Electronic Supplementary Information (ESI) for

N-Annulated Perylene as a Donor in Cyclopentadithiophene Based Sensitizers: The Effect of Linking Mode

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1. Experimental section

1.1 General

All reagents and starting materials were obtained from commercial suppliers and used without further purification unless otherwise noted. Anhydrous dichloromethane (DCM), *N*, *N*-dimethylformamide (DMF) was distilled from CaH_2. Anhydrous toluene and THF were distilled from sodium-benzophenone immediately prior to use. The ^1H NMR and ^{13}C NMR spectra were recorded in solution of $CDCl_3$ or THF-d_8 on Bruker DPX 400 or DRX 500 NMR spectrometers with tetramethylsilane (TMS) as the internal standard. The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t =triplet, m = multiplet. MALDI-TOF mass spectra (MS) were recorded on a Bruker Autoflex instrument using anthracene-1,8,9-triol as matrix. The solvents used for UV-vis PL measurements are of HPLC grade (Merck). The electrochemical measurements were carried out in anhydrous DCM with 0.1 M tetrabutylammonium hexafluorophosphate (Bu_4NPF_6) as the supporting electrolyte at room temperature under the protection of nitrogen. A gold stick was used as working electrode, platinum wire was used as counting electrode, and Ag/AgCl (3M KCl solution) was used as reference electrode. The potential was externally calibrated against the ferrocene/ferrocenium couple. Steady-state UV-vis absorption were recorded on a Shimadzu UV-1700 and UV-3600 spectrometer.

1.2 Cell fabrication

Fluorine-doped tinoxide (FTO, Pilkington TEC-15, 15 Ωsq^{-1}) glass plate was cleaned by 5% Decon 90 solution, deionized water, and ethanol sequentially in an ultrasonic bath sequentially. A compact TiO_2 layer was synthesized onto that cleaned FTO glass by spray

pyrolysis at 500 °C. A transparent mesoporous TiO_2 layer (90 T, Dyesol, ~ 5.3μm) and scattering layer (~4 μm, no scattering layer for TA) were prepared onto the substrate by screen-printing method. Thereafter, the electrode was gradually heated at 125 °C for 5 min, at 325 °C for 5 min, at 375 °C for 5 min, at 450 °C for 15 min and at 500 °C for 15 min. Finally, the TiO_2 electrode was treated by 40 mM $TiCl_4$ aqueous solution at 70 °C for 30 min and then sintered at 500 °C for 30 min. DSCs were assembled by separating the sensitized TiO_2 film and the platinized FTO glass with a hot-melt spacer (25 μm, Surlyn, DuPont) and followed by heating at 110°C for 1 min. The platinized FTO counter electrode was prepared by thermal decomposition of hexachloroplatinic acid at 400 °C for 15 min. The dye loading was performed by immersing the photoanodes in 0.2 mM in a mixture solutions (DCM:EtOH=4:1) of the individual dyes and kept for 18 h in dark at room temperature. The co-sensitized photo-anodes were prepared by dyeing them into appropriate (0.15 mM) of the individual dyes and in a mixture solutions (DCM:EtOH=4:1) containing CDCA (1.5 mM). The redox electrolyte (0.2 M $Co(bpy)_3(PF_6)_2$, 0.02 M $Co(bpy)_3(PF_6)_3$, 0.5M $LiClO_4$, and 0.5M 4-*tert*-butylpyridine in acetonitrile) was injected through a hole at the platinized FTO a partial vacuum. Finally, the hole was sealed with a small piece of hot-melt polymer and a cover glass.

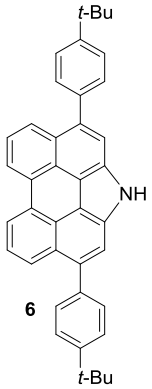
1.3 Cell characterization

Electrochemical impedance spectroscopy (EIS) were measured under 627 nm illumination from a high-power LED using a potentiostat equipped with a frequency response analyzer (Ecochemie, AUTOLAB PGSTAT302N/FRA2) and the Nova 1.6 software package. Different

light intensities were achieved by using neutral density filters mounted in an automated filter wheel system (Newport). The frequency range of the EIS measurement was 10^5 to 0.1Hz with a perturbation of 10 mV. Photocurrent–voltage characteristics were measured with a Keithley 2400 Source Meter under AM 1.5G illumination at 100 mW cm^{-2} from a solar simulator (450 W, Newport class A) calibrated with a silicon reference cell. The active area of the cells was 0.12 cm^2 defined by a mask. The incident photon-to current conversion efficiency (IPCE) spectra were attained under a 300W Xenon lamp and a grating monochromator with a spectral resolution of ~5 nm (Newport/Oriel) controlled by TRACQ basic software (Newport).

2. Synthetic procedure and characterization data

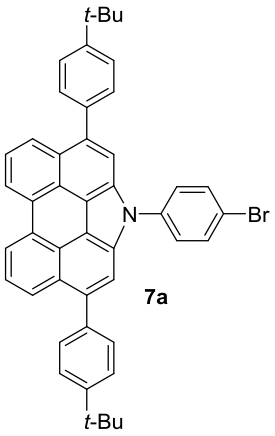
The synthetic route toward **CPD-1** – **CPD-4** is shown in Scheme 1. The building blocks **1**[1], **2**[2] and **3**[3] were synthesized according to literature approaches.



6

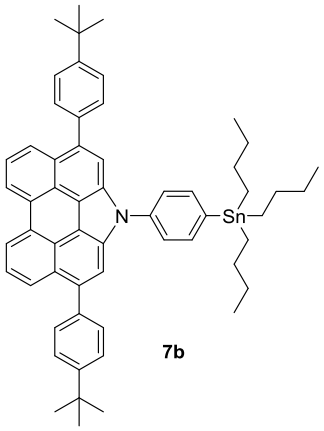
Perylene **5** (500 mg, 1.89 mmol) was dissolved in DMF (10 ml) and cooled to 0 ^{o}C. To this solution was added *N*-bromosuccinimide (NBS) (672 mg, 3.78 mmol) in portion wise and the reaction mixture was stirred at the same temperature for another 30 min. MeOH (200 ml) was added and gray solid precipitated immediately. The solid was filtered, washed with MeOH and dried under vacuum to afford dibromo substituted perylene **6a**, which was subjected into next step directly without further purification. Compound **6a** and 4-*tert*-butylphenylboronic acid (841 mg, 4.73 mmol) were dissolved in a mixture of toluene (30 mL), ethanol (20 mL) and aqueous saturated $NaHCO_3$ solution (12 ml). The solution was degassed by argon bubbling for 20 min before adding $Pd(PPh_3)_4$ (109 mg, 0.095 mmol). The reaction mixture was refluxed for 5 h and cooling down. Water was added and the product was extracted with ethyl acetate (3 x 30 mL). The organic layer was washed with saturated brine and dried over anhydrous Na_2SO_4. The solvent was removed under vacuum, and the residue was purified by column chromatography (silica gel, THF/hexane) to give product **6** as a yellow solid (679 mg, 68% yield for two steps). Characterization for **6**: ^{1}H NMR (500 MHz,

d-THF) δ 8.72 (d, *J* = 7.5 Hz, 2H), 8.11 (d, *J* = 8.2 Hz, 2H), 7.82 (s, 2H), 7.76 – 7.70 (m, 2H), 7.67 – 7.57 (m, 8H), 1.45 (s, 18H); ^{13}C NMR (126 MHz, d-THF) δ 149.79, 139.53, 137.67, 131.40, 131.14, 130.02, 128.21, 125.32, 125.25, 124.46, 124.28, 120.78, 117.56, 115.44, 34.55, 31.13.



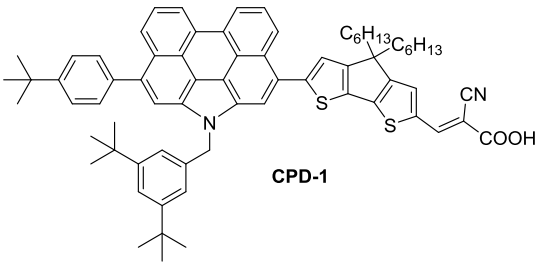
7a

A mixture of compound **6** (679 mg, 1.28 mmol), 1,4-dibromobenzene (1.21g, 5.12 mmol), K_2CO_3 (353 mg, 2.56 mmol), Cu powder (82 mg, 1.28 mmol) and 18-crown-6 (50.2 mg, 0.19 mmol) in mesitylene (15 ml) was stirred and heated at reflux under an N_2 atmosphere for 3 days. The solvent was removed under vacuum and the residue was then dissolved in CH_2Cl_2 (100 mL) and water (100 mL). The organic phase was separated, dried with anhydrous Na_2SO_4 and the solvents were removed to dryness. Purification by column chromatography (silica gel, CH_2Cl_2/hexane) gave compound **7a** as yellow solid (394 mg, 45% yield). Characterization for **7a**: ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.59 (d, *J* = 7.5 Hz, 2H), 8.16 (d, *J* = 8.2 Hz, 2H), 7.91 (d, *J* = 8.6 Hz, 2H), 7.86 (s, 2H), 7.78 – 7.72 (m, 2H), 7.66 – 7.54 (m, 10H), 1.46 (s, 18H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 150.30, 139.54, 139.17, 131.01, 129.98, 129.96, 126.12, 125.46, 125.29, 125.25, 125.21, 124.97, 121.17, 118.17, 114.71, 90.46, 34.76, 31.58.



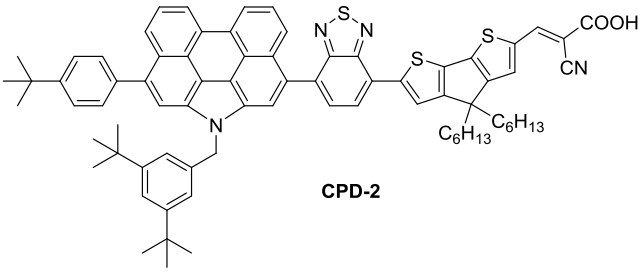
7b

To a solution of compound **7a** (197 mg, 0.29 mmol) in 20 mL of THF at -78 °C was added *n*-BuLi (2.5 M in hexane, 0.13 mL, 0.32 mmol) dropwise. After the mixture was stirred for 30 min, tributylstannyl chloride (0.1 mL, 0.34 mmol) was added to the mixture. Then it was slowly warmed to room temperature and stirred for another 12 h. The mixture was poured into water and extracted with diethyl ether. The organic extracts were dried over $MgSO_4$. Upon evaporation of the solvent, the crude product was quickly passed a short column of deactivated silica gel to afford compound **7b** (169 mg, 65% yield). Characterization for **7b**: ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.67 (d, *J* = 7.5 Hz, 2H), 8.18 (d, *J* = 8.3 Hz, 2H), 7.98 (s, 2H), 7.90 – 7.84 (m, 2H), 7.78 (dd, *J* = 8.2, 7.5 Hz, 2H), 7.72 (d, *J* = 8.2 Hz, 2H), 7.69 – 7.64 (m, 4H), 7.62 – 7.56 (m, 4H), 1.68 – 1.57 (m, 6H), 1.46 (s, 18H), 1.40 (dd, *J* = 14.8, 7.3 Hz, 6H), 1.19 – 1.12 (m, 6H), 0.95 (t, *J* = 7.3 Hz, 9H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 150.07, 140.13, 139.49, 138.89, 137.95, 137.93, 131.50, 130.93, 129.95, 128.51, 125.32, 125.30, 124.96, 124.51, 123.77, 120.95, 117.92, 115.10, 34.66, 31.50, 29.12, 27.42, 13.69, 9.77.



CPD-1

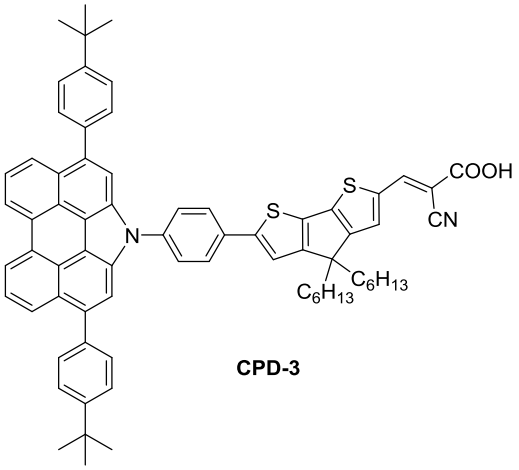
To a solution of N-annulated perylene bronic ester **1** (72.6 mg, 0.1 mmol), 6-bromo-4,4-dihexyl-4H-cyclopenta[2,1-b:3,4-b']dithiophene-2-carbaldehyde **2** (54.4 mg, 0.12 mmol), and tetrakis(triphenylphosphine)palladium (11.6 mg, 0.01 mmol) in toluene (15 mL) was added potassium carbonate aqueous solution (2 M, 0.4 mL) under argon. The reaction mixture was refluxed for 24 h and then water (30 mL) added. The crude compound was extracted into ethyl acetate, washed with brine and water, and dried over anhydrous sodium sulfate. After removing solvent under reduced pressure, the residue was loaded into a two-necked round bottom flask. To a stirred solution of the residue and cyanoacetic acid (10 mg, 0.12 mmol) in chloroform (5mL) was added piperidine (23 mg, 0.28 mmol). The reaction mixture was refluxed under argon for 18 h and then acidified with 2 M hydrochloric acid aqueous solution (3 mL). The crude product was extracted by chloroform, washed with water, and dried over anhydrous sodium sulfate. After removing solvent under reduced pressure, the residue was purified by flash chromatography (silica gel, CH_2Cl_2/MeOH) as eluent to yield **CPD-1** (57 mg, 55% yield for two steps). Characterization for **CPD-1**: ^{1}H NMR (500 MHz, d-THF) δ 8.79 (d, *J* = 7.6 Hz, 1H), 8.76 (d, *J* = 7.6 Hz, 1H), 8.49 (d, *J* = 8.2 Hz, 1H), 8.39 (s, *1*H), 8.14 – 8.10 (m, 1H), 8.12 (s, 1H), 7.87 (s, 1H), 7.85 – 7.82 (m, 2H), 7.82 – 7.74 (m, 1H), 7.61 (d, *J* = 2.1 Hz, 4H), 7.51 (s, 1H), 7.41 (s, 2H), 7.39 – 7.36 (m, 1H), 6.03 (s, 2H), 2.07 (t, *J* = 7.3 Hz, 4H), 1.45 (s, 9H), 1.24 (s, 18H), 1.22 – 0.75 (m, 26H). HRMS (APCI): m/z = 1039.5276 (M^++1); elemental analysis calcd (%) for $C_{70}H_{75}N_2O_2S_2$: 1039.5264 (error = +1.1 ppm).



