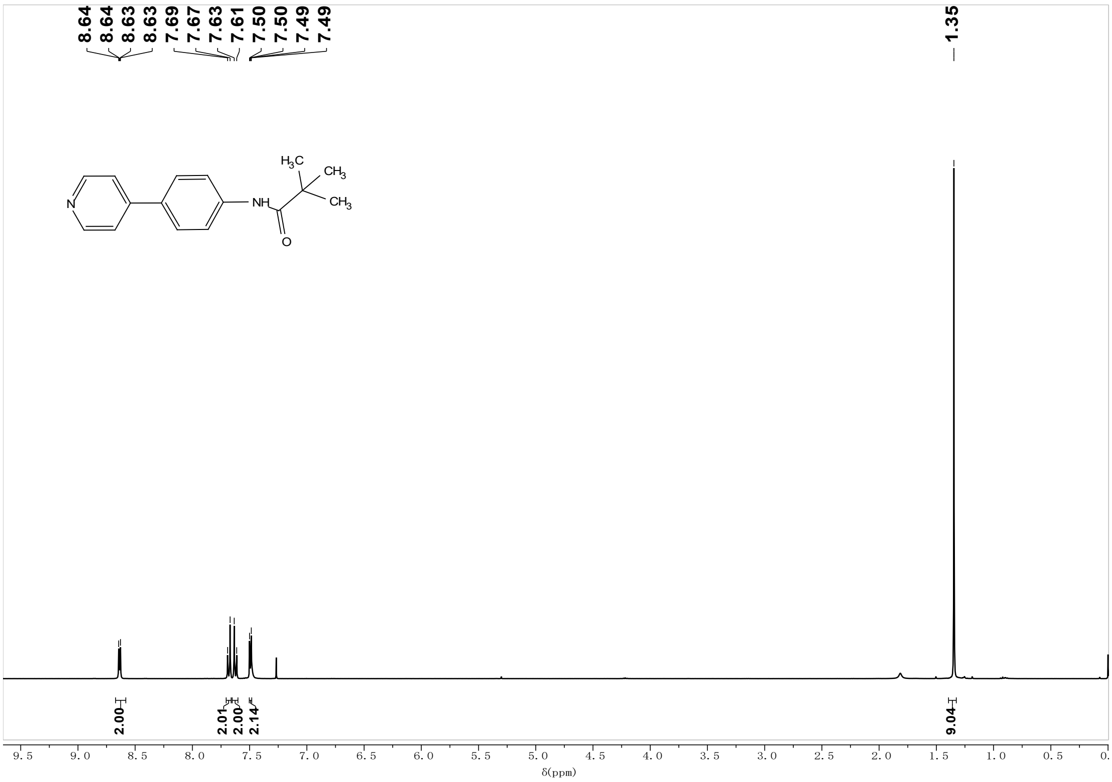


Figure S4. ^{1}H NMR spectrum of compound **2** in $CDCl_3$.

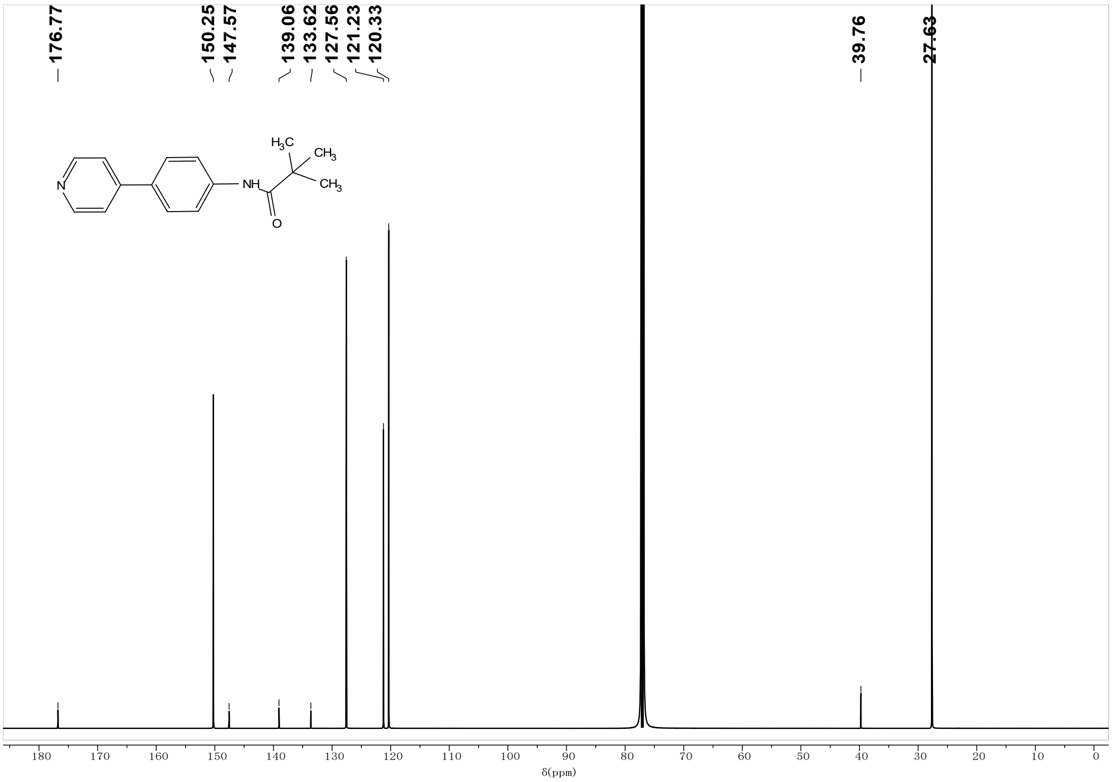


Figure S5. ^{13}C NMR spectrum of compound **2** in $CDCl_3$.

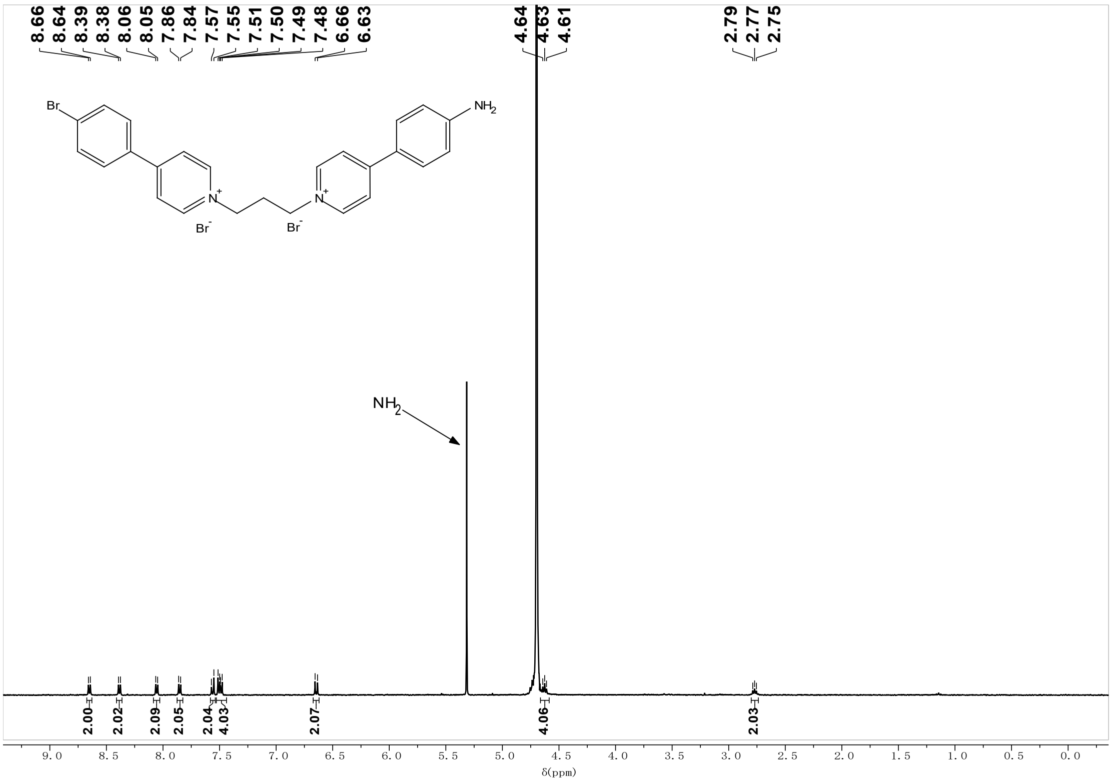


Figure S6. ^{1}H NMR spectrum of compound **Y1** in D_2O.

