High-Yield and Sustainable Synthesis of Quinoidal Compounds Assisted by Keto-Enol Tautomerism

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1. General methods and materials

^{1}H NMR and ^{13}C NMR spectra were measured on a Bruker 400 MHz spectrometer in chloroform-*d* ($CDCl_3$) or dimethyl sulfoxide-d_6 (DMSO-d_6) with tetramethylsilane (TMS) as internal standard at room temperature. The NMR spectra of compound **4** were measured using Low Pressure/Vacuum (LPV) NMR tube under argon. Multiplicities are reported as follows: singlet (s), doublet (d), doublet of doublets (dd), triplet (t), and multiplet (m). Matrix-assisted laser desorption ionization time-of-light (MALDI-TOF) mass spectra were recorded on a Bruker/AutoflexIII Smartbean MALDI mass spectrometer with 2-[(2*E*)-3-(4-tert-buthylphenyl)-2-methylprop-2-enylodene]malononitrile (DCTB) or 2-5-dihydroxybenzoic acid (DHB) as the matrix in a reflection mode. UV-*vis*-NIR absorption spectra were measured on a Shimadzu UV-3600 plus spectrometer. Solution spectra were measured in toluene and thin-films were prepared by spin-casting from their toluene solutions (5 mg/mL) on the quartz substrates. Optical bandgap were calculated from the onset of thin-film absorption spectrum according to the equation: $E_g = 1240/\lambda_{onset}$ eV. Cyclic voltamograms (CV) were measured using a CHI660 electrochemical analyzer with a three-electrode cell at a scan rate of 100 mV s^{-1}. Terabutylammonium hexafluorophosphate (Bu_4NPF_6, 0.1 mol L^{-1}) was used as the supporting electrolyte in anhydrous dichloromethane. A Pt disk with 2 mm diameter, a Pt wire and a saturated calomel electrode (SCE) were used as working, counter and reference electrodes, respectively. The potential was calibrated against ferrocene/ferrocenium (Fc/Fc^+) that was measured under the same conditions. The highest occupied molecular orbital energy level (E_{HOMO}) and the lowest unoccupied molecular orbital energy level (E_{LUMO}) were calculated according to the equations: E_{HOMO} = -(4.80+E_{onset}^{ox}) eV; E_{HOMO} = -(4.80+E_{onset}^{re}) eV, in which E_{onset}^{ox} and E_{onset}^{re} represent the

oxidation and reduction onset-potentials. EPR measurements were carried out at room temperature using a Bruker EMX plus 6/1 spectrometer. Cross-polarized optical microscope images were obtained with Nikon ECLIPSE Ci-POL polarized optical microscopes.

Geometry optimizations and frequency calculations were carried out using the B3LYP[1-2] functional and a mixed basis set of SDD[3-4] for Pd and Br and 6-31G(d) for other atoms. Frequency outcomes were examined to confirm stationary points as minima (no imaginary frequencies) or transition states (only one imaginary frequency). Because the M06-L[5-6] functional includes noncovalent interactions and can give more accurate energies for transition-metal systems, the energy were then refined by single-point calculations with M06-L and a mixed basis set of SDD for Pd and Br and 6-31++G(d,p) for other atoms, in which solvation energy corrections were calculated using the SMD[7] model in 1,4-dioxane. The combined use of two DFT functional has been successfully applied to investigate various catalytic reactions.[8-17] Free energies (kcal/mol) obtained in solution were discussed. All of the calculations were performed with Gaussian 09[18].

Chemical reagents were purchased from Energy Chemical, Innochem or Aldrich, and used as received. All air and water sensitive reactions were performed under argon atmosphere. Tetrahydrofuran (THF) and toluene were distilled in standard method prior to use. Compounds **S1**[19], **S3**[20] and **S5**[21] were prepared according to the references. Compounds **1a-1b** was purchased from Innochem, and compounds **S7**, **2e**, and **2f** were purchased from SunaTech Inc.

2. Organic field-effect transistor (OFET) devices fabrication and measurements

Top-gate and bottom-contact (TGBC) configuration OFETs were fabricated on bare Si/SiO_2 wafers. The substrate was first cleaned with deionized water, acetone and isopropanol in an ultrasonic bath and then dried under a nitrogen flow, followed by heating at 120 °C for 10 min. Gold source/drain electrodes were prepared by vacuum deposition through shadow mask to give a defined channel length (L = 50 μm) and channel width (W = 5.6 mm). Subsequently, the active layers were deposited by spin-coating 5 mg/mL chloroform solution in an argon filled glove-box with 2000 rpm for 40 s, followed by annealing at 120 °C for 10 min. As the gate dielectric, CYTOP (Asahi Glass, type CTL-809M) was spin-cast at 2000 rpm for 120 s and annealed at 100 °C for 40 min. Finally, Al (~80 nm) was vacuum-evaporated as the gate electrode. OTFT devices were measured under ambient conditions with Keysight B1500A source/measure units. The mobility was extracted from the saturation region by using the equation of: $I_{DS} = (\mu C_i W/2L)(V_{GS}-V_T)^2$, where W/L is the channel width/length, I_{DS} is the drain-source current, μ is the field-effect mobility, C_i is the capacitance per unit area of the gate dielectric layer, V_{GS} and V_T are the gate voltage and threshold voltage, respectively.

3. Single crystal OFET devices fabrication and measurements

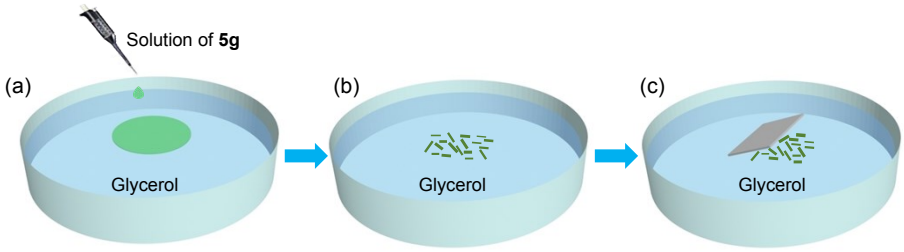


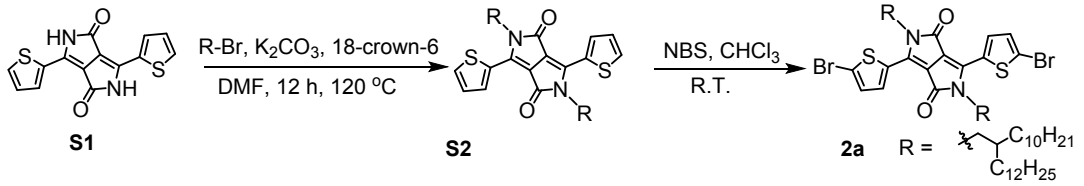
Figure S1. Schematic showing the growth and transfer of micro-wires.

Glass weighing bottles (75 mm×35 mm) were cleaned twice by ethanol and were used as the

containers to grow micro-wires of **5g**. 25 mL of glycerol was added into the glass weighing bottles as a liquid substrate. 50 μL of **5g** solution (0.2 mg mL^{-1} in toluene) was slowly dropped on the glycerol surface (Figure S1a) and then the glass weighing bottles were placed in a cabinet with constant temperature and humidity (temperature: 15°C, humidity: 30%). Micro-wires gradually appeared on the surface of glycerol. After the solvent evaporated completely, micro-wires of **5g** floating on the surface of glycerol were obtained (Figure S1b). SiO_2 (300 nm)/Si wafers were used as the substrates for OFET devices fabrication. They were cleaned by sonification with deionized water, acetone and isopropanol for 10 min successively. Then the substrates were treated with oxygen plasma at 80 W for 15 min followed by modification with octadecyltrichlorosilane (OTS) by a vapor phase method. The OTS modified SiO_2/Si substrates were cleaned by sonification in chloroform, n-hexane and isopropanol, successively. The micro-wires of **5g** floating on the surface of glycerol were transferred to the OTS modified SiO_2/Si substrates by dipping the substrate up-side-down and fishing the micro-wires out (Figure S1c). The SiO_2/Si substrate with micro-wires was gently rinsed by DI water to remove excess glycerol and dried. Bottom-gate/top-contact devices were fabricated on the SiO_2/Si substrate by stamping Au (80 nm) stripes on the micro-wires of **5g** as the source and drain electrodes. The OFET devices were measured using a Keithley 4200 SCS in ambient environment at room temperature. The mobility was extracted from the saturation region by using the equation of: $I_{DS} = (\mu C_i W/2L)(V_{GS}-V_T)^2$, where I_{DS} is the drain-source current, μ is the mobility, C_i is the capacitance per unit area of the gate dielectric layer, V_{GS} and V_T are the gate voltage and threshold voltage, L and W are the channel length and width basing on an individual micro-wire in OFET devices, respectively.

4. Synthetic procedures

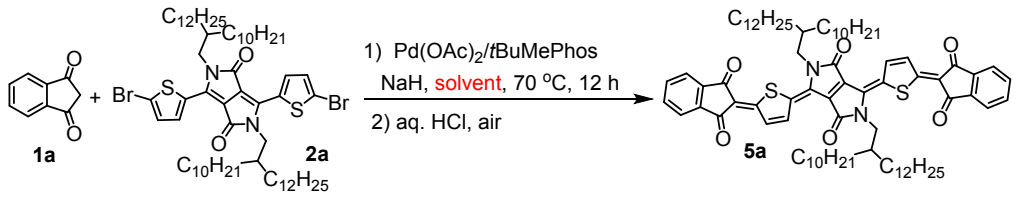
Synthesis of compound 2a



Compound S2: Compound **S1** (6.00 g, 19.98 mmol), anhydrous potassium carbonate (15.84 g, 59.93 mmol), 18-crown-6 (0.14 g, 1.00 mmol) and anhydrous DMF (200 mL) were added to a 500 mL three necked flask. The solution was stirred at 40 °C for 10 min, then 1-bromo-2-dodecyl-tetradecane (25.02 g, 59.93 mmol) was added dropwise. After stirring at 120 °C for 12 h, the solvent was removed under vacuum. The residue was dissolved in dichloromethane (CH_2Cl_2), washed with brine and dried anhydrous $MgSO_4$. After removal of the solvent, the crude product was purified by chromatography on silica gel using petroleum ether (PE)/CH_2Cl_2 = 2/1 (V/V) as the eluent, affording **S2** as a dark red solid in the yield of 33% (6.42 g). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 8.87 (dd, J_1 = 4.0 MHz, J_2 = 1.2 MHz, 2H), 7.62 (dd, J_1 = 5.2 MHz, J_2 = 1.2 MHz, 2H), 7.27 (m, 2H), 4.02 (d, J = 7.6 MHz, 4H), 1.90 (m, 2H), 1.21 (m, 80 H), 0.87 (m, 12H).

Compound 2a: To the solution of **S2** (6.40 g, 6.57 mmol) in chloroform (240 mL), *N*-bromosuccinimide (NBS) (3.51 g, 19.72 mmol) was added slowly at 0 °C. The mixture was stirred at room temperature for overnight in the absence of light. After removal of the solvent, the crude product was purified by chromatography on silica gel using PE/CH_2Cl_2 = 3/1 (V/V) as the eluent, affording compound **2a** as a dark purple solid in the yield of 80% (5.95 g). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 8.63 (d, J = 4.0 MHz, 2H), 7.22 (d, J = 4.4 MHz, 2H), 3.93 (d, J = 8.0 MHz, 2H), 1.87 (m, 2H), 1.22 (m, 80H), 0.87 (m, 12H).

Solvent screening for the synthesis of compound 5a



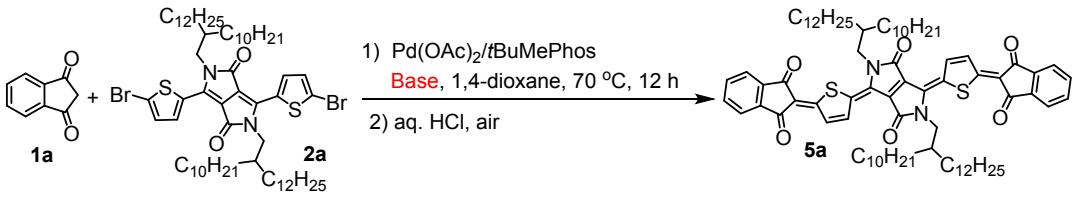
Compound **1a** (38.5 mg, 0.26 mmol), **2a** (140.8 mg, 0.12 mmol), $Pd(OAc)_2$ (0.56 mg, 2.49 μmol, 2 mol%), *t*BuMePhos (1.55 mg, 4.98 μmol, 4 mol%), sodium hydride (60% dispersion in mineral oil, 22.1 mg, 0.55 mmol) and anhydrous **solvent** (1.2 mL) were added in a schlenk tube. The mixture was stirred at 70 °C for 12 h in the absence of light, then the solvent was removed under vacuum. Subsequently, 15 mL HCl aqueous solution (0.05 M) was added, and the mixture was stirred in air for 10 min. The resulting precipitate was collected by filtration, and dissolved in CH_2Cl_2. After stirring in air for 20 min, the solution was washed with brine and dried by anhydrous $MgSO_4$. The crude product was purified by chromatography on silica gel using CH_2Cl_2 as the eluent.

Table S1: Solvent screening for the synthesis of compound 5a

Entry	Cat.	Ligand	Base	Solvent	Temp. [°C]	Time [h]	Yield [%][a]
1	$Pd(OAc)_2$	*t*BuMePhos	NaH	1,4-dioxane	70	12	40
2	$Pd(OAc)_2$	*t*BuMePhos	NaH	THF	70	12	30
3	$Pd(OAc)_2$	*t*BuMePhos	NaH	Toluene	110	12	10
4	$Pd(OAc)_2$	*t*BuMePhos	NaH	NMP	70	12	-[b]
5	$Pd(OAc)_2$	*t*BuMePhos	NaH	DMAc	70	12	-[b]
6	$Pd(OAc)_2$	*t*BuMePhos	NaH	DMAc:Dioxane (1:1)	70	12	-[b]

[a]Isolated yield for compound **5a**; [b]No product.

Base screening for the synthesis of compound 5a



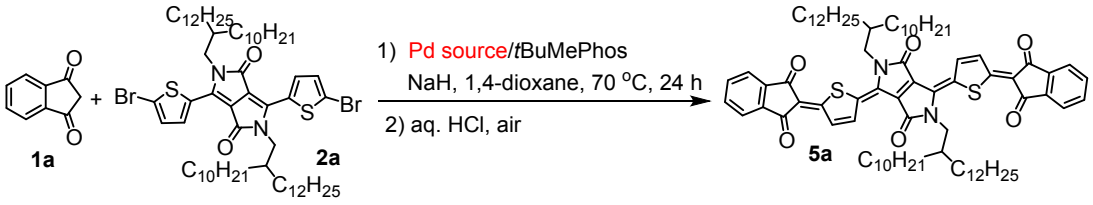
Compound **1a** (38.5 mg, 0.26 mmol), **2a** (140.8 mg, 0.12 mmol), $Pd(OAc)_2$ (0.56 mg, 2.49 μmol, 2 mol%), *t*BuMePhos (1.55 mg, 4.98 μmol, 4 mol%), **base** (0.55 mmol) and anhydrous 1,4-dioxane (1.2 mL) were added in a schlenk tube. The mixture was stirred at 70 °C for 12 h in the absence of light, then the solvent was removed under vacuum. Subsequently, 15 mL HCl aqueous solution (0.05 M) was added, and the mixture was stirred in air for 10 min. The resulting precipitate was collected by filtration, and dissolved in CH_2Cl_2. After stirring in air for 20 min, the solution was washed with brine and dried by anhydrous $MgSO_4$. The crude product was purified by chromatography on silica gel using CH_2Cl_2 as the eluent.

Table S2. Base screening for the synthesis of compound 5a.

Entry	Cat.	Ligand	Base	Solvent	Temp. [℃]	Time [h]	Yield [%][a]
1	$Pd(OAc)_2$	*t*BuMePhos	NaH	1,4-dioxane	70	12	40
2	$Pd(OAc)_2$	*t*BuMePhos	K_3PO_4	1,4-dioxane	70	12	18
3	$Pd(OAc)_2$	*t*BuMePhos	NaO^{t}Bu	1,4-dioxane	70	12	5
4	$Pd(OAc)_2$	*t*BuMePhos	NaHMDS	1,4-dioxane	70	12	-[b]
5	$Pd(OAc)_2$	*t*BuMePhos	Cs_2CO_3	1,4-dioxane	70	12	10
6	$Pd(OAc)_2$	*t*BuMePhos	Et_3N	1,4-dioxane	70	12	-[b]
7	$Pd(OAc)_2$	*t*BuMePhos	Pyridine	1,4-dioxane	70	12	-[b]

[a]Isolated yield for compound **5a**; [b]No product.

Pd source screening for the synthesis of compound 5a



Compound **1a** (38.5 mg, 0.26 mmol), **2a** (140.8 mg, 0.12 mmol), **Pd source** (2 mol%), *t*BuMePhos (1.55 mg, 4.98 μmol, 4 mol%), sodium hydride (60% dispersion in mineral oil, 22.1 mg, 0.55 mmol) and anhydrous 1,4-dioxane (1.2 mL) were added in a schlenk tube. The mixture was stirred at 70 °C for 12 h in the absence of light, then the solvent was removed under vacuum. Subsequently, 15 mL HCl aqueous solution (0.05 M) was added, and the mixture was stirred in air for 10 min. The resulting precipitate was collected by filtration, and dissolved in CH_2Cl_2. After stirring in air for 20 min, the solution was washed with brine and dried by anhydrous $MgSO_4$. The crude product was purified by chromatography on silica gel using CH_2Cl_2 as the eluent.

Table S3: Pd source screening for the synthesis of compound 5a

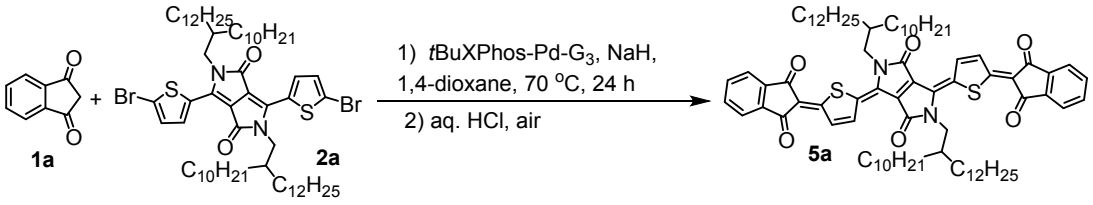
Entry	Cat.	Ligand	Base	Solvent	Temp. [℃]	Time [h]	Yield [%][a]
1	$Pd(OAc)_2$	*t*BuMePhos	NaH	1,4-dioxane	70	12	40
2	$Pd(PPh_3)_4$	*t*BuMePhos	NaH H	1,4-dioxane	70	12	-[b]
3	Herrmann	*t*BuMePhos	NaH	1,4-dioxane	70	12	11
4	$Pd_2(dba)_3$	*t*BuMePhos	NaH	1,4-dioxane	70	12	17

[a]Isolated yield for compound **5a**; [b]No product.

General procedure for the synthesis of compounds 5a-5h with *t*BuXPhos-Pd-G3 as catalyst

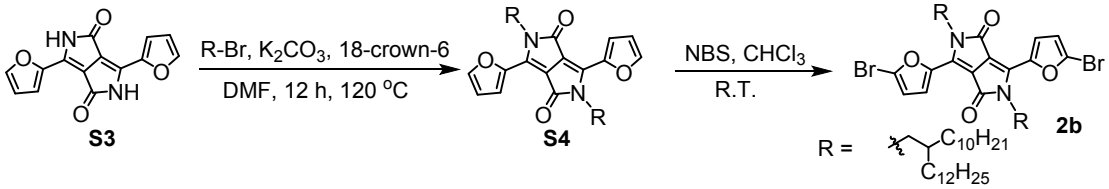
Compound **1a-1b** (2.2 equiv), **2a-2g** (1.0 equiv), *t*BuXPhos-Pd-G3 (2 mol%), sodium hydride (60% dispersion in mineral oil, 4.6 equiv) and anhydrous 1,4-dioxane (0.1 mmol ml^{-1}) were added in a schlenk tube. The mixture was stirred at 70 °C for 12 h in the absence of light, then the solvent was removed under vacuum. Subsequently, 15 mL HCl aqueous solution (0.05 M) was added, and the mixture was stirred in air for 10 min. The resulting precipitate was collected by filtration, and dissolved in CH_2Cl_2. After stirring in air for 20 min, the solution was washed by brine and dried with anhydrous $MgSO_4$. The crude product was purified by chromatography on silica gel to afford the corresponding product.

Synthesis of compound 5a



Compound **5a** was obtained from **1a** (38.5 mg, 0.26 mmol) and **2a** (140.0 mg, 0.12 mmol) as a blue solid following the general procedure (141.8 mg, yield: 91%; eluent: CH_2Cl_2). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 9.49 (d, *J* = 5.6 MHz, 2H), 8.43 (d, *J* = 5.6 MHz), 7.86 (m, 4H), 7.65 (m, 4H), 4.15 (d, *J* = 7.6 MHz, 4H), 2.07 (m, 2H), 1.21 (m, 80H), 0.84 (m, 12H). ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 189.48, 186.79, 161.59, 158.89, 145.79, 141.55, 141.11, 134.55, 134.50, 134.42, 134.39, 133.47, 132.64, 122.86, 122.45, 119.45, 47.32, 38.24, 31.94, 31.92, 31.02, 30.17, 29.76, 29.74, 29.70, 29.67, 29.40, 29.38, 26.11, 22.68, 14.08. HRMS (MALDI-TOF): calcd for $C_{80}H_{110}N_2O_6S_2$ $[M]^+$: 1258.7805, found: 1258.7843.

Synthesis of compound 2b

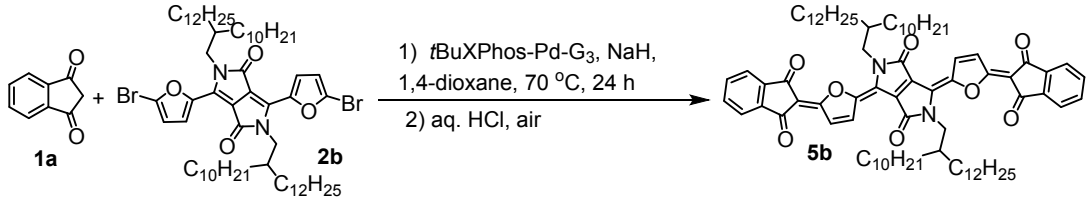


Compound S4: Compound **S4** was obtained from **S3** (200 mg, 0.75 mmol) as a red solid following the same procedure as **S2** (315.9 mg, yield: 45%). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 8.33 (d, *J* = 3.6 MHz, 2H), 7.68 (m, 2H), 7.27 (m, 2H), 4.03 (d, *J* = 7.6 MHz, 4H), 1.79 (m, 2H), 1.22 (m, 80 H), 0.87 (m, 12H).

Compound 2b: Compound **2b** was obtained from **S4** (300.0 mg, 0.32 mmol) as a dark red solid following the same procedure as **2a** (241.5 mg, yield: 69%).^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 8.30 (d, *J* = 3.6 MHz, 2H), 6.62 (d, *J* = 3.6 MHz, 2H), 3.99 (d, *J* = 7.2 MHz, 2H), 1.77 (m, 2H),

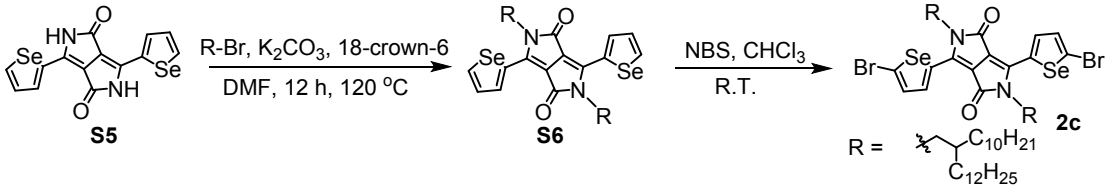
1.22 (m, 80H), 0.87 (m, 12H).

Synthesis of compound 5b



Compound **5b** was obtained from **1a** (38.5 mg, 0.26 mmol) and **2b** (135.0 mg, 0.12 mmol) as a blue solid following the general procedure (134.2 mg, yield: 89%; eluent: CH_2Cl_2). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 9.02 (d, J = 5.6 MHz, 2H), 8.04 (d, J = 5.6 MHz, 2H), 7.90 (m, 4H), 7.74 (m, 4H), 4.38 (d, J = 7.6 MHz, 4H), 1.92 (m, 2H), 1.18 (m, 80 H), 0.84 (m, 12H). ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 188.99, 186.59, 164.94, 160.80, 145.03, 141.79, 141.40, 138.28, 134.72, 134.56, 134.24, 126.75, 122.51, 122.42, 121.57, 108.51, 47.66, 37.94, 31.89, 30.45, 30.04, 29.69, 29.65, 29.61, 29.34, 26.34, 22.65, 14.07. HRMS (MALDI-TOF): calcd for $C_{80}H_{110}N_2O_8$ $[M]^+$: 1226.8262, found: 1226.8284.

Synthesis of compound 2c

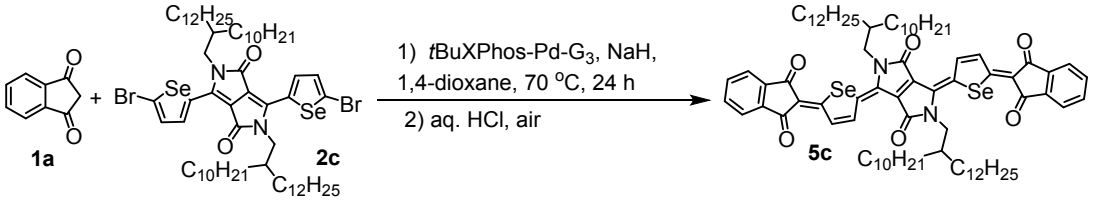


Compound S6: Compound **S6** was obtained from **S5** (500 mg, 1.27 mmol) as a red solid following the same procedure as **S2** (378.0 mg, yield: 28%). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 8.82 (dd, J_1 = 4.0 MHz, J_2 = 0.8 MHz, 2H), 8.38 (dd, J_1 = 5.6 MHz, J_2 = 0.8 MHz, 2H), 7.48 (m, 2H), 3.97 (d, J = 7.6 MHz, 4H), 1.91 (m, 2H), 1.21 (m, 80 H), 0.87 (m, 12H).

Compound 2c: Compound **2c** was obtained from **S6** (350.0 mg, 0.33 mmol) as a dark red solid following the same procedure as **2a** (301.3 mg, yield: 75%). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ

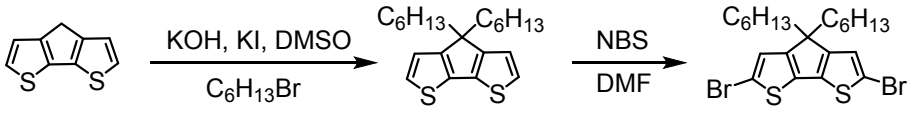
8.40 (d, *J* = 4.4 MHz, 2H), 7.40 (d, *J* = 4.0 MHz, 2H), 3.89 (d, *J* = 8.0 MHz, 2H), 1.88 (m, 2H), 1.21 (m, 80H), 0.88 (t, *J* = 6.4 MHz,12H).

