Sulfur-substituted perylene diimides: efficient tuning of LUMO levels and visible-light absorption via sulfur redox

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1. Supporting Methods

1.1. General materials and methods

Unless otherwise indicated, all other reagents are commercially purchased and used as received. All aqueous solutions were prepared with Milli-Q water. Organic solvents are including 1-methyl-2-pyrrolidinone (NMP), acetic acid, ethanol, acetonitrile, methanol (MeOH), dichloromethane (DCM), acetone and petroleum ether. Organic reagents are including 3,4,9,10-perylenetetracarboxylic dianhydride (**10**), 1,6,7,12-tetrachloroperylene tetracarboxylic acid dianhydride (**11**), *n*-octylamine, potassium carbonate, 18-crown-6, *n*-butyl mercaptan, pentahydrate copper sulfate, 3-chloroperbenzoic acid (*m*-CPBA), pentafluorothiophenol, thiophenol, periodic acid, chromium trioxide. Nitrogen and Argon stored in the high-pressure gas cylinder were purchased from Dehai Gas in Qingdao. Unless otherwise noted, column chromatography was carried out on silica gel (200 - 300 mesh). TLC analysis was performed on precoated silica gel plates (0.2 mm thick). ^{1}H, ^{13}C and ^{19}F NMR spectra were performed on 400 MHz spectrometer (Bruker AVANCE NEO 400 Ascend) in the indicated solvents at room temperature. Spin multiplicities are reported as a singlet (s), doublet (d), triplet (t) and quartet (q) with coupling constants (*J*) given in Hz, or multiplet (m). MALDI-TOF mass spectrometry analysis was performed on a Bruker Microflex-LRF mass spectrometer in positive ion. The liquid UV-vis absorbance was measured by UV spectrometer (HITACHI, 3900). Fluorescence spectra were recorded on fluorescence spectrometer (HITACHI, F-2700). Cyclic

voltammetry (CV) measurements were carried out using a standard one compartment, three-electrode electrochemical cell attached to an CHI 760E Electrochemical Workstation. The Saturated calomel electrode (SCE) was used as reference electrode. Glass-carbon was used as the working electrode, and Pt was used as the counter electrode. Tetrabutylammonium hexafluorophosphate (0.1 M) in DCM was used as electrolyte. The potential range was set between -1.5 V and 1.5 V and the scan rate was 100 mV s^{-1}. The fluorescence quantum yields were measured on Quantaurus-QY C11347-11 with a calibrated integrating sphere system.

1.2 Synthesis

The synthesis of the sulfide and sulfone PDIs (**2**-**9**) is shown in Figure S1. The sulfide PDIs **2** was prepared from **5** (4Cl-PDI) by nucleophilic substitution with butanethiol in the presence of K_2CO_3 as a base. However, for the phenylsulfide and pentafluorophenylsulfide substituted PDIs (**3**, **6**), the nucleophilic substitution is more difficult. First, the copper salts of thiophenol (**13**) and pentafluorothiophenol (**14**) had to be used instead of the thiophenol form to increase the nucleophilicities. Then, more active **4** (4Br-PDI) was used instead of **5** (4Cl-PDI) to increase the activity of the leaving group. The oxidation of **2** by *m*-CPBA at room temperature is relatively easy. However, the same condition is not suitable for **3** and **6**. To obtain **8** from **3**, harsher conditions which involved H_5IO_6 and CrO_3 was necessary. However, for the ultimate goal compound **9** from **6**, even under extremely harsh conditions, no target product

was obtained. We did observe the existence of **9** in the reaction mixture by MALDI-TOF mass spectrometry. However, the synthesis and separation of **9** have so far not been successful. The aromatic core of **9** is probably too electron deficient to exist. The details of all the synthesis procedures were listed below.

Compound 12. This compound was prepared following the literature procedure.[S1]

Compound 1. To a solution of **10** (392 mg, 1.0 mmol) in NMP (50 mL), acetic acid (0.5 mL) and *n*-octylamine (259 mg, 2.0 mmol) were added. The mixture was then stirred for 12 h at 80 °C. The resulting mixture was poured into 1 M HCl aqueous solution (100 mL) and washed with water and concentrated in vacuo. Silica gel column chromatography of the residue (PE/DCM 2:1 - 1:1) gave pure **1** (321 mg, 82%). ^{1}H NMR (400 MHz, $CDCl_3$): 8.70 (d, ^{3}J (H, H) = 8.0 Hz, 4H), 8.63 (d, ^{3}J (H, H) = 8.4 Hz, 4H), 4.21 (t, ^{3}J (H, H) = 7.6 Hz, 4H), 1.54 - 1.51 (m, 20H), 1.30 - 1.25 (m, 4H), 0.90 (t, ^{3}J (H, H) = 6.4 Hz, 6H). MS (MALDI-TOF) calcd for $C_{40}H_{42}N_2O_4$: 614.31, found 614.79.

Compound 4. To a solution of **12** (707 mg, 1.0 mmol) in NMP (70 mL), acetic acid (0.7 mL) and *n*-octylamine (259 mg, 2.0 mmol) were added. The mixture was then stirred for 4 h at 80 °C. The resulting mixture was poured into 1 M HCl aqueous solution (200 mL) and washed with water and concentrated in vacuo. Silica gel column chromatography of the residue (PE/DCM 2:1 - 1:1) gave pure **4** (608 mg, 86%). ^{1}H NMR (400 MHz, $CDCl_3$): 8.83 (s, 4H,), 4.20 (t, ^{3}J (H, H) = 8.0 Hz, 4H), 1.78 - 1.70 (m, 4H), 1.57 - 1.44 (m, 20H), 0.88 (t, ^{3}J (H, H) = 6.4 Hz, 6H). ^{13}C NMR

(100 MHz, $CDCl_3$): 162.20(*C*), 136.11(*CH*), 131.62(*C*), 131.45(*C*), 123.95(*C*), 122.73(*C*), 40.99(CH_2), 31.83(CH_2), 29.32(CH_2), 28.13(CH_2), 27.09(CH_2), 22.65(CH_2), 14.11(CH_3). MS (MALDI-TOF) calcd for $C_{40}H_{38}Br_4N_2O_4$: 929.96, found 929.99.

Compound 5. To a solution of **11** (1 g, 1.9 mmol) in NMP (50 mL), acetic acid (0.5 mL) and *n*-octylamine (488 mg, 3.8 mmol) were added. The mixture was then stirred for 4 h at 80 °C. The resulting mixture was poured into 1 M HCl aqueous solution (300 mL) and washed with water and concentrated in vacuo. Silica gel column chromatography of the residue (PE/DCM 1.5:1 - 1:1) gave pure **5** (890 mg, 89%). ^{1}H NMR (400 MHz, $CDCl_3$): 8.68 (s, 4H), 4.21 (t, ^3J (H, H) = 7.6 Hz, 4H), 1.78 - 1.71 (m, 4H), 1.55 - 1.25 (m, 20H), 0.90 (t, ^3J (H, H) = 6.8 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): 161.26(*C*), 135.37(*C*), 132.94(*C*), 131.44(*CH*), 128.59(*C*), 123.27(*C*), 41.00(CH_2), 31.82(CH_2), 29.20(CH_2), 28.11(CH_2), 27.08(CH_2), 22.65(CH_2), 14.10(CH_3). MS (MALDI-TOF) calcd for $C_{40}H_{38}Cl_4N_2O_4$: 752.16, found 752.25.

Compound 2. To a solution of **5** (500 mg, 0.6 mmol) in acetonitrile (15 mL), potassium carbonate (1.1 g, 8.0 mmol), 18-crown-6 (35 mg, 0.1 mmol) and *n*-butyl mercaptan (6 mg, 67.0 mmol) were added. The mixture was then stirred for 12 h at 120 °C. Silica gel column chromatography of the residue (PE/DCM 4:1 - 2:1) gave pure **2** (390 mg, 78%) as purple solid. ^{1}H NMR (400 MHz, $CDCl_3$): 8.72 (s, 4H), 4.22 (t, ^3J (H, H) = 7.6 Hz, 4H), 2.99 - 2.91 (m, 8H), 1.80 - 1.73 (m, 4H), 1.55 - 1.53 (m, 16H), 1.29 - 1.26 (m, 20H), 0.88 (t, ^3J (H, H) = 6.4 Hz, 6H), 0.74 (t, ^3J (H, H) = 7.2

Hz, 12H). ^{13}C NMR (100 MHz, $CDCl_3$): 163.61(*C*), 139.52(*C*), 131.45(*C*), 131.18(*C*), 129.23(*CH*), 122.69(*C*), 121.22(*C*), 40.74(CH_2), 36.38(CH_2), 31.84(CH_2), 30.84(CH_2), 29.25(CH_2), 28.24(CH_2), 27.19(CH_2), 22.66(CH_2), 21.89(CH_2), 14.11(CH_3), 13.50(CH_3). MS (MALDI-TOF) calcd for $C_{56}H_{74}N_2O_4S_4$: 967.46, found 967.06.

Compounds **13** and **14**. These compounds were prepared following the literature procedure.[S2]

Compound 3. To solution of **4** (930 mg, 1.0 mmol) in NMP (90 mL), **13** (3.7 g, 20.0 mmol) was added. The mixture was then stirred for 3h at 150 °C. The resulting mixture was poured into 1M HCL aqueous solution (500 mL). The precipitate was collected by filtration and washed with water. Silica gel column chromatography of the residue (DCM/PE 1:1.5; R_f 0.35 with DCM/PE 1:1) gave pure **3** (828 mg, 89%) as purple solid. ^{1}H NMR (400 MHz, $CDCl_3$): 8.47 (s, 4H), 7.16 - 7.13 (m, 20H), 4.10 (t, ^3J (H, H) = 7.6 Hz, 4H), 1.68 - 1.58 (m, 4H), 1.33 - 1.28(m, 20H), 0.86 (t, ^3J (H, H) = 8.0 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): 163.04 (*C*), 138.66 (*C*), 137.05 (*C*), 134.60 (*C*), 131.51 (*C*), 129.08 (*CH*), 127.53 (*CH*), 123.62 (*CH*), 121.56 (*C*), 40.64 (CH_2), 31.81 (CH_2), 29.24 (CH_2), 28.13 (CH_2), 27.13 (CH_2), 22.64 (CH_2), 14.10 (CH_3). MS (MALDI-TOF): calcd for $C_{64}H_{58}F_{20}N_2O_4S_4$: 1047.33, found 1047.00.

Compound 6. To solution of **4** (930 mg, 1.0 mmol) in NMP (90 mL), **14** (5.26 g, 20.0 mmol) was added. The mixture was then stirred for 3h at 150 °C. The resulting mixture was poured into 1M HCL aqueous solution (500 mL). The precipitate was collected by filtration and washed with water. Silica gel column chromatography of

the residue (DCM/PE 4:1.5 - 2:1) gave pure **6** (781 mg, 84%) as red solid. ^{1}H NMR (400 MHz, $CDCl_3$): 8.68 (s, 4H), 4.15 (t, ^{3}J (H, H) = 7.6 Hz, 4H), 1.76 - 1.69 (m, 4H), 1.34 - 1.26 (m, 20H), 0.87 (t, ^{3}J (H, H) = 6.8 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): 162.24 (*C*), 148.03(*C*), 147.96(*C*), 145.45(*C*), 135.03(*C*), 133.09(*C*), 128.02(*CH*), 125.00(*C*), 123.40(*C*), 41.07(CH_2), 31.81(CH_2), 29.26(CH_2), 29.19(CH_2), 27.13(CH_2), 22.63(CH_2), 14.07(CH_3). ^{19}F NMR (376 MHz, $CDCl_3$): -130.2 – -133.2 (m, 8F), -147.7 – -149.6 (m, 4F), -157.8 – -160.3 (m, 8F). MS (MALDI-TOF) calcd for $C_{64}H_{38}F_{20}N_2O_4S_4$: 1407.23, found 1407.06.

Compound 7. To a solution of **2** (300 mg, 0.3 mmol) in DCM (10 mL), *m*-CPBA (6 g, 31.0 mmol) was added. After stirring for 8 h at r.t., the mixture was washed with aqueous $Na_2S_2O_3$ (10%, 100 mL), brine (50 mL) and concentrated in vacuo. Silica gel column chromatography of the residue (DCM/PE 1:1 - 10:1) gave pure **7** (237 mg, 79%) as red solid. ^{1}H NMR (400 MHz, $CDCl_3$): 9.13 (s, 4H), 4.24 (t, ^{3}J (H, H) = 7.6 Hz, 4H), 3.51 - 3.01 (m, 8H), 1.80 - 1.72 (m, 4H), 1,54 - 1.52 (m, 16H), 1.35 - 1.25 (m, 20H), 0.90 (t, ^{3}J (H, H) = 6.8 Hz, 6H), 0.84 (t, ^{3}J (H, H) = 7.2 Hz, 12H). ^{13}C NMR (100 MHz, $CDCl_3$): 161.49 (*C*), 145.71(*C*), 130.16(*C*), 129.12(*C*), 127.75(*C*), 127.39(*C*), 124.26(*CH*), 56.62(CH_2), 41.24(CH_2), 31.83(CH_2), 29.19(CH_2), 28.12(CH_2), 27.07(CH_2), 23.45(CH_2), 22.65(CH_2), 21.56(CH_2), 14.11(CH_3), 13.49(CH_3). MS (MALDI-TOF) calcd for $C_{56}H_{74}N_2O_{12}S_4$: 1094.45, found 1094.45.

Compound 8. To a solution of **3** (262 mg, 0.2 mmol) in acetonitrile (20 mL), H_5IO_6 (1.71 g, 7.5 mmol) and CrO_3 (1 mg, 0.01 mmol) were added. The mixture was then

stirred for 12h at r.t. The resulting mixture was filtrated and the filtrate was evaporated. Silica gel column chromatography of the residue (DCM/EtOAc 20:1; R_f 0.31 with DCM/MeOH 50:1) gave pure **8** (53 mg, 20%) as purple solid. ^{1}H NMR (400MHz, $CDCl_3$): 9.23 (s, 4H), 7.44 (t, ^3J (H,H) = 7.6 Hz, 4H), 7.37 (t, ^3J (H,H) = 7.2 Hz, 8H), 7.20 (t, ^3J (H,H) = 8.0 Hz, 8H), 4.18 (t, ^3J (H,H) = 8.4 Hz, 4H), 1.79 - 1.71 (m, 4H), 1.36 - 1.25 (m, 20H), 0.88 (t, ^3J (H,H) = 5.2 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): 161.42 (*C*), 147.58 (*C*), 140.48 (*C*), 133.62 (*CH*), 130.75 (*C*), 129.71 (*CH*), 129.19 (*CH*), 127.86 (*CH*), 126.35 (*CH*), 49.47 (CH_2), 43.60 (CH_2), 30.69 (CH_2), 29.62 (CH_2), 26.49 (CH_2),17.66 (CH_2), 14.12 (CH_3). MS (MALDI-TOF) calcd for $C_{64}H_{58}N_2O_{12}S_4$: 1175.41, found 1175.66.

