

## Electronic supplementary information (ESI)

### **Emissions from the triad of triphenylamine-benzothiadiazole-monocarbaborane and its applications as the fluorescent chemosensor and white OLED**

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## Experimental Procedures

### Material and Instruments

Unless otherwise mentioned, solvents and reagents were purchased from commercial sources and used as received,  $\text{CB}_{11}\text{H}_{11}\text{C}\equiv\text{CH}\cdot\text{Cs}^+$  was synthesized according to previous literature. For the purpose of the measurement of photophysical properties, THF was distilled from sodium. Melting points were measured with a micro melting point apparatus. Infrared spectra were obtained with an FTIR spectrometer. NMR spectra were operated at 400 or 500 MHz for  $^1\text{H}$  NMR, 100 or 125 MHz for  $^{13}\text{C}$  NMR, 160 MHz for  $^{11}\text{B}$  NMR. All the NMR spectra were recorded at room temperature. Chemical shifts were quoted in parts per million (ppm) referenced to the appropriate solvent peak or 0.0 ppm for tetramethylsilane. The following abbreviations are used to describe peak patterns as appropriate: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet. Coupling constants  $J$  were reported in hertz. High-resolution mass spectra (HRMS) data were obtained with an electron ionization time-of-flight (EI-TOF) mass spectrometer. Flash column chromatography was performed employing 300-400 mesh silica gel. Thin layer chromatography (TLC) was performed on silica gel HSGF254. The absorption spectra were measured using UV-vis spectrometer. FL spectra were recorded on a fluorospectro photometer with a xenon lamp excitation source. PL decay dynamics were measured on a timecorrelated single-photon counting (TCSPC) spectrofluorometer at room temperature, and the compounds were excited by a 405 nm picosecond laser diode. Cyclic voltammetry measurements were performed on an electrochemical analyzer in acetonitrile at room temperature. Thermogravimetric Analysis (TGA) was obtained with a thermal analyzer at heating and cooling rates of 10 K/min under an  $\text{N}_2$  atmosphere.

Device Fabrication: Before device fabrication, the ITO glass substrates were pre-cleaned carefully. Then hole transporting material PEDOT:PSS was made with 4000 r/s for 45 s and annealing 25 min at 150 °C. Emission Layer was prepared in chlorobenzene with 30 mg/mL. Then it was made with 2000 r/s for 45 s and annealing 25 min at 50 °C, annealing 25 min at 150 °C for PVK. After the organic film deposition, 30 or 35 nm of TPBi, 1 nm of LiF and 50 nm of aluminum were thermally evaporated onto the organic surface.

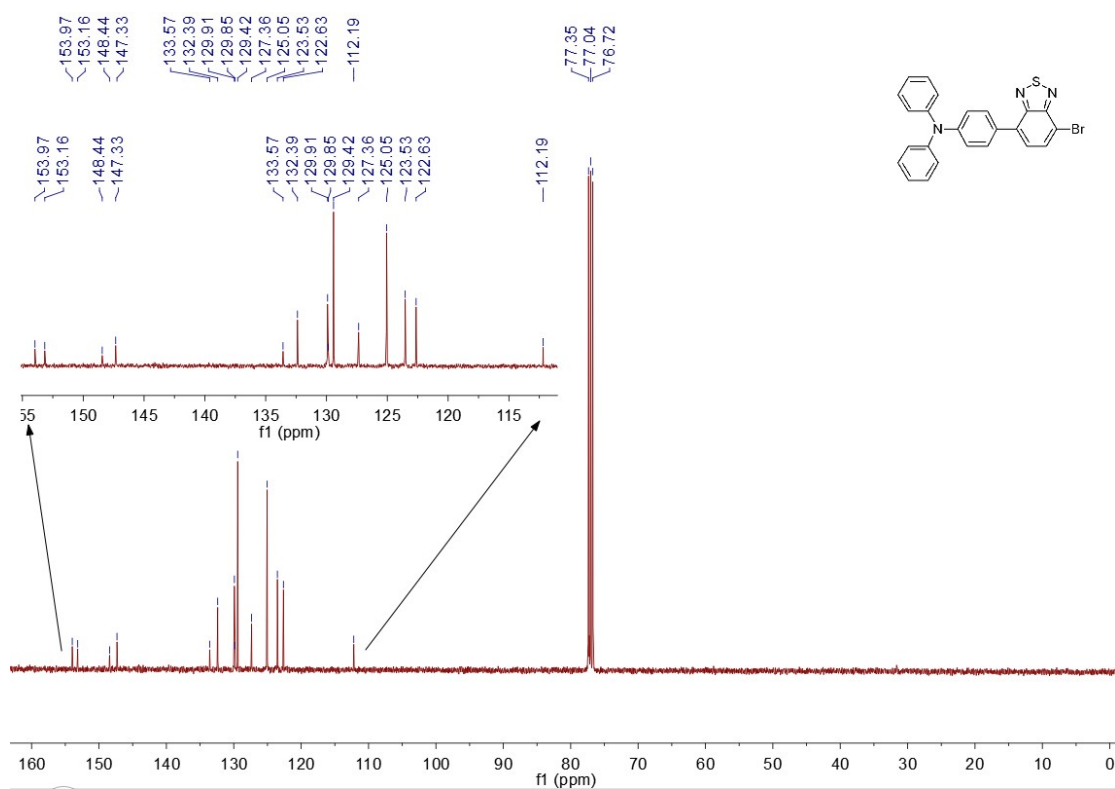
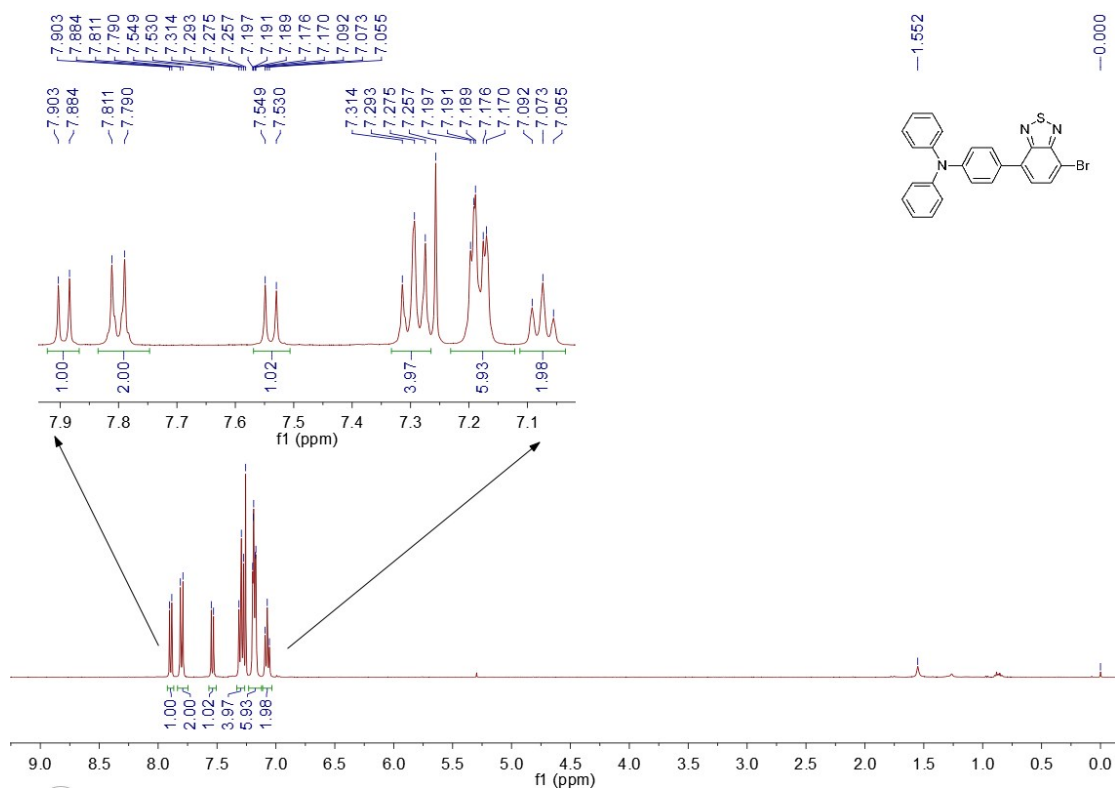
### General procedure for synthesis of organic molecular

#### 1. Synthesis of TPA-BTD-Br

TPA-BTD-Br was synthesized according to Suzuki coupling.<sup>1</sup>

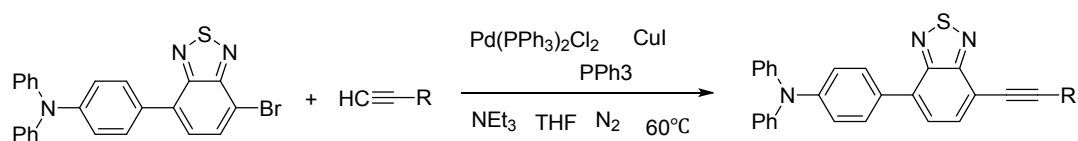
**TPA-BTD-Br:** Orange solid, yield 60%.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.89 (d,  $J$  = 3.8, 1H), 7.80 (d,  $J$  = 4.2, 2H), 7.54 (d,  $J$  = 3.8, 1H), 7.31-7.27 (m, 4H), 7.20-7.17 (m, 6H), 7.09-7.06 (m, 2H).  $^{13}\text{C}$  NMR

(100MHz, CDCl<sub>3</sub>):  $\delta$  154.0, 153.2, 148.4, 147.3, 133.6, 132.4, 129.9, 129.8, 129.4, 127.4, 125.1, 123.5, 122.6, 112.2.