Synthesis of compound 5c



Compound **5c** was obtained from **1a** (38.5 mg, 0.26 mmol) and **2c** (151.0 mg, 0.12 mmol) as a dark blue solid following the general procedure (158.5 mg, yield: 95%; eluent: CH_2Cl_2). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 9.61 (d, *J* = 6.0 MHz, 2H), 8.43 (d, *J* = 6.4 MHz, 2H), 7.84 (m, 4H), 7.64 (m, 4H), 4.07 (d, *J* = 8.0 MHz, 4H), 2.07 (m, 2H), 1.21 (m, 80 H), 0.83 (m, 12H). ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 190.33, 186.07, 162.28, 161.94, 148.71, 141.37, 140.92, 137.55, 135.68, 134.62, 134.33, 133.93, 133.20, 123.06, 122.52, 122.03, 122.01, 47.18, 38.20, 31.92, 31.91, 31.02, 30.10, 29.75, 29.69, 29.39, 29.37, 26.08, 22.67, 14.08. HRMS (MALDI-TOF): calcd for $C_{80}H_{110}N_2O_6Se_2$ $[M]^+$: 1354.6694, found: 1354.6741.

Synthesis of compound 2d

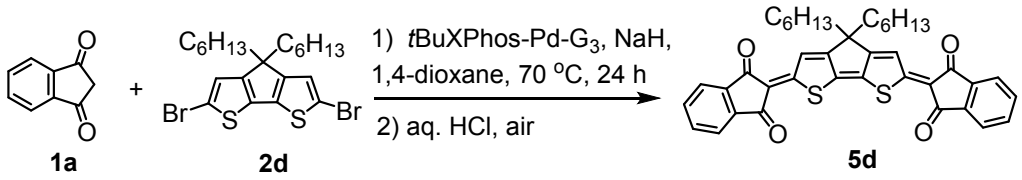


Compound S8: To the solution of **S7** (200.0 mg 1.12 mmol) in anhydrous DMSO (5 mL), KI (5.6 mg, 0.034 mmol) and KOH (188.8 mg 3.37 mmol) were added. After stirring at room temperature for 1 h, 1-bromohexane (555.6mg 3.37 mmol) was added. The mixture was stirred at room temperature for overnight, then poured into water, and extracted with ether. The organic layer was washed with brine and dried with anhydrous $MgSO_4$. After removal of the solvent, the crude

product was purified by chromatography on silica gel using PE as the eluent, affording compound **S8** as a yellow oil (330.5 mg, yield: 85%). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 7.15 (d, J = 4.8 MHz, , 2H), 6.93 (d, J = 4.8 MHz, 2H), 1.82 (m, 4H), 1.13 (m, 12H), 0.94 (m, 4 H), 0.81 (t, J = 6.8 MHz, 6H).

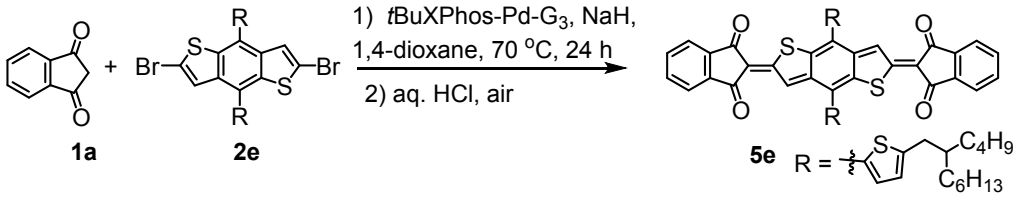
Compound 2d: To the solution of **S8** (300.0 mg, 0.86 mmol) in DMF (8 mL), NBS (323.5 mg, 1.82 mmol) was added in one portion. The mixture was stirred at room temperature for 12 h in the absence of light, then poured into water and extracted with ether. The organic layer was washed with brine and dried with anhydrous $MgSO_4$. After removal of the solvent, the crude product was purified by chromatography on silica gel using PE as the eluent, affording compound **2d** as a yellow oil (375.5 mg, yield: 86%). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 6.93 (s, 2H), 1.75 (m, 4H), 1.13 (m, 12H), 0.90 (m, 4 H), 0.83 (t, J = 6.8 MHz, 6H).

Synthesis of compound 5d



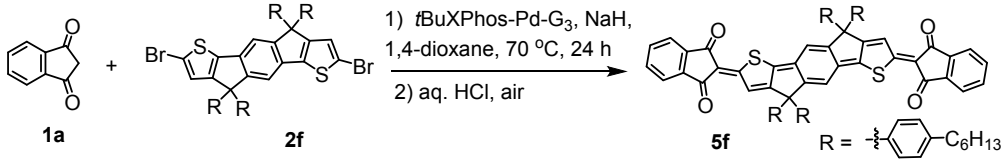
Compound **5d** was obtained from **1a** (76.5 mg, 0.52 mmol) and **2d** (120.0 mg, 0.24 mmol) as a purple solid following the general procedure (128.0 mg, yield: 85%; eluent: PE/DCM = 1/3). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 8.02 (s, 2H), 7.93 (m, 4H), 7.76 (m, 4H), 1.98 (m, 4H), 1.18 (m, 12 H), 1.06 (m, 4H), 0.81 (m, 6H).

Synthesis of compound 5e



Compound **5e** was obtained from **1a** (75.7 mg, 0.31 mmol) and **2e** (120.0 mg, 0.14 mmol) as a dark blue solid following the general procedure (118.8 mg, yield: 86%; eluent: PE/CH_2Cl_2 = 1/3). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 8.77 (s, 2H), 7.80 (m, 4H), 7.53 (m, 4H), 7.41 (d, *J* = 3.6 MHz, 4H), 6.94 (d, *J* = 3.2 MHz, 4H), 2.91 (d, *J* = 6.8 MHz, 2H), 1.78 (m, 2 H), 1.39 (m, 32H), 0.96 (m, 12 H). ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 189.68, 186.92, 157.32, 148.83, 146.82, 144.06, 141.48, 141.18, 134.41, 134.16, 133.63, 133.29, 131.01, 128.71, 126.33, 122.78, 122.20, 39.90, 34.83, 33.36, 32.97, 32.00, 29.74, 28.89, 26.69, 23.08, 22.72, 14.25, 14.26. HRMS (MALDI-TOF): calcd for $C_{60}H_{64}O_4S_4$ $[M]^+$: 976.3721, found: 976.3710.

Synthesis of compound 5f



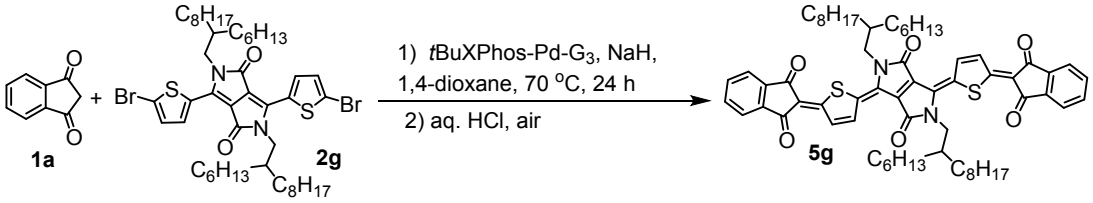
Compound **5f** was obtained from **1a** (41.7 mg, 0.29 mmol) and **2f** (140.0 mg, 0.13 mmol) as a purple solid following the general procedure (142.3 mg, yield: 92%; eluent: PE/DCM = 1/1). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 8.17 (s, 2H), 7.84 (m, 4H), 7.67 (m, 4H), 7.15 (M, 18 H), 2.59 (t, *J* = 7.6 MHz, 8H), 1.59 (m, 8 H), 1.31 (m, 24H), 0.87 (t, *J* = 6.8 MHz, 12H).

Synthesis of compound 2g

Compound S9: Compound **S9** was obtained from **S1** (500 mg, 1.66 mmol) as a red solid following the same procedure as **S2** (475 mg, yield: 38%).[1]H NMR (400 MHz, $CDCl_3$, ppm): δ 8.87 (d, *J* = 2.8 MHz, 2H), 7.62 (d, *J* = 4.8 MHz, 2H), 7.27 (m, 2H), 4.03 (d, *J* = 8.0 MHz, 4H), 1.90 (m, 2H), 1.21 (m, 80 H), 0.84 (m, 12H).

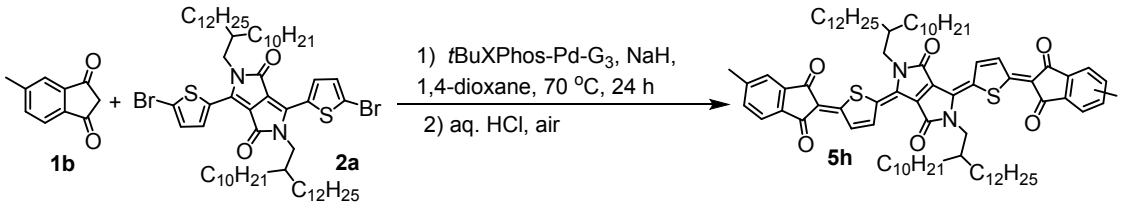
Compound 2g: Compound **2g** was obtained from **S9** (400.0 mg, 0.53 mmol) as a dark red solid following the same procedure as **2a** (411.4 mg, yield: 85%). [1]H NMR (400 MHz, $CDCl_3$, ppm): δ 8.62 (d, *J* = 4.0 MHz, 2H), 7.22 (d, *J* = 4.0 MHz, 2H), 3.93 (d, *J* = 8.0 MHz, 2H), 1.88 (m, 2H), 1.22 (m, 80H), 0.86 (m, 12H).

Synthesis of compound 5g



Compound **5g** was obtained from **1a** (46.1 mg, 0.31 mmol) and **2g** (130.0 mg, 0.14 mmol) as a dark blue solid following the general procedure (133.6 mg, yield: 90%; eluent: DCM). [1]H NMR (400 MHz, $CDCl_3$, ppm): δ 9.45 (d, *J* = 5.6 MHz, 2H), 8.37 (d, *J* = 12.8 MHz), 7.82 (m, 4H), 7.60 (m, 4H), 4.12 (d, *J* = 7.6 MHz, 4H), 2.04 (m, 2H), 1.29 (m, 48H), 0.83 (m, 12H).

Synthesis of compound 5h



Compound **5h** was obtained from **1b** (46.7 mg, 0.29 mmol) and **2a** (150.0 mg, 0.0.13 mmol) as a blue solid following the general procedure (147.1 mg, yield: 86%; eluent: DCM). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 9.45 (dd, J_1 = 6.0 MHz, J_2 = 1.2 MHz, 2H), 8.36 (t, J = 5.2 MHz, 2H), 7.72 (dd, J_1 = 7.6 MHz, J_2 = 4.0 MHz, 2H), 7.62 (s, 2H), 7.40 (dd, J_1 = 11.2 MHz, J_2 = 8.0 MHz, 2H), 4.12 (d, J = 7.6 MHz, 4H), 2.42 (d, J = 11.6 MHz, 6H), 2.04 (m, 2H), 1.21 (m, 80H), 0.83 (m, 12H). ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 189.53, 189.19, 186.86, 186.56, 161.56, 158.25, 146.14, 145.95, 145.52, 141.95, 141.50, 139.41, 139.00, 135.37, 135.31, 133.21, 133.54, 123.10, 122.83, 122.69, 122.42, 119.88, 99.95, 47.23, 38.24, 31.92, 30.96, 30.19, 29.77, 29.71, 29.42, 29.40, 26.08, 22.69, 22.08, 14.11. HRMS (MALDI-TOF): calcd for $C_{82}H_{114}N_2O_6Se_2$ $[M]^+$: 1286.8118, found: 1286.8085.

5. NMR study of the coupling product

Compound **1a** (38.5 mg, 0.26 mmol), **2a** (140 mg, 0.12 mmol), *t*BuXPhos-Pd-G3 (2.0 mg, 2.47 μmol, 2 mol%), sodium hydride (60% dispersion in mineral oil, 22.1 mg, 0.55 mmol) and anhydrous 1,4-dioxane (1.2 mL) were added in a schlenk tube. The mixture was stirred at 70 ^{o}C for 12 h in the absence of light, then the solvent was removed under vacuum. Subsequently, 15 mL HCl aqueous solution (0.05 M, degassed) was added, and the mixture was stirred for 10 min. The resulting precipitate was collected by filtration under argon, and then dried by argon flow. After that, 5 mg of the solid was transferred to a LPV-NMR tube in an argon-filled glovebox.

6. Supplementary Date

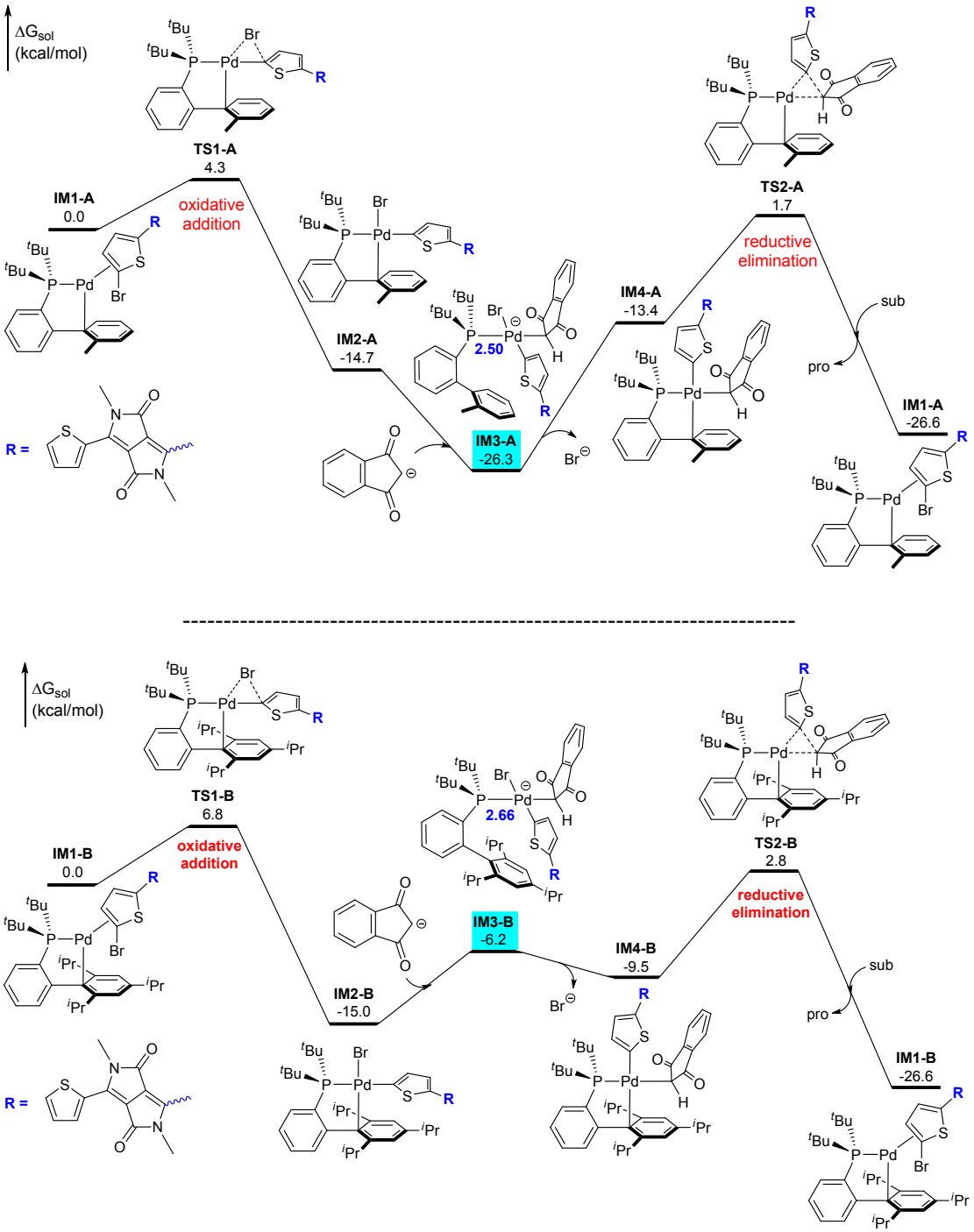


Figure S2. Free-energy profiles for the coupling of **1a** and **2a** with *t*BuMePhos (top) and *t*BuXPhos (bottom) as the ligand.

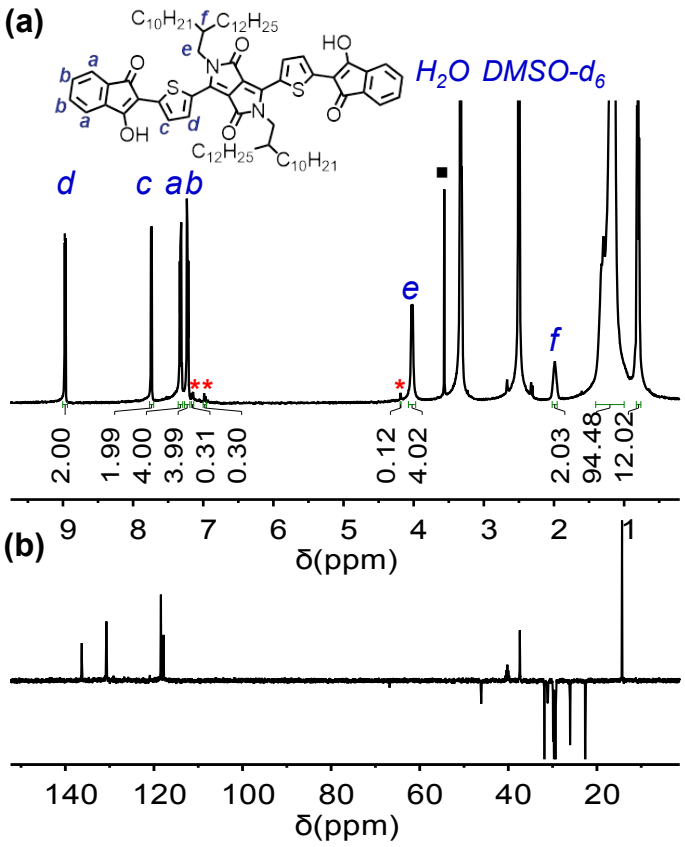


Figure S3. ^{1}H NMR (a) and ^{13}C DEPT-135 NMR (b) spectra of compound **4** in DMSO-d_6; (■) signal for 1,4-dioxane; (*) signal for the residual indandione.

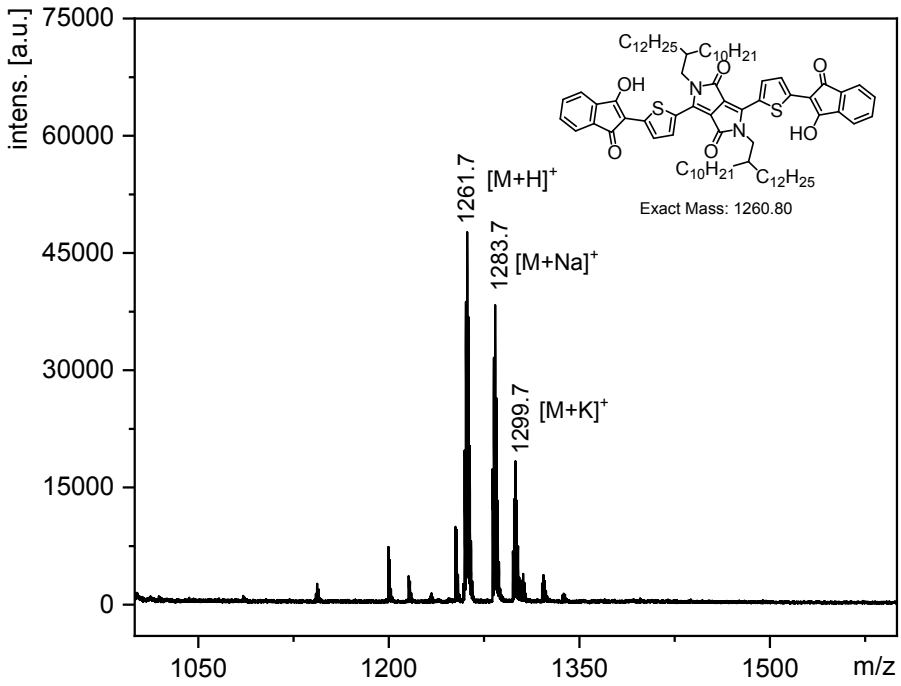


Figure S4. MALDI-TOF mass spectrum of compound **4**.

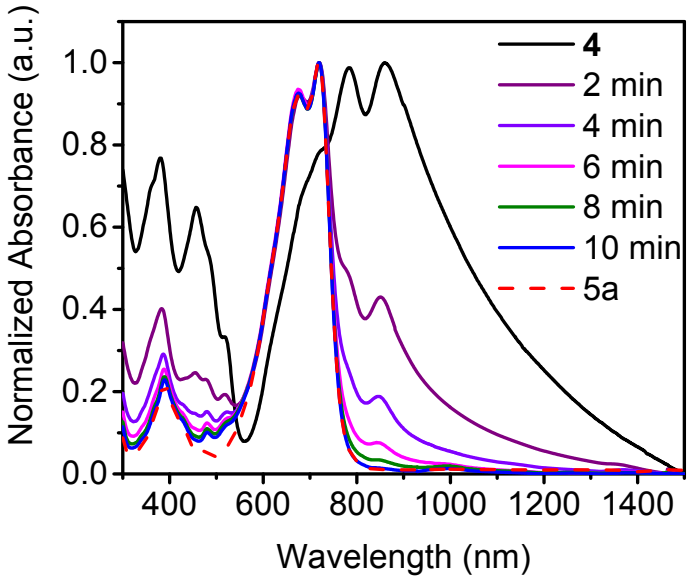


Figure S5. Time dependence of UV-vis-NIR spectra of compound **4** in solution (CH_2Cl_2, 1×10^{-5} mol L^{-1}) under bubbling air with the irradiation of UV light (254 nm).

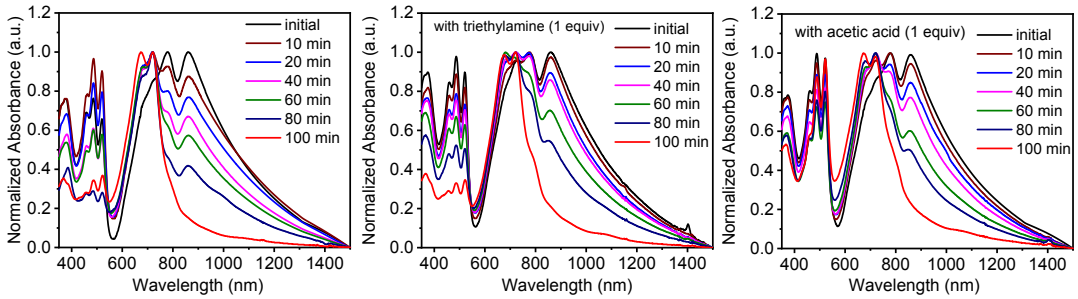


Figure S6. The oxidation process of compound **4** by electrochemical method under argon monitored by solution UV-vis-NIR absorption (in CH_2Cl_2, 1×10^{-5} mol L^{-1}).

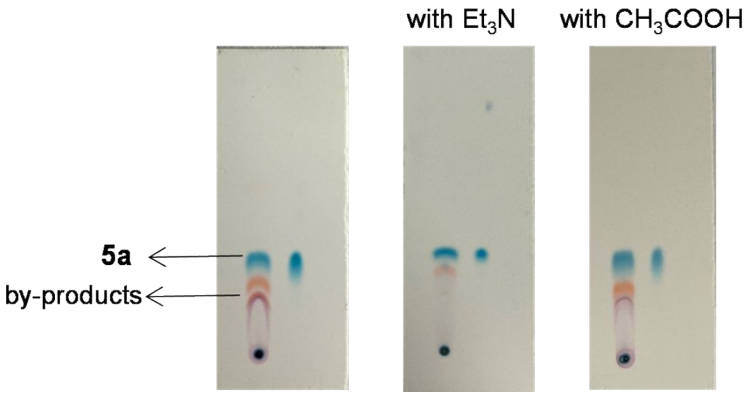


Figure S7. Thin layer chromatography analysis of electrochemical oxidation of compound **4**.

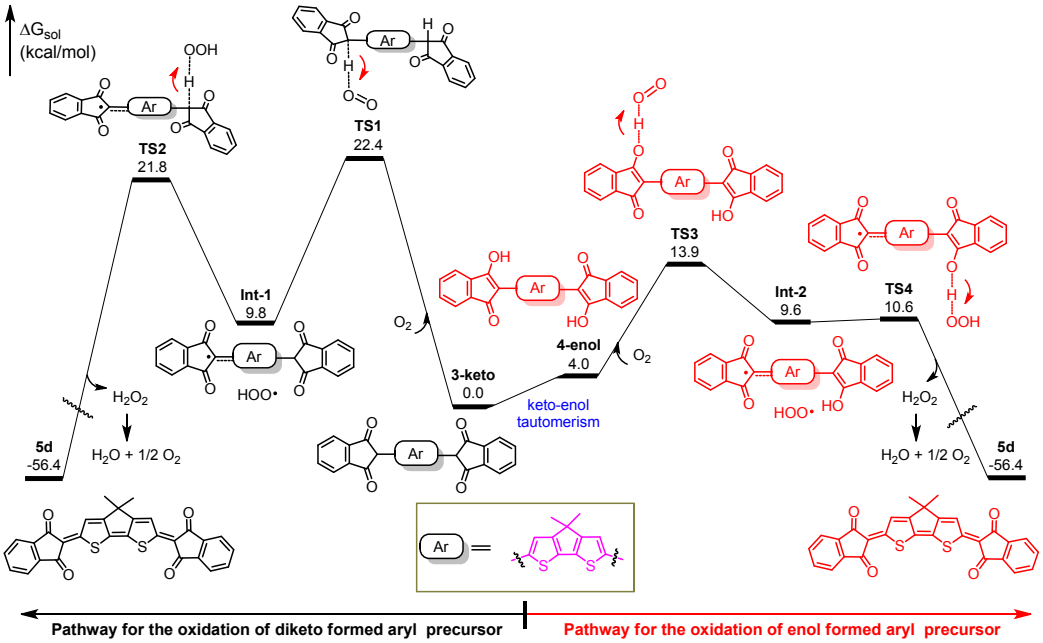


Figure S8. Free energy profiles for the formation of compound **5d**.