CPD-2

To a solution of bromo substituted N-annulated perylene **3** (67.9 mg, 0.1 mmol), 2,1,3-Benzothiadiazole-4,7-bis(boronic acid pinacol ester) **4** (38.8 mg, 0.1 mmol), 6-bromo-4,4-dihexyl-4H-cyclopenta[2,1-b:3,4-b']dithiophene-2-carbaldehyde **2** (45.3 mg, 0.1 mmol), and tetrakis(triphenylphosphine)palladium (11.6 mg, 0.01 mmol) in toluene (15 mL) was added potassium carbonate aqueous solution (2 M, 0.4 mL) under argon. The reaction mixture was refluxed for 24 h and then water (30 mL) added. The crude compound was extracted into ethyl acetate, washed with brine and water, and dried over anhydrous sodium sulfate. After removing solvent under reduced pressure, the residue was loaded into a two-necked round bottom flask. To a stirred solution of the residue and cyanoacetic acid (10 mg, 0.12 mmol) in chloroform (5mL) was added piperidine (23 mg, 0.28 mmol). The reaction mixture was refluxed under argon for 18 h and then acidified with 2 M hydrochloric acid aqueous solution (3 mL). The crude product was extracted by chloroform, washed with water, and dried over anhydrous sodium sulfate. After removing solvent under reduced pressure, the residue was purified by flash chromatography (silica gel, CH_2Cl_2/MeOH) as eluent to yield **CPD-2** (27 mg, 23% yield for two steps). Characterization for **CPD-2**: ^{1}H NMR (500 MHz, d-THF+CS_2) δ 8.73 (d, *J* = 4.5 Hz, 1H), 8.72 (d, *J* = 4.5 Hz, 1H), 8.36 (s, 1H), 8.35 (d, 1H), 8.24 (t, *J* = 6.1 Hz, 1H), 8.19 (s, 1H), 8.13 (d, *J* = 8.4 Hz, 1H), 7.98 (d, *J* = 7.4 Hz, 1H), 7.93 (d, *J* = 8.3 Hz, 1H), 7.87 – 7.79 (m, 2H), 7.79 – 7.73 (m, 1H), 7.73 – 7.67 (m, 1H), 7.59 (dd, *J* = 8.2, 2.2 Hz, 4H), 7.37 (s, 2H), 7.33 (s, 1H), 5.98 (s, 2H), 2.07 (t, *J* = 8.2 Hz, 4H), 1.45 (s, 9H), 1.23 (s, 18H),

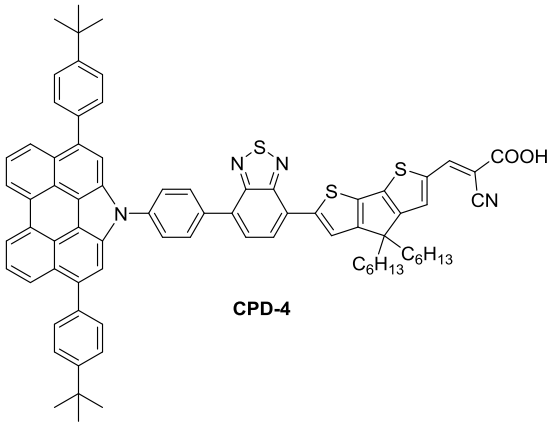
1.30 – 0.84 (m, 26H). HRMS (APCI): m/z=1173.5228 (M^++1); elemental analysis calcd (%) for $C_{76}H_{77}N_4O_2S_3$: 1173.5203 (error=+2.1 ppm).



CPD-3

To a solution of 4-(tributylstannyl)phenyl N-annulated perylene **7b** (89.5 mg, 0.1 mmol), 6-bromo-4,4-dihexyl-4H-cyclopenta[2,1-b:3,4-b']dithiophene-2-carbaldehyde **2** (54.4 mg, 0.12 mmol), and tetrakis(triphenylphosphine)palladium (11.6 mg, 0.01 mmol) in toluene (15 mL) was added potassium carbonate aqueous solution (2 M, 0.4 mL) under argon. The reaction mixture was refluxed for 24 h and then water (30 mL) added. The crude compound was extracted into ethyl acetate, washed with brine and water, and dried over anhydrous sodium sulfate. After removing solvent under reduced pressure, the residue was passed through column chromatography to afford aldehyde intermediate **CPD-3a** (75 mg, 77% yield). Characterization for **CPD-3a**: ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.86 (s, 1H), 8.58 (br, 2H), 8.16 (br, 2H), 7.93 (s, 2H), 7.90 (d, *J* = 8.6 Hz, 2H), 7.85 (d, *J* = 8.5 Hz, 2H), 7.75 (t, *J* = 7.8 Hz, 2H), 7.64 (d, *J* = 6.7 Hz, 4H), 7.61 – 7.52 (m, 5H), 7.29 (s, 1H), 2.01 – 1.86 (m, 4H), 1.46 (s, 18H), 1.29 – 0.78 (m, 26H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 182.47, 167.73, 163.39, 157.78, 157.77, 150.20, 150.18, 150.17, 150.14, 148.24, 148.23, 147.68, 143.41, 139.32, 135.08, 132.37, 130.88, 130.85, 129.88, 128.79, 127.04, 125.34, 124.86, 124.58, 118.05, 118.04, 117.93, 54.22, 37.72,

34.65, 31.58, 31.48, 29.63, 24.62, 22.59, 14.00. The aldehyde intermediate **CPD-3a** was loaded into a two-necked round bottom flask. To a stirred solution of the residue and cyanoacetic acid (10 mg, 0.12 mmol) in chloroform (5mL) was added piperidine (23 mg, 0.28 mmol). The reaction mixture was refluxed under argon for 18 h and then acidified with 2 M hydrochloric acid aqueous solution (3 mL). The crude product was extracted by chloroform, washed with water, and dried over anhydrous sodium sulfate. After removing solvent under reduced pressure, the residue was purified by flash chromatography (silica gel, CH_2Cl_2/MeOH) as eluent to yield **CPD-3** (64.4 mg, 80% yield). Characterization for **CPD-3**: ^{1}H NMR (500 MHz, d-THF+CS_2) δ 8.64 (br, 3H), 8.32 (d, *J* = 2.1 Hz, 1H), 8.10 (br, 2H), 7.94 (br, 6H), 7.73 (br, 3H), 7.62 - 7.42 (m, 8H), 1.98 (br, 4H), 1.45 (s, 18H), 1.40 – 0.83 (m, 26H). HRMS (APCI): m/z=1045.4816 (M^++1); elemental analysis calcd (%) for $C_{71}H_{69}N_2O_2S_2$: 1045.4795 (error=+2.1 ppm).



CPD-4

To a solution of 4-bromophenyl N-annulated perylene **7a** (68.5 mg, 0.1 mmol), 2,1,3-Benzothiadiazole-4,7-bis(boronic acid pinacol ester) **4** (38.8 mg, 0.1 mmol), 6-bromo-4,4-dihexyl-4H-cyclopenta[2,1-b:3,4-b']dithiophene-2-carbaldehyde **2** (45.3 mg, 0.1 mmol), and tetrakis(triphenylphosphine)palladium (11.6 mg, 0.01 mmol) in toluene (15 mL) was added potassium carbonate aqueous solution (2 M, 0.4 mL) under argon. The reaction

mixture was refluxed for 24 h and then water (30 mL) added. The crude compound was extracted into ethyl acetate, washed with brine and water, and dried over anhydrous sodium sulfate. After removing solvent under reduced pressure, the residue was loaded into a two-necked round bottom flask. To a stirred solution of the residue and cyanoacetic acid (10 mg, 0.12 mmol) in chloroform (5mL) was added piperidine (23 mg, 0.28 mmol). The reaction mixture was refluxed under argon for 18 h and then acidified with 2 M hydrochloric acid aqueous solution (3 mL). The crude product was extracted by chloroform, washed with water, and dried over anhydrous sodium sulfate. After removing solvent under reduced pressure, the residue was purified by flash chromatography (silica gel, CH_2Cl_2/MeOH) as eluent to yield **CPD-4** (21.2 mg, 18% yield for two steps). Characterization for **CPD-4**: ^{1}H NMR (500 MHz, d-THF+CS_2) δ 8.70 (d, *J* = 7.2 Hz, 2H), 8.40 (d, *J* = 8.2 Hz, 2H), 8.30 (s, 1H), 8.27 (s, 1H), 8.15 (m, 5H), 8.08 – 7.98 (m, 3H), 7.82 – 7.73 (m, 3H), 7.72 – 7.56 (m, 8H), 2.11 – 1.99 (m, 4H), 1.45 (s, 18H), 1.33 – 0.77 (m, 26H). HRMS (APCI): m/z=1179.4784 (M^++1); elemental analysis calcd (%) for $C_{77}H_{70}N_4O_2S_3$: 1179.4734 (error=+4.3 ppm).

3. Summary of optical and electrochemical properties

Table S1. Summary of Optical and Electrochemical Properties of **CPD-1** – **CPD-4**

Dye	λ_{abs} (nm)	ε ($M^{-1}cm^{-1}$)	E_g^{opt} (eV)	$E_{1/2}^{ox}$ (V)	$E_{1/2}^{red}$ (V)	HOMO (eV)	LUMO (eV)	E_g^{EC} (eV)
CPD-1	404	23120	2.05	1.00	-1.08	-5.01	-3.13	1.88
	488	64080		1.29	-1.53			
					-1.71			
CPD-2	397	20200	1.96	1.05	-0.93	-5.06	-3.25	1.81
	422	31300		1.30	-1.12			
	450	43900			-1.44			
	524	43100						
CPD-3	429	50200	2.29	1.21	-1.47	-5.07	-2.77	2.30
	450	67300		1.51				
CPD-4	402	30100	2.03	1.10	-1.06	-5.12	-3.22	1.90
	424	41400		1.43	-1.38			
	449	50000		1.57				
	516	44600						

Note: The HOMO and LUMO energy levels were calculated by the following equations: HOMO = -[4.8 + E_{ox}^{onset} – $E_{1/2}(Fc^+/Fc)$] eV, LUMO = -[4.8 + E_{red}^{onset} – $E_{1/2}(Fc^+/Fc)$] eV. In our case, $E_{1/2}(Fc^+/Fc)$ is determined to be 0.72 eV.

4. Differential pulse voltammograms of CPD-1 – CPD-4

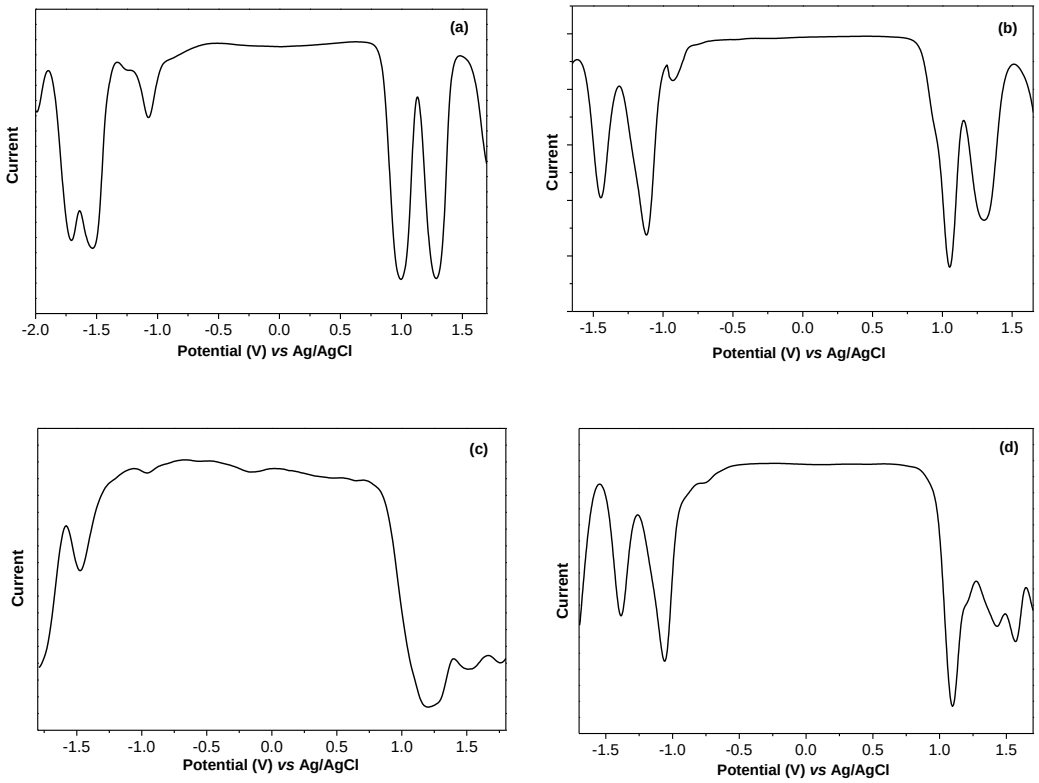


Figure S1. Differential pulse voltammograms recorded in dry THF with 0.1 M Bu_4NPF_6 as supporting electrolyte: (a) **CPD-1**; (b) **CPD-2**; (c) **CPD-3** and (d) **CPD-4**.

5. TD-DFT calculations of CPD-1 – CPD-4

Time-dependent DFT (TD-DFT) calculations have been performed at the B3LYP/6-31G* level of theory,[4] as implemented in the Gaussian 09 program package.[5] The geometries of **CPD-1** – **CPD-4** were fully optimized in gas phase using the default convergence criteria without any constraints and confirmed by frequency calculations. UV-vis-NIR absorption spectra were generated assuming an average UV-vis width of 4000 cm^{-1} at half-height using the SWizard program.

