

Supporting Information for

***C*₂- and *C*₁-Symmetric Configurationally Stable Pyrene-Fused [5]Helicenes Connected via Hexagonal and Heptagonal Rings**

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S1. Materials and characterization

All chemicals and solvents were purchased from commercial sources and were used without further purification unless stated otherwise. The 8-methylnaphthalen-2-ol (**3**) and 2-(2,7-di-*tert*-butylpyren-4-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane were synthesized according to literature known protocols^{1,2}. The reactions and experiments sensitive to dioxygen were performed using Schlenk techniques and nitrogen-saturated solvents. All the glassware and NMR tubes prior to use for experiments were kept in oven at 80 °C for 12 h.

Chromatography:

Open-column chromatography and thin-layer chromatography (TLC) were performed on silica gel (Merck silica gel 100-200 mesh). Chiral stationary phase HPLC separations were performed by SHIMADZU 223.

NMR spectroscopy:

The NMR experiments were performed at 298 K on NMR spectrometers operating at 400 MHz proton and 101 MHz ¹³C frequencies. Standard pulse sequences were used and the data was processed using 2-fold zero-filling in the indirect dimension for all 2D experiments. Chemical shifts (δ) are reported in parts per million (ppm) relative to the solvent residual peak (¹H and ¹³C NMR, respectively): CDCl₃ (δ = 7.26 and 77.16 ppm), CD₂Cl₂ (δ = 5.32 and 53.84 ppm) and *J* values are given in Hz. Structural assignments for compound **1** and **2** were made with additional information from gCOSY, gNOESY, gHSQC and gHMBC experiments.

HRMS:

The ESI-HRMS were measured on Bruker micrOTOF while the MALDI-TOF-HRMS were measured on Bruker ultrafleXtreme. *trans*-2-[3-(4-*tert*-Butylphenyl)-2-methyl-2-propenylidene]malononitrile (DCTB) dissolved in chloroform was used as supporting matrix in the MALDI-TOF-HRMS measurement.

Melting point:

Melting points were measured using an OptiMelt Automated Melting Point System.

UV-vis and Fluorescence spectroscopy:

UV-vis spectra were measured on JASCO V-670 spectrometer, while emission spectra were measured Edinburgh FLS 980 photoluminescence spectrometer. The fluorescence lifetimes

were measured in DCM using a 418.6 nm pulsed laser diode with a pulse frequency of 1/100 ns. The fluorescence quantum yields were measured in DCM using same spectrometer with a 450 W xenon arc lamp as a light source and a calibrated integrating sphere.

Circular dichroism Spectroscopy:

CD spectra were measured on JASCO J-810 spectrometer.

Optical rotation:

Optical rotations were measured on JASCO P-1020 polarimeter with WCG3-100 cell.

Cyclic voltammetry:

Cyclic voltammetry experiments were performed in DCM with 0.1 M [Bu₄N][PF₆] as supporting electrolyte using a Gamry Instruments Reference 600 potentiostat. A standard three-electrode cell configuration was employed using a platinum disk working electrode, a platinum wire counter electrode, and an Ag/AgCl serving as reference electrode. The redox potentials were referenced to the ferrocene (Fc) / ferrocenium (Fc⁺) redox couple.

S2. Synthetic details and analytical data

rac-8,8'-dimethyl-[1,1'-binaphthalene]-2,2'-diol ((±)-4)



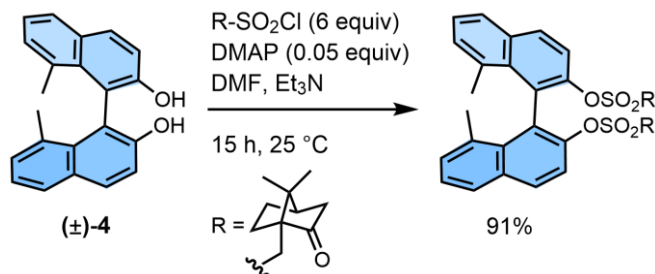
3 (500 mg, 3.16 mmol) was dissolved in dry DCM (8 mL) then Cu-TMEDA (44 mg, 3.0 mol%) was added in portions over 15 min to the flask. The reaction mixture was then stirred for 50 min at 25 °C. The reaction was quenched by 1 M HCl followed by extraction with 25 mL of DCM. The organic layer was dried over anhydrous sodium sulfate. The solvent was removed under reduced pressure using a rotary evaporator. Crude product was purified by column chromatography on silica gel using 20% ethylacetate in petrolether to yield 392 mg (78%) of **(±)-4** as white crystalline solid. Melting Point 255.8 °C.

¹H NMR (400 MHz, CDCl₃, 25 °C): δ [ppm] = 7.94 (d, J = 8.9 Hz, 1H), 7.74 (d, J = 9.3 Hz, 1H), 7.30 (d, J = 8.9 Hz, 1H), 7.19 (d, J = 6.5 Hz, 1H), 5.04 (s, 1H), 1.85 (s, 3H). (1H integrated under the CDCl₃ residual peak at δ 7.26 ppm)

¹³C NMR (101 MHz, CDCl₃, 25 °C): δ [ppm] = 153.4, 134.1, 133.0, 131.1, 130.6, 128.2, 124.0, 116.9, 113.8, 22.7.

HRMS (ESI): m/z : [M-H]⁻ Calcd for [C₂₂H₁₇O₂] 313.1234; Found 313.1231

8,8'-dimethyl-[1,1'-binaphthalene]-2,2'-dicamphorsulfonicester



Rac-**4** (10.0 g, 31.8 mmol, 1.00 equiv) was dissolved in dry DMF (30 mL) and triethylamine (20 mL, 143 mmol, 4.50 equiv) followed by addition of DMAP (200 mg, 1.63 mmol, 0.05 equiv). The reaction mixture was then stirred at 0 °C for 30 min. (1*S*)-(+)-10-Camphorsulfonyl

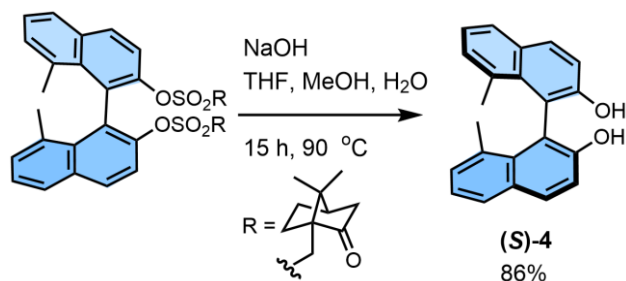
chloride (50.0 g, 199 mmol, 6.27 equiv) was dissolved in 45 mL dry DMF at 0 °C and added to the reaction mixture dropwise via syringe. The reaction mixture was stirred at 0 °C for 20 min, then warmed up to 25 °C and stirred for 15 h. The reaction was quenched with water and the product was extracted with DCM, dried over anhydrous sodium sulfate. The solvent was removed under reduced pressure using a rotary evaporator. Crude product was purified by column chromatography on silica gel using 5% ethylacetate in toluene to isolate both the diastereomers separately. Combined Yield: 21.56 g (91%) as white crystalline solid. Melting Point 166.5 °C.

¹H NMR (400 MHz, CDCl₃, 25 °C): δ [ppm] = 7.95 (d, J = 9.0 Hz, 1H), 7.78 (d, J = 7.9 Hz, 1H), 7.62 (d, J = 8.9 Hz, 1H), 7.43 – 7.37 (m, 1H), 7.30 (d, J = 7.0 Hz, 1H), 2.59 (d, J = 14.8 Hz, 1H), 2.28 – 2.17 (m, 2H), 1.96 (m, 4H), 1.91 – 1.83 (m, 1H), 1.79 (d, J = 18.5 Hz, 1H), 1.47 – 1.16 (m, 3H), 0.82 (s, 3H), 0.61 (s, 3H).

¹³C NMR (101 MHz, CDCl₃, 25 °C): δ [ppm] = 213.4, 146.2, 136.1, 133.1, 132.6, 131.4, 131.3, 127.7, 126.2, 126.0, 120.1, 77.5, 77.2, 76.8, 57.6, 48.7, 47.9, 42.8, 42.4, 26.9, 24.7, 23.5, 19.5, 19.4.

HRMS (ESI): m/z : [2M + Na⁺] Calcd for [C₄₂H₄₆O₈S₂Na] 765.2526; Found 765.2540

(S)-8,8'-dimethyl-[1,1'-binaphthalene]-2,2'-diol ((S)-4)



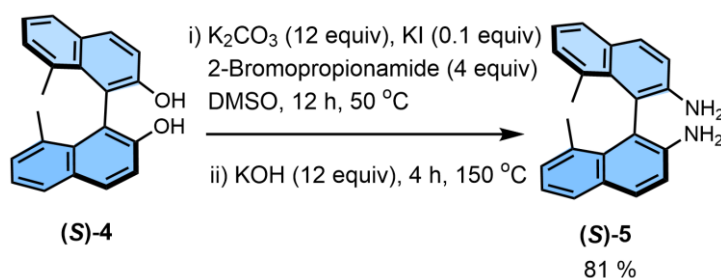
(S)- 8,8'-dimethyl-[1,1'-binaphthalene]-2,2'-dicamphorsulfonate (2.0 g, 2.7 mmol) was dissolved in THF (40 mL), MeOH (20 mL) and 5 M NaOH (20 mL) and refluxed at 90 °C in an oil bath for 15 h. Then 1M Hydrochloric acid was added to the reaction mixture until it was acidic. The reaction mixture was then concentrated by evaporating methanol under reduced pressure using a rotary evaporator and the product was extracted with DCM, dried over anhydrous sodium sulfate. The solvent was then removed under reduced pressure and the crude product was purified by column chromatography on silica gel using 5% ethylacetate in petroleum ether to yield 1.08 g (86%) of **(S)-4** as white crystalline solid. *er* 96:04. Melting point 255.7 °C.

¹H NMR (400 MHz, CDCl₃, 25 °C): δ [ppm] = 7.94 (d, *J* = 8.9 Hz, 1H), 7.74 (d, *J* = 9.3 Hz, 1H), 7.30 (d, *J* = 8.9 Hz, 1H), 7.19 (d, *J* = 6.5 Hz, 1H), 5.04 (s, 1H), 1.85 (s, 3H). (1H integrated under the CDCl₃ residual peak at δ 7.26 ppm)

¹³C NMR (101 MHz, CDCl₃, 25 °C): δ [ppm] = 153.4, 134.1, 133.0, 131.1, 130.6, 128.2, 124.0, 116.9, 113.8, 22.7.

HRMS (ESI): *m/z*: [M-H]⁻ Calcd for [C₂₂H₁₇O₂] 313.1234; Found 313.1231

(*S*)-8,8'-dimethyl-[1,1'-binaphthalene]-2,2'-diamine ((*S*)-5)



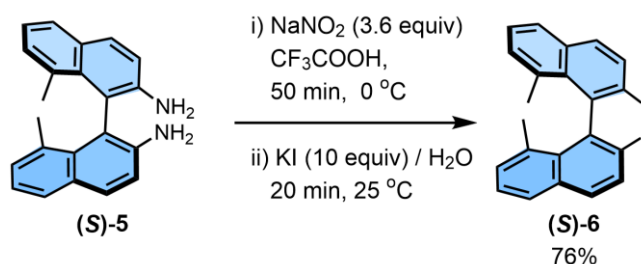
K₂CO₃ (1.58 g, 11.4 mmol, 3.0 equiv) and 2-Bromopropionamide (1.70 g, 11.4 mmol, 3.0 equiv) were dissolved in DMSO (3 mL) and stirred for 20 min at 25 °C. KI (63.1 mg, 0.03 mmol, 0.1 equiv) was added to the solution and stirred for 10 more minutes. (*S*)-4 (1.2 g, 3.8 mmol, 1.0 equiv) was added to the reaction mixture and stirred for 12 h at 50 °C in an oil bath. Once all the starting material was consumed, confirmed by TLC, KOH (1.7 g, 30.4 mmol, 8.0 equiv) was added to the reaction mixture and heated at 150 °C for 4 h in an oil bath. The reaction was then quenched with water and extracted with ethyl acetate. The solvent was removed under reduced pressure using a rotary evaporator and the crude product was purified by column chromatography on silica gel using 40% ethylacetate in petroleum ether to yield 965 mg (81%) as off-white solid. Melting Point 249.8 °C.

¹H NMR (400 MHz, CDCl₃, 25 °C): δ [ppm] = 7.75 (d, *J* = 8.7 Hz, 1H), 7.63 (d, *J* = 7.3 Hz, 1H), 7.15 – 7.07 (m, 2H), 7.05 (d, *J* = 8.7 Hz, 1H), 1.90 (s, 3H). The broad amine peak can be seen around 3.30 ppm.

¹³C NMR (101 MHz, CDCl₃, 25 °C): δ [ppm] = 140.5, 134.2, 133.2, 131.4, 130.9, 130.6, 128.1, 123.3, 118.4, 118.2, 23.1.

HRMS (ESI): *m/z*: [M + H] Calcd for [C₂₂H₂₁N₂] 313.1705; Found 313.1699

Synthesis of (S)- 2,2'-diiodo-8,8'-dimethyl-1,1'-binaphthalene ((S)-6)



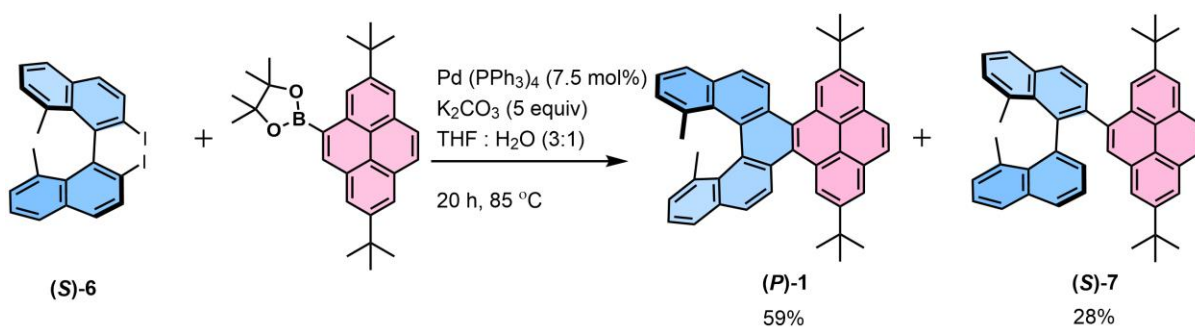
(S)-5 (200 mg, 0.64 mmol, 1 equiv) was dissolved in triflic acid (8 mL) and stirred at 0 °C for 10 minutes followed by addition of NaNO₂ (155 mg, 2.24 mmol, 3.5 equiv). Then the reaction mixture was continued to stir at 0 °C for 50 min followed by dropwise addition using syringe into a solution of 1.06 g KI (6.40 mmol, 10 equiv) in 4 mL H₂O. After 20 min stirring at 25 °C, the reaction was quenched with 10% solution of NaHCO₃ and washed with saturated solution of Na₂S₂O₃. The product was extracted with DCM, dried over anhydrous sodium sulfate. The solvent was removed under reduced pressure using a rotary evaporator and the crude product was purified by column chromatography on silica gel using 1% ethylacetate in petroleum ether to yield 260 mg (76%) of (S)-6 as white solid. Melting Point 189.3 °C. *er* 96:04.

¹H NMR (400 MHz, CDCl₃, 25 °C): δ [ppm] = 7.99 (d, J = 8.6 Hz, 1H), 7.78 (d, J = 8.6 Hz, 1H), 7.61 (d, J = 8.7 Hz, 1H), 7.44 – 7.36 (m, 1H), 7.24 (s, 1H), 1.79 (s, 3H).

¹³C NMR (101 MHz, CDCl₃, 25 °C): δ [ppm] = 148.3, 135.5, 135.0, 134.4, 133.5, 130.9, 130.8, 128.2, 126.4, 104.8, 24.8.

HRMS (MALDI-TOF): m / z: [M] Calcd for [C₂₂H₁₆I₂] 533.9341; Found 533.9362

12, 17-di-tert-butyl-4,5-dimethyldinaphtho[2,1,8-def:1',2'-s]picene ((P)-1) and (S)-2,7-di-tert-butyl-4-(8,8'-dimethyl-[1,1'-binaphthalen]-2-yl)pyrene ((S)-7)



In a Schlenk tube (S)-6 (30.0 mg, 0.056 mmol, 1 equiv) and 2-(2,7-di-tert-butylpyren-4-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (30.0 mg, 0.067 mmol, 1.2 equiv) were dissolved in dry THF (3 mL) and K₂CO₃ (38.7 mg, 0.28 mmol, 5 equiv) was dissolved in water (1 mL) and

both solutions were degassed for 10 min separately and then mixed together. To this mixture Pd(PPh₃)₄ (6.50 mg, 0.0056 mmol, 0.1 equiv) was added under high nitrogen pressure and bubbled with nitrogen for 10 additional min. The reaction flask was then sealed and heated at 85 °C for 20 h in an oil bath. The reaction was quenched by adding water and extracted with DCM, dried over anhydrous sodium sulfate. The solvent was evaporated under reduced pressure using a rotary evaporator. The crude product was purified by column chromatography on silica gel using 1% ethylacetate in petroleum ether to yield 19.5 mg (59%) as a green fluorescent oil of (*P*)-**1**. Melting Point 150.7 °C. *er* 95:05.

Optical rotation: $[\alpha]_D^{25} = +940$

¹H NMR (400 MHz, CDCl₃, 25 °C): δ [ppm] = 9.17 (d, *J* = 1.7 Hz, 1H), 9.03 (d, *J* = 8.8 Hz, 1H), 8.25 (d, *J* = 1.7 Hz, 1H), 8.17 (d, *J* = 8.9 Hz, 1H), 8.12 (s, 1H), 7.93 (d, *J* = 7.6 Hz, 1H), 7.56 – 7.49 (m, 1H), 7.18 (d, *J* = 6.8 Hz, 1H), 1.68 (s, 9H), 1.19 (s, 3H).

¹³C NMR (101 MHz, CD₂Cl₂, 25 °C): δ [ppm] = 148.2, 135.4, 133.0, 132.9, 131.1, 129.4, 129.1, 128.5, 128.2, 127.6, 127.5, 126.1, 125.8, 125.5, 124.9, 123.9, 123.4, 122.0, 35.6, 32.1, 23.1.

HRMS (MALDI-TOF): *m/z*: [M] Calcd for [C₄₆H₄₀] 592.3130; Found 592.3119

The above reaction also produced 9.4 mg (28%) as pale yellow crystalline solid **9**. Melting Point 259.6 °C.

¹H NMR (400 MHz, CDCl₃, 25 °C): δ [ppm] = 8.07 (d, *J* = 1.8 Hz, 1H), 8.04 (d, *J* = 8.5 Hz, 1H), 7.97- 7.94 (m, 2H), 7.93 – 7.86 (m, 2H), 7.81 (d, *J* = 1.8 Hz, 1H), 7.53 (d, *J* = 8.3 Hz, 1H), 7.50 – 7.46 (m, 1H), 7.42 (d, *J* = 1.8 Hz, 1H), 7.39 (s, 1H), 7.38 – 7.29 (m, 3H), 7.25 – 7.18 (m, 2H), 7.05 (dd, *J* = 7.1, 1.4 Hz, 1H), 6.62 – 6.52 (m, 1H), 2.21 (s, 3H), 1.92 (s, 3H), 1.43 (s, 9H), 1.42 (s, 9H).

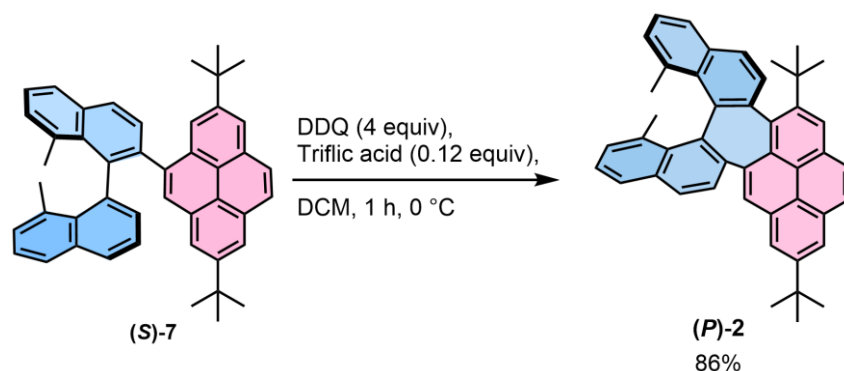
¹³C NMR (101 MHz, CD₂Cl₂, 25 °C): δ [ppm] = 148.2, 147.9, 141.3, 139.9, 138.9, 138.2, 136.7, 135.6, 134.5, 134.4, 134.0, 132.9, 131.1, 130.6, 130.3, 129.7, 129.6, 128.9, 128.6, 128.5, 128.3, 128.0, 127.7, 127.5, 127.1, 127.1, 125.8, 124.9, 123.3, 122.6, 122.1, 121.8, 121.4, 121.3, 35.3, 35.1, 32.0, 31.9, 25.2, 24.2.