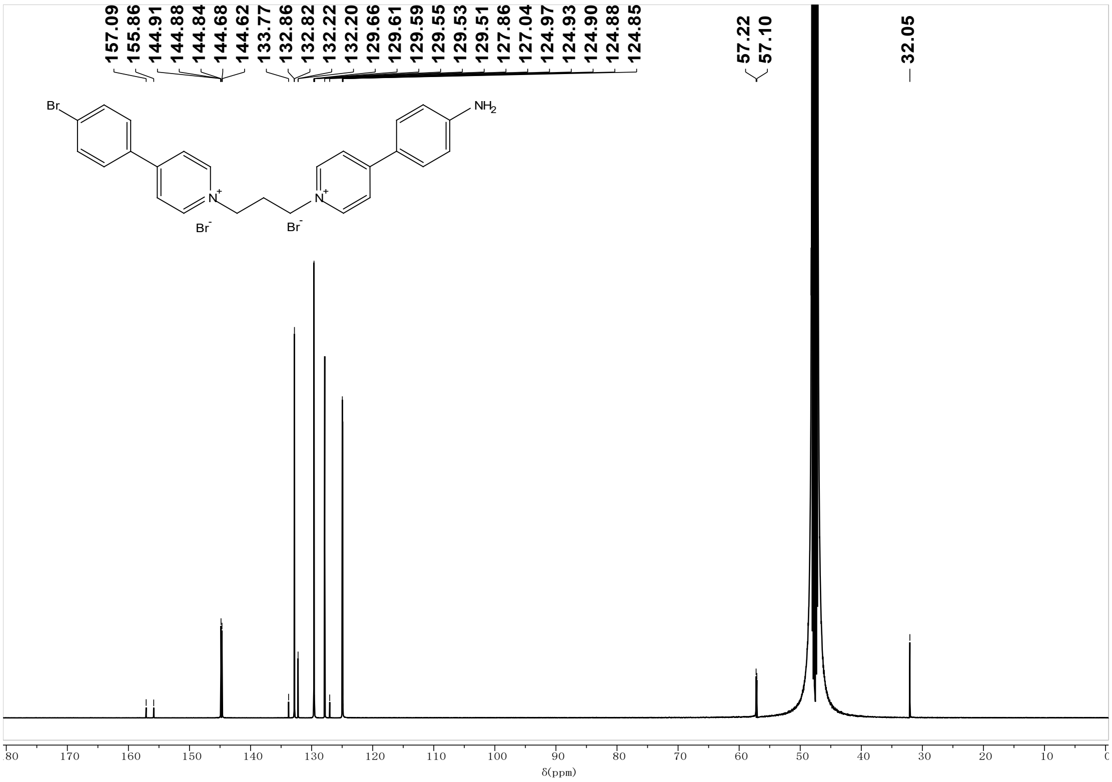
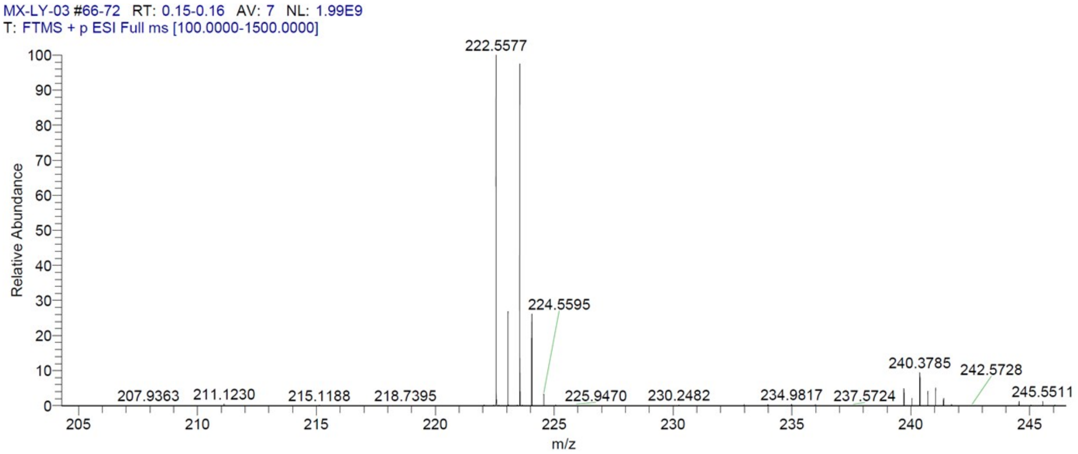


Figure S7. ^{13}C NMR spectrum of compound **Y1** in CD_3OD.



MX-LY-03#49-80 RT: 0.11-0.18 AV: 32
T: FTMS + p ESI Full ms [100.0000-1500.0000]
m/z= 222.13-222.71

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
222.5576	717601664.0	100.00	222.5571	0.44	$C_{25}H_{24}N_3Br$

Figure S8. HRMS spectrum of compound **Y1**.

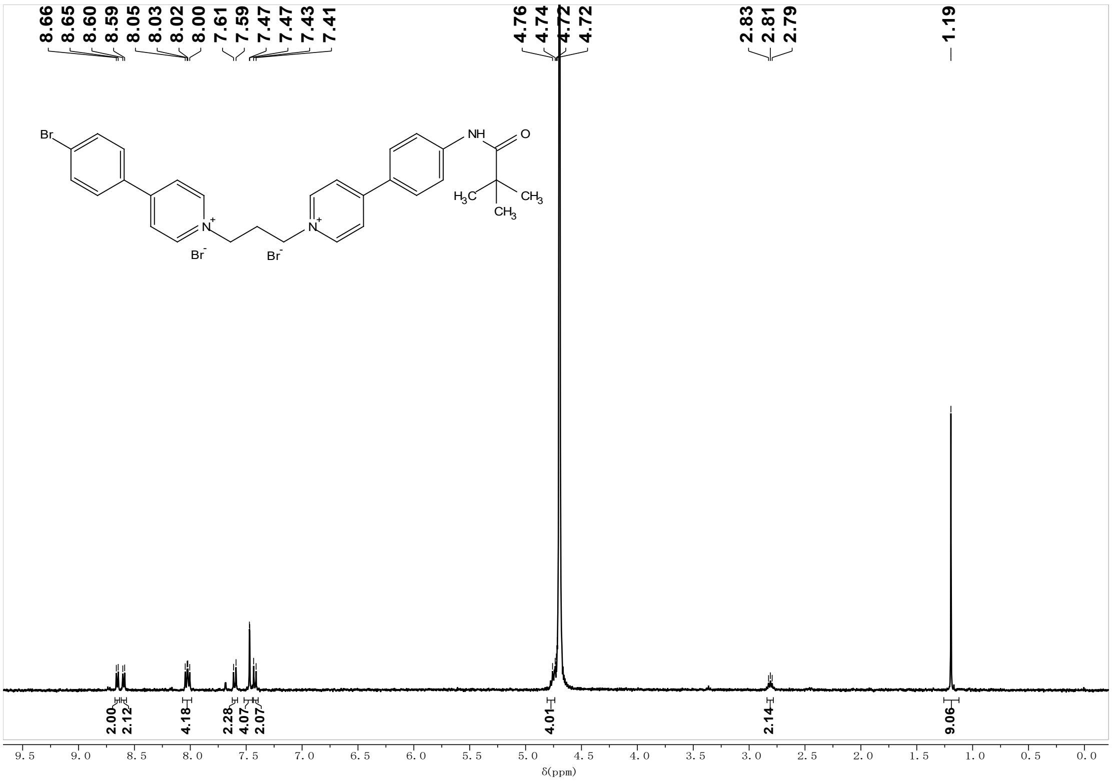


Figure S9. ^1H NMR spectrum of compound **Y2** in D_2O.