## 2. Synthesis of the triads

The triads were synthesized according to Sonogashira coupling:



To a 25 mL shrek tube with magnetic stir bar was added **TPA-BTD-Br** (230mg, 0.5mmol), alkyne (0.3mmol), Pd(PPh<sub>3</sub>)<sub>2</sub>Cl<sub>2</sub> (35mg, 0.05mmol), PPh<sub>3</sub> (25mg, 0.1 mmol), Cul (10mg, 0.05mmol), NEt<sub>3</sub> (505mg, 5mmol) and was suspended in THF (12ml) and refluxed under N<sub>2</sub> for 12h. After cooling to room temperature, the solvent was removed via vacuum. Purification of the residue by flash chromatography on silica gel afforded the desired product.

**Compound 1:** Before purification by flash chromatography on silica gel, A solution of [Et<sub>4</sub>N]<sup>+</sup> Br<sup>-</sup> (0.42 g, 2.0 mmol, 4.0 equiv) in MeCN were added, the reaction mixture was stirred for 2 h for cation exchange. DCM/MeCN = 20:1 as eluent, red solid, yield 47.3%, mp 128-129°C. <sup>1</sup>H {<sup>11</sup>B} NMR (500 MHz, Acetone-*d*<sub>6</sub>): δ 7.96 (d, *J* = 8.5, 2H), 7.77 (d, *J* = 7.0, 2H), 7.70 (d, *J* = 7.5, 2H), 7.33 (t, *J* = 10, 4H), 7.12-7.08 (m, 8H), 3.47 (q, *J* = 7.0, 8H), 2.82 (broad signal, 1H), 1.86 (broad signal, 5H), 1.71 (broad signal, 5H), 1.37 (t, *J* = 9, 12H). <sup>11</sup>B NMR (160 MHz, Acetone-*d*<sub>6</sub>): δ -7.17 (s, 1B), -12.18 (d, *J* = ca. 137.6, 5B), -16.50 (d, *J* = ca. 148.8, 5B). <sup>11</sup>B {<sup>1</sup>H} NMR (160 MHz, Acetone-*d*<sub>6</sub>): δ -7.11 (1B), -12.17 (5B), -16.51 (5B). <sup>13</sup>C NMR (125MHz, Acetone-*d*<sub>6</sub>): δ 155.9, 152.7, 148.1, 147.4, 132.5, 131.9, 130.5, 130.0, 129.5, 127.4, 124.8, 123.6, 122.3, 118.1, 52.1, 49.0, 6.8. High-resolution ESI-MS (negative mode, MeOH): *m/z* calcd for [C<sub>27</sub>H<sub>27</sub>B<sub>11</sub>N<sub>3</sub>S]<sup>-</sup>: 544.3022. Found: 544.3043. IR: 2556, 2168, 1702, 1588, 1513, 1483, 1326, 1278, 1244, 1169, 1072, 1006.

**Compound 2:** DCM/HEX = 1:4 as eluent, yellow solid, yield 90.3%, mp 162-163°C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.89-7.86 (m, 3H), 7.69-7.67 (m, 3H), 7.41-7.38 (m, 3H), 7.32-7.28 (m, 4H), 7.21-7.18 (m, 6H), 7.10-7.06 (m, 2H). <sup>13</sup>C NMR (100MHz, CDCl<sub>3</sub>): δ 155.5, 153.2, 148.4, 147.3, 134.2, 133.1, 132.0, 130.2, 130.0, 129.4, 128.8, 128.4, 126.7, 125.1, 123.5, 122.8, 122.6, 115.1, 95.8, 85.6. HRMS (EI-TOF): calcd. for C<sub>32</sub>H<sub>21</sub>N<sub>3</sub>S [M<sup>+</sup>], 479.1456; found: 479.1457. IR: 2955, 2929, 2859, 2206, 1591, 1510, 1490, 1351, 1328, 1313, 1281, 1192, 1173.

**Compound 3:** DCM/HEX = 1:2 as eluent, Orange solid, yield 88.4%, mp 200-201°C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.88 (d, *J* = 4.4, 2H), 7.84 (d, *J* = 3.6, 1H), 7.67 (d, *J* = 3.6, 1H), 7.62 (d, *J* = 4.4, 2H), 7.32-7.28 (m, 4H), 7.21-7.17 (m, 6H), 7.10-7.06 (m, 2H), 6.92 (d, *J* = 4.4, 2H), 3.85 (s, 3H). <sup>13</sup>C NMR (100MHz, CDCl<sub>3</sub>): δ 160.0, 155.4, 153.1, 148.3, 147.3, 133.7, 133.5, 132.7, 130.3, 129.9, 129.4, 126.7, 125.0, 123.4, 122.6, 115.4, 114.9, 114.0, 96.0, 84.4, 55.3. HRMS (Maldi-TOF): calcd. for C<sub>33</sub>H<sub>23</sub>N<sub>3</sub>OS [M<sup>+</sup>], 509.1562; found: 510.1624. IR: 2946, 2952, 2198, 1588, 1505, 1478, 1433,

1328, 1278, 1268, 1250, 1175, 1104, 1021.

**Compound 4:** EtOAc/HEX = 1:4 as eluent, Red solid, yield 85.4%, mp 243-244°C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.65 (d,  $J$  = 6.0, 2H), 7.91-7.87 (m, 3H), 7.69 (d,  $J$  = 7.6, 1H), 7.52 (d,  $J$  = 6.0, 2H), 7.32-7.28 (m, 4H), 7.21-7.18 (m, 6H), 7.10-7.07 (m, 2H).  $^{13}\text{C}$  NMR (100MHz,  $\text{CDCl}_3$ ):  $\delta$  155.2, 153.0, 149.7, 148.6, 147.2, 135.2, 134.0, 131.0, 130.0, 129.7, 129.4, 126.4, 125.7, 125.1, 123.6, 122.3, 113.6, 92.4, 89.9. HRMS (EI-TOF): calcd. for  $\text{C}_{31}\text{H}_{20}\text{N}_4\text{S}$  [ $\text{M}^+$ ], 480.1409; found: 480.1408. IR: 3032, 2955, 2920, 2860, 2206, 1592, 1543, 1488, 1409, 1354, 1323, 1283, 1214, 1199, 1167.

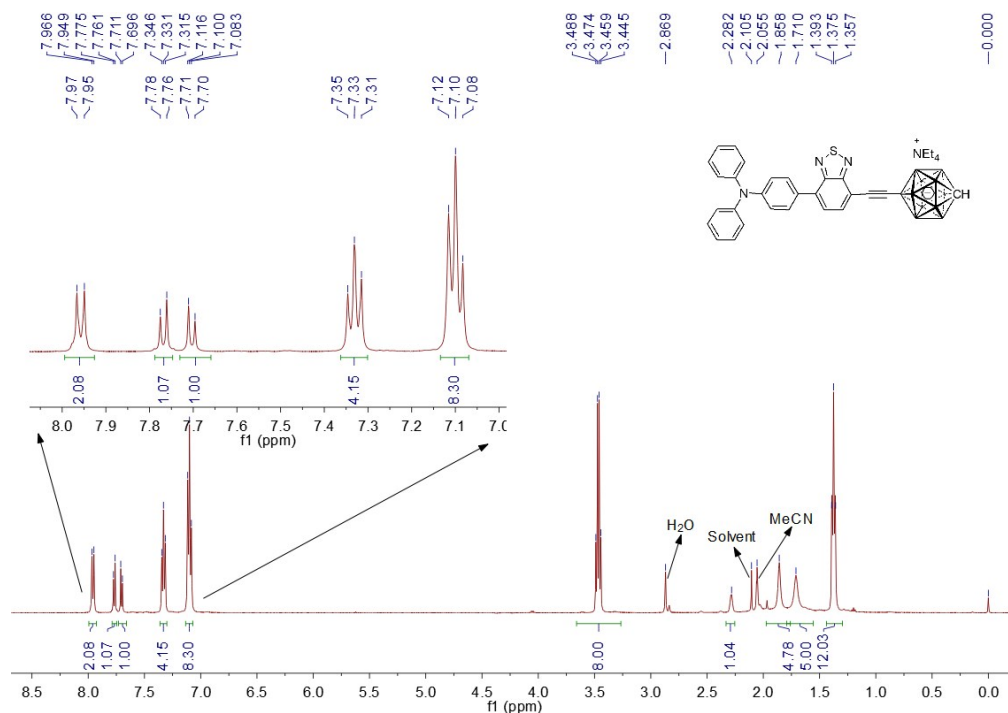


Figure S3  $^1\text{H}$   $\{^{11}\text{B}\}$  NMR of **1** in Acetone- $d_6$ .