Table S2. Energy levels of compound **CPD-1**

	Hartree	eV
LUMO+5	-0.01104	-0.30
LUMO+4	-0.01326	-0.36
LUMO+3	-0.01865	-0.51
LUMO+2	-0.03546	-0.96
LUMO+1	-0.06825	-1.86
LUMO	-0.09493	-2.58
HOMO	-0.17834	-4.85
HOMO-1	-0.20424	-5.56
HOMO-2	-0.21438	-5.83
HOMO-3	-0.23377	-6.36
HOMO-4	-0.24253	-6.60
HOMO-5	-0.24485	-6.66
HOMO-6	-0.24718	-6.73
HOMO-7	-0.24983	-6.80
HOMO-8	-0.25203	-6.86
HOMO-9	-0.26118	-7.11

Table S3. Selected TD-DFT (UB3LYP/6-31G(d,p)) calculated energies, oscillator strength and compositions of major electronic transitions of **CPD-1**

Wavelength (nm)	Osc. Strength (*f*)	Major contributions
608.0	0.8728	H-0->L+0(+99%)
467.3	0.8875	H-0->L+1(+65%) H-1->L+0(+33%)
421.5	0.1785	H-1->L+0(+63%) H-0->L+1(30%)
372.1	0.0858	H-1->L+1(+81%) H-0->L+2(11%)
360.4	0.0402	H-2->L+1(+69%) H-1->L+1(9%)
		H-0->L+2(6%)
316.1	0.0395	H-8->L+0(+41%) H-0->L+4(+15%)
		H-0->L+3(13%) H-6->L+0(+13%)
		H-7->L+0(6%)
298.3	0.0383	H-0->L+8(+37%) H-0->L+5(24%)
293.5	0.0347	H-0->L+6(+45%) H-0->L+7(+9%)
		H-1->L+2(9%) H-11->L+0(9%)
278.2	0.0613	H-2->L+2(+37%) H-6->L+1(10%)
		H-12->L+0(8%) H-1->L+2(+6%)

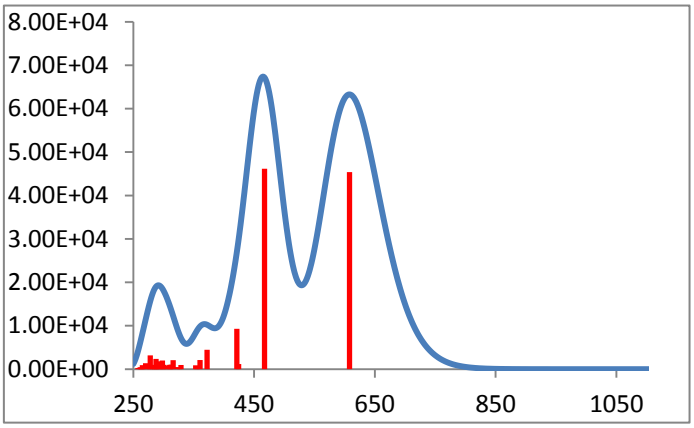


Figure S2. Calculated absorption spectrum for **CPD-1**

Table S4. Energy levels of compound **CPD-2**

	Hartree	eV
LUMO+5	-0.01313	-0.36
LUMO+4	-0.01819	-0.49
LUMO+3	-0.04273	-1.16
LUMO+2	-0.0652	-1.77
LUMO+1	-0.08782	-2.39
LUMO	-0.10785	-2.93
HOMO	-0.17747	-4.83
HOMO-1	-0.19924	-5.42
HOMO-2	-0.21117	-5.75
HOMO-3	-0.23199	-6.31
HOMO-4	-0.23705	-6.45
HOMO-5	-0.23974	-6.52
HOMO-6	-0.24149	-6.57
HOMO-7	-0.24802	-6.75
HOMO-8	-0.25504	-6.94
HOMO-9	-0.25877	-7.04

Table S5. Selected TD-DFT (UB3LYP/6-31G(d,p)) calculated energies, oscillator strength and compositions of major electronic transitions of **CPD-2**

Wavelength (nm)	Osc. Strength (*f*)	Major contributions	
776.0	0.6272	H-0->L+0(+97%)	
541.5	0.9567	H-1->L+0(+74%)	H-0->L+1(17%)
454.4	0.7515	H-1->L+1(+67%)	H-0->L+2(24%)
439.8	0.0565	H-0->L+2(+70%)	H-1->L+1(+20%)
		H-1->L+0(6%)	
398.3	0.0340	H-3->L+0(+93%)	

365.2	0.0294	H-0->L+3(+41%) H-2->L+2(+17%) H-1->L+2(+15%) H-8->L+0(7%) H-4->L+0(+6%)
362.7	0.0310	H-2->L+2(+61%) H-1->L+2(15%) H-0->L+8(6%) H-4->L+0(5%)
331.1	0.0730	H-0->L+4(+37%) H-4->L+1(34%) H-3->L+1(6%) H-11->L+0(6%)
305.9	0.0576	H-0->L+6(+31%) H-0->L+9(+14%) H-0->L+5(+8%) H-8->L+2(8%) H-7->L+2(+5%)

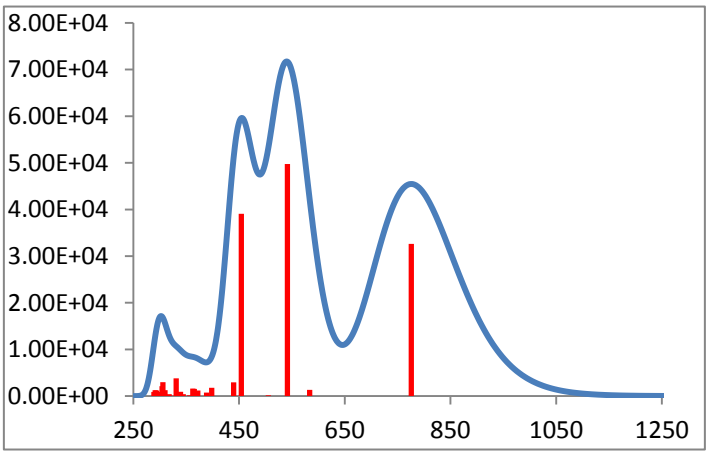


Figure S3. Calculated absorption spectrum for **CPD-2**

Table S6. Energy levels of compound **CPD-3**

	Hartree	eV
LUMO+5	-0.01776	-0.48
LUMO+4	-0.0197	-0.54
LUMO+3	-0.02607	-0.71
LUMO+2	-0.05188	-1.41
LUMO+1	-0.06642	-1.81
LUMO	-0.10021	-2.73
HOMO	-0.17875	-4.86
HOMO-1	-0.19734	-5.37
HOMO-2	-0.21559	-5.87
HOMO-3	-0.23106	-6.29
HOMO-4	-0.23377	-6.36
HOMO-5	-0.2472	-6.73
HOMO-6	-0.24854	-6.76
HOMO-7	-0.24927	-6.78
HOMO-8	-0.25263	-6.87
HOMO-9	-0.25737	-7.00

Table S7. Selected TD-DFT (UB3LYP/6-31G(d,p)) calculated energies, oscillator strength and

compositions of major electronic transitions of **CPD-3**

Wavelength (nm)	Osc. Strength (*f*)	Major contributions
653.6	0.0024	H-0->L+0(+100%)
503.3	1.4112	H-1->L+0(+96%)
442.3	0.5857	H-0->L+1(+98%)
420.2	0.3455	H-2->L+0(+93%)
399.0	0.0747	H-0->L+2(+97%)
350.1	0.0489	H-1->L+2(+66%) H-8->L+0(+19%) H-2->L+1(9%)
333.8	0.0449	H-0->L+4(+60%) H-0->L+5(+26%)
309.7	0.0492	H-11->L+0(+82%) H-1->L+3(8%)
289.9	0.0837	H-0->L+8(+56%) H-1->L+4(+8%) H-2->L+1(+7%)
283.5	0.1009	H-13->L+0(+38%) H-1->L+4(+12%) H-1->L+3(+11%) H-12->L+0(8%) H-1->L+5(7%) H-0->L+10(6%)

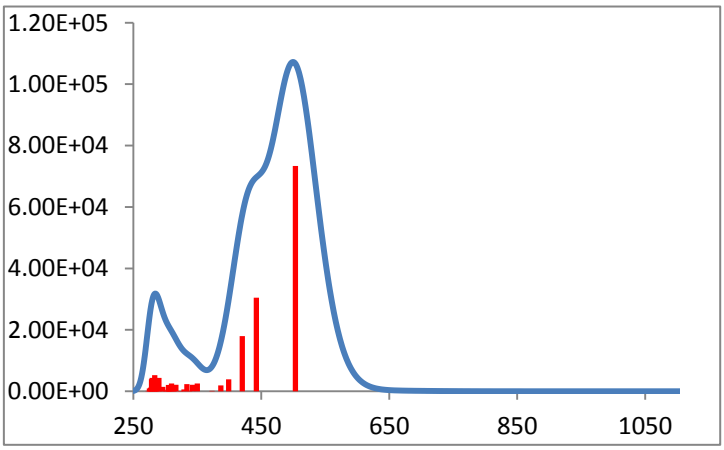


Figure S4. Calculated absorption spectrum for **CPD-3**

Table S8. Energy levels of compound **CPD-4**

	Hartree	eV
LUMO+5	-0.01885	-0.51
LUMO+4	-0.03086	-0.84
LUMO+3	-0.04878	-1.33
LUMO+2	-0.06408	-1.74
LUMO+1	-0.09146	-2.49
LUMO	-0.11226	-3.05
HOMO	-0.17683	-4.81
HOMO-1	-0.19701	-5.36
HOMO-2	-0.20987	-5.71

HOMO-3	-0.2295	-6.25
HOMO-4	-0.23191	-6.31
HOMO-5	-0.23976	-6.52
HOMO-6	-0.24538	-6.68
HOMO-7	-0.24692	-6.72
HOMO-8	-0.24812	-6.75
HOMO-9	-0.25534	-6.95

Table S9. Selected TD-DFT (UB3LYP/6-31G(d,p)) calculated energies, oscillator strength and compositions of major electronic transitions of **CPD-4**

Wavelength (nm)	Osc. Strength (*f*)	Major contributions
822.2	0.0009	H-0->L+0(+99%)
606.7	1.2777	H-1->L+0(+95%)
471.2	0.5214	H-1->L+1(+80%) H-2->L+0(12%)
440.6	0.6218	H-0->L+2(+98%)
416.8	0.0924	H-2->L+1(+75%) H-3->L+0(14%)
		H-5->L+0(+8%)
389.1	0.0898	H-5->L+0(+77%) H-2->L+1(7%)
		H-1->L+3(+6%)
379.9	0.1114	H-1->L+2(+71%) H-2->L+2(18%)
342.6	0.1712	H-1->L+3(+50%) H-5->L+1(14%)
		H-4->L+1(12%) H-11->L+0(10%)
305.5	0.0837	H-2->L+3(+24%) H-15->L+0(+22%)
		H-1->L+4(+16%) H-13->L+0(6%)
		H-3->L+2(6%) H-0->L+8(5%)
301.8	0.0766	H-2->L+3(+36%) H-1->L+4(29%)
		H-15->L+0(16%) H-3->L+2(5%)
		H-0->L+8(5%)

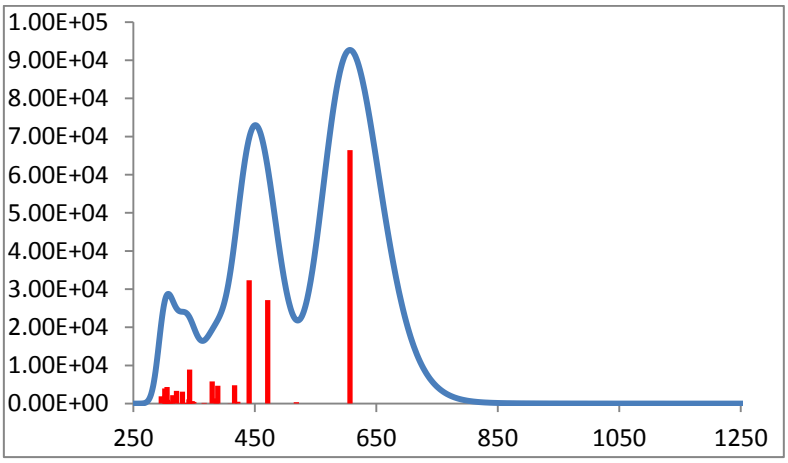


Figure S5. Calculated absorption spectrum for **CPD-4**

6. Reference

1. Jiao, C.; Huang, K.-W.; Guan, Z.; Xu, Q.-H.; Wu, J. *Org. Lett.*, **2010**, *12*, 4046.
2. Gao, P.; Tsao, H. N.; Grätzel, M.; Nazeeruddin, M. K. *Org. Lett.*, **2012**, *14*, 4330.
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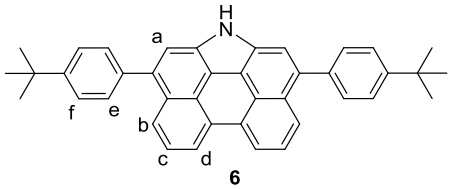
4. (a) Ditchfie, R. W.; Hehre, J.; Pople, J. A. *J. Chem. Phys.* **1971**, *54*, 724. (b) Hehre, W. J.; Ditchfie R.; Pople, J. *J. Chem. Phys.* **1972**, *56*, 2257. (c) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 1372.
5. Gaussian 09; Revision A.2; Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J.; Gaussian, Inc., Wallingford CT, 2009

6. $^{1}H/^{13}C$ NMR spectra and mass spectra of all new compounds



6

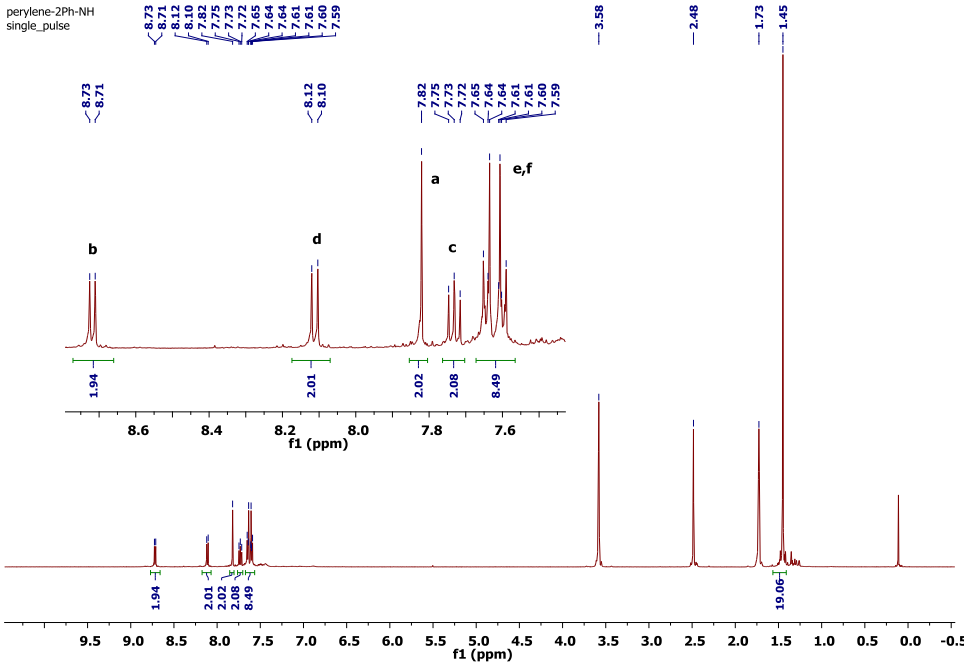


Figure S2. ^{1}H NMR spectrum (500 MHz) of compound **6** in d-THF at 298 K.