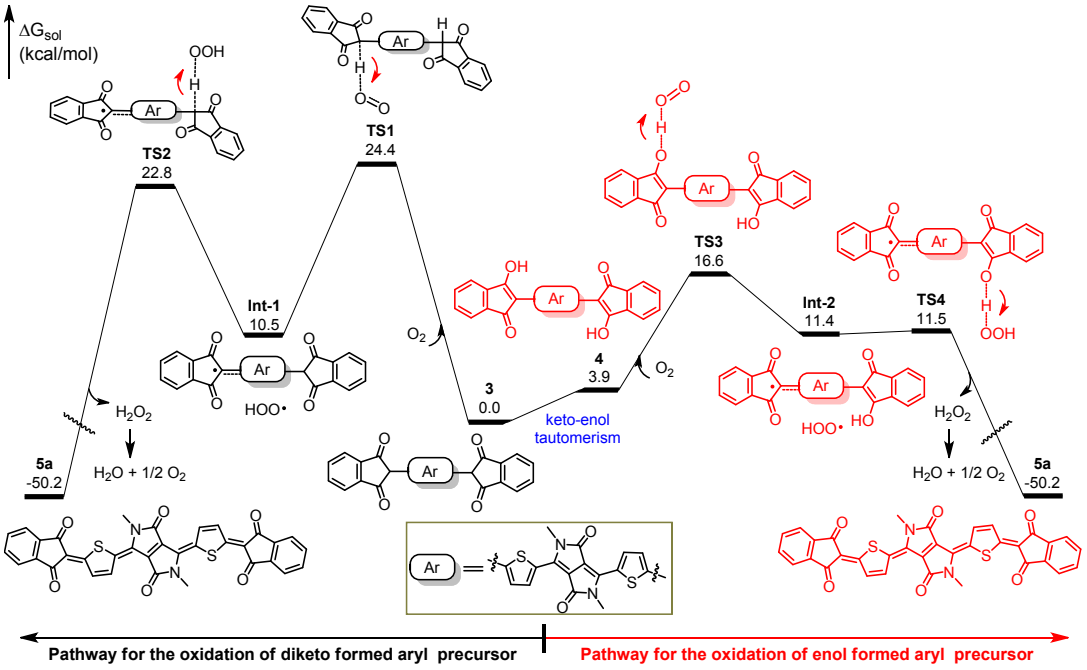


Figure S9. Free-energy profiles for the oxidation of intermediates **3** and **4** to give quinoid **5a** obtained from M06L/SMD-6-31++G(d,p)//M06L-6-31G(d,p) calculations.

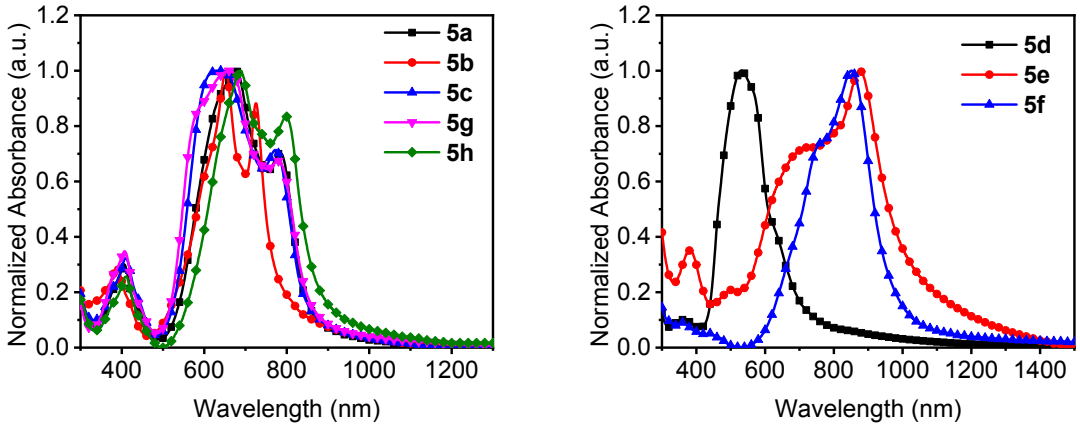


Figure S10. Thin-film absorption spectra of **5a**-**5h**.

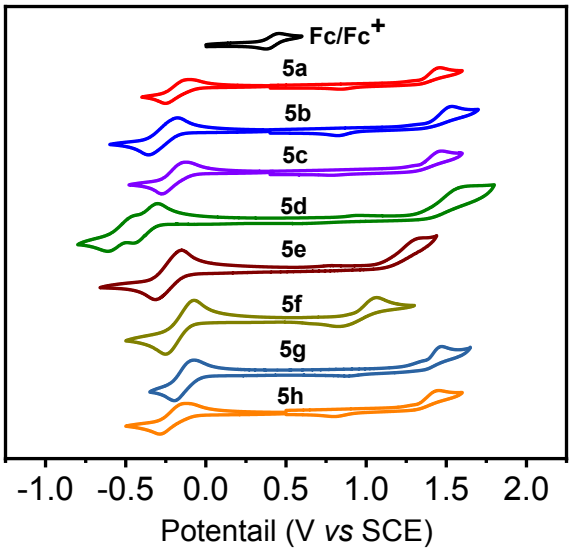


Figure S11. Solution cyclic voltammograms (CVs) of **5a-5h**.

Table S4. **Optical and electrochemical properties of 5a-5h.**

Compound	λ_{max}^{sol}[nm][a]	λ_{max}^{film} [nm][b]	E_g[eV][c]	E_{LUMO}[eV][d]	E_{HOMO}[eV][d]
5a	721, 679	783, 676	1.45	-4.33	-5.74
5b	675, 641	725, 652	1.60	-4.23	-5.81
5c	715, 673	773, 637	1.42	-4.32	-5.69
5d	610, 562, 522	530	1.91	-4.06	-5.73
5e	661, 611	877, 710	1.26	-4.22	-5.62
5f	790, 727	851, 761	1.32	-4.29	-5.29
5g	721, 679	779, 660	1.45	-4.32	-5.74
5h	721, 680	799, 688	1.43	-4.27	-5.68

[a]In toluene solution. [b]Thin-films were prepared by spin-casting from toluene solutions on the quartz substrates [c]Calculated from the onset of thin-film absorption according to the equation of E_g^{opt} =1240/λ_{onset}. [d]The highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) energy levels were calculated according to the equation of E_{HOMO} = -(4.80 + E_{onset}^{ox}) eV and E_{LUMO} = -(4.80 + E_{onset}^{red}) eV, in which E_{onset}^{ox} and E_{onset}^{red} represent the oxidation and reduction onset-potentials.

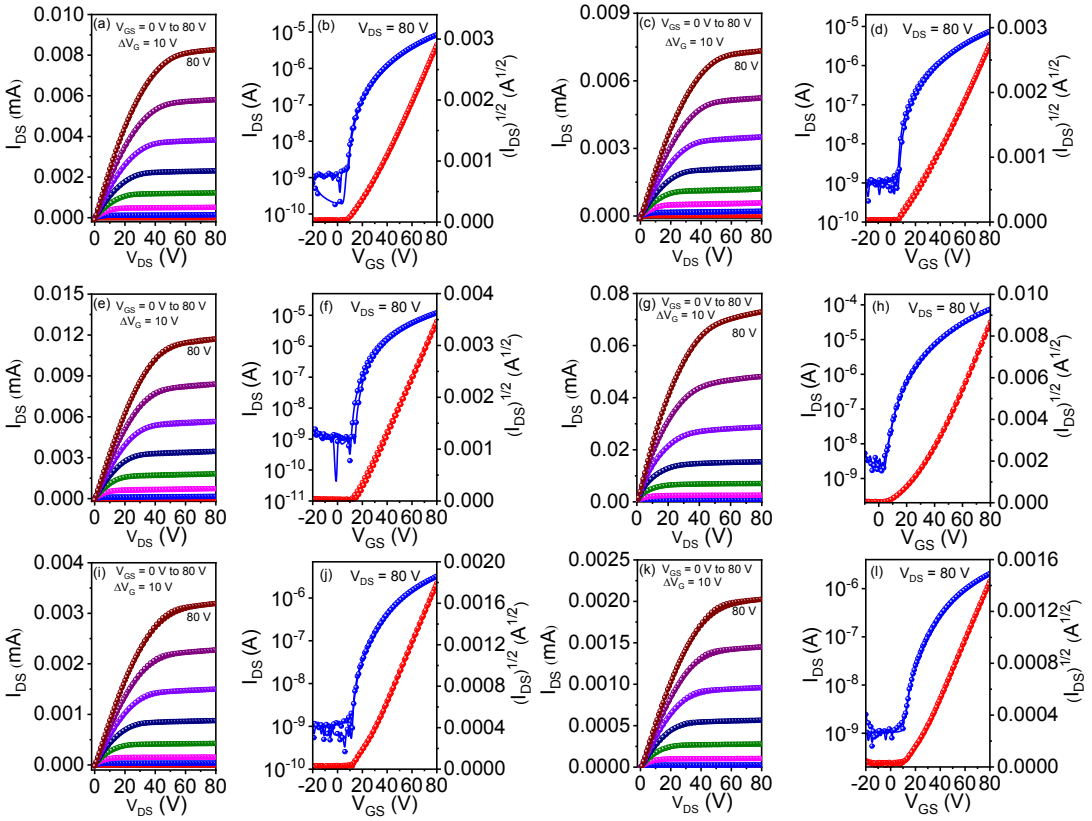


Figure S12. Output (a, c, e, g, i, k) and transfer (b, d, f, h, j, l) curves of the TGBC OFETs based on **5a** (a, b), **5b** (c, d), **5c** (e, f), **5f** (g, h), **5g** (i, j) and **5h** (k, l).

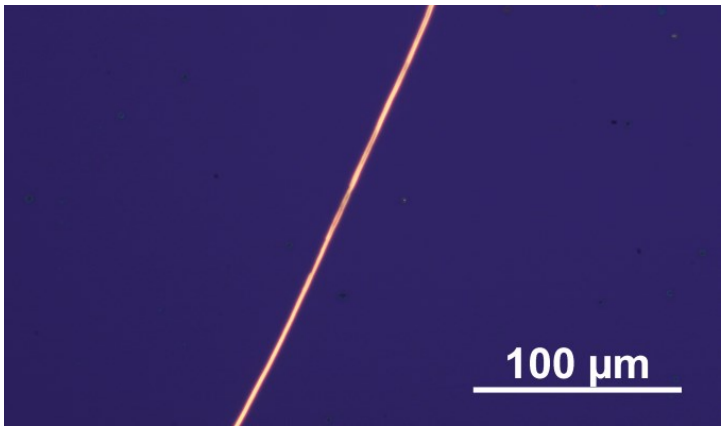


Figure S13. The cross-polarized optical micrograph of the micro-wire of compound **5g** with rotation of 45°.

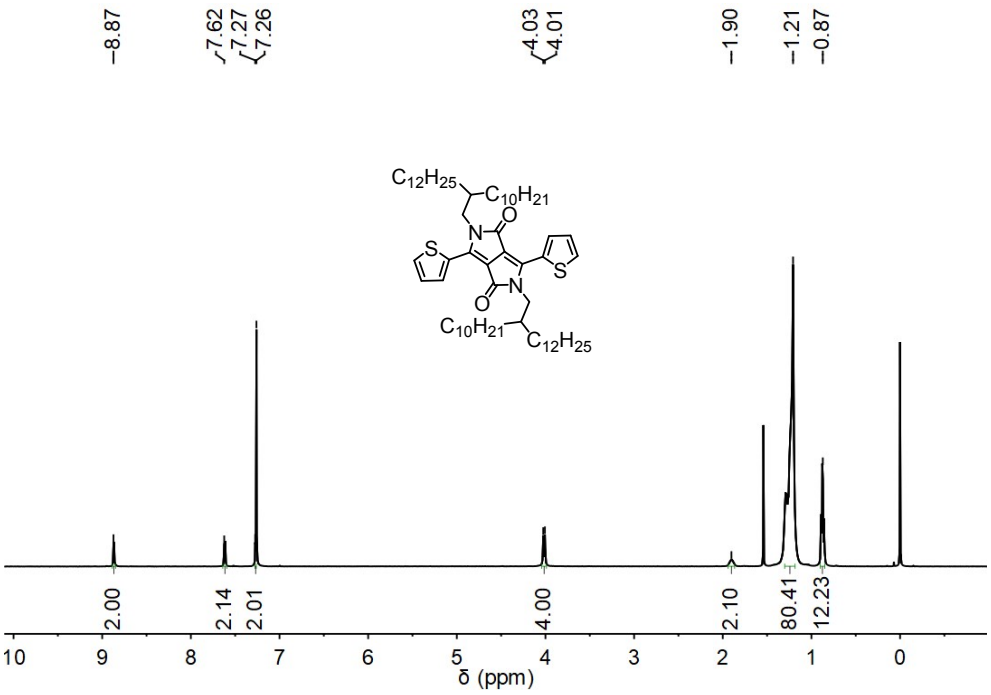


Figure S14. ^{1}H NMR spectrum of compound **S2** (400 MHz, $CDCl_3$).

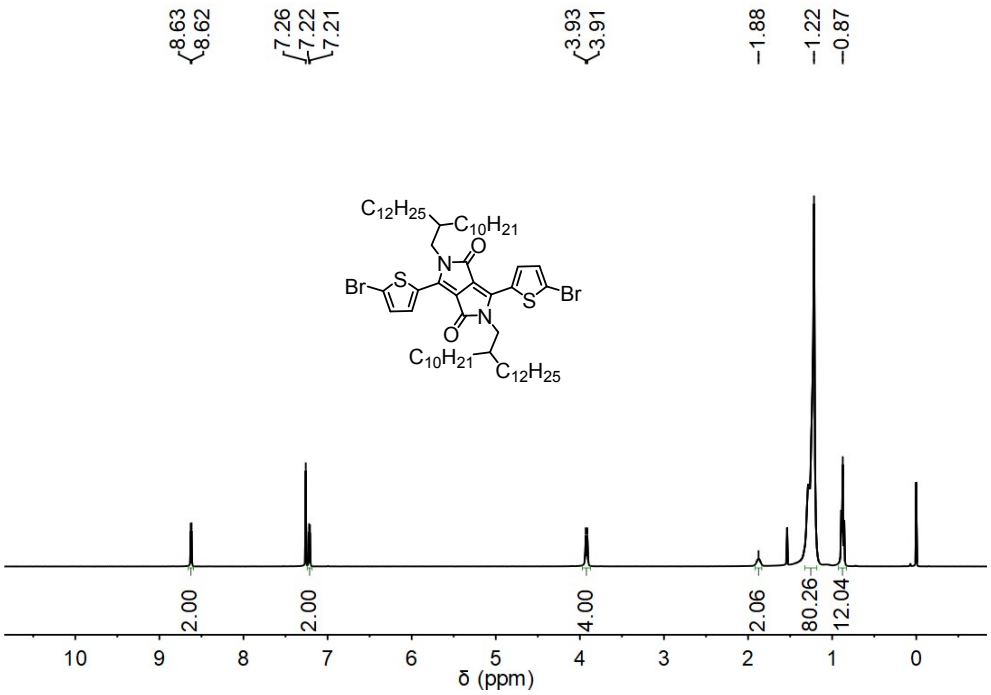


Figure S15. ^{1}H NMR spectrum of compound **2a** (400 MHz, $CDCl_3$).

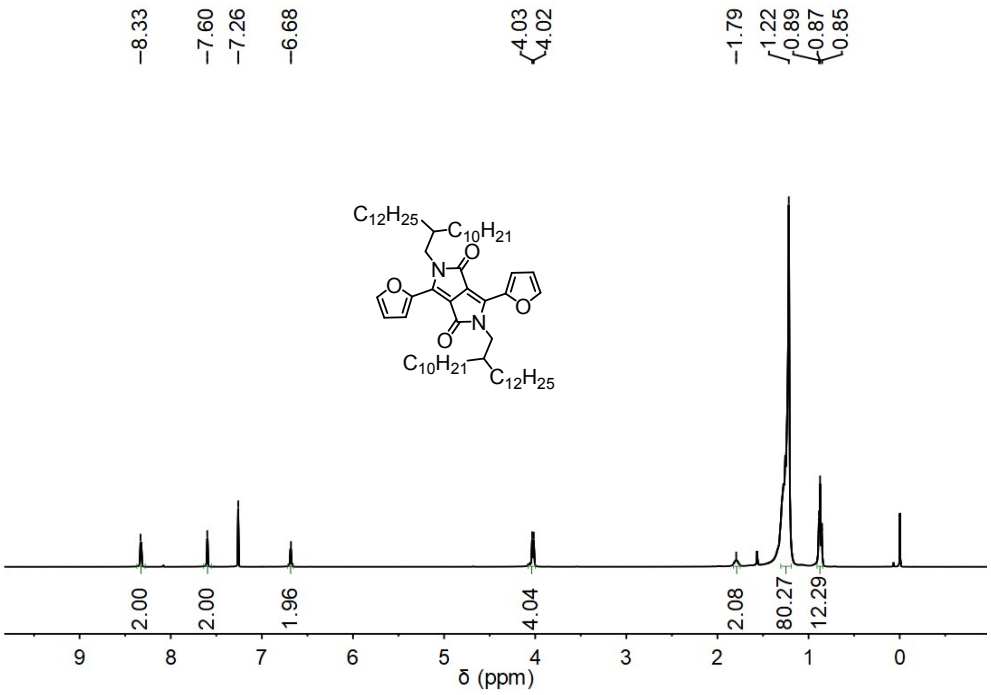


Figure S16. ^{1}H NMR spectrum of compound **S4** (400 MHz, $CDCl_3$).

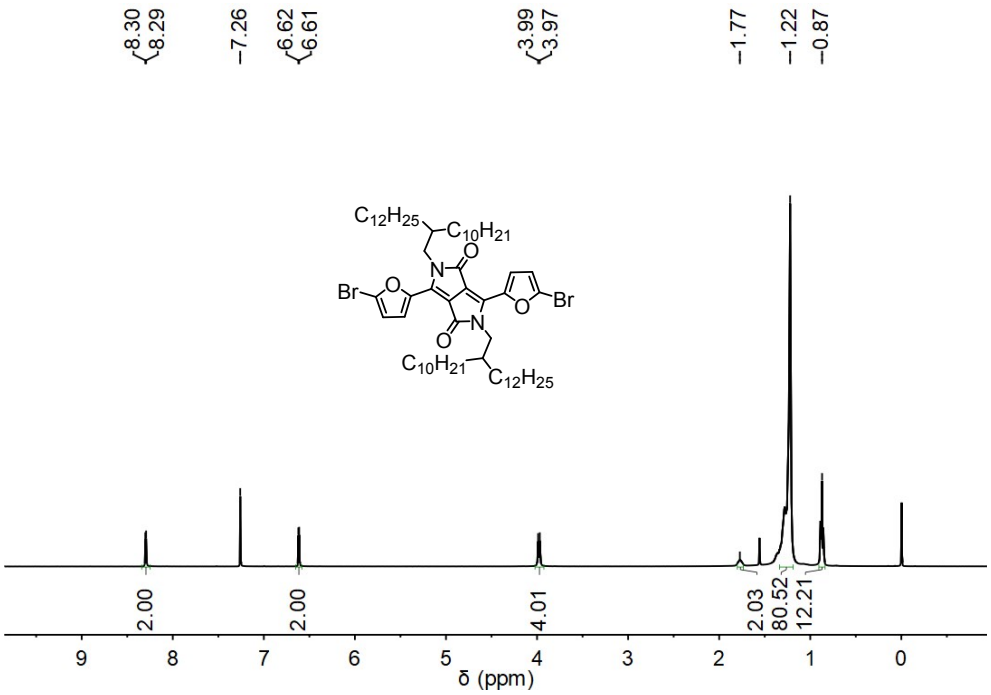


Figure S17. ^{1}H NMR spectrum of compound **2b** (400 MHz, $CDCl_3$).

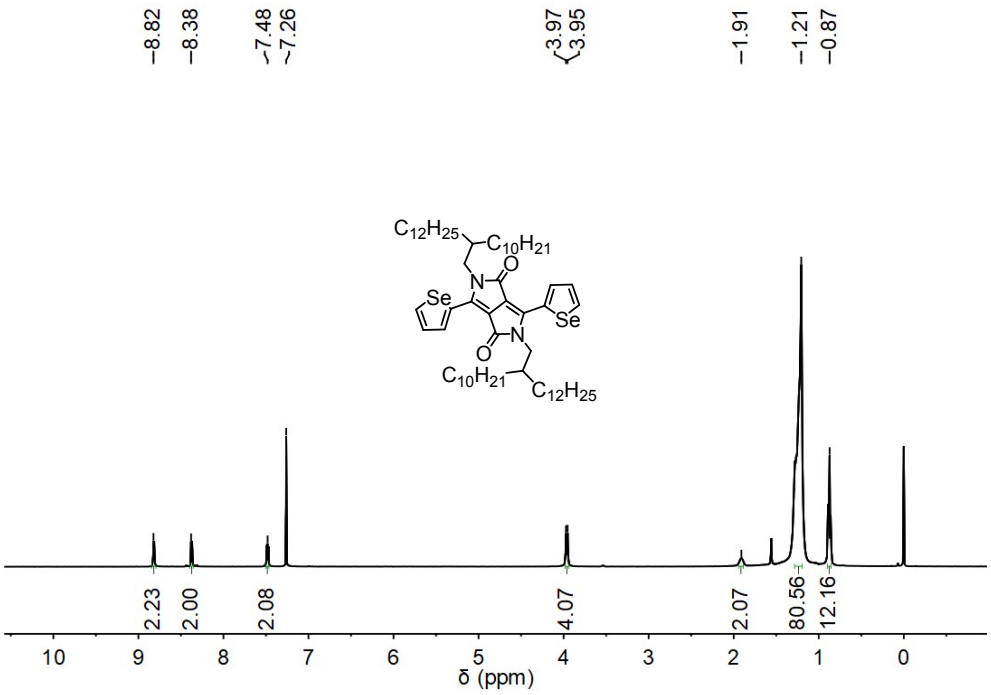


Figure S18. ^{1}H NMR spectrum of compound **S6** (400 MHz, $CDCl_3$).

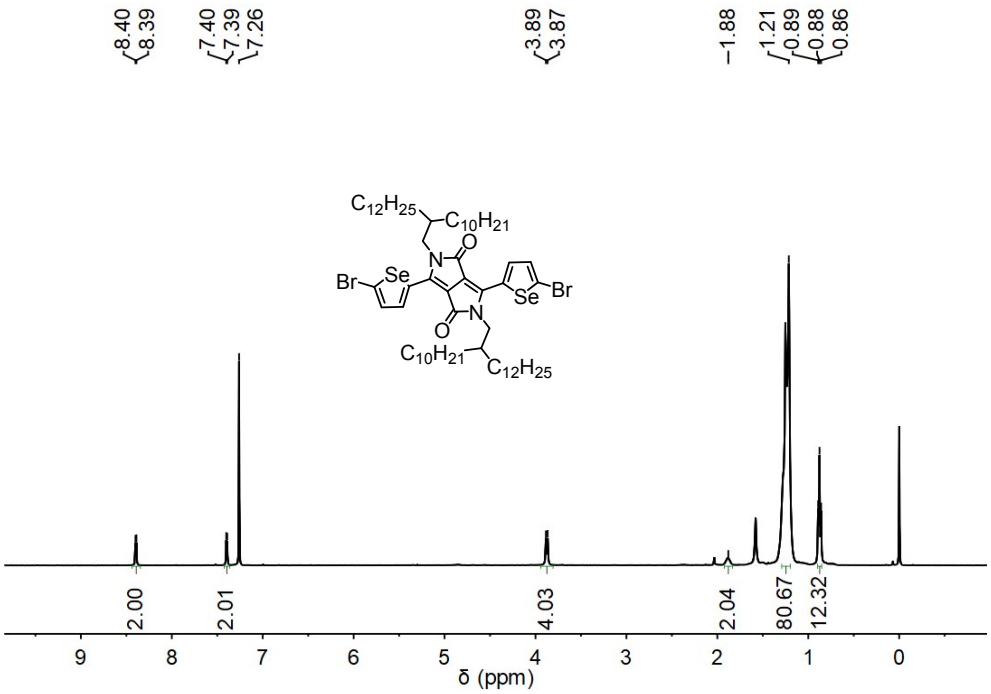


Figure S19. ^{1}H NMR spectrum of compound **2c** (400 MHz, $CDCl_3$).

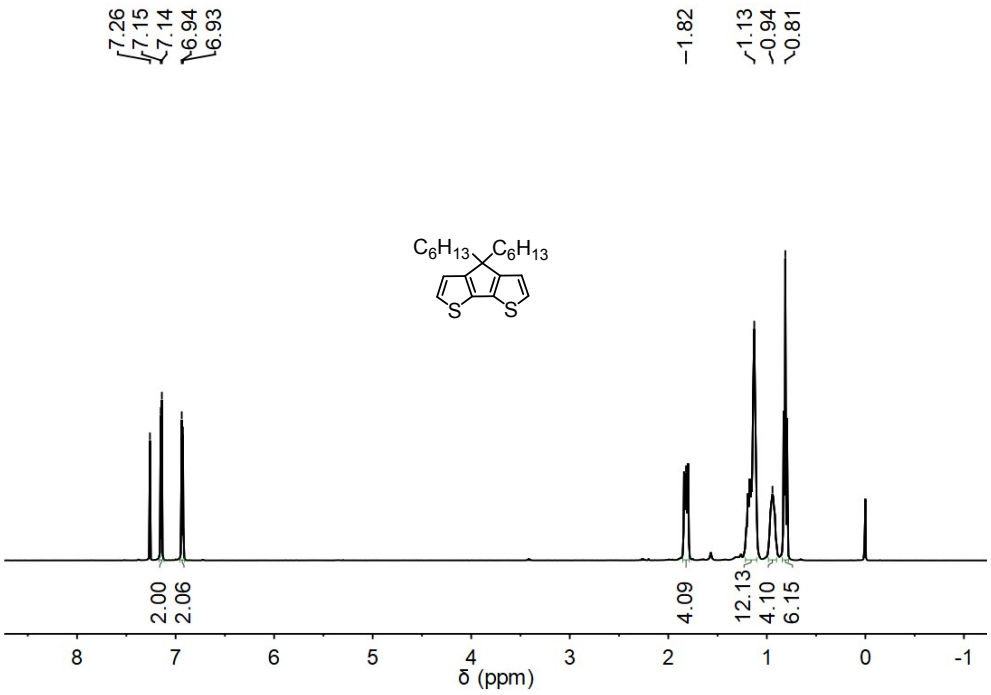


Figure S20. ^{1}H NMR spectrum of compound **S8** (400 MHz, $CDCl_3$).

