Supporting Information

Experimental Section

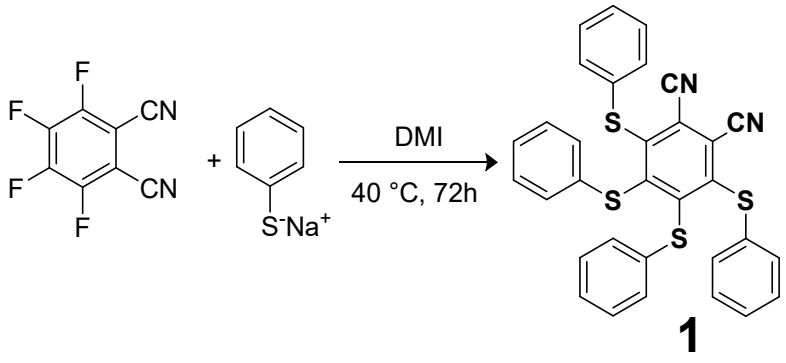
1.1 Materials

3,4,5,6-Tetrafluorophthalonitrile, 4-Bromobenzaldehyde, 4-Bromotriphenylamine, [4-(Diphenylamino)phenyl]boronic acid, 4-Methoxythiophenol, 1,3-Dimethyl-2-imidazolidinone, Lauric acid, and Tetrakis(triphenylphosphine)palladium were purchased from Bide Pharmatech Ltd. P-toluenethiol, Sodium benzenethiolate, 4-Tolylboronic acid, and N, N-Dimethylformamide were purchased from Adamas-beta®. Potassium carbonate, and 1,4-Dioxane were purchased from General-reagent®. 2,3,5,6-Tetrafluoroterephthalonitrile was purchased from Meryer Chemical Technology Co., Ltd. 2-Naphthalenethiol was purchased from Shanghai Yien Chemical Technology Co., Ltd. Other chemicals were purchased commercially and used without further purification.

1.2 Measurements

^{1}H NMR and ^{13}C NMR were measured on a Bruker 400L spectrometer. High-resolution mass spectrometry data were recorded on a matrix-assisted laser desorption ionization time-of-flight (MALDI-TOF) mass spectrometer (5800). Absorption spectra were recorded on a Shimadzu 1800 spectrophotometer. Fluorescence spectra and phosphorescence spectra were recorded in Horiba FluoroMax-4 (Horiba Scientific). Phosphorescence lifetime (the instrument is a single photon counter Fluorohub (Horiba Scientific), the laser source uses Special LED-370 of 1MHz, and the lifetime analysis software is DataStation v6.6 (Horiba Scientific)). The photos were taken by the Redmi K40 phone.

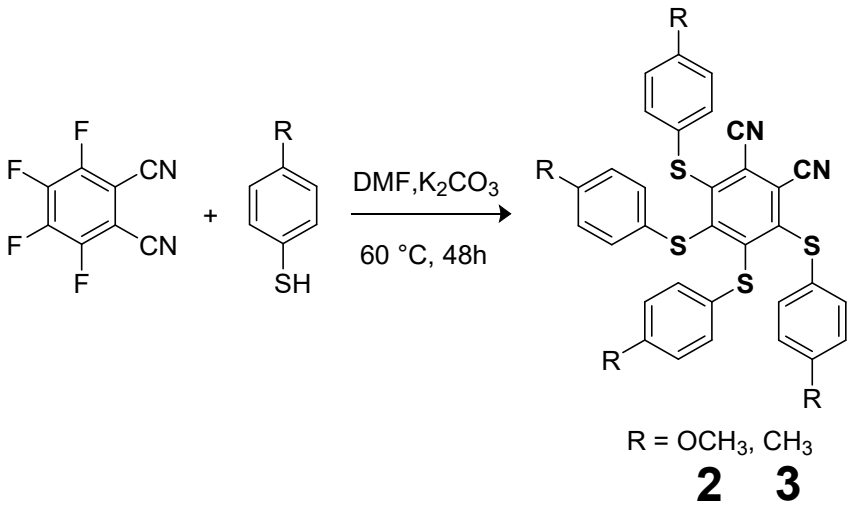
1.3 Synthesis



Scheme S1 The synthesis route of compound **1**.

Synthesis of compound **1**: 3,4,5,6-Tetrafluorophthalonitrile (800 mg, 4 mmol), sodium benzenethiolate (3.17 g, 24 mmol), and DMI (20.0 mL) were stirred under nitrogen at 40 °C for 72 hours. After cooling the solution to room temperature, it was poured into water and extracted with EA. The EA layer was dried over

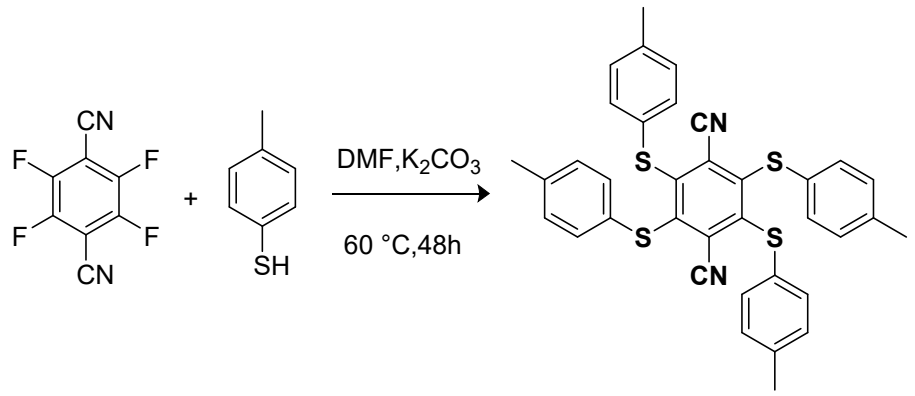
anhydrous Na_2SO_4 and filtered. The solvent was evaporated, and the product was purified by silica gel column chromatography using PE as the eluent, and recrystallized from acetone, and ethanol to give the product (896 mg, 40 %). ^{1}H NMR (400 MHz, DMSO-d_6, δ): 7.35-7.18 (m, 16H), 7.02-6.99 (m, 4H). ^{13}C NMR (101 MHz, DMSO-d_6, δ): 151.70, 144.53, 136.00, 134.91, 130.08, 129.90, 128.94, 128.49, 127.84, 127.53, 123.60, 114.97, 40.64, 40.43, 40.22, 40.01, 39.80, 39.60, 39.39. MS (MALDI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{32}H_{20}N_2S_4$, 560.0509; found, 560.1956.



Scheme S2 The synthesis route of compounds **2** and **3**.

Synthesis of compound **2**: 3,4,5,6-Tetrafluorophthalonitrile (800 mg, 4 mmol), 4-Methoxythiophenol (3.36 g, 24 mmol), potassium carbonate (6.63 g, 48 mmol) and DMF (20.0 mL) were mixed in Stir at 60 °C for 48 hours under nitrogen protection. After cooling the solution to room temperature, it was poured into water and extracted with EA. The EA layer was dried over anhydrous Na_2SO_4 and filtered. The solvent was evaporated and the product was purified by silica gel column chromatography using DCM/PE (1/4) as eluent and washed with ethanol to give the product (1.72 g, 63 %). ^{1}H NMR (400 MHz, DMSO-d_6, δ): 7.24-7.12 (m, 4H), 6.92 (dd, J = 14.1, 8.9 Hz, 8H), 6.84-6.76 (m, 4H), 3.74 (d, J = 8.4 Hz, 12H). ^{13}C NMR (101 MHz, DMSO-d_6, δ): 159.57, 159.19, 151.64, 144.92, 132.31, 131.37, 126.24, 124.95, 121.57, 115.70, 115.51, 115.07, 55.75, 55.68, 40.61, 40.40, 40.19, 39.98, 39.78, 39.57, 39.36. MS (MALDI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{36}H_{28}N_2O_4S_4$, 680.0932; found, 680.2872.

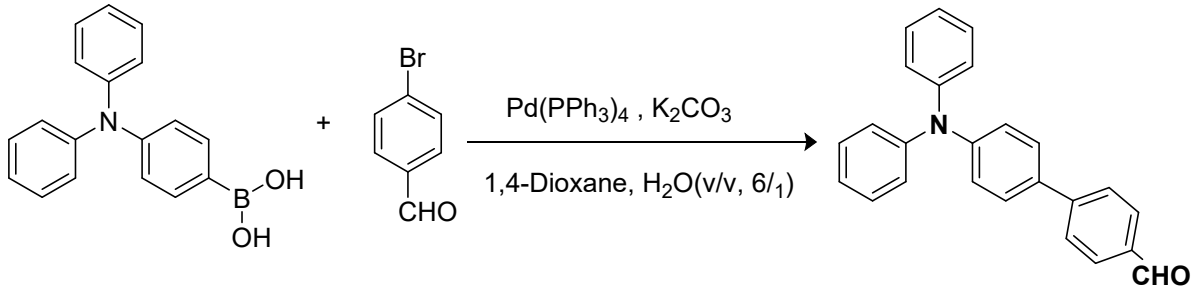
Synthesis of compound **3**: The synthetic procedure is similar to compound **2**. ^{1}H NMR (400 MHz, DMSO-d_6, δ): 7.19-6.92 (m, 12H), 6.88 (d, J = 8.0 Hz, 4H), 2.26 (d, J = 11.7 Hz, 12H). ^{13}C NMR (101 MHz, DMSO-d_6, δ): 151.86, 144.67, 137.59, 137.16, 132.51, 131.35, 130.69, 130.51, 129.56, 128.97, 122.65, 115.03, 40.64, 40.43, 40.22, 40.01, 39.80, 39.60, 39.39, 21.06. MS (MALDI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{36}H_{28}N_2S_4$, 616.1135; found, 616.2560.



4

Scheme S3 The synthesis route of compound **4**.

Synthesis of compound **4**: 2,3,5,6-Tetrafluoroterephthalonitrile (800 mg, 4 mmol), p-toluenethiol (2.98 g, 24 mmol), potassium carbonate (6.63 g, 48 mmol) and DMF (35.0 mL) were mixed in Stir at 60 °C for 48 hours under nitrogen protection. After cooling the solution to room temperature, it was poured into water, and a precipitate formed, which was filtered. The precipitate was washed successively with ethanol, methanol, toluene, acetonitrile, acetone, chloroform, and n-hexane to obtain the product (1.73 g, 70 %). ^{1}H NMR (400 MHz, Chloroform-*d*, δ): 7.10-7.03 (m, 16H), 2.31 (s, 12H). ^{13}C NMR (101 MHz, Chloroform-*d*, δ): 146.79, 138.23, 131.11, 130.67, 130.25, 128.12, 114.36, 77.35, 77.04, 76.72, 21.19. MS (MALDI-TOF) *m*/*z*: $[M + H]^+$ calcd for $C_{36}H_{28}N_2S_4$, 616.1135; found, 616.3096.