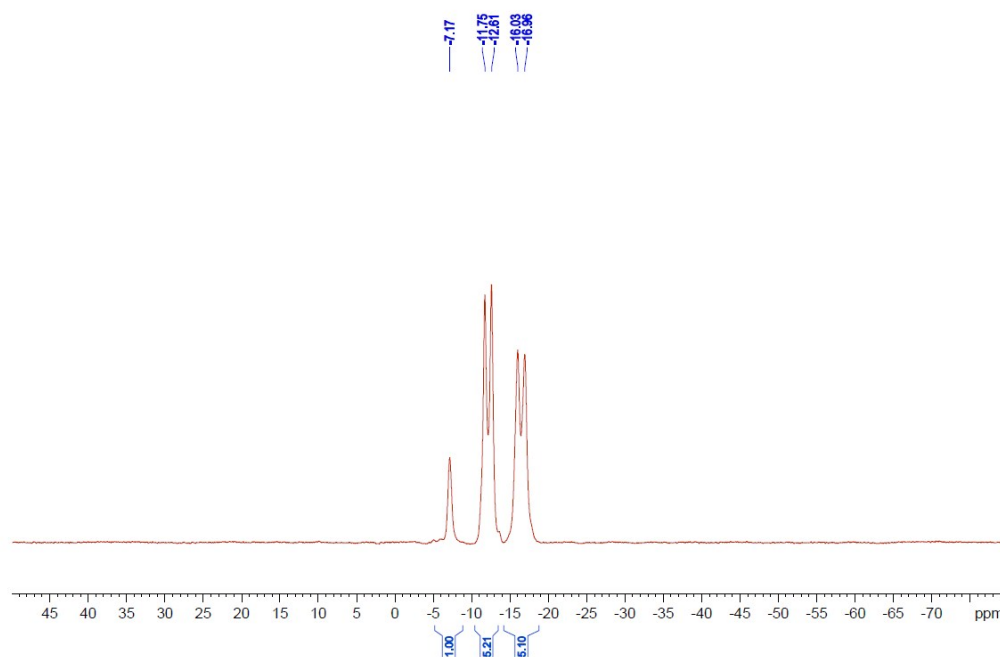


Figure S4  $^{11}\text{B}$  NMR of **1** in Acetone- $d_6$ .

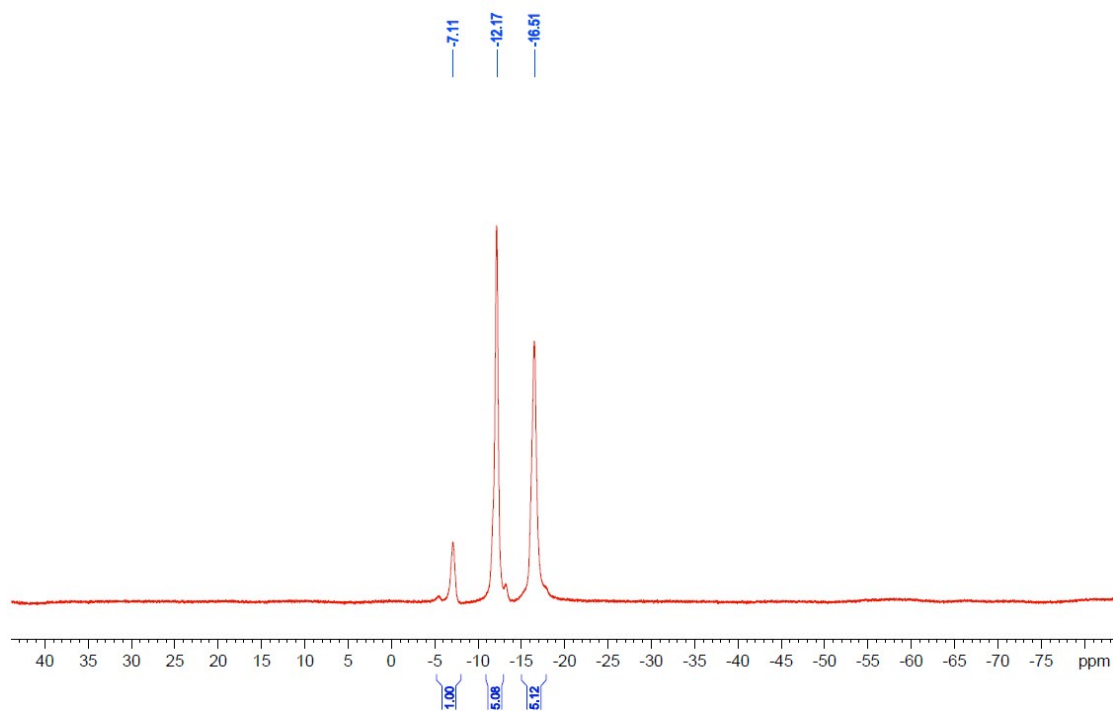


Figure S5  $^1\text{H}$  NMR of **1** in Acetone- $d_6$ .

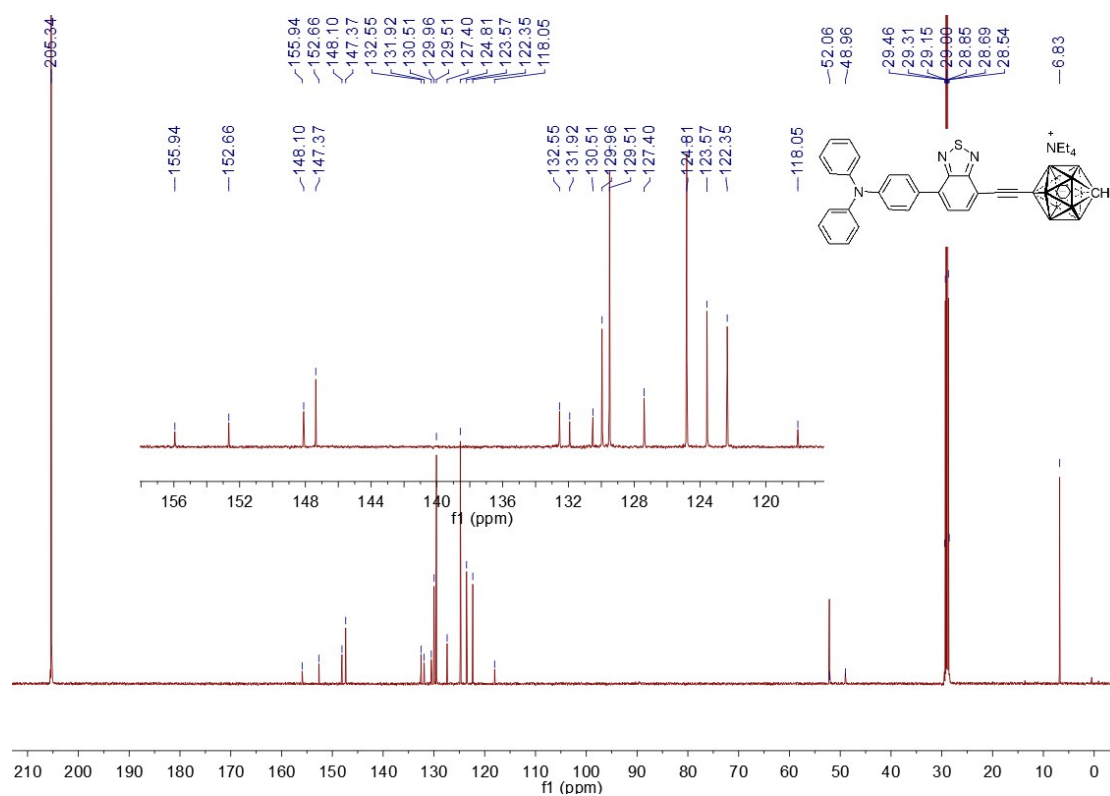
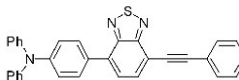


Figure S6  $^{13}\text{C}$  NMR of **1** in Acetone- $d_6$ .

[illegible]

**Figure S8**  $^{13}\text{C}$  NMR of **2** in  $\text{CDCl}_3$ .



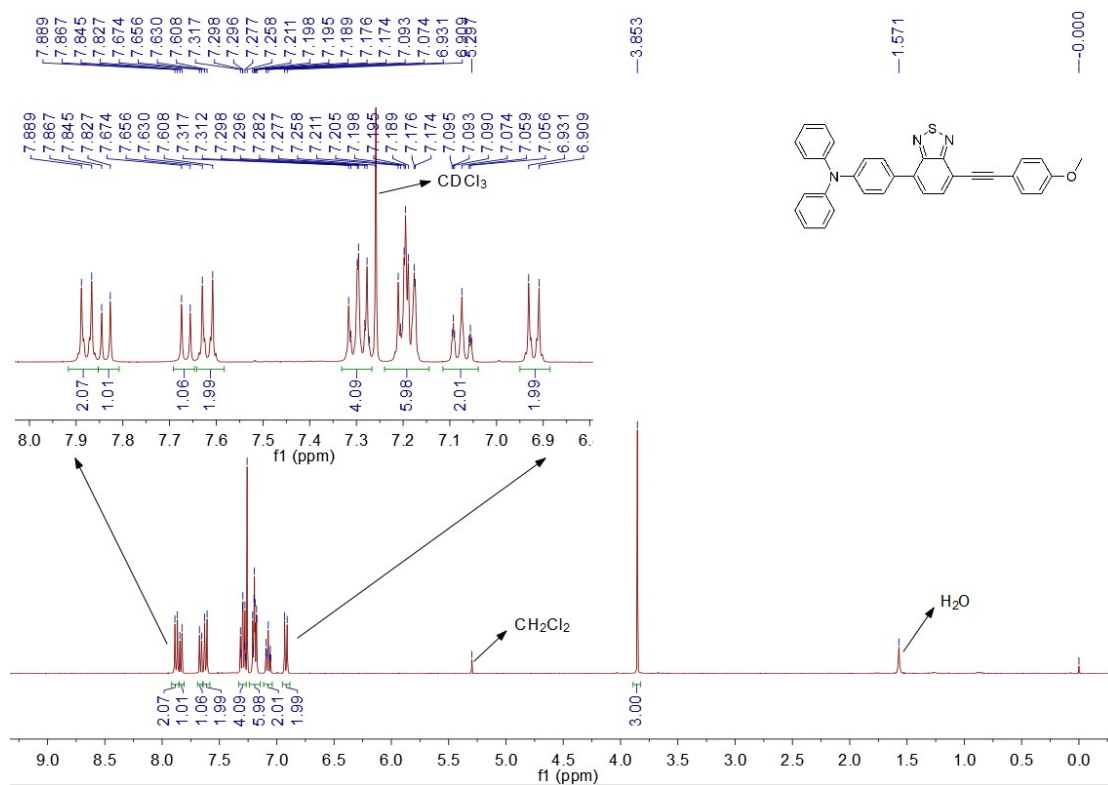


Figure S9 <sup>1</sup>H NMR of **3** in CDCl<sub>3</sub>.