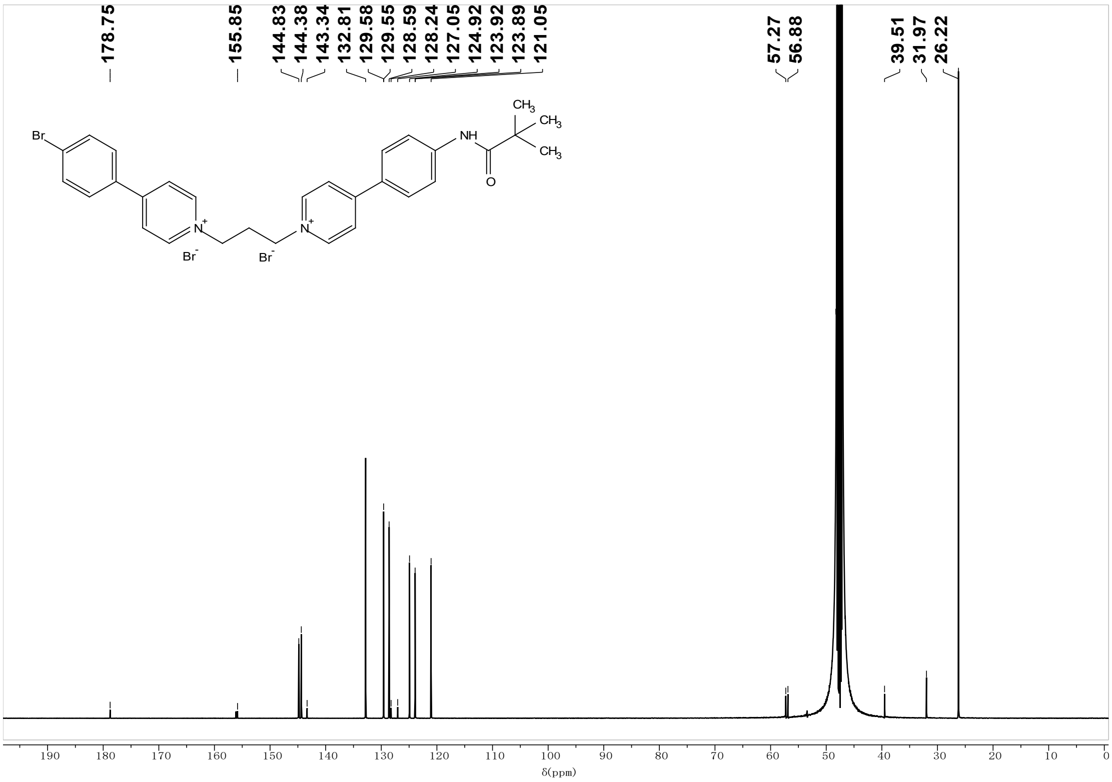
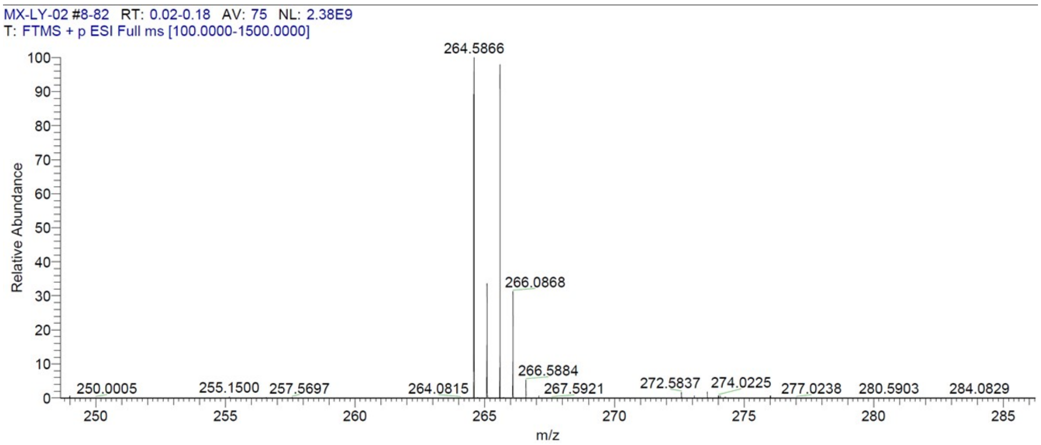
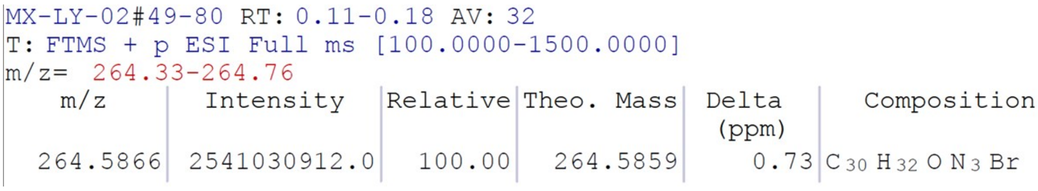


Figure S10. ^{13}C NMR spectrum of compound **Y2** in CD_3OD.





MX-LY-02#49-80 RT: 0.11-0.18 AV: 32
T: FTMS + p ESI Full ms [100.0000-1500.0000]
m/z= 264.33-264.76

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
264.5866	2541030912.0	100.00	264.5859	0.73	$C_{30}H_{32}ON_3Br$

Figure S11. HRMS spectrum of compound **Y2**.

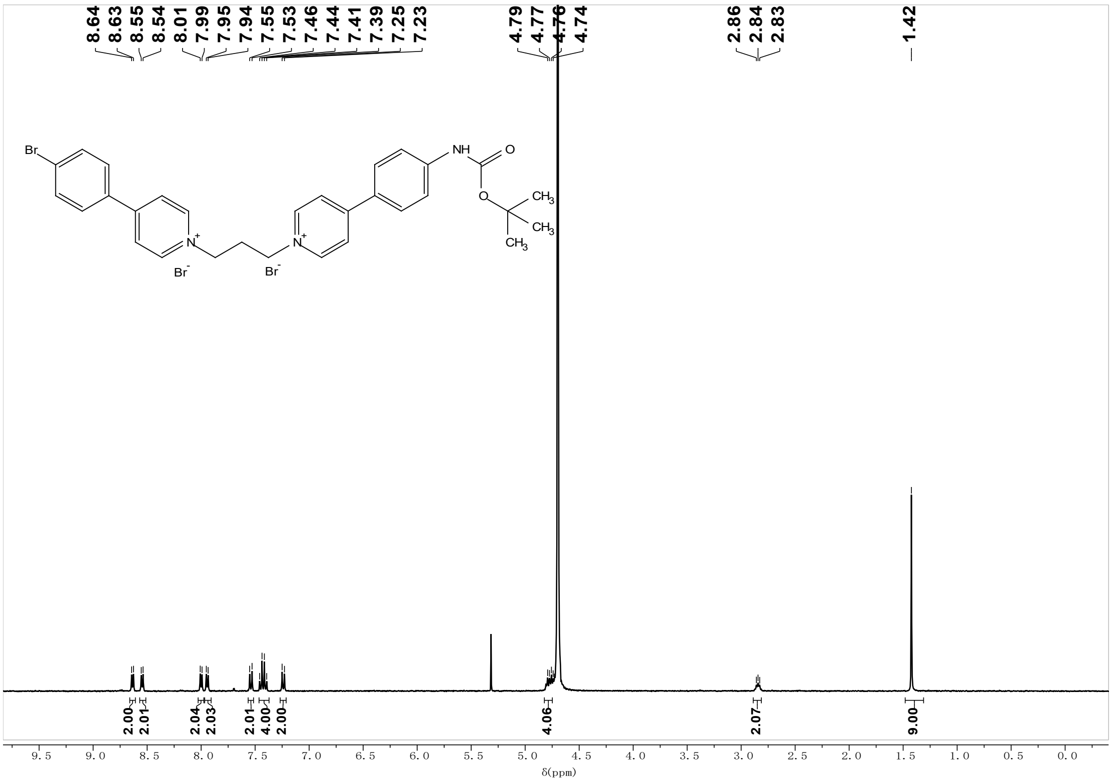


Figure S12. ^{1}H NMR spectrum of compound **Y3** in D_2O.

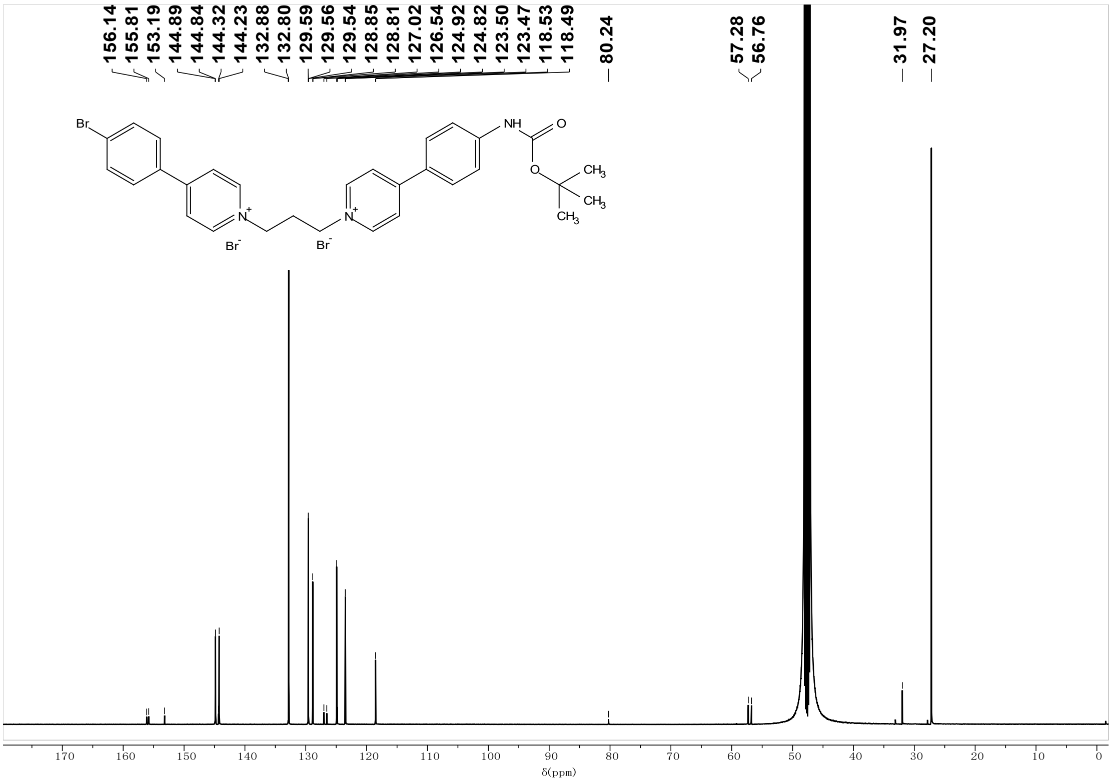
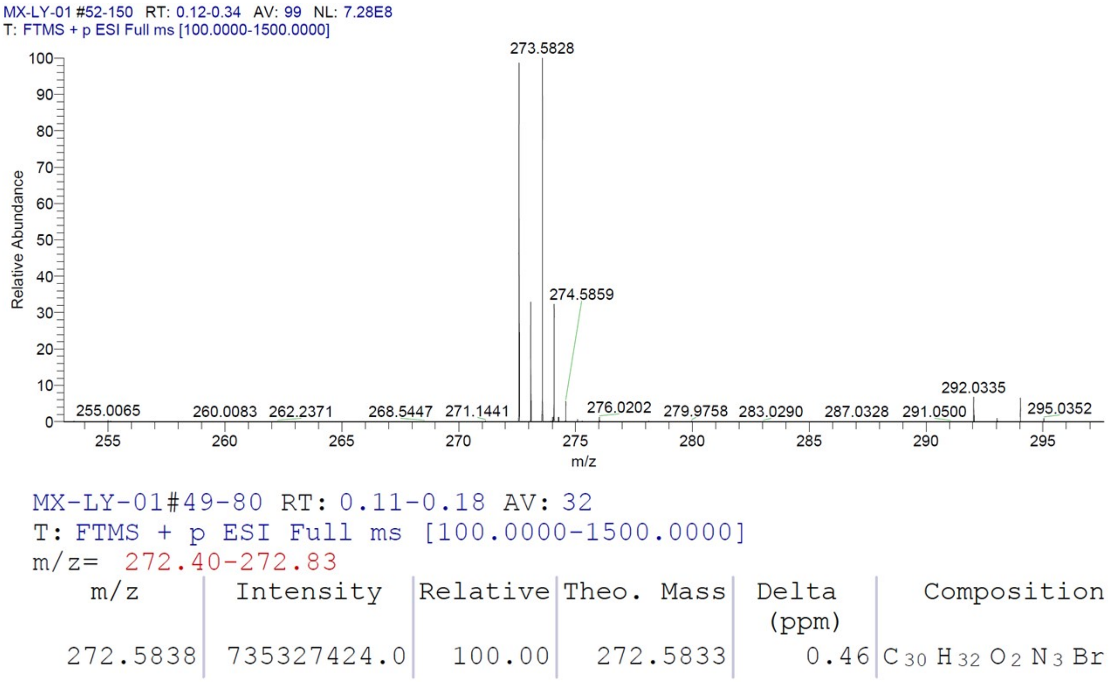