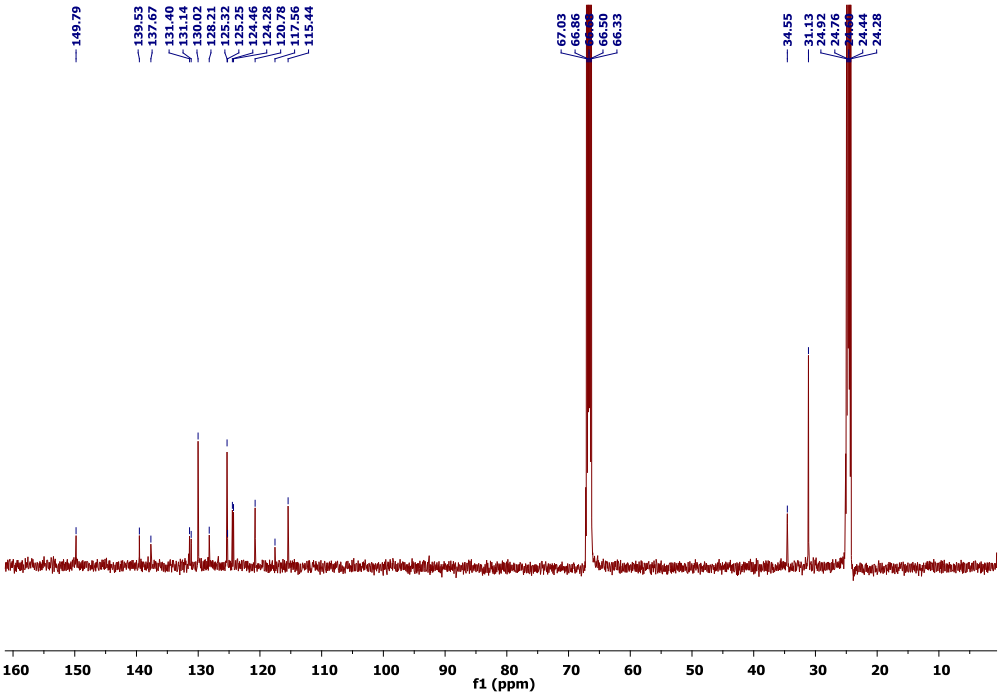


Figure S3. ^{13}C NMR spectrum (125 MHz) of compound **6** in d-THF at 298 K.

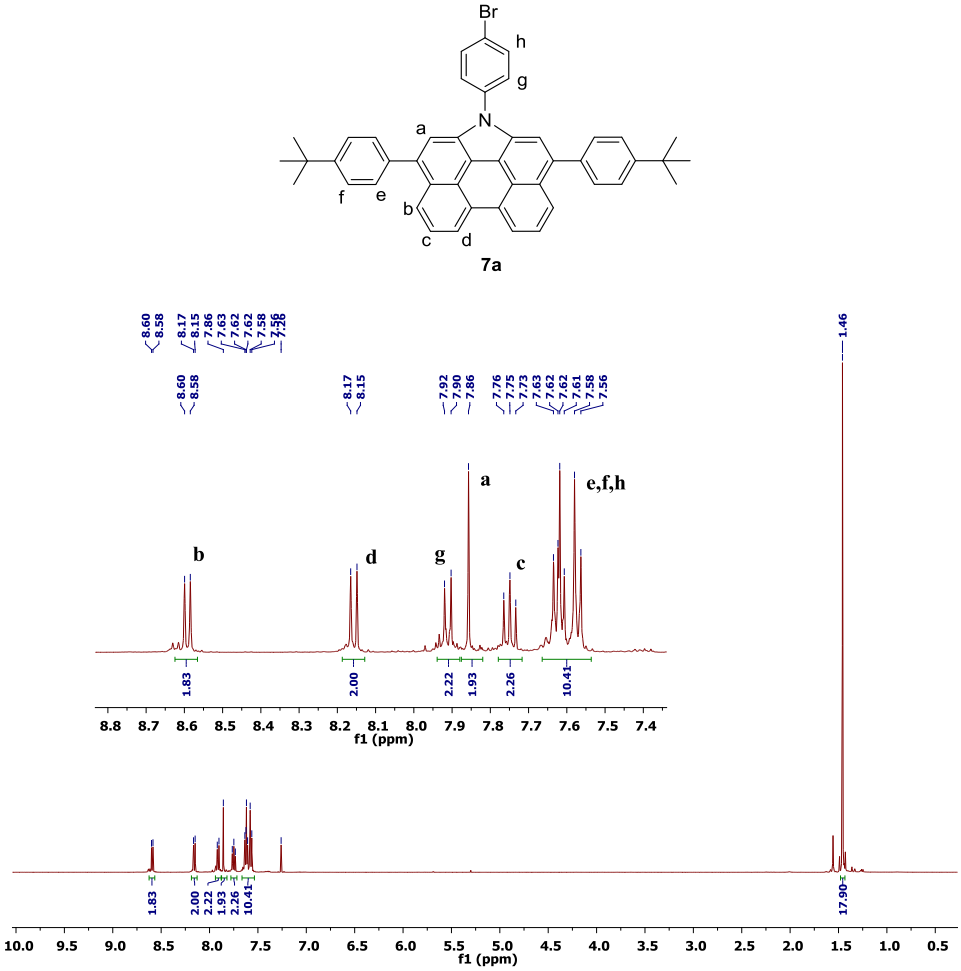


Figure S4. ^{1}H NMR spectrum (500 MHz) of compound **7a** in $CDCl_3$ at 298 K.

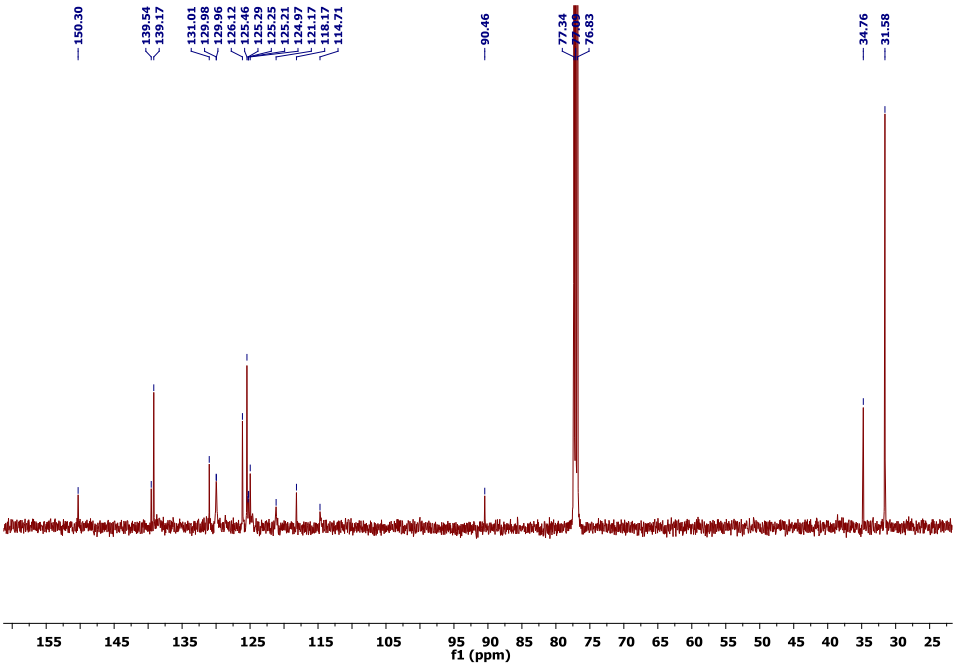


Figure S5. ^{13}C NMR spectrum (125 MHz) of compound **7a** in $CDCl_3$ at 298 K.

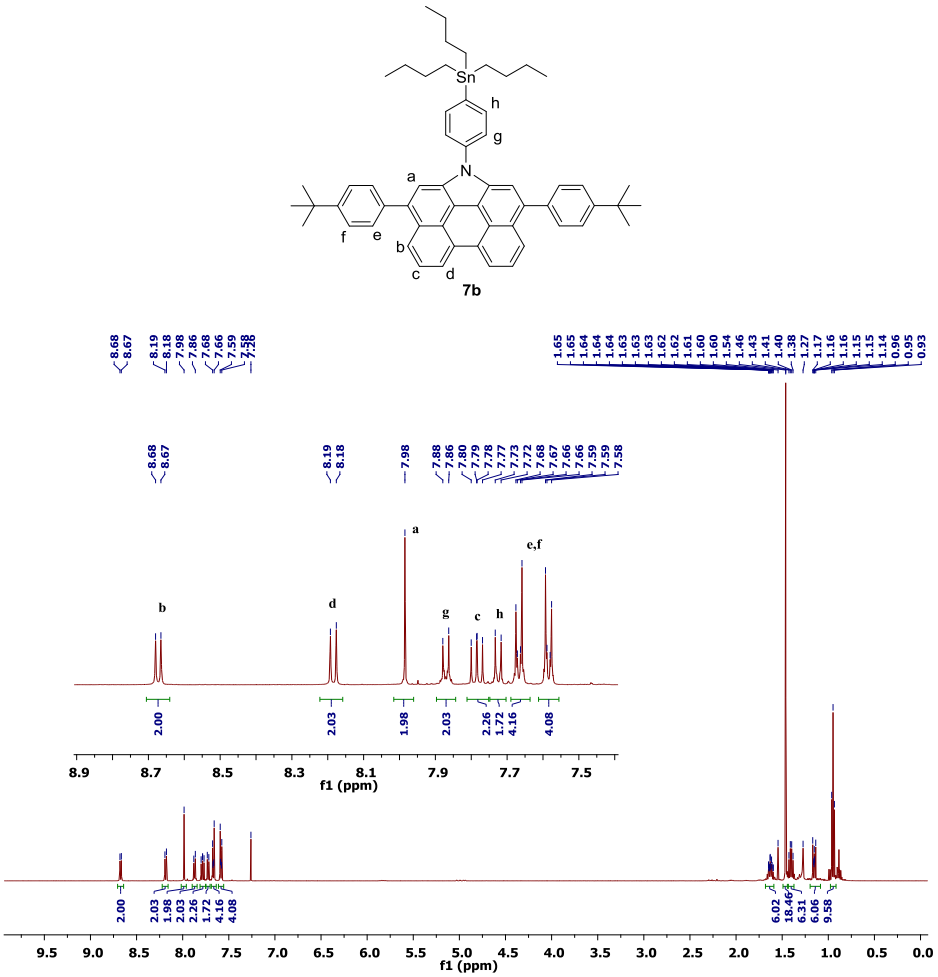


Figure S6. ^{1}H NMR spectrum (500 MHz) of compound **7b** in $CDCl_3$ at 298 K.

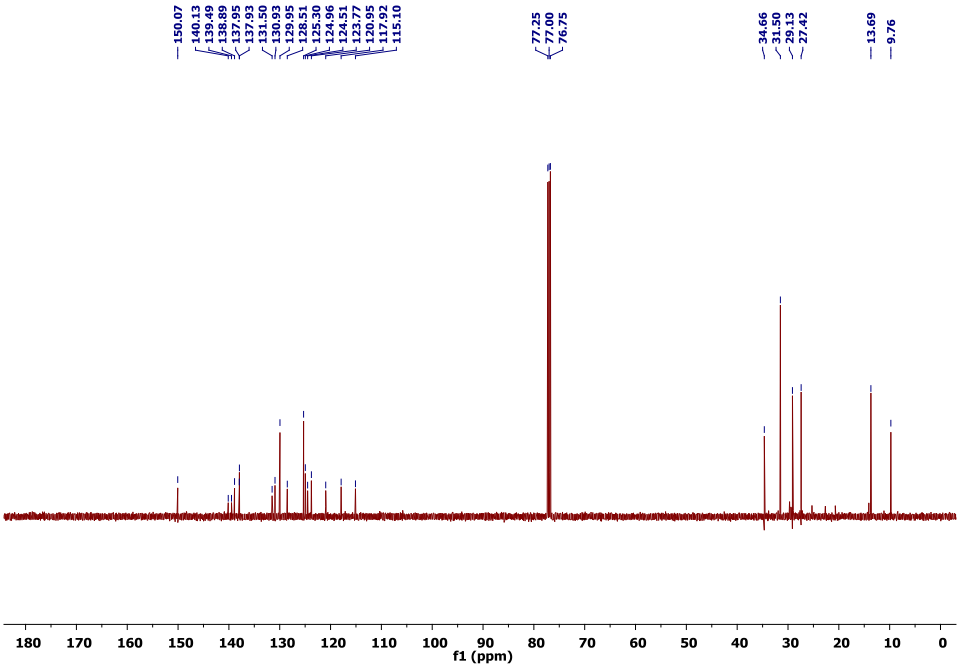


Figure S7. ^{13}C NMR spectrum (125 MHz) of compound **7b** in $CDCl_3$ at 298 K.