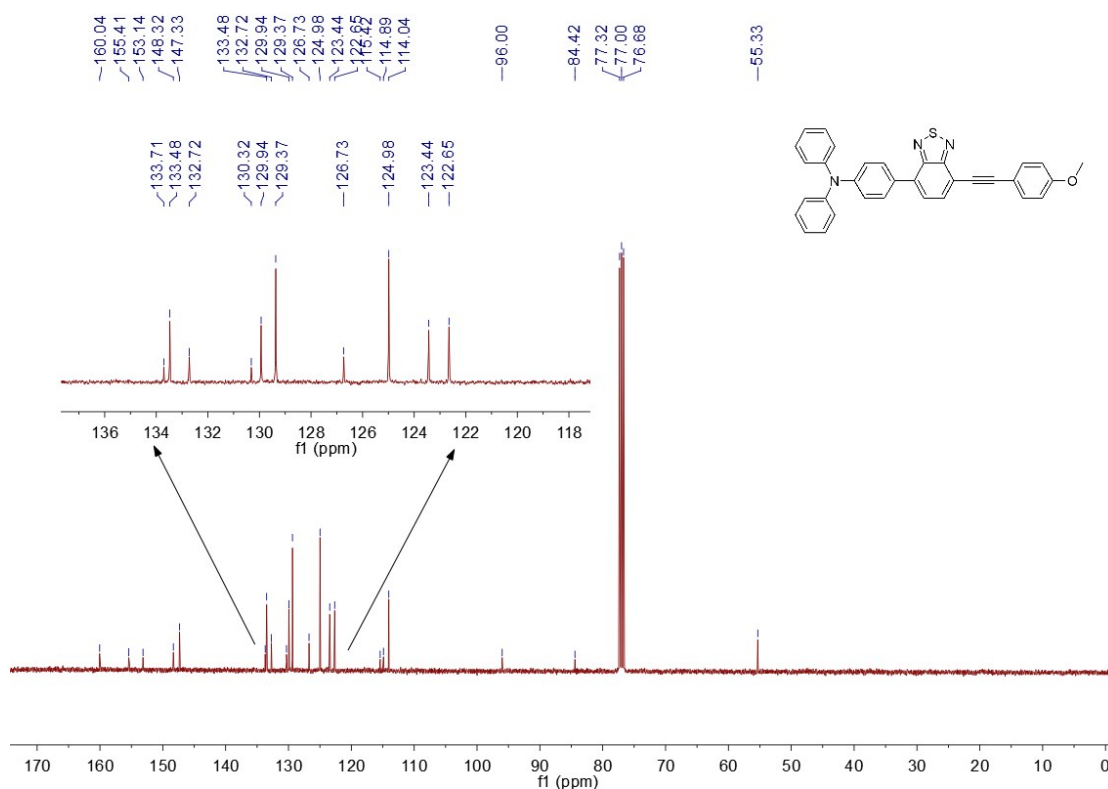


Figure S10 <sup>13</sup>C NMR of **3** in CDCl<sub>3</sub>.

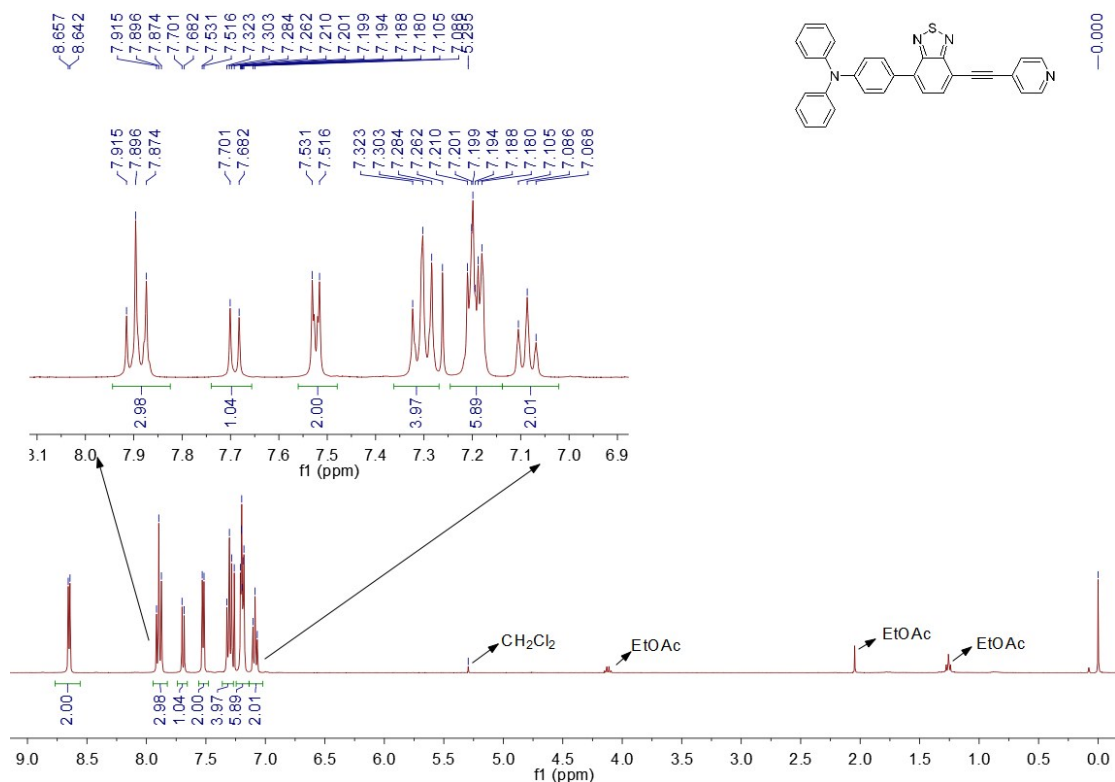


Figure S11 <sup>1</sup>H NMR of 4 in CDCl<sub>3</sub>.

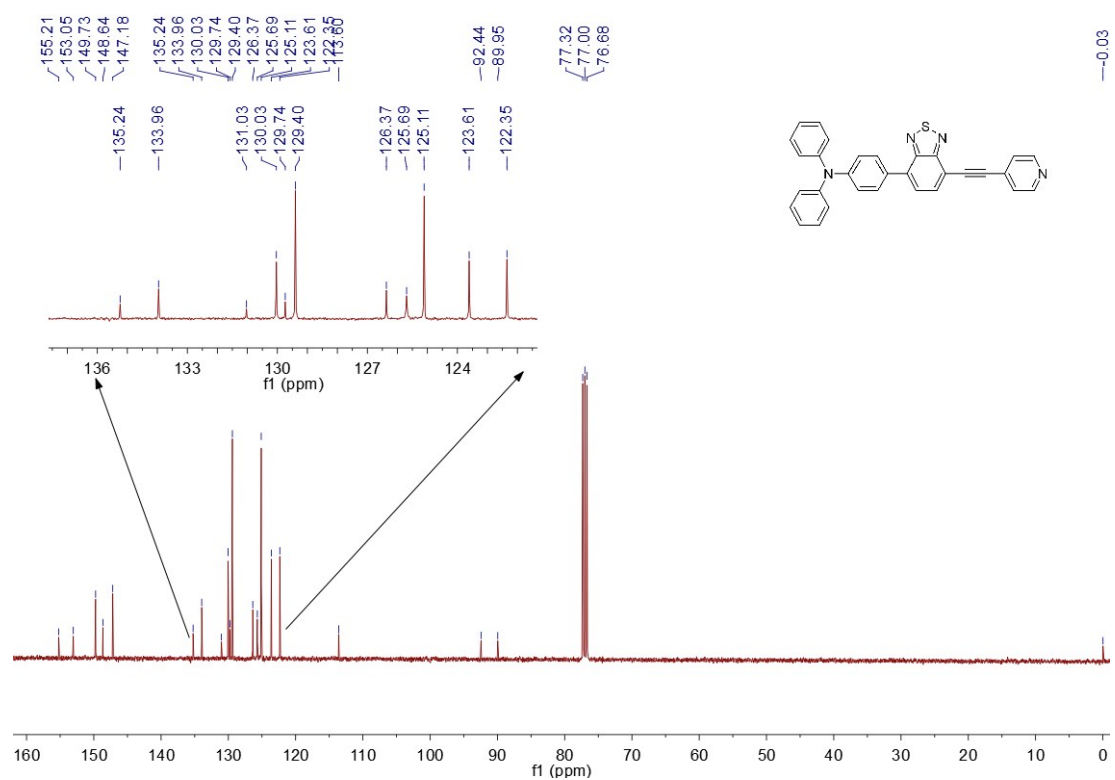
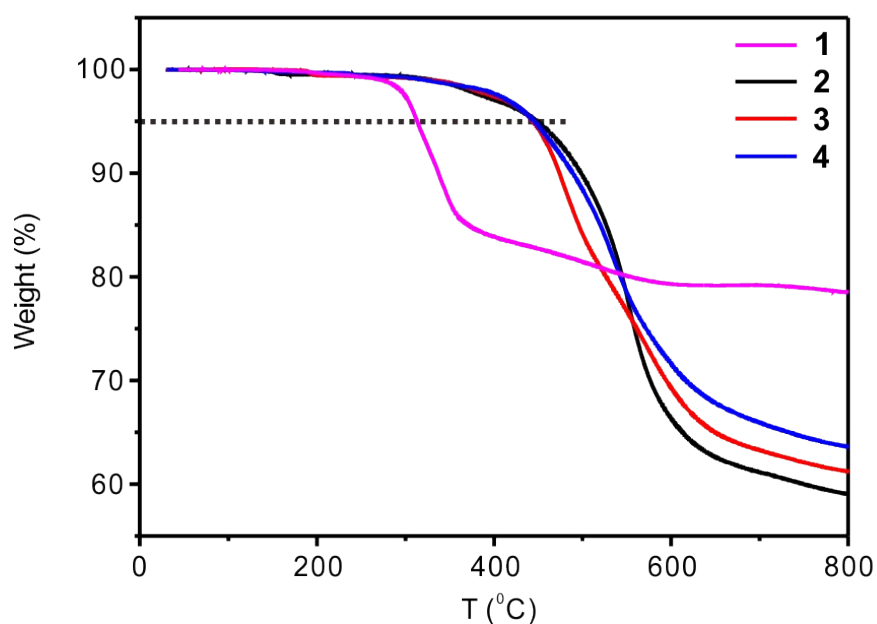