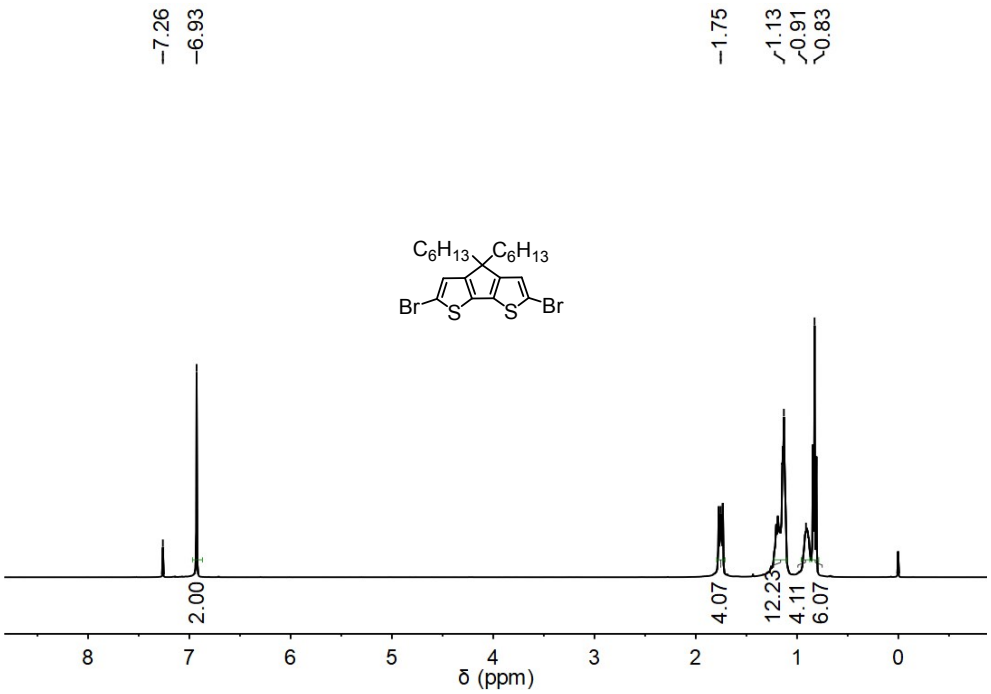


Figure S21. ^{1}H NMR spectrum of compound **2d** (400 MHz, $CDCl_3$).

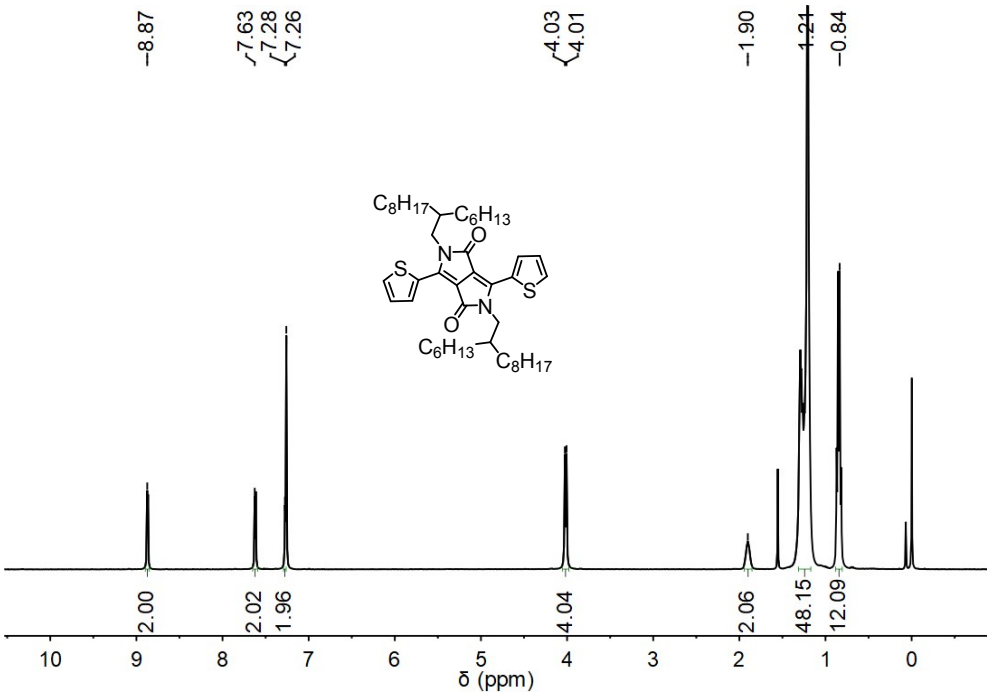


Figure S22. ^{1}H NMR spectrum of compound **S9** (400 MHz, $CDCl_3$).

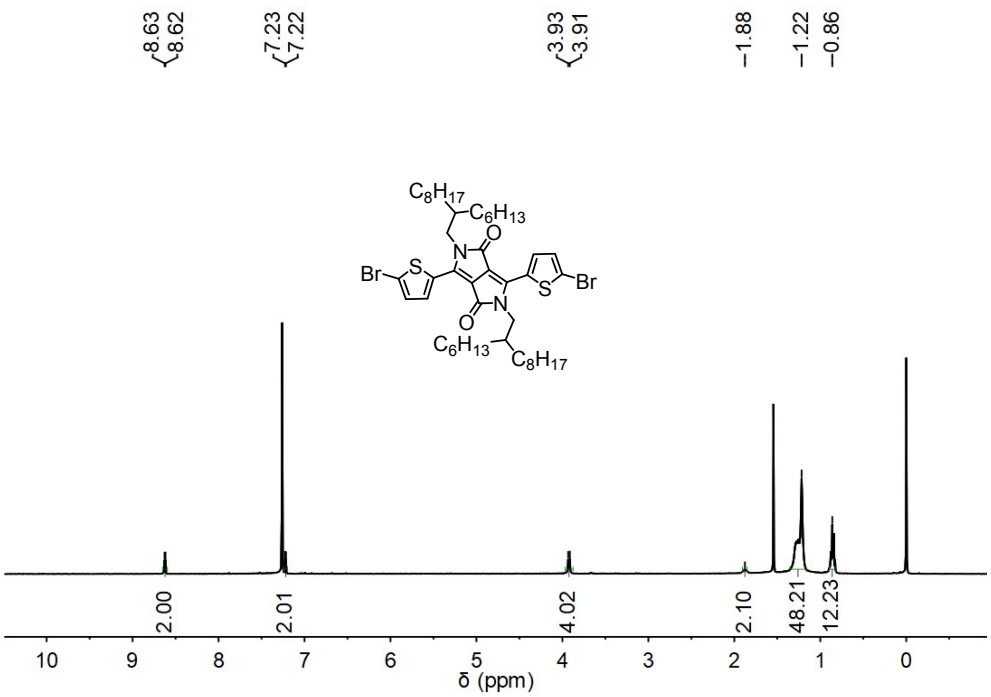


Figure S23. ^{1}H NMR spectrum of compound **2g** (400 MHz, $CDCl_3$).

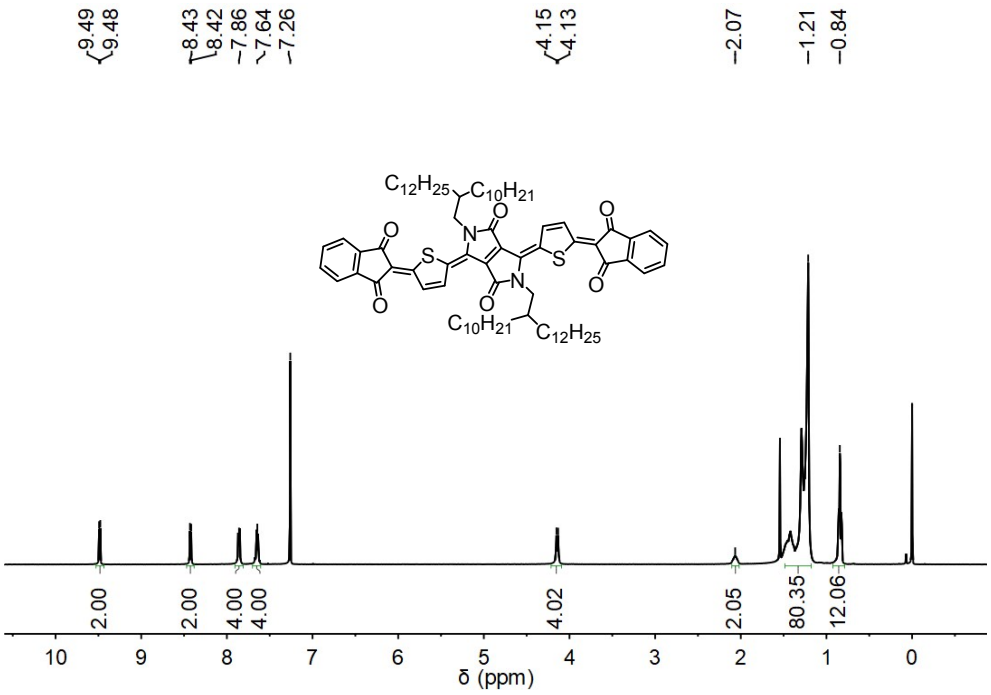


Figure S24. ^{1}H NMR spectrum of compound **5a** (400 MHz, $CDCl_3$).

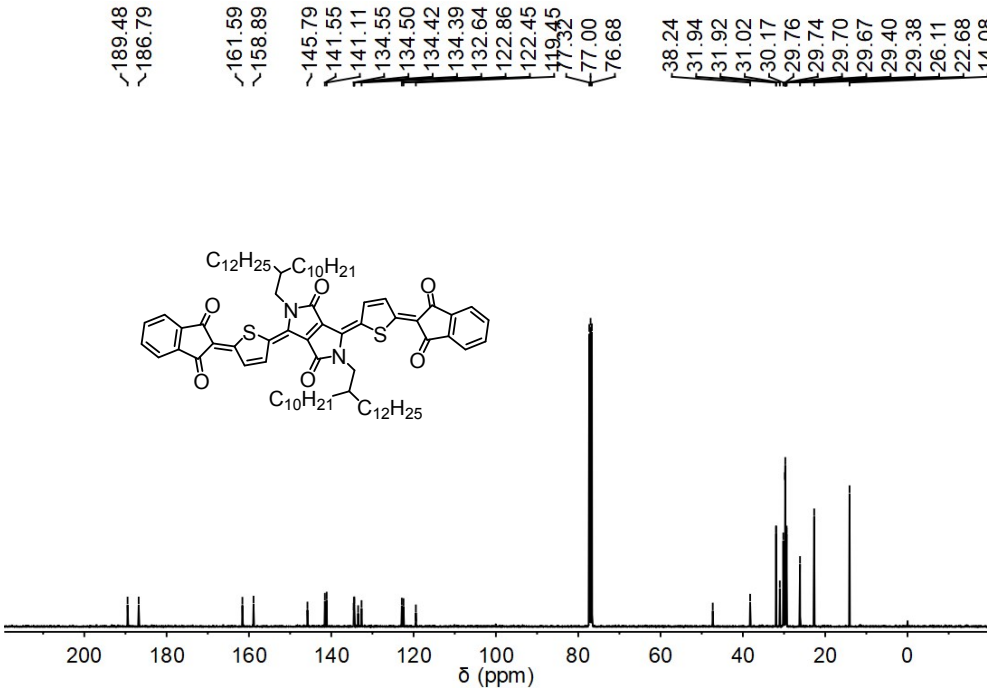


Figure S25. ^{13}C NMR spectrum of compound **5a** (100 MHz, $CDCl_3$).

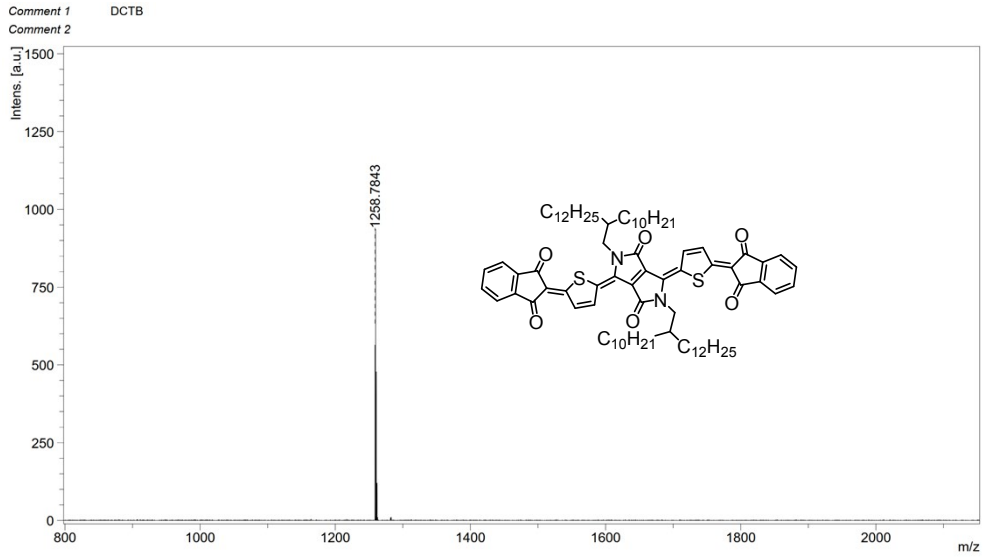


Figure S26. MALDI-TOF mass spectrum of compound **5a**.

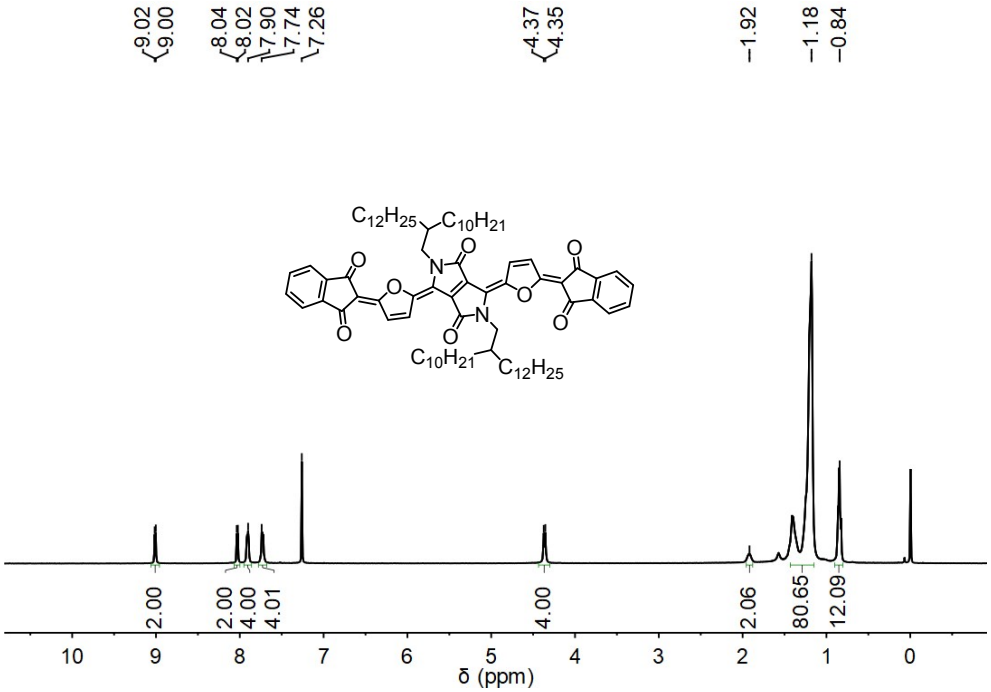


Figure S27. ^{1}H NMR spectrum of compound **5b** (400 MHz, $CDCl_3$).

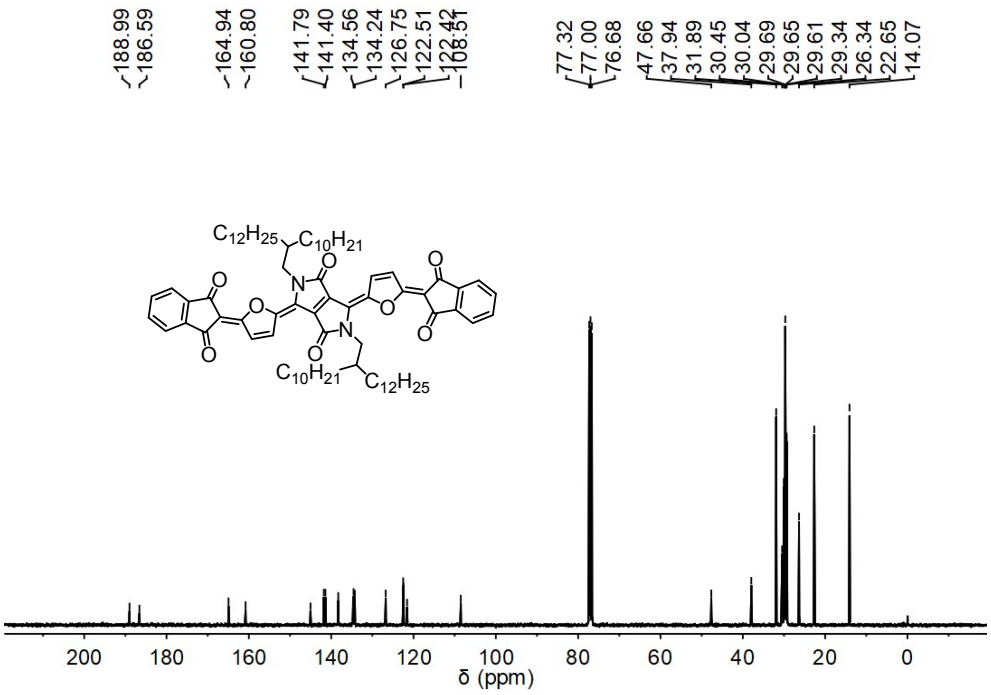


Figure S28. ^{13}C NMR spectrum of compound **5b** (100 MHz, $CDCl_3$).

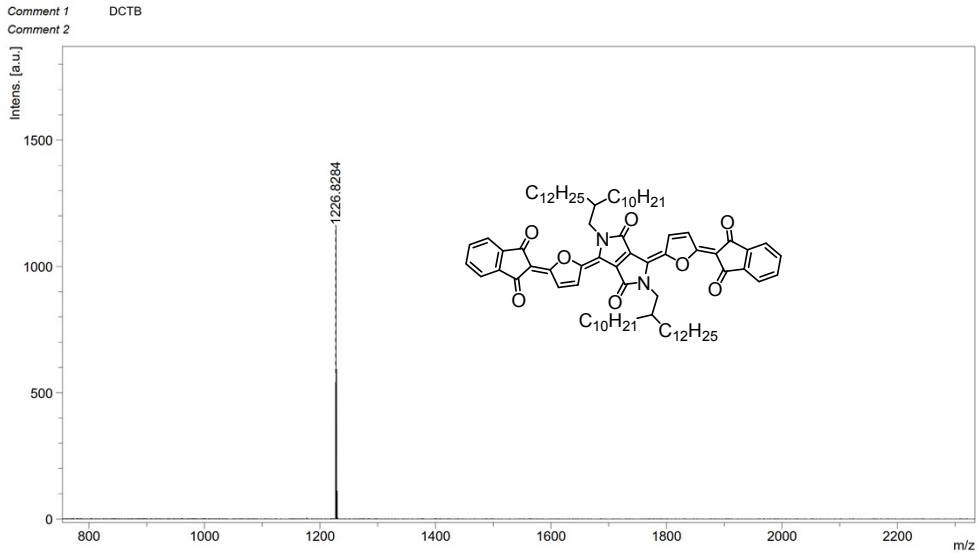


Figure S29. MALDI-TOF mass spectrum of compound **5b**.

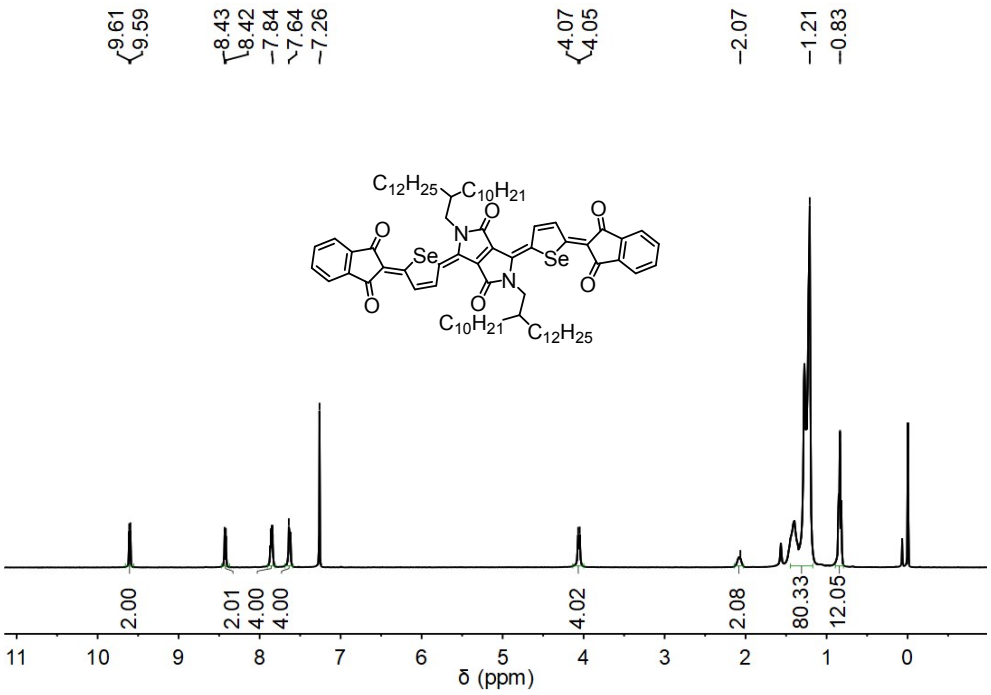


Figure S30. ^{1}H NMR spectrum of compound **5c** (400 MHz, $CDCl_3$).

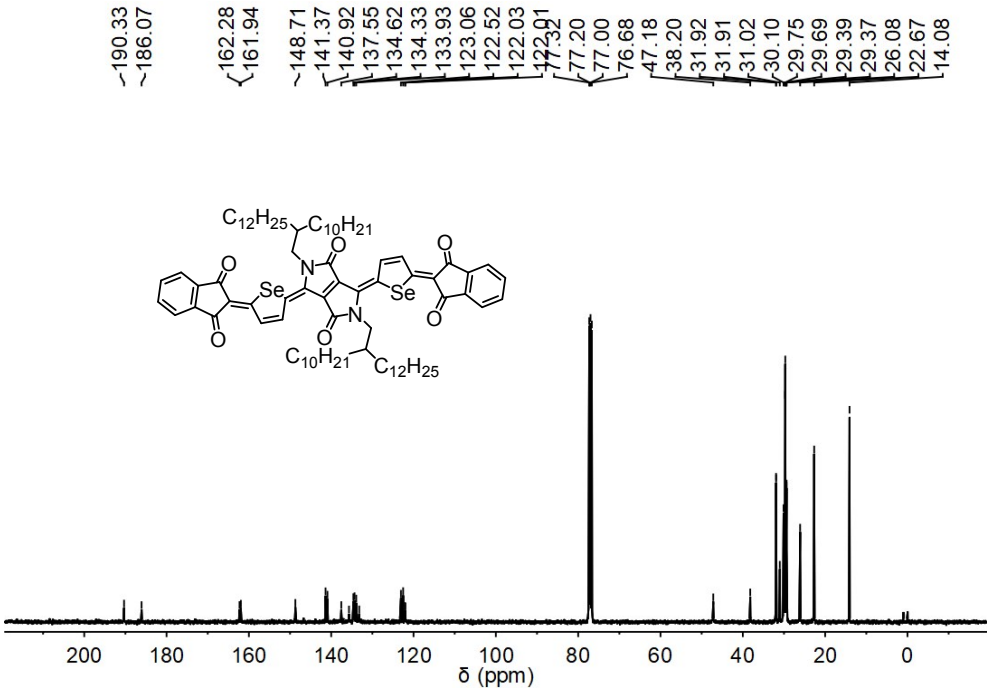


Figure S31. ^{13}C NMR spectrum of compound **5c** (100 MHz, $CDCl_3$).

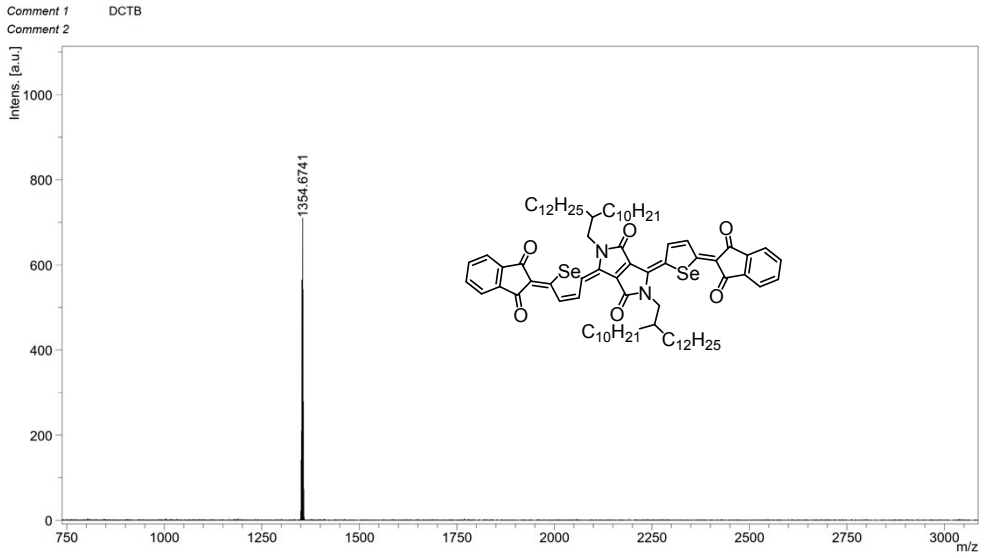


Figure S32. MALDI-TOF mass spectrum of compound **5c**.

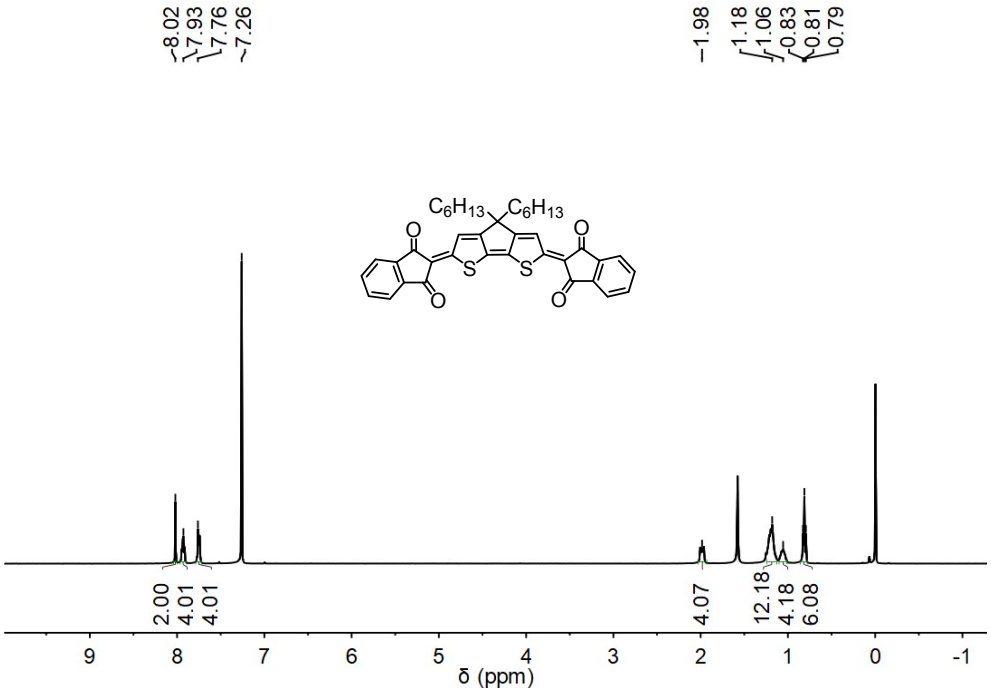


Figure S33. ^{1}H NMR spectrum of compound **5d** (400 MHz, $CDCl_3$).