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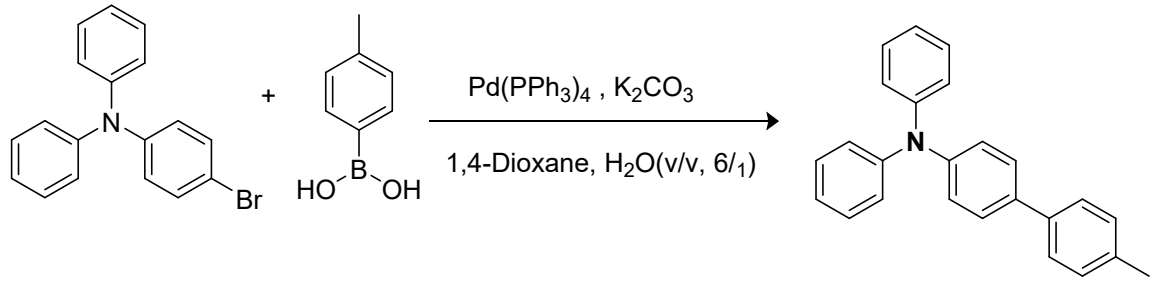

6

Scheme S4 The synthesis route of compounds **5** and **6**.

Synthesis of compound **5**: Compound **5** was synthesized according to the literature.[1] ^{1}H NMR (400 MHz, DMSO-d_6, δ): 10.02 (s, 1H), 7.96 (d, J = 8.3 Hz, 2H), 7.87 (d, J = 8.3 Hz, 2H), 7.71 (d, J = 8.7 Hz, 2H), 7.41-7.29 (m, 4H), 7.16-6.97 (m, 8H).

Synthesis of compound **6**: Compound **6** was synthesized according to the literature.[1] ^{1}H NMR (400 MHz, DMSO-d_6, δ): δ 7.68-7.42 (m, 4H), 7.41-7.15 (m, 6H), 7.13 – 6.88 (m, 8H), 2.33 (s, 3H).

Computational Section

In order to simulate the structure and phosphorescence wavelength of compound **2**, we employed the ONIOM simulation[2] of the large fragment extracted from X-ray crystal structure containing 6 molecules where the one molecule was fully surrounded by other ones. We optimized the target (internal) molecule in a T_1 state at high-level B3LYP/6-311G(d,p),[3-6] while the surrounding molecule was optimized by molecular mechanics method employing UFF force field.[7] These calculations simulate the behaviour of compound **2** in a crystal state (before grinding). Then, we optimized individual molecule **2** without surrounding by using the same B3LYP/6-311G(d,p) method as for the target molecule in ONIOM method. the phosphorescence wavelengths for all optimized structures were calculated by using long-range-corrected CAM-B3LYP functional[8] and 6-311G(d,p) basis set motivated by charge-transfer nature of lowest excited states in persulfurated benzenes that was the common feature of these compounds.[9,10]

Supporting Figures

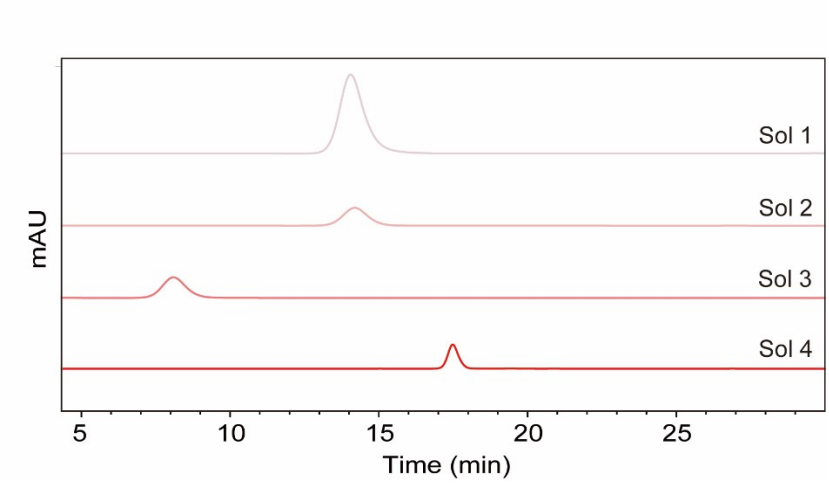

Figure S1. HPLC of compounds **1-4** in acetonitrile.

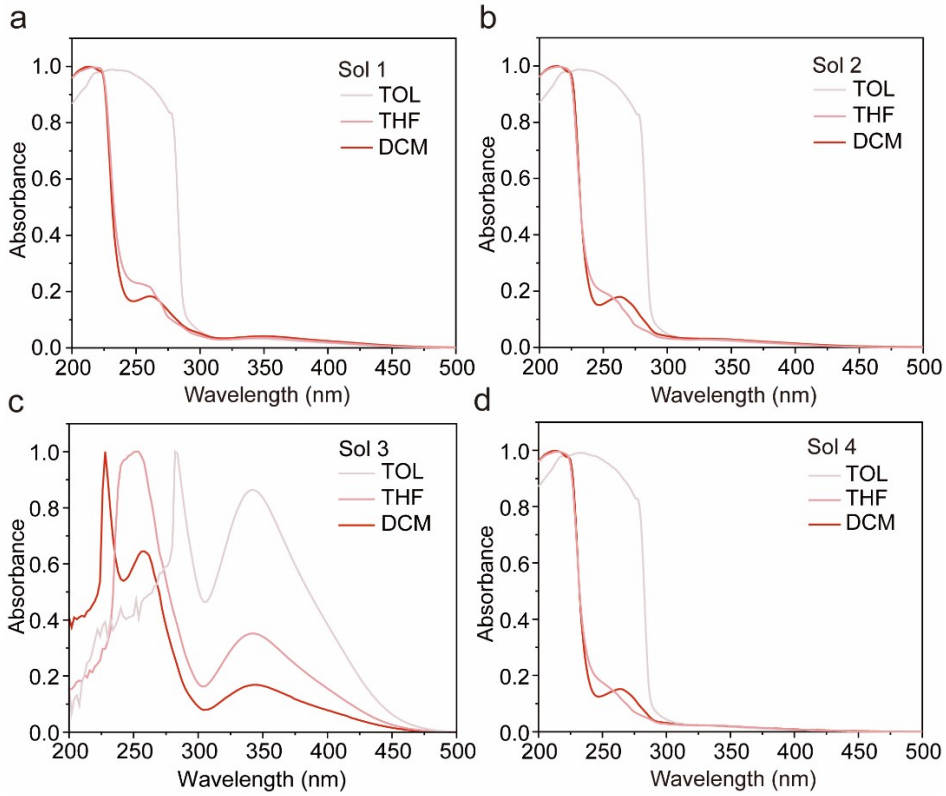

Figure S2. a-d) Absorption spectra of compounds **1-4** in different solvents at room temperature. The concentration is 100 μM.

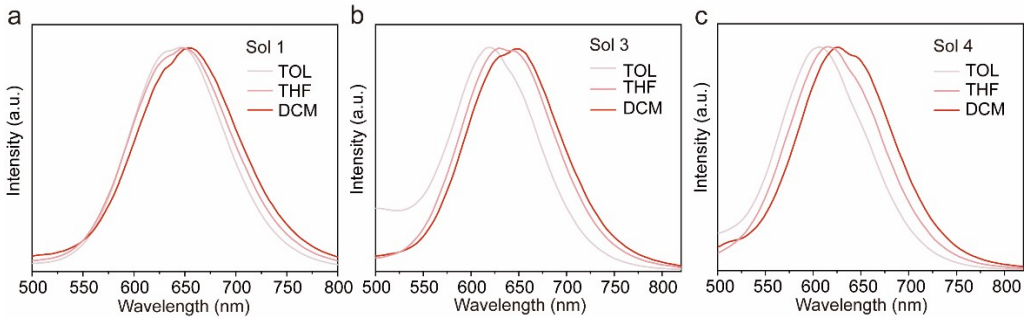

Figure S3. a-c) Normalized photoluminescent spectra of **1**, **3** and **4** in different solvents upon 420 nm excitation at room temperature. The concentration is 100 μM.

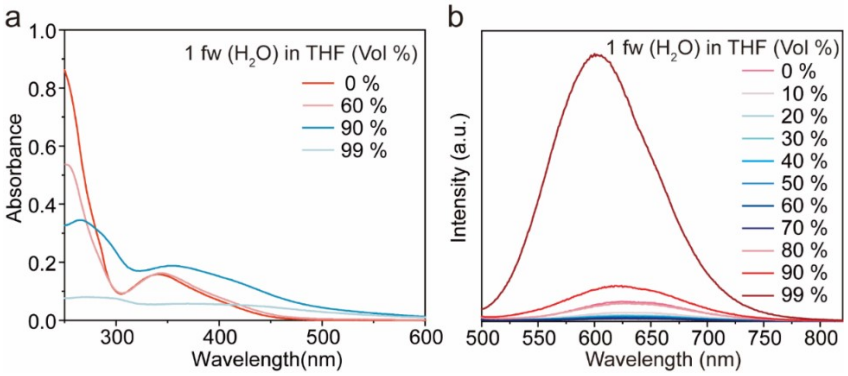

Figure S4. a) Absorption and b) photoluminescent spectra of **1** in THF/H_2O with different water fractions. The excitation wavelength is 420 nm. All the measurements were performed with a concentration of 10 μM.

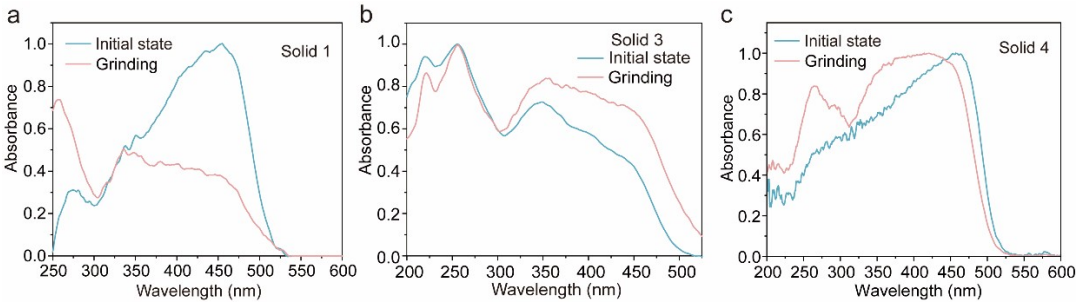

Figure S5. a-c) Normalized absorption spectra of compounds **1**, **3** and **4** before and after grinding of the solid powders.