HRMS (MALDI-TOF): *m/z*: [M] Calcd for [C₄₆H₄₂] 594.3287; Found 594.3228

Table S1. Optimization of Suzuki coupling with different reaction conditions.

Catalyst	Base (3 equiv)	Temp / °C	Solvent system	Yield ^a / % 1:7
Pd(PPh ₃) ₄ (10%)	K ₂ CO ₃	100	Toluene: EtOH:H ₂ O (5:3:1)	0:62
Pd(PPh ₃) ₄ (7.5%)	K ₂ CO ₃ (5 equiv)	85	THF:H ₂ O (3:1)	59:28
Pd(PPh ₃) ₄ (10%)	NHCO ₃	85	THF:H ₂ O (3:1)	32:20
Pd(PPh ₃) ₂ Cl ₂ (10%)	K ₂ CO ₃	85	THF:H ₂ O (3:1)	31:16
Pd(PPh ₃) ₂ Cl ₂ (10%)	NHCO ₃	85	THF:H ₂ O (3:1)	36:15
PdCl ₂ (PCy) ₃ (10%)	Cs ₂ CO ₃	110	Dioxane	40:13

^aIsolated yield after column chromatography.

Synthesis of 11,16-di-*tert*-butyl-4,5-dimethyldinaphtho[2',1':4,5;1'',2'':6,7]cyclohepta[1,2,3-*cd*]pyrene ((*P*)-2):

In a Schlenk tube (*S*)-7 (8.00 mg, 0.013 mmol, 1 equiv) was dissolved in dry DCM and stirred at 0 °C for 10 min. Then the solution was added dropwise to a flask containing DDQ (15.0 mg, 0.067 mmol, 5 equiv) and stirred at 0 °C for 20 min. Then triflic acid (0.14 mL, 1.50 μmol, 0.12 equiv) was added to the reaction mixture and continued to stir at 0 °C for 30 min under nitrogen atmosphere. The reaction was quenched by saturated NaHCO₃ solution in water, extracted with DCM and dried over anhydrous sodium sulfate. The solvent was then evaporated under reduced pressure using a rotary evaporator. The crude product was purified by column chromatography on silica gel using 1% ethylacetate in petroleum ether to yield 6.8 mg (86%) as green fluorescent solid. Melting Point 332.1 °C. *er* 96:04.

Optical rotation: $[\alpha]_D^{25} = +308$

¹H NMR (400 MHz, CDCl₃, 25 °C): δ [ppm] = 8.39 (d, J = 8.2 Hz, 2H), 8.24 (d, J = 1.7 Hz, 1H), 8.18 (d, J = 1.8 Hz, 1H), 7.97 (dt, J = 17.8, 8.9 Hz, 3H), 7.79 (d, J = 6.7 Hz, 1H), 7.63 (d, J = 8.7 Hz, 2H), 7.41 – 7.35 (m, 2H), 7.30 – 7.25 (m, 1H), 7.14 (d, J = 8.4 Hz, 1H), 7.02 (d, J = 7.9 Hz, 1H), 6.73 (d, J = 8.5 Hz, 1H), 1.62 (s, 9H), 1.56 (s, 9H), 1.38 (s, 3H), 1.26 (s, 3H).

¹³C NMR (101 MHz, CD₂Cl₂, 25 °C): δ [ppm] = 149.6, 148.6, 143.5, 143.2, 141.0, 136.9, 136.8, 135.5, 135.3, 135.1, 134.7, 134.5, 134.5, 133.6, 132.3, 131.4, 131.2, 131.0, 130.9, 130.4, 129.9, 129.7, 129.3, 128.2, 127.6, 127.5, 127.4, 127.2, 126.9, 126.8, 126.0, 125.7, 123.4, 123.1, 121.9, 121.6, 38.1, 35.5, 34.9, 32.0, 23.5, 22.4.

HRMS (MALDI): m / z: [M] Calcd for [C₄₆H₄₀] 592.3130; Found 592.3162

S3. Cyclic Voltammetry

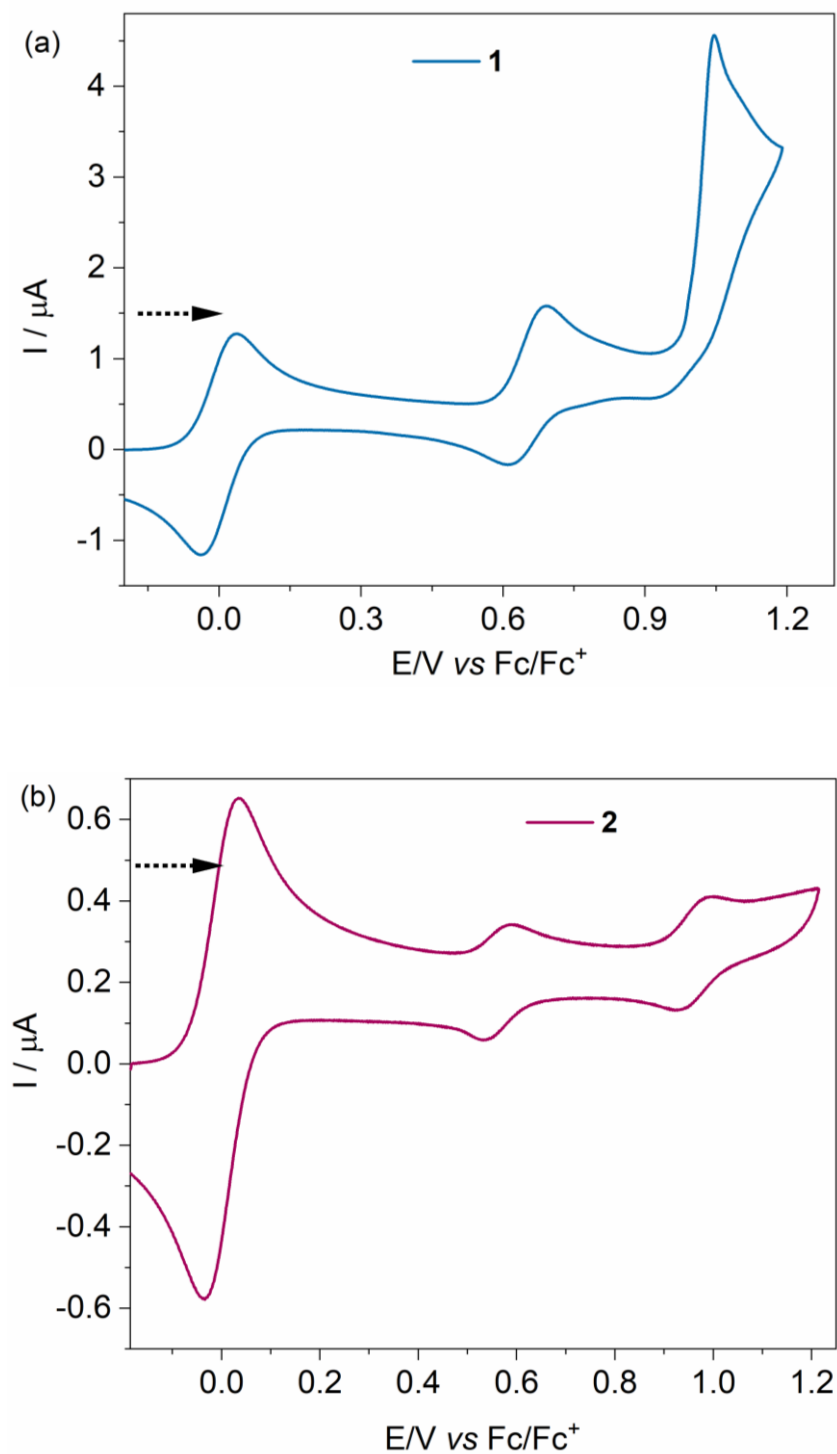


Figure S1. Cyclic voltammograms of (a) **1** and (b) **2** in DCM at 0.2 V/s scan rate, with 0.1 M $(n\text{-C}_4\text{H}_9)_4\text{NBF}_4$ as supporting electrolyte, versus ferrocene/ferrocenium (Fc/Fc^+) at room temperature.

S4. Fluorescence lifetime

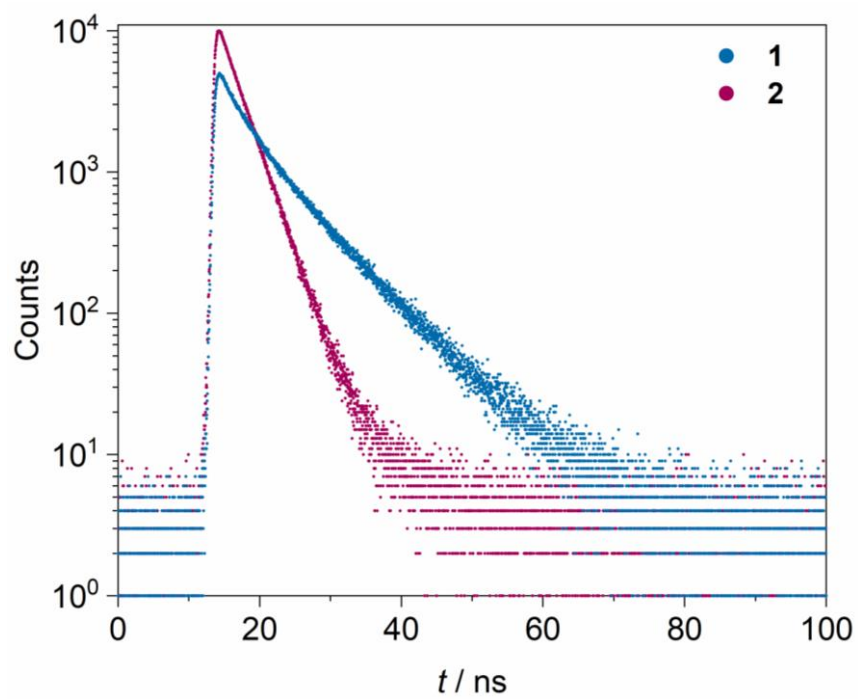


Figure S2. Fluorescence decay profile of **1** and **2** in DCM.

S5. Chiral-Stationary-Phase HPLC and CD

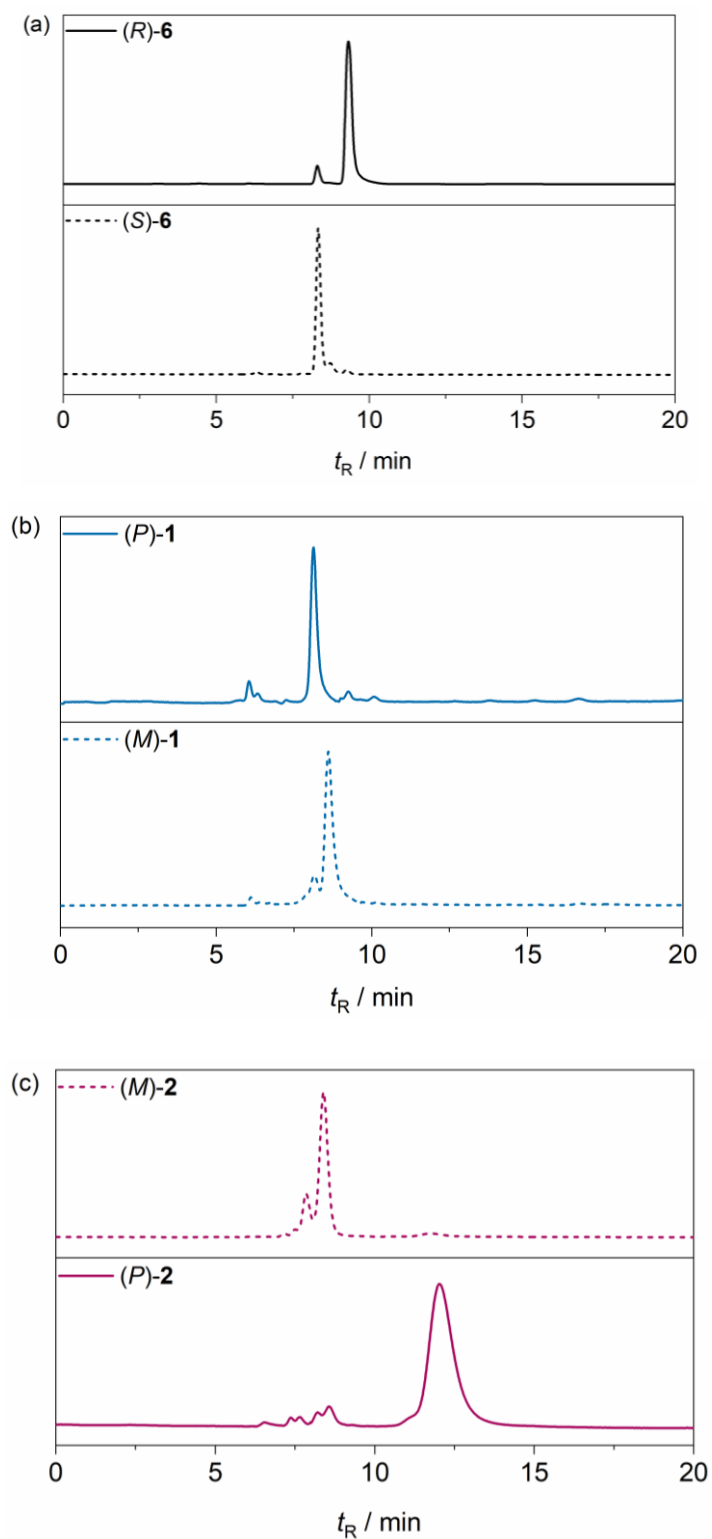


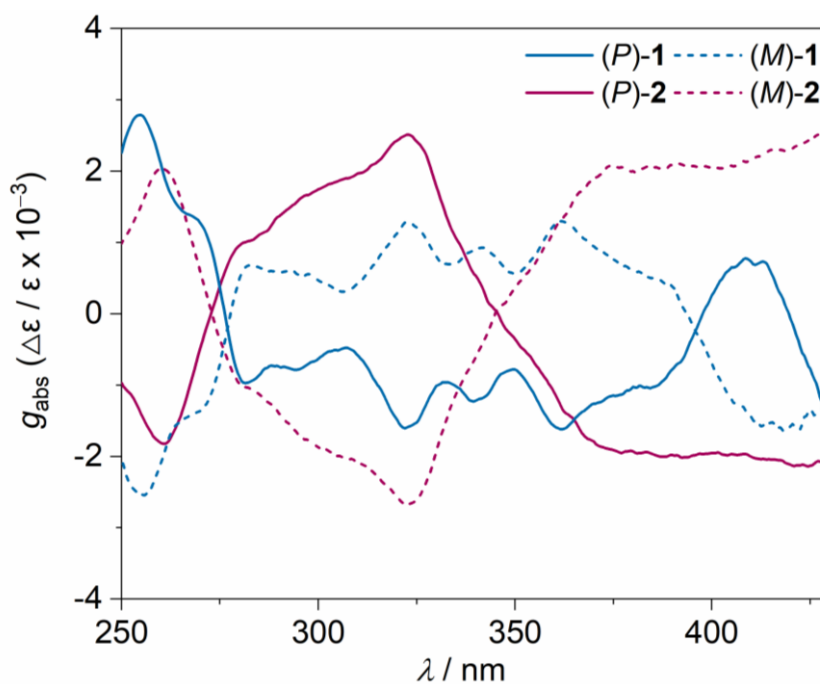
Figure S3. HPLC chromatogram of (a) **6**, (b) **1** and (c) **2** using chiral stationary phase column.

Table S2. Overview of Parameters for HPLC Separation of Enantiomers of 1, 2 and 6.

Compound	Eluent <i>n</i> -hexane/ <i>i</i> PrOH	First fraction	Second fraction	α^b	R_S^c	<i>er</i>
6	97:3	(<i>S</i>)	(<i>R</i>)	1.12	1.22	95.84 : 4.16
1	97:3	(<i>P</i>)	(<i>M</i>)	1.05	0.61	95.31 : 4.69
2	97:3	(<i>M</i>)	(<i>P</i>)	1.43	2.33	95.91 : 4.09

^aPhenomenex Lux i-Amylose-3 5 μm (250 x 4.6 mm). Sample injection: 5 μL of a 1 mg/mL solution in hexane. Separation conditions: Eluent, flow rate: 0.5 mL/min, 25 $^\circ\text{C}$. ^bSelectivity parameter: $\alpha = t_{R2} / t_{R1}$, where t_{R1} , and t_{R2} are elution times for first and second fraction, respectively. ^cResolution parameter: $R_S = 2(t_{R2} - t_{R1}) / (w_1 + w_2)$, where w_1 and w_2 are peak widths for first and second fraction, respectively.

Absorption dissymmetry factor

**Figure S4.** Absorption dissymmetry factor of 1 and 2.

S6. Determination and Analysis of Activation Parameters of Enantiomerization

The values of the Gibbs activation energies ($\Delta G^\ddagger(T)$) for enantiomerization of **1** and **2** calculated by following the decay of the enantiomeric excess (ee) of the enantioenriched samples dissolved in diethylene glycol dibutyl ether (1-(2-(2-butoxyethoxy)ethoxy)butane) at 493 K for **1** and 503 K for **2** over time (t) by HPLC on a chiral stationary phase. To estimate the $\Delta G^\ddagger(T)$ value, the $\ln(ee_t/ee_0)$ values were plotted against the t and the data set was linearly fitted (Figures S5 (a) and (b)). Following the equations $\ln(ee_t/ee_0) = -k_{\text{rac}}t$, where k_{rac} is the rate constant of racemization, and $k_{\text{rac}} = 2k_e$, where k_e is the rate constant of enantiomerization, the k_e values were obtained and used to calculate the corresponding $\Delta G^\ddagger(T)$ values by using the Eyring equation $\Delta G^\ddagger(T) = -RT \ln(k_e h / \kappa k_B T)$, where R is the gas constant ($R = 8.31446 \text{ J K}^{-1}$), h is the Planck constant ($h = 6.62607 \times 10^{-34} \text{ J s}$), k_B is the Boltzmann constant ($k_B = 1.38064852 \times 10^{-23} \text{ J K}^{-1}$), and κ is the transmission coefficient ($\kappa = 0.5$ or 1). The transmission coefficient $\kappa = 0.5$ was used because the enantiomerization process is defined as a reversible first order reaction.

The $\Delta G^\ddagger(T)$ value for **1** was determined at 493 K, where racemization could be followed within a ~10–12 h period of time. Because the $\Delta G^\ddagger(T)$ values of **1** and **2** differ significantly, it was not possible to follow the racemization process for both compounds at the same temperature i.e., at 493 K without the process for **2** being too slow. Hence the $\Delta G^\ddagger(T)$ value for **2** was determined at 503 K, where the racemization was followed up to 3 days.