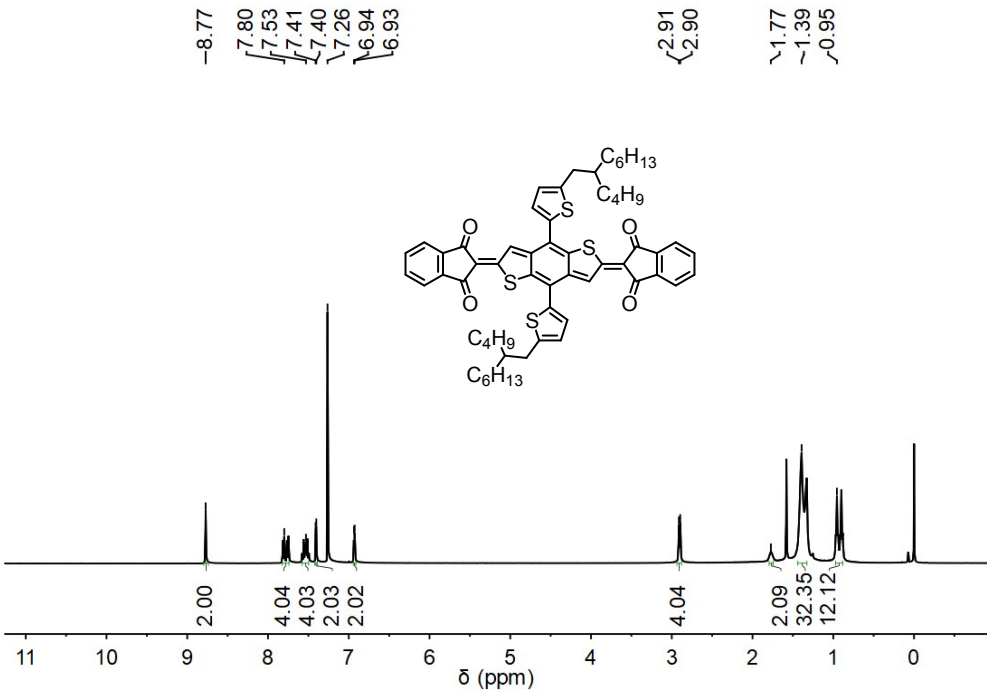


Figure S34. ^{1}H NMR spectrum of compound **5e** (400 MHz, $CDCl_3$).

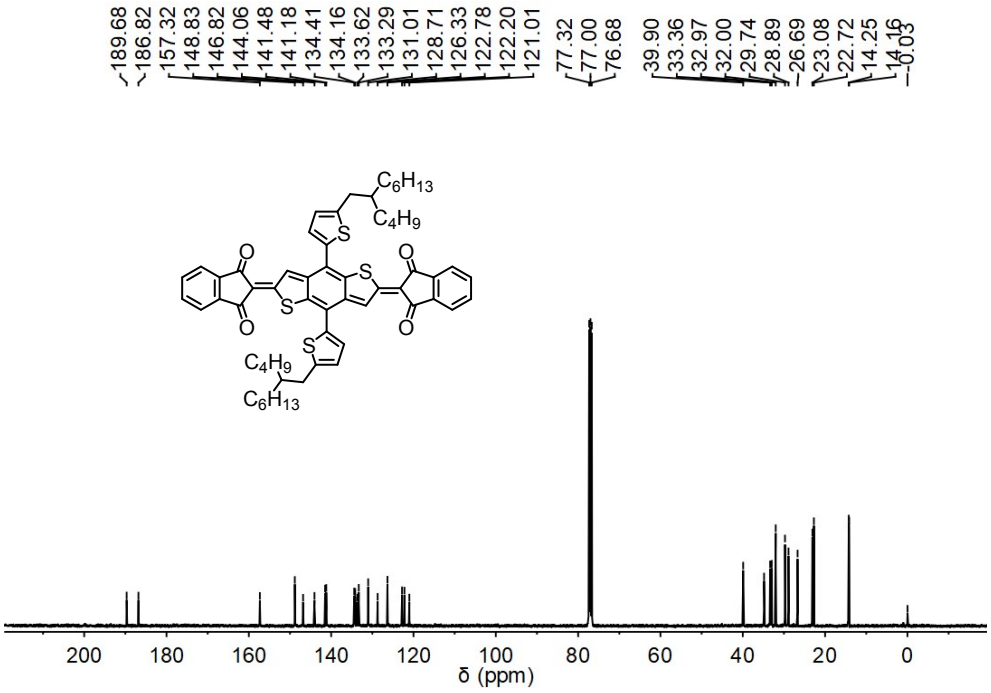


Figure S35. ^{13}C NMR spectrum of compound **5e** (100 MHz, $CDCl_3$).

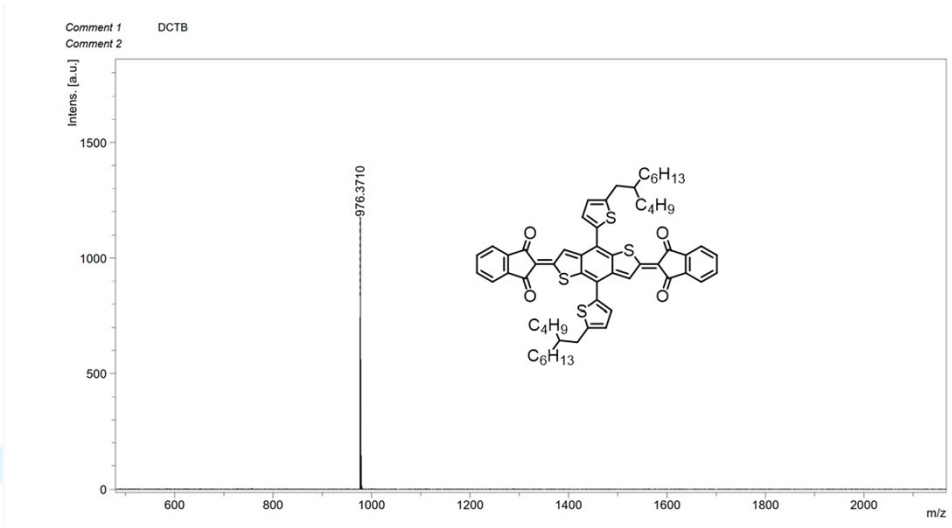


Figure S36. MALDI-TOF mass spectrum of compound **5e**.

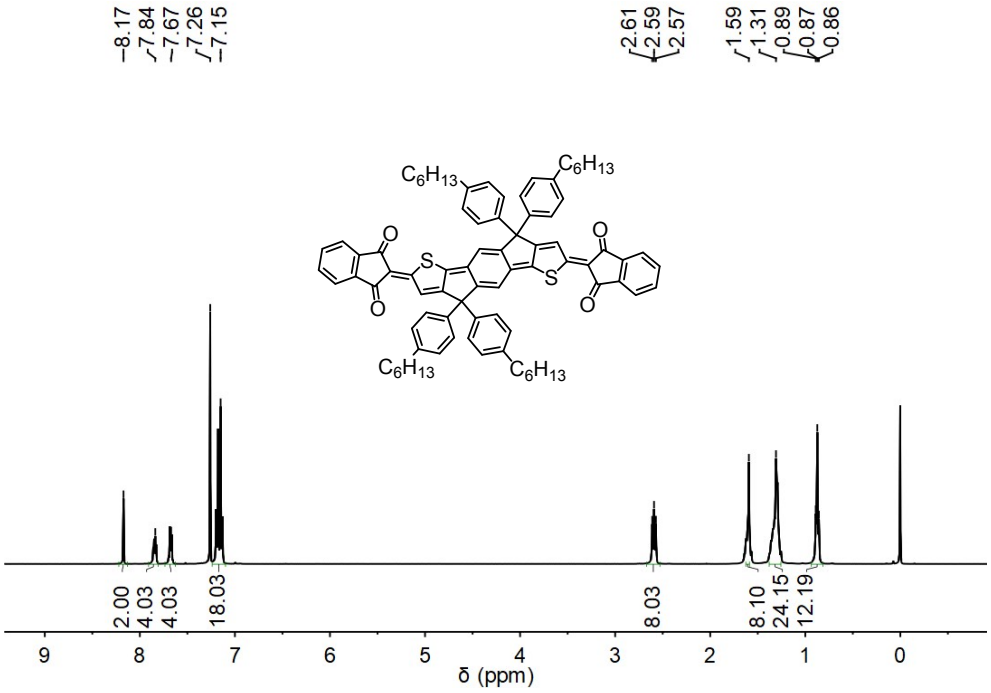


Figure S37. ^{1}H NMR spectrum of compound **5f** (400 MHz, $CDCl_3$).

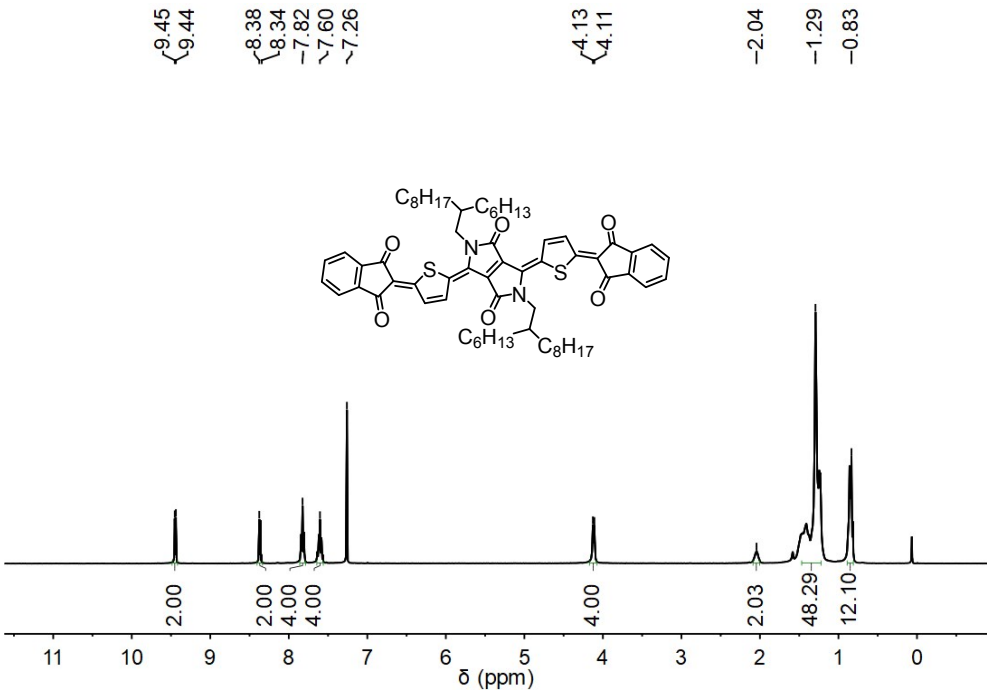


Figure S38. ^{1}H NMR spectrum of compound **5g** (400 MHz, $CDCl_3$).

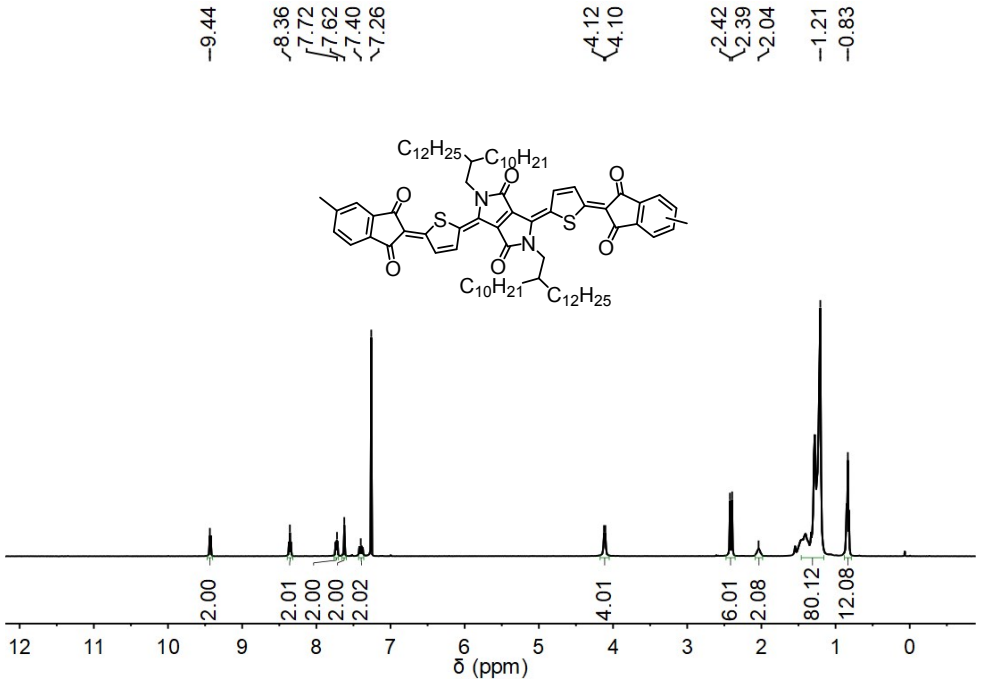


Figure S39. ^{1}H NMR spectrum of compound **5h** (400 MHz, $CDCl_3$).

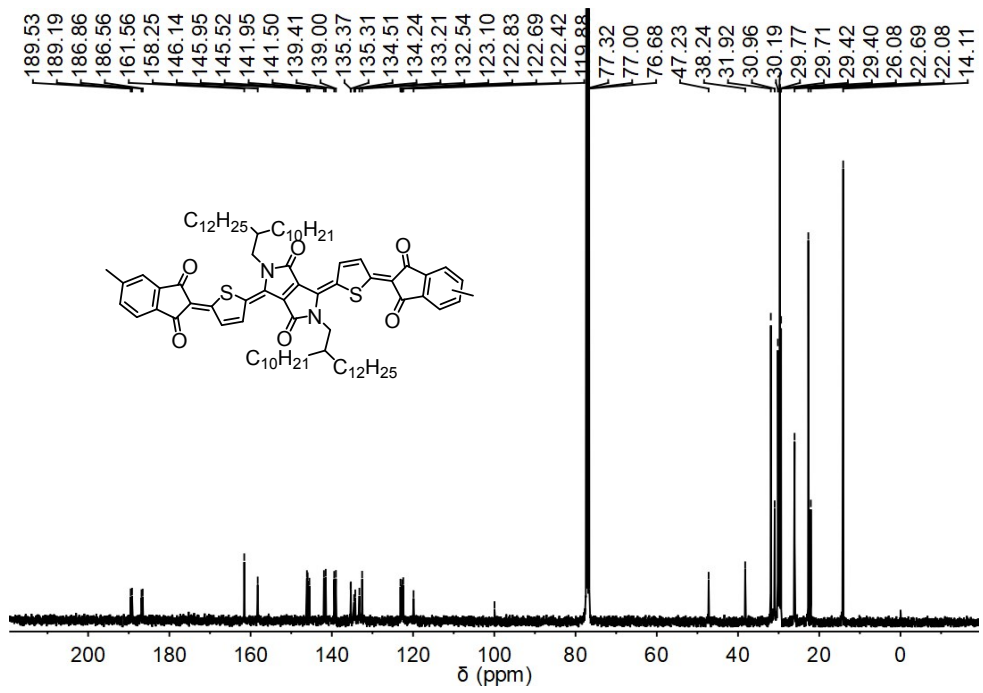


Figure S40. ^{13}C NMR spectrum of compound **5g** (100 MHz, $CDCl_3$).

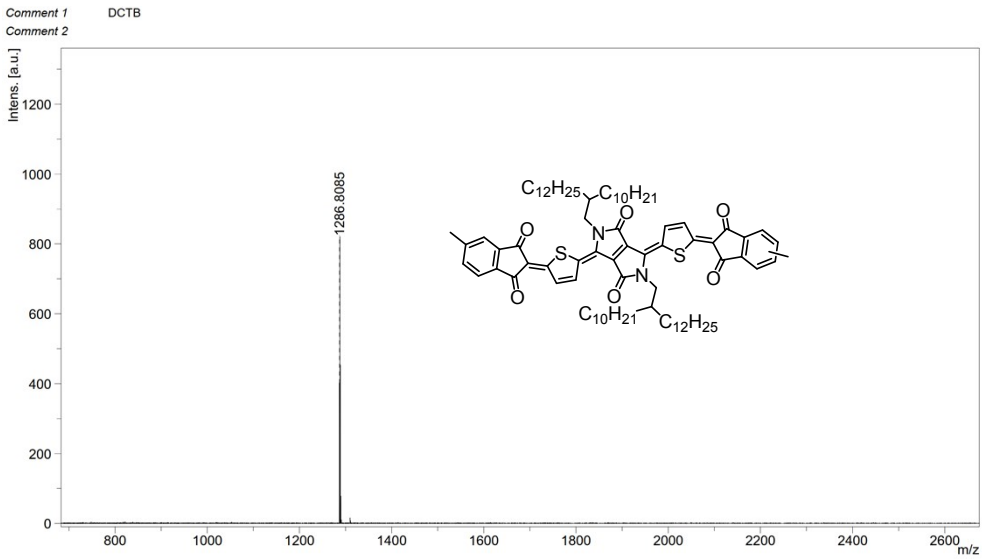


Figure S41 MALDI-TOF mass spectrum of compound **5g**.

7. X-ray crystallography

The single crystals of compound **5g** was grown by slow diffusion of methanol into their toluene solution. The data were collected on a "Bruker APEX-II CCD" diffractometer. In the Olex2, the structure was solved with the ShelXT structure solution program using Intrinsic Phasing and refined with the ShelXL refinement package using Least Squares minimisation.

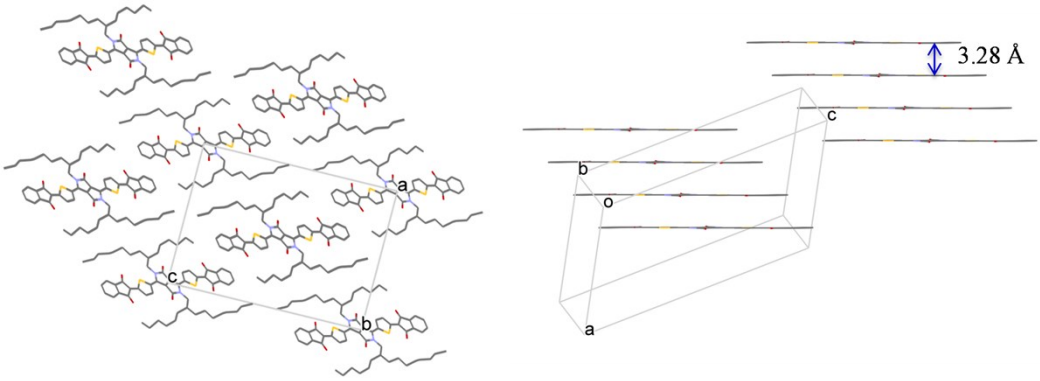


Figure S42. The molecular packing arrangement of compound **5g**.

Table S5. Crystal data and structure refinement for compound **5g**.

Identification code	190708dyf_2_0m	
Empirical formula	$C_{64}\ H_{78}\ N_2\ O_6\ S_2$	
Formula weight	1035.40	
Temperature	170.01 K	
Wavelength	1.34139 Å	
Crystal system	Monoclinic	
Space group	P 1 21/n 1	
Unit cell dimensions	a = 19.8786(11) Å	a= 90°.
	b = 5.1836(3) Å	b= 90.923(4)°.
	c = 27.5685(17) Å	g = 90°.
Volume	2840.4(3) $Å^3$	
Z	2	
Density (calculated)	1.211 Mg/m^3	
Absorption coefficient	0.818 mm^{-1}	
F(000)	1112	
Crystal size	0.1 x 0.02 x 0.01 mm^3	
Theta range for data collection	2.789 to 55.037°.	
Index ranges	-24<=h<=24, -3<=k<=6, -33<=l<=32	
Reflections collected	19822	
Independent reflections	5234 [R(int) = 0.0500]	
Completeness to theta = 53.594°	96.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7508 and 0.5864	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5234 / 83 / 336	
Goodness-of-fit on F^2	0.886	
Final R indices [I>2sigma(I)]	R1 = 0.0946, wR2 = 0.2388	
R indices (all data)	R1 = 0.1385, wR2 = 0.2707	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.673 and -0.484 $e.Å^{-3}$	

8. Cartesian coordinates (Å) and energies for the optimized structures

IM1-A

B3LYP SCF energy in gas phase: -2973.018581 a.u.

M06-L SCF energy in 1,4-dioxane: -2003.093021 a.u.

C	-2.693413	-1.534824	-0.135221
C	-3.567730	-0.488125	-0.451911
C	-4.785342	-0.661928	0.262592
C	-5.633279	0.412275	0.000103
N	-3.363178	-2.356805	0.768878
C	-4.681275	-1.868061	1.054052
O	-5.452697	-2.448656	1.814765
C	-2.926192	-3.619873	1.338793
H	-2.095967	-3.481706	2.038963
H	-3.783522	-4.020384	1.883469
H	-2.628186	-4.325403	0.557419
C	-1.370039	-1.752118	-0.645283
C	-0.822565	-1.042932	-1.698391
S	-0.176244	-2.876112	0.053402
C	0.545609	-1.345069	-1.987526
H	-1.396180	-0.302858	-2.245735
C	1.103521	-2.234867	-1.013728
H	0.987652	-1.170594	-2.963443
C	-6.955266	0.627755	0.532225
C	-7.614927	-0.241730	1.390461
S	-7.972567	2.030398	0.203544
C	-8.902514	0.210489	1.770651
H	-7.161089	-1.169286	1.725396
C	-9.235051	1.417726	1.211854
H	-9.559463	-0.340545	2.434516
H	-10.148836	1.984945	1.330079
N	-4.949990	1.253539	-0.880231
C	-5.401037	2.490992	-1.489385
H	-4.588701	2.820248	-2.140430
H	-6.303313	2.338092	-2.090400
H	-5.592785	3.264432	-0.738250
C	-3.649682	0.740848	-1.198386
O	-2.878334	1.324170	-1.966875
Pd	1.891465	-0.302538	-0.630915
Br	2.473259	-3.595170	-1.523725
P	3.370388	0.268045	1.137680
C	2.620456	-0.003197	2.900357
C	3.568754	0.143682	4.105468
C	1.462155	1.007140	3.040562
C	2.011171	-1.421665	2.934196
H	4.379378	-0.590350	4.087816
H	4.004756	1.142372	4.191149
H	2.995280	-0.032692	5.025520
H	0.754463	0.918109	2.208481
H	0.912331	0.796891	3.967312
H	1.813992	2.042235	3.086520
H	1.481114	-1.556743	3.886822
H	1.296265	-1.571731	2.122107
H	2.768634	-2.206923	2.866884
C	5.137300	-0.493482	1.005248
C	6.237289	0.185687	1.842429
C	5.061505	-1.988346	1.375453
C	5.532933	-0.377320	-0.482142
H	6.393802	1.225623	1.542728
H	6.033903	0.161891	2.916103
H	7.183744	-0.347098	1.678811
H	4.267641	-2.506628	0.828747
H	6.013648	-2.469463	1.115201
H	4.904870	-2.139978	2.447786
H	6.508059	-0.858630	-0.634979
H	4.802405	-0.864617	-1.135611
H	5.631829	0.669619	-0.789879
C	3.629041	2.108498	0.992525
C	3.059018	2.811370	-0.096925
C	4.337095	2.846152	1.962062
C	3.217127	4.208793	-0.162081
C	2.318402	2.208079	-1.266249
C	4.480039	4.229060	1.883826
H	4.788335	2.331347	2.800168
C	3.913077	4.917428	0.812120

H	2.784481	4.740010	-1.005571
C	3.069636	1.732808	-2.368011
C	0.924404	2.427676	-1.441622
H	5.030615	4.761514	2.654680
H	4.015252	5.996234	0.730939
C	2.482477	1.514841	-3.613573
H	4.138862	1.592367	-2.247279
C	0.351495	2.188866	-2.702749
C	1.118200	1.760815	-3.784453
H	3.092236	1.168793	-4.443787
H	-0.717280	2.341650	-2.820754
H	0.650106	1.608110	-4.753511
C	0.052377	2.985235	-0.339141
H	0.074711	4.083582	-0.335095
H	-0.985819	2.674422	-0.489669
H	0.378303	2.654254	0.650045

TS1-A

B3LYP SCF energy in gas phase: -2973.009332 a.u.

M06-L SCF energy in 1,4-dioxane: -2972.964389 a.u.