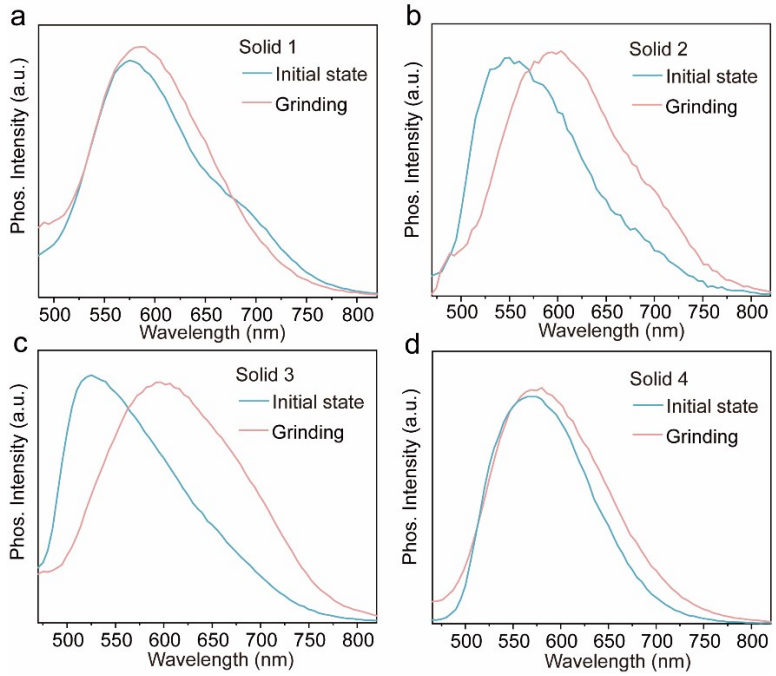

Figure S6. a-d) Phosphorescence spectra of compounds **1-4** before and after grinding (λ_{ex} = 420 nm) at room temperature.

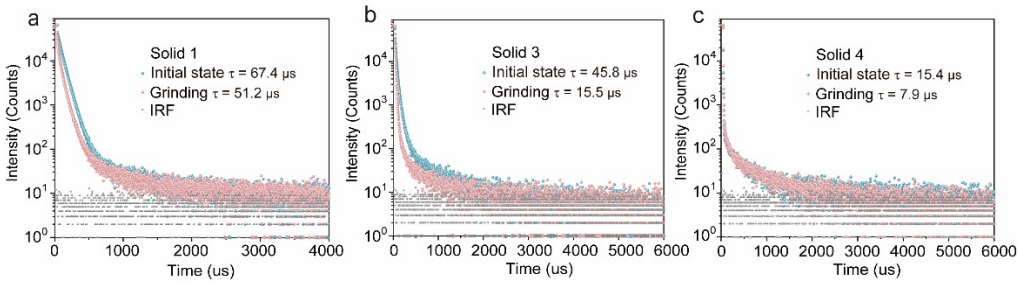

Figure S7. a-c) Phosphorescence lifetimes of **1**, **3** and **4** in solid powder before and after grinding at room temperature.

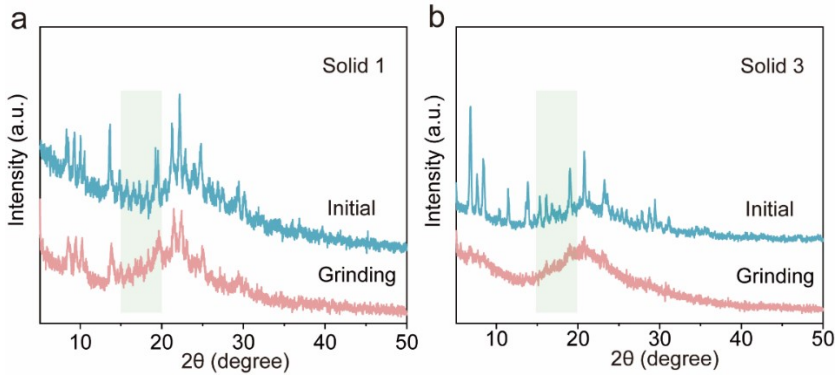

Figure S8. PXRD spectra of compounds **1** and **3** before and after grinding.

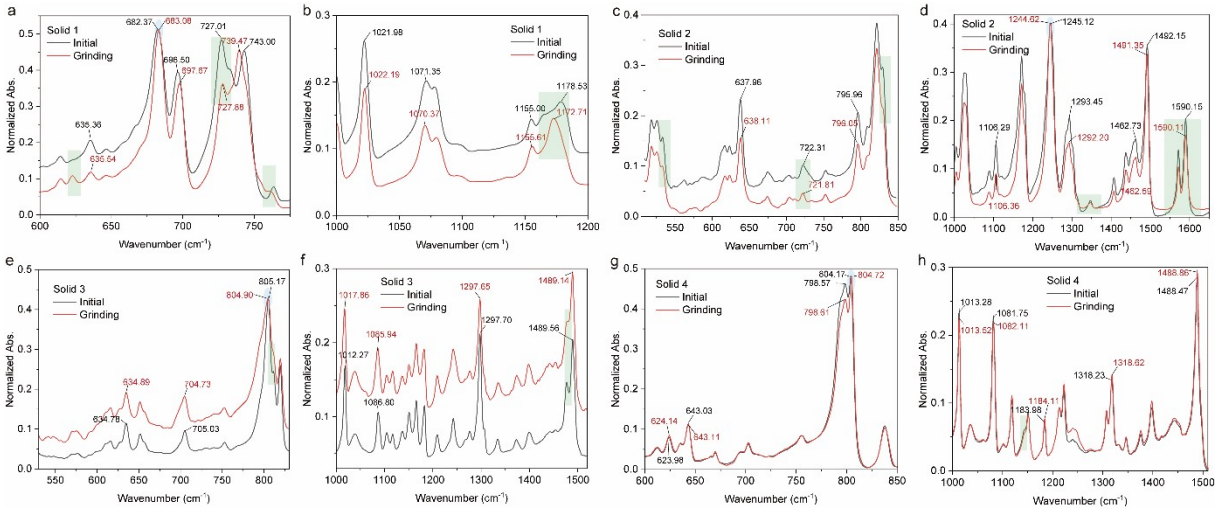

Figure S9. The infrared-absorption spectrum of solid a, b) **1**, c, d) **2**, e, f) **3**, and g, h) **4**.

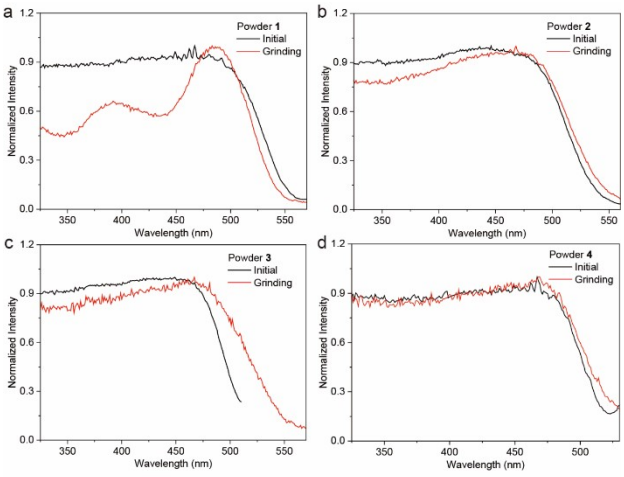

Figure S10. The excitation spectra of compound a) 1, b) 2, c) 3, and d) 4 in solid state before and after grinding.

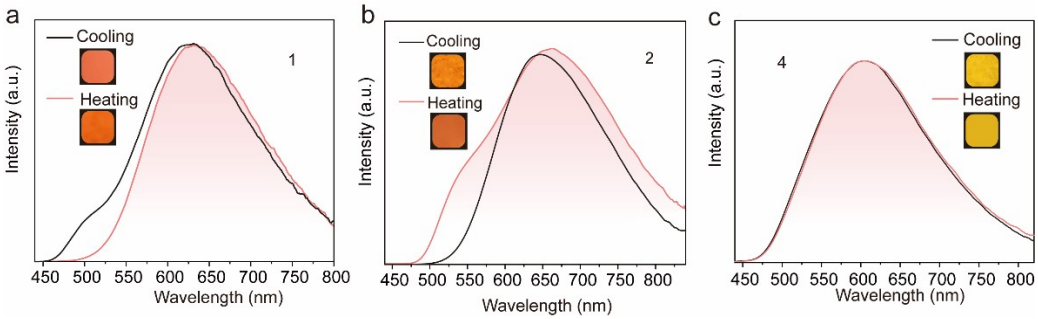

Figure S11. The emission spectra of a) 1@LA (mass ratios of 200:1), b) 2@LA (mass ratios of 100:1) and c) 4@LA (mass ratios of 100:1) at 30 °C and 60 °C under 420 nm photoexcitation. The insets are their corresponding photographs taken under 365 nm UV light.

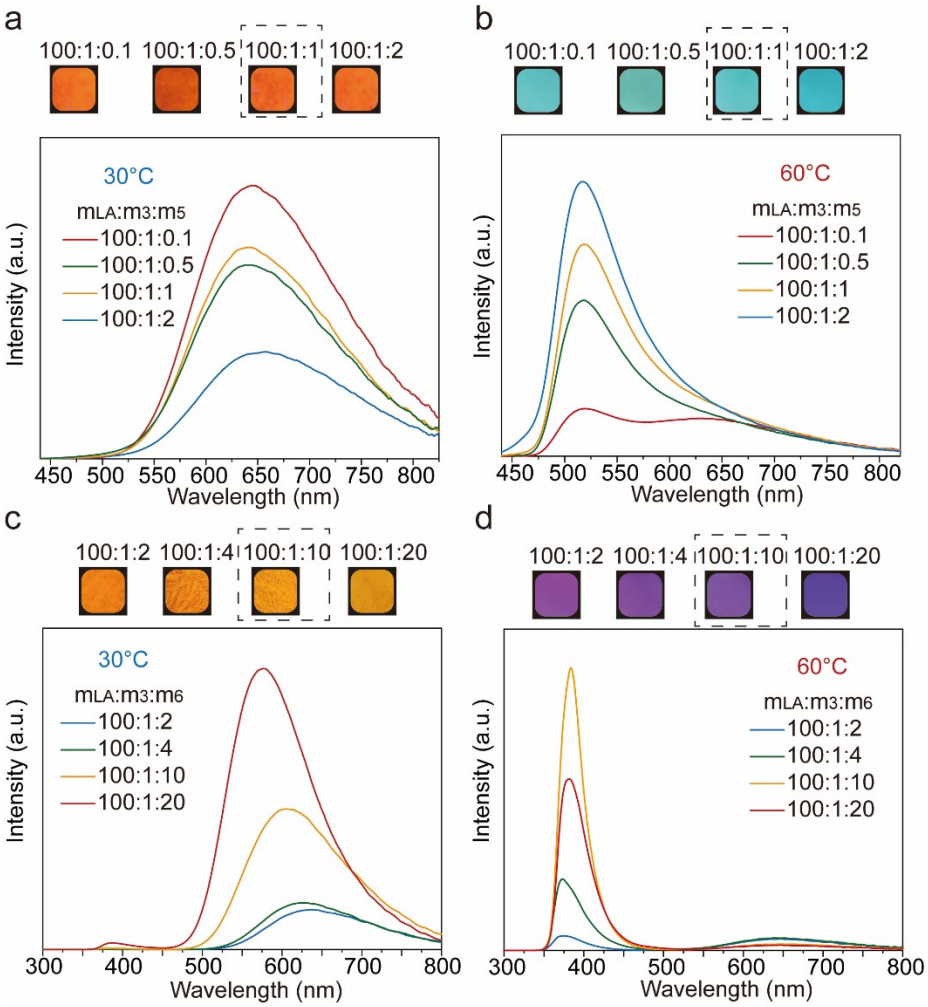

Figure S12. Emission spectra of 3-5@LA with different doping ratios at a) 30 °C and b) 60 °C. Emission spectra of 3-6@LA with different doping ratios at c) 30 °C and d) 60 °C under 280 nm UV excitation. The corresponding photo taken under 365 nm UV light.