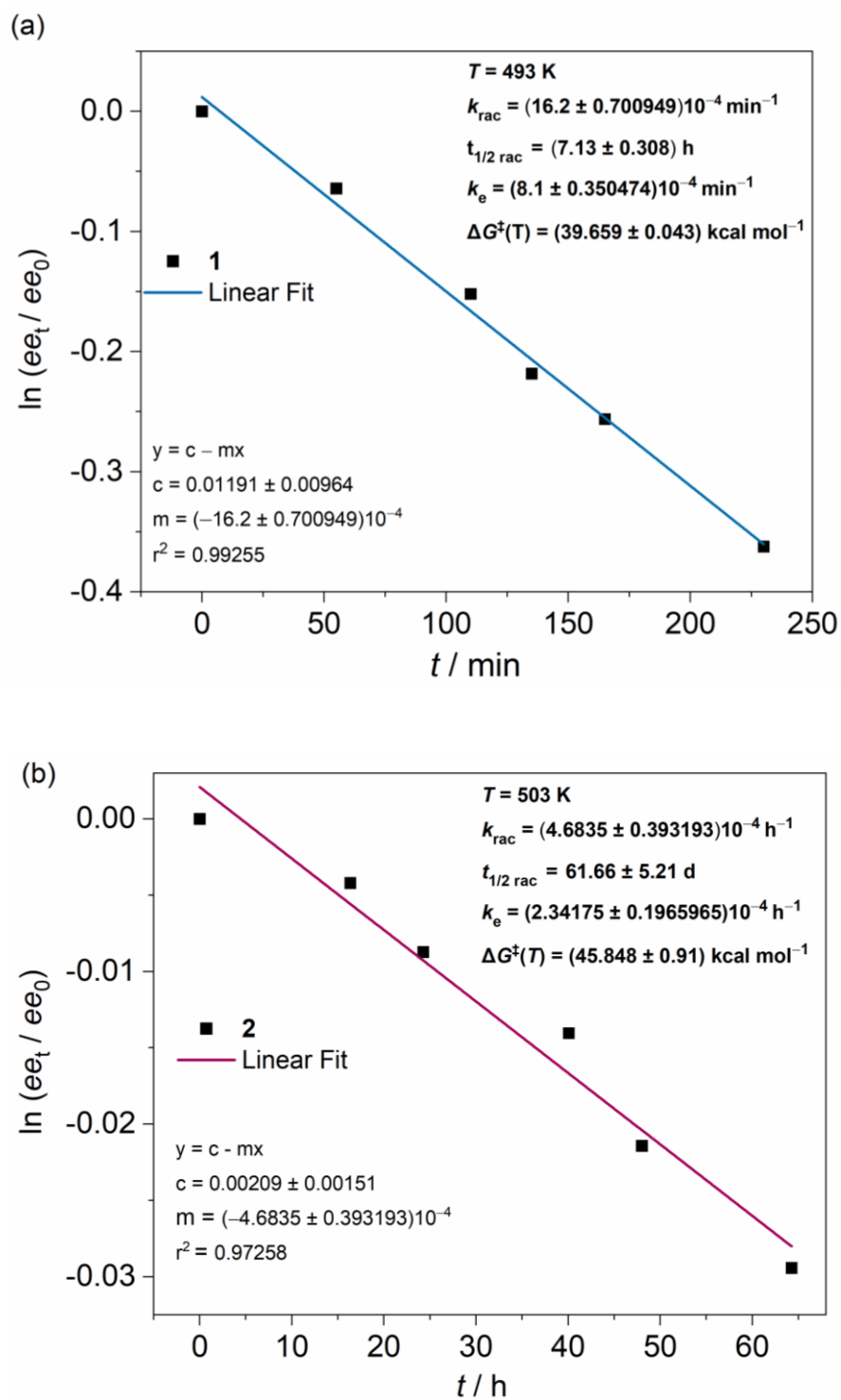


Figure S5. Plot of $\ln(ee_t/ee_0)$ against t for (a) **1** and (b) **2** and fitted linearly to obtain the k_{rac} , $t_{1/2\text{-rac}}$, k_e and ΔG^\ddagger values.

S7. Quantum Chemical Calculations

DFT calculations were performed using Gaussian 16 suite.³ Geometries were optimized using B3LYP functional and 6-31G(d,p) basis set in the gas phase unless stated otherwise. Frequency analysis was performed to verify the stationary state geometry. In all cases no imaginary frequency was found. TD-DFT calculations were performed on B3LYP/6-31G(d,p) optimized geometries at the B3LYP/6-31g(d,p) level. The effect of the solvent was accounted for using PCM (with dichloromethane as the solvent). SpecDis and Avogadro software were used to analyze the TD-DFT calculated spectra and to generate graphical images of frontier molecular orbitals (FMOs), respectively.

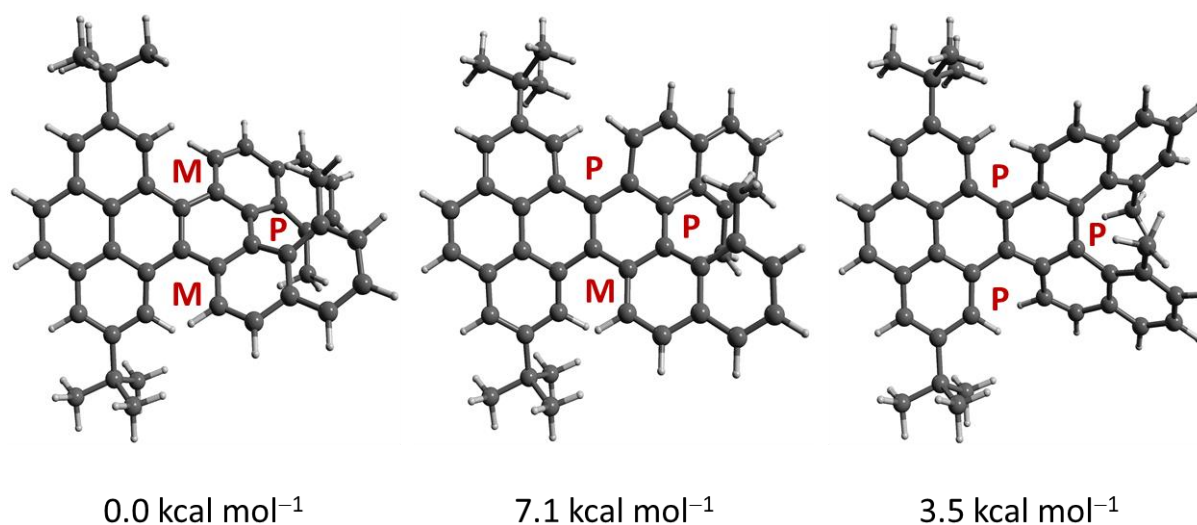


Figure S6. Relative Gibbs's free energies of diastereomers of **1**.

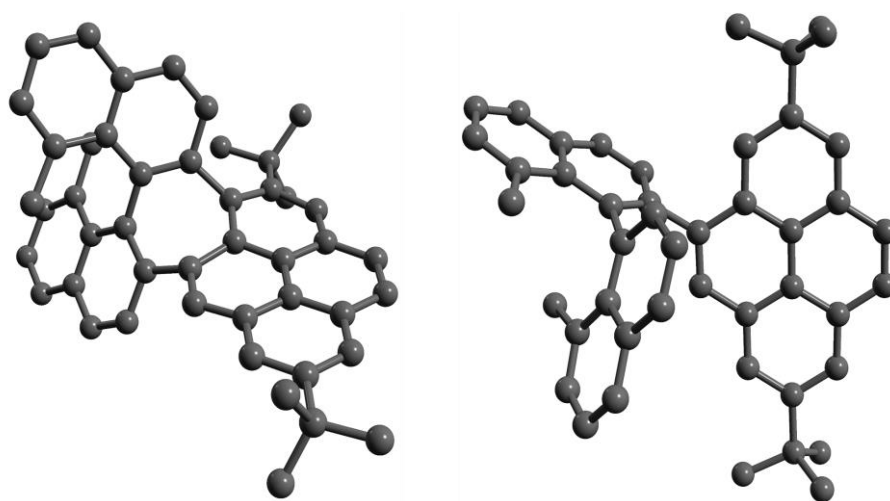
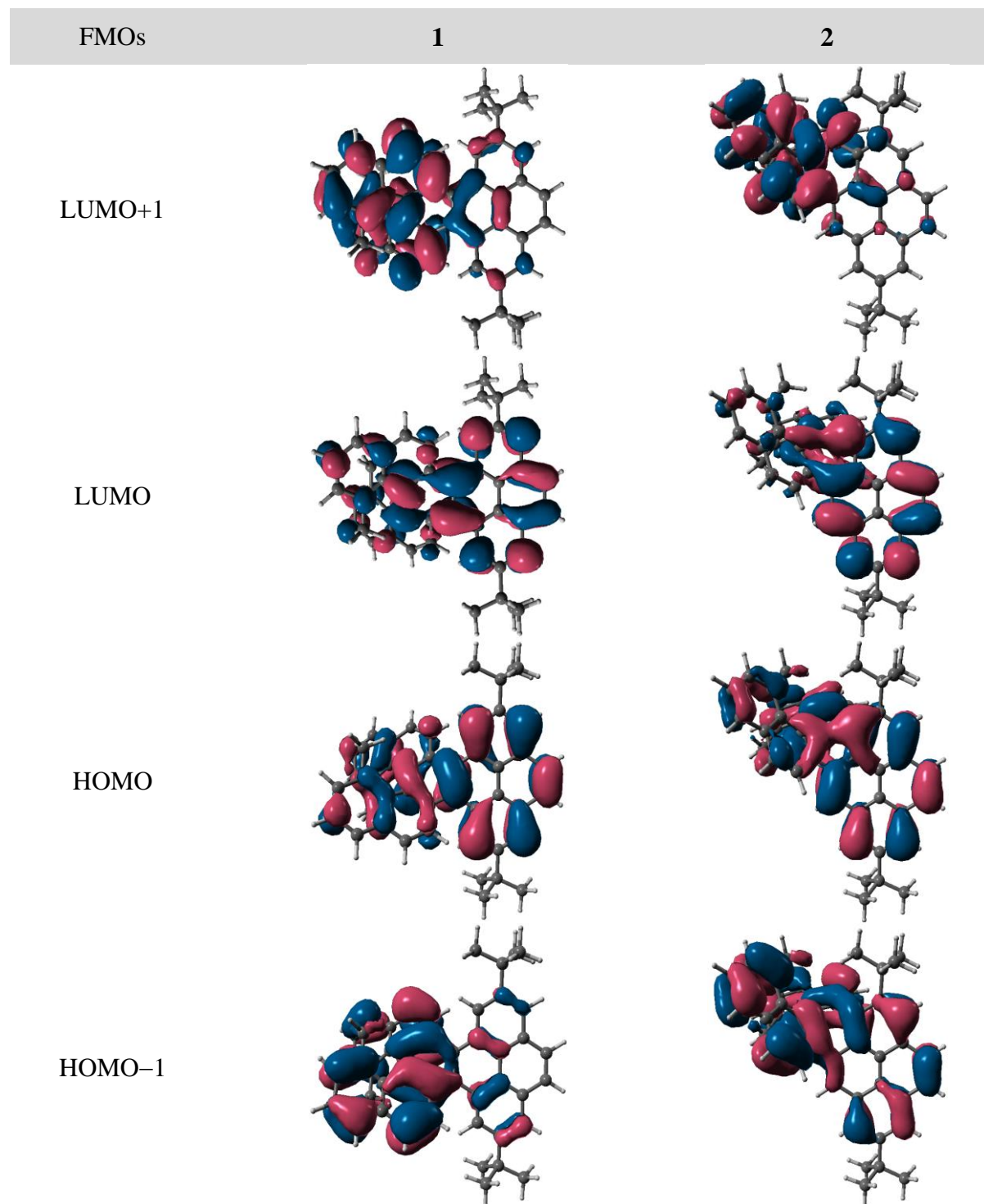


Figure S7. Optimized geometries of **2** and **7**. Hydrogen atoms are omitted for clarity

Table S3. Frontier molecular orbitals of **1** and **2**.



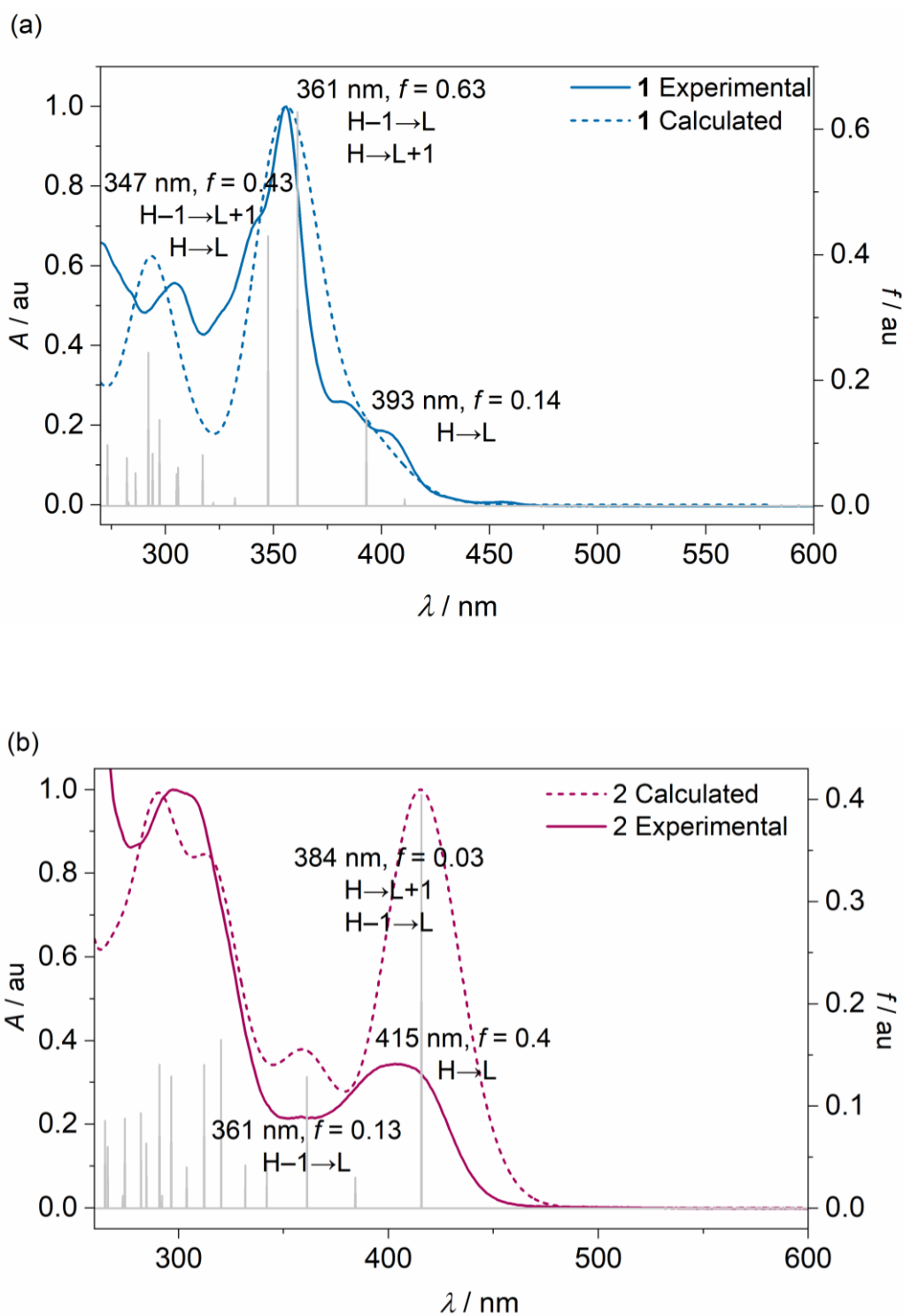


Figure S8. Comparison of experimental (solid) and TD-DFT calculated (dashed, shifted by 62 eV) UV-vis spectra of (a) **1** and (b) **2** along with assignments of key transitions. H = HOMO, L = LUMO, f = oscillator strength.

Table S4. Summary of TD-DFT calculated key low energy transitions.

Excited singlet state	Wavelength / nm	Energy / eV	Major transitions	Contribution	oscillator strength (<i>f</i>)
1					
1	410.73	3.02	HOMO→LUMO+1	0.41	0.01
			HOMO-1→LUMO	0.56	
2	393.03	3.15	HOMO→LUMO	0.65	0.14
3	361.09	3.43	HOMO-1→LUMO	0.41	0.63
			HOMO→LUMO+1	0.57	
4	347.51	3.57	HOMO-1→LUMO+1	0.65	0.43
			HOMO→LUMO	0.23	
2					
1	415.67	2.98	HOMO→LUMO	0.68	0.40
2	384.18	3.23	HOMO→LUMO+1	0.68	0.03
			HOMO-1→LUMO	0.16	
3	361.25	3.43	HOMO-1→LUMO	0.61	0.13

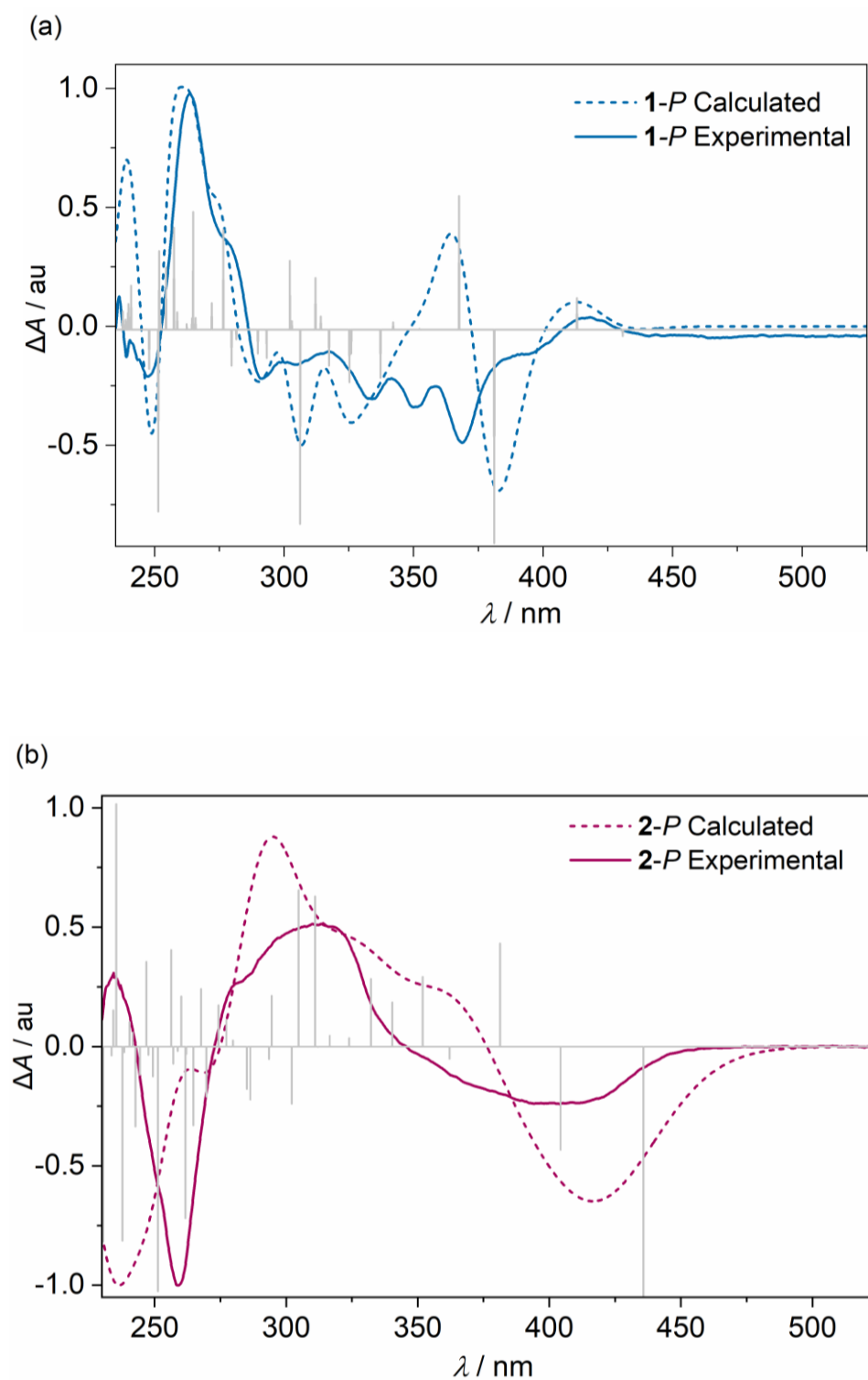


Figure S9. Comparison of experimental (solid) and TD-DFT calculated (dashed, shifted by 62 eV) CD spectra for *P*-enantiomer of (a) **1** and (b) **2**.