C	-3.003681	-1.315121	0.254311
C	-4.027908	-0.610516	-0.393712
C	-5.136051	-0.479072	0.485624
C	-6.137313	0.265376	-0.139517
N	-3.477025	-1.621447	1.530722
C	-4.807834	-1.130202	1.735374
O	-5.423450	-1.302312	2.785394
C	-2.835261	-2.413144	2.564969
H	-1.957927	-1.904871	2.979369
H	-3.576510	-2.537242	3.357061
H	-2.539374	-3.396497	2.186227
C	-1.723505	-1.663577	-0.275809
C	-1.343462	-1.463441	-1.608949
S	-0.351080	-2.255115	0.665930
C	-0.014457	-1.790437	-1.889308
H	-2.037537	-1.063167	-2.341036
C	0.715998	-2.161398	-0.745541
H	0.423638	-1.778858	-2.879701
C	-7.415020	0.638761	0.410550
C	-7.870880	0.278255	1.672086
S	-8.627468	1.627274	-0.403959
C	-9.159362	0.784497	1.971188
H	-7.273777	-0.329799	2.344677
C	-9.694283	1.529129	0.951224
H	-9.672064	0.602493	2.909209
H	-10.654775	2.025922	0.913639
N	-5.658726	0.591057	-1.408588
C	-6.320492	1.326550	-2.470964
H	-5.627009	1.326869	-3.314313
H	-7.254375	0.841819	-2.773063
H	-6.526406	2.361465	-2.178202
C	-4.340855	0.069705	-1.626445
O	-3.731376	0.234488	-2.686382
Pd	2.224151	-0.906710	-0.265654
Br	2.143361	-3.723356	-0.925671
P	4.143457	0.392665	0.377141
C	4.700638	-0.254158	2.122277
C	6.188393	-0.121588	2.505796
C	3.840071	0.474999	3.175376
C	4.341205	-1.757737	2.180628
H	6.843553	-0.677493	1.829521
H	6.537803	0.912558	2.551767
H	6.328321	-0.546410	3.508886
H	2.771078	0.378469	2.955975
H	4.016977	0.021631	4.159530
H	4.078268	1.539861	3.246858
H	4.572501	-2.142092	3.183341
H	3.275744	-1.926442	1.990212
H	4.905176	-2.354325	1.458467
C	5.535668	0.127248	-0.933697
C	6.828996	0.938936	-0.736480
C	5.874309	-1.375580	-0.997026
C	4.917449	0.545069	-2.285627
H	6.643153	2.016112	-0.763510
H	7.347196	0.701075	0.195678
H	7.518407	0.705538	-1.558947
H	4.977299	-1.991264	-1.124048
H	6.531314	-1.559334	-1.857432
H	6.405208	-1.720010	-0.104292
H	5.640607	0.349713	-3.088684
H	4.001643	-0.013202	-2.507164
H	4.679805	1.613543	-2.306161
C	4.039340	2.251760	0.533003
C	2.936733	3.002397	0.051643

C	5.093436	2.955604	1.151627
C	2.946935	4.401960	0.215571
C	1.723854	2.473756	-0.663715
C	5.081429	4.338144	1.311884
H	5.954111	2.412136	1.516978
C	3.995056	5.071124	0.838163
H	2.098963	4.965886	-0.163184
C	1.723847	2.457739	-2.066584
C	0.519987	2.210793	0.030581
H	5.916889	4.833987	1.798709
H	3.964223	6.151884	0.947221
C	0.567202	2.162623	-2.788982
H	2.639956	2.704606	-2.595730
C	-0.630492	1.921099	-0.713581
C	-0.619269	1.892782	-2.108876
H	0.593111	2.160442	-3.875631
H	-1.558936	1.718294	-0.185480
H	-1.533369	1.659208	-2.646947
C	0.447147	2.261629	1.539781
H	0.866000	3.192423	1.938669
H	-0.589543	2.181546	1.881271
H	1.010451	1.436640	1.992096

IM2-A

B3LYP SCF energy in gas phase: -2973.040818 a.u.

M06-L SCF energy in 1,4-dioxane: -2972.998497 a.u.

C	-3.582051	-0.200732	0.359522
C	-4.768550	-0.188823	-0.382945
C	-5.875997	-0.056770	0.500383
C	-7.057023	-0.025911	-0.239098
N	-3.950425	-0.077506	1.699929
C	-5.372948	0.014292	1.853792
O	-5.914528	0.122044	2.953188
C	-3.102210	-0.101848	2.877216
H	-2.438289	0.768365	2.915315
H	-3.775349	-0.073141	3.736463
H	-2.500137	-1.014981	2.915626
C	-2.244184	-0.318483	-0.139055
C	-1.910967	-0.532803	-1.473516
S	-0.755772	-0.166563	0.806352
C	-0.518623	-0.575484	-1.711619
H	-2.669953	-0.644476	-2.242353
C	0.259043	-0.361288	-0.588626
H	-0.095194	-0.771902	-2.690859
C	-8.399639	0.099966	0.272228
C	-8.730469	0.201973	1.616408
S	-9.864112	0.149341	-0.709259
C	-10.123985	0.316419	1.847123
H	-7.972705	0.193141	2.393819
C	-10.863377	0.303218	0.692655
H	-10.562350	0.404598	2.835176
H	-11.937248	0.373156	0.580317
N	-6.691660	-0.138952	-1.579912
C	-7.540037	-0.181280	-2.755607
H	-6.865845	-0.292942	-3.607549
H	-8.226808	-1.033909	-2.728061
H	-8.115380	0.743219	-2.873027
C	-5.265545	-0.246569	-1.734082
O	-4.728946	-0.363093	-2.836531
Pd	2.273439	-0.371650	-0.368631
Br	1.861878	-2.826620	-0.022643
P	4.675216	-0.469548	0.115009
C	5.041990	-1.136247	1.891985
C	6.350760	-0.623177	2.525436
C	3.864846	-0.645333	2.764085
C	5.062547	-2.678873	1.903771
H	7.242438	-0.899823	1.954970
H	6.348521	0.460677	2.665610
H	6.449756	-1.080629	3.518442
H	2.909174	-1.050364	2.419110
H	4.022931	-0.979705	3.797822
H	3.799101	0.448910	2.779164
H	5.113014	-3.013539	2.948248
H	4.164105	-3.110180	1.457490
H	5.942201	-3.082805	1.393259
C	5.794850	-1.291391	-1.221754
C	7.278141	-1.456986	-0.836715
C	5.216850	-2.680278	-1.570732
C	5.702601	-0.410974	-2.486588
H	7.785120	-0.501896	-0.676238
H	7.412010	-2.078654	0.052431
H	7.798092	-1.959218	-1.663105
H	4.170199	-2.624977	-1.877805
H	5.799272	-3.098739	-2.402368
H	5.276566	-3.384068	-0.737750

H	6.293046	-0.876641	-3.285875
H	4.671135	-0.336153	-2.847093
H	6.094729	0.598422	-2.326446
C	5.178613	1.311824	0.174847
C	4.183073	2.290166	-0.021696
C	6.502084	1.736788	0.406785
C	4.542109	3.651579	0.039690
C	2.751802	2.035653	-0.431963
C	6.842309	3.084983	0.461053
H	7.280796	1.002530	0.563499
C	5.851525	4.051047	0.281817
H	3.774550	4.401791	-0.129257
C	2.522662	1.733625	-1.806125
C	1.679270	2.622981	0.321799
H	7.872450	3.377132	0.644441
H	6.097910	5.108590	0.317499
C	1.321185	2.080872	-2.440926
H	3.360179	1.396412	-2.407706
C	0.497054	2.941934	-0.339188
C	0.320920	2.703015	-1.710430
H	1.191204	1.872064	-3.498329
H	-0.311729	3.396438	0.226202
H	-0.610161	2.989815	-2.189788
C	1.817170	2.907122	1.799569
H	1.873037	1.971737	2.369245
H	2.720535	3.479783	2.032050
H	0.952679	3.466673	2.167893

IM3-A

B3LYP SCF energy in gas phase: -3469.545875 a.u.

M06-L SCF energy in 1,4-dioxane: -3469.527456 a.u.

C	3.396650	-0.320519	-0.175839
C	4.583036	-0.239346	0.578428
C	5.650190	-0.819476	-0.160363
C	6.825750	-0.750899	0.582591
N	3.739489	-0.951797	-1.376661
C	5.126628	-1.283048	-1.428571
O	5.644859	-1.837924	-2.398641
C	2.886458	-1.240717	-2.515963
H	2.438379	-0.327351	-2.918786
H	3.531327	-1.694852	-3.270842
H	2.088208	-1.941806	-2.253177
C	2.099278	0.139453	0.180597
C	1.795874	0.822821	1.362467
S	0.610937	-0.032883	-0.766808
C	0.439882	1.177480	1.477547
H	2.556729	1.048378	2.104275
C	-0.373024	0.778512	0.414865
H	0.051570	1.741823	2.318247
C	8.131993	-1.226255	0.195148
C	8.436033	-1.834578	-1.014372
S	9.586613	-1.124632	1.190862
C	9.799404	-2.206611	-1.134370
H	7.678643	-1.996583	-1.775192
C	10.546807	-1.891129	-0.030069
H	10.210301	-2.692395	-2.013305
H	11.601472	-2.059861	0.142464
N	6.493103	-0.127708	1.786694
C	7.347480	0.202973	2.907823
H	6.700069	0.694416	3.638151
H	7.787764	-0.691269	3.363497
H	8.150318	0.890936	2.619460
C	5.094975	0.217812	1.840601
O	4.598258	0.781667	2.819717
Pd	-2.320324	1.123366	0.065896
Br	-4.803854	1.857198	-0.593160
P	-3.240901	-0.795729	1.375887
C	-2.127204	-2.304770	1.911919
C	-2.933361	-3.461795	2.539342
C	-1.450045	-2.856084	0.642664
C	-1.005968	-1.872508	2.877762
H	-3.398415	-3.199356	3.491232
H	-3.717675	-3.822311	1.867430
H	-2.248078	-4.299779	2.729615
H	-0.882874	-2.094111	0.106662
H	-0.752290	-3.653297	0.935814
H	-2.171693	-3.287129	-0.048502
H	-0.346760	-2.734884	3.048008
H	-0.396462	-1.068430	2.460030
H	-1.375291	-1.554565	3.855267
C	-3.863825	0.069830	3.038565
C	-4.101042	-0.841891	4.264321
C	-2.745621	1.075668	3.410708
C	-5.139484	0.912147	2.814555
H	-4.875972	-1.598229	4.111343

H	-3.196443	-1.352350	4.600561
H	-4.437036	-0.205732	5.094562
H	-2.611054	1.829848	2.628971
H	-3.038525	1.594100	4.334235
H	-1.780237	0.598098	3.592416
H	-5.315229	1.495726	3.729394
H	-5.031739	1.605550	1.980990
H	-6.033886	0.313860	2.629994
C	-4.705427	-1.673734	0.567102
C	-4.781319	-2.077813	-0.800197
C	-5.832939	-1.920814	1.372568
C	-6.003004	-2.590182	-1.276828
C	-3.677528	-2.088564	-1.825346
C	-7.021987	-2.456015	0.883126
H	-5.789832	-1.687937	2.425164
C	-7.120015	-2.768310	-0.468090
H	-6.060794	-2.853030	-2.329368
C	-3.193172	-0.898424	-2.383651
C	-3.197857	-3.326119	-2.326173
H	-7.861051	-2.611443	1.556720
H	-8.043910	-3.157672	-0.888459
C	-2.217721	-0.903408	-3.383844
H	-3.601824	0.045921	-2.046809
C	-2.217190	-3.312257	-3.326475
C	-1.722508	-2.118244	-3.852707
H	-1.854295	0.046393	-3.764727
H	-1.836709	-4.262362	-3.697731
H	-0.959054	-2.141556	-4.627142
C	-3.700892	-4.666624	-1.826006
H	-4.660195	-4.941487	-2.283258
H	-2.984431	-5.458637	-2.070502
H	-3.859716	-4.676265	-0.742941
C	0.447008	4.048331	-0.512636
C	0.485366	3.464226	-1.780760
C	1.625130	3.546232	-2.577573
C	2.733430	4.228811	-2.069723
C	2.694685	4.815756	-0.793758
C	1.547242	4.732070	-0.001084
C	-0.914199	3.832639	0.092439
C	-1.695742	2.984897	-0.858651
C	-0.846610	2.830054	-2.077963
H	1.636507	3.091764	-3.564522
H	3.639775	4.309254	-2.665422
H	3.572257	5.339440	-0.421943
H	1.500818	5.182478	0.986484
O	-1.131665	2.325791	-3.159698
O	-1.268410	4.312500	1.163702
H	-2.706366	3.338889	-1.057776

IM4-A

B3LYP SCF energy in gas phase: -3456.035650 a.u.

M06-L SCF energy in 1,4-dioxane: -3455.993167 a.u.

C	3.282539	-0.127273	-0.414894
C	4.448722	-0.412129	0.303570
C	5.557993	-0.430768	-0.587171
C	6.718090	-0.730953	0.124720
N	3.664527	0.034221	-1.746962
C	5.077184	-0.140940	-1.919273
O	5.629100	-0.034619	-3.013657
C	2.841005	0.387906	-2.888706
H	2.097881	-0.386454	-3.105446
H	3.521961	0.475773	-3.737713
H	2.330167	1.343163	-2.731929
C	1.948635	-0.016543	0.098661
C	1.604596	-0.110339	1.442211
S	0.479487	0.238103	-0.852130
C	0.216929	0.019078	1.687276
H	2.349985	-0.272637	2.215569
C	-0.554208	0.185601	0.550050
H	-0.200479	0.013718	2.686786
C	8.054975	-0.850307	-0.402976
C	8.401495	-0.665363	-1.734279
S	9.490429	-1.256029	0.537872
C	9.784119	-0.845524	-1.987306
H	7.662447	-0.409435	-2.487265
C	10.499384	-1.166792	-0.862575
H	10.232169	-0.740106	-2.969285
H	11.560756	-1.356217	-0.771336
N	6.338420	-0.897525	1.455795
C	7.164812	-1.202389	2.608263
H	6.487179	-1.228626	3.464365
H	7.924560	-0.431615	2.775636
H	7.653858	-2.177277	2.508922
C	4.923550	-0.707124	1.631742
O	4.377755	-0.799440	2.731705

Pd	-2.534096	0.443561	0.350743
P	-3.207630	-1.909492	0.296289
C	-3.355556	-2.711301	2.049848
C	-3.481209	-4.246784	2.070348
C	-4.594375	-2.103148	2.739975
C	-2.115546	-2.302093	2.870935
H	-2.601000	-4.743578	1.654444
H	-4.368827	-4.609043	1.544142
H	-3.572965	-4.573828	3.114441
H	-4.515632	-1.013964	2.818499
H	-4.658121	-2.497819	3.762138
H	-5.527093	-2.353048	2.225293
H	-2.195440	-2.737594	3.875674
H	-2.056088	-1.216364	2.977793
H	-1.178031	-2.649358	2.430433
C	-2.174908	-3.010509	-0.906866
C	-2.785693	-4.365941	-1.319844
C	-0.789273	-3.277838	-0.280709
C	-2.022645	-2.171475	-2.194891
H	-3.692334	-4.246121	-1.917559
H	-3.005449	-5.021471	-0.474050
H	-2.051318	-4.886298	-1.948594
H	-0.312263	-2.373960	0.099647
H	-0.131918	-3.703507	-1.049560
H	-0.847893	-4.006954	0.533649
H	-1.401626	-2.725527	-2.910895
H	-1.543440	-1.208830	-2.009668
H	-2.993705	-1.990717	-2.669700
C	-4.920355	-1.949238	-0.416439
C	-5.532717	-0.746697	-0.830014
C	-5.622494	-3.156590	-0.607210
C	-6.776688	-0.807074	-1.488599
C	-5.076789	0.651116	-0.497465
C	-6.862300	-3.196965	-1.238552
H	-5.191453	-4.087932	-0.265653
C	-7.433676	-2.013252	-1.704966
H	-7.240928	0.122155	-1.806473
C	-4.825784	1.607659	-1.521586
C	-5.371979	1.115520	0.810047
H	-7.372208	-4.147220	-1.370254
H	-8.394500	-2.025087	-2.212025
C	-4.961654	2.966856	-1.215573
C	-5.503620	2.475560	1.088573
C	-5.327057	3.401938	0.059876
H	-4.772029	3.696318	-1.997780
H	-5.754603	2.801551	2.093300
C	-0.070271	3.699999	-0.174307
C	-0.013570	3.576195	1.218639
C	1.068374	4.073039	1.942373
C	2.097884	4.697317	1.234636
C	2.039170	4.825644	-0.163838
C	0.950924	4.329111	-0.884534
C	-1.348002	3.102990	-0.678490
C	-2.064305	2.515779	0.502945
C	-1.258871	2.901804	1.710048
H	1.098423	3.972545	3.023301
H	2.957920	5.092518	1.768786
H	2.853721	5.319839	-0.686951
H	0.889835	4.426192	-1.964730
O	-1.558683	2.748808	2.886887
O	-1.719922	3.134705	-1.847207
H	-3.101866	2.837770	0.580641
H	-5.448140	4.464102	0.253984
H	-5.608942	0.387355	1.578066
C	-4.434489	1.210883	-2.925276
H	-5.151200	1.594659	-3.661831
H	-4.372349	0.127375	-3.046645
H	-3.455540	1.646600	-3.154575

TS2-A

B3LYP SCF energy in gas phase: -3456.010370 a.u.

M06-L SCF energy in 1,4-dioxane: -3455.965465 a.u.

C	3.340050	0.052926	0.411617
C	4.452525	-0.200332	-0.403190
C	5.587541	-0.455039	0.414301
C	6.692440	-0.717296	-0.395150
N	3.786382	-0.045013	1.731976
C	5.183136	-0.358190	1.799045
O	5.782580	-0.485289	2.865966
C	3.037703	0.154810	2.958895
H	2.237770	-0.584901	3.069427
H	3.753685	0.029170	3.773713
H	2.607016	1.159943	3.008123
C	2.009137	0.352198	-0.009731
C	1.610240	0.497612	-1.337958

S	0.604095	0.578877	1.047160	H	-0.650068	-3.038563	2.938964
C	0.246663	0.792518	-1.500708	H	-0.590530	-3.774377	1.336558
H	2.313762	0.390331	-2.159147	H	-2.616462	-1.878763	3.801093
C	-0.487146	0.834440	-0.308788	H	-2.408413	-0.642250	2.541797
H	-0.209170	0.987879	-2.463974	H	-3.977488	-1.443753	2.758311
C	8.033161	-1.026122	0.035845	C	-4.782212	-2.316235	-0.050056
C	8.444801	-1.102626	1.359406	C	-5.657145	-1.213899	-0.207610
S	9.394094	-1.366477	-1.033619	C	-5.353349	-3.603203	0.033083
C	9.816785	-1.425776	1.505704	C	-7.045866	-1.448014	-0.259947
H	7.758804	-0.928037	2.182496	C	-5.265600	0.225209	-0.411889
C	10.460306	-1.597866	0.307416	C	-6.727598	-3.816455	-0.024468
H	10.309089	-1.526841	2.466783	H	-4.711889	-4.464723	0.155038
H	11.498383	-1.846221	0.130254	C	-7.584427	-2.726409	-0.167866
N	6.249676	-0.624810	-1.714319	H	-7.707136	-0.595870	-0.391465
C	7.001061	-0.799021	-2.942674	C	-5.585215	1.221202	0.549006
H	6.290246	-0.631624	-3.754752	C	-4.854556	0.627329	-1.702241
H	7.816407	-0.072468	-3.024375	H	-7.121634	-4.826744	0.043475
H	7.409395	-1.811764	-3.027004	H	-8.660468	-2.868712	-0.217600
C	4.850778	-0.301102	-1.783252	C	-5.497913	2.567093	0.169312
O	4.256906	-0.166165	-2.854975	C	-4.780530	1.975948	-2.059253
Pd	-2.434516	0.251865	-0.225890	C	-5.111900	2.949672	-1.117935
P	-2.932243	-2.080547	0.047273	H	-5.748826	3.331405	0.900922
C	-2.201507	-3.194212	-1.350695	H	-4.458523	2.256379	-3.056687
C	-2.277330	-4.718690	-1.142557	C	-0.482364	4.188537	0.842866
C	-2.966368	-2.822966	-2.639497	C	-0.444617	4.346415	-0.548675
C	-0.719405	-2.806127	-1.546777	C	0.261745	5.393807	-1.136728
H	-1.752257	-5.043510	-0.239721	C	0.939254	6.277878	-0.294285
H	-3.302820	-5.094811	-1.106913	C	0.900242	6.120442	1.101726
H	-1.788297	-5.211311	-1.993464	C	0.183865	5.074507	1.687405
H	-2.897131	-1.750005	-2.850524	C	-1.325797	3.008500	1.194791
H	-2.518307	-3.355886	-3.487915	C	-1.741875	2.361993	-0.105833
H	-4.023925	-3.100933	-2.588950	C	-1.268714	3.286569	-1.203074
H	-0.334400	-3.324917	-2.434627	H	0.279741	5.506681	-2.216487
H	-0.592878	-1.732492	-1.700238	H	1.505472	7.101598	-0.720432
H	-0.092564	-3.100046	-0.701291	H	1.436373	6.825631	1.731032
C	-2.463970	-2.719997	1.807366	H	0.141731	4.944073	2.764532
C	-3.135786	-4.026479	2.271125	O	-1.531413	3.215644	-2.392145
C	-0.934352	-2.893716	1.888248	O	-1.645307	2.660348	2.319843
C	-2.892579	-1.595983	2.776541	H	-2.848163	2.283321	-0.135420
H	-4.220479	-3.925103	2.359708	H	-5.070321	4.002784	-1.381533
H	-2.918013	-4.876161	1.617785	H	-4.661241	-0.135887	-2.450014
H	-2.749614	-4.277566	3.267981	C	-5.996461	0.876871	1.962903
H	-0.397563	-2.016757	1.517782	H	-6.474755	1.734021	2.446660

H	-6.689348	0.031439	2.001549
H	-5.120457	0.608459	2.566032

IM1-B

B3LYP SCF energy in gas phase: -3287.518286 a.u.

M06-L SCF energy in 1,4-dioxane: -3287.468758 a.u.

C	-3.106350	-1.442278	-0.750066
C	-3.965985	-0.366467	-0.488693
C	-5.214108	-0.866038	-0.024482
C	-6.057663	0.201438	0.276798
N	-3.816010	-2.602961	-0.449180
C	-5.144533	-2.310087	0.006017
O	-5.946963	-3.188461	0.314796
C	-3.404383	-3.986430	-0.615872
H	-2.590297	-4.250763	0.066611
H	-4.279091	-4.593876	-0.375037
H	-3.094467	-4.187351	-1.645827
C	-1.765675	-1.384218	-1.255485
C	-1.159944	-0.222353	-1.696650
S	-0.626341	-2.756017	-1.319800
C	0.204949	-0.363127	-2.092537
H	-1.693396	0.722211	-1.721762
C	0.702644	-1.683828	-1.847971
H	0.685806	0.332112	-2.773478
C	-7.406834	0.130728	0.778979
C	-8.096549	-1.046767	1.035023
S	-8.428429	1.516967	1.160174
C	-9.409365	-0.836125	1.524284
H	-7.647556	-2.021084	0.868948
C	-9.731846	0.491098	1.644753
H	-10.090917	-1.640871	1.776939
H	-10.659247	0.929641	1.988711
N	-5.339220	1.366204	-0.000560
C	-5.764677	2.748006	0.123994
H	-4.917673	3.354726	-0.202450
H	-6.627361	2.963218	-0.515009
H	-6.009009	3.002325	1.160612
C	-4.022354	1.072244	-0.482638
O	-3.217935	1.958769	-0.791810
Pd	1.615610	-0.442846	-0.411774
Br	1.947486	-2.557477	-3.155604
P	3.261078	-1.190436	1.135672
C	2.606760	-2.370214	2.533928
C	3.661612	-3.121116	3.371701
C	1.734360	-1.536741	3.492978
C	1.687045	-3.409219	1.854006
H	4.284660	-3.787992	2.771436
H	4.316027	-2.450845	3.936190
H	3.138154	-3.746850	4.107187
H	0.918295	-1.039341	2.963441
H	1.283086	-2.208655	4.234982
H	2.311509	-0.781137	4.034328
H	1.222713	-4.034742	2.628604
H	0.890971	-2.925053	1.282121
H	2.227436	-4.074096	1.175295
C	4.839944	-1.969095	0.335082
C	6.105054	-2.005749	1.214140
C	4.504520	-3.395961	-0.146030
C	5.158398	-1.114315	-0.906724
H	6.438544	-1.001161	1.489098
H	5.980559	-2.591928	2.127498
H	6.915580	-2.471764	0.637891
H	3.595713	-3.417920	-0.753995
H	5.329261	-3.759311	-0.773328
H	4.392191	-4.103110	0.680075
H	6.008489	-1.559273	-1.441269
H	4.308892	-1.070176	-1.593480
H	5.440095	-0.093894	-0.632982
C	3.850933	0.351278	2.008123
C	3.366058	1.631567	1.628907
C	4.745746	0.272069	3.093593
C	3.807244	2.754810	2.356834
C	2.388932	1.956985	0.513213
C	5.168664	1.396214	3.797933
H	5.122155	-0.694982	3.399754
C	4.694147	2.651757	3.424430
H	3.429741	3.732268	2.071112
C	2.883305	2.518530	-0.706513
C	0.995469	2.068234	0.800715
H	5.858791	1.288134	4.630285
H	5.005535	3.544377	3.960287
C	1.990410	3.128762	-1.590562
C	0.146822	2.682595	-0.138040
C	0.617985	3.227418	-1.330058
H	2.384396	3.564207	-2.504725

H	-0.915629	2.748808	0.075817
C	0.411507	1.710829	2.168443
C	-0.867904	0.859477	2.080429
C	0.146587	2.991787	2.988757
H	1.160206	1.130344	2.712720
H	-0.694982	-0.060113	1.510870
H	-1.205896	0.586149	3.087639
H	-1.685386	1.398579	1.591195
H	1.059716	3.582589	3.118094
H	-0.599218	3.626472	2.496267
H	-0.233647	2.734869	3.984994
C	4.374944	2.567332	-1.040090
C	4.945328	3.988330	-0.843576
C	4.685558	2.070554	-2.465570
H	4.897680	1.911116	-0.337771
H	4.813087	4.338208	0.184975
H	6.018344	4.004247	-1.070439
H	4.450444	4.705632	-1.508948
H	4.250414	1.084836	-2.653439
H	4.299735	2.758673	-3.226390
H	5.769963	2.000392	-2.612641
C	-0.332063	3.949339	-2.278417
C	-0.247613	3.426976	-3.724610
C	-0.097273	5.473111	-2.235697
H	-1.350480	3.756945	-1.919147
H	-0.460539	2.353569	-3.775497
H	-0.977797	3.943154	-4.358939
H	0.744436	3.594897	-4.161015
H	-0.200431	5.861355	-1.216343
H	0.908423	5.728994	-2.591598
H	-0.820973	5.994010	-2.874196

TS1-B

B3LYP SCF energy in gas phase: -3287.508575 a.u.

M06-L SCF energy in 1,4-dioxane: -3287.455374 a.u.