Table S1 Photophysical date of compounds **1-4**

Compound	Sol (DCM)		Solid (before grinding)		Solid (after grinding)	
	λ_{abs}[a] [nm]	λ_{em}[b] [nm]	$\lambda_{em\ (prompt)}$[c] [nm]	$\lambda_{em\ (delay)}$[d] [nm]	$\lambda_{em\ (prompt)}$ [nm]	$\lambda_{em\ (delay}$ [nm]
1	330	650	550	555	575	575
2	350	655	548	544	582	592
3	345	655	500	510	582	595
4	340	615	525	555	565	575

[a] Absorption peak. [b] Maximum photoluminescence peak. [c] Maximum fluorescence peaks. [d] Maximum phosphorescence peak.

Table S2. Relation between starting geometry, curvature of the central ring and phosphorescence wavelength of compound 2.

Method	**λ_{phos},nm**	**Central core**	**Deviation from planarity**	**Starting geometry**	**Experiment**
ONIOM GD3-B3LYP/6-311G(d,p):UFF	640	Slightly distorted	21	Start from X-ray for crystal packing of 6 molecules	Before grinding (548 nm)
Individual GD3-B3LYP/6-311G(d,p) GD3	696	Slightly distorted	26	Start from ideal planar central core	After grinding (582 nm)

Single-crystal structural parameters

Samples	**2**
Empirical formula	C36 H28 N2 O4 S4
Formula weight	680.84
Temperature/K	293
Crystal system	triclinic
Space group	P -1
a/Å	10.0346(13)
b/Å	10.9918(9)
c/Å	17.534(2)
α/°	90.506(9)
β/°	106.183(11)
γ/°	114.022(11)
Volume/Å^3	1679.9(4)
Z	2
ρ_{calc}g/cm^3	1.346
CCDC number	2343600

Cartesian coordinates of the calculated structures

Optimized structure of crystal fragment of compound 2 in ONIOM approach (GD3-UB3LYP/6-311G(d) for target molecule and UFF for surrounding).

16	9.936483000	1.184641000	0.722209000
16	5.941246000	1.615069000	-4.334473000
16	6.943666000	4.353868000	-2.774492000
16	8.674158000	4.047000000	0.020039000
8	12.535166000	5.944384000	-3.910471000
8	14.376947000	4.110917000	-1.903325000
8	3.353861000	6.021845000	1.771509000
8	0.874961000	4.043181000	-2.411304000
7	6.868129000	-1.871553000	-3.802168000
7	9.427210000	-2.104607000	-0.711982000
6	8.949401000	-1.091486000	-0.997515000
6	7.132694000	-0.925151000	-3.191578000
6	7.467703000	0.264412000	-2.435964000
6	6.932294000	1.503829000	-2.820062000
6	7.368730000	2.727640000	-2.100447000

6	8.201739000	2.598237000	-0.968384000
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6	8.359641000	0.182126000	-1.349345000
6	11.291375000	2.060806000	-0.094005000
6	12.074553000	2.942733000	0.669237000
1	11.868370000	3.072409000	1.621952000
6	13.087173000	3.631548000	0.111159000
1	13.597584000	4.249708000	0.677661000
6	13.402324000	3.459985000	-1.261564000
6	12.639936000	2.545764000	-2.000216000
1	12.842965000	2.388252000	-2.949060000
6	11.578388000	1.862963000	-1.397599000
1	11.056009000	1.227630000	-1.934141000
6	15.161876000	5.069541000	-1.185944000
1	15.836930000	5.469961000	-1.816398000
1	15.661718000	4.626751000	-0.430039000
1	14.580042000	5.815202000	-0.835187000
6	8.631985000	4.872067000	-3.137883000
6	9.526094000	4.008027000	-3.798501000
1	9.226780000	3.115585000	-4.081344000
6	10.788691000	4.390064000	-4.055835000
1	11.396097000	3.770674000	-4.518980000
6	11.255556000	5.652762000	-3.659441000
6	10.342590000	6.527256000	-3.018447000
1	10.606118000	7.426576000	-2.727304000
6	9.027170000	6.107989000	-2.782911000
1	8.399580000	6.715003000	-2.330622000
6	13.053036000	7.212491000	-3.493956000
1	14.025722000	7.262857000	-3.748685000
1	12.985945000	7.312690000	-2.492419000
1	12.567237000	7.965352000	-3.957075000
6	7.040926000	4.643236000	0.509672000
6	5.925164000	3.796018000	0.639076000
1	6.006081000	2.836739000	0.446095000
6	4.736955000	4.279678000	1.042032000
1	3.971152000	3.669238000	1.114181000
6	4.568512000	5.634156000	1.374986000
6	5.685123000	6.498322000	1.269918000
1	5.621733000	7.453109000	1.484713000
6	6.913663000	5.996023000	0.839623000
1	7.687764000	6.597556000	0.767203000
6	3.146303000	7.387237000	2.148002000
1	3.720223000	7.623303000	2.942156000
1	2.182779000	7.511501000	2.410366000
1	3.340528000	8.005078000	1.375992000
6	4.430279000	2.401187000	-3.714763000
6	3.597943000	2.933724000	-4.628249000
1	3.835306000	2.912325000	-5.582201000
6	2.386207000	3.514536000	-4.242711000
1	1.806063000	3.889010000	-4.939893000
6	2.020550000	3.537092000	-2.876370000
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6	-8.842904000	-1.025590000	-0.839288000
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6	-7.908018000	-1.327467000	1.388428000
6	-6.231752000	1.150995000	3.235274000
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1	-5.958753000	1.293960000	5.286459000
6	-4.264459000	1.906371000	4.380651000
1	-3.813224000	2.091324000	5.232458000
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1	-6.763061000	1.351531000	-1.357986000
6	-6.008353000	3.211531000	-1.181035000
1	-5.094152000	2.903138000	-0.994046000
6	-6.282131000	4.586884000	-1.214917000
6	-7.607881000	4.994837000	-1.501529000
1	-7.858357000	5.942245000	-1.545356000
6	-8.600556000	4.030778000	-1.713057000
1	-9.522954000	4.319425000	-1.893076000
6	-5.516153000	6.831393000	-0.967643000
1	-4.658752000	7.309910000	-0.746644000
1	-6.199701000	7.076335000	-0.267892000
1	-5.819604000	7.133821000	-1.880021000
6	-11.212597000	2.273764000	0.945077000
6	-11.912212000	1.107708000	1.296648000
1	-11.449395000	0.384201000	1.774642000
6	-13.215903000	0.970281000	0.999030000
1	-13.683484000	0.146279000	1.262262000
6	-13.923220000	1.973059000	0.315099000
6	-13.239001000	3.166114000	-0.028584000
1	-13.687765000	3.902384000	-0.496964000
6	-11.889935000	3.314920000	0.303743000
1	-11.414725000	4.142010000	0.066646000
6	-15.961648000	2.719134000	-0.678148000

1	-16.014343000	3.576813000	-0.150026000
1	-16.898231000	2.374643000	-0.811211000
1	-15.557976000	2.888350000	-1.586990000
6	-11.120011000	-1.537846000	-2.170378000
6	-11.891284000	-1.062803000	-3.164460000
1	-11.484177000	-0.792195000	-4.017414000
6	-13.273907000	-0.926710000	-2.987988000
1	-13.805629000	-0.559169000	-3.726341000
6	-13.868911000	-1.319271000	-1.763123000
6	-13.034366000	-1.848581000	-0.766696000
1	-13.422779000	-2.142899000	0.087699000
6	-11.707734000	-1.945535000	-0.956955000
1	-11.147476000	-2.318065000	-0.241465000
6	-16.049217000	-0.661142000	-2.473272000
1	-15.784628000	0.287553000	-2.691182000
1	-16.984799000	-0.647304000	-2.101836000
1	-16.050652000	-1.227097000	-3.308132000
16	10.128089000	-5.408291000	3.509735000
16	6.549633000	-9.658891000	0.209796000
16	6.851776000	-6.520516000	-0.872184000
16	8.000355000	-4.366008000	1.253685000
8	11.836317000	-4.639831000	-3.468648000
8	13.124814000	-2.684568000	-0.819121000
8	2.809719000	-4.362693000	4.122889000
8	1.532015000	-6.683859000	1.283503000
7	8.681257000	-11.448237000	2.628085000
7	10.943994000	-8.791854000	4.612394000
6	10.220137000	-8.428041000	3.785925000
6	8.617772000	-10.322705000	2.366336000
6	8.538264000	-8.914095000	2.039165000
6	7.658354000	-8.484403000	1.034509000
6	7.646978000	-7.051305000	0.663708000
6	8.330284000	-6.130487000	1.471592000
6	9.202312000	-6.589824000	2.483197000
6	9.314186000	-7.972970000	2.750878000
6	11.063531000	-4.600301000	2.191888000
6	11.243847000	-3.208340000	2.257244000
1	10.858445000	-2.704970000	3.008923000
6	11.911735000	-2.549556000	1.292970000
1	11.995084000	-1.574169000	1.367683000
6	12.472355000	-3.255945000	0.197261000
6	12.327912000	-4.649503000	0.171771000
1	12.722638000	-5.171331000	-0.561614000
6	11.608694000	-5.303572000	1.178399000
1	11.512344000	-6.280488000	1.139995000
6	13.243166000	-1.258463000	-0.852034000
1	13.740396000	-0.993936000	-1.686436000
1	13.763785000	-0.923931000	-0.055677000
1	12.331050000	-0.830594000	-0.881715000
6	8.355144000	-5.936953000	-1.682618000
6	9.527804000	-6.717170000	-1.683511000
1	9.533466000	-7.594279000	-1.240176000
6	10.645808000	-6.279646000	-2.289231000
1	11.456206000	-6.836729000	-2.269615000
6	10.677022000	-5.031664000	-2.931734000
6	9.484460000	-4.268345000	-2.955649000
1	9.440071000	-3.392916000	-3.396763000
6	8.336037000	-4.752711000	-2.318769000