NICS Calculations: The Nucleus Independent Chemical Shift (NICS) calculations were performed on B3LYP/6-31G(d,p) optimized geometry at GIAO-B3LYP/6-311+G(2d,p) level. Considering the non-planarity of molecule the NICS (1)_{zz} values were obtained by placing dummy atom at 1 Å above and below the each ring.

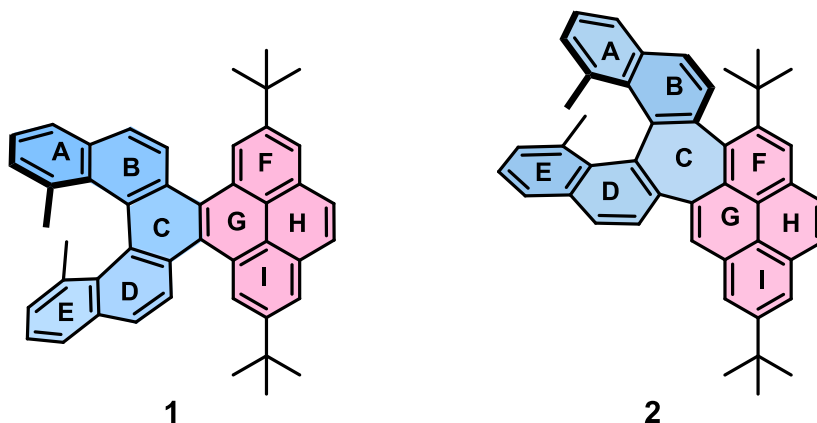


Table S5. The calculated NICS(0) and NICS(1)_{zz} values for **1** and **2**.

Ring	1			2		
	NICS(1) _{zz} (Up)	NICS(1) _{zz} (Down)	NICS(0)	NICS(1) _{zz} (Up)	NICS(1) _{zz} (Down)	NICS(0)
A	-3.83	-8.91	-8.28	-10.15	-8.40	-7.64
B	-7.09	-1.27	-5.64	-6.14	-5.39	-6.94
C	-2.93	-3.38	-3.41	12.12	14.94	7.61
D	-	-	-	-10.17	-9.09	-7.04
E	-	-	-	-10.72	-13.19	-7.59
F	-2.43	-0.84	-9.60	-30.88	-27.69	-9.57
G	-3.05	-3.17	1.42	-9.65	-14.90	-2.45
H	-2.50	-2.47	-3.37	-14.66	-14.81	-3.13
I	-	-	-	-32.28	-30.18	-10.06

S8. X-Ray Crystallography

The single crystals of **2** were grown by slow diffusion of hexane to solution of **2** in chloroform in an NMR tube. Single Crystal X-ray diffraction data were collected at 100 K on a Bruker D8 Quest Kappa diffractometer with a Photon II CPAD area detector and multi-layered mirror monochromated CuK α radiation. The structures were solved using direct methods, expanded with Fourier techniques and refined with the Shelx software package.⁴ All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included in the structure factor calculation on geometrically idealized positions. Crystallographic data have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC 2052372 for **2**. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.ac.uk/data.request/cif.

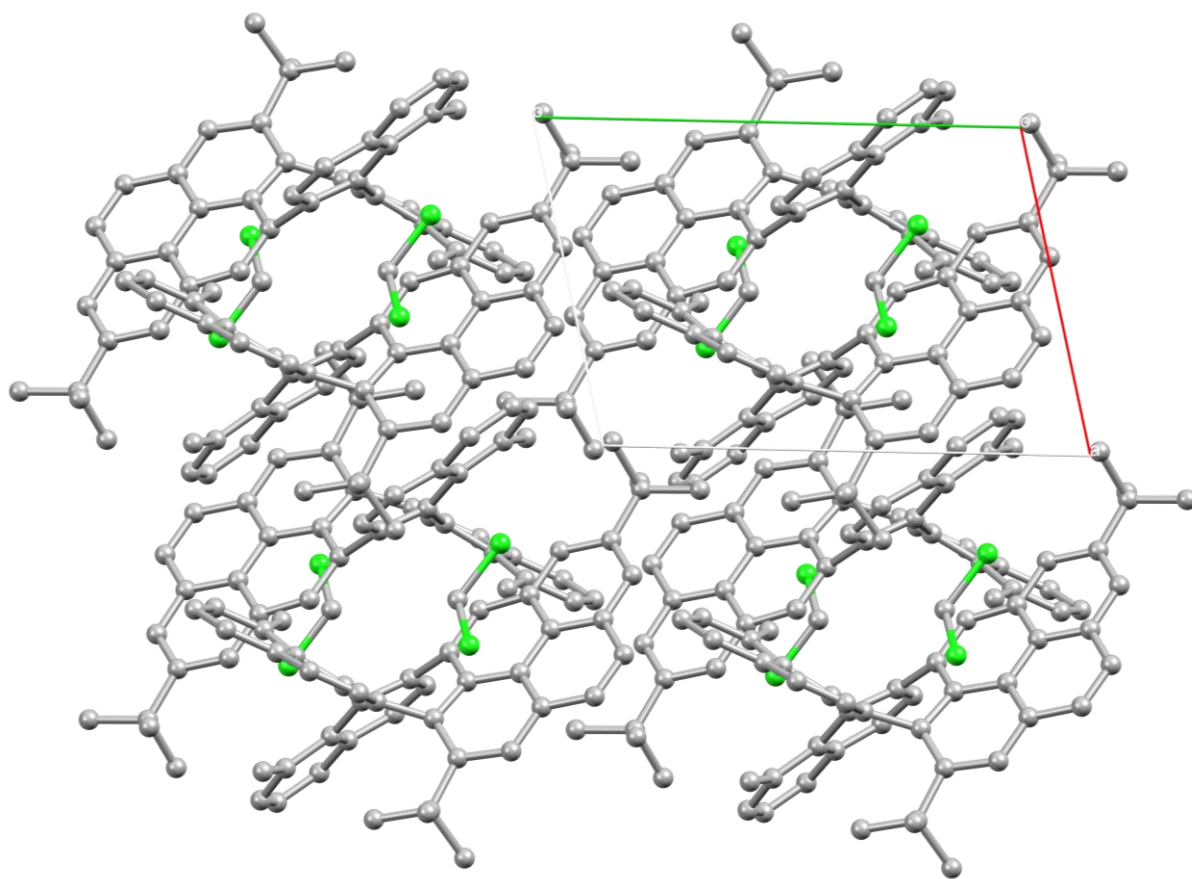


Figure S10. Crystal packing of **2**. Hydrogen atoms are omitted for clarity.

Table S6. Crystallographic table for 2.

CCDC number	2052372
Chemical formula	C ₄₆ H ₄₀ ·CH ₂ Cl ₂
M_r	677.70
Crystal system, space group	Triclinic, <i>P</i> -1
Temperature (K)	100
a, b, c (Å)	8.4265 (6), 12.964 (1), 17.6847 (13)
α, β, γ (°)	110.250 (4), 97.265 (4), 99.701 (4)
V (Å ³)	1750.5 (2)
Z	2
Radiation type	Cu $K\alpha$
μ (mm ⁻¹)	1.91
Crystal size (mm)	0.23 × 0.03 × 0.02
T_{\min}, T_{\max}	0.639, 0.754
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	29713, 6872, 6142
R_{int}	0.031
($\sin \theta/\lambda$) _{max} (Å ⁻¹)	0.618
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.035, 0.095, 1.04
No. of reflections/parameters	6872/ 450

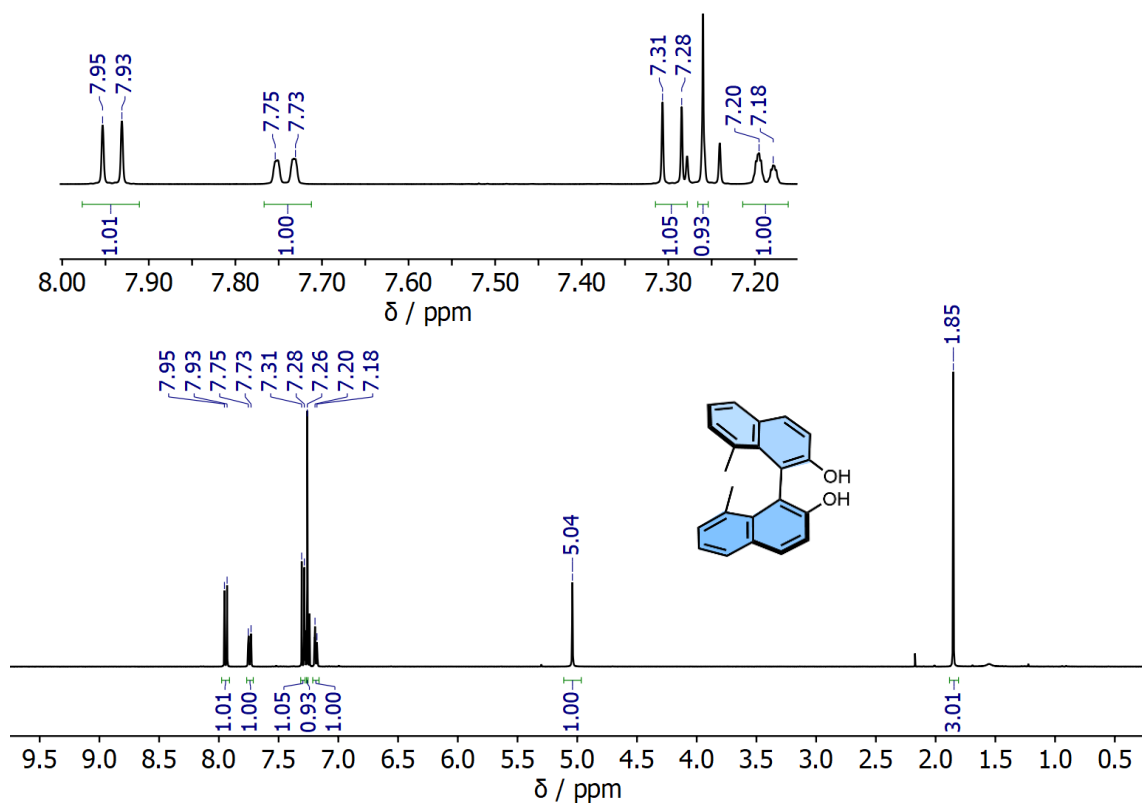


Figure S12. ^1H NMR spectrum of **4** (400 MHz, CDCl_3).

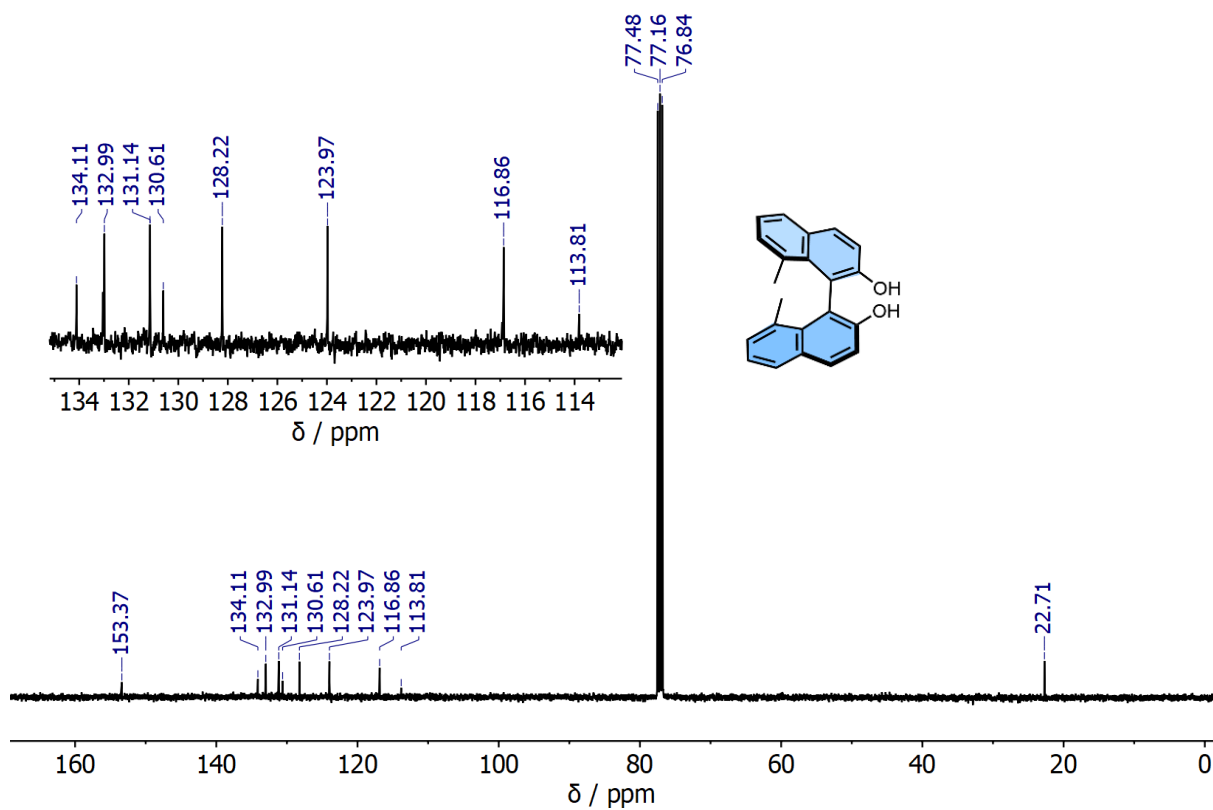


Figure S13. ^{13}C NMR spectrum of **4** (101 MHz, CDCl_3).

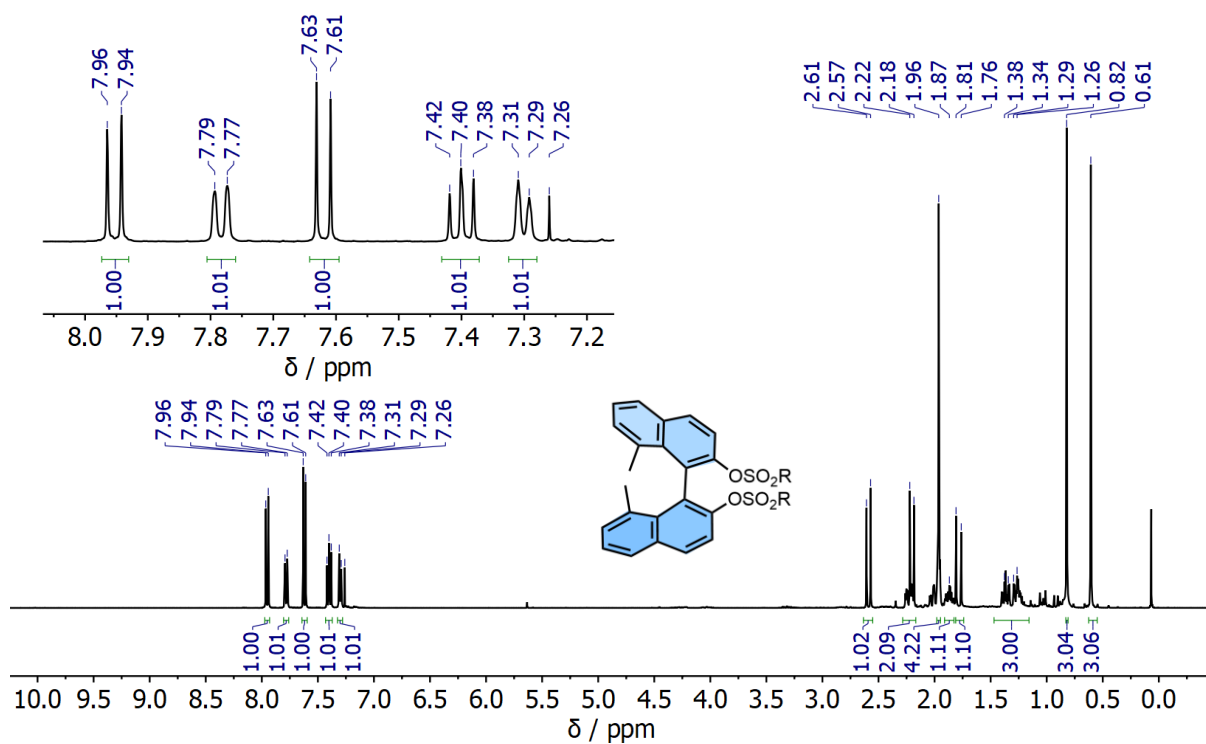


Figure S14. ^1H NMR spectrum of 8,8'-dimethyl-[1,1'-binaphthalene]-2,2'-dicamphorsulfonic ester (400 MHz, CDCl_3) (R = Camphor).

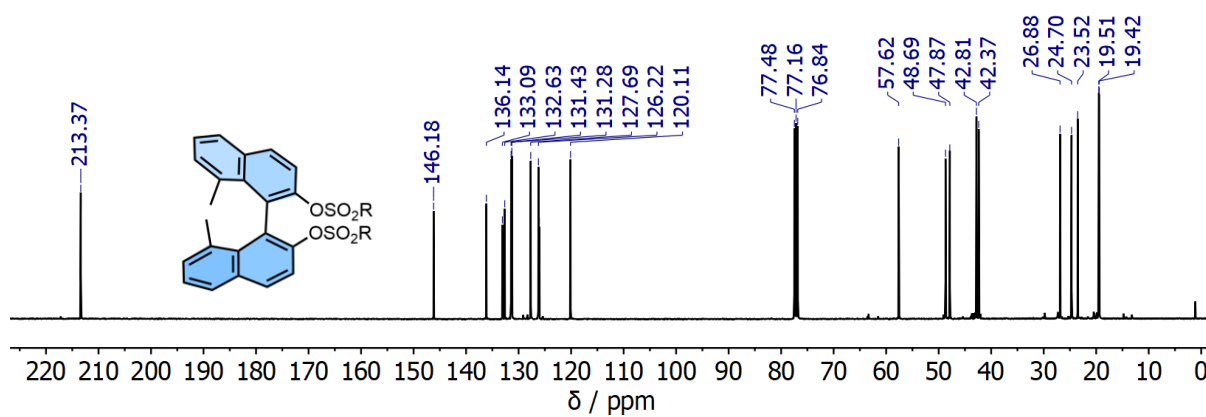


Figure S15. ^{13}C NMR spectrum of 8,8'-dimethyl-[1,1'-binaphthalene]-2,2'-dicamphorsulfonic ester (101 MHz, CDCl_3) (R = Camphor).

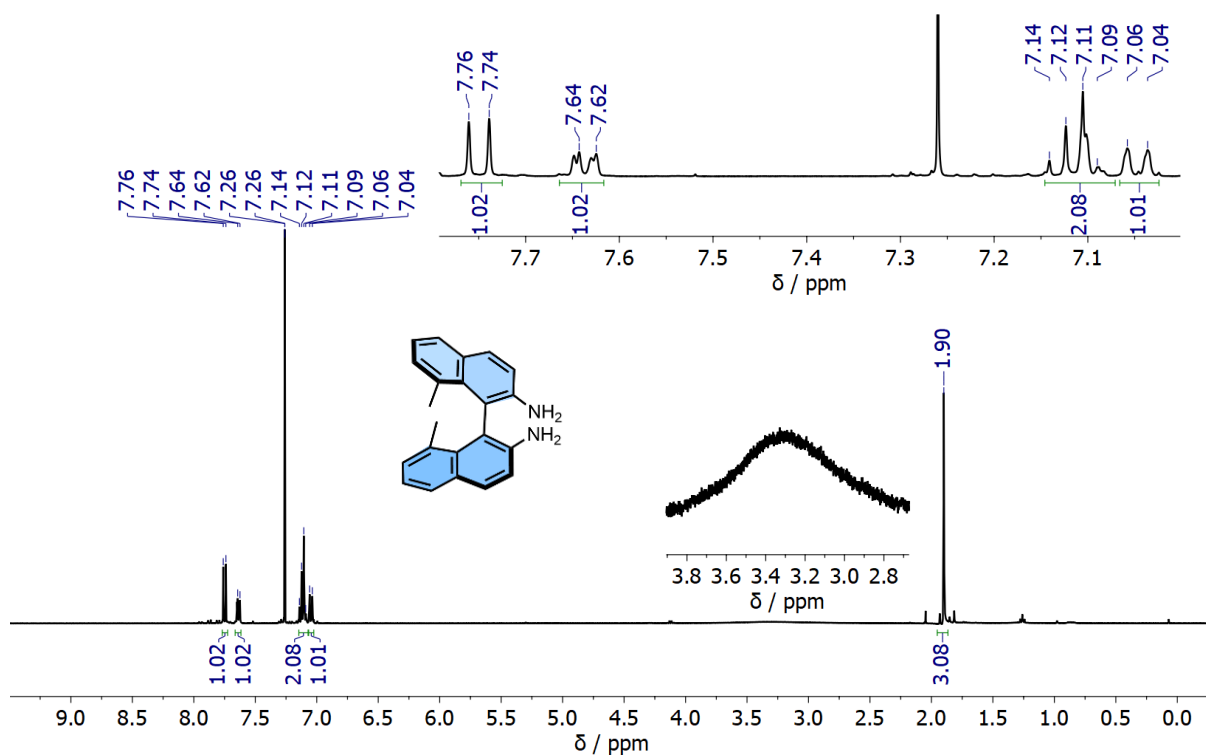


Figure S16. ^1H NMR spectrum of **5** (400 MHz, CDCl_3).