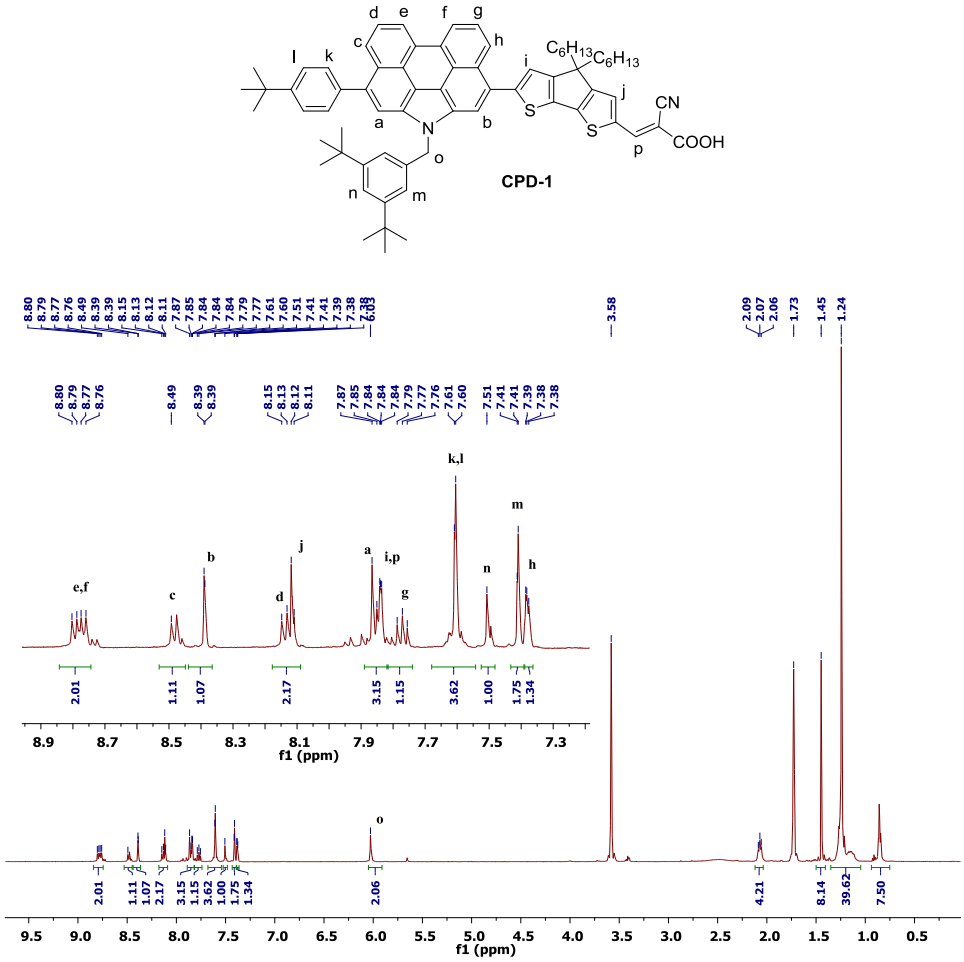


Figure S8. ^{1}H NMR spectrum (500 MHz) of compound **CPD-1** in d-THF at 298 K.

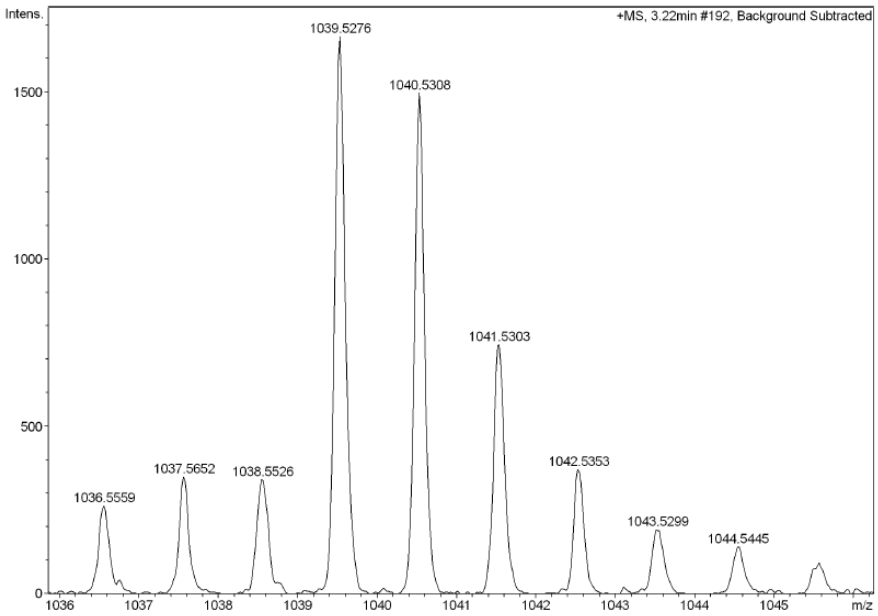


Figure S9. HRMS spectrum (APCI) of compound **CPD-1**.

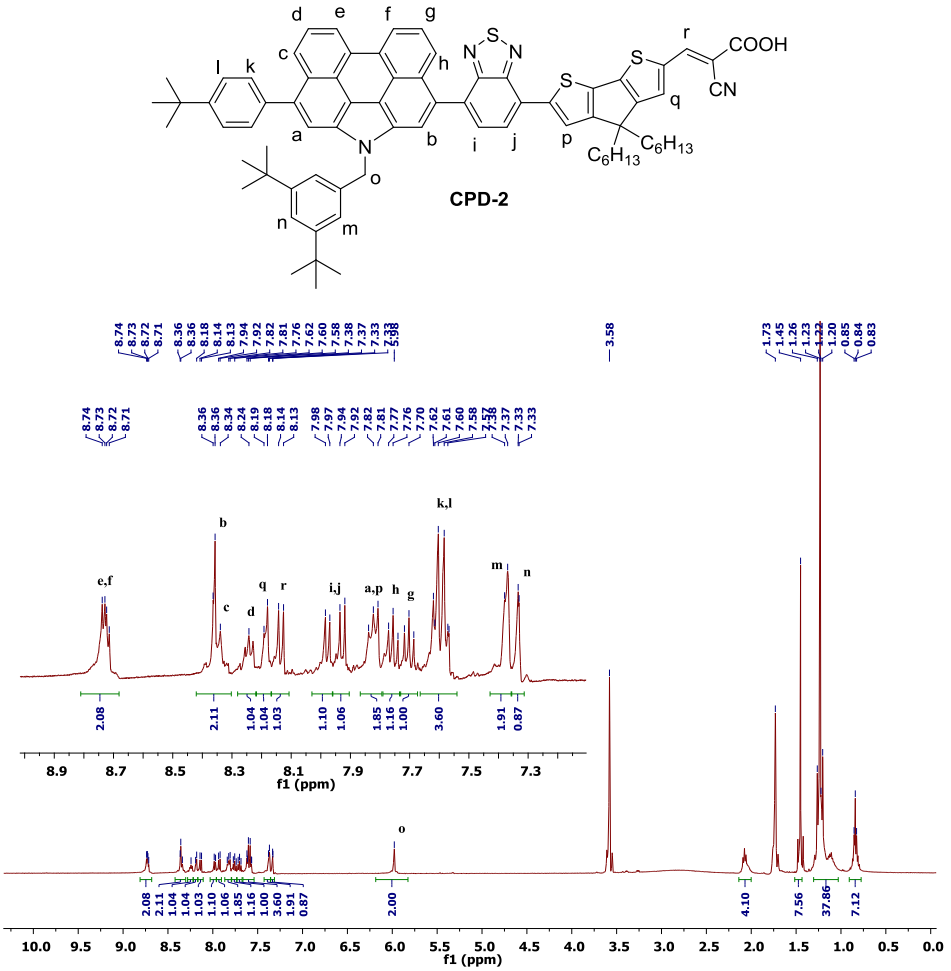


Figure S10. ^{1}H NMR spectrum (500 MHz) of compound **CPD-2** in d-THF+CS_2 at 298 K.

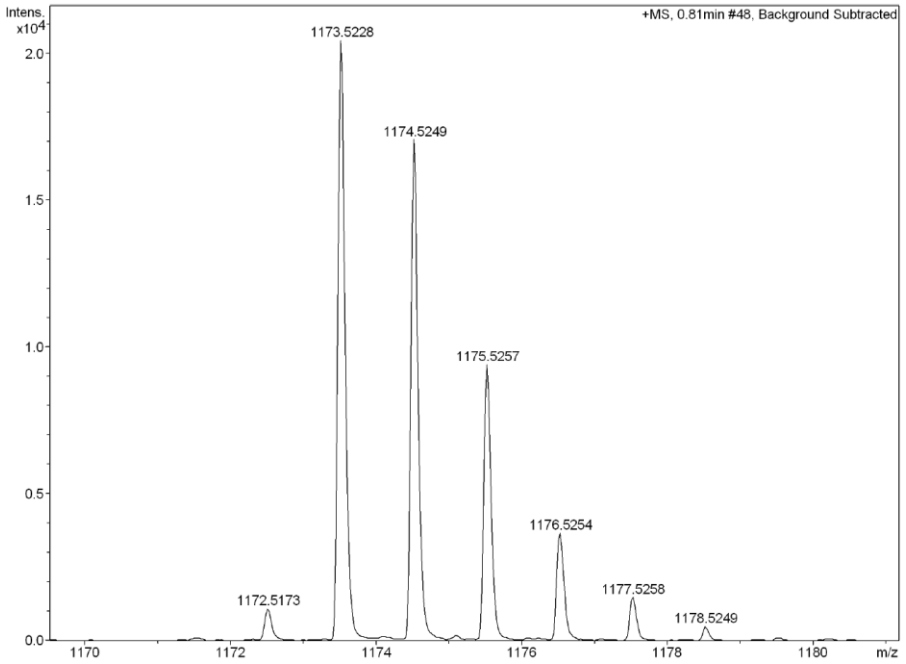


Figure S11. HRMS spectrum (APCI) of compound **CPD-2**.

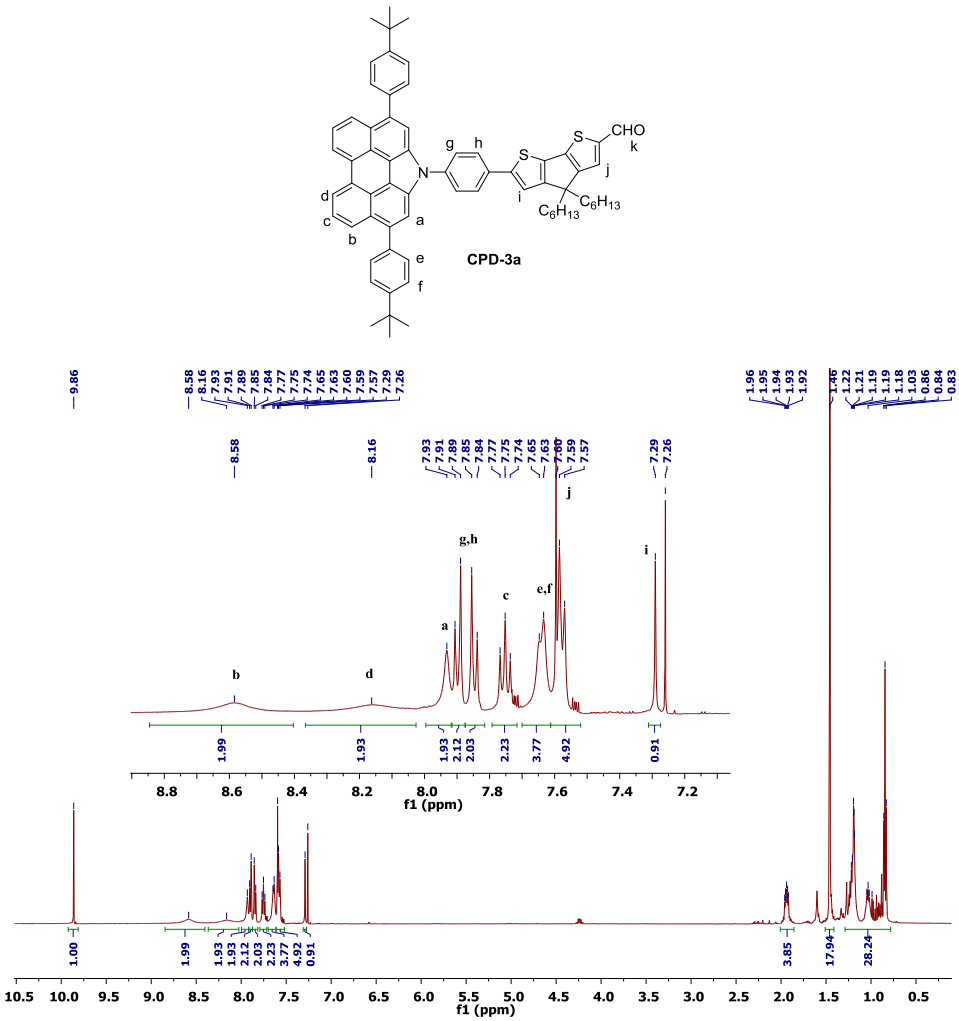


Figure S12. ^{1}H NMR spectrum (500 MHz) of compound **CPD-3a** in d-THF at 298 K.

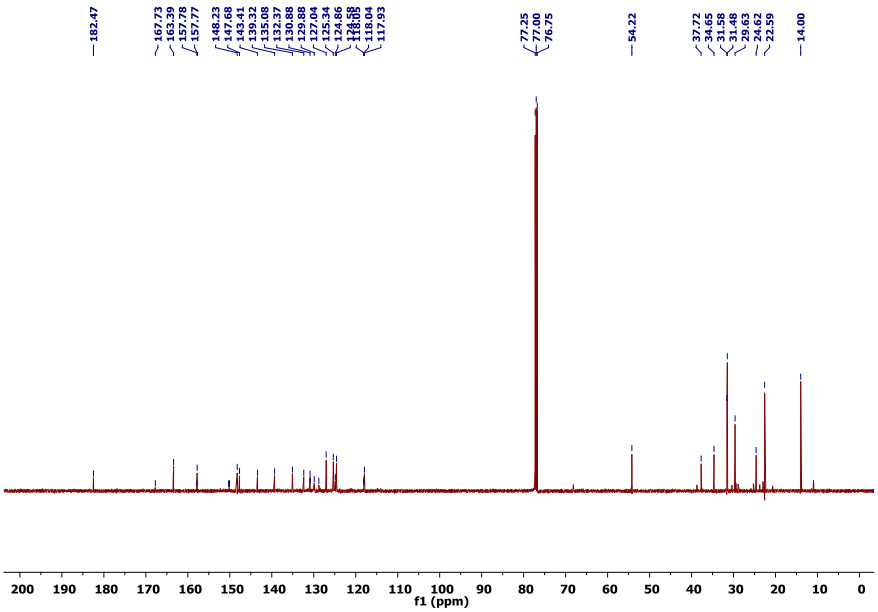


Figure S13. ^{13}C NMR spectrum (125 MHz) of compound **CPD-3a** in d-THF at 298 K.