Figure S12 <sup>13</sup>C NMR of 4 in CDCl<sub>3</sub>.

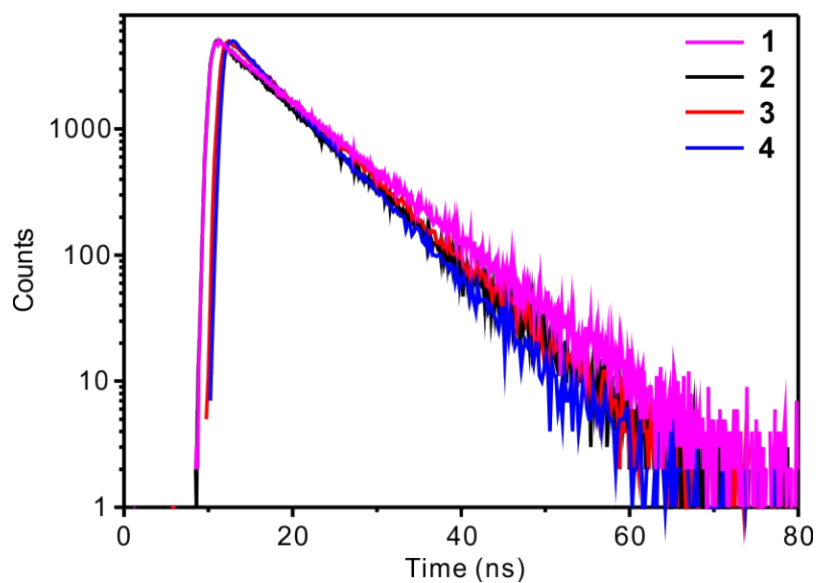
## Additional photophysical properties of four compounds in solution and crystalline state

**Table S1** Single crystal data of four compounds

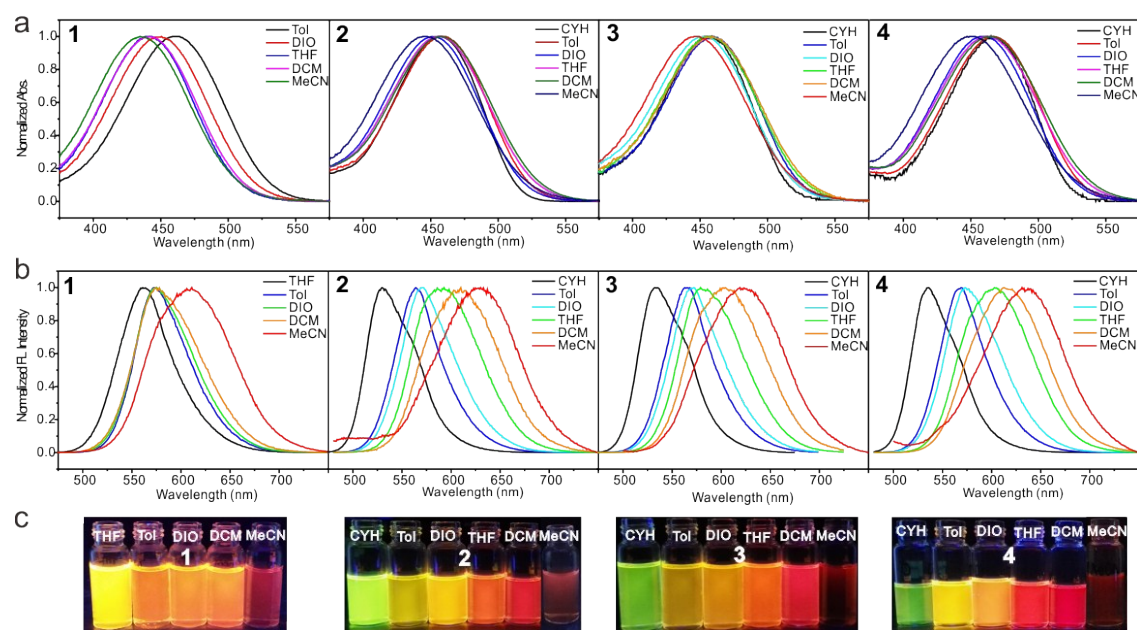
Compounds	1	2	3	4
Formula	$C_{35}H_{47}B_{11}N_4S$	$C_{32}H_{21}N_3S$	$C_{33}H_{23}N_3OS$	$C_{31}H_{20}N_4S$
CCDC	1850554	1850551	1850552	1850553
a [Å]	38.0550	10.1337	9.3757	9.2421
b [Å]	8.6859	12.1832	9.5330	25.8803
c [Å]	48.844	39.958	28.1021	10.1049
$\alpha$ [°]	90	90	90	90
$\beta$ [°]	90	94.845	90	99.171
$\gamma$ [°]	90	90	90	90
Z	16	8	4	4
V [Å <sup>3</sup> ]	16144.9	4915.6	2511.7	2386.1
D [g cm <sup>-3</sup> ]	1.110	1.296	1.348	1.338
Space group	P n a 21	P 1 21 / n 1	P 21 21 21	P 1 21 / n 1
Hall group	P 2c -2n	-P 2yn	P 2ac 2ab	-P 2yn
Mu [mm <sup>-1</sup> ]	0.598	0.893	0.162	0.164
R (reflections)	0.0995	0.0816	0.0390	0.0485
wR2 (reflections)	0.2705	0.2462	0.0906	0.1254



**Figure S13** Thermogravimetric Analysis of four compounds.



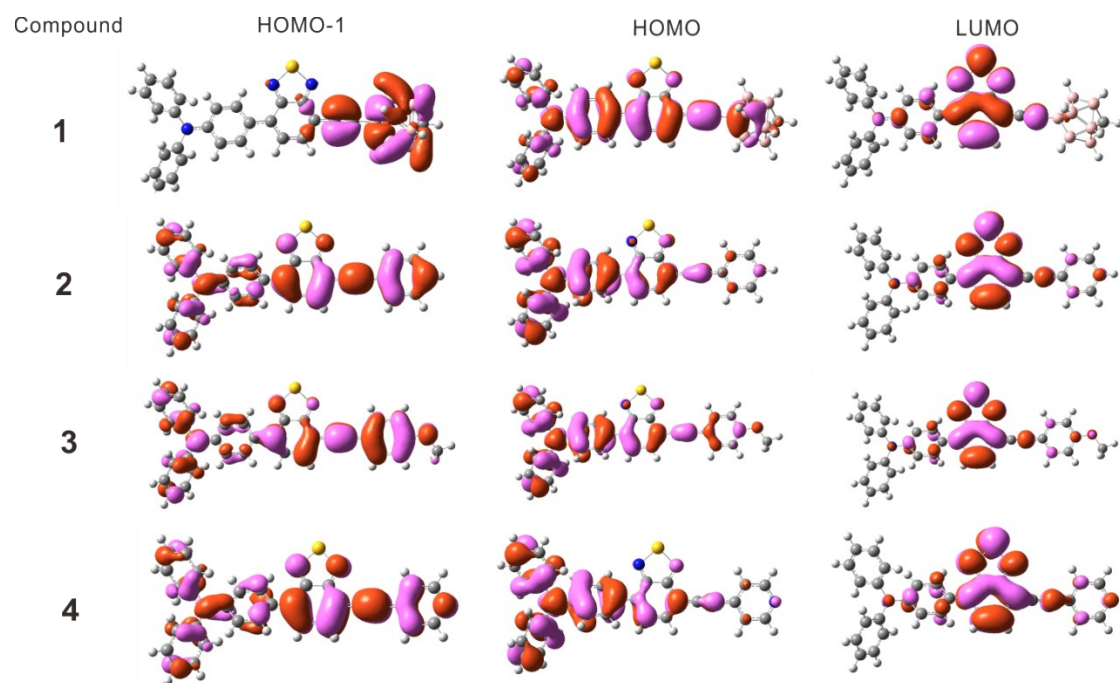
**Figure S14** Fluorescence decay traces of four compounds in THF at  $2 \times 10^{-5}$  M.



**Figure S15** Photophysical properties in different solvent: (a) Absorption of **1- 4** (b) emission spectra of **1- 4** (excited at its corresponding maximum absorption wavelength), (c) photos of **1- 4** under UV lamp (365 nm).