1	7.520166000	-4.206368000	-2.317306000
6	11.911875000	-3.352928000	-4.092813000
1	12.850397000	-3.211683000	-4.428435000
1	11.703084000	-2.622124000	-3.429141000
1	11.285152000	-3.301929000	-4.881422000
6	6.396337000	-4.396407000	2.072419000
6	6.260476000	-4.927948000	3.364414000
1	7.039937000	-5.315052000	3.819152000
6	5.080194000	-4.897140000	4.003609000
1	5.014955000	-5.276989000	4.908682000
6	3.939012000	-4.335187000	3.409765000
6	4.054244000	-3.787948000	2.105459000
1	3.288333000	-3.380662000	1.645887000
6	5.287985000	-3.815593000	1.447111000
1	5.373370000	-3.428628000	0.547323000
6	1.614446000	-3.826212000	3.551635000
1	1.723284000	-2.842681000	3.358272000
1	0.862092000	-3.935583000	4.211557000
1	1.370607000	-4.328351000	2.713064000
6	5.007734000	-8.766359000	0.521326000
6	4.097107000	-8.673662000	-0.465471000
1	4.275805000	-9.084451000	-1.340544000
6	2.903681000	-7.967152000	-0.268630000
1	2.269613000	-7.902130000	-1.014901000
6	2.640384000	-7.368278000	0.988107000
6	3.600053000	-7.515442000	2.000715000
1	3.432949000	-7.126439000	2.887757000
6	4.743232000	-8.186570000	1.778306000
1	5.395539000	-8.276893000	2.507863000
6	0.524246000	-6.527140000	0.280112000
1	0.880130000	-5.997055000	-0.498931000
1	-0.250902000	-6.024674000	0.676678000
1	0.183488000	-7.423416000	-0.031165000
16	-4.089827000	-11.108298000	2.193887000
16	-5.015444000	-7.942294000	-3.367160000
16	-5.037662000	-6.288267000	-0.383580000
16	-5.185888000	-8.091784000	2.295514000
8	-0.703141000	-4.543717000	-4.033049000
8	0.760180000	-8.088957000	3.770581000
8	-10.762025000	-6.531282000	0.976351000
8	-10.660949000	-6.567329000	-2.222632000
7	-3.904252000	-11.360630000	-4.070705000
7	-3.335443000	-13.316762000	-0.618709000
6	-3.679862000	-12.211994000	-0.604515000
6	-4.072964000	-10.816469000	-3.063348000
6	-4.284234000	-10.135390000	-1.802143000
6	-4.683798000	-8.789831000	-1.797094000
6	-4.835280000	-8.089939000	-0.489379000
6	-4.781533000	-8.848774000	0.694876000
6	-4.352541000	-10.192165000	0.649141000
6	-4.110215000	-10.828356000	-0.586853000
6	-2.603399000	-10.203988000	2.675782000
6	-2.536095000	-9.633052000	3.958098000
1	-3.297632000	-9.730907000	4.572478000
6	-1.456239000	-8.929281000	4.346806000
1	-1.457767000	-8.530967000	5.244015000
6	-0.346749000	-8.776237000	3.475355000
6	-0.411868000	-9.387889000	2.215765000

1	0.346852000	-9.320592000	1.594755000
6	-1.558634000	-10.090615000	1.831467000
1	-1.590207000	-10.507597000	0.942479000
6	0.849449000	-7.417555000	5.031437000
1	1.737762000	-6.946500000	5.083034000
1	0.799928000	-8.078393000	5.791634000
1	0.121497000	-6.724440000	5.117360000
6	-3.696045000	-5.740332000	-1.461784000
6	-2.489637000	-6.457852000	-1.585994000
1	-2.344049000	-7.272487000	-1.056562000
6	-1.528723000	-6.045718000	-2.433283000
1	-0.701935000	-6.571234000	-2.520019000
6	-1.690441000	-4.878674000	-3.196983000
6	-2.883078000	-4.134508000	-3.026406000
1	-3.048661000	-3.302180000	-3.519181000
6	-3.866900000	-4.594994000	-2.144659000
1	-4.699590000	-4.085093000	-2.042054000
6	-0.843062000	-3.366926000	-4.837567000
1	-0.015387000	-3.261002000	-5.400682000
1	-0.934392000	-2.546463000	-4.259223000
1	-1.636318000	-3.450356000	-5.454930000
6	-6.885302000	-7.613914000	1.918429000
6	-7.761208000	-8.477467000	1.240889000
1	-7.453172000	-9.368493000	0.963199000
6	-9.026451000	-8.105520000	0.975163000
1	-9.620654000	-8.730951000	0.503639000
6	-9.512901000	-6.838196000	1.339731000
6	-8.654784000	-5.969078000	2.056883000
1	-8.947312000	-5.079620000	2.350755000
6	-7.350816000	-6.369474000	2.353407000
1	-6.756814000	-5.763694000	2.845630000
6	-11.278120000	-5.232487000	1.289982000
1	-11.317133000	-5.096093000	2.288435000
1	-12.213818000	-5.159614000	0.925663000
1	-10.717436000	-4.513749000	0.858590000
6	-6.726027000	-7.499388000	-3.017264000
6	-7.145408000	-6.251040000	-3.288554000
1	-6.514476000	-5.587709000	-3.646009000
6	-8.472552000	-5.878670000	-3.041724000
1	-8.742897000	-4.954633000	-3.228577000
6	-9.385426000	-6.829297000	-2.523340000
6	-8.919223000	-8.134673000	-2.302322000
1	-9.537884000	-8.820973000	-1.966012000
6	-7.633463000	-8.457417000	-2.527894000
1	-7.331130000	-9.377560000	-2.360259000
6	-11.151786000	-5.232054000	-2.387583000
1	-10.632858000	-4.590714000	-1.807780000
1	-12.115956000	-5.203252000	-2.099463000
1	-11.103629000	-4.949867000	-3.354629000
16	-2.967208000	11.267480000	-1.715343000
16	-0.285138000	11.388815000	4.149827000
16	-0.914067000	8.502843000	2.687083000
16	-1.800941000	8.542987000	-0.461634000
8	-6.385159000	6.186055000	2.577574000
8	-8.506980000	9.346094000	-0.738656000
8	3.974743000	8.133972000	-1.793801000
8	5.290854000	10.351282000	2.376342000
7	-1.423185000	14.773089000	3.251519000

7	-3.123348000	14.667659000	-0.384569000
6	-2.711531000	13.694981000	0.088334000
6	-1.510328000	13.770141000	2.680706000
6	-1.619038000	12.515012000	1.965972000
6	-1.120131000	11.339499000	2.546464000
6	-1.279890000	10.054812000	1.827926000
6	-1.787593000	10.065100000	0.516589000
6	-2.271776000	11.266117000	-0.041324000
6	-2.196712000	12.477029000	0.680732000
6	-4.645624000	10.672033000	-1.356817000
6	-5.427983000	10.269140000	-2.453701000
1	-5.044185000	10.300612000	-3.358619000
6	-6.692453000	9.839429000	-2.290923000
1	-7.196511000	9.564112000	-3.086981000
6	-7.270030000	9.780469000	-0.997606000
6	-6.489139000	10.196837000	0.087937000
1	-6.862387000	10.178401000	0.997231000
6	-5.177533000	10.642603000	-0.113286000
1	-4.666824000	10.942093000	0.667286000
6	-9.328208000	8.899663000	-1.823464000
1	-10.215995000	8.601073000	-1.454455000
1	-9.495473000	9.650690000	-2.475620000
1	-8.903861000	8.114365000	-2.292793000
6	-2.584435000	7.794161000	2.668026000
6	-3.742633000	8.601179000	2.697080000
1	-3.664449000	9.578491000	2.748133000
6	-4.969713000	8.051293000	2.667448000
1	-5.761566000	8.633908000	2.684322000
6	-5.136231000	6.659509000	2.619643000
6	-3.973145000	5.853510000	2.624034000
1	-4.024986000	4.875510000	2.596486000
6	-2.709313000	6.454280000	2.659244000
1	-1.909724000	5.884895000	2.660843000
6	-6.589675000	4.769532000	2.533303000
1	-7.578654000	4.587719000	2.502253000
1	-6.171959000	4.373926000	1.705628000
1	-6.215602000	4.329658000	3.360102000
6	-0.017285000	8.415830000	-0.743119000
6	0.811507000	9.546617000	-0.873319000
1	0.440604000	10.448595000	-0.762622000
6	2.112368000	9.418402000	-1.190271000
1	2.663650000	10.226996000	-1.289230000
6	2.691136000	8.160021000	-1.423302000
6	1.882235000	7.008813000	-1.269625000
1	2.243276000	6.106283000	-1.396231000
6	0.532906000	7.145625000	-0.936726000
1	-0.029936000	6.346547000	-0.848066000
6	4.573526000	6.880918000	-2.143370000
1	4.099995000	6.468063000	-2.932769000
1	5.532602000	7.044587000	-2.401035000
1	4.563717000	6.245486000	-1.362990000
6	1.403582000	11.037120000	3.587713000
6	2.274505000	10.544840000	4.488478000
1	1.978890000	10.357851000	5.407347000
6	3.606047000	10.294436000	4.135586000
1	4.209909000	9.929990000	4.817879000
6	4.047930000	10.566161000	2.817863000
6	3.117555000	11.089993000	1.908509000

1	3.401279000	11.296364000	0.989689000
6	1.845108000	11.323194000	2.276250000
1	1.232208000	11.713620000	1.617081000
6	6.264363000	9.810521000	3.276764000
1	5.979647000	8.900843000	3.606554000
1	7.136008000	9.705418000	2.784097000
1	6.415576000	10.434968000	4.054248000
16	-2.411343000	2.136352000	-2.243729000
16	1.898530000	1.988540000	2.388689000
16	0.840568000	-0.948686000	1.112039000
16	-0.839394000	-0.739962000	-1.759832000
8	-3.952335000	-3.509576000	3.397275000
8	-6.222607000	-2.282437000	-3.208700000
8	4.413211000	-3.283442000	-2.807020000
8	6.920848000	-0.965533000	1.469294000
7	0.605060000	5.246717000	1.963729000
7	-2.530384000	5.107717000	-0.283068000
6	-1.900175000	4.134011000	-0.188394000
6	0.381630000	4.239855000	1.441114000
6	0.033376000	3.012192000	0.815902000
6	0.729861000	1.836835000	1.086824000
6	0.370816000	0.596964000	0.422377000
6	-0.581654000	0.659717000	-0.674113000
6	-1.309347000	1.811937000	-0.898201000
6	-1.094048000	2.997680000	-0.070612000
6	-3.446181000	0.715369000	-2.483521000
6	-3.823258000	0.444148000	-3.798928000
1	-3.383251000	1.007681000	-4.613031000
6	-4.750848000	-0.550490000	-4.079958000
1	-5.021838000	-0.738134000	-5.108920000
6	-5.307957000	-1.294516000	-3.035322000
6	-4.913849000	-1.037485000	-1.713054000
1	-5.345369000	-1.632206000	-0.918257000
6	-3.999265000	-0.038367000	-1.436349000
1	-3.698559000	0.147386000	-0.414002000
6	-6.621803000	-2.599586000	-4.537619000
1	-7.374599000	-3.377826000	-4.447741000
1	-7.065799000	-1.733459000	-5.040326000
1	-5.778148000	-2.974889000	-5.127522000
6	-0.712187000	-1.672786000	1.592459000
6	-1.716030000	-0.925989000	2.226121000
1	-1.605495000	0.146670000	2.312355000
6	-2.811573000	-1.564963000	2.774935000
1	-3.580538000	-1.015461000	3.303792000
6	-2.911896000	-2.964062000	2.718895000
6	-1.957146000	-3.703665000	2.013223000
1	-2.044037000	-4.776289000	1.912768000
6	-0.868517000	-3.049464000	1.446837000
1	-0.117397000	-3.612340000	0.907859000
6	-4.003666000	-4.925540000	3.510109000
1	-4.838840000	-5.143010000	4.172428000
1	-4.174935000	-5.390113000	2.534217000
1	-3.082011000	-5.326237000	3.947287000
6	0.782393000	-1.449797000	-1.965938000
6	1.895887000	-0.708128000	-2.378752000
1	1.801183000	0.360859000	-2.522161000
6	3.105074000	-1.341872000	-2.618010000
1	3.975045000	-0.786878000	-2.947877000