Compound 9. The aromatic core of **9** is probably too electron deficient to exist. However, we did observe the existence of **9** in the reaction mixture by MALDI-TOF mass spectrometry. MS (MALDI-TOF) calcd for $C_{64}H_{38}F_{20}N_2O_{12}S_4$: 1535.22, found 1535.52.

1.3 Electrochemistry

The reduction potentials of **1** – **8** were determined using cyclic voltammetry and differential pulse voltammetry (DPV, scan rate 100 mV/s) vs Fc^+ / Fc in DCM (supporting electrolyte: 100 mM Bu_4NPF_6, working electrode: Pt, counter electrode: Pt wire, reference electrode: SCE). LUMO energies vs vacuum were calculated from reduction peak in DPV using the equation S1.[S3]

$$E_{LUMO} = -5.1\ eV - E_{DPV}\ vs\ (Fc^{+}/Fc) \quad (S1)$$

1.4 Density functional theory (DFT) calculation details

Geometry optimization of dye **1-9** at the lowest singlet ground state (S_0) was performed using B3LYP as the density functional and 6-31+G** as the basis set for C H O N F Cl and LanL2DZ for Br. Time-dependent DFT was performed at the S_0 optimum geometry to calculate the contribution of molecular orbitals to excitations to different excited state, using the keyword td=(nstates=5). Visualization of frontier orbitals was performed with the Multiwfn software package,[S4] while visualization of the optimized molecular geometries was performed by the CYLViewer software.[S5]

1.5 References

[S1] L. Zhang, Y. Xu, F. Zhu and J. Sun, *Asian J. Chem.*, 2010, **22**, 7135-7144.

[S2] M. E. Peach, *Can. J. Chem.*, 1968, **46**, 2699-2706.

[S3] C. M. Cardona, W. Li, A. E. Kaifer, D. Stockdale and G. C. Bazan, *Adv. Mater.*, 2011, **23**, 2367-2371.

[S4] T. Lu and F. Chen, *J. Comput. Chem.*, 2012, **33**, 580-592.

[S5] CYLview, 1.0b; Legault, C. Y., Universite de Sherbrooke, 2009 (http://www.cylview.org)

2. Supporting Figures and Legends

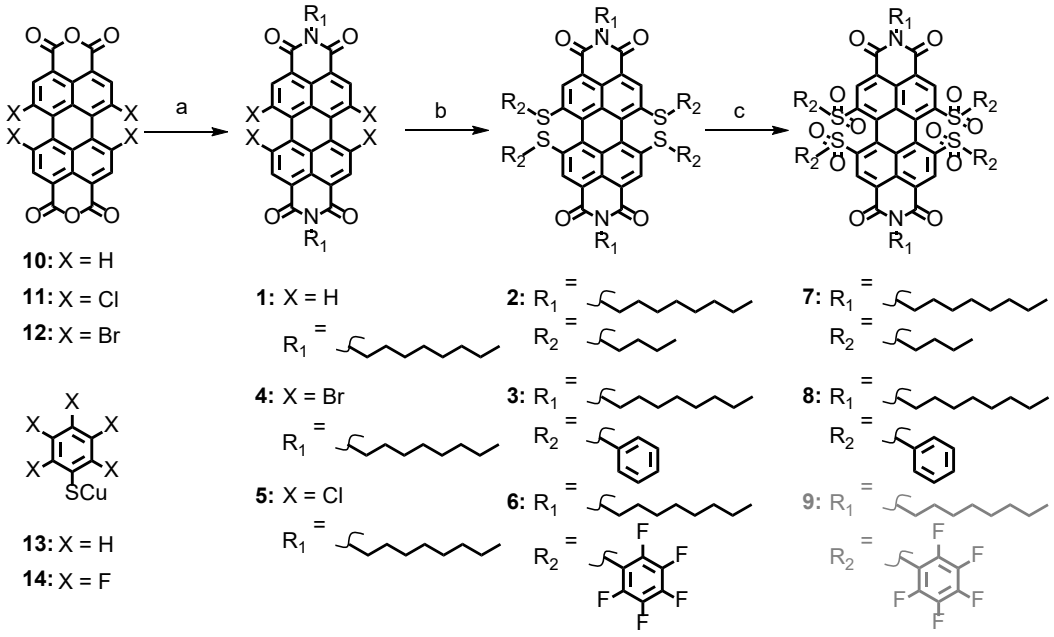

Figure S1. The synthesis scheme of different substituted PDIs.

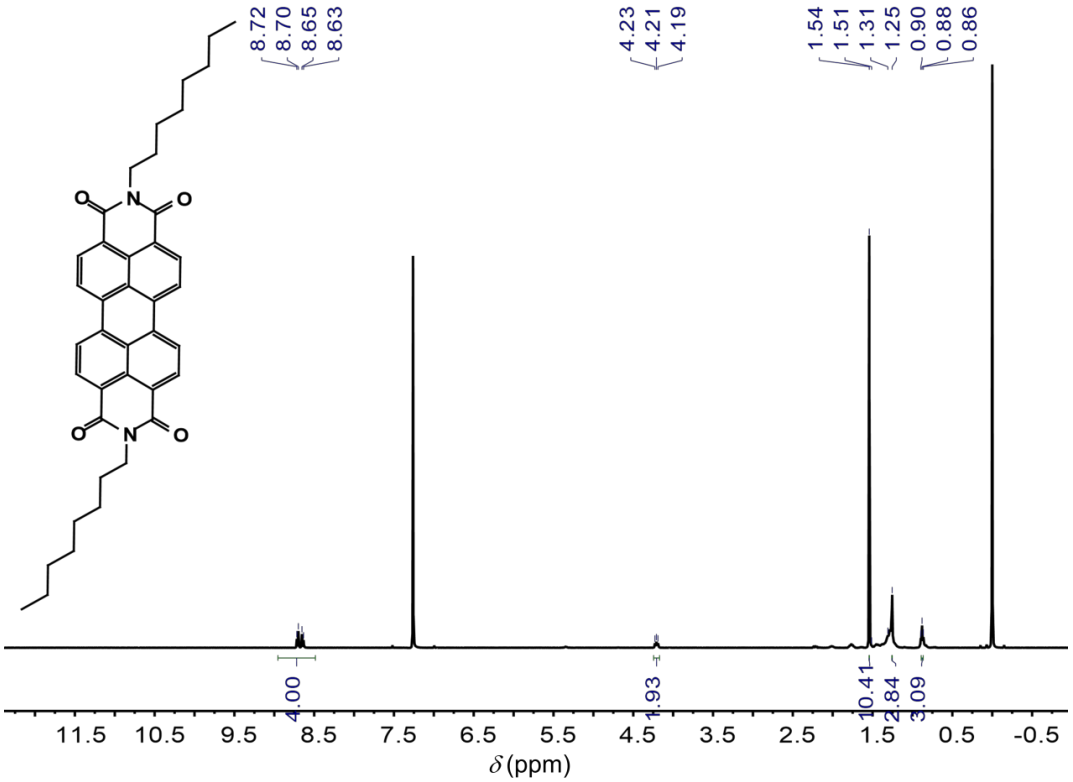

Figure S2. ^{1}H-NMR (400 MHz) spectrum of compound **1** in $CDCl_3$.

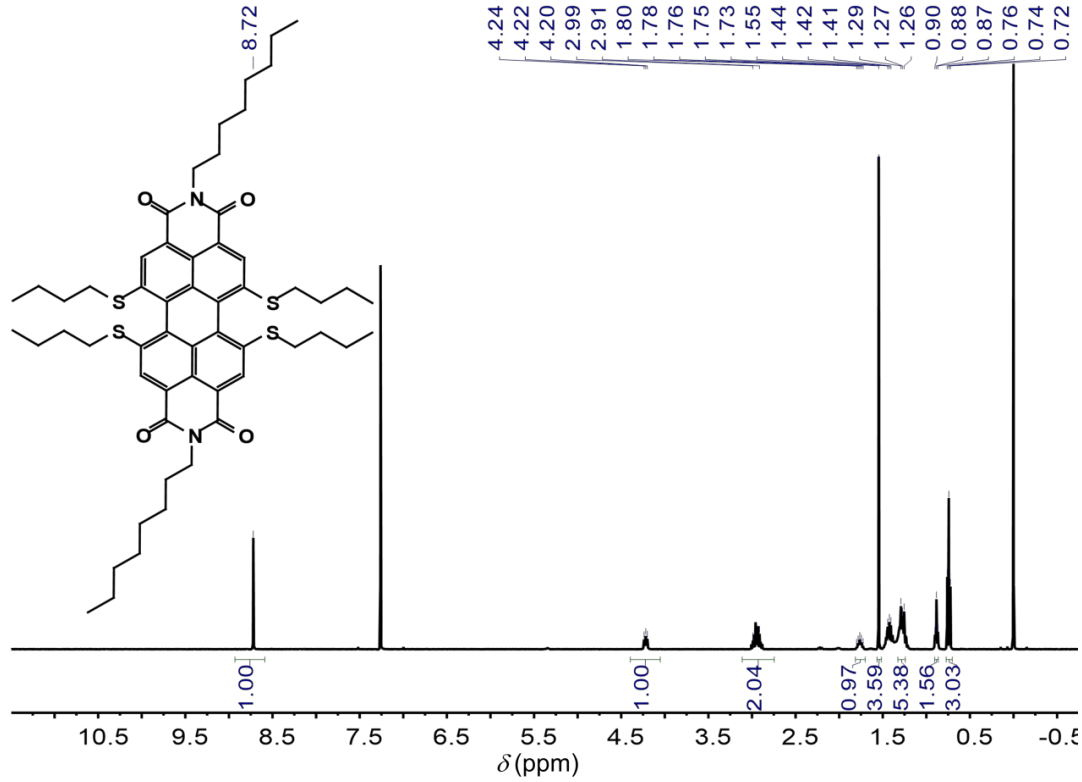

Figure S3. ^{1}H-NMR (400 MHz) spectrum of compound **2** in $CDCl_3$.

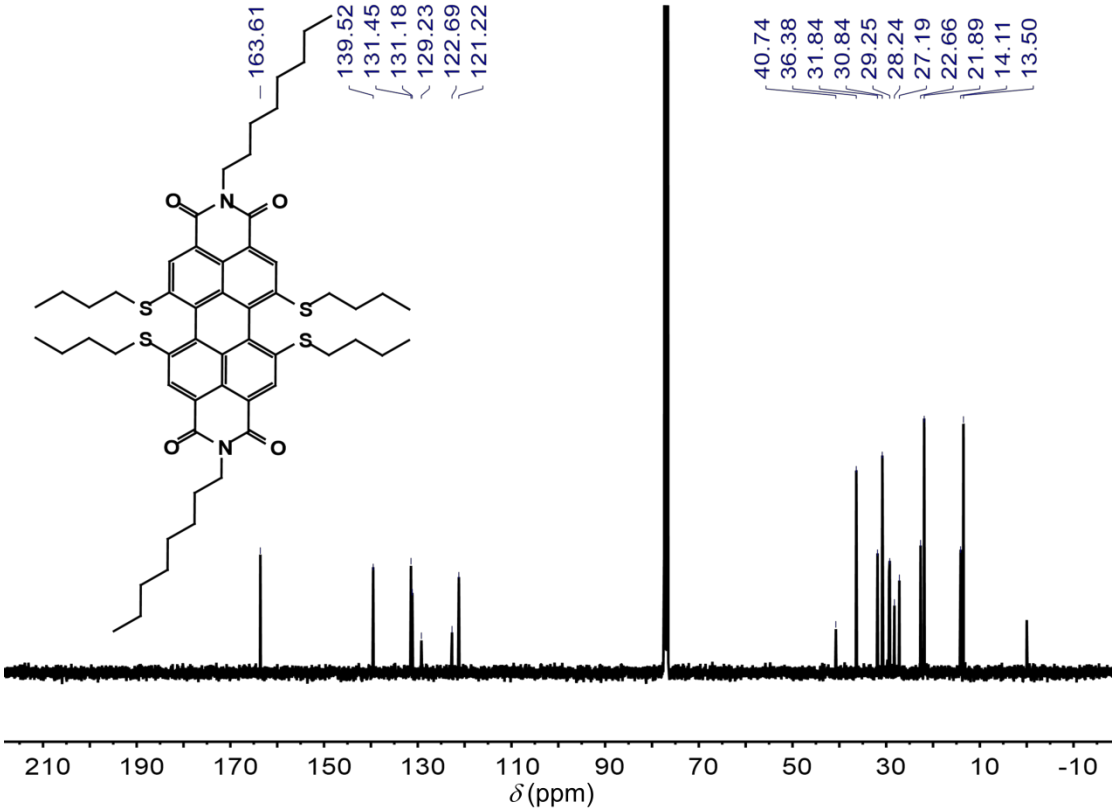

Figure S4. ^{13}C-NMR (100 MHz) spectrum of compound **2** in $CDCl_3$.