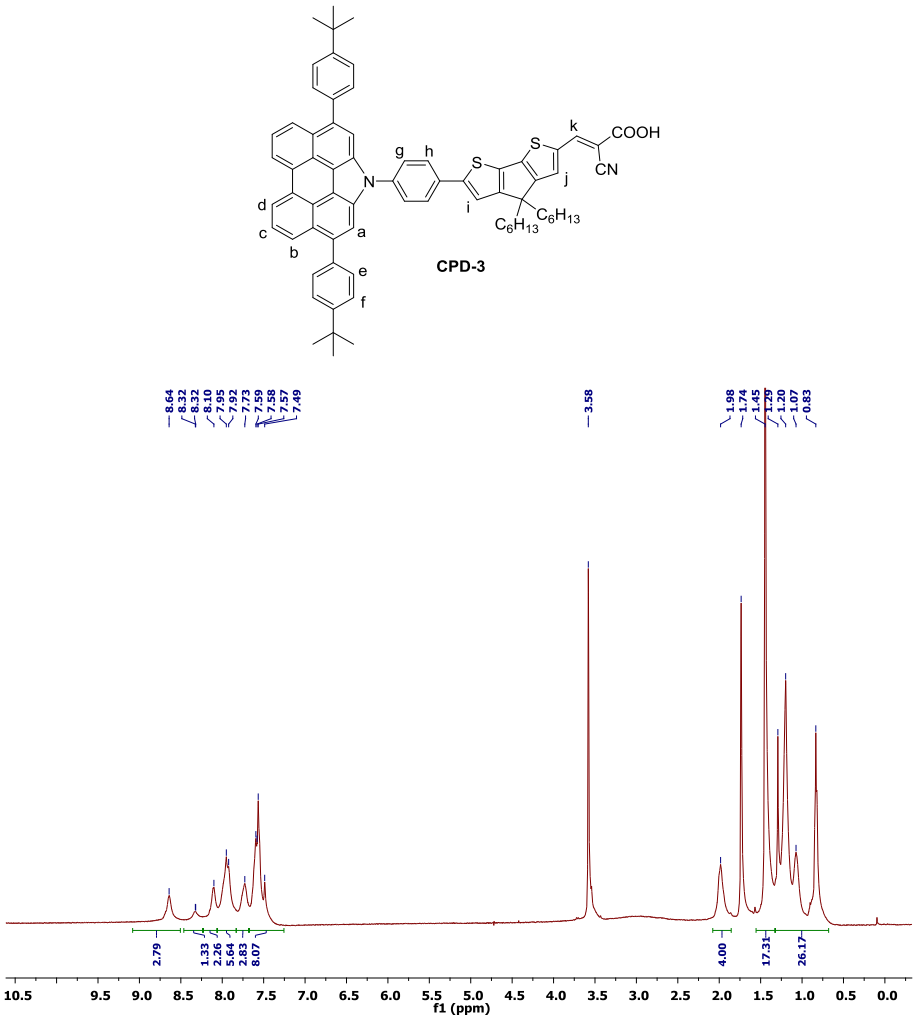


Figure S14. ^{1}H NMR spectrum (500 MHz) of compound **CPD-3** in d-THF+CS_2 at 298 K.

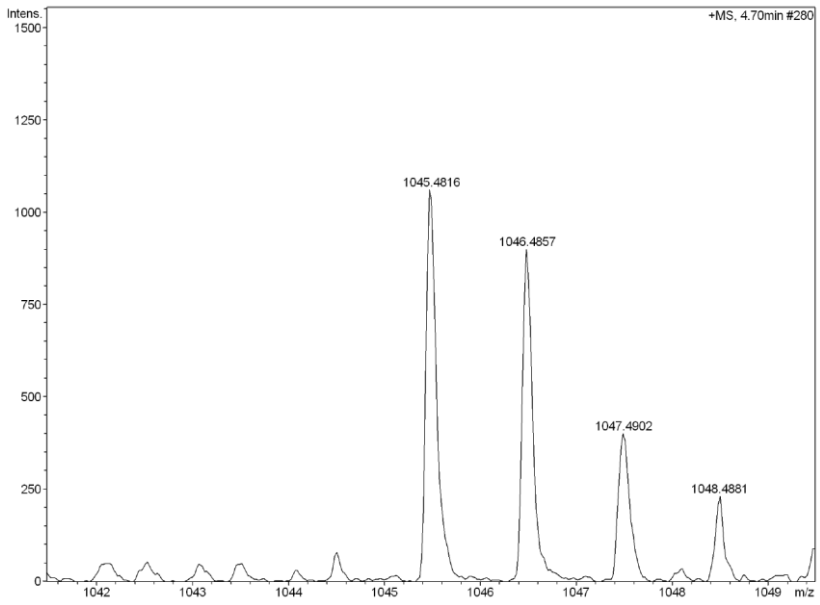


Figure S15. HRMS spectrum (APCI) of compound **CPD-3**.

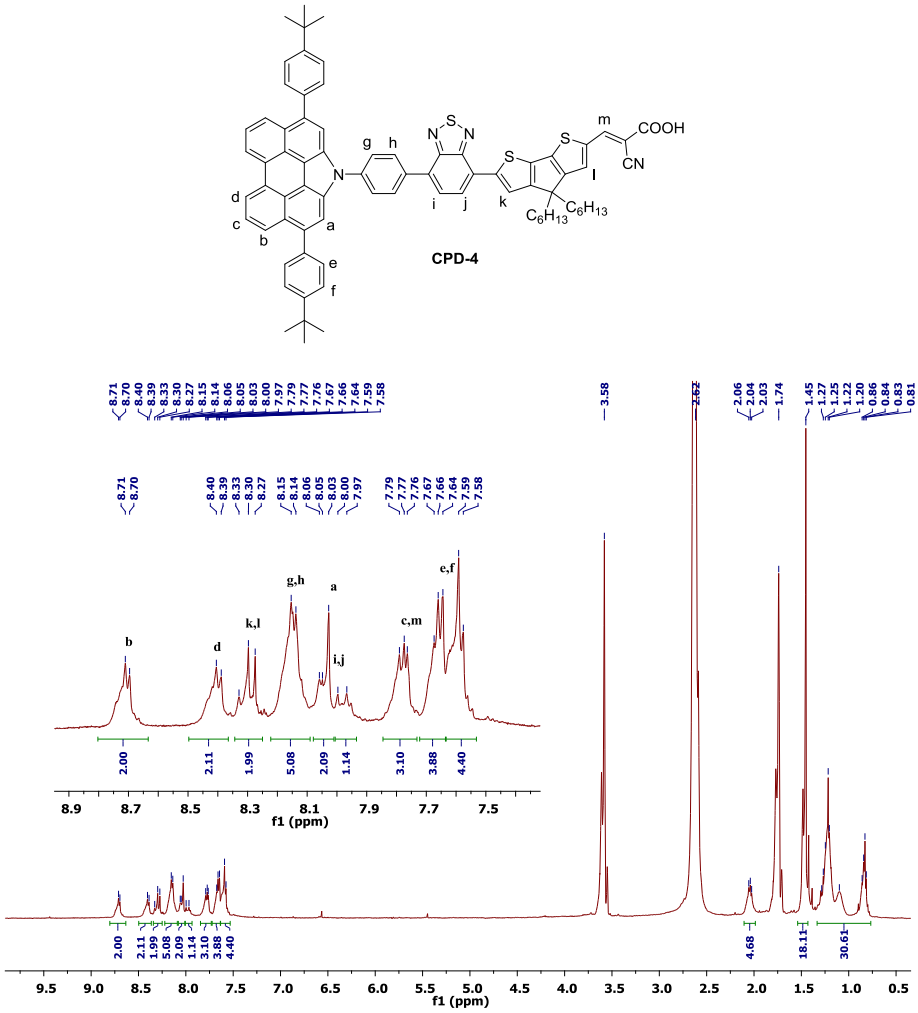


Figure S16. ^{1}H NMR spectrum (500 MHz) of compound **CPD-4** in d-THF+CS_2 at 298 K.

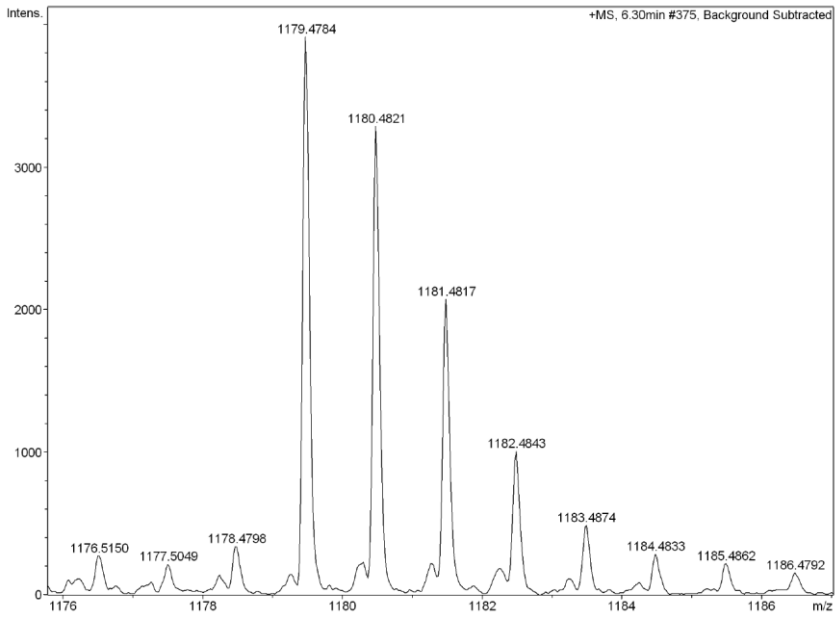


Figure S17. HRMS spectrum (APCI) of compound **CPD-4**.

8. Appendix: Cartesian coordinates of CPD-1 – CPD-4

CPD-1:

H	0.07860706	0.87799084	0.47589072
C	-0.30031659	-0.07524705	0.11951511
C	0.62097822	-1.03662546	-0.33959426
C	-2.02031250	-1.67106728	-0.26991981
C	0.20540565	-2.35973609	-0.81172684
C	-1.67354452	-0.39416219	0.15319973
C	-1.18255480	-2.66704684	-0.74781776
C	1.02858278	-3.36732850	-1.36719868
C	0.47035598	-4.57550470	-1.77108482
H	2.09121677	-3.20060748	-1.50266406
H	1.12196319	-5.33434708	-2.19639562
C	-0.90614425	-4.85772168	-1.66447658
H	-1.26704552	-5.82571032	-2.00046755
C	-1.78771174	-3.90455337	-1.15624757
H	-3.48692269	-6.07828557	-1.80499790
C	-3.99055970	-5.20701077	-1.39567264
C	-3.26843277	-4.07180361	-1.02849542
C	-6.12723150	-4.17631705	-0.74351613
C	-4.05352366	-2.99193602	-0.50218041
C	-5.39295171	-5.24034253	-1.25668139
C	-5.46482938	-2.99727699	-0.32499289
C	-3.39025498	-1.82597588	-0.15191799
H	-5.92188882	-6.13604542	-1.57178289
H	-7.20710536	-4.25375556	-0.67934156
C	-3.93838112	-0.65244503	0.34475693
C	-5.34092570	-0.64318600	0.53699982
H	-5.85969266	0.22015483	0.94074967
C	-6.08231726	-1.79033934	0.22243909
N	-2.86974039	0.24490455	0.54227902
C	-7.55028760	-1.74395457	0.46739305
C	-10.35621594	-1.58712271	0.99933313
C	-8.20545253	-2.72192219	1.22976602
C	-8.32900669	-0.68190527	-0.02265279
C	-9.69385456	-0.60875648	0.23833013
C	-9.57492219	-2.64316202	1.48759483
H	-7.63330382	-3.54510435	1.64848866
H	-7.85666731	0.08576988	-0.62996920
H	-10.25329805	0.22924889	-0.16886099
H	-10.02728550	-3.42272836	2.09072711
C	-11.86730004	-1.46774159	1.26579748
C	-12.40724954	-2.63881198	2.10854179

H	-11.92930787	-2.68727955	3.09358789
H	-12.25955585	-3.60280671	1.60846032
H	-13.48363591	-2.51215317	2.27004907
C	-12.62951002	-1.45263779	-0.08088285
H	-12.32323741	-0.61346674	-0.71430229
H	-13.70891651	-1.36212313	0.09245842
H	-12.45183426	-2.37686766	-0.64247056
C	-12.15222209	-0.15252780	2.02949280
H	-11.82599347	0.72633461	1.46352852
H	-11.63268682	-0.13988256	2.99447836
H	-13.22725445	-0.04651470	2.22042151
C	-2.98377758	1.59300365	1.08498730
H	-1.96110735	1.95361022	1.24263633
H	-3.45227769	1.54193643	2.07589382
C	-3.75447489	2.56316203	0.20319285
C	-5.10681626	4.40639506	-1.36810374
C	-4.68508733	3.42509262	0.77555376
C	-3.50659216	2.62617129	-1.17488319
C	-4.17861536	3.54368507	-1.98354791
C	-5.37953527	4.37140660	0.00108259
H	-2.78570217	1.93889181	-1.60346076
C	2.04418866	-0.68007587	-0.32197356
C	3.13270229	-1.42367450	0.10975337
H	3.02097212	-2.42435394	0.51121696
C	4.35346814	-0.71801238	0.03052464
C	4.20151722	0.56689188	-0.47381239
S	2.55519380	0.92680779	-0.86666500
C	5.47847506	1.20772495	-0.50978555
C	6.45244113	0.32292491	-0.02559157
C	7.72942214	0.88995868	0.00731199
H	8.62145105	0.39208015	0.36544212
C	7.75831347	2.20964751	-0.46628523
C	5.81836936	-1.01950657	0.34895145
S	6.12694913	2.73571713	-0.94858088
C	8.82205129	3.13647390	-0.61279444
H	8.56546526	4.12013506	-1.00230148
C	10.16278858	2.99487108	-0.33778063
C	10.73450972	1.79560177	0.17148543
N	11.16366951	0.79439655	0.58714972
C	11.03622892	4.16162512	-0.59721151
O	10.65851347	5.23335644	-1.03282082
O	12.33300941	3.91279500	-0.29415148
H	12.81630001	4.73436564	-0.49895583
C	6.29689260	-2.17469644	-0.58878610