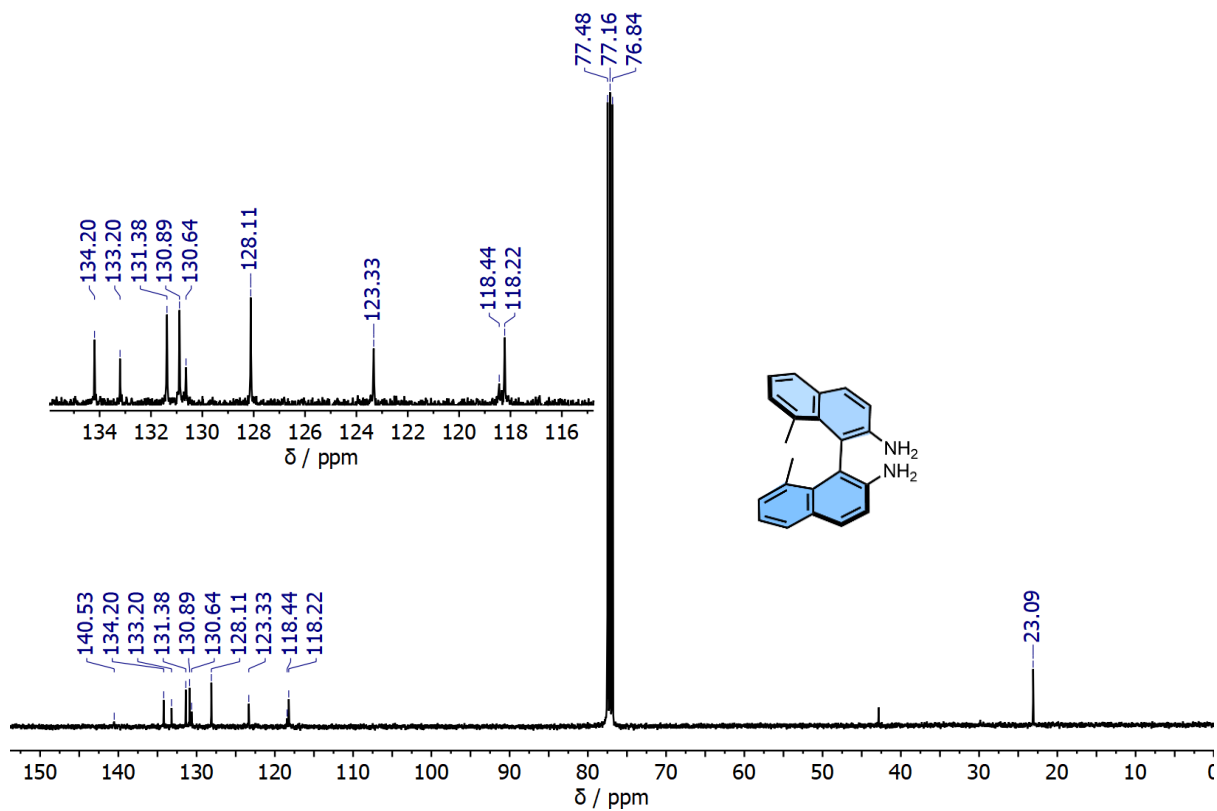


Figure S17. ^{13}C NMR spectrum of **5** (101 MHz, CDCl_3).

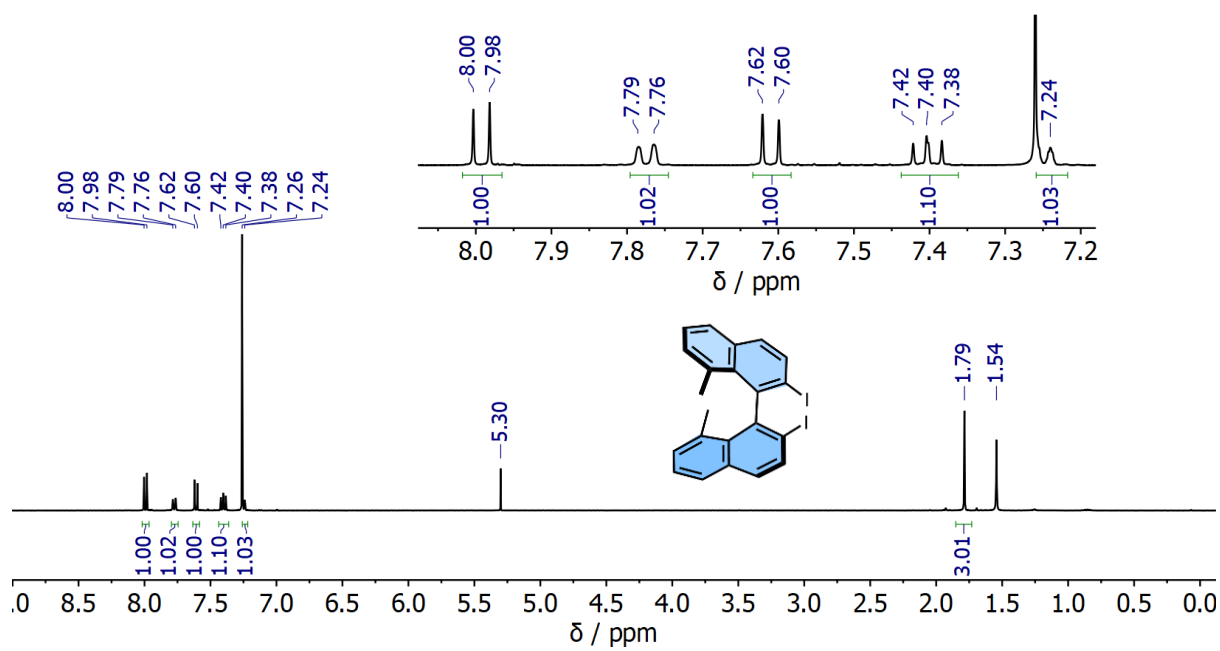


Figure S18. ^1H NMR spectrum of **6** (400 MHz, CDCl_3).

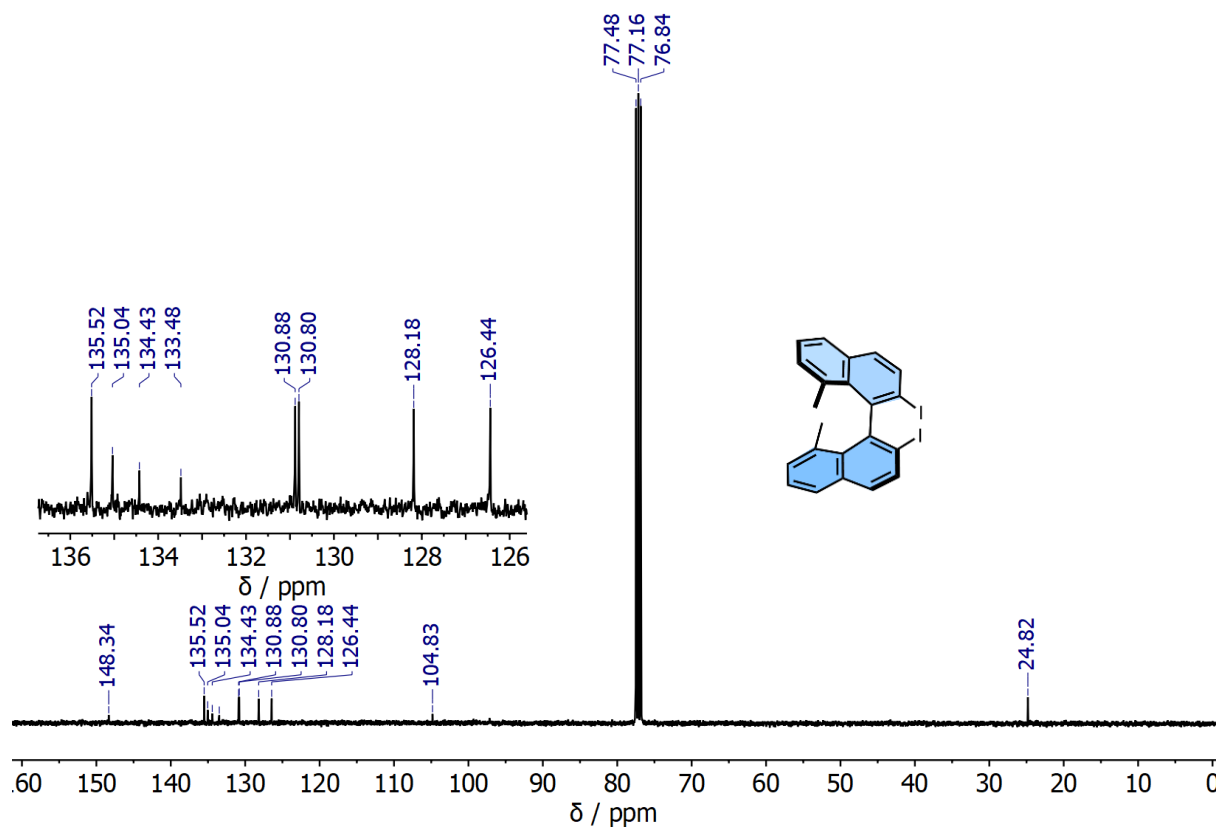


Figure S19. ^{13}C NMR spectrum of **6** (101 MHz, CDCl_3).

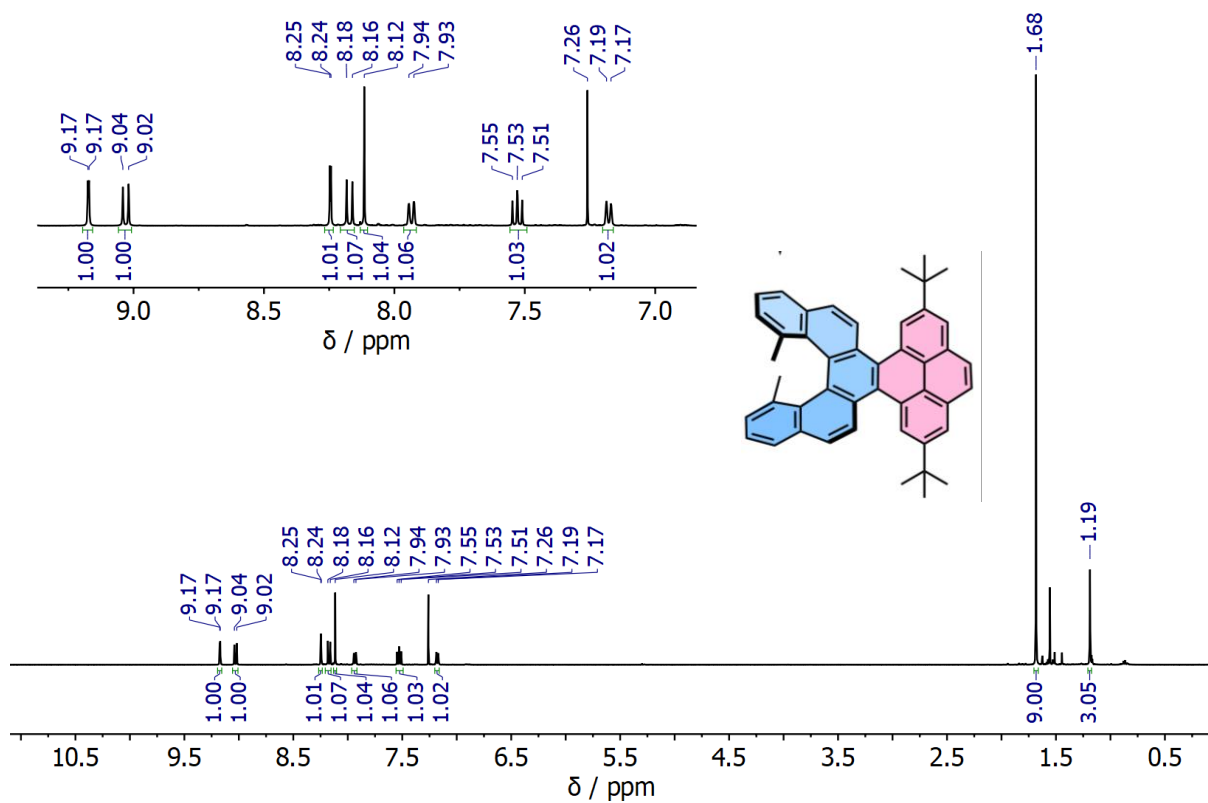


Figure S20. ^1H NMR spectrum of **1** (400 MHz, CDCl_3).

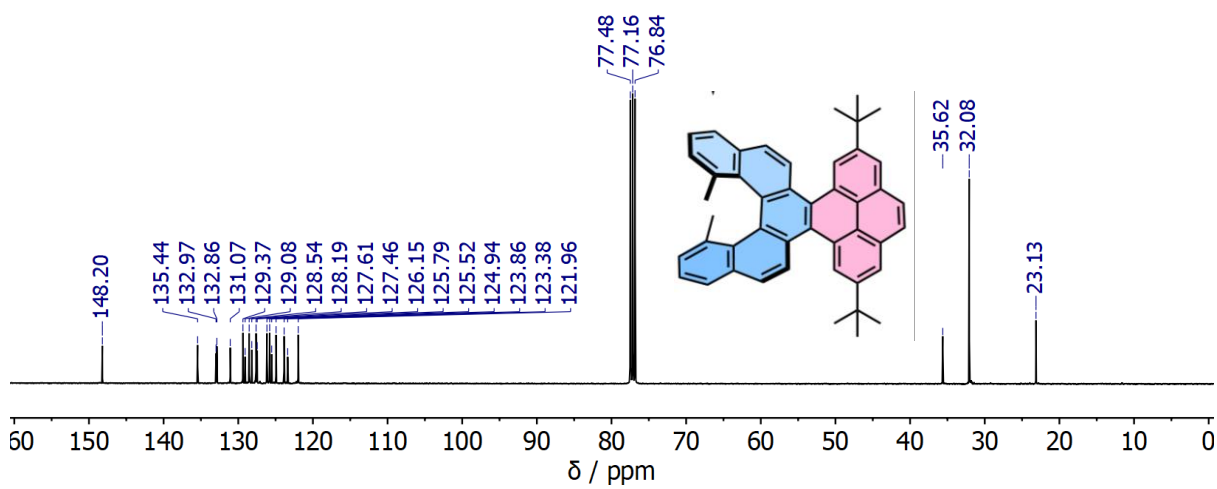


Figure S21. ^{13}C NMR spectrum of **1** (101 MHz, CDCl_3).

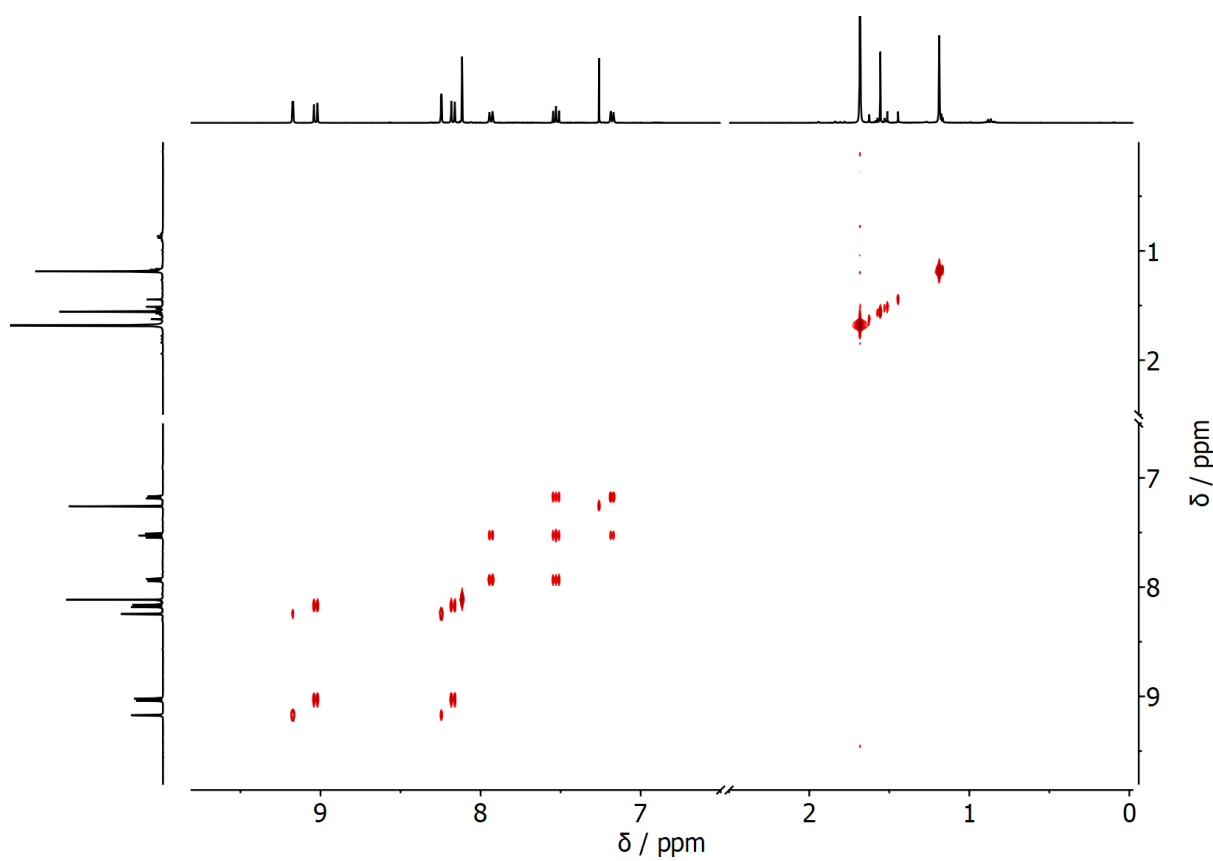


Figure S22. $^1\text{H} - ^1\text{H}$ COSY NMR spectrum of **1** (CDCl_3).