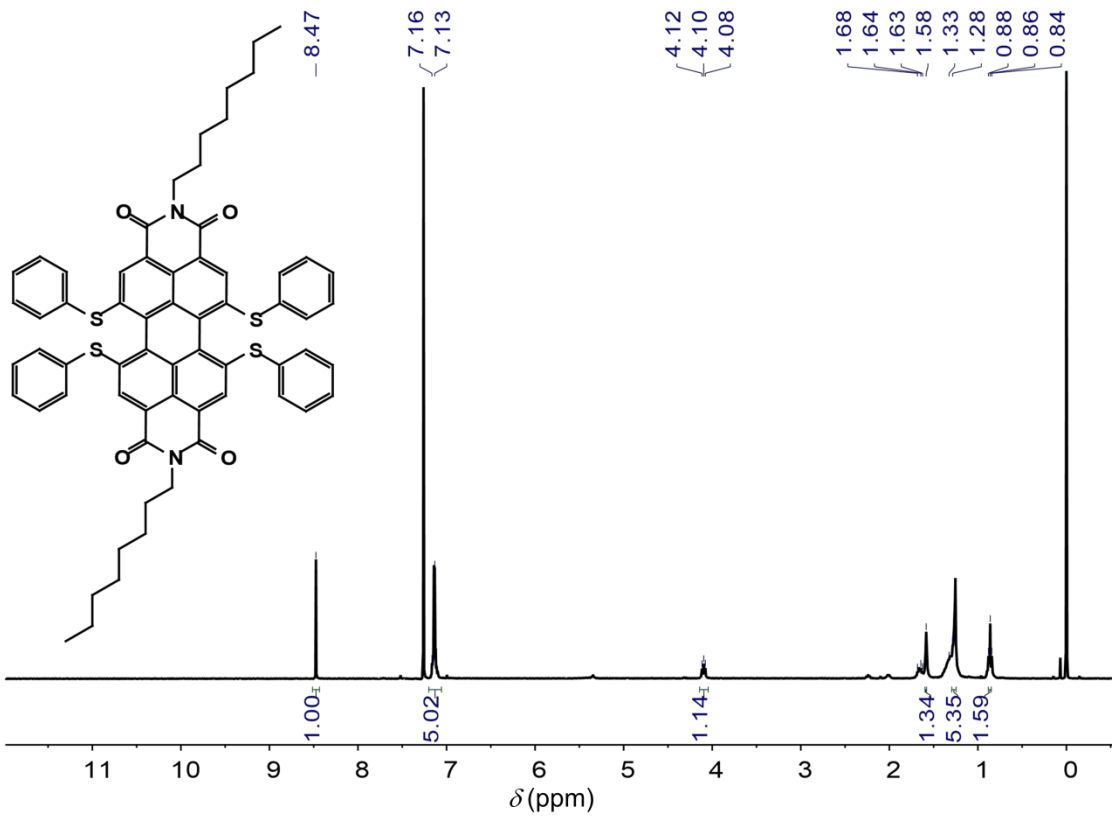

Figure S5. ^{1}H-NMR (400 MHz) spectrum of compound **3** in $CDCl_3$.

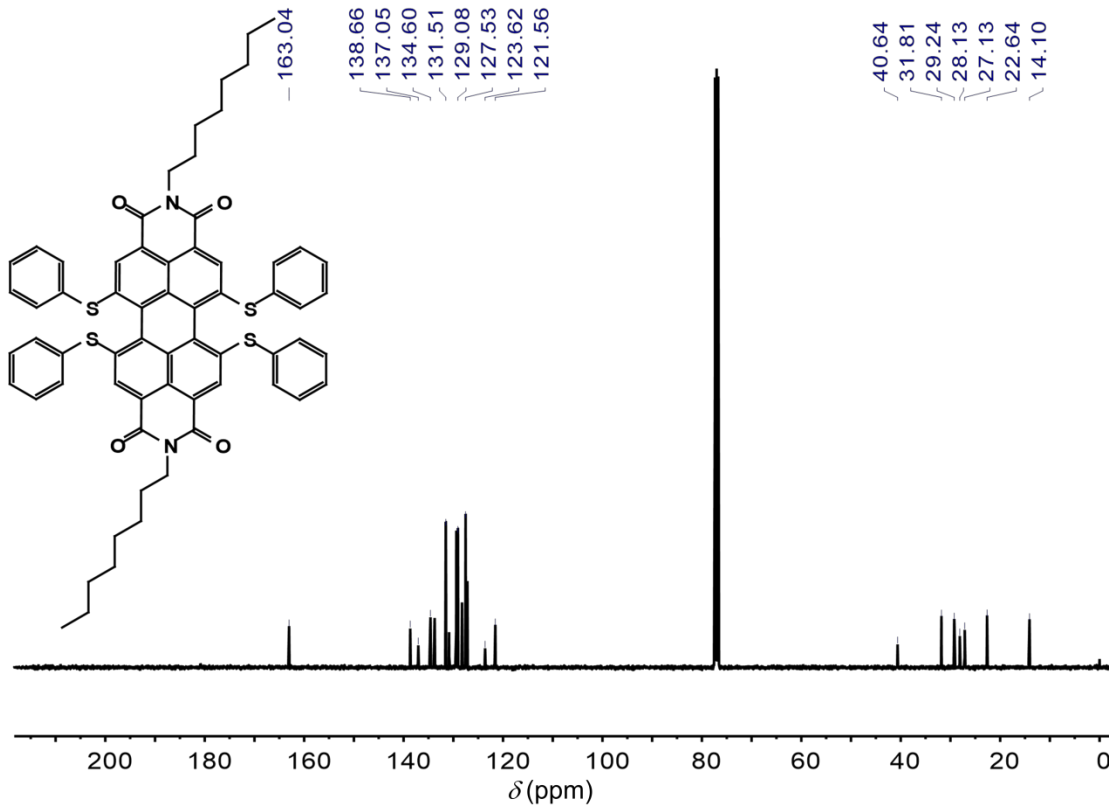

Figure S6. ^{13}C-NMR (100 MHz) spectrum of compound **3** in $CDCl_3$.

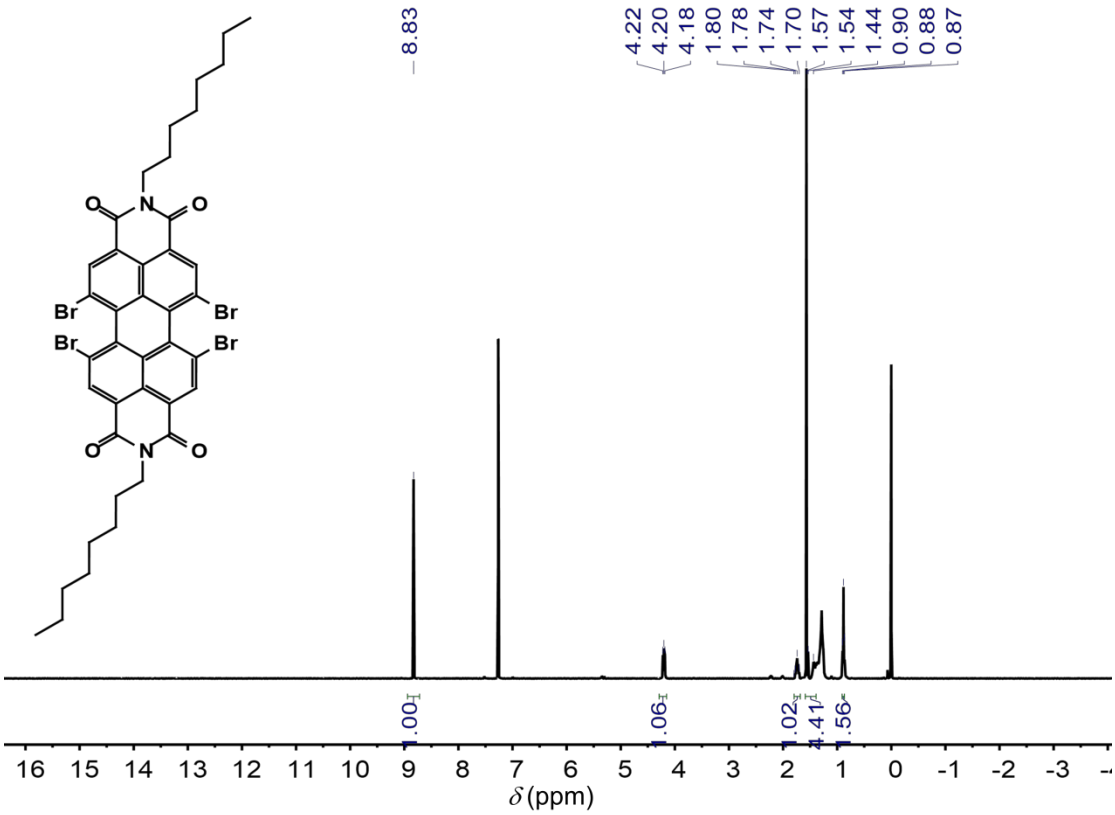

Figure S7. ^{1}H-NMR (400 MHz) spectrum of compound **4** in $CDCl_3$.

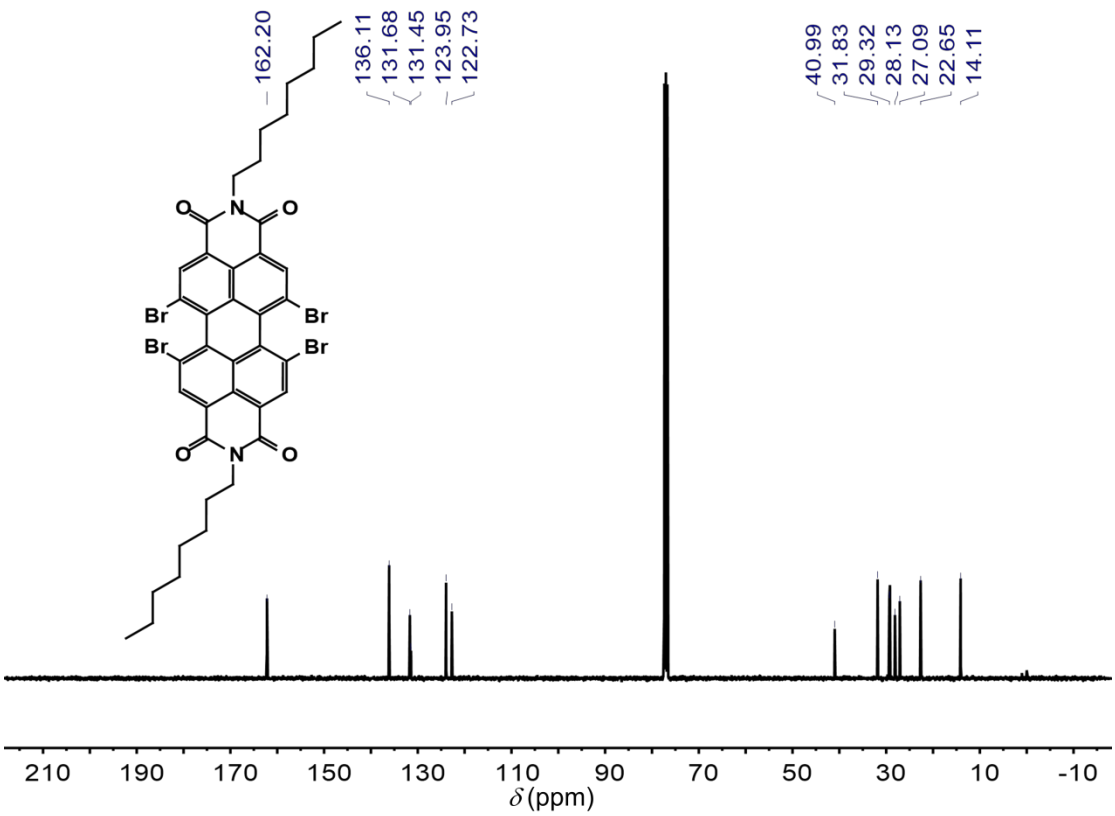

Figure S8. ^{13}C-NMR (100 MHz) spectrum of compound **4** in $CDCl_3$.

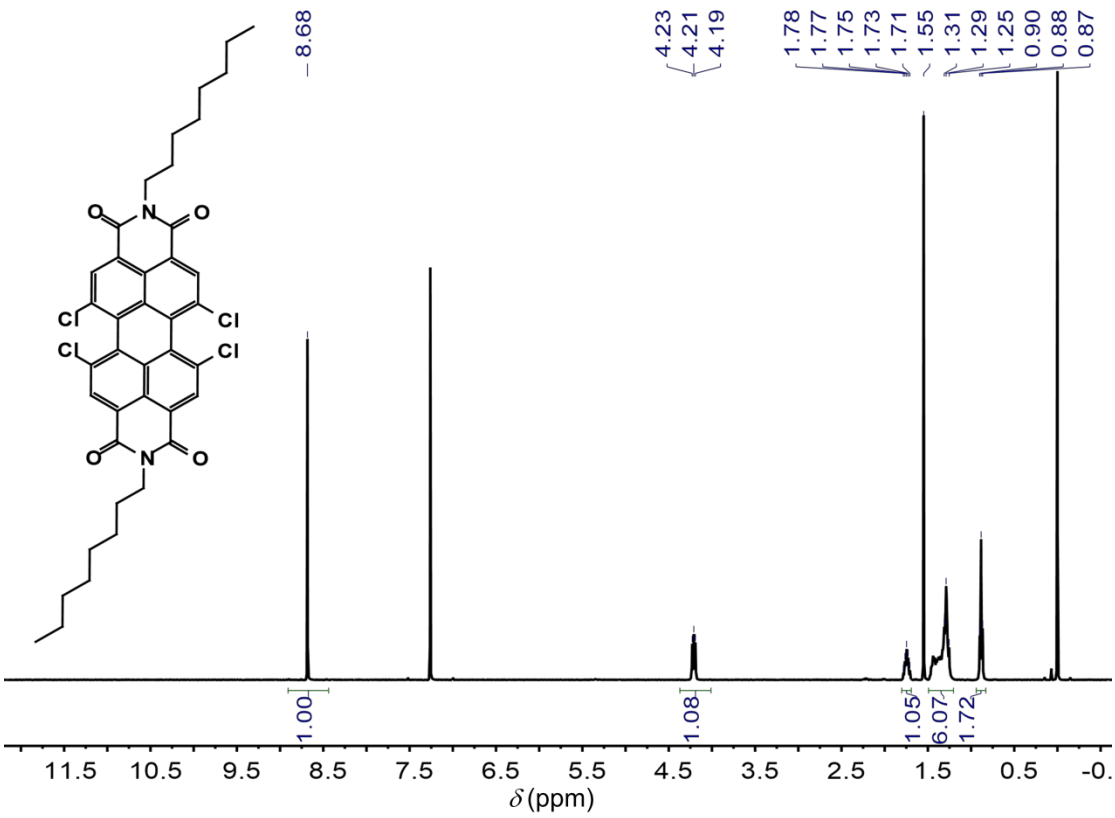

Figure S9. ^{1}H-NMR (400 MHz) spectrum of compound **5** in $CDCl_3$.