H	6.07987961	-1.88074412	-1.62395159
H	5.66432968	-3.04896345	-0.37877658
C	6.04055470	-1.38891235	1.84194285
H	7.11833773	-1.50211089	2.01077413
H	5.59933576	-2.38156455	2.01256291
C	7.77067971	-2.59062788	-0.48357471
H	8.00414435	-2.91267304	0.53950210
H	8.41867805	-1.73034524	-0.69429481
C	8.12383356	-3.72868530	-1.45263913
H	7.90071703	-3.41270863	-2.48243778
H	7.47320013	-4.59321128	-1.25225214
C	9.59148094	-4.16600658	-1.36156792
H	9.81460493	-4.47728546	-0.33019312
H	10.24154762	-3.30222796	-1.56313191
C	9.95118695	-5.30693342	-2.32198706
H	9.72985645	-4.99615825	-3.35310658
H	9.30092511	-6.17006305	-2.11907233
C	11.41804136	-5.73796840	-2.22225811
H	11.66009550	-6.08796263	-1.21117261
H	12.09229382	-4.90396066	-2.45214562
H	11.64471015	-6.55235371	-2.91994080
C	5.47785169	-0.39937800	2.87134491
H	5.89185139	0.60064834	2.68498135
H	4.39059460	-0.31235705	2.74579457
C	5.79132100	-0.81319654	4.31575326
H	6.88103142	-0.89281240	4.44316407
H	5.38920566	-1.82008401	4.50360010
C	5.23004745	0.15825643	5.36204733
H	5.62630369	1.16654529	5.17059763
H	4.13898760	0.23327350	5.24084878
C	5.55192417	-0.24500390	6.80676885
H	6.64214446	-0.31771515	6.92720425
H	5.15748162	-1.25323755	6.99797917
C	4.98799039	0.72913810	7.84616605
H	5.38939654	1.73966369	7.70078222
H	5.23798477	0.41539064	8.86610435
H	3.89509674	0.79509502	7.77650442
H	-5.63093103	5.12300131	-1.98908880
H	-4.87058505	3.35959381	1.84500886
C	-3.94328824	3.64236560	-3.50311758
C	-5.27235574	3.37171389	-4.24793342
H	-5.12175456	3.44084560	-5.33214432
H	-6.04954706	4.09277068	-3.97374610
H	-5.65053800	2.36852025	-4.02080590

C	-3.43754275	5.06172855	-3.85596890
H	-3.27098188	5.14862350	-4.93658069
H	-2.49036508	5.27797247	-3.34858879
H	-4.15576539	5.83626725	-3.56705096
C	-2.89997211	2.62505603	-4.00315699
H	-2.77079092	2.73332790	-5.08587842
H	-3.21001155	1.59200533	-3.80987111
H	-1.92017918	2.78157090	-3.53786001
C	-6.39896735	5.30917131	0.67545771
C	-7.52334063	4.46638936	1.32365674
H	-8.05080943	3.87012861	0.57035181
H	-8.25542893	5.11983821	1.81375898
H	-7.13369080	3.77792341	2.08090932
C	-7.04828355	6.28829765	-0.32077636
H	-7.60378446	5.76414780	-1.10673903
H	-6.30480370	6.93556721	-0.79970593
H	-7.75713256	6.93543904	0.20794152
C	-5.68819261	6.14104551	1.76979884
H	-4.88762479	6.75304276	1.33890997
H	-5.24357320	5.50577209	2.54302940
H	-6.40215390	6.81265082	2.26180876

CPD-2:

H	1.96891791	0.27839170	-0.92713156
C	2.45694243	-0.63681488	-0.61130728
C	1.66381518	-1.69938097	-0.14584492
C	4.36021041	-2.01777603	-0.24528778
C	2.23828933	-2.96362201	0.31894244
C	3.85742908	-0.79435849	-0.66740098
C	3.65324755	-3.10374844	0.24666268
C	1.54937088	-4.06057518	0.89081629
C	2.25344396	-5.18670403	1.30337390
H	0.47430318	-4.02863954	1.03016279
H	1.70141732	-6.01493374	1.74011088
C	3.65385807	-5.29941376	1.19243646
H	4.13259925	-6.21069471	1.53951685
C	4.40858737	-4.25142904	0.66739016
H	6.36746712	-6.18905025	1.33640901
C	6.75806513	-5.26397725	0.92155487
C	5.89902407	-4.23314797	0.54128360
C	8.75038439	-3.97239851	0.27637661
C	6.54356826	-3.06645173	0.00884019
C	8.15424103	-5.11919652	0.79039224
C	7.94560608	-2.89025767	-0.15372136

C	5.73939770	-1.99787272	-0.35535166
H	8.79092366	-5.93828204	1.11461966
H	9.83179557	-3.91063010	0.22060461
C	6.13654555	-0.76283245	-0.84704778
C	7.52840310	-0.57267424	-1.02206418
H	7.93855352	0.35014386	-1.42039004
C	8.40806201	-1.61411238	-0.69670814
N	4.96428204	-0.01201995	-1.05901390
C	9.86137224	-1.37754651	-0.91947681
C	12.63290299	-0.86050485	-1.40080205
C	10.64614162	-2.25342343	-1.68331378
C	10.49203558	-0.23328916	-0.40258947
C	11.84084012	0.01491959	-0.63846632
C	11.99848059	-1.99863689	-1.91693587
H	10.18891041	-3.13608468	-2.12173490
H	9.91734744	0.45891668	0.20729219
H	12.28376063	0.90963882	-0.20895413
H	12.55478712	-2.70575243	-2.52254051
C	14.12272962	-0.55155777	-1.63383190
C	14.81388141	-1.62088897	-2.50066680
H	14.36169485	-1.69459039	-3.49628820
H	14.77557882	-2.61130150	-2.03312302
H	15.86958807	-1.36013563	-2.63569948
C	14.85410254	-0.49049711	-0.27144166
H	14.43584380	0.28271509	0.38145812
H	15.91737515	-0.26395084	-0.41810822
H	14.78058828	-1.44836929	0.25607643
C	14.26143952	0.81310731	-2.34957374
H	13.82889507	1.62851421	-1.76028536
H	13.75620241	0.79900907	-3.32206250
H	15.31915467	1.04943994	-2.51924302
C	4.91222415	1.36237332	-1.54042518
H	3.90961735	1.51325852	-1.95797345
H	5.61335663	1.45984334	-2.37715639
C	5.21183779	2.42125182	-0.48890007
C	5.68704927	4.41725330	1.37194040
C	6.04680449	3.49356017	-0.80889869
C	4.62236694	2.35284444	0.77679474
C	4.85148272	3.34864979	1.73224556
C	6.29903339	4.51670359	0.11548549
H	3.98354065	1.50882128	1.00988481
C	-4.18305263	-1.01896588	-0.41109495
C	-4.99835329	0.00573174	0.05629973
H	-4.58954056	0.85558175	0.58565283

C	-6.36156134	-0.19755239	-0.23548002
C	-6.59657240	-1.37558139	-0.93264385
S	-5.14602098	-2.26252060	-1.24166088
C	-7.99541293	-1.49329000	-1.19491783
C	-8.65765074	-0.37741571	-0.66322757
C	-10.04226005	-0.43307806	-0.84731023
H	-10.74534526	0.31193434	-0.49775030
C	-10.45962294	-1.58074520	-1.53608835
C	-7.65769270	0.58261330	-0.01359679
S	-9.06533582	-2.60899852	-1.94311045
C	-11.74715595	-2.02453557	-1.93715809
H	-11.79709399	-2.97874944	-2.45878554
C	-12.97641581	-1.43088627	-1.77204479
C	-13.15951977	-0.17524828	-1.12784054
N	-13.26724708	0.85612616	-0.59515397
C	-14.15622691	-2.15136057	-2.30494542
O	-14.11802603	-3.22620064	-2.87361073
O	-15.31095348	-1.47723866	-2.09088423
H	-16.01738114	-2.02898489	-2.47448677
C	-7.55179623	1.93202156	-0.79514813
H	-7.29180288	1.69706808	-1.83548651
H	-6.69463794	2.48201606	-0.38227130
C	-7.95793760	0.82842382	1.49126495
H	-8.93397964	1.32303108	1.57084959
H	-7.21817358	1.54831028	1.86953286
C	-8.78433657	2.84652746	-0.78372732
H	-9.03228135	3.14372237	0.24342447
H	-9.65722470	2.30567341	-1.17110561
C	-8.56961787	4.11098693	-1.62913744
H	-8.32280055	3.81845973	-2.66043657
H	-7.69326230	4.65843164	-1.25092581
C	-9.78544800	5.04614132	-1.64506700
H	-10.02791485	5.34744495	-0.61516007
H	-10.66320420	4.49509329	-2.01302785
C	-9.57850393	6.30070146	-2.50367357
H	-9.33321651	5.99817221	-3.53178944
H	-8.70334858	6.85367634	-2.13307980
C	-10.79828722	7.22743910	-2.52213080
H	-11.04847879	7.57426378	-1.51190496
H	-11.68070542	6.71259340	-2.92127648
H	-10.61928984	8.11263723	-3.14322821
C	-7.95581534	-0.42063537	2.38274488
H	-8.67183639	-1.15414081	1.98831246
H	-6.96910784	-0.90039904	2.34325243

C	-8.30900517	-0.11090106	3.84408996
H	-9.30004218	0.36459830	3.88750269
H	-7.59896873	0.62798771	4.24482990
C	-8.30437111	-1.35575837	4.74040646
H	-9.01036796	-2.09598608	4.33541493
H	-7.31215339	-1.82948851	4.69882924
C	-8.66321430	-1.06363063	6.20311430
H	-9.65554033	-0.59257274	6.24531232
H	-7.95827188	-0.32377646	6.60860663
C	-8.65439355	-2.31492385	7.08712802
H	-9.37413842	-3.05987856	6.72602985
H	-8.91578356	-2.07472110	8.12401692
H	-7.66490215	-2.78867065	7.09406580
C	0.19519771	-1.51733214	-0.17279945
C	-2.73992437	-1.16827636	-0.30996894
C	-0.44492940	-0.33549822	0.34498448
C	-0.66444660	-2.45388877	-0.72073608
C	-2.06839644	-2.28614505	-0.78611682
C	-1.89312568	-0.15993809	0.28435920
H	-0.24433643	-3.35758087	-1.15034297
H	-2.63683110	-3.08671837	-1.25130230
N	0.18396828	0.68772455	0.93546696
N	-2.30522752	0.99089205	0.82470906
S	-0.96600334	1.77471588	1.36650309
H	5.87077580	5.20026529	2.10176414
H	6.50011498	3.52309604	-1.79482032
C	7.21054491	5.71841662	-0.20087475
C	8.37934595	5.76431423	0.81181267
H	8.02374984	5.86695413	1.84223680
H	9.03473737	6.61781051	0.59919082
H	8.98194638	4.85055615	0.75618681
C	6.39094254	7.02669153	-0.09588105
H	5.96766963	7.16326091	0.90468567
H	5.56103195	7.02815783	-0.81181606
H	7.02712519	7.89415439	-0.31052288
C	7.81059666	5.64307570	-1.61781407
H	7.03435291	5.64202020	-2.39155444
H	8.42939479	4.74837049	-1.75226115
H	8.44977616	6.51532030	-1.79478714
C	4.21565600	3.31024367	3.13551303
C	5.32757313	3.35083123	4.21069832
H	4.88628635	3.32467934	5.21440586
H	5.93597335	4.25854998	4.13961991
H	5.99812902	2.48964536	4.11247117

C	3.29006563	4.53791421	3.31027868
H	2.83505255	4.53403735	4.30836852
H	2.48259367	4.52883191	2.56898137
H	3.83669169	5.48012297	3.19619371
C	3.37824312	2.03732338	3.36604301
H	2.95187309	2.05696044	4.37551271
H	3.98696139	1.12995044	3.28314817
H	2.54666408	1.95095086	2.65771554

CPD-3:

H	3.28909471	3.09841080	-0.18951990
C	4.29112144	2.69081876	-0.10741287
C	5.37338485	3.57991393	-0.05573779
C	5.86522806	0.90506881	-0.06184360
C	6.75706985	3.12219869	0.01467723
C	4.53825916	1.29700627	-0.09669788
C	6.98768963	1.71846412	-0.00480543
C	7.91352196	3.93193386	0.12821990
C	9.17058087	3.34145700	0.17647979
H	7.82602266	5.01148396	0.18654354
H	10.04545273	3.98056057	0.26359698
C	9.36348572	1.94521860	0.12289400
H	10.37793856	1.55841593	0.16212682
C	8.27362252	1.08098746	0.03567362
H	10.49584840	-0.67483563	0.03904900
C	9.52570548	-1.16195253	-0.00315577
C	8.35096940	-0.41220179	-0.00812089
C	8.28817479	-3.28427632	-0.12159799
C	7.13665351	-1.17610539	-0.07127956
C	9.47911608	-2.57011500	-0.06866295
C	7.05046799	-2.59573791	-0.10519117
C	5.93738392	-0.47962824	-0.11199969
H	10.41805157	-3.11751917	-0.08281156
H	8.31485533	-4.36666089	-0.18469388
C	4.65843260	-1.00294493	-0.19004940
C	4.55212951	-2.41439666	-0.19279044
H	3.59228681	-2.92005188	-0.19287142
C	5.71852452	-3.19056389	-0.14745864
N	3.76576074	0.10477472	-0.17942671
C	5.55373513	-4.67056172	-0.13503653
C	5.14742463	-7.50170590	-0.08286502
C	6.13858896	-5.47486724	0.85375909
C	4.75907139	-5.31348887	-1.09892999
C	4.56327191	-6.69075410	-1.07071992