Figure S13. ^{13}C NMR spectrum of compound **Y3** in CD_3OD.

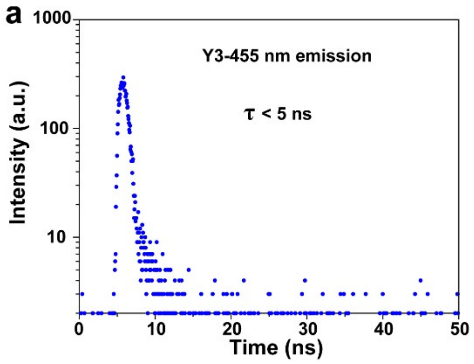


MX-LY-01#49-80 RT: 0.11-0.18 AV: 32
T: FTMS + p ESI Full ms [100.0000-1500.0000]
m/z= 272.40-272.83

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
272.5838	735327424.0	100.00	272.5833	0.46	$C_{30}H_{32}O_2N_3Br$

Figure S14. HRMS spectrum of compound **Y3**.

a



b

Luminescence	Emission wavelength	Lifetime
Fluorescence	455 nm	< 5 ns
Phosphorescence	580 nm	20 µs

Figure S15. (a) Lifetime of **Y3** at 455 nm in aqueous solution at room temperature. (b) A comprehensive summary of the fluorescence and phosphorescence emission characteristics along with the lifetime properties of Y3 molecule.

N ...	Cursor1-2: 400.07 - 421.20(...	Cursor3-4: 410.64 - 957.25(...	QuantumYield	QY(Corrected)	Factor a	Abs	Peak Wavele...	Peak Co...	Peak FW...	Peak Wavele...	Peak Co...	Peak FW...	RMS
1	106698439	---	---	---	---	---	410.64	43412.68	5.72	410.64	43412.68	5.72	---
6	8906693	1466632	0.015	---	---	0.917	411.39	3688.68	5.60	411.39	3688.68	5.60	---
3	8912025	1430718	0.015	---	---	0.916	411.39	3691.87	5.61	411.39	3691.87	5.61	---
4	8903273	1415094	0.014	---	---	0.917	411.39	3684.68	5.61	411.39	3684.68	5.61	---

N ...	Cursor1-2: 390.25 - 411.39(...	Cursor3-4: 413.65 - 957.25(...	QuantumYield	QY(Corrected)	Factor a	Abs	Peak Wavele...	Peak Co...	Peak FW...	Peak Wavele...	Peak Co...	Peak FW...	RMS
1	105770839	---	---	---	---	---	400.82	43389.84	5.79	413.65	246.89	41.86	---
2	4779059	1024777	0.010	---	---	0.955	403.84	2503.36	3.94	413.65	15.68	27.10	---
3	4698807	1052617	0.010	---	---	0.956	403.84	2456.05	3.96	413.65	18.42	26.79	---
4	4601188	977154	0.010	---	---	0.956	403.84	2379.85	3.98	950.74	18.35	0.88	---

Figure S16. The absolute quantum yield measurement of (a) **Y3** and (b) **Y2** molecule (0.1 mM) in water at room temperature.

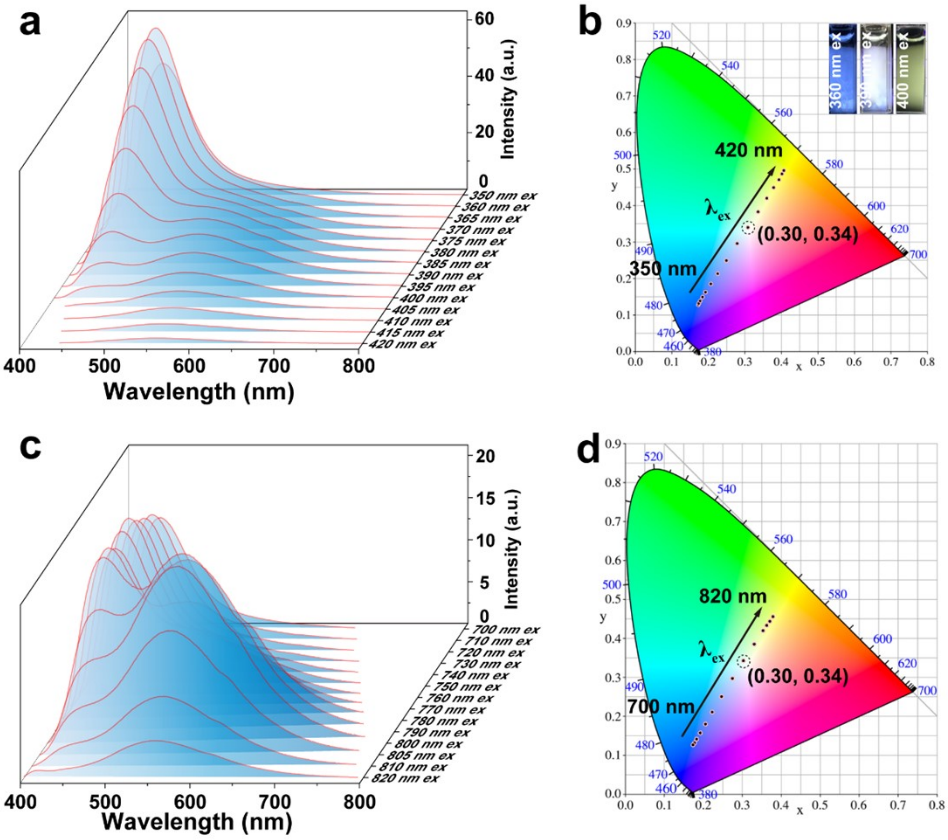


Figure S17. (a) PL spectra of **Y2** (1×10^{-4} M, excited by 350 nm to 420 nm) at aqueous solutions. (b) Chromaticity coordinate (CIE) of **Y2** with varying excitation wavelength in aqueous solution in accordance with (a). Inset images: The luminescent color of the **Y2** molecule upon excitation at wavelengths of 360 nm, 390 nm, and 400nm, respectively. (c) PL spectra of **Y2** (1×10^{-4} M, excited by 700 nm to 820 nm). (d) CIE of **Y2** with varying NIR excitation wavelength in accordance with (c).

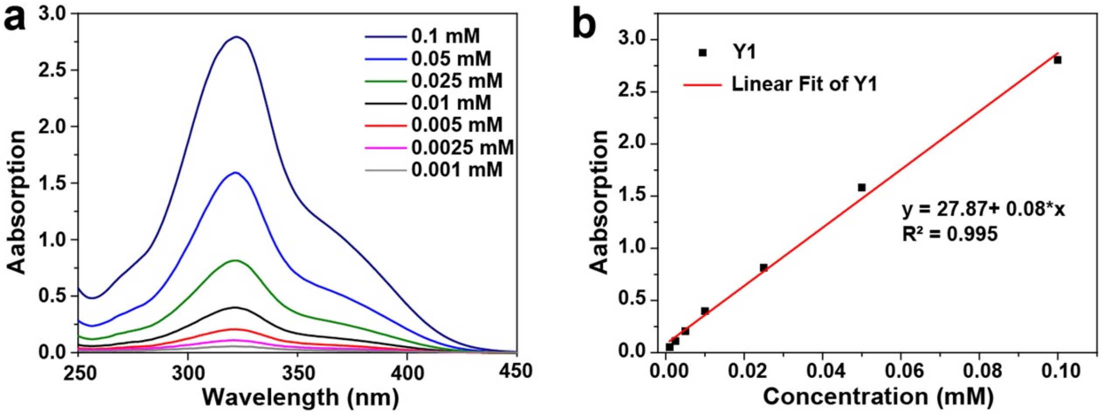


Figure S18. Absorption spectra of **Y3** aqueous solutions at various concentration respectively range from (a) 1.0 μM to 0.1 mM (1-mm optical length), 25 ^{o}C. (b) absorption intensities at 323 nm wavelength of **Y3** aqueous solutions at various concentrations respectively corresponding to (a).