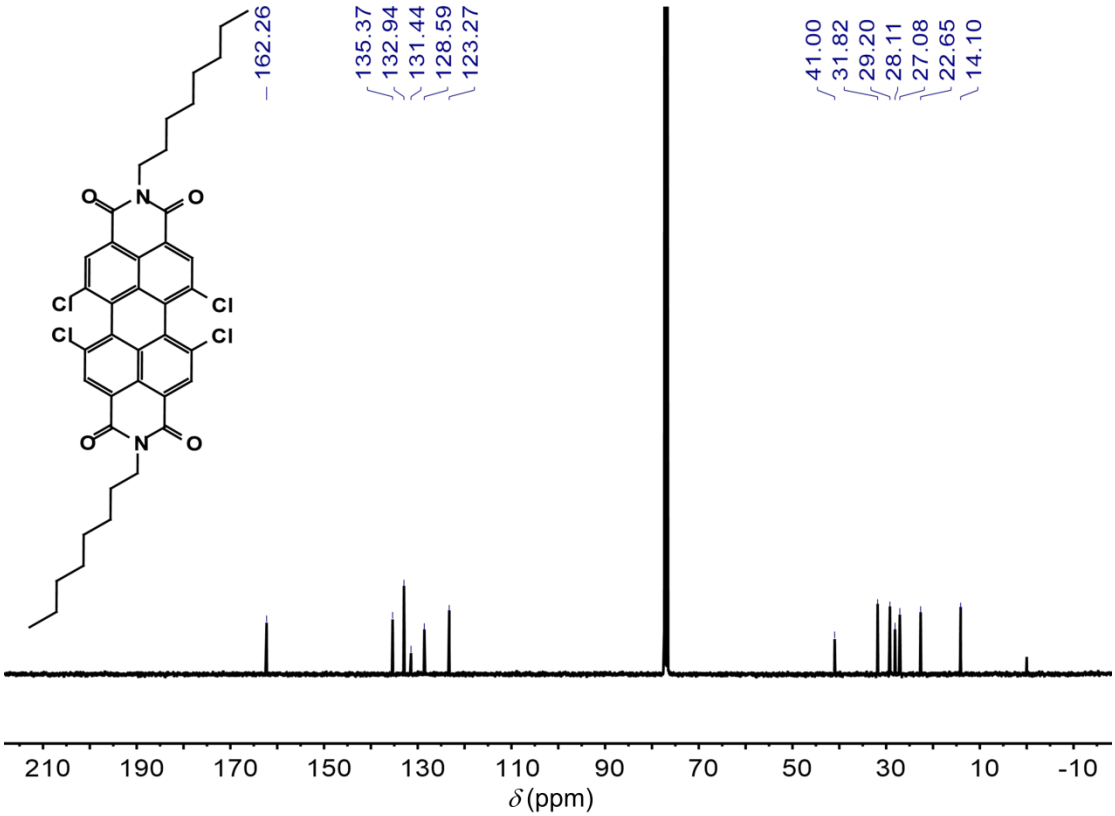

Figure S10. ^{13}C-NMR (100 MHz) spectrum of compound **5** in $CDCl_3$.

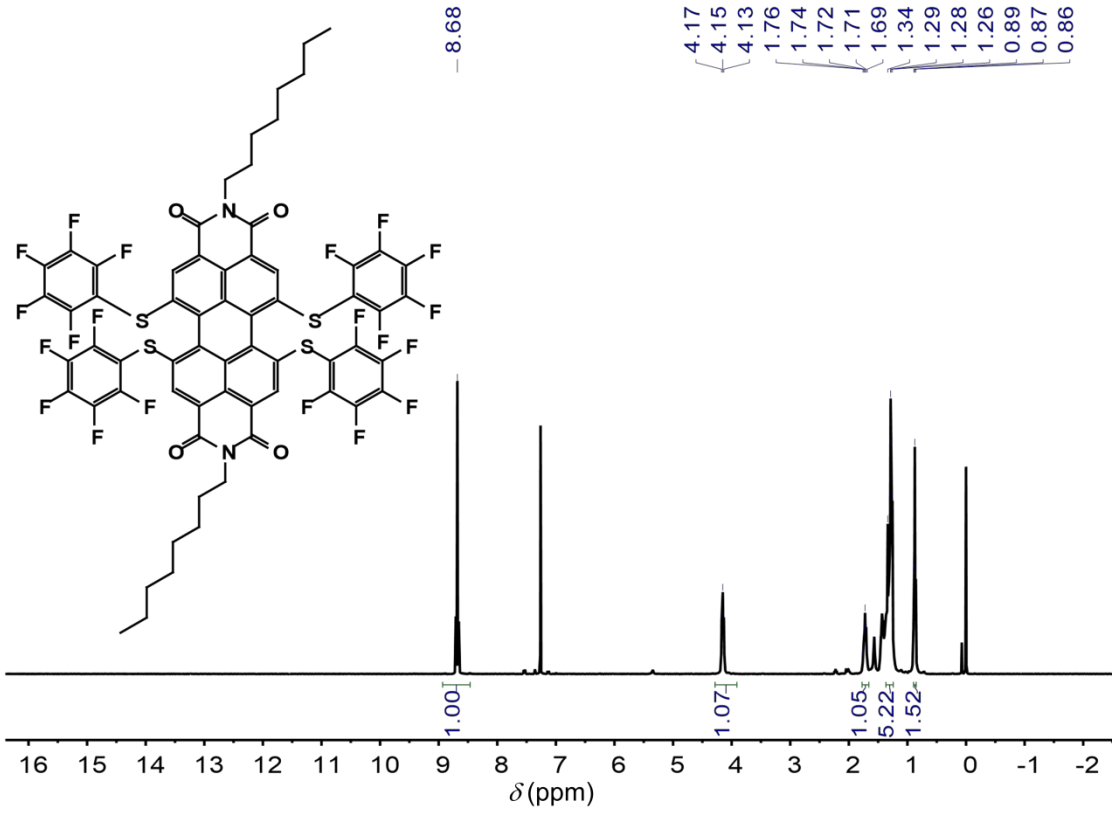

Figure S11. ^{1}H-NMR (400 MHz) spectrum of compound **6** in $CDCl_3$.

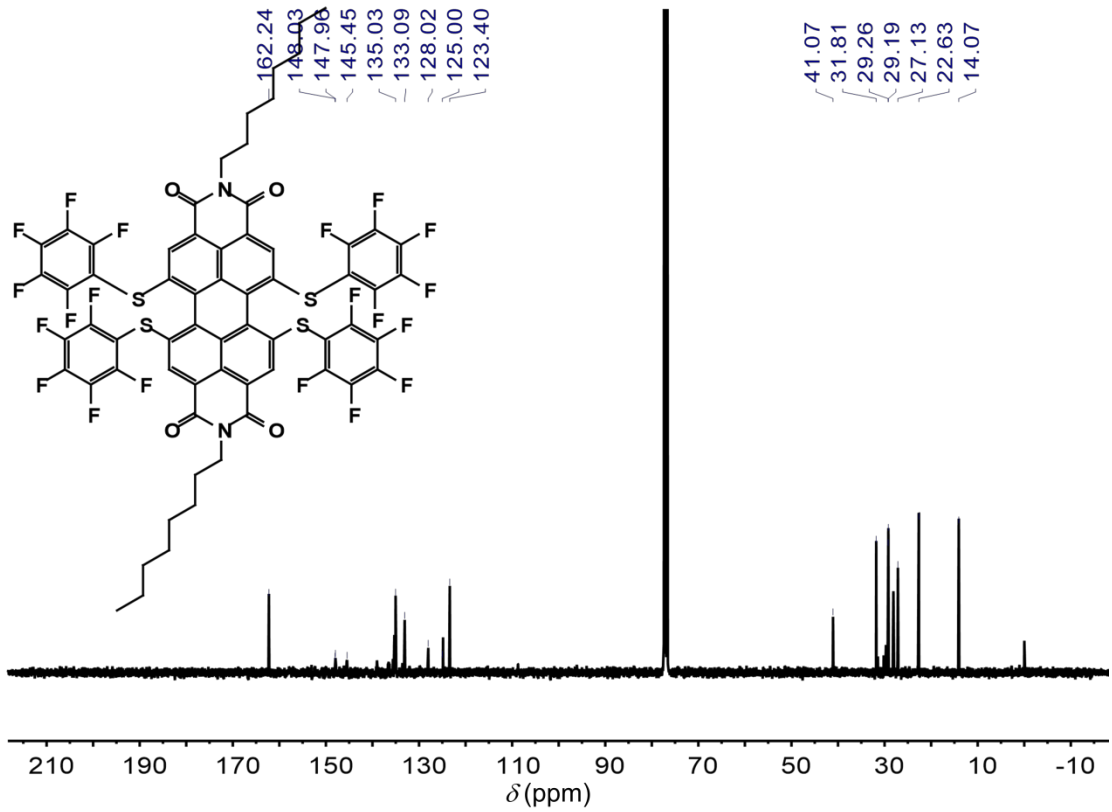

Figure S12. ^{13}C-NMR (100 MHz) spectrum of compound **6** in $CDCl_3$.

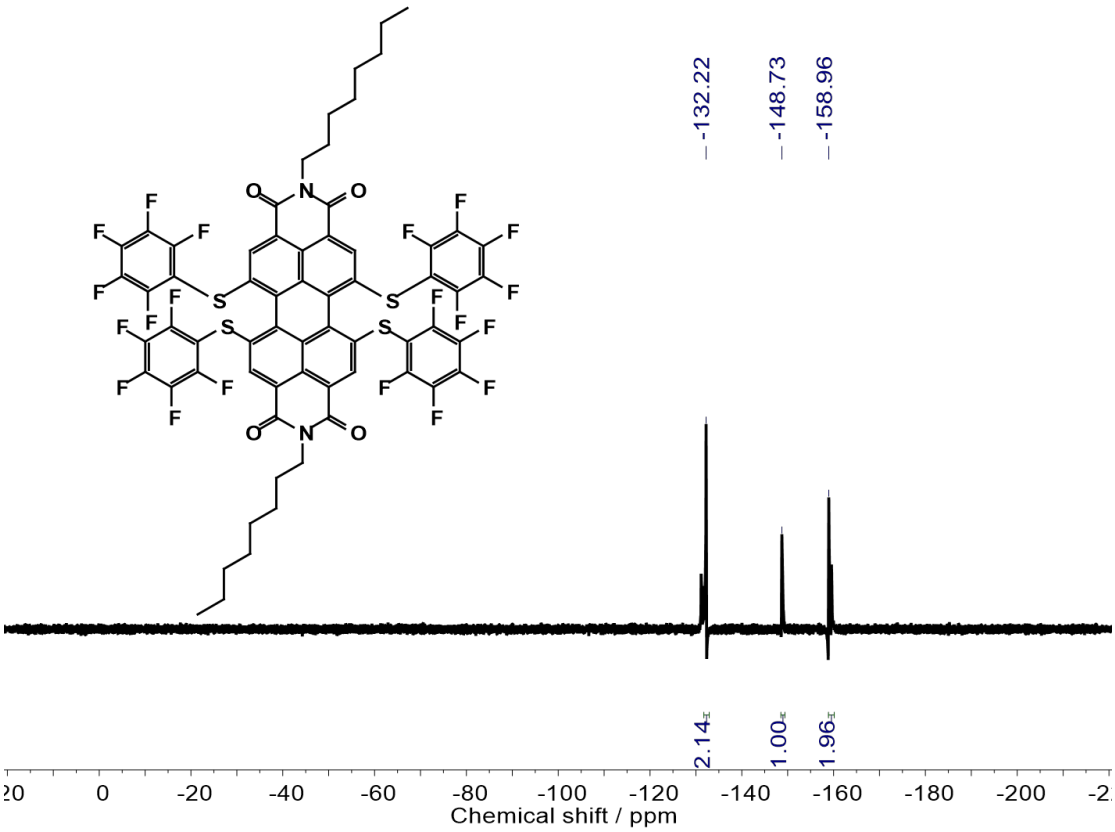

Figure S13. ^{19}F-NMR (376 MHz) spectrum of compound **6** in $CDCl_3$.

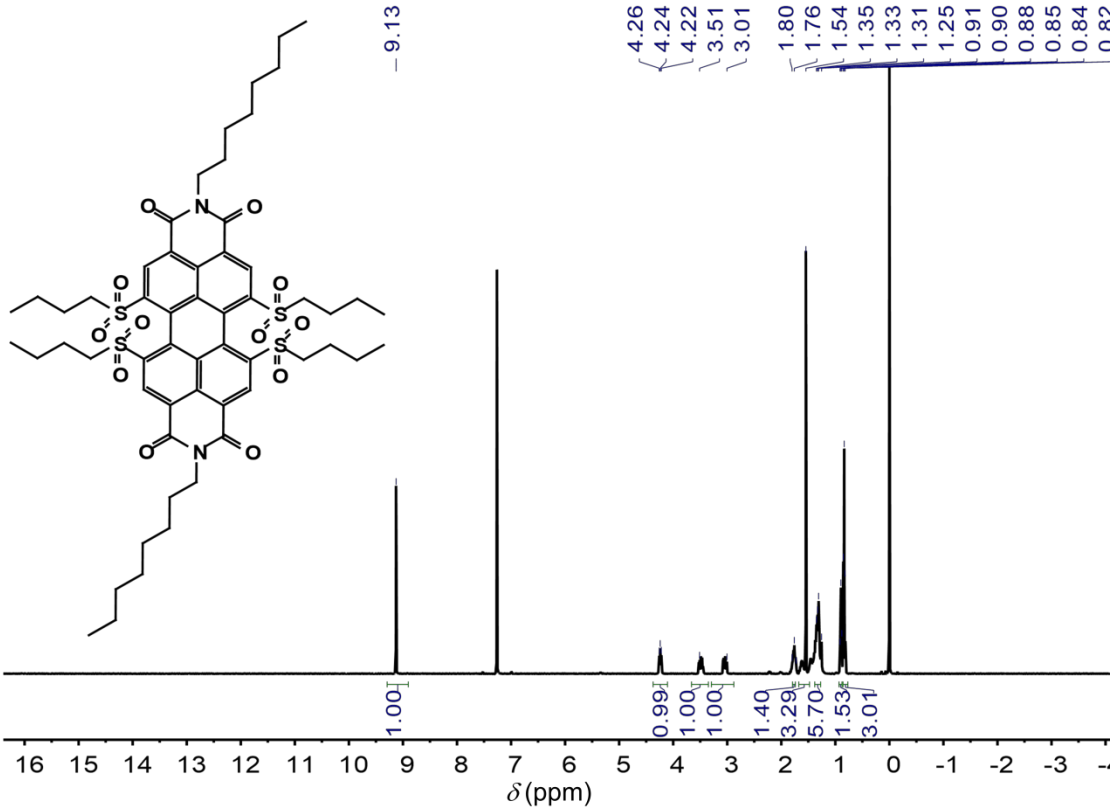

Figure S14. ^{1}H-NMR (400 MHz) spectrum of compound **7** in $CDCl_3$.