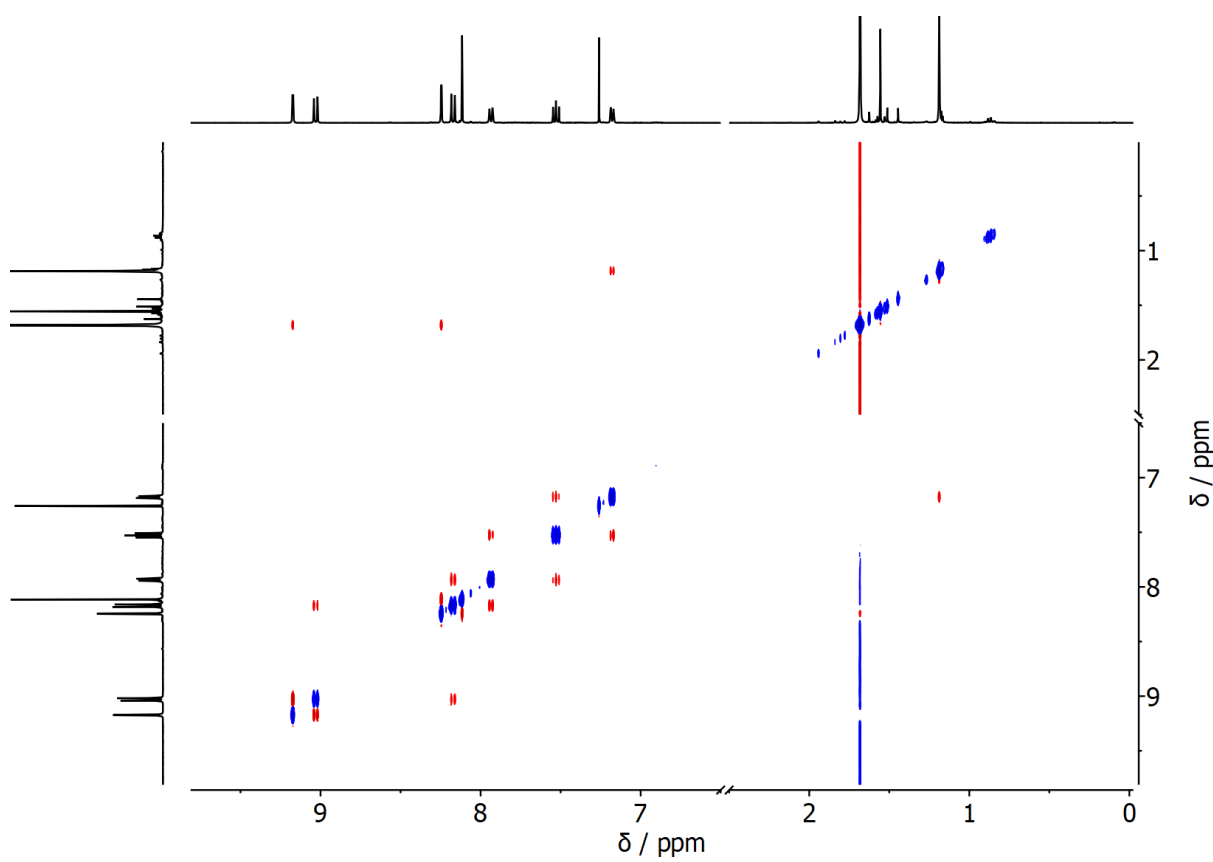


Figure S23. $^1\text{H} - ^1\text{H}$ NOESY NMR spectrum of **1** (CDCl_3).

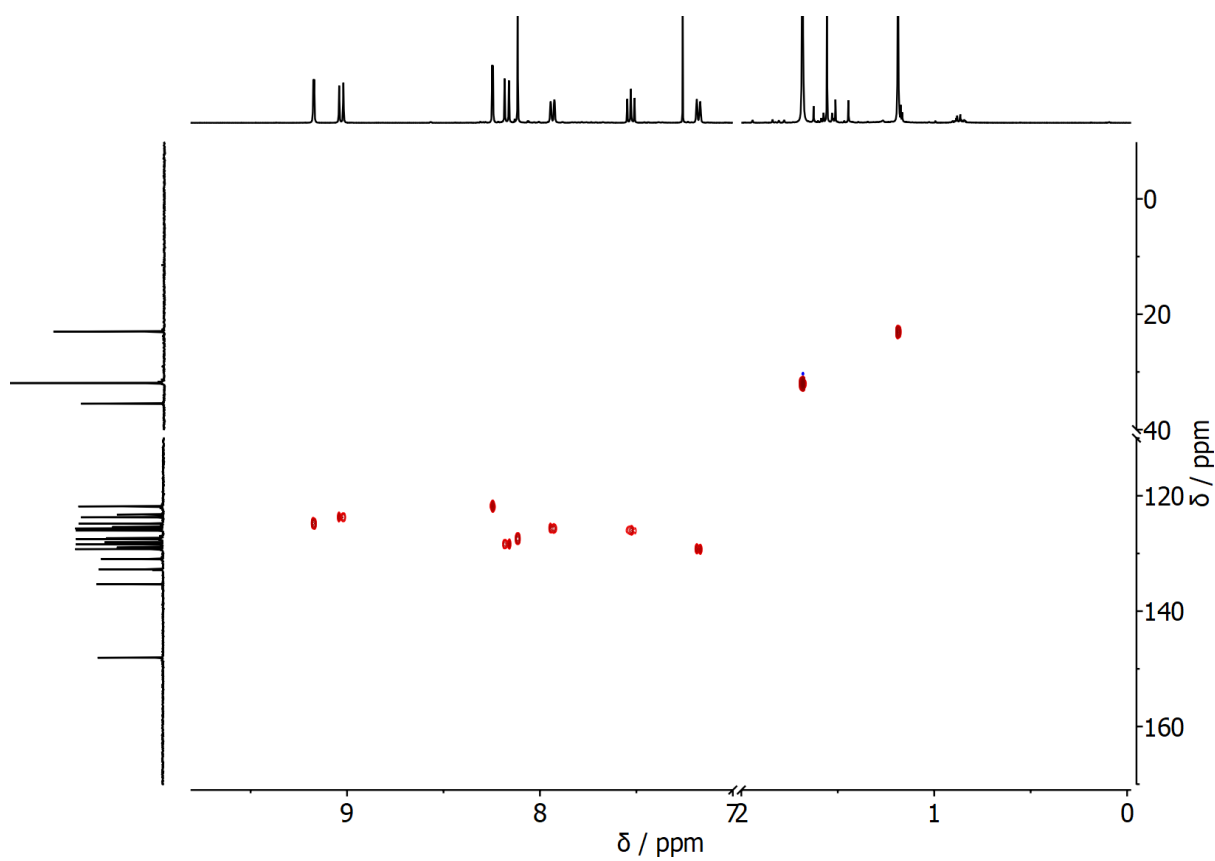


Figure S24. ^1H – ^{13}C HSQC NMR spectrum **1** (CDCl_3).

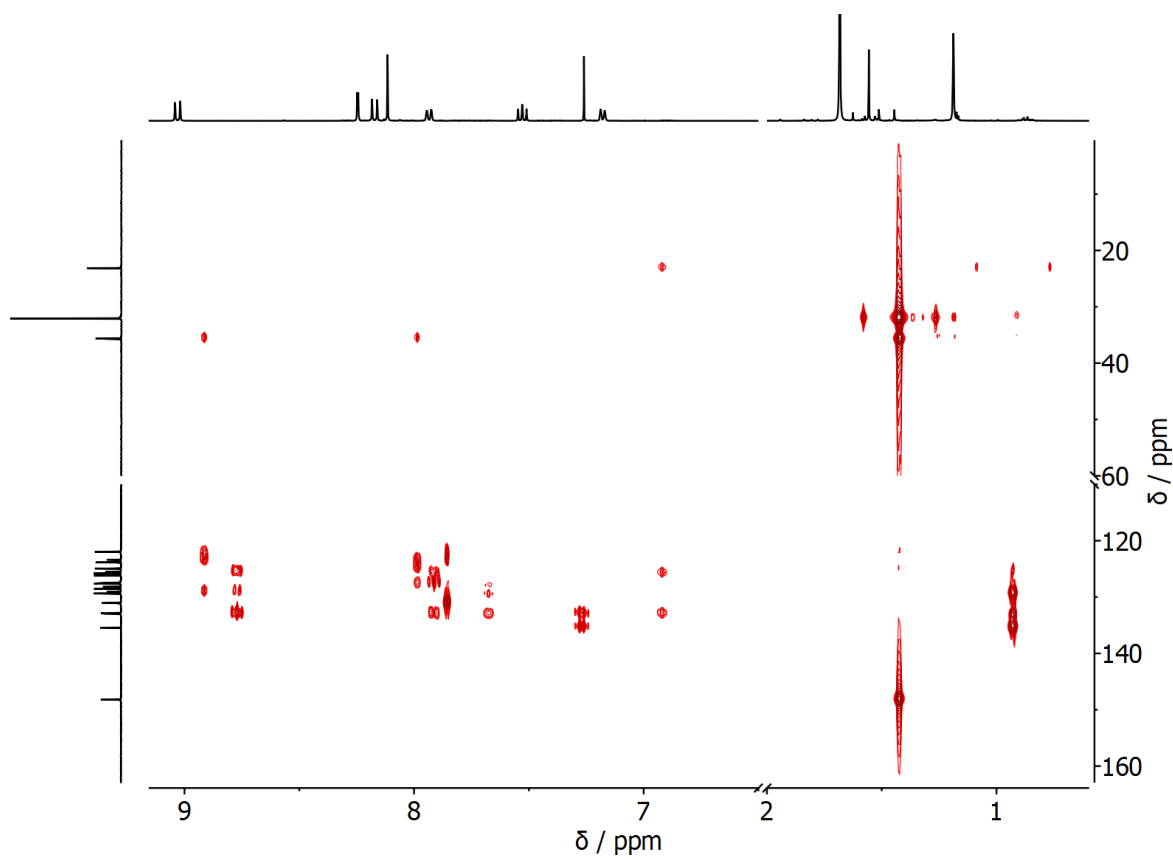


Figure S25. ^1H – ^{13}C HMBC NMR spectrum of **1** (CDCl_3).

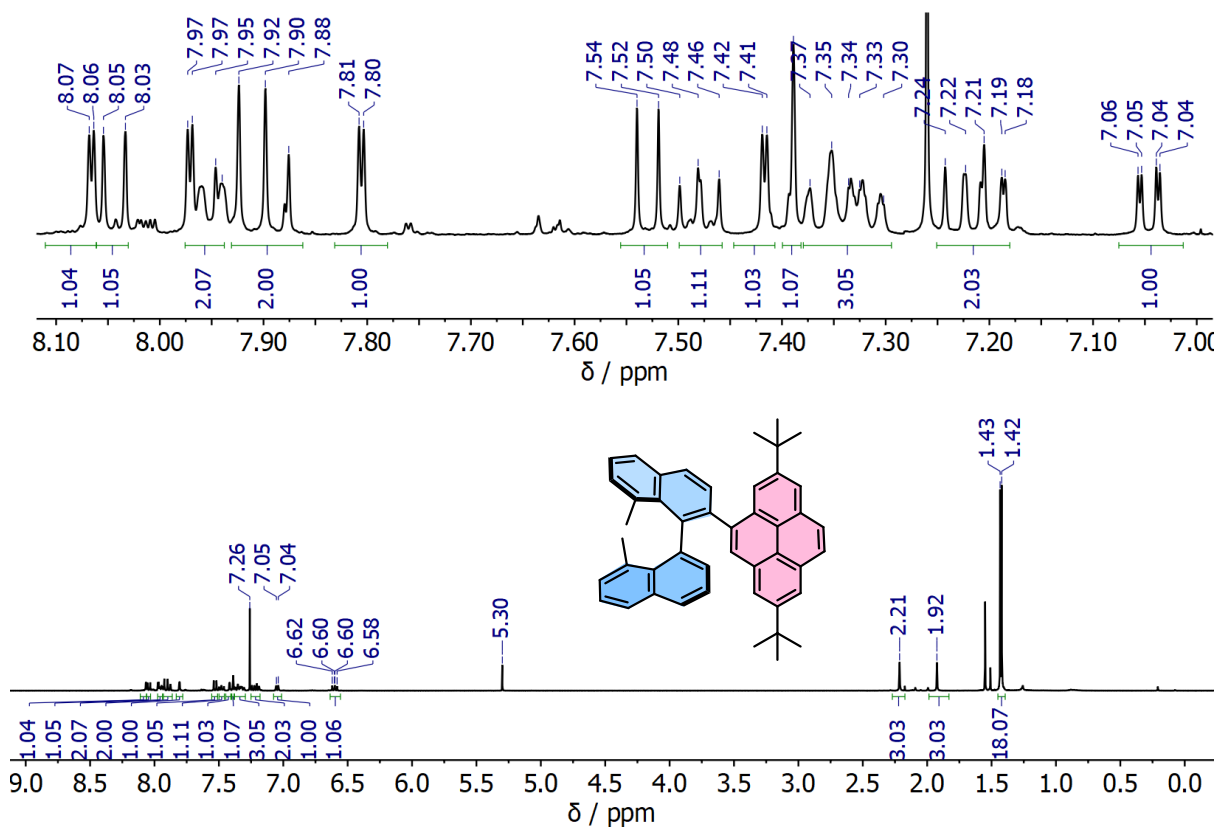


Figure S26. ^1H NMR spectrum of **7** (400 MHz, CDCl_3).

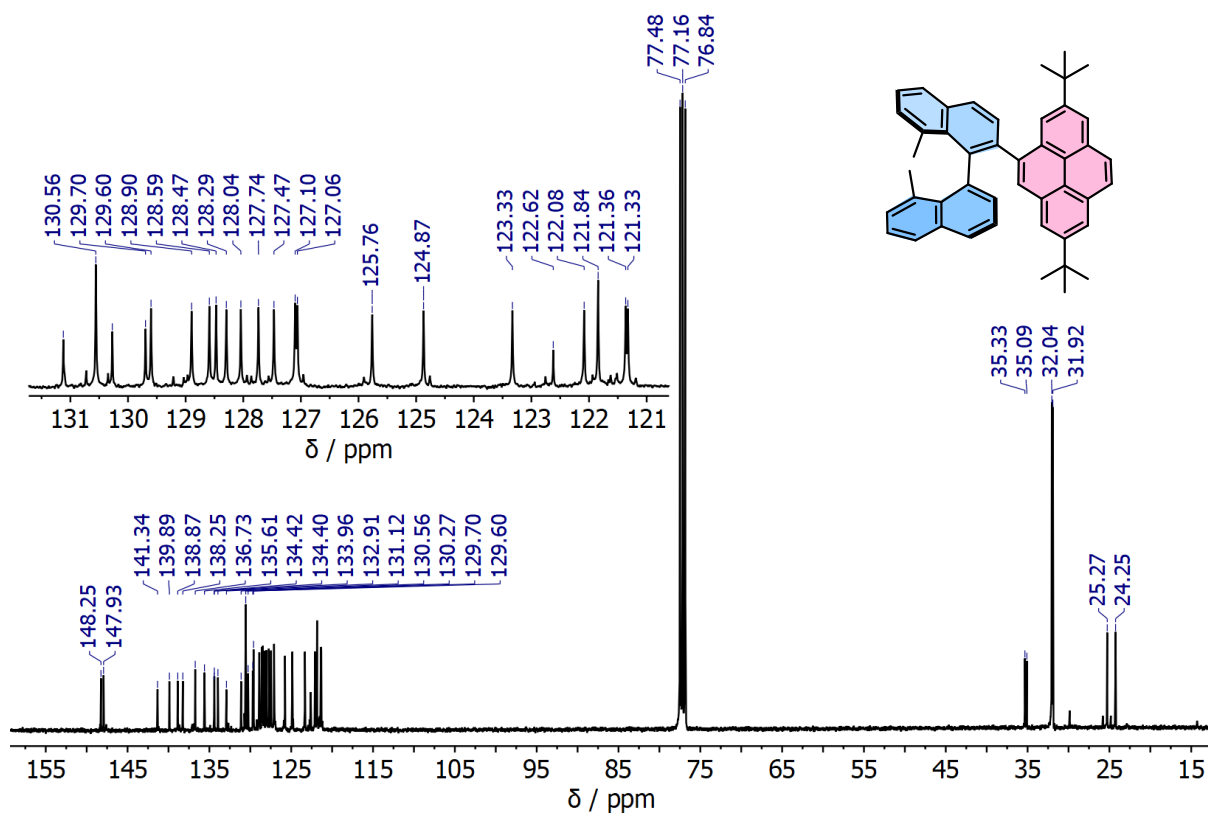


Figure S27. ^{13}C NMR spectrum of **7** (101 MHz, CDCl_3).

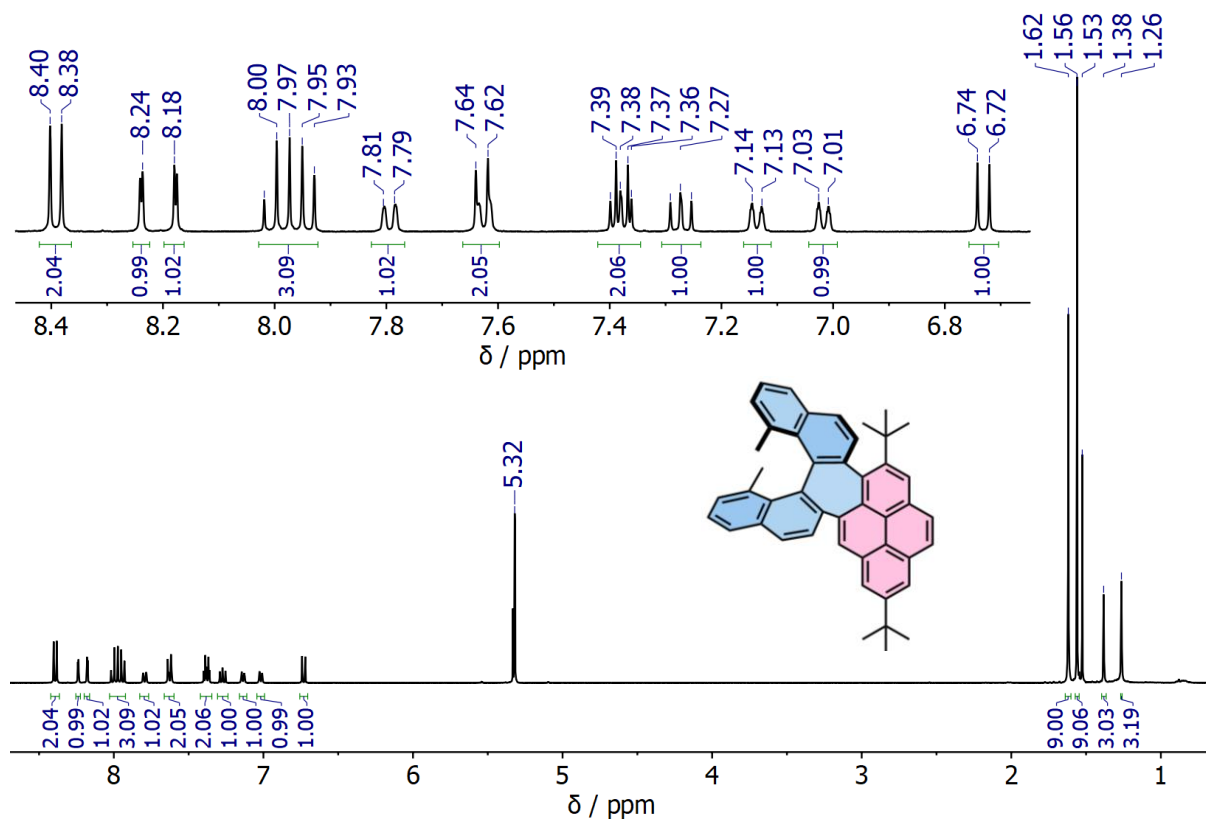


Figure S28. ^1H NMR spectrum of **2** (400 MHz, CD_2Cl_2).