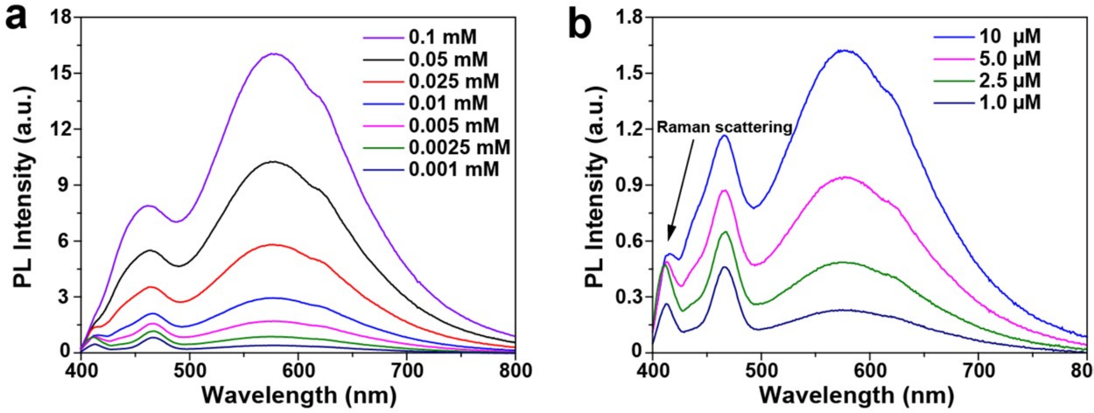


Figure S19. (a) PL spectra of aqueous **Y3** solutions at various concentrations (from 1 μM~0.1 mM). (b) Partial magnification of PL spectra at extremely diluted concentration (from 1~10 μM). Excitation wavelength 400 nm, 25 ^{o}C.

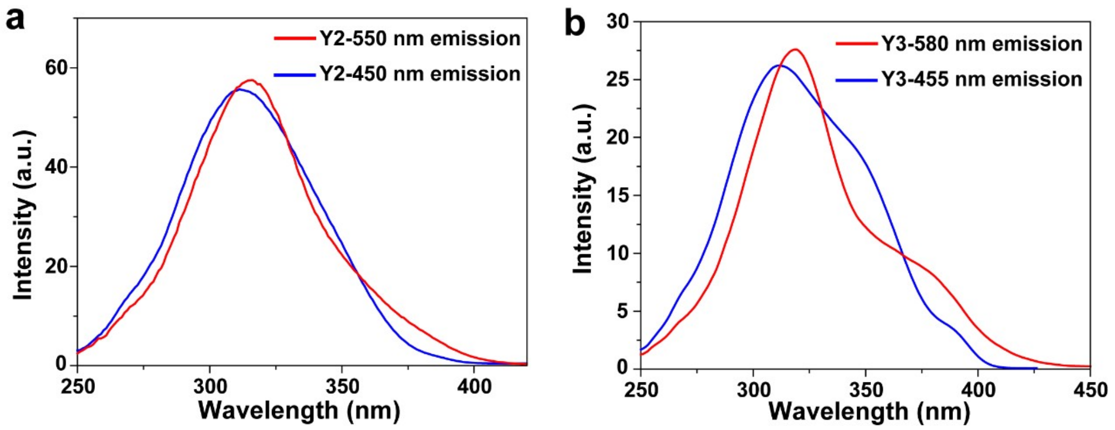


Figure S20. Excitation spectra of (a) **Y2** (1×10^{-4} M) at 550 nm and 450 nm, (b) **Y3** (1×10^{-4} M) at 580 nm and 455 nm in aqueous solution at room temperature.

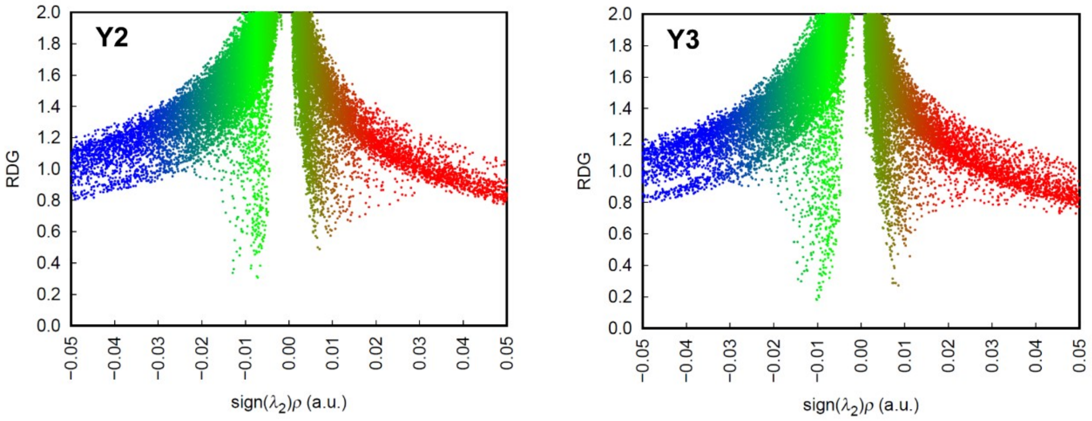


Figure S21. Plots of reduced density gradient vs the electron density (ρ) multiplied by the sign of the second Hessian eigenvalue (λ_2).

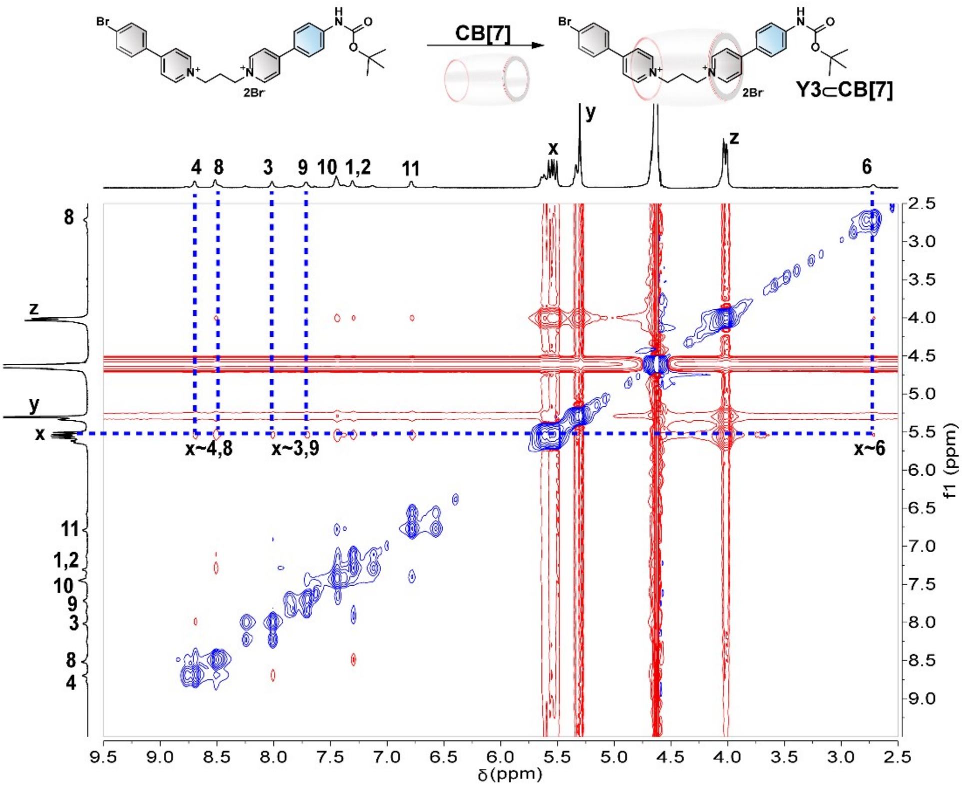


Figure S22. Partial 2D ROESY NMR spectrum of the complex **Y3**⊂CB[7] ([**Y3**] = [CB[7]] = 1 mM, in D_2O at 298 K).

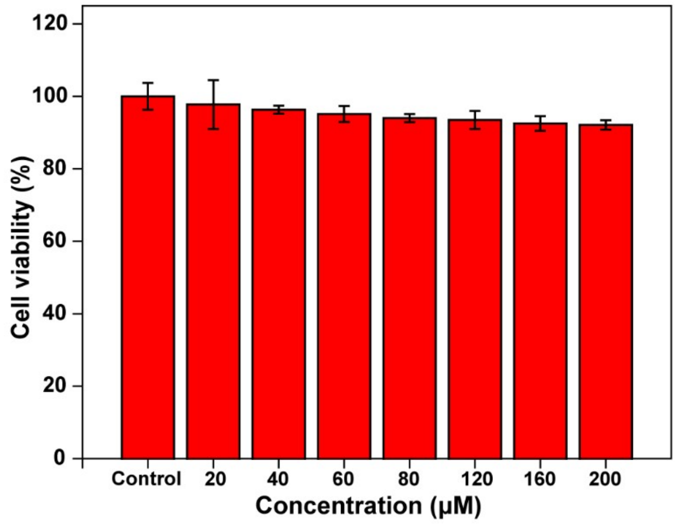


Figure S23. Cell toxicity of **Y3** towards HeLa cells with an incubation time of 24 h. Error bar represents s.d.