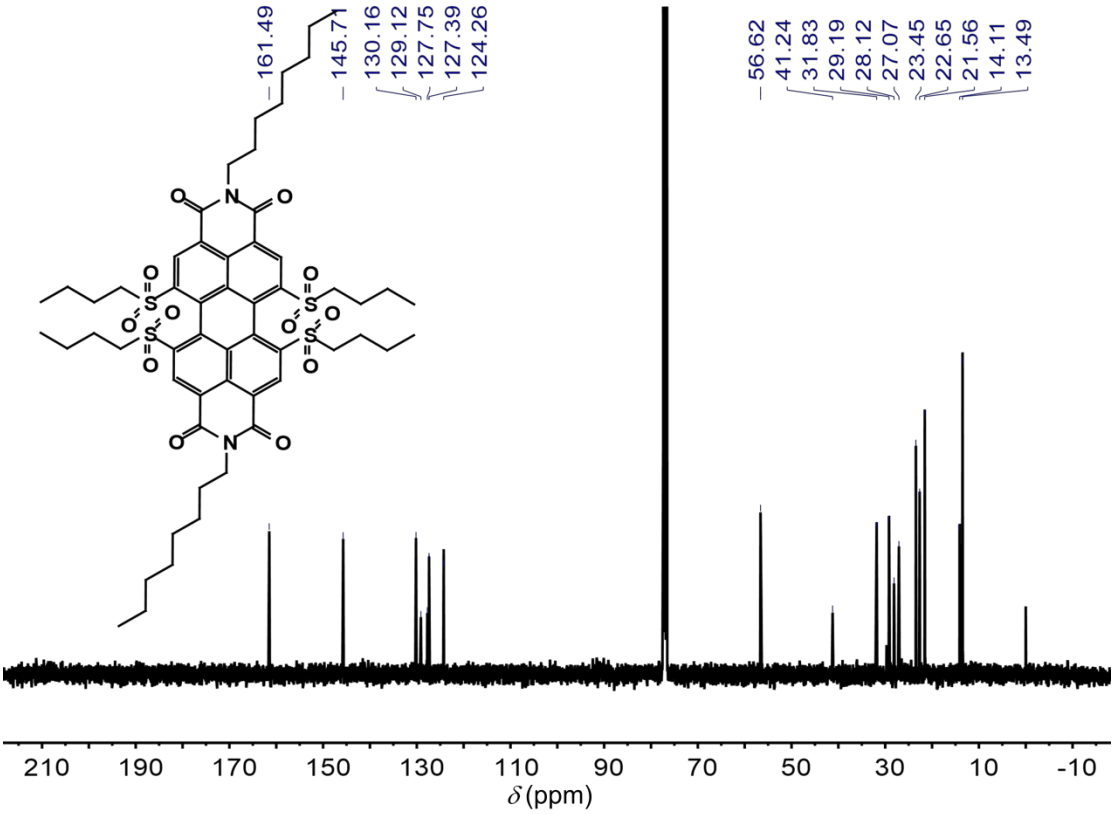

Figure S15. ^{13}C-NMR (100 MHz) spectrum of compound **7** in $CDCl_3$.

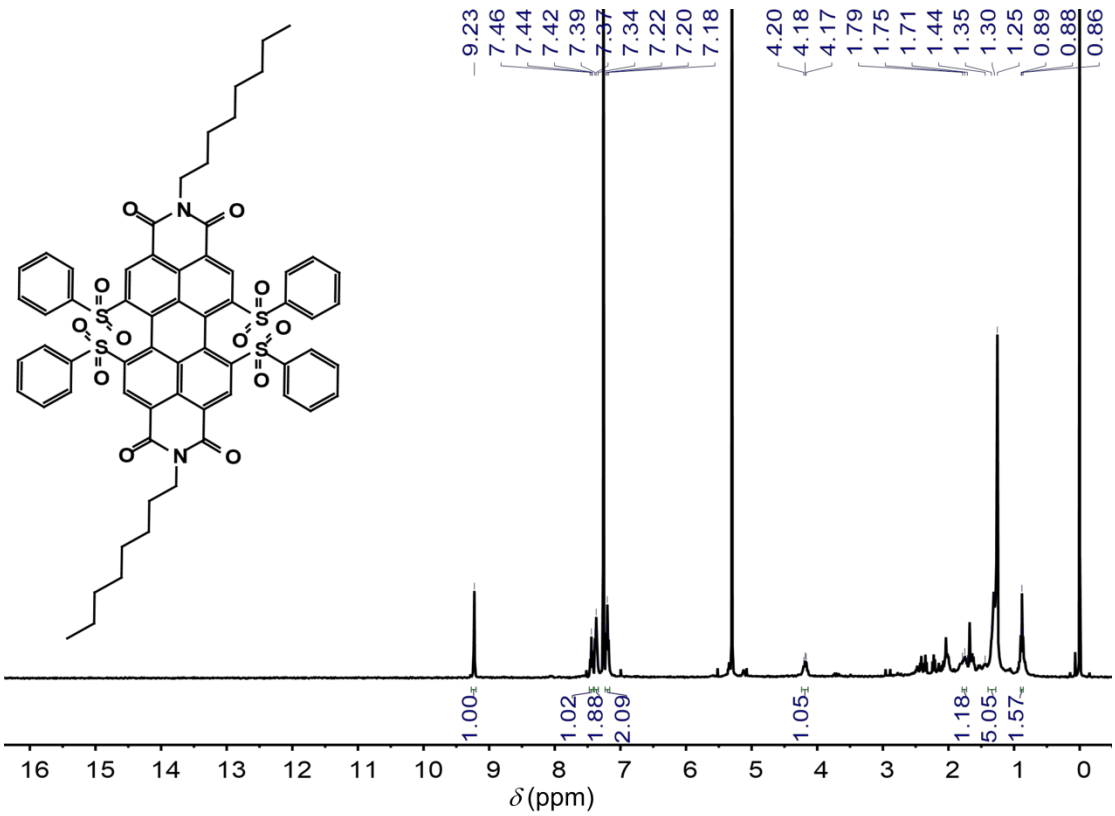

Figure S16. ^{1}H-NMR (400 MHz) spectrum of compound **8** in $CDCl_3$.

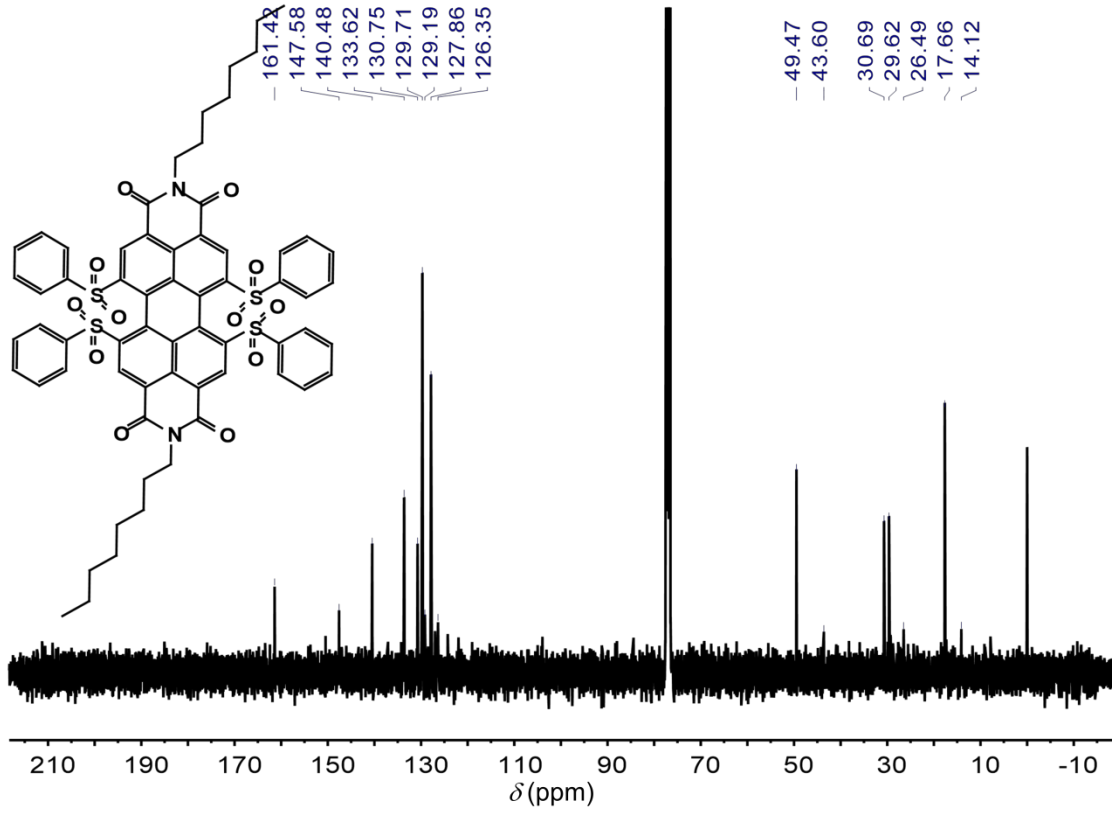

Figure S17. ^{13}C-NMR (100 MHz) spectrum of compound **8** in $CDCl_3$.

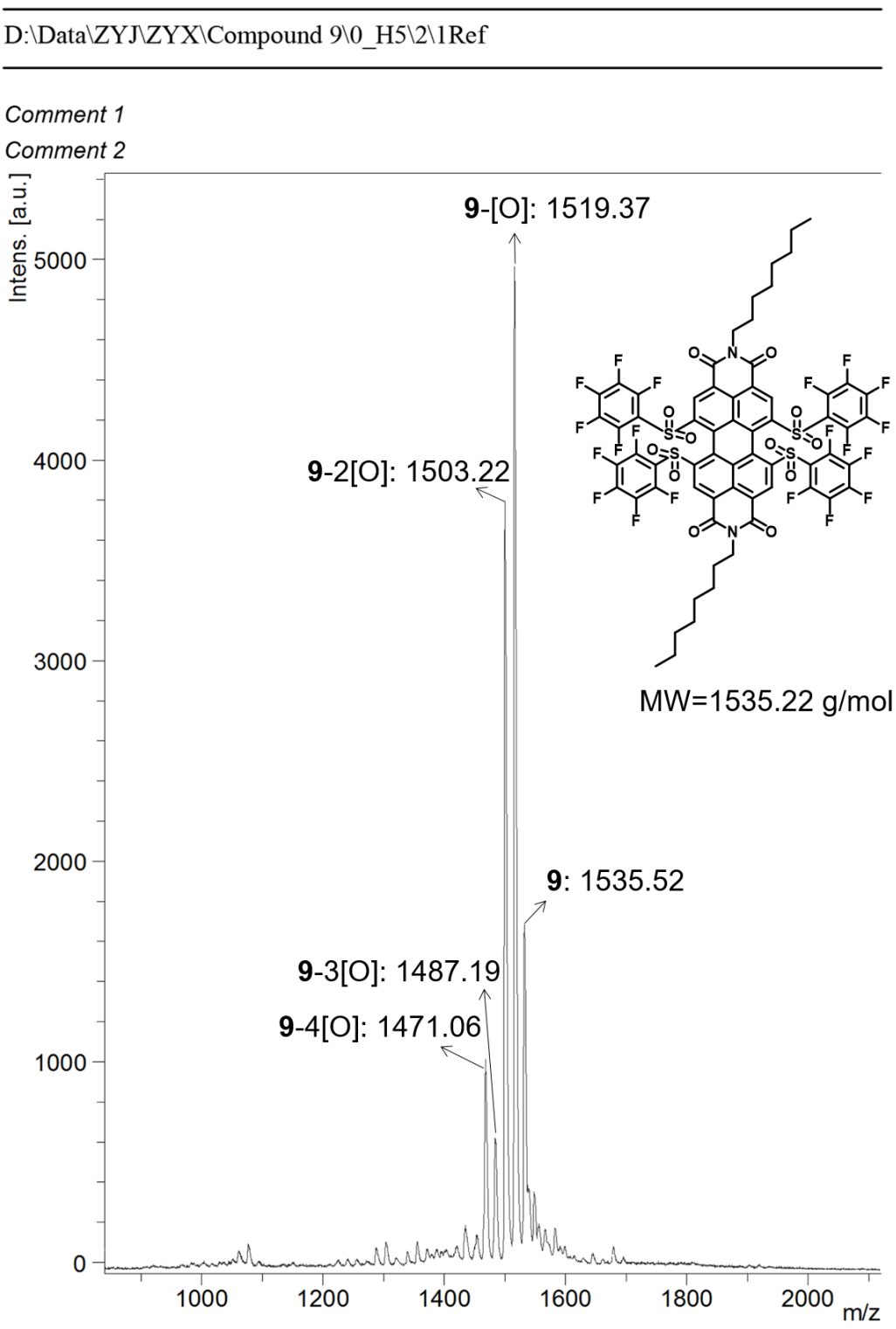

Figure S18. MALDI-TOF mass spectrum of compound **9**.