**Table S2** Solvent effect on absorption and emission of four compounds.

	<b>1</b>			<b>2</b>			<b>3</b>			<b>4</b>		
	Abs (nm )	FL (nm )	Stoke s (nm)	Abs (nm )	FL (nm )	Stoke s (nm)	Abs (nm )	FL (nm )	Stoke s (nm)	Abs (nm )	FL (nm )	Stoke s (nm)
CYH				454	531	77	454	535	81	465	536	71
Tol	460	573	113	459	564	105	458	565	107	467	569	102
DIO	453	572	119	451	571	120	453	570	117	459	573	114
THF	440	564	124	456	593	137	454	581	127	462	603	141
DCM	441	575	134	457	610	153	459	604	145	464	613	149
MeC N	435	608	173	446	630	184	450	617	167	451	631	180

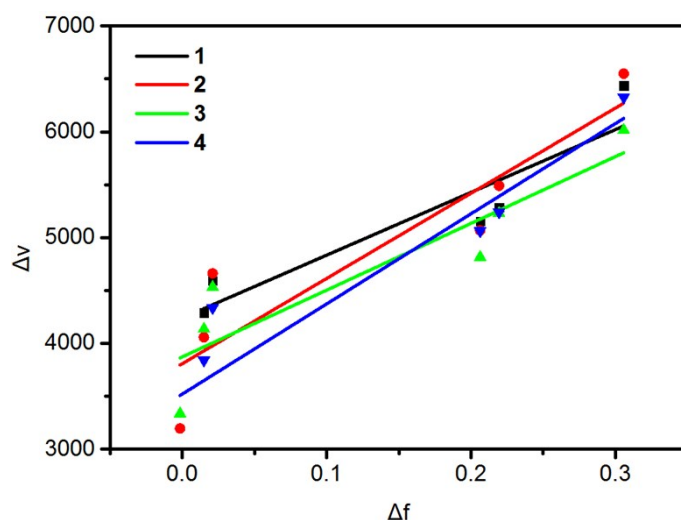
**Figure S16** HOMO/LUMO orbitals calculated by Gaussian in gas phase.

**Table S3** Calculated excitation energy (E), dominant contributing transitions and associated percent contribution and assignment of compounds **1-4** in different solvents.<sup>a</sup>

Compound	S <sub>n</sub>	Solvent	λ(nm)	f	Dominant transitions (percent contribution <sup>b</sup> )	assignment
<b>1</b>	S <sub>1</sub>	Tol	413	0.75	HOMO → LUMO (72.1%) HOMO-1 → LUMO (24.1%)	ICT
		DIO	412	0.74	HOMO → LUMO (73.7%) HOMO-1 → LUMO (22.5%)	
		THF	412	0.73	HOMO → LUMO (70.0%) HOMO-1 → LUMO (29.2%)	
		DCM	413	0.73	HOMO → LUMO (67.1%) HOMO-1 → LUMO (29.1%)	
		MeCN	415	0.70	HOMO → LUMO (69.1%) HOMO-1 → LUMO (27.1%)	
<b>2</b>	S <sub>1</sub>	CYH	430	0.94	HOMO → LUMO (75.1%) HOMO-1 → LUMO (19.4%)	ICT
		Tol	432	0.94	HOMO → LUMO (74.9%) HOMO-1 → LUMO (19.5%)	
		DIO	431	0.93	HOMO → LUMO (75.1%) HOMO-1 → LUMO (19.3%)	
		THF	433	0.89	HOMO → LUMO (75.5%) HOMO-1 → LUMO (19.1%)	
		DCM	433	0.89	HOMO → LUMO (75.4%) HOMO-1 → LUMO (19.1%)	
		MeCN	433	0.86	HOMO → LUMO (75.8%) HOMO-1 → LUMO (18.9%)	
<b>3</b>	S <sub>1</sub>	CYH	435	0.99	HOMO → LUMO (75.6%) HOMO-1 → LUMO (16.2%)	ICT
		Tol	436	0.99	HOMO → LUMO (75.3%) HOMO-1 → LUMO (16.4%)	
		DIO	435	0.98	HOMO → LUMO (75.6%) HOMO-1 → LUMO (16.2%)	
		THF	437	0.95	HOMO → LUMO (75.4%) HOMO-1 → LUMO (16.2%)	
		DCM	438	0.95	HOMO → LUMO (75.3%) HOMO-1 → LUMO (16.3%)	
		MeCN	437	0.92	HOMO → LUMO (75.6%) HOMO-1 → LUMO (16.0%)	

<b>4</b>	$S_1$	CYH	433	0.92	HOMO → LUMO (77.8%) HOMO-1 → LUMO (18.9%)	ICT
		Tol	435	0.93	HOMO → LUMO (77.7%) HOMO-1 → LUMO (17.7%)	
		DIO	433	0.92	HOMO → LUMO (77.9%) HOMO-1 → LUMO (17.5%)	
		THF	435	0.89	HOMO → LUMO (78.1%) HOMO-1 → LUMO (17.4%)	
		DCM	435	0.89	HOMO → LUMO (78.0%) HOMO-1 → LUMO (17.4%)	
		MeCN	434	0.87	HOMO → LUMO (78.2%) HOMO-1 → LUMO (17.3%)	

<sup>a</sup> Computed at the TDDFT/CAM-B3LYP/6-31+G\*. <sup>b</sup> The actual percent contribution=(configuration coefficient)<sup>2</sup>×2×100%.



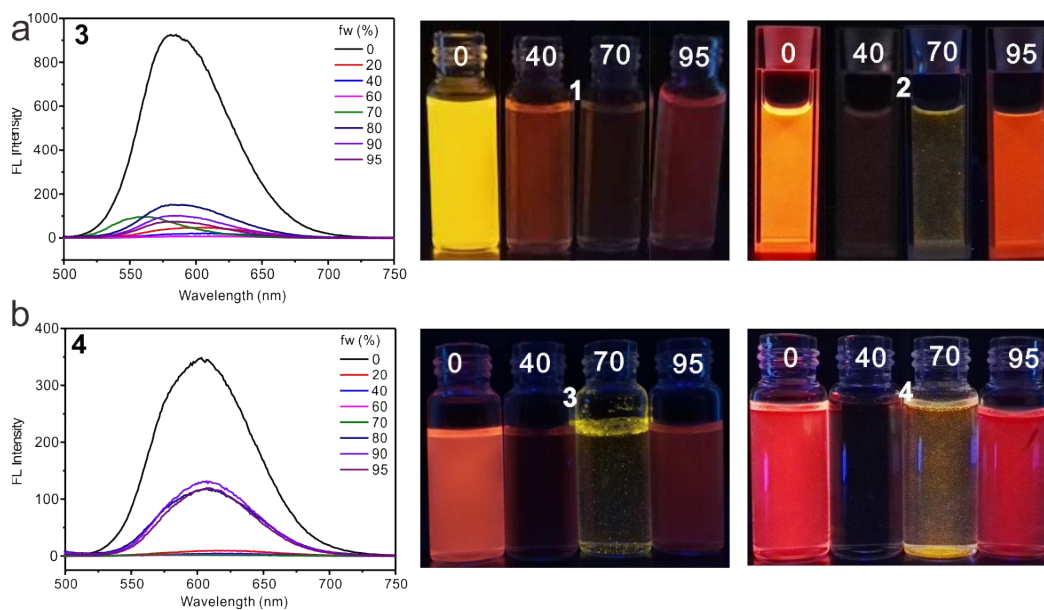
**Figure S17** Fluorescence Stokes shifts as a function of orientational polarizability  $\Delta f$  in various solvents.

**Table S4** Parameter of four compounds in different solvents.

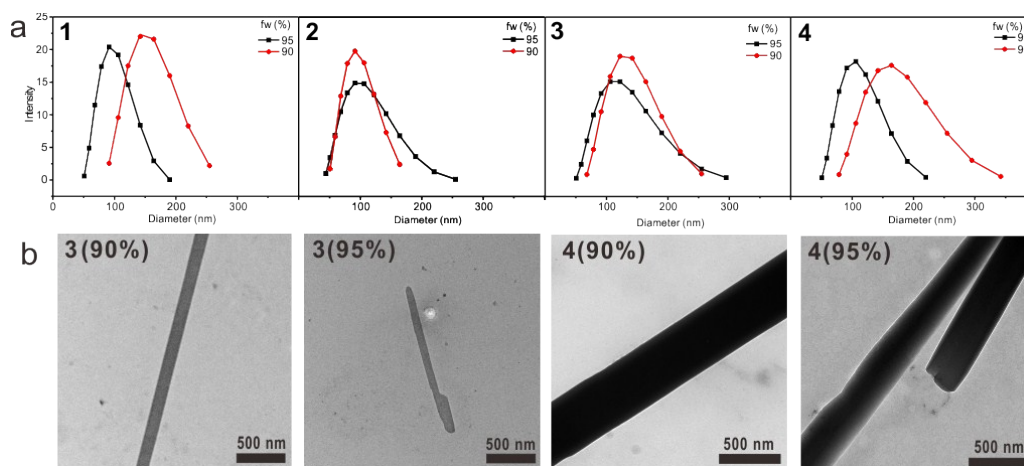
compound	$\alpha$ ( $\text{\AA}$ ) <sup>a</sup>	$R^2$	$\mu_g$ (D) <sup>a</sup>	Slope	$\Delta\mu_{eg}$ (D) <sup>b</sup>	$\mu_e$ (D) <sup>c</sup>
<b>1</b>	6.18	0.8671	29.58	5939	11.84	41.42
<b>2</b>	6.10	0.8383	2.52	8060	13.53	16.05
<b>3</b>	6.33	0.8206	3.83	6315	12.67	16.50
<b>4</b>	6.32	0.8656	6.29	8527	14.67	20.96

<sup>a</sup> Dipole moments in ground state ( $\mu_g$ ) are calculated based on Gaussian 09 applying B3LYP 6-31+G as method; <sup>b</sup> dipole moment changes obtained by the modified Lippert-Mataga equation; <sup>c</sup> dipole moments in excited states, calculated from the equation of  $\mu_e = \Delta\mu_{eg} + \mu_g$ .