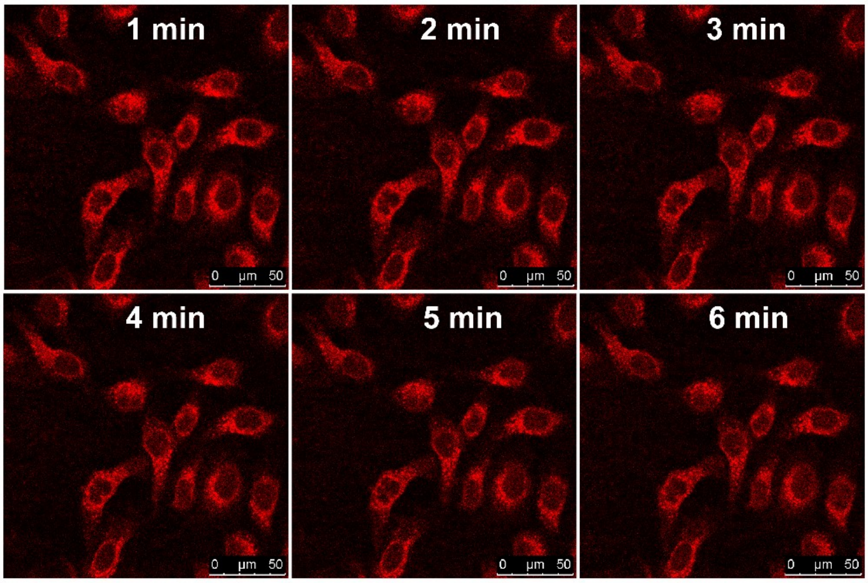


Figure S24. Intracellular photobleaching of RTP probe **Y3** at 405 nm laser (intensity 30 %) in HeLa cells. Phosphorescence images of HeLa cells stained with 100 μM **Y3** were captured after every 1 min irradiation.

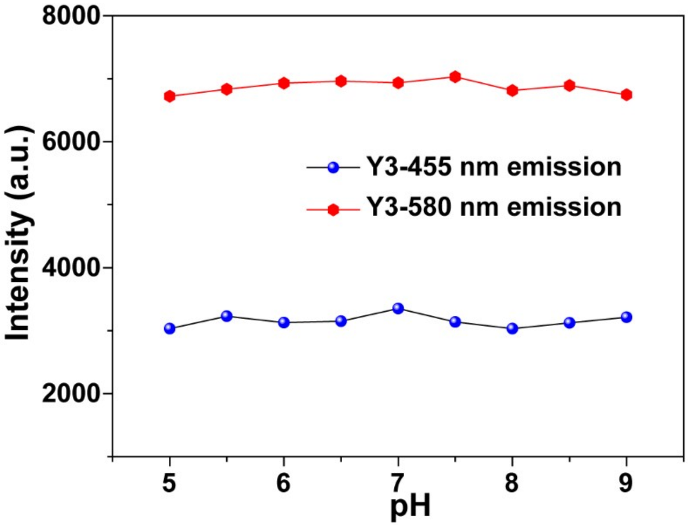


Figure S25. Fluorescence spectra of **Y3** (5×10^{-5} M) in PBS buffer (10 mM) at various pH's. λ_{ex} = 405 nm.

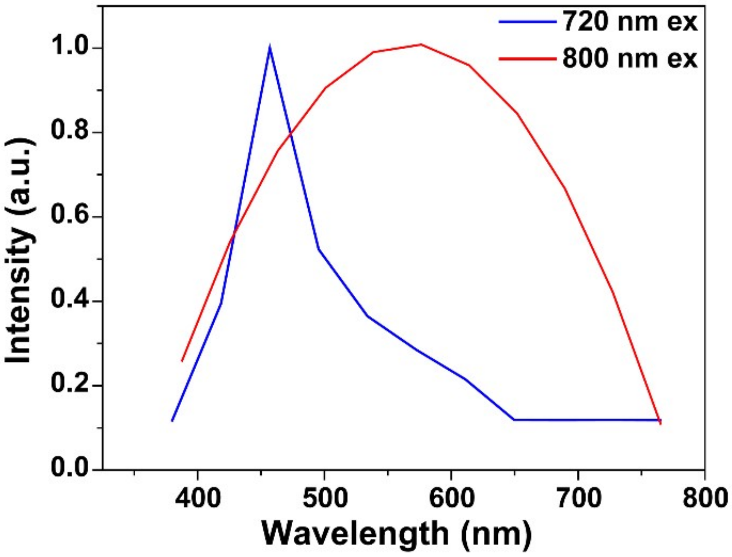


Figure S26. Emission spectra of **Y3** molecule at different excitation intensities (mW) by an 800 nm and 700 nm femtosecond pulsed laser light.

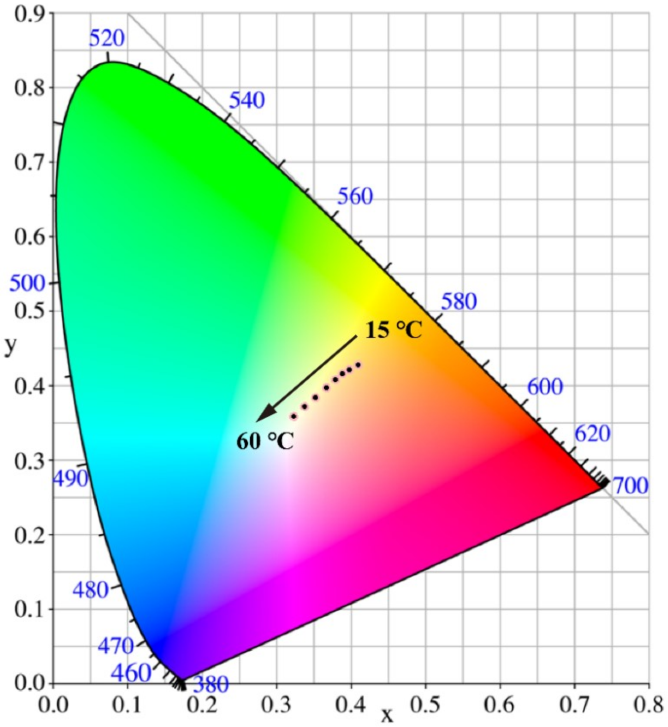
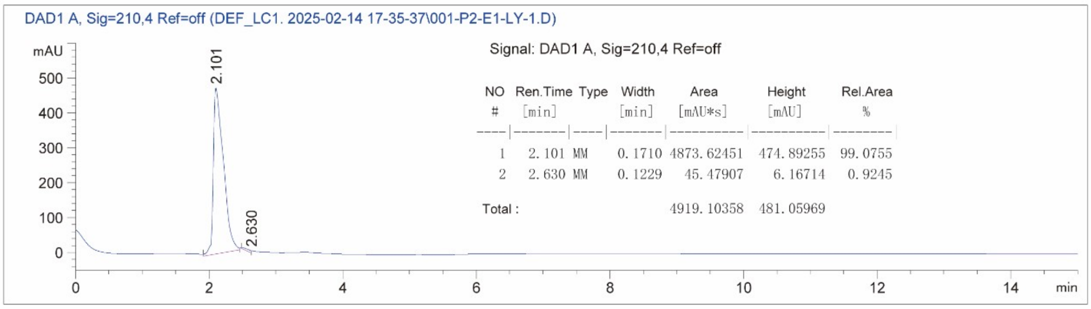


Figure S27. CIE of **Y3** with varying temperature (15 °C to 60 °C) in aqueous solution in accordance with Figure 7a.