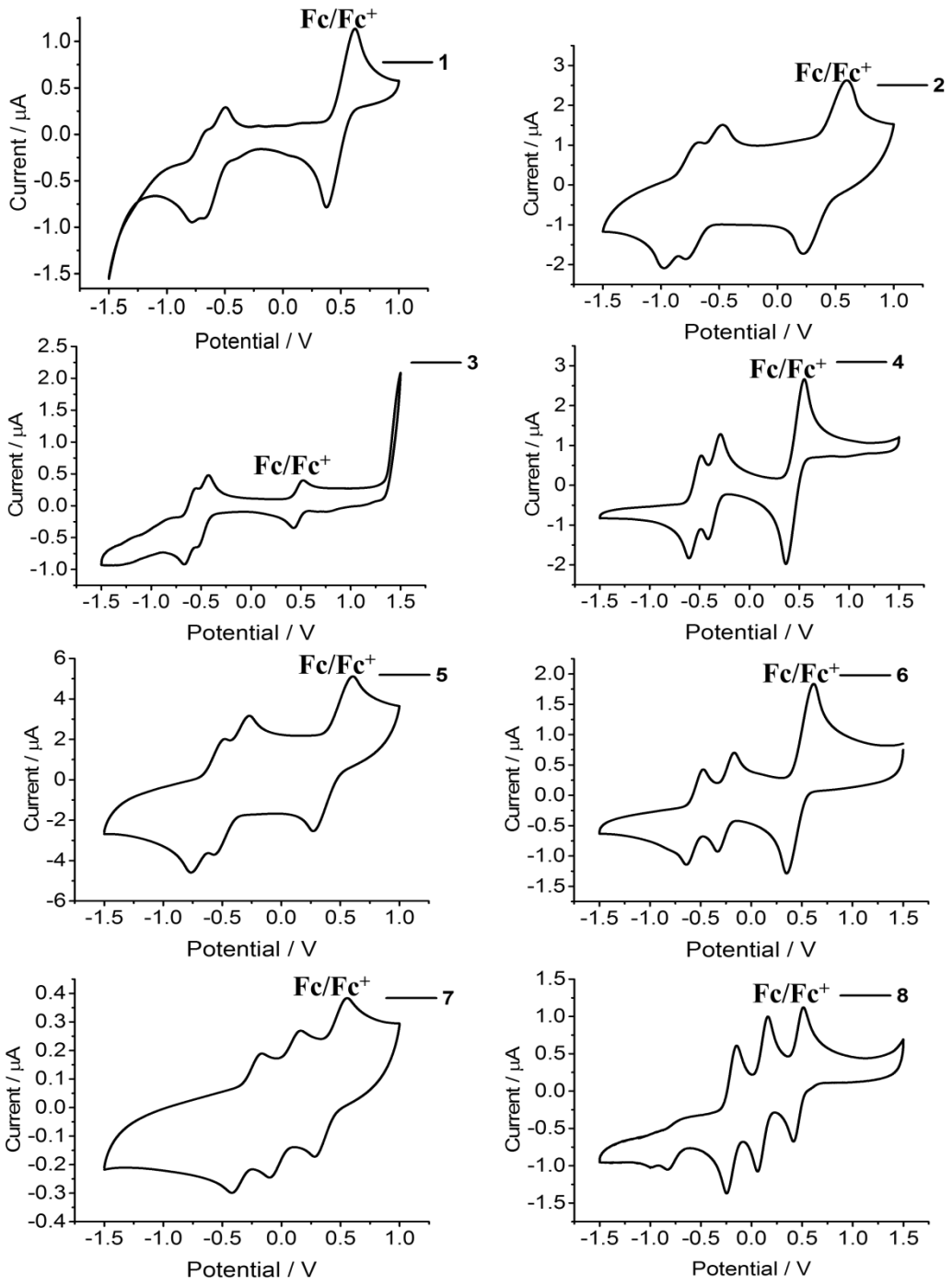

Figure S19. The CV curves of the compounds **1-8** measured in DCM at 298 K.

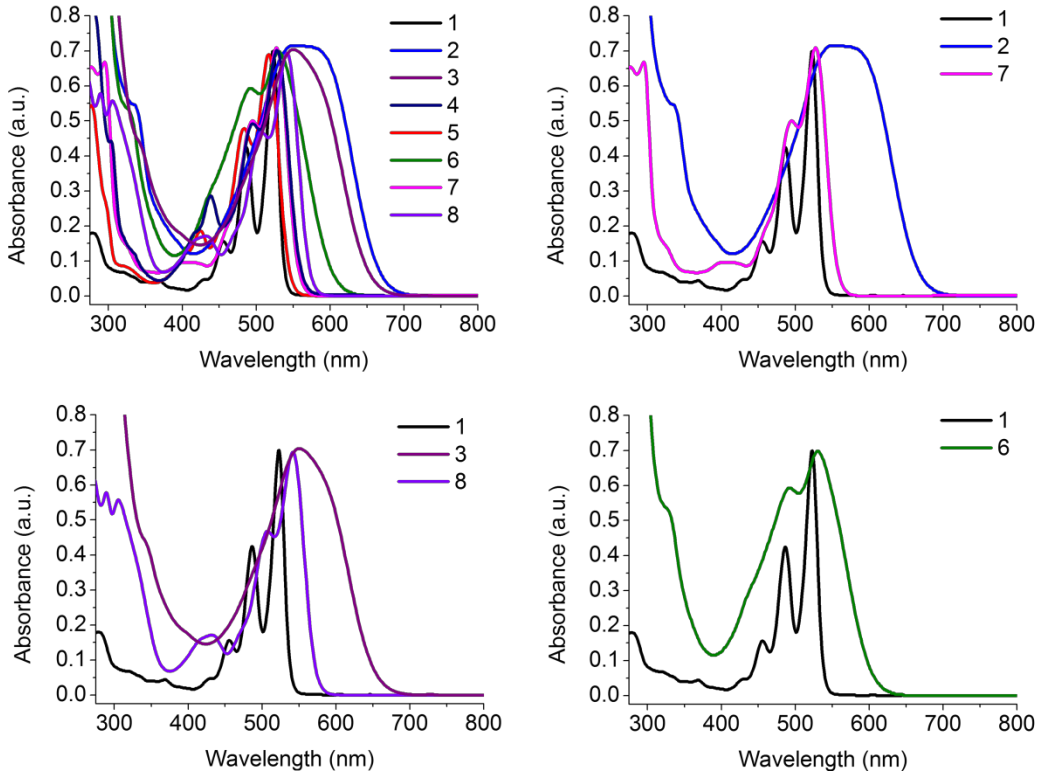

Figure S20. UV-Vis spectra of compounds **1-8** (3×10^{-5} M in DCM).

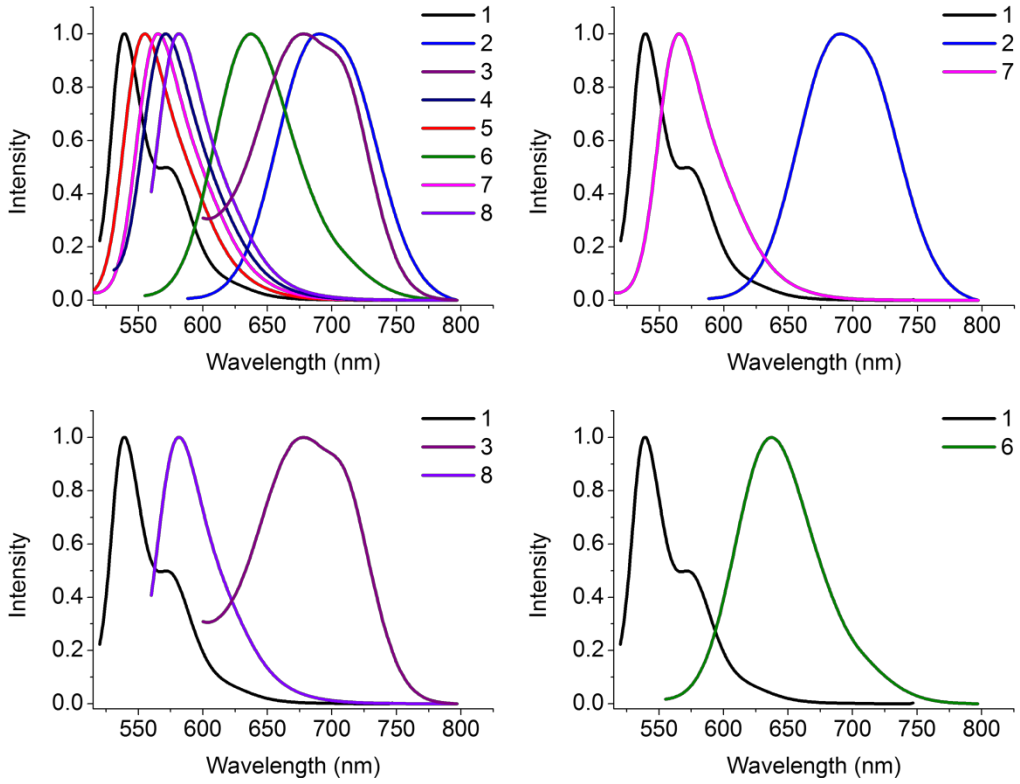

Figure S21. Fluorescence spectra of compounds **1-8** (3×10^{-5} M in DCM).

Molecular coodinates:

Dye **1**, singlet ground state

C	0.00387000	1.48180900	2.43153400
C	0.00079400	0.73580200	1.24999000
C	0.00041800	1.43350600	0.00000000
C	-0.00000100	2.86424600	0.00000000
C	0.00156000	3.57664500	1.22479500
C	0.00543300	2.88184200	2.42334900
H	0.00585700	0.98313300	3.39272800
C	0.00079400	0.73580200	-1.24999000
C	0.00156000	3.57664500	-1.22479500
H	0.00924000	3.44175900	3.35229400
C	0.00543300	2.88184200	-2.42334900
C	0.00387000	1.48180900	-2.43153400
H	0.00924000	3.44175900	-3.35229400
H	0.00585700	0.98313300	-3.39272800
C	-0.00079400	-0.73580200	1.24999000
C	-0.00041800	-1.43350600	0.00000000
C	-0.00387000	-1.48180900	2.43153400
C	-0.00079400	-0.73580200	-1.24999000
C	0.00000100	-2.86424600	0.00000000
C	-0.00543300	-2.88184200	2.42334900
H	-0.00585700	-0.98313300	3.39272800
C	-0.00387000	-1.48180900	-2.43153400
C	-0.00156000	-3.57664500	-1.22479500
C	-0.00156000	-3.57664500	1.22479500
H	-0.00924000	-3.44175900	3.35229400
C	-0.00543300	-2.88184200	-2.42334900
H	-0.00585700	-0.98313300	-3.39272800
H	-0.00924000	-3.44175900	-3.35229400
C	0.00384000	5.05951900	1.24162100
O	0.02767200	5.70327100	2.28531400
C	0.00384000	5.05951900	-1.24162100
O	0.02767200	5.70327100	-2.28531400
N	-0.02591100	5.70998400	0.00000000
C	-0.00384000	-5.05951900	-1.24162100
O	-0.02767200	-5.70327100	-2.28531400
C	-0.00384000	-5.05951900	1.24162100
O	-0.02767200	-5.70327100	2.28531400
N	0.02591100	-5.70998400	0.00000000
C	-0.03398900	7.17959400	0.00000000
H	0.98969100	7.56645000	0.00000000

H	-0.54225900	7.52065200	-0.89975300
H	-0.54225900	7.52065200	0.89975300
C	0.03398900	-7.17959400	0.00000000
H	-0.98969100	-7.56645000	0.00000000
H	0.54225900	-7.52065200	-0.89975300
H	0.54225900	-7.52065200	0.89975300

Dye **2**, singlet ground state

C	-2.30990700	1.42299400	0.76090100
C	-1.23108300	0.71322100	0.19275200
C	0.00335400	1.41417400	0.00011200
C	0.00660600	2.83286100	-0.00043200
C	-1.15200900	3.53205700	0.40437000
C	-2.25654900	2.82903700	0.84761000
C	1.23436700	0.70728700	-0.19180500
C	1.16789900	3.52789700	-0.40566900
H	-3.08486700	3.39292800	1.25750200
C	2.26884000	2.81827500	-0.84821000
C	2.31615400	1.41218000	-0.76033400
H	3.09973100	3.37769300	-1.25882100
C	-1.23436700	-0.70728700	-0.19180500
C	-0.00335400	-1.41417400	0.00011200
C	-2.31615400	-1.41218000	-0.76033400
C	1.23108300	-0.71322100	0.19275200
C	-0.00660600	-2.83286100	-0.00043200
C	-2.26884000	-2.81827500	-0.84821000
C	2.30990700	-1.42299400	0.76090100
C	1.15200900	-3.53205700	0.40437000
C	-1.16789900	-3.52789700	-0.40566900
H	-3.09973100	-3.37769300	-1.25882100
C	2.25654900	-2.82903700	0.84761000
H	3.08486700	-3.39292800	1.25750200
C	-1.15554200	5.01025400	0.42379600
O	-2.12342700	5.66954600	0.78891400
C	1.18525800	5.00764600	-0.42947100
O	2.16431800	5.64643300	-0.80006700
N	0.01409000	5.65471100	-0.00192700
C	1.15554200	-5.01025400	0.42379600
O	2.12342700	-5.66954600	0.78891400
C	-1.18525800	-5.00764600	-0.42947100
O	-2.16431800	-5.64643300	-0.80006700
N	-0.01409000	-5.65471100	-0.00192700
C	-0.01409000	7.12207700	0.00875600
H	-0.81106900	7.47868100	-0.64686500

H	0.95372200	7.47558500	-0.33695200
H	-0.21698500	7.47701200	1.02105200
C	0.01409000	-7.12207700	0.00875600
H	0.81106900	-7.47868100	-0.64686500
H	-0.95372200	-7.47558500	-0.33695200
H	0.21698500	-7.47701200	1.02105200
S	-3.65193100	-0.53274200	-1.53762300
S	-3.64901200	0.54925700	1.53859000
S	3.65193100	0.53274200	-1.53762300
S	3.64901200	-0.54925700	1.53859000
C	5.09404100	-1.58276300	1.11579600
H	5.06783000	-2.55276900	1.61439900
H	5.96833300	-1.03146700	1.46905000
H	5.15456700	-1.70883900	0.03294100
C	5.10142300	1.55880100	-1.11187800
H	5.08031000	2.52966900	-1.60904400
H	5.97347500	1.00388600	-1.46500900
H	5.16132100	1.68294200	-0.02877200
C	-5.09404100	1.58276300	1.11579600
H	-5.15456700	1.70883900	0.03294100
H	-5.06783000	2.55276900	1.61439900
H	-5.96833300	1.03146700	1.46905000
C	-5.10142300	-1.55880100	-1.11187800
H	-5.16132100	-1.68294200	-0.02877200
H	-5.08031000	-2.52966900	-1.60904400
H	-5.97347500	-1.00388600	-1.46500900