C	-3.374283	-1.419044	-0.727214
C	-4.297645	-0.384200	-0.532448
C	-5.486237	-0.917399	0.034342
C	-6.380617	0.121307	0.294257
N	-3.988254	-2.591593	-0.288076
C	-5.315417	-2.345743	0.194184
O	-6.045023	-3.242184	0.612381
C	-3.489184	-3.952929	-0.366153
H	-2.655506	-4.120105	0.324466
H	-4.319741	-4.599612	-0.076090
H	-3.171744	-4.200482	-1.383837
C	-2.056875	-1.311444	-1.271566
C	-1.551069	-0.161070	-1.885159
S	-0.788141	-2.533069	-1.129994
C	-0.205182	-0.246500	-2.260480
H	-2.163591	0.724352	-2.017622
C	0.403657	-1.436466	-1.839691
H	0.332473	0.522745	-2.799540
C	-7.693842	0.011735	0.876093
C	-8.296296	-1.181628	1.252792
S	-8.773672	1.362585	1.222166
C	-9.589770	-1.010152	1.803845
H	-7.798631	-2.138553	1.129274
C	-9.983613	0.302617	1.852228
H	-10.207050	-1.831280	2.151099
H	-10.915342	0.711883	2.219841
N	-5.754016	1.299390	-0.113664
C	-6.265527	2.657521	-0.089816
H	-5.481315	3.282659	-0.521572
H	-7.174986	2.755812	-0.691416
H	-6.468424	2.993833	0.932286
C	-4.444449	1.046198	-0.641081
O	-3.718058	1.945956	-1.070109
Pd	1.935183	-1.179438	-0.565343
Br	1.878802	-2.377694	-3.123379
P	3.729263	-1.058904	1.016223
C	3.360254	-2.304203	2.467327
C	4.564783	-2.884519	3.235754
C	2.430814	-1.597953	3.473763
C	2.573250	-3.487225	1.856109
H	5.239765	-3.457621	2.594623
H	5.147634	-2.123709	3.761016
H	4.186830	-3.575891	4.000909
H	1.528484	-1.217034	2.988037
H	2.113788	-2.323270	4.234793
H	2.924317	-0.768314	3.988154
H	2.276075	-4.173605	2.660772
H	1.664564	-3.144566	1.349797
H	3.162625	-4.059041	1.134691
C	5.371643	-1.566793	0.125781

C	6.683251	-1.415276	0.920084
C	5.233459	-3.024243	-0.362429
C	5.473629	-0.659608	-1.116548
H	6.880351	-0.373237	1.186352
H	6.711263	-2.017000	1.831777
H	7.514247	-1.751163	0.285366
H	4.305087	-3.179768	-0.922249
H	6.068821	-3.251950	-1.037551
H	5.272415	-3.749327	0.455724
H	6.362488	-0.940757	-1.697306
H	4.599828	-0.760605	-1.767497
H	5.579968	0.392878	-0.840633
C	4.102495	0.574229	1.852439
C	3.432489	1.798232	1.570177
C	5.081624	0.579588	2.869127
C	3.783666	2.935227	2.329267
C	2.355097	2.089159	0.544576
C	5.412356	1.716580	3.599754
H	5.604209	-0.337808	3.101513
C	4.751583	2.911418	3.327496
H	3.263362	3.864360	2.116645
C	2.708157	2.705265	-0.684571
C	0.988722	2.030911	0.918646
H	6.173684	1.662710	4.373214
H	4.982467	3.815618	3.884298
C	1.698650	3.226365	-1.503206
C	0.020120	2.562191	0.058181
C	0.347431	3.178459	-1.151391
H	1.985702	3.717452	-2.428792
H	-1.027882	2.513782	0.343083
C	0.534000	1.490240	2.273181
C	-0.569215	0.423126	2.144729
C	0.073771	2.635821	3.198670
H	1.394486	1.017340	2.754234
H	-0.254708	-0.393830	1.484426
H	-0.806533	0.000537	3.129110
H	-1.495334	0.841398	1.735784
H	0.871941	3.370735	3.351240
H	-0.790069	3.161651	2.775572
H	-0.218285	2.243933	4.180791
C	4.160994	2.914267	-1.114394
C	4.591988	4.384945	-0.931948
C	4.424758	2.461564	-2.563517
H	4.796451	2.311517	-0.458373
H	4.493814	4.706071	0.110084
H	5.639272	4.518836	-1.229976
H	3.978871	5.053212	-1.548154
H	4.081393	1.436562	-2.733379
H	3.917669	3.108526	-3.288353
H	5.497949	2.505578	-2.785279
C	-0.737133	3.850698	-1.986913
C	-0.618138	3.578583	-3.496405
C	-0.753349	5.370006	-1.714572
H	-1.700255	3.445402	-1.654086
H	-0.634671	2.505745	-3.717809
H	-1.457039	4.040425	-4.029831
H	0.305111	3.994213	-3.917831
H	-0.885155	5.579339	-0.647236
H	0.186931	5.836988	-2.033719
H	-1.572738	5.853265	-2.260689

IM2-B

B3LYP SCF energy in gas phase: -3287.539204 a.u.

M06-L SCF energy in 1,4-dioxane: -3287.493428 a.u.

C	-3.762911	-0.995266	0.061639
C	-4.895373	-0.408748	-0.512989
C	-6.052544	-0.812958	0.208831
C	-7.172396	-0.173502	-0.319406
N	-4.212177	-1.768943	1.131447
C	-5.637390	-1.702036	1.272372
O	-6.247162	-2.321812	2.142158
C	-3.442787	-2.659516	1.981859
H	-2.783265	-2.105310	2.658386
H	-4.168756	-3.217665	2.576418
H	-2.842852	-3.353420	1.385494
C	-2.399617	-0.836925	-0.347518
C	-1.994036	-0.224686	-1.529509
S	-0.968504	-1.265216	0.598949
C	-0.591502	-0.114335	-1.658119
H	-2.708165	0.145254	-2.258031
C	0.122091	-0.590214	-0.571999
H	-0.113186	0.302150	-2.537274
C	-8.536520	-0.295635	0.132041
C	-8.958657	-1.117385	1.168006
S	-9.913773	0.581099	-0.534972

C	-10.351887	-1.041660	1.415865	C	6.397978	1.116394	0.843209
H	-8.264814	-1.742865	1.721215	C	4.443272	3.015606	1.270066
C	-11.000525	-0.169931	0.579750	C	2.564332	1.633391	0.497579
H	-10.855184	-1.614839	2.186781	C	6.754242	2.358073	1.360839
H	-12.053932	0.075175	0.548931	H	7.179545	0.386560	0.680185
N	-6.719138	0.622747	-1.371670	C	5.766281	3.318123	1.575685
C	-7.484181	1.461509	-2.274479	H	3.671897	3.761028	1.440815
H	-6.761747	1.882043	-2.977433	C	2.014246	2.358656	-0.621085
H	-8.230365	0.882828	-2.829016	C	1.708804	1.399952	1.634188
H	-7.982704	2.279261	-1.743021	H	7.793913	2.571060	1.593336
C	-5.295253	0.516463	-1.542116	H	6.020962	4.294096	1.979633
O	-4.686964	1.129750	-2.420934	C	0.685076	2.775938	-0.585543
Pd	2.126554	-0.675844	-0.316664	C	0.383082	1.839837	1.594990
Br	1.815686	-2.911143	-1.427702	C	-0.148929	2.547908	0.515519
P	4.566785	-0.879636	-0.112976	H	0.292358	3.321188	-1.436659
C	5.246497	-2.156729	1.180965	H	-0.251890	1.654658	2.457048
C	6.768372	-2.404132	1.133246	C	2.242812	0.844931	2.953579
C	4.891768	-1.648317	2.591797	C	1.449283	-0.375345	3.455290
C	4.516668	-3.502837	0.978591	C	2.280448	1.945136	4.036144
H	7.107146	-2.805821	0.176429	H	3.273559	0.526984	2.788548
H	7.351000	-1.507718	1.361301	H	1.432795	-1.176484	2.708649
H	7.017996	-3.148529	1.900787	H	1.902425	-0.767304	4.373833
H	3.811885	-1.547996	2.721419	H	0.409310	-0.118786	3.684841
H	5.240156	-2.385502	3.326782	H	2.888368	2.798751	3.719100
H	5.368355	-0.692199	2.828429	H	1.274468	2.313545	4.266617
H	4.854516	-4.199857	1.757246	H	2.712559	1.547885	4.962205
H	3.432738	-3.395908	1.061679	C	2.870873	2.795063	-1.809120
H	4.725603	-3.959854	0.009969	C	3.082287	4.324289	-1.820068
C	5.483672	-1.118899	-1.806091	C	2.287272	2.329447	-3.156907
C	6.928176	-0.583257	-1.841737	H	3.857730	2.338112	-1.696380
C	5.483961	-2.608492	-2.211511	H	3.567296	4.671206	-0.902118
C	4.668394	-0.345423	-2.861312	H	3.717507	4.611201	-2.666475
H	6.972212	0.495529	-1.667975	H	2.129695	4.856495	-1.920856
H	7.590210	-1.078534	-1.126684	H	2.124177	1.247959	-3.170289
H	7.337590	-0.770207	-2.843078	H	1.330294	2.817705	-3.372963
H	4.479163	-3.036580	-2.193391	H	2.974899	2.582119	-3.972657
H	5.861283	-2.682119	-3.239924	C	-1.573854	3.083901	0.607107
H	6.139929	-3.218169	-1.585139	C	-2.195878	3.500549	-0.732514
H	5.133379	-0.491627	-3.845267	C	-1.632526	4.255237	1.613659
H	3.636850	-0.702163	-2.919696	H	-2.186892	2.267962	1.014603
H	4.659967	0.729250	-2.661597	H	-2.194448	2.681688	-1.457050
C	5.063464	0.791121	0.526302	H	-3.239222	3.795168	-0.578672
C	4.061342	1.763171	0.747476	H	-1.676643	4.362175	-1.170845

H	-1.247313	3.967741	2.597851
H	-1.037422	5.104195	1.254998
H	-2.666159	4.596810	1.740401

IM3-B

B3LYP SCF energy in gas phase: -3784.025744 a.u.

M06-L SCF energy in 1,4-dioxane: -3783.993039 a.u.

C	4.001625	0.325508	-0.105032
C	5.207298	0.676716	0.533989
C	6.301690	0.145430	-0.202072
C	7.497078	0.474079	0.431859
N	4.362225	-0.417992	-1.234707
C	5.777004	-0.562856	-1.350769
O	6.311601	-1.176539	-2.275610
C	3.496119	-0.973410	-2.258058
H	2.900943	-0.193213	-2.742187
H	4.154832	-1.437511	-2.994788
H	2.821551	-1.730202	-1.847122
C	2.674630	0.645646	0.293230
C	2.353212	1.437620	1.400480
S	1.162743	0.111788	-0.472700
C	0.971590	1.593314	1.604568
H	3.120960	1.880300	2.028660
C	0.154603	0.909441	0.703065
H	0.557969	2.234170	2.374786
C	8.832752	0.124721	0.011969
C	9.149948	-0.604251	-1.125302
S	10.313380	0.558905	0.870853
C	10.543125	-0.806190	-1.298491
H	8.380882	-0.971921	-1.797669
C	11.300624	-0.240371	-0.306712
H	10.967378	-1.353697	-2.133726
H	12.376714	-0.241822	-0.194500
N	7.150085	1.212450	1.564329
C	8.012824	1.812485	2.560285
H	7.345790	2.314436	3.265354
H	8.601575	1.059968	3.097200
H	8.691497	2.551198	2.119243
C	5.722610	1.372878	1.680742
O	5.209830	1.999708	2.611974
Pd	-1.843837	1.007319	0.522197
Br	-4.371155	1.666730	0.123593
P	-2.474923	-1.002242	2.143203
C	-1.015835	-1.664632	3.262542
C	-1.337406	-2.858563	4.187286
C	0.090727	-2.150094	2.314645
C	-0.459827	-0.503639	4.111683
H	-2.086584	-2.640413	4.947850
H	-1.661389	-3.738031	3.624360
H	-0.412411	-3.131992	4.713968
H	0.430123	-1.370902	1.635840
H	0.953568	-2.482404	2.908373
H	-0.249798	-3.002117	1.725270
H	0.475251	-0.831997	4.586069
H	-0.226804	0.370588	3.502529
H	-1.139399	-0.199249	4.911521
C	-3.843779	-0.322424	3.404218
C	-3.909806	-0.912498	4.834603
C	-3.526441	1.182290	3.588324
C	-5.249360	-0.477290	2.783912
H	-4.168048	-1.973556	4.880341
H	-2.993741	-0.757455	5.407863
H	-4.709883	-0.377701	5.364280
H	-3.584210	1.732047	2.650023
H	-4.266940	1.613751	4.276558
H	-2.536436	1.345330	4.024485
H	-5.957928	0.109366	3.385339
H	-5.293669	-0.094927	1.764243
H	-5.591201	-1.516354	2.790632
C	-3.178969	-2.634801	1.452805
C	-3.040522	-3.190283	0.142656
C	-3.900462	-3.400260	2.395394
C	-3.635209	-4.448626	-0.104069
C	-2.299285	-2.657396	-1.069983
C	-4.477618	-4.635637	2.122539
H	-4.007589	-3.019165	3.397978
C	-4.343595	-5.171781	0.847047
H	-3.528766	-4.859657	-1.102533
C	-2.949824	-1.813046	-2.015607
C	-1.027418	-3.200322	-1.395182
H	-5.018814	-5.164792	2.902891
H	-4.778739	-6.134522	0.590737
C	-2.247548	-1.422661	-3.161013
C	-0.387192	-2.788614	-2.572399
C	-0.960910	-1.878202	-3.454341

H	-2.723329	-0.736522	-3.850194
H	0.589110	-3.202612	-2.813278
C	-2.970772	4.211978	-1.659342
C	-2.649786	4.793799	-0.431579
C	-3.244018	5.984495	-0.020772
C	-4.174918	6.581432	-0.874142
C	-4.493157	5.998657	-2.112703
C	-3.889456	4.806874	-2.520315
C	-2.151173	2.969227	-1.855239
C	-1.335033	2.765267	-0.607567
C	-1.597893	3.972083	0.254889
H	-2.980144	6.424981	0.936671
H	-4.659014	7.510875	-0.582695
H	-5.218760	6.486485	-2.759800
H	-4.123141	4.344638	-3.475166
O	-1.050448	4.298196	1.301705
O	-2.114248	2.331408	-2.900477
H	-0.279417	2.642590	-0.846679
C	-0.223050	-1.416609	-4.704059
C	0.135009	0.080455	-4.623498
C	-1.011057	-1.727365	-5.991221
H	0.717618	-1.984512	-4.753016
H	0.780714	0.280807	-3.762086
H	0.661576	0.401317	-5.532073
H	-0.756212	0.703467	-4.497011
H	-1.251795	-2.794620	-6.063444
H	-1.953109	-1.168132	-6.025208
H	-0.427576	-1.446907	-6.877234
C	-0.352384	-4.316646	-0.589335
C	1.154166	-4.086123	-0.353438
C	-0.545361	-5.686012	-1.279067
H	-0.839032	-4.380212	0.388187
H	1.359244	-3.083562	0.029814
H	1.538891	-4.816943	0.368727
H	1.729625	-4.216007	-1.277701
H	-1.602667	-5.945172	-1.387047
H	-0.098116	-5.680431	-2.280283
H	-0.060329	-6.480740	-0.697325
C	-4.424009	-1.404027	-1.895937
C	-5.365077	-2.566632	-2.292240
C	-4.804157	-0.186974	-2.759171
H	-4.624281	-1.138294	-0.853051
H	-5.277635	-3.431737	-1.632405
H	-6.407568	-2.225559	-2.257192
H	-5.155678	-2.896348	-3.318369
H	-4.105294	0.642603	-2.643137
H	-4.859651	-0.458320	-3.822716
H	-5.793946	0.171226	-2.457993

IM4-B

B3LYP SCF energy in gas phase: -3770.535365 a.u.

M06-L SCF energy in 1,4-dioxane: -3770.483507 a.u.

C	-4.067015	-0.120512	-0.378309
C	-5.181665	-0.094214	0.466897
C	-6.365088	-0.240717	-0.309295
C	-7.474526	-0.241454	0.534650
N	-4.554675	-0.275680	-1.676187
C	-5.986406	-0.354644	-1.699760
O	-6.625300	-0.484067	-2.743058
C	-3.813386	-0.305158	-2.923505
H	-3.157049	-1.179713	-2.983034
H	-4.559520	-0.366202	-3.718384
H	-3.216177	0.602755	-3.054290
C	-2.688072	-0.015568	-0.001725
C	-2.236135	0.218831	1.291813
S	-1.289729	-0.185329	-1.075009
C	-0.827100	0.262592	1.404982
H	-2.921418	0.347530	2.124734
C	-0.150092	0.032918	0.218081
H	-0.321701	0.472977	2.340964
C	-8.858545	-0.373105	0.151584
C	-9.311505	-0.504396	-1.153909
S	-10.226439	-0.398106	1.264607
C	-10.720225	-0.621655	-1.252820
H	-8.628705	-0.515255	-1.997909
C	-11.350161	-0.581454	-0.035676
H	-11.247718	-0.731601	-2.193981
H	-12.409077	-0.647646	0.176530
N	-6.989085	-0.092314	1.833121
C	-7.727236	-0.015421	3.079558
H	-6.978769	0.118441	3.863540
H	-8.414399	0.837189	3.090212
H	-8.288593	-0.935365	3.274412
C	-5.554738	0.008578	1.854991
O	-4.920140	0.155750	2.899994

Pd	1.833192	-0.018441	-0.013887	C	4.927430	2.678926	0.724294
P	2.180400	-2.440353	-0.208715	H	5.504796	2.662147	-1.345373
C	1.301311	-3.635344	1.044149	H	4.277562	2.349101	2.735437
C	1.471513	-5.147988	0.790968	C	-0.180829	3.251325	-1.322694
C	1.864008	-3.305369	2.440724	C	-0.237994	3.527872	0.047809
C	-0.211599	-3.323211	1.067016	C	-1.249348	4.324100	0.580704
H	1.162090	-5.451467	-0.212372	C	-2.208225	4.836951	-0.295944
H	2.491959	-5.496106	0.965028	C	-2.148990	4.562317	-1.673040
H	0.830447	-5.686281	1.501244	C	-1.131197	3.765900	-2.202778
H	1.696100	-2.256697	2.701212	C	1.017162	2.399457	-1.607033
H	1.342131	-3.919108	3.186304	C	1.669980	2.086518	-0.293414
H	2.933610	-3.522691	2.521670	C	0.930230	2.887553	0.735976
H	-0.667559	-3.903908	1.879648	H	-1.280481	4.533396	1.645899
H	-0.412030	-2.268766	1.257647	H	-3.012378	5.459387	0.087586
H	-0.717551	-3.607222	0.143143	H	-2.907073	4.979107	-2.331036
C	1.860173	-3.023495	-2.035799	H	-1.070286	3.549658	-3.265485
C	2.720609	-4.215998	-2.496370	O	1.223460	3.054399	1.913433
C	0.376232	-3.386765	-2.244506	O	1.381913	2.052982	-2.726265
C	2.191871	-1.820167	-2.941618	H	2.745607	2.263575	-0.290526
H	3.790716	-3.995385	-2.463832	C	4.011980	-0.308688	2.915279
H	2.535011	-5.123927	-1.915410	C	2.774250	0.194747	3.679611
H	2.462931	-4.441722	-3.539437	C	5.246499	-0.330046	3.842164
H	-0.298749	-2.595322	-1.912532	H	3.816866	-1.340590	2.615440
H	0.207550	-3.534055	-3.319370	H	1.890968	0.209224	3.034700
H	0.096794	-4.318752	-1.745119	H	2.573378	-0.459756	4.536464
H	1.997524	-2.096457	-3.986588	H	2.910999	1.211221	4.062615
H	1.587631	-0.938804	-2.707423	H	6.125062	-0.743127	3.335394
H	3.244589	-1.536756	-2.871144	H	5.499234	0.678973	4.187747
C	4.008367	-2.695898	0.073790	H	5.045297	-0.946960	4.726056
C	4.872393	-1.608369	0.351757	C	5.380572	0.101642	-2.064454
C	4.561490	-3.994145	0.063810	C	6.913512	0.092751	-2.248216
C	6.226506	-1.882076	0.637144	C	4.713673	0.839279	-3.243610
C	4.547487	-0.126509	0.387389	H	5.050477	-0.941685	-2.085904
C	5.902213	-4.240722	0.342326	H	7.414384	-0.496243	-1.473689
H	3.935012	-4.839524	-0.179593	H	7.173819	-0.338579	-3.222164
C	6.744259	-3.172372	0.641909	H	7.318497	1.110940	-2.214434
H	6.880634	-1.045076	0.862168	H	3.634968	0.959654	-3.106599
C	4.986068	0.687636	-0.708026	H	5.141212	1.840053	-3.378098
C	4.302485	0.497809	1.650954	H	4.891463	0.287905	-4.174865
H	6.280132	-5.259157	0.324227	C	5.183995	4.165752	0.931046
H	7.793343	-3.337587	0.871346	C	4.268986	5.043858	0.056430
C	5.157589	2.059823	-0.511086	C	6.668186	4.516501	0.707113
C	4.475300	1.881623	1.776015	H	4.946300	4.388742	1.979320

H	3.214331	4.852800	0.276842
H	4.468390	6.105359	0.244541
H	4.434376	4.857625	-1.011500
H	7.321348	3.916753	1.350852
H	6.969226	4.341554	-0.332690
H	6.847700	5.574617	0.930372

TS2-B

B3LYP SCF energy in gas phase: -3770.510995 a.u.

M06-L SCF energy in 1,4-dioxane: -3770.459932 a.u.

C	-4.044125	0.132697	-0.398797
C	-5.149636	-0.023383	0.448940
C	-6.324586	-0.189667	-0.334255
C	-7.423323	-0.356569	0.508106
N	-4.534859	0.064891	-1.705304
C	-5.953634	-0.134518	-1.730563
O	-6.591809	-0.218896	-2.779116
C	-3.807918	0.192776	-2.954646
H	-3.075439	-0.611515	-3.080629
H	-4.555051	0.120973	-3.747762
H	-3.297558	1.158502	-3.026079
C	-2.681084	0.322007	-0.017683
C	-2.231662	0.435551	1.297530
S	-1.294144	0.428219	-1.116060
C	-0.843628	0.614265	1.419044
H	-2.916868	0.389005	2.139676
C	-0.145505	0.591551	0.206028
H	-0.347104	0.776619	2.368112
C	-8.796581	-0.557151	0.117494
C	-9.251179	-0.603995	-1.193363
S	-10.148970	-0.783863	1.227138
C	-10.648327	-0.816088	-1.298711
H	-8.577559	-0.487690	-2.036735
C	-11.268655	-0.932438	-0.081609
H	-11.174765	-0.879893	-2.244774
H	-12.317762	-1.095999	0.126464
N	-6.936845	-0.293113	1.813493
C	-7.665100	-0.395937	3.063693
H	-6.920638	-0.281220	3.854503
H	-8.415895	0.395459	3.160232
H	-8.152018	-1.371260	3.169194
C	-5.515060	-0.083261	1.840553
O	-4.881585	0.009503	2.893835
Pd	1.733111	-0.164736	0.042745
P	2.046276	-2.515005	-0.312026
C	1.099376	-3.692522	0.907427
C	0.959959	-5.170609	0.488116
C	1.821178	-3.638431	2.268318
C	-0.317244	-3.108423	1.107361
H	0.409318	-5.295970	-0.447120
H	1.920303	-5.684915	0.397784
H	0.391855	-5.695938	1.267247
H	1.887324	-2.614693	2.645251
H	1.243029	-4.219854	2.998287
H	2.829113	-4.061906	2.225752
H	-0.845408	-3.714677	1.855289
H	-0.284434	-2.078522	1.469303
H	-0.915935	-3.122023	0.193677
C	1.635747	-3.002620	-2.140259
C	2.233621	-4.332350	-2.637994
C	0.104468	-3.031167	-2.322072
C	2.195831	-1.873097	-3.027239
H	3.327021	-4.318280	-2.630445
H	1.893184	-5.199611	-2.066689
H	1.917055	-4.485994	-3.678222
H	-0.366439	-2.114193	-1.957804
H	-0.118582	-3.116072	-3.393880
H	-0.364919	-3.885260	-1.826926
H	1.931392	-2.075219	-4.074021
H	1.786340	-0.895130	-2.756126
H	3.286031	-1.818794	-2.970302
C	3.862481	-2.907720	-0.082996
C	4.824335	-1.906749	0.221403
C	4.301805	-4.244802	-0.162911
C	6.158319	-2.306716	0.440514
C	4.606429	-0.412818	0.356597
C	5.626386	-4.615472	0.051256
H	3.588716	-5.022117	-0.399875
C	6.565600	-3.634675	0.360517
H	6.888098	-1.540373	0.684582
C	4.974258	0.449693	-0.717275
C	4.370622	0.152055	1.643264
H	5.915685	-5.660385	-0.020005
H	7.604864	-3.896803	0.539217
C	5.051273	1.828618	-0.490984

C	4.457893	1.540474	1.805801
C	4.799597	2.400802	0.760110
H	5.339535	2.471867	-1.316475
H	4.269198	1.966644	2.787191
C	0.159549	3.877421	-1.110440
C	0.106502	4.100024	0.272126
C	-0.521824	5.227159	0.797758
C	-1.106462	6.125322	-0.097804
C	-1.052477	5.902936	-1.484470
C	-0.414163	4.776499	-2.007751
C	0.903188	2.613936	-1.389103
C	1.237039	1.994494	-0.053137
C	0.823179	3.003985	0.991511
H	-0.552217	5.389161	1.870945
H	-1.610808	7.010924	0.279036
H	-1.515186	6.620995	-2.156048
H	-0.362110	4.595148	-3.077038
O	1.062206	2.968570	2.186653
O	1.201087	2.181625	-2.491623
H	2.331059	1.816765	0.027065
C	4.134487	-0.708483	2.883334
C	2.899676	-0.267927	3.691053
C	5.390591	-0.728572	3.779551
H	3.962147	-1.735039	2.550331
H	2.006343	-0.233784	3.058058
H	2.718652	-0.969106	4.514737
H	3.028363	0.727771	4.128815
H	6.264892	-1.103351	3.236334
H	5.628793	0.275755	4.149040
H	5.228739	-1.377136	4.648937
C	5.375648	-0.076600	-2.095517
C	6.909018	-0.050569	-2.274275
C	4.698977	0.688743	-3.250258
H	5.063119	-1.123452	-2.158197
H	7.416765	-0.658904	-1.519128
H	7.183908	-0.439539	-3.262179
H	7.293846	0.973262	-2.197411
H	3.619205	0.783343	-3.104657
H	5.108977	1.699836	-3.356763
H	4.878868	0.169040	-4.198961
C	4.976361	3.892113	1.022053
C	4.357056	4.790428	-0.062018
C	6.469933	4.227393	1.218349
H	4.460707	4.113315	1.966005
H	3.291233	4.580358	-0.200049
H	4.458045	5.845051	0.219155
H	4.852992	4.662410	-1.031295
H	6.908762	3.628233	2.023744
H	7.039348	4.026168	0.302640
H	6.599890	5.286709	1.470489

3

B3LYP SCF energy in gas phase: -2664.853382 a.u.

M06-L SCF energy in 1,4-dioxane: -2664.780303 a.u.