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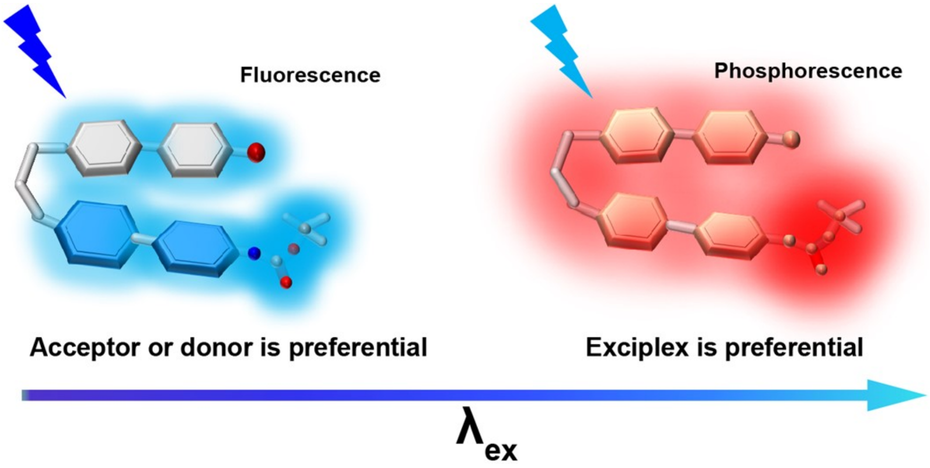
Signal: DAD1 A, Sig=210,4 Ref=off

NO  Ren.Time Type  Width     Area        Height     Rel.Area
 #   [min]         [min]   [mAU*s]      [mAU]         %
----|--------|----|-------|----------|----------|---------
  1   2.101 MM    0.1710 4873.62451  474.89255  99.0755
  2   2.630 MM    0.1229   45.47907    6.16714   0.9245