Dye **3**, singlet ground state

C	-2.31054300	1.42925400	0.75396300
C	-1.23505500	0.71322600	0.19065000
C	0.00018300	1.41566200	-0.00032400
C	0.00027900	2.83606600	-0.00062300
C	-1.15199600	3.53696900	0.42356600
C	-2.25187000	2.83318800	0.87343200
C	1.23512700	0.71286600	-0.19077700
C	1.15220300	3.53805500	-0.42479700
H	-3.08416800	3.37906500	1.30221100
C	2.25159600	2.83277100	-0.87435200
C	2.31038600	1.42897200	-0.75439400
H	3.08398500	3.37806700	-1.30350500
C	-1.23512700	-0.71286600	-0.19077700
C	-0.00018300	-1.41566200	-0.00032400
C	-2.31038600	-1.42897200	-0.75439400
C	1.23505500	-0.71322600	0.19065000

C	-0.00027900	-2.83606600	-0.00062300
C	-2.25159600	-2.83277100	-0.87435200
C	2.31054300	-1.42925400	0.75396300
C	1.15199600	-3.53696900	0.42356600
C	-1.15220300	-3.53805500	-0.42479700
H	-3.08398500	-3.37806700	-1.30350500
C	2.25187000	-2.83318800	0.87343200
H	3.08416800	-3.37906500	1.30221100
C	-1.15617100	5.01645100	0.44937600
O	-2.11745600	5.67086700	0.83641500
C	1.16370000	5.01916000	-0.45430400
O	2.13338200	5.65749300	-0.84607400
N	0.00157800	5.66388900	-0.00147500
C	1.15617100	-5.01645100	0.44937600
O	2.11745600	-5.67086700	0.83641500
C	-1.16370000	-5.01916000	-0.45430400
O	-2.13338200	-5.65749300	-0.84607400
N	-0.00157800	-5.66388900	-0.00147500
C	-0.02940500	7.13144400	0.01052800
H	-0.84424600	7.48608700	-0.62373500
H	0.92828600	7.48706600	-0.36028600
H	-0.20652100	7.48541700	1.02797000
C	0.02940500	-7.13144400	0.01052800
H	0.84424600	-7.48608700	-0.62373500
H	-0.92828600	-7.48706600	-0.36028600
H	0.20652100	-7.48541700	1.02797000
S	-3.65177000	-0.56237800	-1.52898900
S	-3.65172500	0.56234800	1.52838700
S	3.65177000	0.56237800	-1.52898900
S	3.65172500	-0.56234800	1.52838700
C	5.13947400	-1.33543500	0.91330500
C	6.32007000	-1.00906500	1.59377500
C	5.19066600	-2.14813700	-0.22399700
C	7.54381600	-1.49098200	1.13328700
H	6.28200300	-0.36808900	2.46899900
C	6.41988000	-2.63902500	-0.66629300
H	4.28714100	-2.38446400	-0.77168700
C	7.59998300	-2.31115600	0.00394400
H	8.45409800	-1.22319900	1.66055300
H	6.45000100	-3.27371500	-1.54685200
H	8.55333900	-2.69030600	-0.34998500
C	5.13951600	1.33475500	-0.91297300
C	6.32044500	1.00713200	-1.59227500
C	5.19034900	2.14816000	0.22383000

C	7.54414700	1.48850500	-1.13112200
H	6.28266300	0.36556500	-2.46707800
C	6.41956400	2.63843000	0.66684000
H	4.28655900	2.38554300	0.77062700
C	7.59998300	2.30933200	-0.00223200
H	8.45466300	1.21973000	-1.65747700
H	6.44940100	3.27364000	1.54703400
H	8.55331800	2.68801600	0.35225000
C	-5.13947400	1.33543500	0.91330500
C	-6.32007000	1.00906500	1.59377500
C	-5.19066600	2.14813700	-0.22399700
C	-7.54381600	1.49098200	1.13328700
H	-6.28200300	0.36808900	2.46899900
C	-6.41988000	2.63902500	-0.66629300
H	-4.28714100	2.38446400	-0.77168700
C	-7.59998300	2.31115600	0.00394400
H	-8.45409800	1.22319900	1.66055300
H	-6.45000100	3.27371500	-1.54685200
H	-8.55333900	2.69030600	-0.34998500
C	-5.13951600	-1.33475500	-0.91297300
C	-6.32044500	-1.00713200	-1.59227500
C	-5.19034900	-2.14816000	0.22383000
C	-7.54414700	-1.48850500	-1.13112200
H	-6.28266300	-0.36556500	-2.46707800
C	-6.41956400	-2.63843000	0.66684000
H	-4.28655900	-2.38554300	0.77062700
C	-7.59998300	-2.30933200	-0.00223200
H	-8.45466300	-1.21973000	-1.65747700
H	-6.44940100	-3.27364000	1.54703400
H	-8.55331800	-2.68801600	0.35225000

Dye **4**, singlet ground state

C	-2.28505800	1.43532000	0.75354300
C	-1.22796400	0.71148300	0.18989600
C	0.00419300	1.41858000	-0.00005400
C	0.00843300	2.83657900	-0.00012600
C	-1.14742100	3.53741800	0.41121400
C	-2.25673400	2.83676800	0.84855400
C	1.23199400	0.70410400	-0.18951200
C	1.16791600	3.53187100	-0.41148300
H	-3.10183500	3.38176100	1.25154700
C	2.27258600	2.82343600	-0.84881000
C	2.29284000	1.42191100	-0.75377200
H	3.12084600	3.36311200	-1.25214500

C	-1.23199400	-0.70410400	-0.18951200
C	-0.00419300	-1.41858000	-0.00005400
C	-2.29284000	-1.42191100	-0.75377200
C	1.22796400	-0.71148300	0.18989600
C	-0.00843300	-2.83657900	-0.00012600
C	-2.27258600	-2.82343600	-0.84881000
C	2.28505800	-1.43532000	0.75354300
C	1.14742100	-3.53741800	0.41121400
C	-1.16791600	-3.53187100	-0.41148300
H	-3.12084600	-3.36311200	-1.25214500
C	2.25673400	-2.83676800	0.84855400
H	3.10183500	-3.38176100	1.25154700
C	-1.14840500	5.01942000	0.43396300
O	-2.11317200	5.67358800	0.80883100
C	1.18485900	5.01553600	-0.43727200
O	2.16097000	5.64804700	-0.81869600
N	0.01852700	5.66211200	0.00084200
C	1.14840500	-5.01942000	0.43396300
O	2.11317200	-5.67358800	0.80883100
C	-1.18485900	-5.01553600	-0.43727200
O	-2.16097000	-5.64804700	-0.81869600
N	-0.01852700	-5.66211200	0.00084200
C	-0.00843300	7.13095600	0.01324200
H	-0.80358700	7.48825400	-0.64430600
H	0.96028900	7.48465900	-0.32998400
H	-0.21335700	7.48310300	1.02598800
C	0.00843300	-7.13095600	0.01324200
H	0.80358700	-7.48825400	-0.64430600
H	-0.96028900	-7.48465900	-0.32998400
H	0.21335700	-7.48310300	1.02598800
Br	3.79140400	0.53983100	-1.62732700
Br	3.78907400	-0.56177800	1.62634500
Br	-3.78907400	0.56177800	1.62634500
Br	-3.79140400	-0.53983100	-1.62732700

Dye **5**, singlet ground state

C	-2.30165400	1.43947000	0.72234400
C	-1.22979300	0.71249900	0.18215500
C	0.00323200	1.41985100	0.00044700
C	0.00641900	2.83879400	0.00005000
C	-1.15454300	3.54082600	0.39486900
C	-2.27070700	2.84274900	0.81243200
C	1.23286900	0.70679400	-0.18083400
C	1.16994700	3.53680100	-0.39521500

H	-3.12663100	3.38470100	1.19634900
C	2.28249800	2.83236800	-0.81255300
C	2.30748300	1.42907400	-0.72176200
H	3.14071400	3.37000300	-1.19722900
C	-1.23286900	-0.70679400	-0.18083400
C	-0.00323200	-1.41985100	0.00044700
C	-2.30748300	-1.42907400	-0.72176200
C	1.22979300	-0.71249900	0.18215500
C	-0.00641900	-2.83879400	0.00005000
C	-2.28249800	-2.83236800	-0.81255300
C	2.30165400	-1.43947000	0.72234400
C	1.15454300	-3.54082600	0.39486900
C	-1.16994700	-3.53680100	-0.39521500
H	-3.14071400	-3.37000300	-1.19722900
C	2.27070700	-2.84274900	0.81243200
H	3.12663100	-3.38470100	1.19634900
C	-1.15743900	5.02293200	0.41618700
O	-2.12865800	5.67571100	0.77575700
C	1.18640100	5.02057400	-0.42068300
O	2.16785200	5.65304700	-0.78744000
N	0.01418100	5.66692500	-0.00010500
C	1.15743900	-5.02293200	0.41618700
O	2.12865800	-5.67571100	0.77575700
C	-1.18640100	-5.02057400	-0.42068300
O	-2.16785200	-5.65304700	-0.78744000
N	-0.01418100	-5.66692500	-0.00010500
C	-0.01418100	7.13559900	0.01070400
H	-0.80033600	7.49151600	-0.65800100
H	0.95878300	7.48954500	-0.31941600
H	-0.23310800	7.48833500	1.02010500
C	0.01418100	-7.13559900	0.01070400
H	0.80033600	-7.49151600	-0.65800100
H	-0.95878300	-7.48954500	-0.31941600
H	0.23310800	-7.48833500	1.02010500
Cl	-3.68951400	-0.63769200	-1.43600800
Cl	3.68726000	-0.65409300	1.43621700
Cl	3.68951400	0.63769200	-1.43600800
Cl	-3.68726000	0.65409300	1.43621700

Dye **6**, singlet ground state

C	-2.30282600	1.43975100	0.75846800
C	-1.23676800	0.71387800	0.19436800
C	0.00024300	1.41527400	-0.00018100
C	0.00043000	2.83538000	-0.00042800

C	-1.13805000	3.54001300	0.45122000
C	-2.23163700	2.83892300	0.90944400
C	1.23688100	0.71340000	-0.19431500
C	1.13864700	3.54097000	-0.45199200
H	-3.05316700	3.38605100	1.35647600
C	2.23161100	2.83831400	-0.91005500
C	2.30272000	1.43922600	-0.75880600
H	3.05326300	3.38482000	-1.35744100
C	-1.23688100	-0.71340000	-0.19431500
C	-0.00024300	-1.41527400	-0.00018100
C	-2.30272000	-1.43922600	-0.75880600
C	1.23676800	-0.71387800	0.19436800
C	-0.00043000	-2.83538000	-0.00042800
C	-2.23161100	-2.83831400	-0.91005500
C	2.30282600	-1.43975100	0.75846800
C	1.13805000	-3.54001300	0.45122000
C	-1.13864700	-3.54097000	-0.45199200
H	-3.05326300	-3.38482000	-1.35744100
C	2.23163700	-2.83892300	0.90944400
H	3.05316700	-3.38605100	1.35647600
C	-1.13558700	5.02169000	0.49312000
O	-2.07961700	5.66842800	0.92801100
C	1.14356400	5.02435100	-0.49739200
O	2.09549400	5.65509600	-0.93750400
N	0.00209400	5.67005500	-0.00076400
C	1.13558700	-5.02169000	0.49312000
O	2.07961700	-5.66842800	0.92801100
C	-1.14356400	-5.02435100	-0.49739200
O	-2.09549400	-5.65509600	-0.93750400
N	-0.00209400	-5.67005500	-0.00076400
C	-0.02767200	7.13887100	0.01381800
H	-0.86802000	7.49312900	-0.58608600
H	0.91363400	7.49466300	-0.39640400
H	-0.16097600	7.49052000	1.03847500
C	0.02767200	-7.13887100	0.01381800
H	0.86802000	-7.49312900	-0.58608600
H	-0.91363400	-7.49466300	-0.39640400
H	0.16097600	-7.49052000	1.03847500
S	-3.64811700	-0.57462900	-1.53702000
S	-3.64823600	0.57504000	1.53643800
S	3.64811700	0.57462900	-1.53702000
S	3.64823600	-0.57504000	1.53643800
C	5.14864900	-1.30742500	0.91807200
C	6.31374500	-0.91316000	1.59409200

C	5.32778100	-2.12967100	-0.20201600
C	7.58400900	-1.30071500	1.19088700
C	6.59589000	-2.54119800	-0.61197700
C	7.73003300	-2.12740200	0.07859400
C	5.14859900	1.30663500	-0.91836500
C	6.31371000	0.91207500	-1.59418300
C	5.32773400	2.12894700	0.20167800
C	7.58399800	1.29937500	-1.19081200
C	6.59587600	2.54021700	0.61180200
C	7.73003300	2.12612100	-0.07856800
C	-5.14864900	1.30742500	0.91807200
C	-6.31374500	0.91316000	1.59409200
C	-5.32778100	2.12967100	-0.20201600
C	-7.58400900	1.30071500	1.19088700
C	-6.59589000	2.54119800	-0.61197700
C	-7.73003300	2.12740200	0.07859400
C	-5.14859900	-1.30663500	-0.91836500
C	-6.31371000	-0.91207500	-1.59418300
C	-5.32773400	-2.12894700	0.20167800
C	-7.58399800	-1.29937500	-1.19081200
C	-6.59587600	-2.54021700	0.61180200
C	-7.73003300	-2.12612100	-0.07856800
F	6.72131300	3.32604600	1.68665300
F	8.94505300	2.51087800	0.32138900
F	8.66325200	0.87309500	-1.85768100
F	4.29112700	2.55106400	0.94372300
F	6.20595800	0.08880500	-2.65472400
F	8.66325200	-0.87472600	1.85794900
F	8.94502500	-2.51239300	-0.32120400
F	6.72130600	-3.32696000	-1.68688200
F	4.29118400	-2.55148600	-0.94425400
F	6.20602000	-0.08994100	2.65467200
F	-6.72130600	3.32696000	-1.68688200
F	-4.29118400	2.55148600	-0.94425400
F	-8.94502500	2.51239300	-0.32120400
F	-8.66325200	0.87472600	1.85794900
F	-6.20602000	0.08994100	2.65467200
F	-6.72131300	-3.32604600	1.68665300
F	-4.29112700	-2.55106400	0.94372300
F	-6.20595800	-0.08880500	-2.65472400
F	-8.66325200	-0.87309500	-1.85768100
F	-8.94505300	-2.51087800	0.32138900