C	-1.696891	-0.389568	-0.283577
C	-0.576383	0.411990	-0.059447
C	0.576362	-0.412184	0.060015
C	1.696880	0.389389	0.284062
N	-1.248986	-1.709394	-0.303339
C	0.169651	-1.789668	-0.093849
O	0.774999	-2.859941	-0.074177
C	-2.010359	-2.929561	-0.503556
H	-2.494900	-2.945341	-1.485137
H	-1.288540	-3.746928	-0.447908
H	-2.766976	-3.065108	0.275786
C	-3.056513	0.050862	-0.465398
C	-3.466545	1.376161	-0.435212
S	-4.438622	-1.007962	-0.735149
C	-4.857002	1.538642	-0.632939
H	-2.770067	2.192913	-0.272979
C	-5.531385	0.351029	-0.803510
H	-5.355393	2.499348	-0.661252
C	3.056531	-0.050987	0.465804
C	3.466604	-1.376278	0.435803
S	4.438643	1.007941	0.735125
C	4.857099	-1.538668	0.633338
H	2.770137	-2.193084	0.273805
C	5.531468	-0.350997	0.803570
H	5.355530	-2.499349	0.661755
N	1.248975	1.709214	0.303782
C	2.010334	2.929365	0.504152
H	1.288484	3.746722	0.448758
H	2.495002	2.944945	1.485671
H	2.766847	3.065104	-0.275261
C	-0.169667	1.789481	0.094323

O	-0.775038	2.859742	0.074711
C	6.997015	-0.153971	1.092127
C	7.640600	1.098957	0.452349
C	7.925243	-1.309449	0.643734
C	8.915928	0.681905	-0.182107
C	9.078641	-0.703837	-0.073585
C	9.869328	1.474262	-0.823151
C	10.201336	-1.342484	-0.601846
C	10.992835	0.839192	-1.352421
H	9.728293	2.547768	-0.902498
C	11.157008	-0.553921	-1.242811
H	10.313527	-2.418624	-0.512679
H	11.754517	1.425000	-1.859312
H	12.042525	-1.018705	-1.667252
C	-6.996896	0.154099	-1.092328
C	-7.640627	-1.098850	-0.452744
C	-7.925123	1.309586	-0.643957
C	-8.915988	-0.681781	0.181636
C	-9.078621	0.703978	0.073203
C	-9.869486	-1.474137	0.822534
C	-10.201335	1.342642	0.601405
C	-10.993010	-0.839050	1.351749
H	-9.728514	-2.547657	0.901810
C	-11.157104	0.554080	1.242226
H	-10.313464	2.418794	0.512308
H	-11.754768	-1.424858	1.858526
H	-12.042636	1.018876	1.666620
O	7.181466	2.223211	0.481105
O	7.762385	-2.494006	0.855923
O	-7.762210	2.494147	-0.856086
O	-7.181568	-2.223133	-0.481577
H	7.140731	-0.045101	2.181704
H	-7.140441	0.045335	-2.181936

4

B3LYP SCF energy in gas phase: -2664.835688 a.u.

M06-L SCF energy in 1,4-dioxane: -2664.775799 a.u.

C	1.729667	0.361774	0.000092
C	0.570206	-0.422321	0.000328
C	-0.570207	0.422301	0.000347
C	-1.729667	-0.361794	0.000305
N	1.309753	1.692057	-0.000023
C	-0.120435	1.796008	0.000123
O	-0.705052	2.878788	0.000062
C	2.113635	2.901626	-0.000232
H	2.744112	2.965823	-0.892727
H	1.406222	3.733314	-0.000495
H	2.743946	2.966269	0.892355
C	3.088122	-0.100168	0.000037
C	3.462293	-1.442907	0.000071
S	4.514693	0.932728	-0.000026
C	4.852204	-1.636239	0.000038
H	2.729918	-2.244266	0.000124
C	5.585358	-0.454233	-0.000018
H	5.322695	-2.611059	0.000041
C	-3.088121	0.100152	0.000286
C	-3.462286	1.442892	0.000370
S	-4.514696	-0.932740	0.000143
C	-4.852196	1.636229	0.000279
H	-2.729910	2.244250	0.000454
C	-5.585355	0.454227	0.000126
H	-5.322685	2.611051	0.000314
N	-1.309753	-1.692078	0.000289
C	-2.113635	-2.901647	0.000398
H	-1.406221	-3.733334	0.000492
H	-2.744046	-2.965972	0.892933
H	-2.744011	-2.966163	-0.892150
C	0.120435	-1.796029	0.000287
O	0.705052	-2.878809	0.000268
C	-7.014129	0.290970	-0.000002
C	-7.715540	-1.026571	-0.000321
C	-7.991696	1.257127	0.000131
C	-9.190982	-0.733829	-0.000357
C	-9.343084	0.663864	-0.000077
C	-10.279007	-1.581103	-0.000604
C	-10.606595	1.237215	-0.000039
C	-11.566306	-1.006401	-0.000567
H	-10.138392	-2.657974	-0.000818
C	-11.722815	0.378054	-0.000289
H	-10.758899	2.315026	0.000175
H	-12.443321	-1.646882	-0.000756
H	-12.721295	0.805909	-0.000265
C	7.014130	-0.290970	-0.000065
C	7.715531	1.026578	-0.000156
C	7.991705	-1.257119	-0.000020

C	9.190974	0.733847	-0.000180
C	9.343088	-0.663844	-0.000089
C	10.278993	1.581130	-0.000280
C	10.606604	-1.237184	-0.000090
C	11.566297	1.006439	-0.000280
H	10.138372	2.658000	-0.000352
C	11.722817	-0.378015	-0.000186
H	10.758917	-2.314994	-0.000028
H	12.443306	1.646929	-0.000353
H	12.721301	-0.805862	-0.000192
O	-7.199677	-2.131760	-0.000529
O	-7.758982	2.581758	0.000419
O	7.758999	-2.581750	0.000079
O	7.199659	2.131759	-0.000212
H	-8.600334	3.066427	0.000454
H	8.600353	-3.066415	0.000158

O_2

B3LYP SCF energy in gas phase: -150.316605 a.u.

M06-L SCF energy in 1,4-dioxane: -150.319562 a.u.

O	0.000000	0.000000	0.607148
O	0.000000	0.000000	-0.607148

TS1

B3LYP SCF energy in gas phase: -2815.136497 a.u.

M06-L SCF energy in 1,4-dioxane: -2815.075540 a.u.

C	2.138634	-0.365113	-0.484079
C	0.989802	0.431876	-0.314362
C	-0.152085	-0.388126	-0.280249
C	-1.304717	0.414896	-0.109205
N	1.699311	-1.679712	-0.554491
C	0.271584	-1.766242	-0.433563
O	-0.330270	-2.835285	-0.469747
C	2.477257	-2.895860	-0.727026
H	3.182317	-3.039682	0.097303
H	1.758644	-3.717440	-0.731628
H	3.022111	-2.889935	-1.676028
C	3.496938	0.085611	-0.570234
C	3.894613	1.416350	-0.486379
S	4.902105	-0.959422	-0.774766
C	5.290556	1.590700	-0.590797
H	3.183584	2.225475	-0.352125
C	5.983361	0.408488	-0.742532
H	5.785578	2.553032	-0.562283
C	-2.648822	-0.026377	-0.023170
C	-3.048685	-1.374365	-0.106106
S	-4.057405	1.019632	0.186667
C	-4.422214	-1.554931	0.002614
H	-2.332946	-2.178161	-0.244690
C	-5.139232	-0.358822	0.159329
H	-4.928072	-2.511154	-0.035527
N	-0.852464	1.731783	-0.040518
C	-1.627300	2.950364	0.134533
H	-0.906618	3.770067	0.137738
H	-2.333982	3.095932	-0.687901
H	-2.170220	2.945037	1.084403
C	0.569139	1.813125	-0.161494
O	1.181912	2.875872	-0.127677
C	-6.556793	-0.213765	0.346007
C	-7.532343	-1.283393	-0.102522
C	-7.237946	1.106487	0.099568
C	-8.826263	-0.582673	-0.356572
C	-8.656514	0.803151	-0.238200
C	-10.061833	-1.131141	-0.689553
C	-9.716185	1.681417	-0.449723
C	-11.129398	-0.254250	-0.898856
H	-10.178964	-2.206563	-0.780780
C	-10.959106	1.135096	-0.780244
H	-9.569745	2.753384	-0.358874
H	-12.107576	-0.649427	-1.158779
H	-11.808072	1.791500	-0.950113
C	7.465737	0.232526	-0.935192
C	8.070903	-1.063189	-0.345685
C	8.358074	1.353485	-0.344424
C	9.315015	-0.695773	0.373039
C	9.478535	0.694813	0.376441
C	10.238705	-1.534366	0.998510
C	10.572343	1.291617	1.004532
C	11.333626	-0.940857	1.626870
H	10.097473	-2.610690	0.991532
C	11.498551	0.456408	1.629716
H	10.685470	2.371279	1.002172
H	12.071825	-1.563226	2.124659
H	12.361176	0.887562	2.129828

O	8.190878	2.549867	-0.465432
O	7.602619	-2.177838	-0.464929
O	-6.720547	2.210727	0.164868
O	-7.324772	-2.477337	-0.232117
H	7.686048	0.203054	-2.017023
H	-6.765870	-0.319424	1.706706
O	-7.032351	-0.449734	2.902231
O	-8.157332	-1.053959	2.989067

Int-1

B3LYP SCF energy in gas phase: -2815.172195 a.u.

M06-L SCF energy in 1,4-dioxane: -2815.100577 a.u.

C	2.232185	-0.280106	-0.487073
C	1.108877	0.575216	-0.376068
C	-0.060546	-0.186052	-0.324157
C	-1.191443	0.681676	-0.209533
N	1.734443	-1.573376	-0.503354
C	0.304868	-1.589709	-0.403869
O	-0.345865	-2.630495	-0.398820
C	2.459536	-2.830509	-0.604425
H	3.143044	-2.964956	0.239165
H	1.705663	-3.619405	-0.584630
H	3.019743	-2.892136	-1.542211
C	3.606405	0.107151	-0.567020
C	4.061721	1.423854	-0.538535
S	4.968482	-1.006739	-0.693372
C	5.464380	1.532043	-0.622606
H	3.384968	2.268521	-0.457216
C	6.107416	0.314262	-0.703784
H	6.001769	2.471781	-0.628361
C	-2.537828	0.311056	-0.129074
C	-2.998493	-1.038636	-0.153484
S	-3.909872	1.427223	0.016578
C	-4.360992	-1.163632	-0.061545
H	-2.309713	-1.872918	-0.238144
C	-5.052053	0.082430	0.040984
H	-4.905920	-2.098497	-0.063042
N	-0.669776	1.978786	-0.194486
C	-1.389442	3.240225	-0.096495
H	-0.632298	4.025771	-0.121570
H	-2.074658	3.373688	-0.938552
H	-1.947454	3.308164	0.841833
C	0.747988	1.985827	-0.294712
O	1.417200	3.013292	-0.301391
C	-6.417368	0.287466	0.147014
C	-7.461442	-0.741240	0.177554
C	-7.056897	1.609715	0.246644
C	-8.765817	-0.021420	0.297867
C	-8.527627	1.362916	0.338431
C	-10.058046	-0.533774	0.366099
C	-9.571018	2.271814	0.447769
C	-11.112045	0.382787	0.476409
H	-10.241492	-1.605619	0.334790
C	-10.874490	1.763667	0.516724
H	-9.371809	3.338803	0.477810
H	-12.133370	0.016235	0.531741
H	-11.714655	2.447473	0.602582
C	7.583677	0.066603	-0.855532
C	8.118472	-1.232621	-0.208572
C	8.513858	1.167759	-0.285239
C	9.368815	-0.896418	0.513959
C	9.594459	0.485067	0.472589
C	10.245848	-1.752906	1.180980
C	10.705534	1.054213	1.095926
C	11.358127	-1.187007	1.804399
H	10.056889	-2.821536	1.208820
C	11.585400	0.200823	1.762204
H	10.866833	2.127078	1.058807
H	12.061221	-1.823895	2.333593
H	12.459935	0.610363	2.259734
O	8.397700	2.365544	-0.445020
O	7.597528	-2.327024	-0.292055
O	-6.490332	2.698377	0.252447
O	-7.300745	-1.967383	0.115921
H	7.825092	-0.011095	-1.930485
H	-8.346588	-3.329348	0.134527
O	-8.848216	-4.196101	0.134869
O	-10.130987	-3.859875	0.235477

TS2

B3LYP SCF energy in gas phase: -2815.137609 a.u.

M06-L SCF energy in 1,4-dioxane: -2815.077847 a.u.

C	2.155178	-0.363483	-0.003047
C	0.993279	0.449010	0.092219

C	-0.150284	-0.364392	0.049692
C	-1.305273	0.438466	0.143553
N	1.696833	-1.679239	-0.104234
C	0.274289	-1.750824	-0.076812
O	-0.344820	-2.807273	-0.150928
C	2.474234	-2.903959	-0.222298
H	3.121427	-3.050697	0.647271
H	1.750564	-3.719360	-0.272564
H	3.080918	-2.904826	-1.132498
C	3.496708	0.066233	0.003735
C	3.894328	1.427018	0.115775
S	4.913686	-0.987587	-0.122051
C	5.256694	1.610906	0.102882
H	3.166687	2.227447	0.202397
C	6.001000	0.400654	-0.021325
H	5.765585	2.563514	0.177548
C	-2.669950	-0.007583	0.141227
C	-3.061150	-1.343236	0.035851
S	-4.076211	1.044666	0.252415
C	-4.453689	-1.516223	0.052866
H	-2.341720	-2.151210	-0.051961
C	-5.161404	-0.324478	0.155456
H	-4.953879	-2.473913	-0.013702
N	-0.867642	1.749886	0.243167
C	-1.649836	2.970412	0.366369
H	-0.929421	3.788488	0.420174
H	-2.297456	3.118615	-0.502895
H	-2.256140	2.964828	1.277076
C	0.565261	1.829443	0.217091
O	1.167944	2.896307	0.292590
C	-6.608076	-0.156274	0.255157
C	-7.552378	-1.229303	-0.268445
C	-7.247422	1.168285	-0.116261
C	-8.777635	-0.525656	-0.735097
C	-8.607230	0.861923	-0.635408
C	-9.964935	-1.074069	-1.215912
C	-9.617636	1.742634	-1.014812
C	-10.980746	-0.194832	-1.596681
H	-10.083934	-2.150572	-1.289973
C	-10.809582	1.196673	-1.496479
H	-9.472112	2.815419	-0.934752
H	-11.918930	-0.588453	-1.977522
H	-11.618825	1.854591	-1.800470
C	7.376526	0.262691	-0.063208
C	8.088600	-1.019328	-0.193290
C	8.372250	1.356348	0.015503
C	9.547983	-0.696815	-0.192953
C	9.713092	0.690909	-0.070368
C	10.643741	-1.547064	-0.290665
C	10.978780	1.265136	-0.041722
C	11.920158	-0.973924	-0.262531
H	10.502604	-2.619599	-0.384947
C	12.085536	0.414116	-0.139439
H	11.092698	2.340799	0.053852
H	12.797831	-1.610259	-0.336569
H	13.088823	0.830985	-0.120185
O	8.176732	2.560648	0.127913
O	7.580653	-2.133633	-0.283671
O	-6.734006	2.268143	-0.012865
O	-7.370134	-2.435560	-0.257199
H	-6.890176	-0.265567	1.507957
O	-7.213916	-0.560817	2.719965
O	-8.294229	-1.417112	2.613199
H	-7.876717	-2.300130	2.537638

TS3

B3LYP SCF energy in gas phase: -2815.143313 a.u.

M06-L SCF energy in 1,4-dioxane: -2815.088909 a.u.

C	2.156861	-0.529046	-0.012829
C	0.964048	0.228091	-0.051583
C	-0.142449	-0.632239	-0.026186
C	-1.339849	0.132291	-0.064672
N	1.767560	-1.862560	0.035736
C	0.341165	-1.998634	0.029985
O	-0.219119	-3.090721	0.067181
C	2.598827	-3.053326	0.085610
H	3.219680	-3.069681	0.986786
H	1.912272	-3.901743	0.108143
H	3.237818	-3.131376	-0.799458
C	3.491849	-0.031004	-0.020897
C	3.835738	1.324289	-0.073528
S	4.950816	-1.020970	0.034757
C	5.215228	1.557730	-0.069728
H	3.081938	2.104375	-0.112714
C	5.982666	0.395435	-0.014000

H	5.672200	2.537684	-0.106081
C	-2.663001	-0.356451	-0.056582
C	-3.007867	-1.726073	-0.008447
S	-4.125908	0.637161	-0.102728
C	-4.371733	-1.960458	-0.008797
H	-2.251224	-2.503452	0.023940
C	-5.153562	-0.785616	-0.053449
H	-4.837175	-2.936807	0.024347
N	-0.940264	1.467195	-0.113061
C	-1.770108	2.660962	-0.164456
H	-1.082761	3.508326	-0.191283
H	-2.393237	2.674972	-1.063628
H	-2.406566	2.742563	0.721662
C	0.481044	1.598399	-0.107616
O	1.051725	2.683668	-0.145360
C	-6.560849	-0.707031	-0.052433
C	-7.345706	0.465634	-0.087431
C	-7.485715	-1.873914	-0.002005
C	-8.780910	0.105482	-0.064810
C	-8.871573	-1.297330	-0.007709
C	-9.924581	0.896065	-0.110793
C	-10.094682	-1.942467	0.014590
C	-11.167323	0.242645	-0.087040
H	-9.864323	1.978006	-0.171095
C	-11.255006	-1.150860	-0.022277
H	-10.144698	-3.026479	0.055122
H	-12.077729	0.834562	-0.118432
H	-12.231824	-1.626032	-0.002876
C	7.414919	0.306939	0.003482
C	8.218037	-0.808112	0.058253
C	8.333218	1.494219	-0.038520
C	9.648628	-0.455911	0.056108
C	9.734129	0.945504	-0.002752
C	10.796028	-1.235799	0.099262
C	10.950944	1.595972	-0.019738
C	12.040698	-0.578903	0.082223
H	10.762301	-2.322668	0.145016
C	12.120427	0.811898	0.023723
H	10.995166	2.680021	-0.065362
H	12.952359	-1.168342	0.115234
H	13.093506	1.293740	0.011696
O	-6.855755	1.654897	-0.174990
H	-7.428413	2.503389	0.295866
O	-7.206344	-3.062553	0.042503
O	8.034104	2.673541	-0.091210
O	7.750933	-2.065913	0.107437
H	8.485890	-2.699994	0.140986
O	-7.964778	3.529460	0.896272
O	-8.843520	4.003514	0.083318

Int-2

B3LYP SCF energy in gas phase: -2815.164239 a.u.

M06-L SCF energy in 1,4-dioxane: -2815.098815 a.u.

C	2.159845	-0.552098	0.000080
C	0.956101	0.200014	0.000047
C	-0.139597	-0.661815	0.000048
C	-1.351093	0.102121	-0.000002
N	1.776496	-1.887356	0.000119
C	0.353300	-2.029371	0.000090
O	-0.203428	-3.123811	0.000117
C	2.614334	-3.075245	0.000266
H	3.244261	-3.118108	0.894049
H	1.933069	-3.928051	0.000419
H	3.244193	-3.118392	-0.893552
C	3.488008	-0.046280	0.000063
C	3.823837	1.314367	0.000091
S	4.954723	-1.028230	-0.000050
C	5.200192	1.556243	0.000060
H	3.064620	2.090146	0.000124
C	5.976592	0.396958	-0.000001
H	5.651090	2.539669	0.000090
C	-2.659294	-0.387851	0.000034
C	-2.995416	-1.774803	0.000117
S	-4.134919	0.599594	0.000127
C	-4.343713	-2.022112	0.000113
H	-2.229163	-2.543292	0.000143
C	-5.149829	-0.842495	0.000054
H	-4.806402	-3.000660	0.000157
N	-0.949184	1.441088	-0.000060
C	-1.783305	2.634045	-0.000199
H	-1.099536	3.484561	-0.000320
H	-2.413097	2.678829	-0.893409
H	-2.413066	2.679068	0.893021
C	0.465242	1.574288	-0.000019
O	1.039473	2.657605	-0.000069

C	-6.533388	-0.780404	-0.000021
C	-7.318802	0.447162	-0.000104
C	-7.460932	-1.935367	0.000032
C	-8.756485	0.056266	-0.000085
C	-8.839619	-1.346199	0.000013
C	-9.900257	0.849405	-0.000294
C	-10.066910	-1.994330	-0.000047
C	-11.139408	0.195614	-0.000368
H	-9.831505	1.935051	-0.000509
C	-11.223324	-1.203654	-0.000224
H	-10.116109	-3.079089	0.000022
H	-12.052749	0.784153	-0.000576
H	-12.200344	-1.679436	-0.000286
C	7.408272	0.319034	-0.000028
C	8.220500	-0.791750	-0.000090
C	8.317596	1.514422	0.000029
C	9.647813	-0.428219	-0.000092
C	9.722252	0.975188	-0.000026
C	10.801494	-1.200310	-0.000142
C	10.934138	1.635317	-0.000014
C	12.040776	-0.533556	-0.000127
H	10.776276	-2.288351	-0.000191
C	12.109538	0.859251	-0.000065
H	10.969948	2.720616	0.000036
H	12.957122	-1.116576	-0.000166
H	13.078868	1.348695	-0.000055
O	-6.848997	1.596008	-0.000033
H	-7.529522	3.167197	0.000655
O	-7.193628	-3.130591	0.000056
O	8.008790	2.692346	0.000066
O	7.762495	-2.053500	-0.000146
H	8.501768	-2.683535	-0.000188
O	-7.811761	4.128495	0.000605
O	-9.141508	4.104265	-0.000127

TS4

B3LYP SCF energy in gas phase: -2815.151888 a.u.

M06-L SCF energy in 1,4-dioxane: -2815.095918 a.u.

C	1.285937	0.110173	-0.031469
C	0.086730	-0.642317	-0.006945
C	-1.014180	0.225219	-0.026621
C	-2.216473	-0.532804	-0.001599
N	0.903392	1.446148	-0.066048
C	-0.520944	1.590179	-0.064956
O	-1.076122	2.684574	-0.092485
C	1.742099	2.633869	-0.099853
H	2.367454	2.655091	-0.997434
H	1.060479	3.486145	-0.117572
H	2.376732	2.699286	0.788990
C	2.614543	-0.393511	-0.023087
C	2.947996	-1.759701	0.014886
S	4.077741	0.591866	-0.057357
C	4.316739	-2.002339	0.016546
H	2.187369	-2.533439	0.039809
C	5.099998	-0.835277	-0.019952
H	4.774538	-2.982448	0.042769
C	-3.539252	-0.035179	-0.009989
C	-3.865782	1.344195	-0.048577
S	-5.006031	-1.023047	0.025811
C	-5.221249	1.594565	-0.049781
H	-3.098149	2.111063	-0.074171
C	-6.022279	0.419553	-0.011816
H	-5.681564	2.573960	-0.076440
N	-1.828924	-1.869709	0.033219
C	-2.666295	-3.059639	0.067097
H	-1.983938	-3.911166	0.085155
H	-3.292135	-3.080733	0.963993
H	-3.300718	-3.125252	-0.821552
C	-0.406924	-2.009896	0.031831
O	0.154111	-3.099912	0.059345
C	-7.407202	0.345111	-0.003336
C	-8.181982	-0.905431	0.037052
C	-8.346749	1.488771	-0.033363
C	-9.624022	-0.512320	0.031267
C	-9.719700	0.886770	-0.010092
C	-10.760938	-1.312009	0.059461
C	-10.955387	1.523210	-0.024401
C	-12.007648	-0.676115	0.045255
H	-10.673293	-2.393875	0.091261
C	-12.103523	0.723219	0.003771
H	-11.015727	2.606941	-0.056494
H	-12.916179	-1.271782	0.066478
H	-13.085013	1.189384	-0.006466
C	6.514934	-0.761393	-0.027154
C	7.305181	0.402557	-0.062651

C	7.429667	-1.933197	0.007245
C	8.741870	0.035853	-0.058726
C	8.821193	-1.368179	-0.012865
C	9.896072	0.812790	-0.080786
C	10.036641	-2.025972	0.013044
C	11.132683	0.147497	-0.050955
H	9.849549	1.896938	-0.115766
C	11.206153	-1.246994	-0.005706
H	10.073684	-3.110618	0.047997
H	12.048986	0.730769	-0.068413
H	12.177715	-1.732682	0.011082
O	-7.729951	-2.046951	0.069054
O	-8.090343	2.686610	-0.069924
O	7.143983	-3.120210	0.045018
O	6.810530	1.595498	-0.085040
H	7.510833	2.438025	-0.146685
O	8.302333	3.528995	-0.243437
O	7.746718	4.371919	0.706610
H	8.273230	5.186488	0.588223

5a

B3LYP SCF energy in gas phase: -2663.661943 a.u.

M06-L SCF energy in 1,4-dioxane: -2663.589519 a.u.

C	-1.752511	-0.414395	0.000108
C	-0.556032	0.400281	0.000185
C	0.556033	-0.400250	0.000186
C	1.752513	0.414423	0.000143
N	-1.289558	-1.736231	0.000058
C	0.119722	-1.806409	0.000109
O	0.747897	-2.857175	0.000100
C	-2.072650	-2.964879	0.000040
H	-2.699364	-3.034464	-0.893373
H	-1.354555	-3.786347	0.000021
H	-2.699357	-3.034496	0.893457
C	-3.064644	0.020253	0.000097
C	-3.456524	1.405718	0.000174
S	-4.503442	-1.025493	-0.000011
C	-4.804205	1.600278	0.000157
H	-2.717635	2.200514	0.000234
C	-5.572209	0.384314	0.000060
H	-5.305533	2.559939	0.000210
C	3.064643	-0.020231	0.000115
C	3.456512	-1.405699	0.000169
S	4.503449	1.025504	-0.000004
C	4.804192	-1.600269	0.000125
H	2.717617	-2.200490	0.000227
C	5.572206	-0.384311	0.000029
H	5.305513	-2.559934	0.000156
N	1.289562	1.736260	0.000121
C	2.072656	2.964907	0.000180
H	1.354561	3.786376	0.000264
H	2.699399	3.034439	0.893577
H	2.699333	3.034575	-0.893254
C	-0.119719	1.806440	0.000150
O	-0.747890	2.857208	0.000156
C	6.939545	-0.268899	-0.000033
C	7.672193	1.010637	-0.000130
C	7.921750	-1.381333	-0.000010
C	9.125746	0.667289	-0.000170
C	9.270546	-0.728405	-0.000101
C	10.234392	1.507006	-0.000259
C	10.528459	-1.321199	-0.000120
C	11.502047	0.915027	-0.000278
H	10.109147	2.585580	-0.000311
C	11.647185	-0.481050	-0.000209
H	10.626942	-2.402578	-0.000066
H	12.389155	1.542426	-0.000347
H	12.644472	-0.912359	-0.000226
C	-6.939548	0.268891	0.000025
C	-7.672186	-1.010650	-0.000070
C	-7.921761	1.381318	0.000093
C	-9.125742	-0.667313	-0.000121
C	-9.270552	0.728380	-0.000047
C	-10.234381	-1.507038	-0.000236
C	-10.528469	1.321164	-0.000093
C	-11.502041	-0.915069	-0.000278
H	-10.109129	-2.585612	-0.000294
C	-11.647189	0.481007	-0.000208
H	-10.626961	2.402542	-0.000032
H	-12.389144	-1.542475	-0.000369
H	-12.644480	0.912309	-0.000243
O	7.178125	2.133982	-0.000171
O	7.709019	-2.586996	0.000055
O	-7.709039	2.586983	0.000077
O	-7.178110	-2.133991	-0.000135

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