Total :                  4919.10358  481.05969
```

Figure S28. HPLC Spectra of the Y3 Molecule. High Performance Liquid Chromatography (HPLC) Conditions: Column: Agilent Inert Sustain C18 (150 mm×4.6 mm×5 µm); Detection: 210 nm; Flow rate: 1 mL/min; Temperature: 35 °C; Injection load: 2 µL; Solvent: MeOH; Concentration: 0.2 mg/mL; Run time: 15 min; Mobile phase A: water; Mobile phase B: MeOH; Gradient program: Mobile phase A/Mobile phase B = 20/80; tR = 2.101 min, purity: 99.07%.



Scheme S1. Possible mechanism of excitation-dependent luminescence.

Coordinates of optimized Y1 molecule

C	-3.03144	0.64665	0.13415
C	-4.20887	-0.02608	-0.11141
C	-5.41062	0.38655	0.49706
C	-5.33446	1.49899	1.35804
C	-4.13288	2.13827	1.57472
H	-2.0898	0.34953	-0.30947
H	-4.17446	-0.89243	-0.75989
H	-6.21531	1.89236	1.84957
H	-4.04263	2.99837	2.22605
C	-6.68392	-0.31269	0.24626
C	-7.69159	-0.34653	1.22745
C	-6.91748	-0.95825	-0.98186

C	-8.89374	-1.00787	0.99573
H	-7.53192	0.11651	2.1956
C	-8.12037	-1.6127	-1.22874
H	-6.1724	-0.92615	-1.77003
C	-9.0978	-1.63334	-0.23406
H	-9.65837	-1.03918	1.76343
H	-8.29592	-2.09481	-2.18358
C	-1.72365	2.45068	1.17764
H	-1.74065	2.84255	2.19638
H	-0.91945	1.7156	1.1125
C	-1.55835	3.57543	0.14713
H	-2.39747	4.27453	0.22783
H	-1.58437	3.16217	-0.86692
C	-0.28204	4.4019	0.34679
H	-0.28497	5.25085	-0.33895
H	-0.21365	4.79576	1.36228
C	1.73367	3.18993	1.11509
C	1.34116	3.37755	-1.19136
C	2.88632	2.47323	0.88564
H	1.39978	3.44259	2.11329
C	2.48442	2.66546	-1.47023
H	0.69291	3.75981	-1.9698
C	3.30868	2.18018	-0.42965
H	3.47247	2.17132	1.74416
H	2.71867	2.47256	-2.50939
C	4.53361	1.42406	-0.69992
C	5.22626	1.56474	-1.92024
C	5.06558	0.52856	0.24801
C	6.38814	0.85629	-2.16798
H	4.87803	2.26356	-2.67355
C	6.22166	-0.20009	0.00532
H	4.55021	0.36174	1.18845
C	6.90924	-0.04226	-1.21293
H	6.91094	1.00034	-3.10944
H	6.58568	-0.89039	0.75082
N	-2.99742	1.71549	0.96687
N	0.96598	3.6346	0.08812
Br	-10.74816	-2.53423	-0.5627
N	8.08044	-0.71501	-1.5663
H	8.43749	-0.51142	-2.49208
H	7.82292	-1.91854	-1.07657

Coordinates of the excited state of Y1 molecule

C	-1.03545	2.95884	-2.47812

C	-1.00951	3.89629	-3.48771
C	-1.63807	5.14599	-3.32144
C	-2.28362	5.37259	-2.09017
C	-2.28306	4.40334	-1.10989
H	-0.5731	1.98504	-2.57738
H	-0.52032	3.6321	-4.41681
H	-2.77261	6.31469	-1.87556
H	-2.76445	4.54592	-0.15074
C	-1.62221	6.16487	-4.38677
C	-1.80186	5.79961	-5.73323
C	-1.42734	7.52304	-4.07621
C	-1.78187	6.75744	-6.74257
H	-1.9257	4.75707	-6.00726
C	-1.41857	8.49074	-5.07607
H	-1.3144	7.8398	-3.04453
C	-1.59328	8.09684	-6.40261
H	-1.90635	6.46451	-7.77874
H	-1.28256	9.53646	-4.82516
C	-1.63972	2.20169	-0.21689
H	-2.55824	2.3261	0.35965
H	-1.67151	1.2214	-0.69554
C	-0.39566	2.37285	0.66399
H	-0.28542	1.49924	1.31553
H	-0.51768	3.24417	1.31668
C	0.90759	2.49359	-0.1357
H	1.75678	2.49007	0.5503
H	1.03317	1.65512	-0.82291
C	0.82008	3.71473	-2.28822
C	1.25688	4.92213	-0.32426
C	0.89006	4.86356	-3.03916
H	0.63823	2.7451	-2.73422
C	1.33683	6.09577	-1.03214
H	1.39446	4.88527	0.74915
C	1.15233	6.11993	-2.43814
H	0.76888	4.76699	-4.1102
H	1.52536	7.0035	-0.47388
C	1.23318	7.35059	-3.2117
C	0.97013	8.61141	-2.62514
C	1.57679	7.33936	-4.58461
C	1.05044	9.78299	-3.35212
H	0.72936	8.68302	-1.56971
C	1.6467	8.50223	-5.32656
H	1.75645	6.39855	-5.09436
C	1.38848	9.75783	-4.72633

H	0.85994	10.73602	-2.86673
H	1.89597	8.45636	-6.38291
N	-1.66516	3.21315	-1.30515
N	0.99564	3.7386	-0.94075
Br	-1.57372	9.41813	-7.7801
N	1.50511	10.91558	-5.44118
H	1.0992	11.76231	-5.06629
H	1.52298	10.86575	-6.45084

Coordinates of optimized Y2 molecule

C	-2.93597	0.85386	-0.08305
C	-4.12457	0.15119	-0.33112
C	-5.25488	0.42116	0.44261
C	-5.16828	1.39117	1.44052
C	-3.95605	2.0636	1.64363
H	-2.06635	0.65036	-0.67219
H	-4.16398	-0.58528	-1.1062
H	-6.02016	1.61977	2.04604
H	-3.88579	2.80928	2.40722
C	-6.57522	-0.33611	0.20313
C	-7.69704	-0.05462	0.99529
C	-6.6561	-1.30618	-0.80473
C	-8.89901	-0.74201	0.779
H	-7.63573	0.68537	1.76584
C	-7.85848	-1.99406	-1.02074
H	-5.80016	-1.52164	-1.40953
C	-8.97985	-1.71119	-0.22917
H	-9.75504	-0.52675	1.38382
H	-7.91997	-2.73502	-1.79024
C	-1.6232	2.50444	1.13365
H	-1.56528	2.77609	2.16693
H	-0.79312	1.87755	0.88268
C	-1.58864	3.77554	0.26608
H	-2.4267	4.39388	0.51011
H	-1.63475	3.50229	-0.76775
C	-0.28704	4.55443	0.5357
H	-0.27328	5.43835	-0.06726
H	-0.24409	4.82552	1.56981
C	1.43059	2.94132	1.14762
C	1.37439	3.75744	-1.0466
C	2.56127	2.16188	0.86039
H	1.00497	2.91646	2.12927
C	2.50089	2.99791	-1.39

H	0.90518	4.37393	-1.78495
C	3.10974	2.19742	-0.42295
H	2.99939	1.54678	1.61829
H	2.89167	3.03301	-2.38556
C	4.36522	1.3718	-0.76745
C	4.89504	1.41105	-2.06436
C	4.97971	0.58362	0.21529
C	6.04171	0.6679	-2.37721
H	4.42471	2.00908	-2.81583
C	6.1284	-0.15786	-0.09714
H	4.57316	0.54867	1.20462
C	6.65963	-0.11564	-1.39331
H	6.44571	0.69897	-3.36754
H	6.59994	-0.75627	0.65439
N	-2.88015	1.78154	0.88861
N	0.87779	3.72104	0.20143
Br	-10.61932	-2.646	-0.52389
N	7.86447	-0.89371	-1.72048
H	7.83723	-1.16105	-2.68409
C	7.91439	-2.09866	-0.87954
O	6.89103	-2.79925	-1.09097
C	9.17419	-2.91471	-1.22389
C	10.4225	-2.02987	-1.04959
H	11.29206	-2.64952	-0.98036
H	10.51657	-1.37601	-1.89132
H	10.3262	-1.4493	-0.15597
C	9.27128	-4.13037	-0.2835
H	8.49605	-4.82836	-0.52167
H	10.22458	-4.60066	-0.4058
H	9.16069	-3.80673	0.73037
C	9.08858	-3.39993	-2.68294
H	9.15001	-2.5596	-3.34246
H	9.89757	-4.07083	-2.88375
H	8.15866	-3.9065	-2.83637

Coordinates of the excited state of Y2 molecule

C	4.47966	1.25838	1.61403
C	3.11777	1.46389	1.56683
C	2.45498	1.59518	0.33062
C	3.2533	1.51286	-0.82719
C	4.6128	1.30876	-0.7297
H	5.02029	1.16316	2.54699
H	2.58296	1.54879	2.50439

H	2.81963	1.58343	-1.81673
H	5.25228	1.23574	-1.60026
C	0.9986	1.80992	0.25329
C	0.2243	1.1482	-0.71719
C	0.35353	2.67981	1.15149
C	-1.15021	1.35032	-0.79534
H	0.69491	0.49326	-1.443
C	-1.02201	2.88053	1.08991
H	0.9175	3.18309	1.92997
C	-1.76155	2.21425	0.11302
H	-1.7356	0.84565	-1.55536
H	-1.51136	3.54187	1.79571
C	6.67418	0.91318	0.55636
H	7.1425	1.41968	-0.2897
H	7.03395	1.3845	1.47273
C	6.96011	-0.59418	0.53546
H	8.00436	-0.77439	0.81195
H	6.82644	-0.98753	-0.47803
C	6.10324	-1.39061	1.52712
H	6.43656	-2.4296	1.54637
H	6.19032	-0.99528	2.5406
C	3.77352	-0.62867	1.86493
C	4.2137	-2.1955	0.17369
C	2.43378	-0.62691	1.54871
H	4.1768	-0.03287	2.6737
C	2.88452	-2.22743	-0.17866
H	4.96133	-2.793	-0.33265
C	1.93408	-1.43406	0.50321
H	1.77435	-0.01238	2.1481
H	2.59636	-2.86279	-1.00643
C	0.51253	-1.45374	0.15105
C	0.08513	-1.79703	-1.14827
C	-0.48053	-1.13075	1.09604
C	-1.25879	-1.82399	-1.47443
H	0.80558	-2.08432	-1.90689
C	-1.83128	-1.13851	0.77707
H	-0.19918	-0.82826	2.09963
C	-2.24497	-1.4934	-0.52091
H	-1.55901	-2.1117	-2.47818
H	-2.55956	-0.86597	1.52548
N	5.21498	1.18163	0.47807
N	4.65605	-1.40152	1.18256
Br	-3.64803	2.48901	0.01807
N	-3.57087	-1.54147	-0.95546

C	-4.79735	-1.34349	-0.33509
O	-5.83121	-1.46176	-0.97501
C	-5.41227	-1.02288	0.88109
C	-6.17892	0.18675	0.34218
H	-5.51265	1.05121	0.25094
H	-6.62263	-0.02431	-0.63191
H	-6.97911	0.4468	1.04323
C	-6.27003	-2.2882	0.95077
H	-5.66886	-3.13921	1.28846
H	-7.07846	-2.13508	1.67358
H	-6.70947	-2.52613	-0.01907
C	-4.78891	-0.71128	2.24268
H	-4.19379	-1.55745	2.60068
H	-4.14428	0.17156	2.18261
H	-5.57954	-0.51193	2.97273
H	-3.70166	-1.78862	-1.92901

Coordinates of optimized Y3 molecule

C	-3.36243	0.52566	-0.02422
C	-4.58402	-0.10329	-0.13293
C	-5.74425	0.48642	0.40655
C	-5.58288	1.72906	1.04995
C	-4.34017	2.31842	1.13552
H	-2.45007	0.09407	-0.41586
H	-4.61686	-1.072	-0.61527
H	-6.42807	2.2584	1.47153
H	-4.18206	3.27296	1.62079
C	-7.06252	-0.16549	0.30693
C	-8.03718	0.03139	1.30222
C	-7.3729	-0.99569	-0.78551
C	-9.28247	-0.58344	1.21545
H	-7.81865	0.64183	2.17238
C	-8.61942	-1.60558	-0.88864
H	-6.65323	-1.14574	-1.58368
C	-9.56321	-1.39476	0.11636
H	-10.02164	-0.43618	1.99441
H	-8.85411	-2.23151	-1.74185
C	-1.92457	2.39671	0.67445
H	-1.90313	2.96896	1.60397
H	-1.17093	1.6106	0.74565
C	-1.70194	3.29976	-0.54562
H	-2.5012	4.04634	-0.60063
H	-1.75638	2.70681	-1.4652

C	-0.38216	4.07813	-0.49393
H	-0.33283	4.77405	-1.33321
H	-0.29822	4.65804	0.42649
C	1.59238	2.9848	0.51938
C	1.14961	2.6264	-1.75749
C	2.70275	2.17159	0.45696
H	1.29607	3.49036	1.42958
C	2.24728	1.80467	-1.86844
H	0.50241	2.84291	-2.59778
C	3.07208	1.54432	-0.75189
H	3.29597	2.05625	1.35514
H	2.44425	1.34994	-2.83089
C	4.25102	0.67558	-0.84764
C	4.92254	0.49497	-2.07093
C	4.74654	-0.00965	0.28045
C	6.04289	-0.31997	-2.16062
H	4.60004	1.02886	-2.95872
C	5.85401	-0.83895	0.19294
H	4.23046	0.06176	1.23238
C	6.53196	-0.99693	-1.02985
H	6.55363	-0.41326	-3.11228
H	6.18942	-1.37911	1.06811
N	-3.24587	1.72103	0.60385
N	0.82148	3.20566	-0.57452
Br	-11.27356	-2.23196	-0.01642
N	7.63974	-1.86737	-1.16661
C	8.71903	-1.92833	-0.2907
O	9.66962	-2.6719	-0.48887
O	8.58321	-1.08046	0.7391
C	9.62331	-0.96172	1.78997
C	9.78675	-2.29743	2.51966
H	8.82034	-2.64546	2.90023
H	10.2058	-3.06106	1.86275
H	10.45919	-2.16161	3.37352
C	10.93097	-0.46383	1.16858
H	10.75897	0.46329	0.61115
H	11.65276	-0.2526	1.96487
H	11.35979	-1.20815	0.49598
C	9.02756	0.0968	2.72067
H	8.8604	1.03588	2.18351
H	8.07303	-0.24255	3.13577
H	9.71591	0.28956	3.54946
H	7.73864	-2.38654	-2.01554

Coordinates of the excited state of Y3 molecule

C	-5.22321	7.90514	0.6347
C	-4.97577	8.86624	1.59088
C	-3.68071	9.03532	2.11905
C	-2.67919	8.17589	1.62613
C	-2.97533	7.22758	0.67094
H	-6.20814	7.74314	0.21588
H	-5.80886	9.46296	1.94037
H	-1.65372	8.25317	1.96477
H	-2.22728	6.55627	0.26858
C	-3.38919	10.05967	3.13828
C	-2.20761	10.82075	3.07605
C	-4.28949	10.29826	4.19285
C	-1.92736	11.78662	4.0377
H	-1.479	10.64165	2.2923
C	-4.02497	11.26958	5.15346
H	-5.22312	9.74867	4.25336
C	-2.8424	12.00398	5.06762
H	-1.00778	12.35836	3.98788
H	-4.73191	11.45543	5.95388
C	-4.5174	6.10145	-0.88262
H	-3.85561	5.24978	-0.71424
H	-5.54494	5.76451	-0.73441
C	-4.30729	6.70759	-2.27646
H	-4.72706	6.03895	-3.03547
H	-3.23656	6.79824	-2.48879
C	-4.99788	8.06437	-2.4612
H	-4.9092	8.38129	-3.50171
H	-6.06091	8.00978	-2.22033
C	-5.04661	9.57706	-0.50374
C	-3.22955	9.70604	-1.98382
C	-4.50912	10.57154	0.28176
H	-5.99673	9.11118	-0.27584
C	-2.65341	10.70248	-1.2308
H	-2.77105	9.32485	-2.8876
C	-3.27875	11.17712	-0.05547
H	-5.07594	10.89447	1.14559
H	-1.69832	11.09414	-1.5569
C	-2.68885	12.24047	0.76093
C	-1.29765	12.47132	0.76798
C	-3.48812	13.07194	1.56921
C	-0.74522	13.48283	1.53278
H	-0.63838	11.88064	0.14065

C	-2.94455	14.07988	2.35338
H	-4.5602	12.91176	1.62239
C	-1.55518	14.30656	2.34302
H	0.32791	13.64979	1.50256
H	-3.59021	14.68264	2.97354
N	-4.23299	7.09793	0.18207
N	-4.41236	9.14505	-1.62306
Br	-2.46933	13.33395	6.38492
N	-0.89712	15.29031	3.08352
C	-1.32083	16.30233	3.93475
O	-0.50216	17.04457	4.45554
O	-2.6474	16.33688	4.08306
C	-3.30588	17.34806	4.95484
C	-2.84188	17.16137	6.40094
H	-3.00475	16.1275	6.72362
H	-1.78506	17.40702	6.51525
H	-3.42716	17.81748	7.05392
C	-3.02559	18.75284	4.41662
H	-3.32235	18.82526	3.36479
H	-3.61364	19.48008	4.98649
H	-1.96937	19.01102	4.50641
C	-4.78628	16.99296	4.80677
H	-5.10252	17.07222	3.76175
H	-4.97865	15.97336	5.15597
H	-5.39178	17.68195	5.40383
H	0.1111	15.30654	2.98752

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