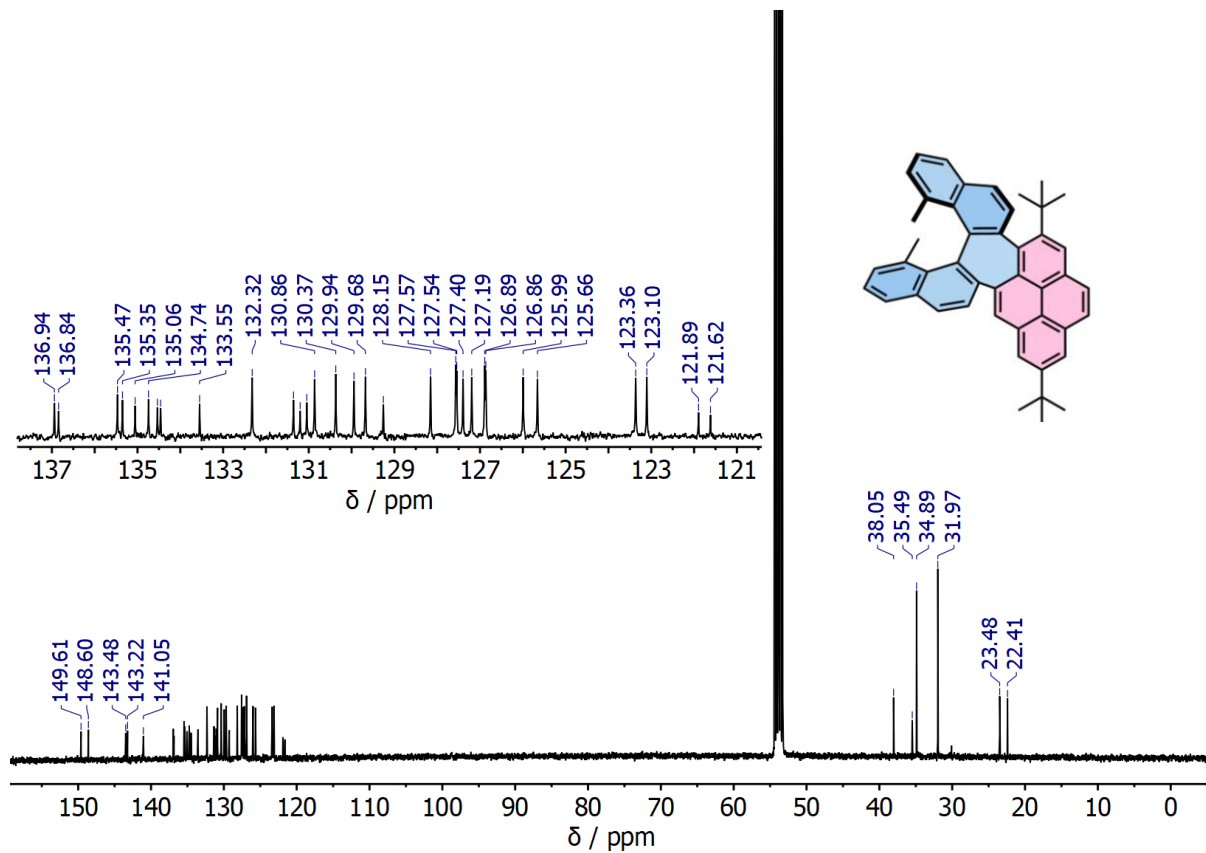


Figure S29. ^{13}C NMR spectrum of **2** (101 MHz, CD_2Cl_2).

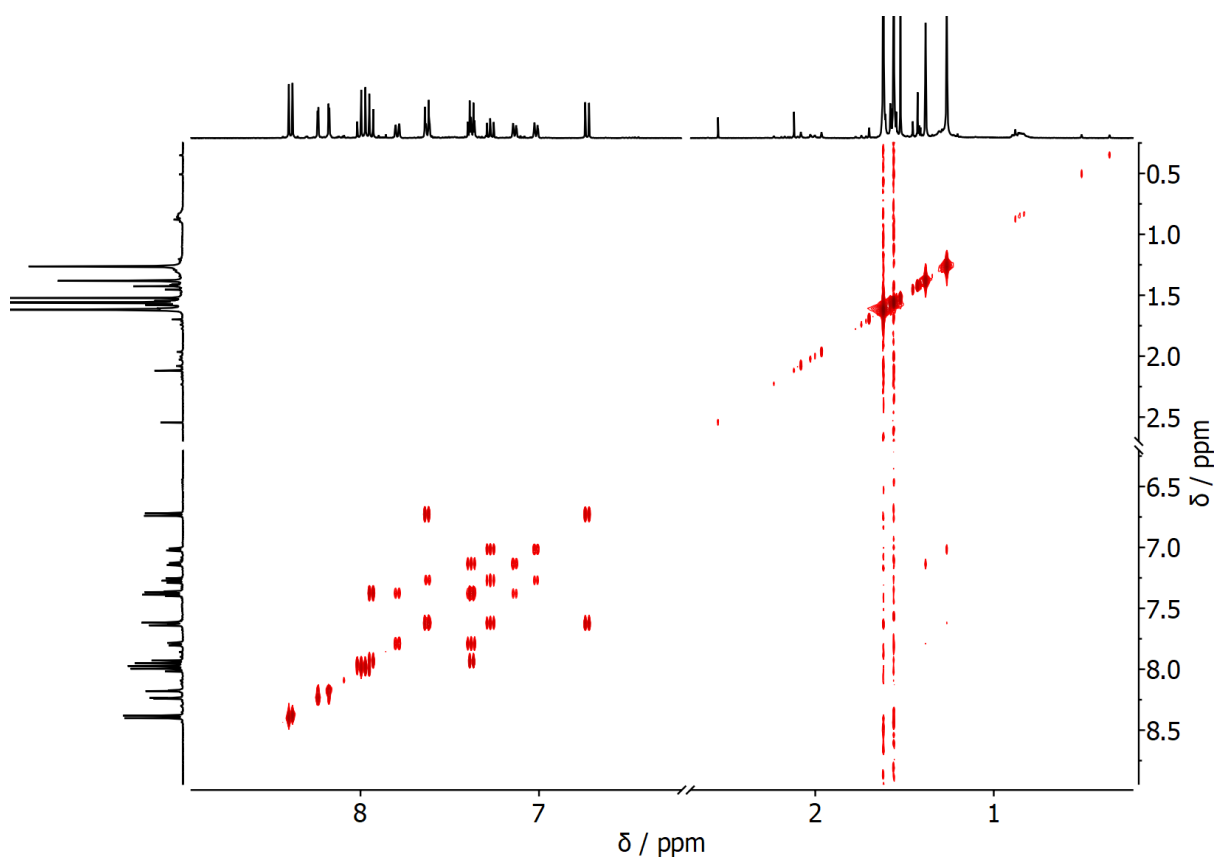


Figure S30. $^1\text{H} - ^1\text{H}$ COSY NMR spectrum of **2** (CD_2Cl_2).

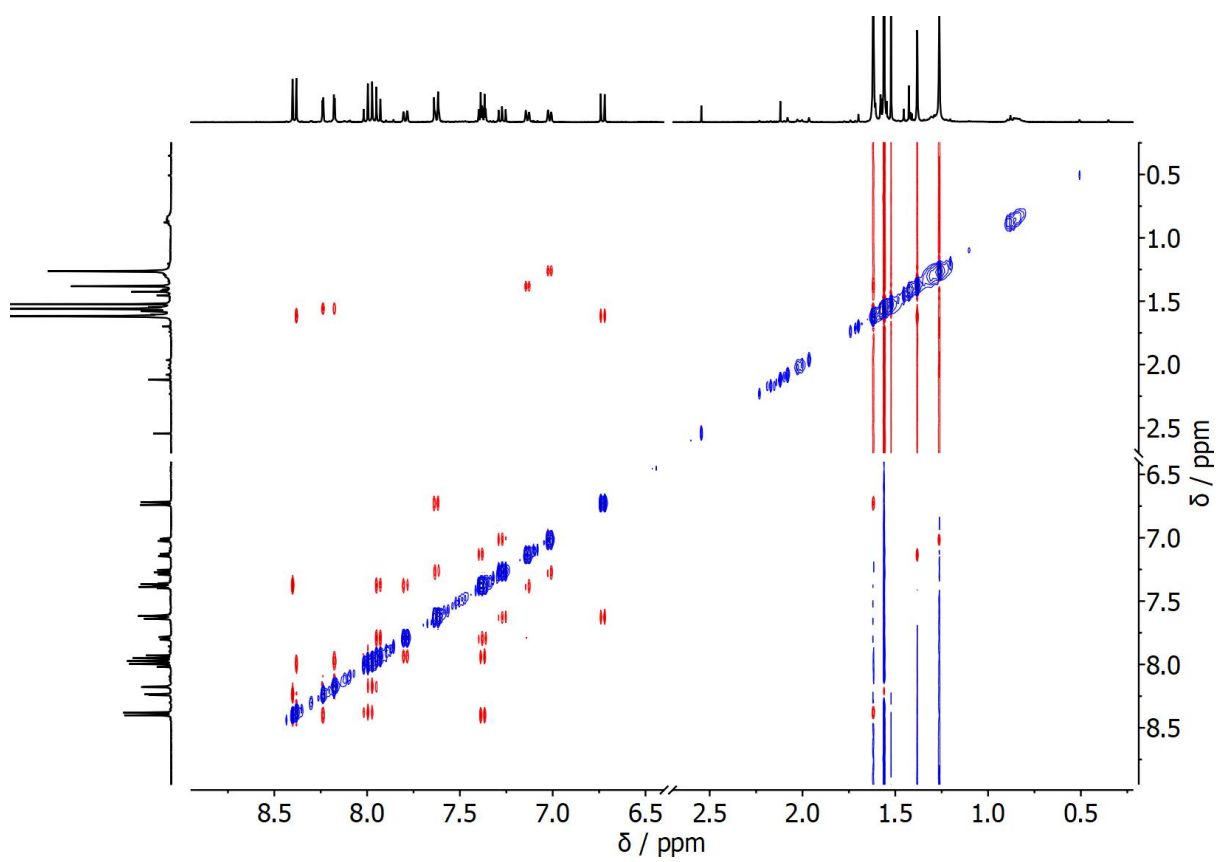


Figure S31. $^1\text{H} - ^1\text{H}$ NOESY NMR spectrum of **2** (CD_2Cl_2).

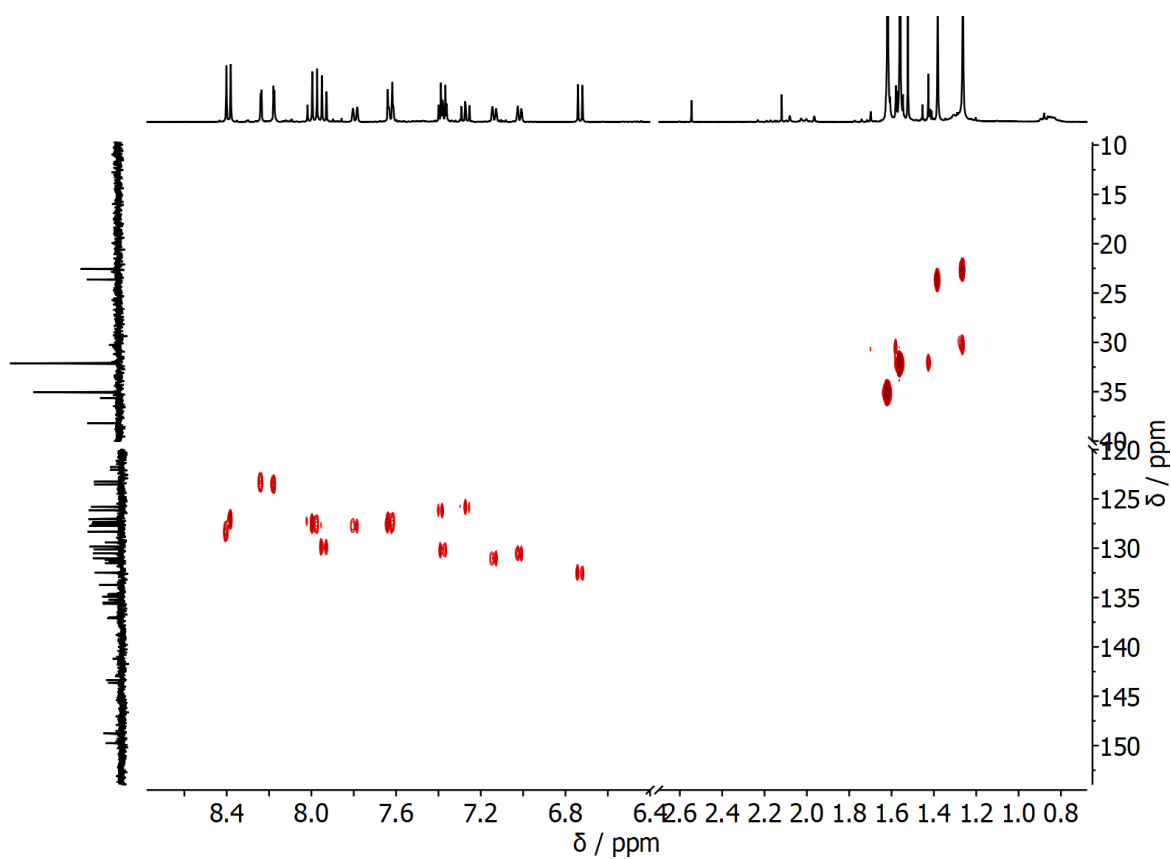


Figure S32. $^1\text{H} - ^{13}\text{C}$ HSQC NMR spectrum of **2** (CD_2Cl_2).

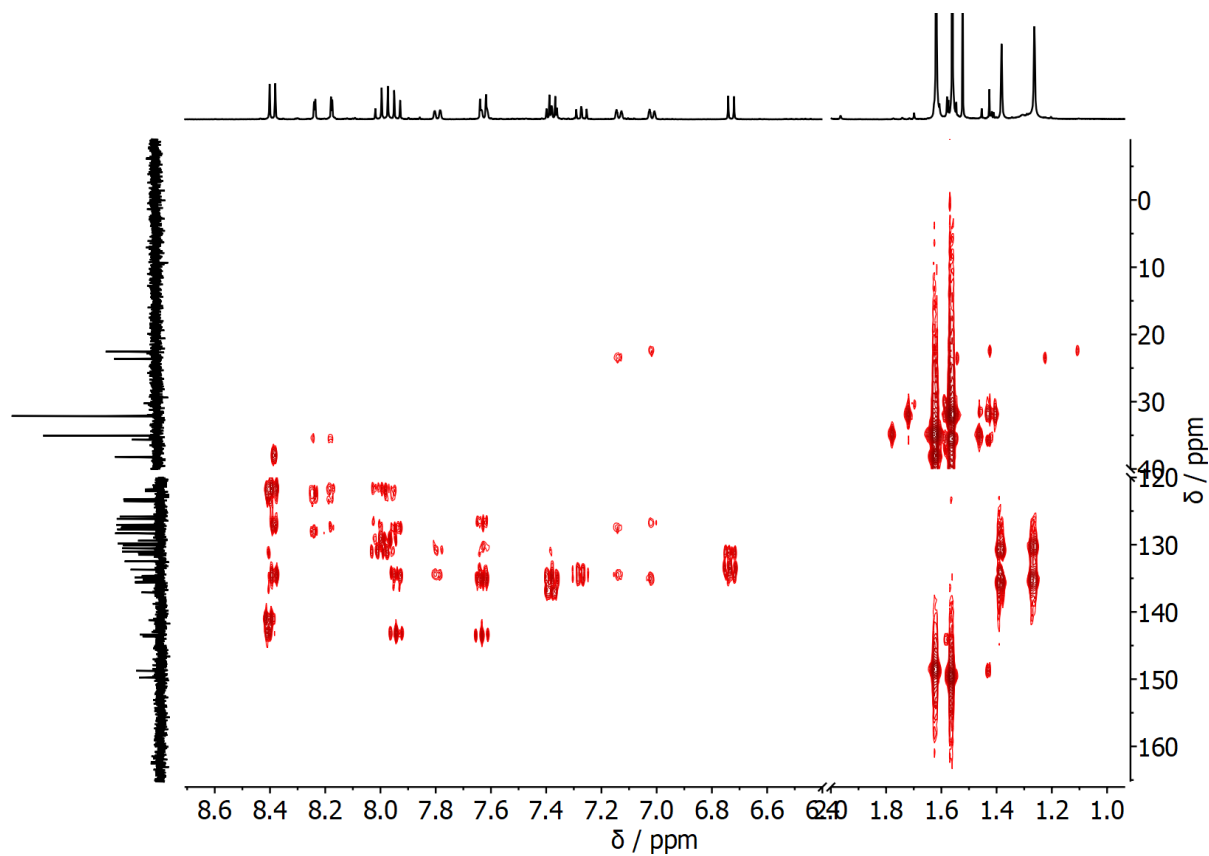


Figure S33. $^1\text{H} - ^{13}\text{C}$ HMBC NMR spectrum of **2** (CD_2Cl_2).

S10. High resolution mass spectrometry (HRMS)

-MS, 0.2-2.5min #8-100

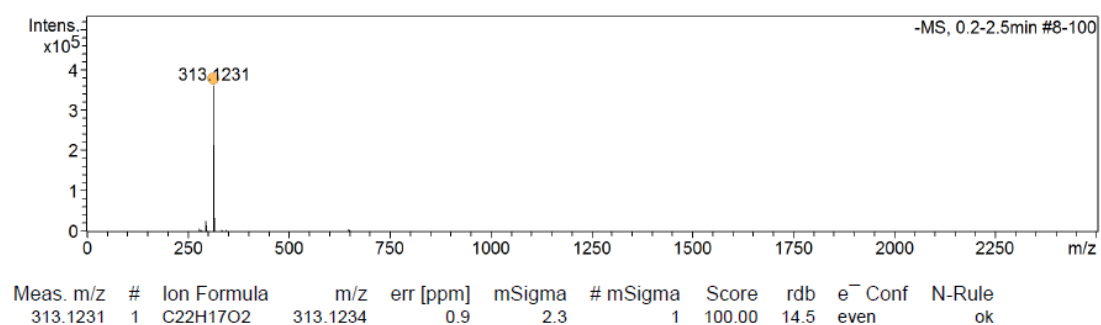


Figure S34. ESI-HRMS of **4**.

+MS, 0.2-2.5min #12-154

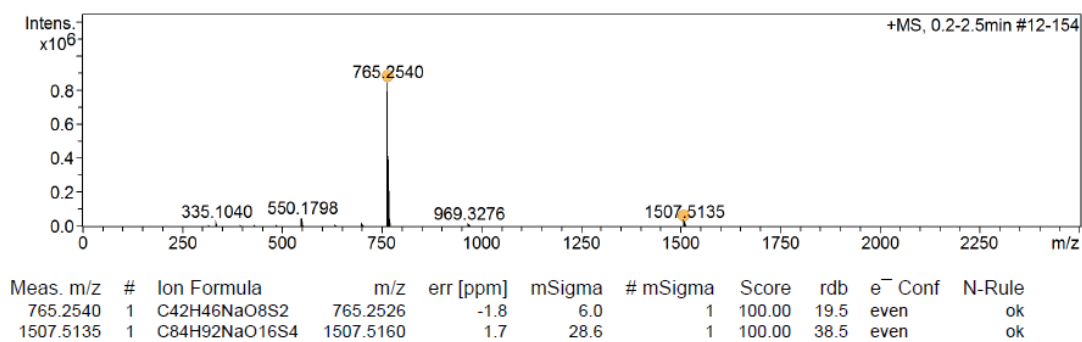


Figure S35. ESI-HRMS of **8,8'-dimethyl-[1,1'-binaphthalene]-2,2'-dicamphorsulfonicester**.

+MS, 1.5min #92

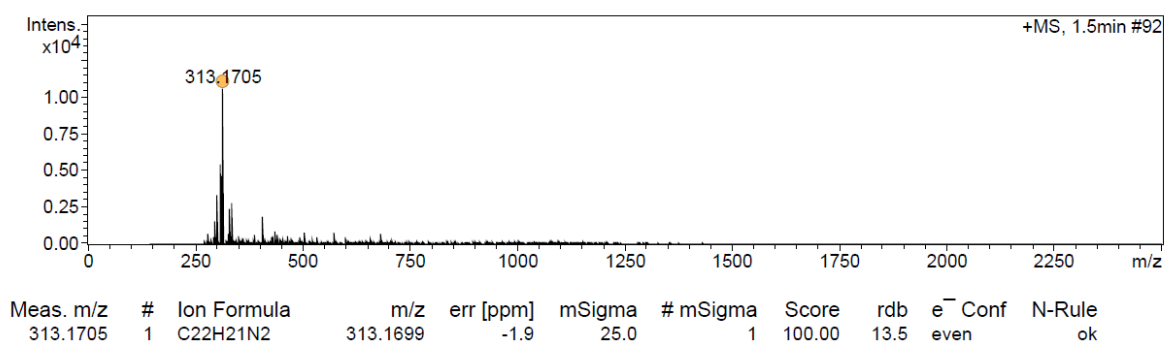


Figure S36. ESI-HRMS of **5**.