6	3.209103000	-2.735271000	-2.491035000
6	2.101166000	-3.477002000	-2.075742000
1	2.161331000	-4.549014000	-1.958590000
6	0.903038000	-2.827308000	-1.801144000
1	0.050518000	-3.396684000	-1.453004000
6	4.490777000	-4.701855000	-2.883163000
1	3.731424000	-5.106356000	-3.561809000
1	5.476360000	-4.930398000	-3.281077000
1	4.376138000	-5.163318000	-1.895855000
6	3.274273000	0.925125000	2.052021000
6	4.067467000	0.618664000	3.162618000
1	3.737723000	0.899371000	4.156354000
6	5.288200000	-0.022716000	3.007863000
1	5.886701000	-0.231007000	3.883175000
6	5.726331000	-0.381988000	1.727946000
6	4.902954000	-0.135024000	0.618253000
1	5.241982000	-0.451964000	-0.359988000
6	3.699815000	0.526863000	0.774021000
1	3.084307000	0.726863000	-0.091134000
6	7.849209000	-1.110378000	2.540674000
1	7.483671000	-1.813123000	3.297261000
1	8.758112000	-1.504380000	2.092678000
1	8.066620000	-0.145488000	3.010578000

Optimized structure of single molecule of compound 2 calculated by GD3-UB3LYP/6-311G(d) method is a gas phase.

16	2.101898000	0.658455000	2.652071000
16	-1.538180000	2.108444000	-2.469942000
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6	1.175301000	2.359638000	0.646110000
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1	4.587767000	2.044735000	3.066138000
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6	3.898110000	-0.393693000	0.798771000
1	3.076019000	-0.995531000	0.430883000
6	8.518980000	0.869219000	0.411656000
1	9.336209000	0.552956000	-0.234171000
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1	8.795740000	0.696370000	1.457841000
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6	1.755293000	-0.834651000	-2.389366000
1	1.492149000	0.167916000	-2.703103000
6	3.053312000	-1.287031000	-2.540876000
1	3.820932000	-0.657130000	-2.972180000
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6	1.130391000	-2.940252000	-1.394412000
1	0.387323000	-3.574421000	-0.925897000
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6	-4.979589000	2.381231000	-0.327661000
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1	-7.154874000	-0.984336000	-0.228763000
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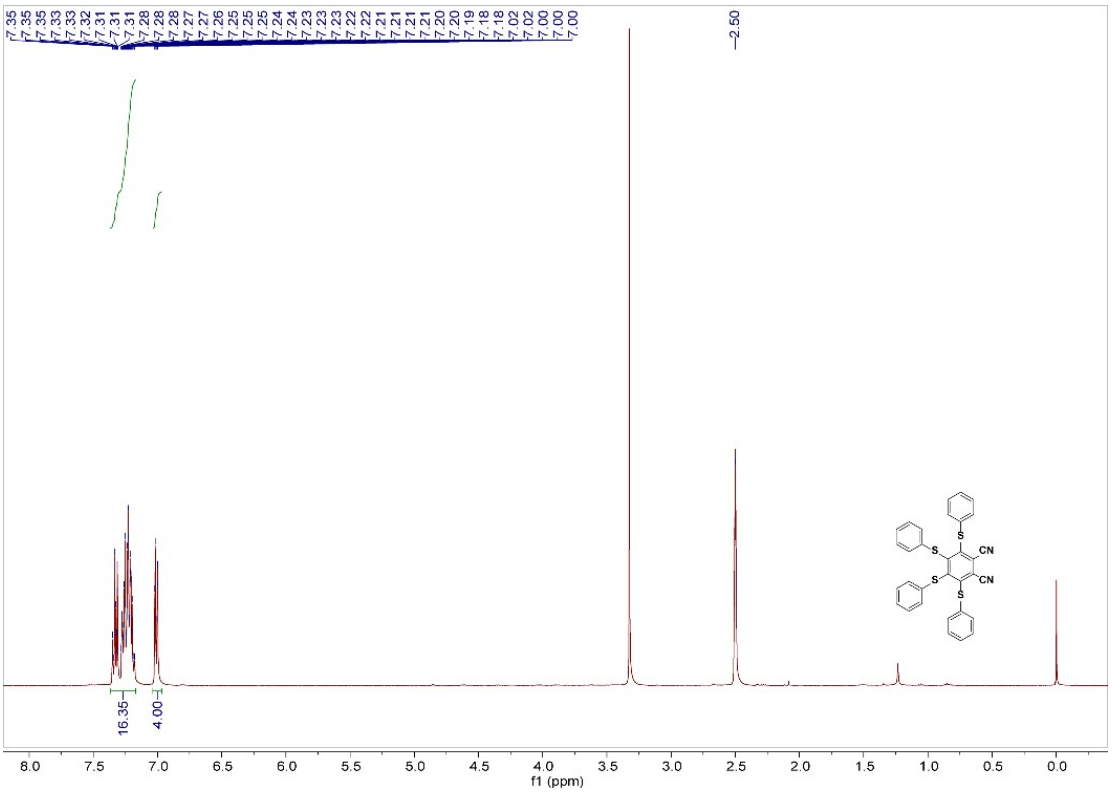

Figure S13. ^{1}H NMR spectrum of compound **1** in DMSO-d_6.

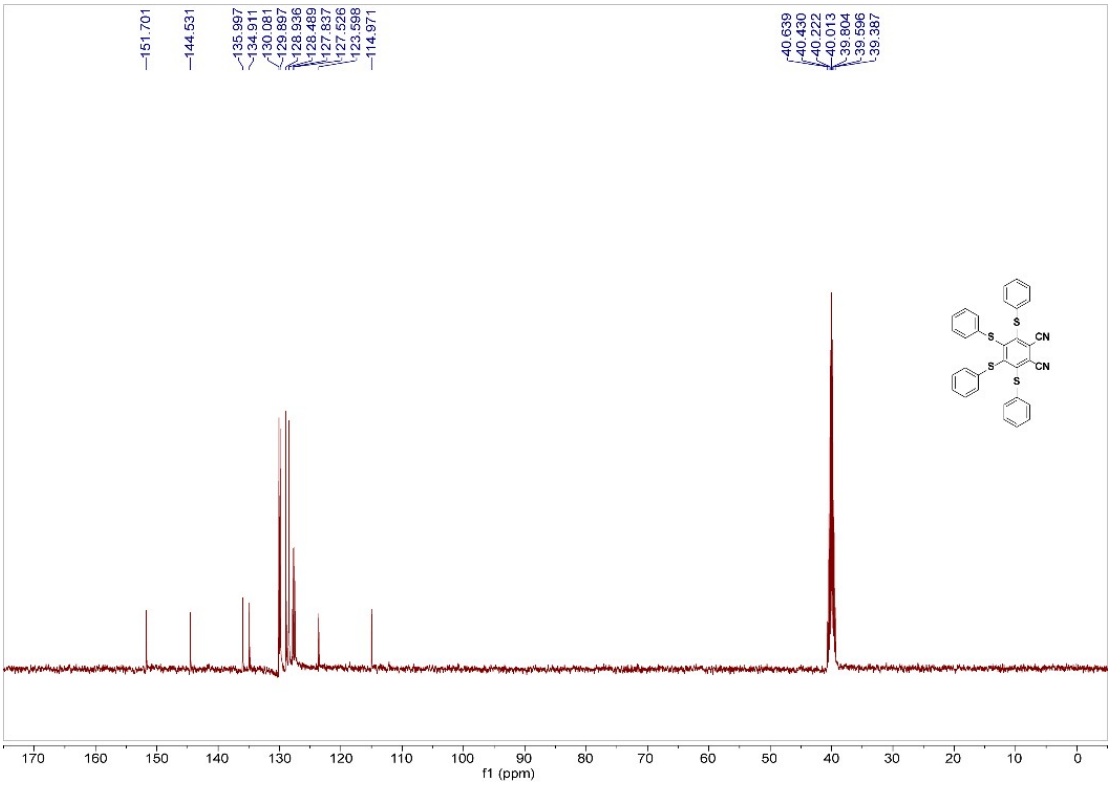

Figure S14. ^{13}C NMR spectrum of compound **1** in DMSO-d_6.

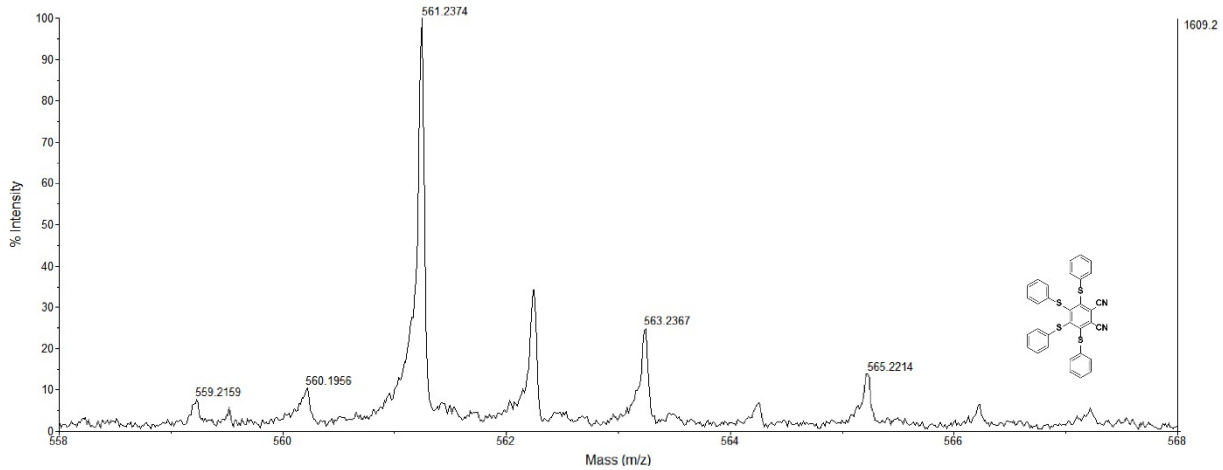

Figure S15. MALDI TOF-MS spectrum of compound **1**.