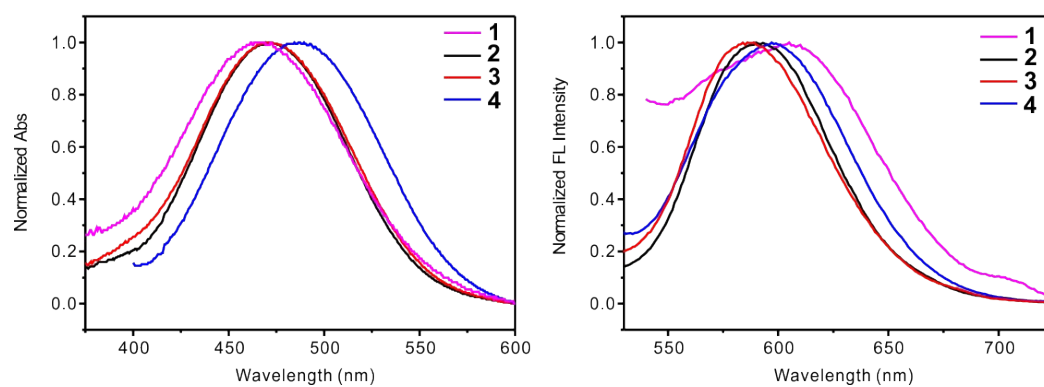




**Figure S18** Emission spectrum in aqueous THF solutions **3** (a) and **4** (b), and photos of **1- 4** in aqueous THF solution (fw = 0%, 40%, 70%, 95%) under UV lamp (365nm).



**Figure S19** (a) DLS of **1- 4**; (b) TEM images of **3** and **4** in aqueous THF solution (fw = 90%, 95%).

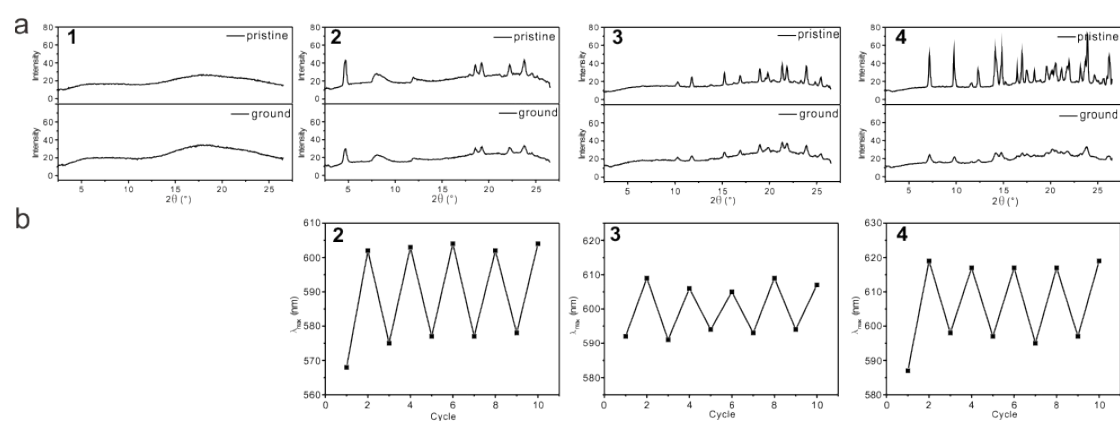


**Figure S20** Absorption (left) and emission (right) of these compounds in films.



**Table S5** Emission in different solid states.

	crystalline		pristine powder		ground powder	
	$\lambda_{em}$ ( nm)	FWHM ( nm)	$\lambda_{em}$ ( nm)	FWHM ( nm)	$\lambda_{em}$ ( nm)	FWHM ( nm)
<b>1</b>	575	62	628	67	630	69
<b>2</b>	568	46	568	49	602	54
<b>3</b>	597	49	592	50	609	57
<b>4</b>	598	50	587	58	619	60

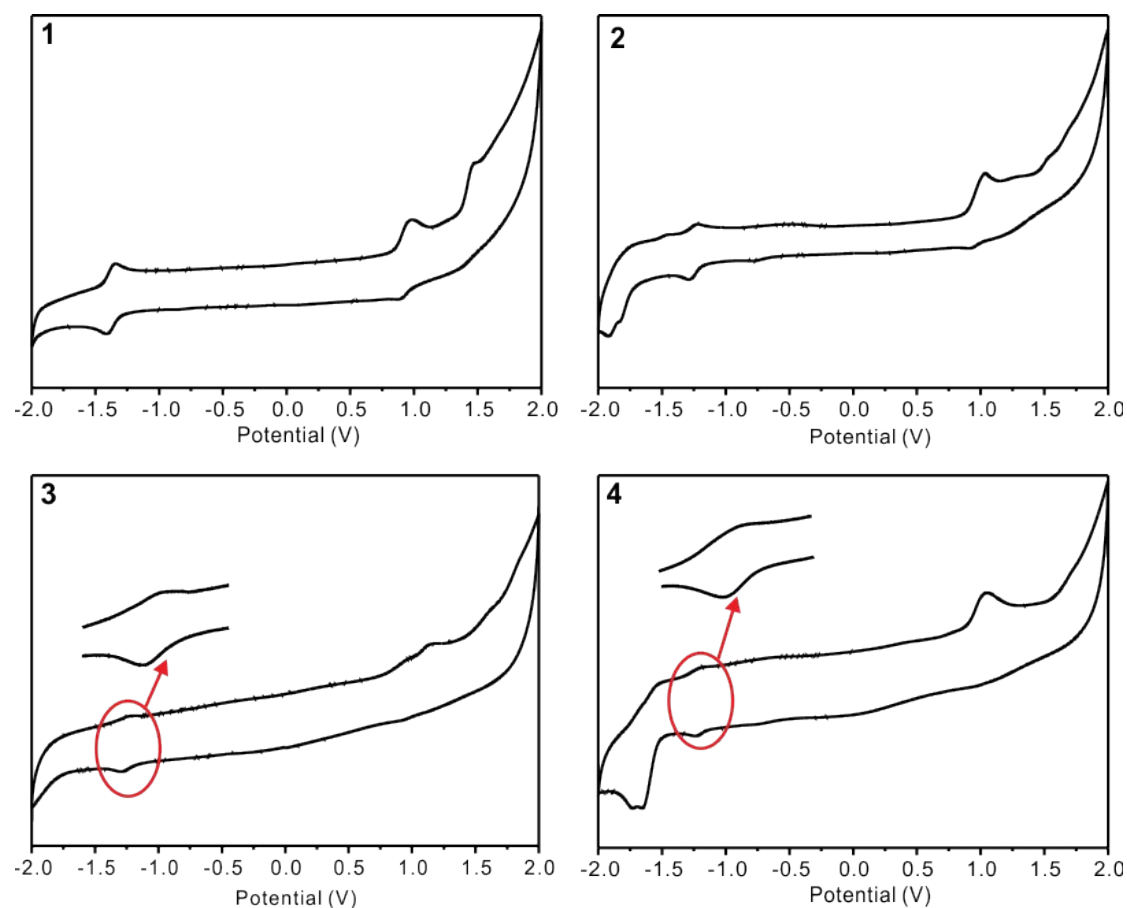
**Figure S21** XRD analysis in the cycle of pristine and ground (a), repeatable cycles, monitored by emission spectra (b).**Table S6** Representative bond length and dihedral angel in the single crystals.

	$l_1$ (Å)	$\alpha$ (°)	$l_2$ (Å)
<b>1</b>	1.467	26.18	1.418
<b>2</b>	1.484	33.54	1.442
<b>3</b>	1.475	36.45	1.437
<b>4</b>	1.473	39.57	1.426

**Table S7** HOMO/LUMO levels calculated from theoretical calculation and CV as well as UV measurements

Compound	HOMO		LUMO		$E_g$		
	CV <sup>a</sup>	Cald <sup>b</sup>	CV <sup>c</sup>	Cald <sup>b</sup>	CV	Cald	UV <sup>d</sup>
	(eV)	(eV)	(eV)	(eV)	(eV)	(eV)	(eV)
<b>1</b>	-5.320	-6.255	-3.031	-3.974	2.289	2.281	2.487
<b>2</b>	-5.368	-5.242	-3.143	-3.054	2.225	2.188	2.396
<b>3</b>	-5.205	-5.176	-3.088	-2.982	2.117	2.194	2.394
<b>4</b>	-5.401	-5.377	-3.176	-3.246	2.225	2.131	2.359

<sup>a</sup> Potentials vs reference electrode SCE, working electrode glassy carbon, auxiliary electrode Pt, 0.1 M Bu<sub>4</sub>N<sup>+</sup>PF<sub>6</sub><sup>-</sup>-MeCN, scan rate 100 mV/s, HOMO =  $E_{\text{ref}} - E_{\text{ox}}$ . <sup>b</sup> Obtained from DFT using the B<sub>3</sub>LYP functional and the 6-31+G basis set. <sup>c</sup> LUMO =  $E_{\text{ref}} - E_{\text{red}}$ . <sup>d</sup>  $E_g = 1241 / \lambda_{(\text{UV onset in THF})}$ .