Dye **7,** singlet ground state

C	-2.25881600	1.43225300	0.83018100
C	-1.22766300	0.70895500	0.21940600
C	0.00469700	1.40818800	-0.00056900
C	0.00947500	2.82746500	-0.00044700
C	-1.11333700	3.53279800	0.48184100
C	-2.18639900	2.82790900	0.98457100
C	1.23223600	0.70069500	-0.22020800
C	1.13664000	3.52670400	-0.48205500
H	-2.97889200	3.38088500	1.47384500
C	2.20466900	2.81366800	-0.98468100
C	2.26792300	1.41758000	-0.83090500
H	3.00106700	3.36132900	-1.47347200
C	-1.23223600	-0.70069500	-0.22020800
C	-0.00469700	-1.40818800	-0.00056900
C	-2.26792300	-1.41758000	-0.83090500
C	1.22766300	-0.70895500	0.21940600
C	-0.00947500	-2.82746500	-0.00044700
C	-2.20466900	-2.81366800	-0.98468100
C	2.25881600	-1.43225300	0.83018100
C	1.11333700	-3.53279800	0.48184100
C	-1.13664000	-3.52670400	-0.48205500
H	-3.00106700	-3.36132900	-1.47347200
C	2.18639900	-2.82790900	0.98457100
H	2.97889200	-3.38088500	1.47384500
C	-1.11171800	5.01451300	0.51132800
O	-2.05137300	5.66268700	0.95285200
C	1.15228000	5.01009600	-0.51363400
O	2.10469700	5.63634100	-0.95849500
N	0.02023300	5.65903700	-0.00025100
C	1.11171800	-5.01451300	0.51132800
O	2.05137300	-5.66268700	0.95285200
C	-1.15228000	-5.01009600	-0.51363400
O	-2.10469700	-5.63634100	-0.95849500
N	-0.02023300	-5.65903700	-0.00025100
C	-0.00469700	7.12801800	0.01482600
H	-0.85382000	7.48437700	-0.57119600
H	0.93068000	7.48082800	-0.41120600
H	-0.11931000	7.48000100	1.04163600
C	0.00469700	-7.12801800	0.01482600
H	0.85382000	-7.48437700	-0.57119600
H	-0.93068000	-7.48082800	-0.41120600
H	0.11931000	-7.48000100	1.04163600
S	-3.63243200	-0.65756200	-1.76365300
S	-3.62853200	0.68071000	1.76211600

S	3.63243200	0.65756200	-1.76365300
S	3.62853200	-0.68071000	1.76211600
C	5.12726600	-1.51018000	1.19892400
H	5.09848300	-2.55156300	1.51746800
H	5.94254100	-0.98582500	1.70196400
H	5.18640700	-1.41945800	0.11562200
C	5.13683300	1.47720400	-1.20126300
H	5.11504800	2.51861900	-1.52020200
H	5.94835700	0.94713400	-1.70438200
H	5.19580300	1.38643600	-0.11795900
C	-5.12726600	1.51018000	1.19892400
H	-5.18640700	1.41945800	0.11562200
H	-5.09848300	2.55156300	1.51746800
H	-5.94254100	0.98582500	1.70196400
C	-5.13683300	-1.47720400	-1.20126300
H	-5.19580300	-1.38643600	-0.11795900
H	-5.11504800	-2.51861900	-1.52020200
H	-5.94835700	-0.94713400	-1.70438200
O	3.73476500	-0.77594100	-1.43015400
O	3.39790900	1.05744900	-3.16014700
O	3.39223000	-1.07899900	3.15877500
O	3.73973200	0.75208400	1.42846200
O	-3.73973200	-0.75208400	1.42846200
O	-3.39223000	1.07899900	3.15877500
O	-3.73476500	0.77594100	-1.43015400
O	-3.39790900	-1.05744900	-3.16014700

Dye **8**, singlet ground state

C	-2.25603600	1.42369500	0.84267300
C	-1.22910500	0.70500000	0.21976100
C	0.00005200	1.40722800	-0.00064500
C	0.00014600	2.82674700	-0.00075900
C	-1.11903400	3.52770500	0.49828700
C	-2.18185200	2.81770800	1.01781600
C	1.22905600	0.70479500	-0.22042400
C	1.11912000	3.52885200	-0.49923700
H	-2.96622800	3.35267900	1.54004000
C	2.18155900	2.81761500	-1.01850700
C	2.25577000	1.42369000	-0.84342300
H	2.96622600	3.35225400	-1.54049100
C	-1.22905600	-0.70479500	-0.22042400
C	-0.00005200	-1.40722800	-0.00064500
C	-2.25577000	-1.42369000	-0.84342300
C	1.22910500	-0.70500000	0.21976100

C	-0.00014600	-2.82674700	-0.00075900
C	-2.18155900	-2.81761500	-1.01850700
C	2.25603600	-1.42369500	0.84267300
C	1.11903400	-3.52770500	0.49828700
C	-1.11912000	-3.52885200	-0.49923700
H	-2.96622600	-3.35225400	-1.54049100
C	2.18185200	-2.81770800	1.01781600
H	2.96622800	-3.35267900	1.54004000
C	-1.12307300	5.00899100	0.52400600
O	-2.06142500	5.65607800	0.96992100
C	1.13069400	5.01180300	-0.52760000
O	2.07778500	5.64293900	-0.97691600
N	0.00166200	5.65657800	-0.00088500
C	1.12307300	-5.00899100	0.52400600
O	2.06142500	-5.65607800	0.96992100
C	-1.13069400	-5.01180300	-0.52760000
O	-2.07778500	-5.64293900	-0.97691600
N	-0.00166200	-5.65657800	-0.00088500
C	-0.02802000	7.12510900	0.01405100
H	-0.88416100	7.47885200	-0.56341100
H	0.90192600	7.48082300	-0.42144300
H	-0.13402600	7.47744000	1.04173100
C	0.02802000	-7.12510900	0.01405100
H	0.88416100	-7.47885200	-0.56341100
H	-0.90192600	-7.48082300	-0.42144300
H	0.13402600	-7.47744000	1.04173100
S	-3.58815000	-0.63883800	-1.78853700
S	-3.58814000	0.63859600	1.78797400
S	3.58815000	0.63883800	-1.78853700
S	3.58814000	-0.63859600	1.78797400
O	3.49239000	-0.82242800	-1.62706900
O	3.46032900	1.21053100	-3.14001300
O	3.46032900	-1.21070000	3.13928600
O	3.49195400	0.82267900	1.62687300
O	-3.49195400	-0.82267900	1.62687300
O	-3.46032900	1.21070000	3.13928600
O	-3.49239000	0.82242800	-1.62706900
O	-3.46032900	-1.21053100	-3.14001300
C	5.16834900	-1.20573900	1.13709100
C	6.28697900	-0.60266700	1.71914400
C	5.29457700	-2.23243600	0.20391400
C	7.55654000	-1.04752800	1.36030100
H	6.16319000	0.20219200	2.43493500
C	6.57416700	-2.67084500	-0.14234200

H	4.42806100	-2.66544000	-0.27434700
C	7.70115200	-2.08581800	0.43587100
H	8.43124100	-0.58042200	1.80057100
H	6.68261500	-3.46840700	-0.87008300
H	8.69260300	-2.43285300	0.16206100
C	5.16806900	1.20669800	-1.13754700
C	6.28701800	0.60431300	-1.71970300
C	5.29375700	2.23328500	-0.20417800
C	7.55635000	1.04972600	-1.36072300
H	6.16365000	-0.20044100	-2.43568800
C	6.57312400	2.67226800	0.14220500
H	4.42703700	2.66584900	0.27411600
C	7.70041700	2.08790300	-0.43607700
H	8.43128900	0.58315000	-1.80108300
H	6.68114100	3.46977000	0.87007400
H	8.69169100	2.43537500	-0.16217500
C	-5.16834900	1.20573900	1.13709100
C	-6.28697900	0.60266700	1.71914400
C	-5.29457700	2.23243600	0.20391400
C	-7.55654000	1.04752800	1.36030100
H	-6.16319000	-0.20219200	2.43493500
C	-6.57416700	2.67084500	-0.14234200
H	-4.42806100	2.66544000	-0.27434700
C	-7.70115200	2.08581800	0.43587100
H	-8.43124100	0.58042200	1.80057100
H	-6.68261500	3.46840700	-0.87008300
H	-8.69260300	2.43285300	0.16206100
C	-5.16806900	-1.20669800	-1.13754700
C	-6.28701800	-0.60431300	-1.71970300
C	-5.29375700	-2.23328500	-0.20417800
C	-7.55635000	-1.04972600	-1.36072300
H	-6.16365000	0.20044100	-2.43568800
C	-6.57312400	-2.67226800	0.14220500
H	-4.42703700	-2.66584900	0.27411600
C	-7.70041700	-2.08790300	-0.43607700
H	-8.43128900	-0.58315000	-1.80108300
H	-6.68114100	-3.46977000	0.87007400
H	-8.69169100	-2.43537500	-0.16217500

Dye **9**, singlet ground state

C	2.40082600	1.17433800	-0.85365900
C	1.30913800	0.55859800	-0.22433600
C	0.16317100	1.39512500	0.00059200
C	0.32839000	2.80766900	0.00072700

C	1.49055100	3.38357900	-0.55269300
C	2.45754700	2.56031600	-1.08057200
C	-1.14480500	0.84552400	0.22498700
C	-0.66900100	3.63743900	0.55374400
H	3.28178400	3.00308900	-1.62528600
C	-1.79971400	3.05840000	1.08130600
C	-2.06457900	1.69684100	0.85444100
H	-2.49963000	3.67914200	1.62609900
C	1.14480500	-0.84552400	0.22498700
C	-0.16317100	-1.39512500	0.00059200
C	2.06457900	-1.69684100	0.85444100
C	-1.30913800	-0.55859800	-0.22433600
C	-0.32839000	-2.80766900	0.00072700
C	1.79971400	-3.05840000	1.08130600
C	-2.40082600	-1.17433800	-0.85365900
C	-1.49055100	-3.38357900	-0.55269300
C	0.66900100	-3.63743900	0.55374400
H	2.49963000	-3.67914200	1.62609900
C	-2.45754700	-2.56031600	-1.08057200
H	-3.28178400	-3.00308900	-1.62528600
C	1.64961200	4.85770900	-0.61294000
O	2.60831400	5.38792200	-1.15544900
C	-0.48997800	5.11094500	0.61764700
O	-1.30913800	5.83347100	1.16593600
N	0.65683900	5.62775000	0.00073700
C	-1.64961200	-4.85770900	-0.61294000
O	-2.60831400	-5.38792200	-1.15544900
C	0.48997800	-5.11094500	0.61764700
O	1.30913800	-5.83347100	1.16593600
N	-0.65683900	-5.62775000	0.00073700
C	0.85477300	7.08415100	-0.01763900
H	1.79306200	7.33044300	0.48257100
H	0.01401800	7.54043400	0.49795400
H	0.90944600	7.43053600	-1.05114100
C	-0.85477300	-7.08415100	-0.01763900
H	-1.79306200	-7.33044300	0.48257100
H	-0.01401800	-7.54043400	0.49795400
H	-0.90944600	-7.43053600	-1.05114100
S	3.53062300	-1.11157400	1.72683600
S	3.69171100	0.26592000	-1.72614000
S	-3.53062300	1.11157400	1.72683600
S	-3.69171100	-0.26592000	-1.72614000
O	-3.66801200	-0.32849000	1.48969900
O	-3.40281900	1.63490500	3.09055200

O	-3.68812100	-0.80462900	-3.08986400
O	-3.49244300	1.16689300	-1.48899900
O	3.49244300	-1.16689300	-1.48899900
O	3.68812100	0.80462900	-3.08986400
O	3.66801200	0.32849000	1.48969900
O	3.40281900	-1.63490500	3.09055200
C	-5.33786700	-0.69390800	-1.05070500
C	-6.39651000	0.05203800	-1.58738600
C	-5.65437500	-1.70735200	-0.14227100
C	-7.71441500	-0.17570400	-1.21212900
C	-6.97341100	-1.94002300	0.24642100
C	-8.00599900	-1.17606100	-0.28716000
C	-5.03306700	1.90855200	1.05108600
C	-6.23563200	1.42776200	1.58759800
C	-5.10636700	2.96768300	0.14260500
C	-7.46503700	1.95419500	1.21210400
C	-6.33572300	3.49918800	-0.24630800
C	-7.51712700	2.99485400	0.28710700
C	5.33786700	0.69390800	-1.05070500
C	6.39651000	-0.05203800	-1.58738600
C	5.65437500	1.70735200	-0.14227100
C	7.71441500	0.17570400	-1.21212900
C	6.97341100	1.94002300	0.24642100
C	8.00599900	1.17606100	-0.28716000
C	5.03306700	-1.90855200	1.05108600
C	6.23563200	-1.42776200	1.58759800
C	5.10636700	-2.96768300	0.14260500
C	7.46503700	-1.95419500	1.21210400
C	6.33572300	-3.49918800	-0.24630800
C	7.51712700	-2.99485400	0.28710700
F	-6.37805800	4.50155800	-1.12710100
F	-8.69098500	3.50237100	-0.08257600
F	-8.59594300	1.45138600	1.71954300
F	-6.23563200	0.42469900	2.47456000
F	-6.16431300	1.02787800	-2.47431700
F	-8.69823100	0.57508600	-1.71973400
F	-9.26548400	-1.39825100	0.08229800
F	-7.24663000	-2.90540100	1.12718100
F	-4.72988600	-2.51186300	0.38517500
F	8.69098500	-3.50237100	-0.08257600
F	6.37805800	-4.50155800	-1.12710100
F	8.59594300	-1.45138600	1.71954300
F	6.16431300	-1.02787800	-2.47431700
F	7.24663000	2.90540100	1.12718100

F	4.72988600	2.51186300	0.38517500
F	9.26548400	1.39825100	0.08229800
F	8.69823100	-0.57508600	-1.71973400
F	4.02071800	-3.53639200	-0.38468400
F	6.23563200	-0.42469900	2.47456000
F	-4.02071800	3.53639200	-0.38468400