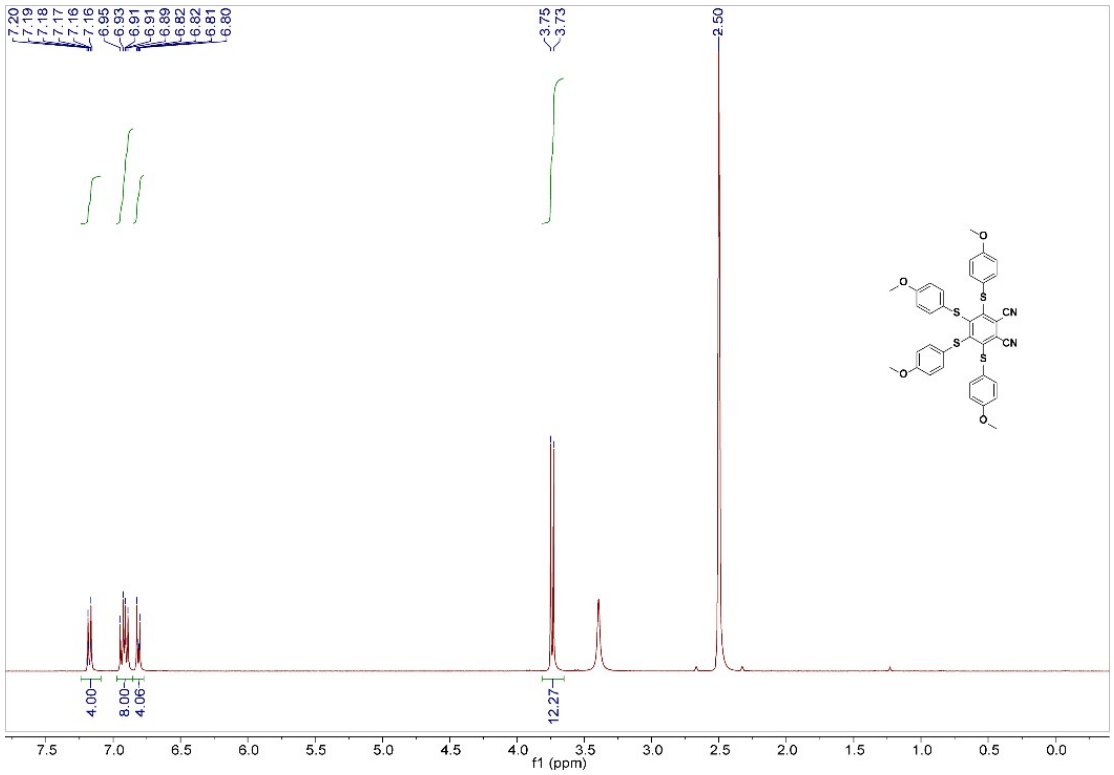

Figure S16. ^{1}H NMR spectrum of compound **2** in DMSO-d_6.

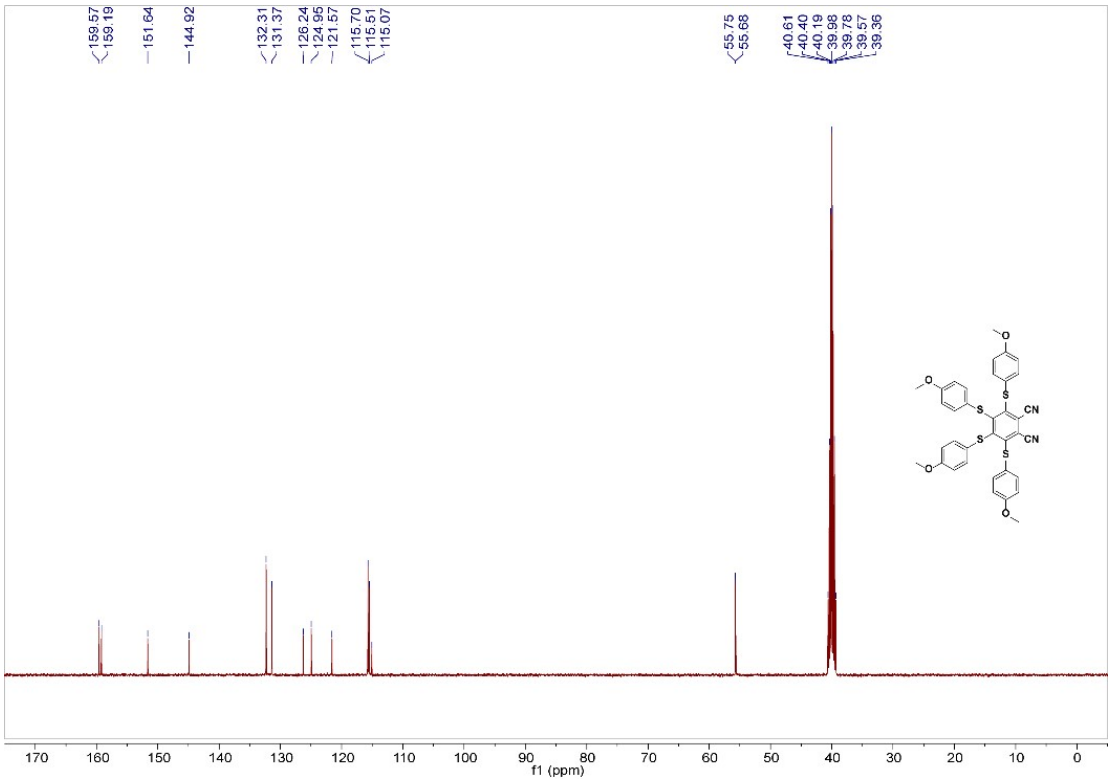

Figure S17. ^{13}C NMR spectrum of compound **2** in DMSO-d_6.

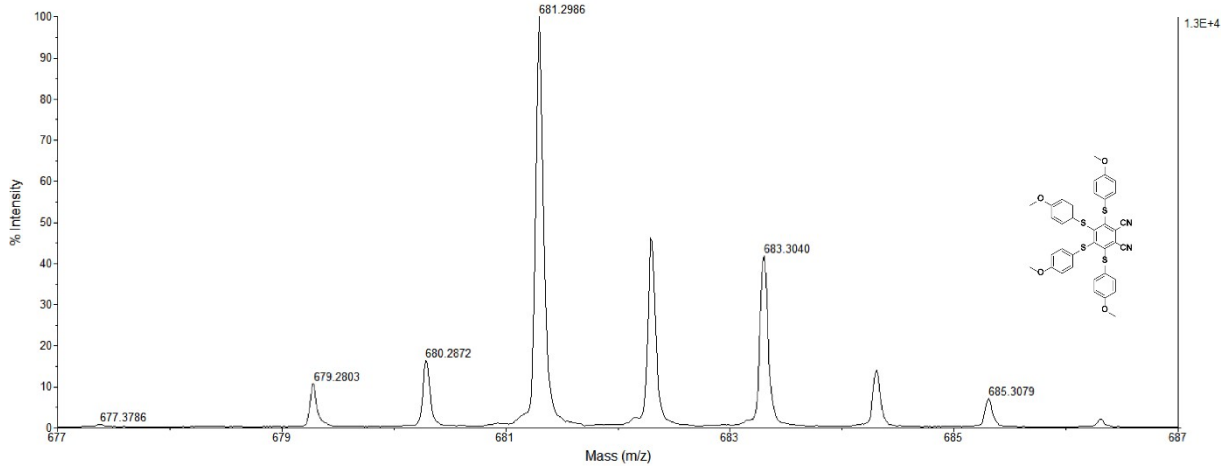

Figure S18. MALDI TOF-MS spectrum of compound **2**.

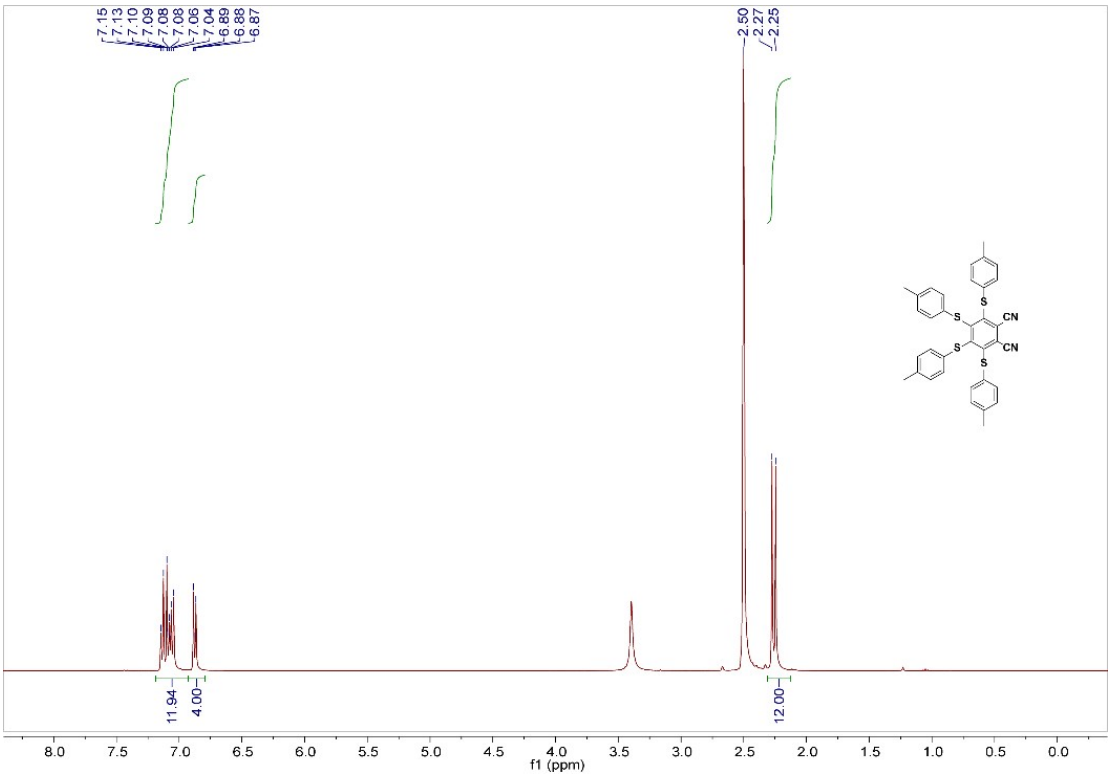

Figure S19. ^{1}H NMR spectrum of compound **3** in DMSO-d_6.