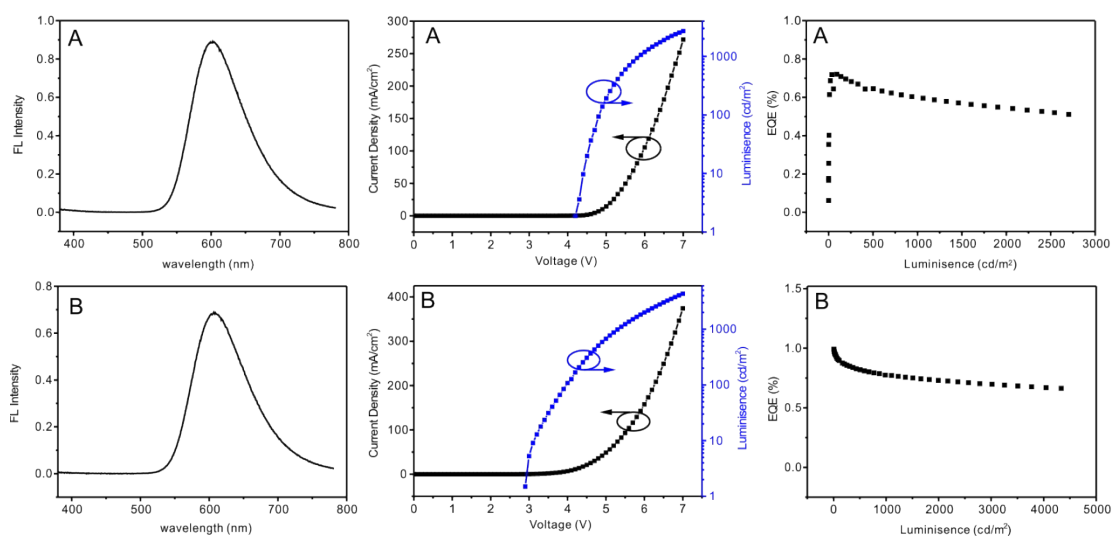


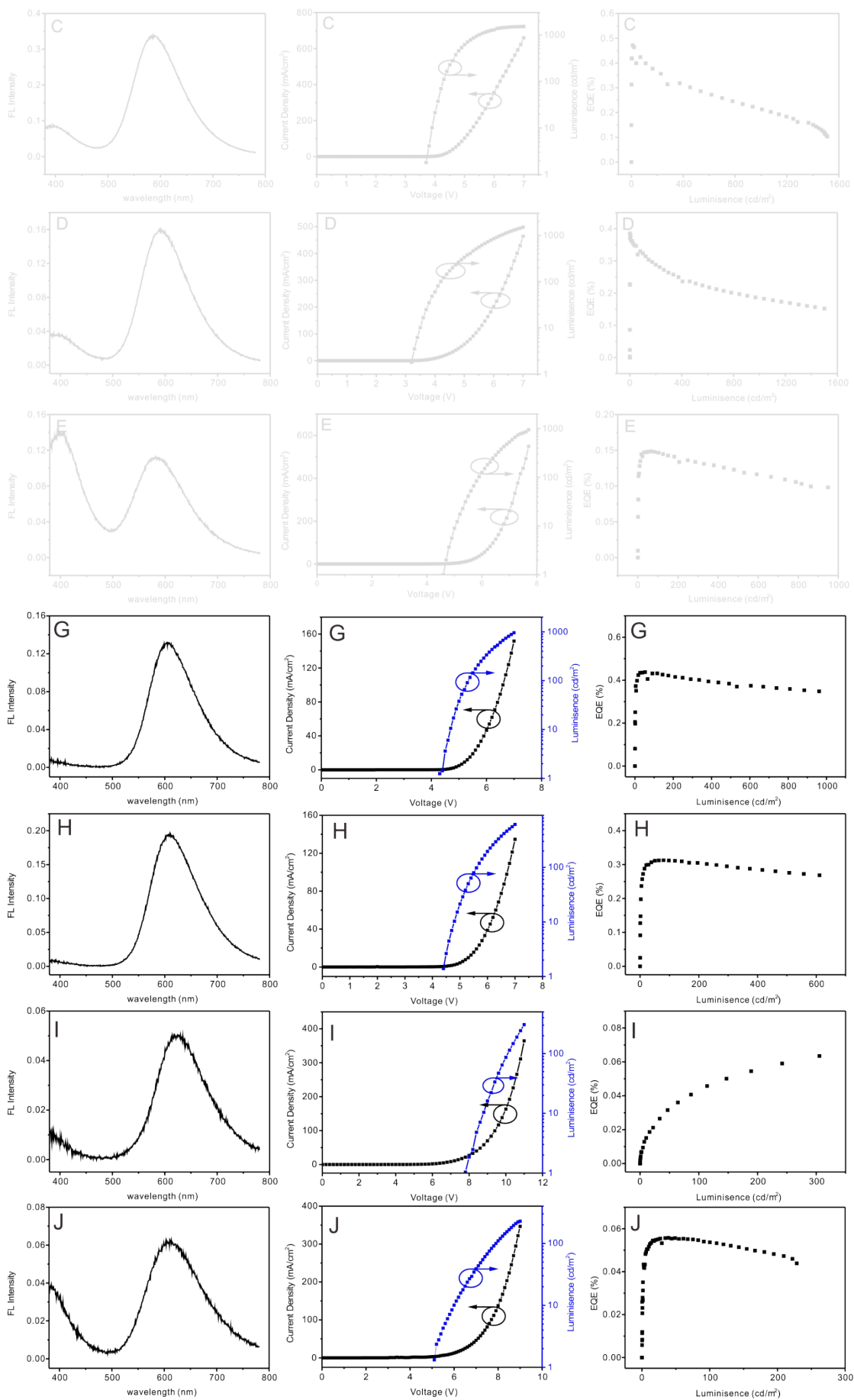
**Figure S22** Cyclic voltammograms of four compounds.

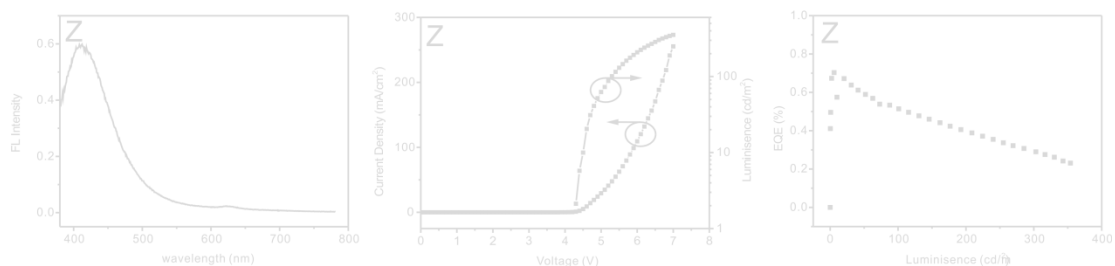
**Table S8** Device performance.

Device	Emitter	$V_{\text{turn-on}}^a$ (V)	$\text{CIE}_{1931}^b$ [x, y]	$\lambda_{\text{EL}}^c$ [nm]	Device performances at 100 cd		
					$\text{m}^{-2}$		
					EQE [%]	CE [cd A <sup>-1</sup> ]	PE [lm W <sup>-1</sup> ]
A	<b>2</b>	4.2	(0.58, 0.41)	602	0.71	1.35	0.86
B	<b>3</b>	2.9	(0.60, 0.40)	606	0.90	1.55	1.22
C	<b>2/PVK(1/8)</b>	3.7	(0.48, 0.43)	390, 586	0.40	0.88	0.64
D	<b>3/PVK(1/8)</b>	3.2	(0.50, 0.43)	396, 590	0.32	0.68	0.51
E	<b>4/PVK(1/16)</b>	4.6	(0.38, 0.34)	399, 581	0.15	0.28	0.15
F	<b>1/PVK(1/16)</b>	3.6	(0.34, 0.31)	400, 576	0.18	0.32	0.20
G	<b>2/PVK(1/2)</b>	4.3	(0.57, 0.42)	604	0.43	0.77	0.45
H	<b>3/PVK(1/2)</b>	4.4	(0.58, 0.41)	610	0.31	0.51	0.29
I	<b>4/PVK(1/2)</b>	7.8	(0.58, 0.38)	619	0.05	0.06	0.02
J	<b>1/PVK(1/2)</b>	4.9	(0.50, 0.38)	610	0.05	0.08	0.03
Z	<b>PVK</b>	4.3	(0.17, 0.10)	412	0.51	0.21	0.13

<sup>a</sup>  $V_{\text{on}}$  = turn-on voltage at 1 cd  $\text{m}^{-2}$ ; <sup>b</sup> CIE=Commission Internationale de l'Eclairage coordinates; <sup>c</sup> peak electroluminescence at terminal voltage.







**Figure S23** EL spectra at 7V (first column); Current density-Luminance-Voltage (L-J-V) characteristics (second column); EQE (third column) of different devices.

## References

- 1 (a) Y.-M. Zhang, F. Meng, J.-H. Tang, Y. Wang, C. You, H. Tan, Y. Liu, Y.-W. Zhong, S. Su and W. Zhu, *Dalton Trans.*, 2016, **45**, 5071–5080; (b) Y. Zhang, Z. Yin, F. Meng, J. Yu, C. You, S. Yang, H. Tan, W. Zhu and S. Su, *Org. Electron.*, 2017, **50**, 317–324.