C	5.93896897	-6.85620761	0.87684815
H	6.73995509	-5.01268386	1.63163924
H	4.30448908	-4.72320238	-1.89040119
H	3.94524932	-7.14052031	-1.84324533
H	6.40791632	-7.42702788	1.67090187
C	4.90421545	-9.02143316	-0.08872009
C	5.62272306	-9.73402256	1.07284069
H	5.27778473	-9.37325528	2.04859016
H	6.70957444	-9.60186170	1.02365684
H	5.41884710	-10.80977021	1.02810754
C	5.42363409	-9.62166600	-1.41692427
H	4.91976560	-9.18614535	-2.28611788
H	5.25101566	-10.70470440	-1.43946498
H	6.49935413	-9.44643774	-1.53216894
C	3.38790334	-9.30135628	0.04033776
H	2.81886214	-8.85450848	-0.78161824
H	2.99311461	-8.89662147	0.97920653
H	3.19778169	-10.38160994	0.02879739
C	-1.92671784	-0.14633947	-0.47895366
C	-2.84430633	0.25110580	0.48126283
H	-2.54094704	0.63341828	1.44964134
C	-4.18370365	0.06279943	0.07840901
C	-4.28897913	-0.47642631	-1.19640589
S	-2.74469289	-0.75610168	-1.92433526
C	-5.67208477	-0.63536627	-1.52364977
C	-6.45198816	-0.18882959	-0.44836602
C	-7.82321474	-0.34538648	-0.67341460
H	-8.60209792	-0.08677465	0.03238645
C	-8.11415475	-0.89781027	-1.92824365
C	-5.56178381	0.33384354	0.68188734
S	-6.61540862	-1.23144565	-2.82823489
C	-9.34705947	-1.21584839	-2.55697104
H	-9.29237112	-1.65478957	-3.55171134
C	-10.63516532	-1.05627605	-2.10393086
C	-10.95487887	-0.49577243	-0.83547379
N	-11.17422363	-0.03024043	0.21057604
C	-11.73035622	-1.49396617	-3.00095944
O	-11.57385326	-1.98261805	-4.10399880
O	-12.95345100	-1.29074285	-2.45689714
H	-13.59612788	-1.60775995	-3.11802978
C	-5.71033841	1.87811829	0.87498731
H	-5.49010204	2.35946863	-0.08671996
H	-4.91757576	2.19796543	1.56616833
C	-5.78791987	-0.41902068	2.02171551

H	-6.81636294	-0.22942170	2.35271188
H	-5.13473461	0.03912950	2.77850286
C	-7.05998265	2.39262735	1.39390290
H	-7.28544963	1.95500999	2.37496855
H	-7.86639502	2.07717862	0.71957165
C	-7.08531543	3.92357409	1.51625357
H	-6.86827274	4.36974862	0.53447956
H	-6.27348588	4.24927068	2.18392700
C	-8.42096579	4.46856787	2.03782309
H	-8.63663388	4.02403927	3.02075507
H	-9.23294055	4.13938831	1.37313933
C	-8.45233341	5.99778305	2.15708127
H	-8.23849849	6.44186140	1.17437151
H	-7.64028351	6.32633343	2.82166020
C	-9.78886305	6.53423897	2.67966529
H	-10.01371845	6.13494939	3.67633728
H	-10.61559307	6.25049577	2.01706853
H	-9.78033864	7.62777444	2.75288893
C	-5.54640835	-1.93419084	1.99344896
H	-6.18964340	-2.39555244	1.23217249
H	-4.51150082	-2.14000389	1.69000484
C	-5.81728566	-2.59536295	3.35205124
H	-6.85429140	-2.39053547	3.65653810
H	-5.17846784	-2.13008425	4.11782792
C	-5.58071211	-4.11097128	3.34977398
H	-6.22162238	-4.57767496	2.58706523
H	-4.54447961	-4.31752742	3.04281038
C	-5.84675242	-4.77342538	4.70778833
H	-6.88188096	-4.56669921	5.01433908
H	-5.20555643	-4.30713252	5.46953027
C	-5.60963386	-6.28696233	4.69785593
H	-6.26417225	-6.78577835	3.97252966
H	-5.80465092	-6.72955835	5.68134775
H	-4.57374834	-6.52417180	4.42518924
C	2.35740413	0.03504530	-0.25395453
C	-0.46634735	-0.09386125	-0.41176606
C	1.56067720	0.87358192	0.53961703
C	1.73361787	-0.86845153	-1.12589694
C	0.34728369	-0.93806624	-1.19066483
C	0.17600863	0.81838221	0.44827666
H	2.03203714	1.56296766	1.23201705
H	2.33891249	-1.50636539	-1.76106334
H	-0.11012078	-1.66384818	-1.85730291
H	-0.41853066	1.49948720	1.04913022

C	5.06351560	5.03647985	-0.08280075
C	4.38750852	7.81477356	-0.16536810
C	5.63436152	5.89901185	-1.03497098
C	4.14982601	5.59450696	0.82117037
C	3.82084881	6.95056028	0.78028579
C	5.30170319	7.24951585	-1.07184913
H	6.32933821	5.49993394	-1.76857886
H	3.70186703	4.95992526	1.58162555
H	3.11301312	7.32786774	1.51040565
H	5.76182265	7.87256559	-1.83435541
C	4.04867827	9.31410522	-0.24288529
C	5.34084992	10.14615707	-0.06377839
H	5.11425247	11.21785668	-0.12007004
H	6.08160435	9.92164987	-0.83824192
H	5.80353494	9.94676319	0.90952233
C	3.42514184	9.62894552	-1.62356842
H	3.18890277	10.69735545	-1.70158896
H	2.49789652	9.06401574	-1.77293402
H	4.10487821	9.37735064	-2.44437623
C	3.04775351	9.74479227	0.84599497
H	2.84038468	10.81682817	0.75349581
H	3.44176018	9.57061326	1.85380424
H	2.09251098	9.21533254	0.75532319

CPD-4:

H	-5.51709997	-2.88464958	-0.03047220
C	-6.49577726	-2.41890609	0.01694944
C	-7.63125066	-3.24045543	0.03617761
C	-7.96022740	-0.54106054	-0.00497122
C	-8.98654038	-2.69903634	0.06432871
C	-6.65897224	-1.01282582	0.01122275
C	-9.13117500	-1.28442973	0.02791639
C	-10.19292888	-3.43581596	0.15428469
C	-11.41264063	-2.76967882	0.16615082
H	-10.17286057	-4.51802719	0.22402558
H	-12.32671464	-3.35383430	0.23494702
C	-11.51872427	-1.36481932	0.10054341
H	-12.50814152	-0.91628692	0.11222400
C	-10.37613084	-0.56928390	0.03603456
H	-12.48394076	1.32110713	0.06854477
C	-11.48576467	1.74748052	0.02167050
C	-10.36028018	0.92597737	-0.00642205
C	-10.11783513	3.79034843	-0.04795978
C	-9.10108312	1.61327820	-0.06870413

C	-11.35068562	3.15130800	0.00670334
C	-8.92714558	3.02491408	-0.10191357
C	-7.94600656	0.84467233	-0.06819443
H	-12.25217187	3.75717405	0.04858220
H	-10.07562240	4.87401810	-0.03459816
C	-6.63506375	1.28849248	-0.09484930
C	-6.44267861	2.69037844	-0.12171597
H	-5.45383440	3.13556806	-0.15218447
C	-7.56037668	3.53588466	-0.13959011
N	-5.81332620	0.12889741	-0.04894321
C	-7.30900923	5.00290777	-0.19497652
C	-6.75882608	7.80682765	-0.32312170
C	-6.44950584	5.62220939	0.72244064
C	-7.88623107	5.81603559	-1.18598393
C	-7.61568724	7.17953771	-1.24466019
C	-6.18164462	6.99095318	0.65853915
H	-5.99757969	5.02633492	1.51126892
H	-8.53831709	5.36824802	-1.93075502
H	-8.08096396	7.76352534	-2.03438280
H	-5.51554657	7.41757302	1.40064455
C	-6.49360181	9.31951950	-0.42171177
C	-5.54646291	9.82104353	0.68496050
H	-4.56219980	9.34217120	0.62866809
H	-5.95760807	9.64216405	1.68496885
H	-5.39410807	10.90109001	0.57882915
C	-7.83090040	10.08715820	-0.29336024
H	-8.54017852	9.80541836	-1.07857685
H	-7.65951058	11.16782101	-0.37134864
H	-8.30648125	9.88700352	0.67357178
C	-5.84853818	9.64156201	-1.79090226
H	-6.49400102	9.34617093	-2.62462592
H	-4.89284799	9.11756001	-1.90656319
H	-5.65919237	10.71837082	-1.88004378
C	4.30947660	0.35047287	-0.26356841
C	5.27251585	-0.59109235	0.08030508
H	4.99897114	-1.57362572	0.43998713
C	6.58915138	-0.12096450	-0.09285600
C	6.63989635	1.17795593	-0.58234189
S	5.06951205	1.85220360	-0.83608790
C	8.00582237	1.56659338	-0.73670020
C	8.83236665	0.50487295	-0.34286515
C	10.19223460	0.81931210	-0.42884138
H	11.00193934	0.15537610	-0.15439234
C	10.42665149	2.11667413	-0.90465953

C	7.99233502	-0.69963036	0.09014360
S	8.89072363	2.95135346	-1.23490340
C	11.63102340	2.82871200	-1.15039320
H	11.53203699	3.85020987	-1.51351677
C	12.93757627	2.42890476	-1.00200805
C	13.31370694	1.13287441	-0.54996368
N	13.58050043	0.06079333	-0.17796086
C	13.99254350	3.41337476	-1.34112072
O	13.78708736	4.54478536	-1.73767127
O	15.23801412	2.91455586	-1.16100830
H	15.85195578	3.63036651	-1.40876998
C	8.15403984	-1.90880712	-0.88685362
H	7.91830741	-1.55699637	-1.89954523
H	7.37853333	-2.64332570	-0.62883738
C	8.27453874	-1.12515210	1.55831656
H	9.32136739	-1.44535688	1.62791409
H	7.66697658	-2.01597618	1.77276910
C	9.51863514	-2.61132871	-0.90345624
H	9.74608568	-3.02319597	0.08814623
H	10.31240149	-1.88794065	-1.12979480
C	9.57426178	-3.74773182	-1.93563983
H	9.37321025	-3.33967696	-2.93703639
H	8.76592501	-4.46586435	-1.73190346
C	10.91858900	-4.48660706	-1.94740089
H	11.11409756	-4.89979701	-0.94673618
H	11.72779839	-3.76740987	-2.14055771
C	10.98690208	-5.61681670	-2.98285944
H	10.79962705	-5.20262104	-3.98380594
H	10.17361068	-6.33201526	-2.79308467
C	12.32858559	-6.35652956	-2.97910513
H	12.52676343	-6.81198749	-2.00102917
H	13.15825101	-5.67351588	-3.19851003
H	12.34724999	-7.15574717	-3.72887875
C	8.00727116	-0.05739127	2.62773735
H	8.58844769	0.84599734	2.39852363
H	6.95059653	0.23935520	2.59819295
C	8.35974839	-0.53700678	4.04249650
H	9.42032295	-0.82692061	4.07566853
H	7.78818071	-1.44859867	4.27286199
C	8.08887145	0.51662018	5.12410762
H	8.65716215	1.42953197	4.89174873
H	7.02739465	0.80459084	5.09347952
C	8.44442009	0.04735888	6.54076389
H	9.50511106	-0.23966946	6.57128186

H	7.87640398	-0.86481186	6.77342211
C	8.17114952	1.10601892	7.61399874
H	8.75507714	2.01634412	7.43071804
H	8.43182366	0.73927167	8.61335887
H	7.11186441	1.39088990	7.62951978
C	-4.40035287	0.11328738	-0.06584647
C	-1.57033258	0.07424573	-0.10284675
C	-3.68826727	-0.74242158	0.78525852
C	-3.69131632	0.94775556	-0.94113549
C	-2.30194984	0.92872671	-0.94981716
C	-2.29848442	-0.76845271	0.75775477
H	-4.22804673	-1.36990987	1.48682737
H	-4.23255884	1.58156481	-1.63576966
H	-1.77559403	1.55682619	-1.66227802
H	-1.77036043	-1.43758354	1.42537291
C	-7.41225399	-4.71325534	0.01528319
C	-6.91544143	-7.52899854	-0.05848593
C	-8.02049074	-5.53733460	-0.94791251
C	-6.55157910	-5.32865128	0.93414469
C	-6.30935711	-6.70316886	0.89706340
C	-7.77585930	-6.90640679	-0.97971872
H	-8.67480979	-5.09393779	-1.69324061
H	-6.07643514	-4.72384309	1.70226912
H	-5.63904898	-7.12565244	1.63773920
H	-8.26330526	-7.49957575	-1.74883077
C	-6.67858466	-9.04795150	-0.13036422
C	-8.02476274	-9.78848119	0.05271208
H	-7.87432775	-10.87361793	-0.00487005
H	-8.75039731	-9.51128550	-0.71904745
H	-8.46951018	-9.55805758	1.02753400
C	-6.07859254	-9.41202222	-1.50963503
H	-5.90784493	-10.49345779	-1.57739028
H	-5.11944509	-8.90532077	-1.66590392
H	-6.74331399	-9.12807079	-2.33222154
C	-5.70840961	-9.54146221	0.95963442
H	-5.57089439	-10.62486240	0.86841619
H	-6.09099804	-9.34116126	1.96691490
H	-4.72094242	-9.07467310	0.86907611
C	-0.09357122	0.10161382	-0.11806203
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C	0.72112765	-1.06101523	0.12130333
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C	2.02425178	1.33519733	-0.42154057
C	2.17870778	-0.99340307	0.07779146

H	0.06138176	2.18713206	-0.53074518
H	2.46237372	2.30970963	-0.61760982
N	0.26128392	-2.29083762	0.37831699
N	2.76543462	-2.17150302	0.30837405
S	1.56644447	-3.26710818	0.55514447