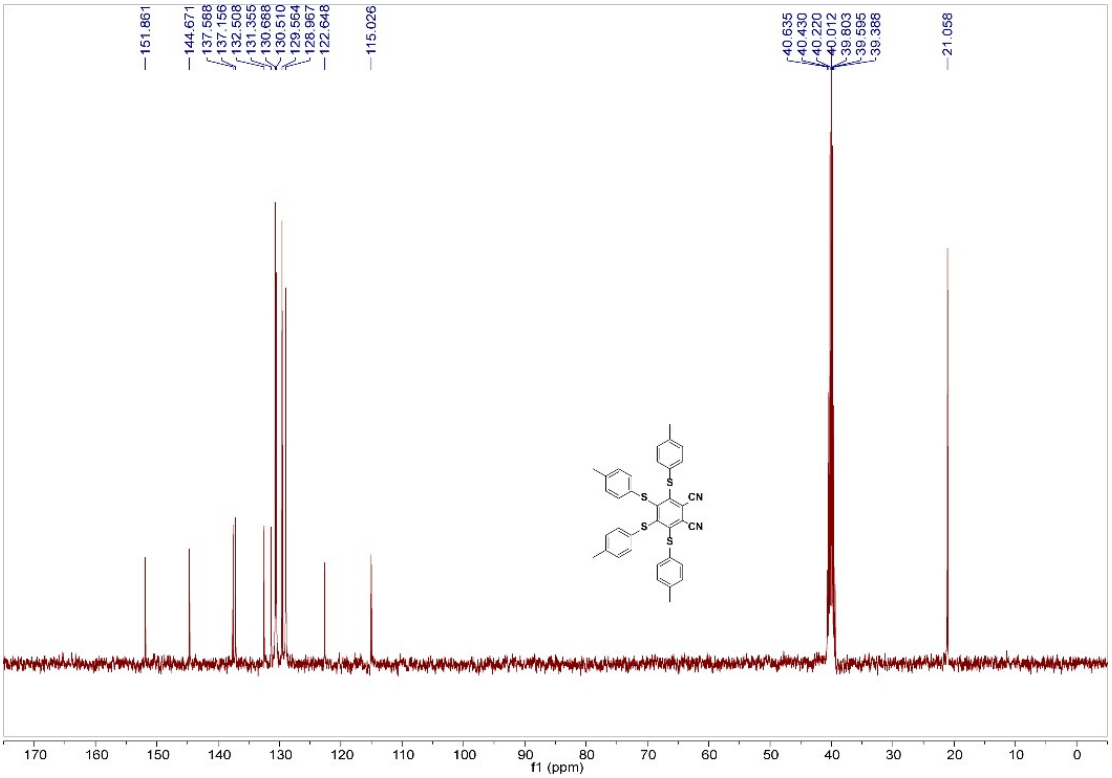

Figure S20. ^{13}C NMR spectrum of compound **3** in DMSO-d_6.

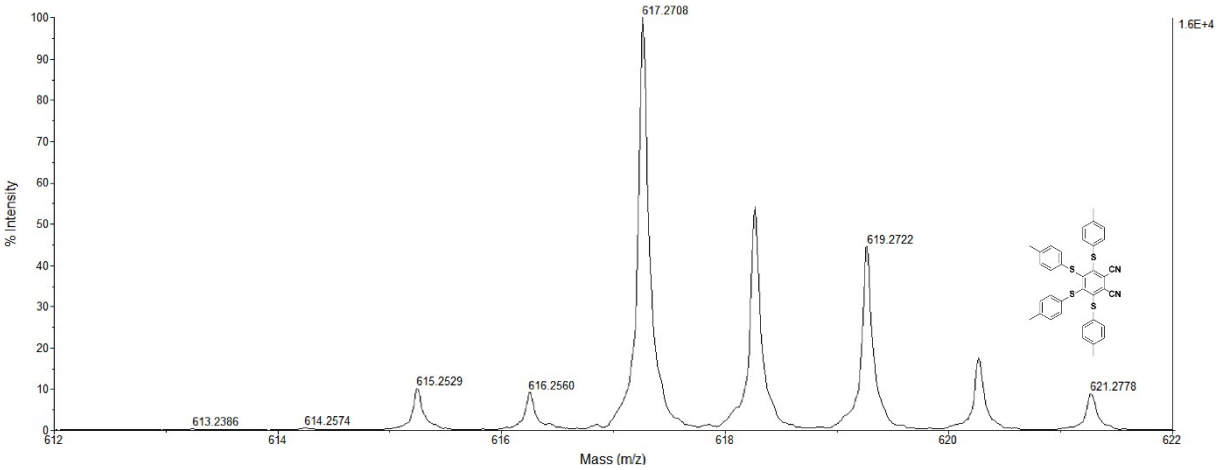

Figure S21. MALDI TOF-MS spectrum of compound **3**.

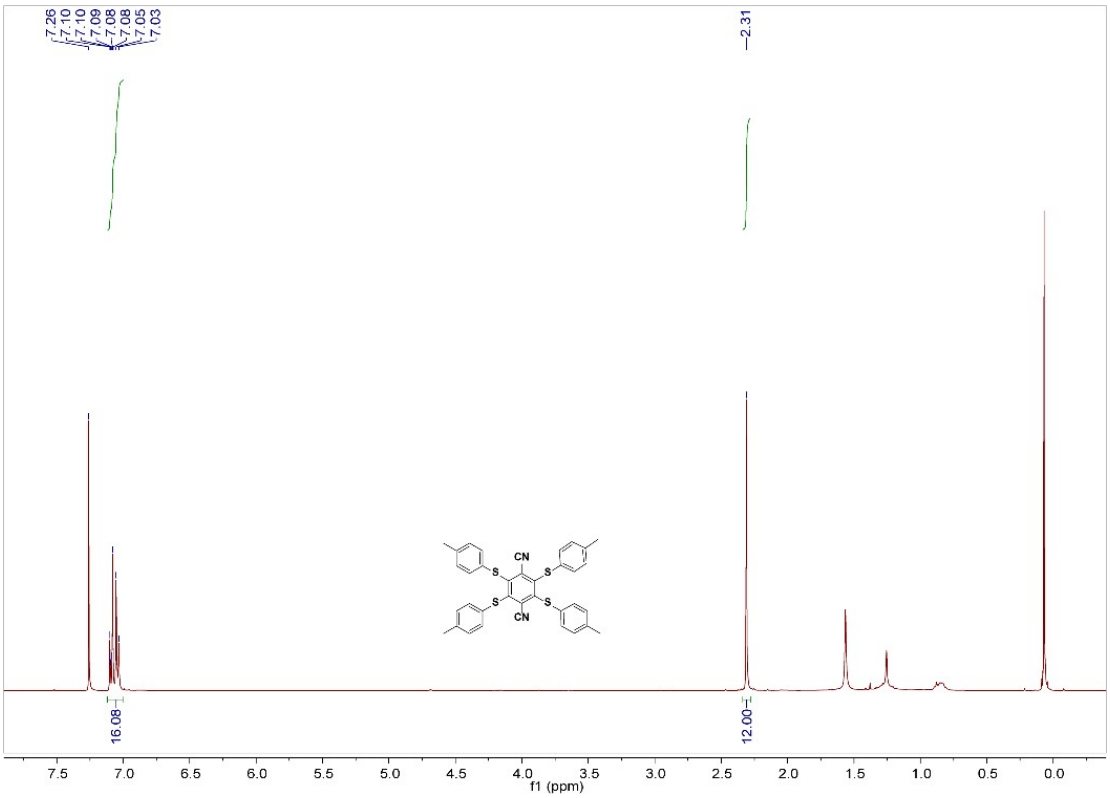

Figure S22. ^{1}H NMR spectrum of compound **4** in $CDCl_3$.

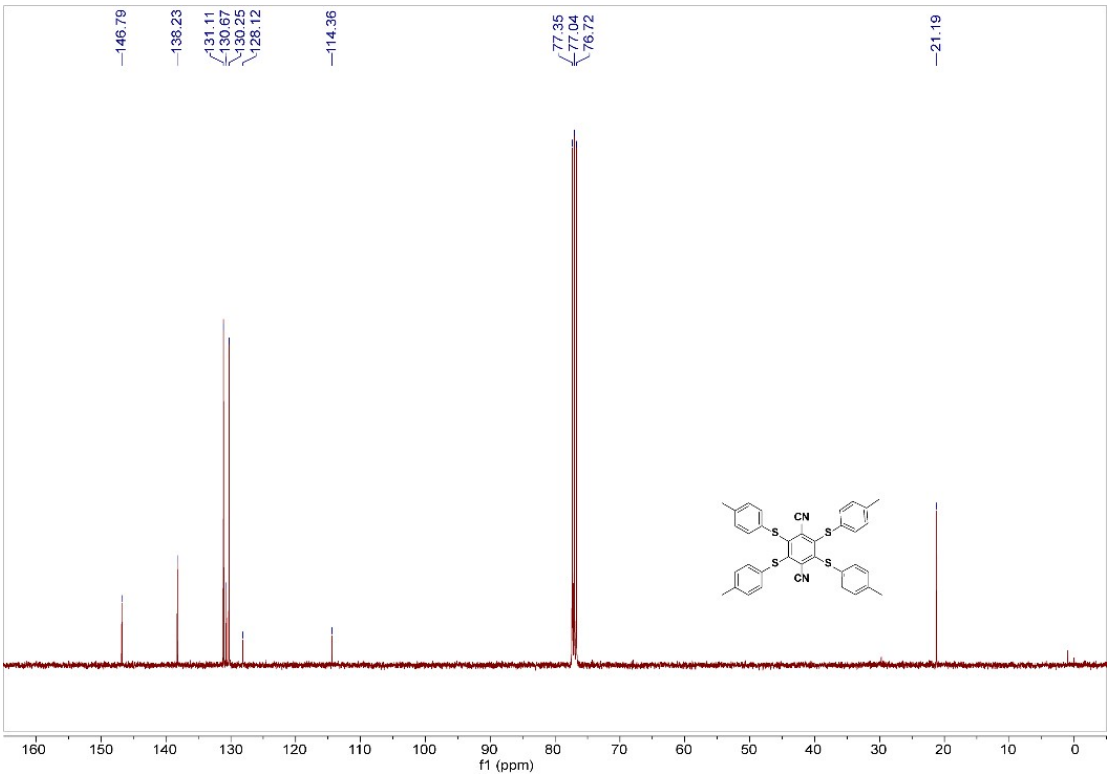

Figure S23. ^{13}C NMR spectrum of compound **4** in $CDCl_3$.

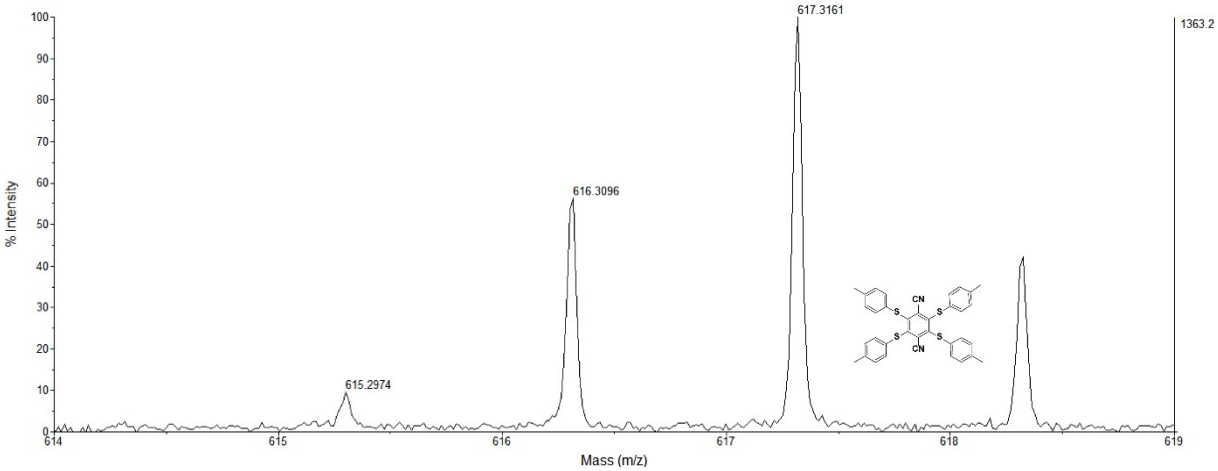

Figure S24. MALDI TOF-MS spectrum of compound **4**.

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