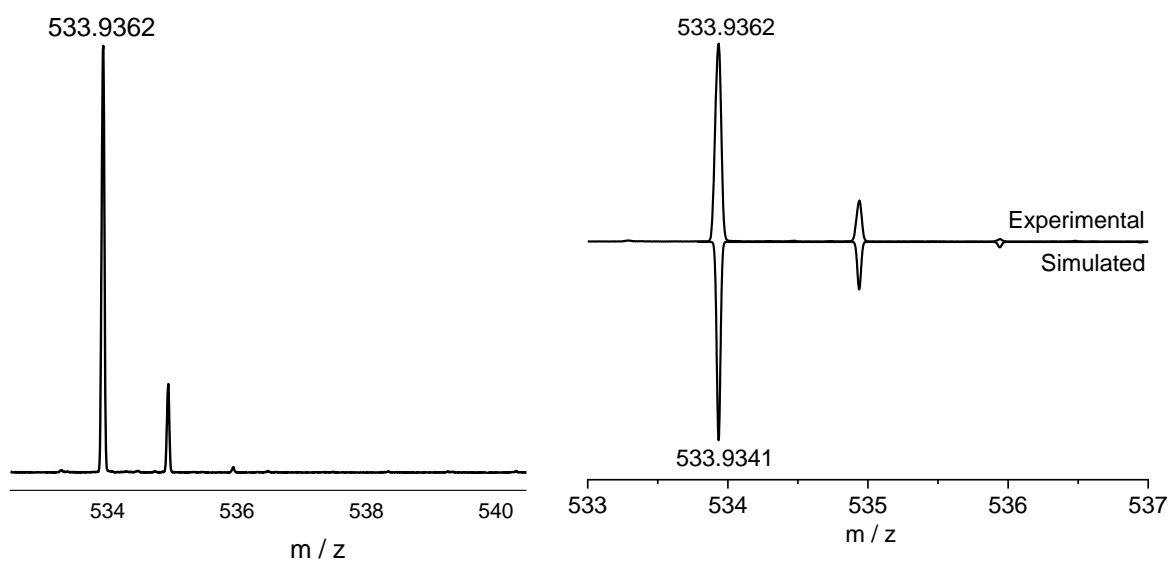


Figure S37. MALDI-TOF HRMS of **6**.

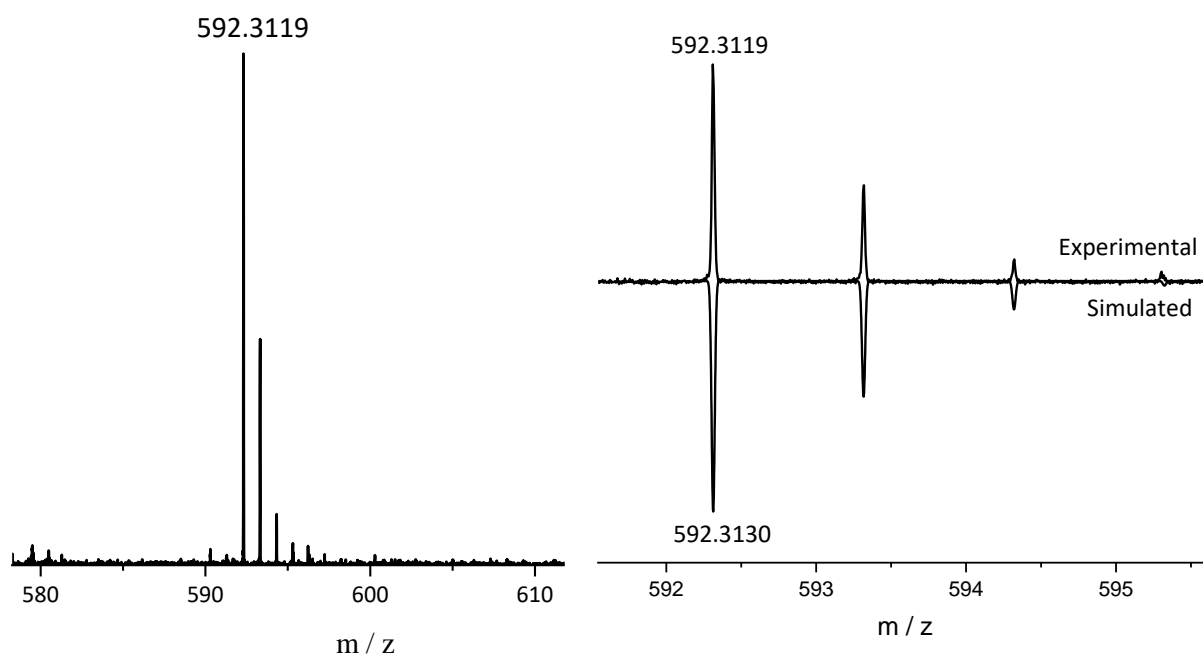


Figure S38. MALDI-TOF HRMS of **1**.

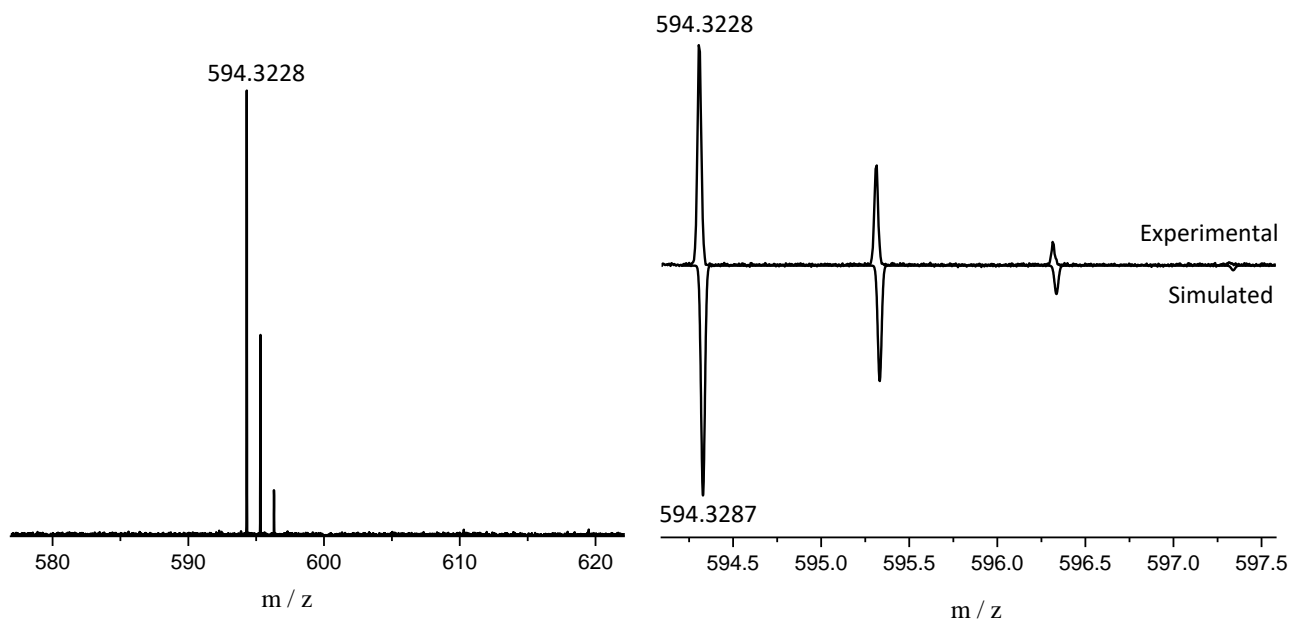


Figure S39. MALDI-TOF HRMS of **7**.

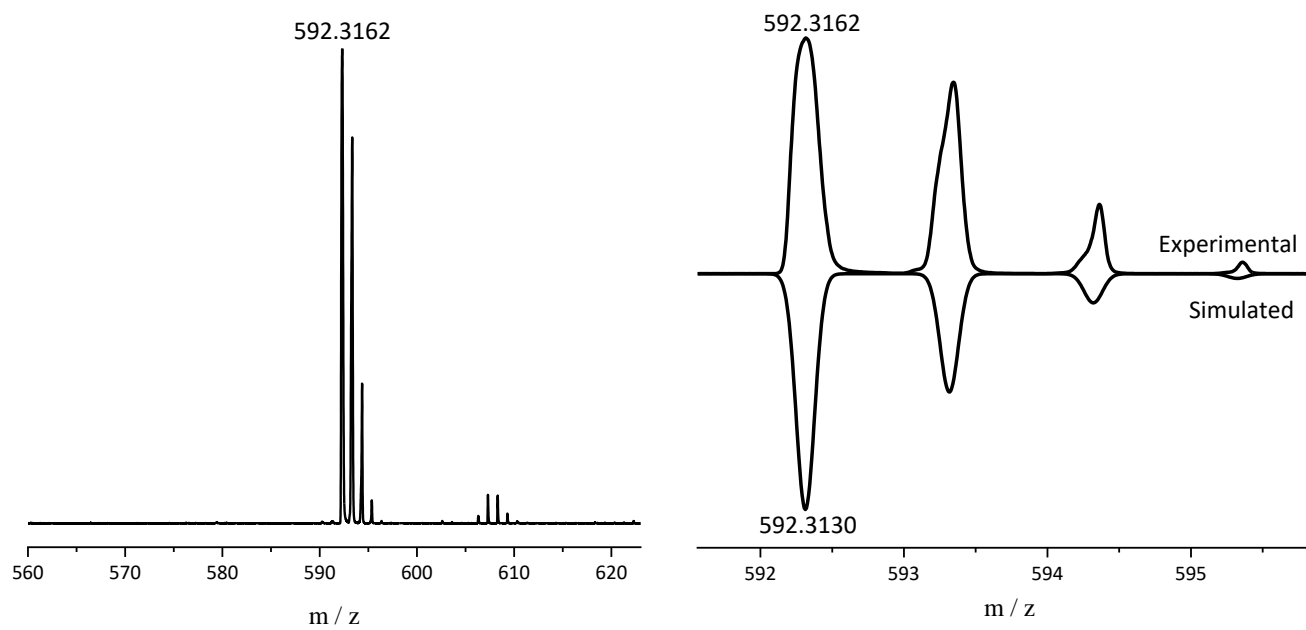


Figure S40. MALDI-TOF HRMS of **2**.

1 (PPM)

C	-3.906109000	3.078185000	-0.052114000	H	4.963184000	-1.702826000	-0.983593000
C	-3.972780000	1.727196000	-0.438892000	H	3.529433000	-1.388455000	-1.958495000
C	-5.217524000	1.110158000	-0.798984000	H	-3.196359000	-6.139085000	1.751472000
C	-5.309375000	-0.238855000	-0.951350000	H	-2.085932000	-4.764231000	1.808248000
C	-2.796684000	0.925592000	-0.401707000	H	-3.797282000	-4.527268000	2.182642000
C	-2.892778000	-0.490976000	-0.541342000	H	-4.886465000	-6.373227000	-0.057422000
C	-4.169897000	-1.087368000	-0.742046000	H	-5.099534000	-5.144738000	-1.308771000
C	-1.749495000	-1.315778000	-0.301191000	H	-5.577882000	-4.805032000	0.365671000
C	-1.994529000	-2.674690000	-0.053904000	H	-1.374661000	-5.334367000	-0.622153000
C	-3.251106000	-3.284361000	-0.235118000	H	-2.530529000	-6.668121000	-0.656683000
C	-4.312641000	-2.482723000	-0.640077000	H	-2.596689000	-5.406578000	-1.900369000
C	-1.546985000	1.525558000	-0.075595000	H	-3.900996000	6.806956000	1.334856000
C	-2.729328000	3.631612000	0.445027000	H	-4.342552000	5.898783000	-0.114075000
C	-1.569144000	2.834162000	0.425951000	H	-4.786429000	5.287221000	1.491206000
C	2.033585000	-0.779507000	0.065425000	H	-2.174590000	6.004448000	2.926118000
C	2.155285000	0.581986000	-0.390514000	H	-1.267191000	4.514834000	2.636662000
C	0.812348000	-1.443743000	-0.235997000	H	-2.974299000	4.429865000	3.088083000
C	0.960474000	1.350343000	-0.480407000	H	-1.869468000	5.945899000	-0.831589000
C	-0.327764000	0.726966000	-0.246820000	H	-1.547418000	6.904357000	0.624189000
C	-0.418302000	-0.681524000	-0.285569000	H	-0.604390000	5.446519000	0.301094000
C	0.920643000	-2.852189000	-0.506874000				
C	3.071409000	-1.532903000	0.758544000				
C	3.075397000	-2.956987000	0.601040000				
C	2.032170000	-3.563217000	-0.164778000				
C	4.091420000	-3.741280000	1.186518000				
C	5.052077000	-3.151359000	1.981368000				
C	4.980307000	-1.773240000	2.239573000				
C	4.017691000	-0.950499000	1.661915000				
C	3.419889000	1.160099000	-0.846389000				
C	3.495201000	2.588597000	-0.945446000				
C	2.284481000	3.341852000	-0.958627000				
C	1.072715000	2.731663000	-0.847284000				
C	4.559110000	0.421583000	-1.317502000				
C	5.748424000	1.104804000	-1.553520000				
C	5.863663000	2.498192000	-1.427134000				
C	4.727903000	3.237648000	-1.181469000				
C	3.978324000	0.492523000	2.116720000				
C	4.537177000	-1.034891000	-1.736334000				
C	-3.404261000	-4.792465000	0.043314000				
C	-3.100401000	-5.069022000	1.535085000				
C	-4.827179000	-5.299008000	-0.259446000				
C	-2.415638000	-5.593364000	-0.836781000				
C	-2.653731000	5.061442000	1.014362000				
C	-4.003202000	5.798228000	0.922132000				
C	-2.240970000	4.995260000	2.504100000				
C	-1.604605000	5.883839000	0.229158000				
H	-4.819907000	3.660537000	-0.090586000				
H	-6.098061000	1.739366000	-0.898437000				
H	-6.265179000	-0.705533000	-1.174550000				
H	-1.191621000	-3.287613000	0.324365000				
H	-5.296449000	-2.905355000	-0.810401000				
H	-0.655185000	3.244348000	0.834300000				
H	0.130676000	-3.338216000	-1.061888000				
H	2.112448000	-4.615304000	-0.423680000				
H	4.085403000	-4.815518000	1.022738000				
H	5.830943000	-3.749999000	2.444436000				
H	5.685422000	-1.330773000	2.938472000				
H	2.343491000	4.405397000	-1.174432000				
H	0.177633000	3.302455000	-1.044558000				
H	6.607382000	0.535479000	-1.899862000				
H	6.817560000	2.985136000	-1.606915000				
H	4.749509000	4.323753000	-1.206992000				
H	2.960878000	0.889061000	2.131369000				
H	4.385787000	0.566361000	3.129284000				
H	4.571041000	1.149885000	1.474015000				
H	5.136694000	-1.143648000	-2.645888000				

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction=	0.721851 (Hartree/Particle)
Thermal correction to Energy=	0.759656
Thermal correction to Enthalpy=	0.760600
Thermal correction to Gibbs Free Energy=	0.654991
Sum of electronic and zero-point Energies=	-1776.403764
Sum of electronic and thermal Energies=	-1776.365959
Sum of electronic and thermal Enthalpies=	-1776.365015
Sum of electronic and thermal Free Energies=	-1776.470624

1(PPP)

C	5.500051000	-3.269601000	-0.126375000	C	-2.195361000	-5.410247000	1.692411000
C	5.417773000	-2.215212000	0.795316000	H	-2.725768000	-4.978944000	2.547535000
C	4.404320000	-3.560240000	-0.912590000	H	-1.171243000	-5.026246000	1.706838000
C	3.246925000	-2.755863000	-0.843630000	H	-2.146175000	-6.495754000	1.834694000
C	3.229377000	-1.569142000	-0.040578000	C	-2.151014000	5.714283000	0.812488000
C	4.310426000	-1.374270000	0.877716000	H	-2.114512000	6.803271000	0.696135000
C	2.053083000	-3.148875000	-1.524914000	H	-1.119780000	5.354156000	0.872190000
C	2.047510000	-0.706754000	-0.132001000	H	-2.640602000	5.491585000	1.766328000
C	0.871068000	-2.526859000	-1.259548000	C	-2.196485000	5.409720000	-1.692821000
C	0.812915000	-1.327485000	-0.468245000	H	-1.172294000	5.025911000	-1.707236000
C	2.047401000	0.707143000	0.132170000	H	-2.147514000	6.495217000	-1.835263000
C	0.812730000	1.327698000	0.468479000	H	-2.726846000	4.978195000	-2.547862000
C	-0.443541000	0.684281000	0.162166000	C	-4.326913000	5.699233000	-0.415877000
C	-0.443428000	-0.684235000	-0.161933000	H	-4.887521000	5.513620000	0.506225000
C	3.229127000	1.569701000	0.040656000	H	-4.914368000	5.317104000	-1.256946000
C	0.870793000	2.527014000	1.259885000	H	-4.243519000	6.783791000	-0.538670000
C	2.052738000	3.149216000	1.525132000	H	4.777748000	-0.854045000	2.898025000
C	3.246564000	2.756432000	0.843687000	H	4.807931000	0.535934000	1.813374000
C	4.310164000	1.374910000	-0.877662000	H	3.265151000	-0.137596000	2.330482000
C	4.403846000	3.560983000	0.912536000	H	3.265021000	0.137864000	-2.330202000
C	5.499567000	3.270475000	0.126251000	H	4.777501000	0.854435000	-2.897909000
C	5.417396000	2.216016000	-0.795373000	H	4.807906000	-0.535370000	-1.813038000
H	6.391608000	-3.888352000	-0.167373000				
H	6.231333000	-2.066513000	1.500846000				
H	4.399051000	-4.430798000	-1.562907000				
C	4.283187000	-0.397229000	2.035006000				
H	2.090034000	-3.997966000	-2.201664000				
H	-0.037529000	-2.877861000	-1.731837000				
H	-0.037785000	2.877822000	1.732343000				
H	2.089634000	3.998270000	2.201932000				
C	4.283031000	0.397689000	-2.034802000				
H	4.398504000	4.431548000	1.562840000				
H	6.391042000	3.889347000	0.167176000				
H	6.230951000	2.067373000	-1.500919000				
C	-1.705193000	-1.434207000	-0.075336000				
C	-2.932932000	-0.713408000	-0.004447000				
C	-1.761189000	-2.826793000	0.082922000				
C	-2.933066000	0.712988000	0.004665000				
C	-4.165781000	-1.423203000	0.054729000				
C	-2.967232000	-3.544491000	0.187101000				
H	-0.833578000	-3.375610000	0.166124000				
C	-4.166057000	1.422536000	-0.054546000				
C	-1.705455000	1.434028000	0.075491000				
C	-5.393693000	-0.679953000	0.035970000				
C	-4.158752000	-2.827531000	0.133403000				
C	-4.159307000	2.826856000	-0.133348000				
C	-5.393825000	0.679047000	-0.035736000				
C	-1.761741000	2.826581000	-0.082994000				
H	-6.330012000	-1.230796000	0.068746000				
H	-5.115313000	-3.336123000	0.178357000				
C	-2.967929000	3.544034000	-0.187208000				
H	-5.115968000	3.335254000	-0.178339000				
H	-6.330251000	1.229706000	-0.068526000				
H	-0.834257000	3.375572000	-0.166371000				
C	-2.920279000	5.073598000	-0.367095000				
C	-2.919275000	-5.074071000	0.366763000				
C	-2.149935000	-5.714432000	-0.812945000				
H	-2.113208000	-6.803430000	-0.696747000				
H	-1.118777000	-5.354088000	-0.872645000				
H	-2.639610000	-5.491698000	-1.766730000				
C	-4.325786000	-5.699990000	0.415512000				
H	-4.886470000	-5.514345000	-0.506538000				
H	-4.913277000	-5.318102000	1.256664000				
H	-4.242172000	-6.784550000	0.538137000				

- Thermochemistry -			

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.			
Zero-point correction=		0.721781 (Hartree/Particle)	
Thermal correction to Energy=		0.759613	
Thermal correction to Enthalpy=		0.760557	
Thermal correction to Gibbs Free Energy=		0.655259	
Sum of electronic and zero-point Energies=		-1776.409579	
Sum of electronic and thermal Energies=		-1776.371748	
Sum of electronic and thermal Enthalpies=		-1776.370804	
Sum of electronic and thermal Free Energies=		-1776.476102	

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C	3.354811000	-0.964969000	-0.928686000	H	-3.956518000	5.188444000	0.430485000
C	2.281617000	-0.075607000	-0.742375000	H	-3.283501000	4.102897000	-0.789681000
C	2.542534000	1.246777000	-0.295055000	H	-3.423790000	3.570495000	0.895151000
C	3.887768000	1.646820000	-0.044734000	H	7.461868000	-2.410992000	0.340183000
C	4.920741000	0.722895000	-0.246249000	H	6.997768000	-0.780411000	0.842258000
C	4.679985000	-0.589168000	-0.686346000	H	5.947667000	-2.149667000	1.225716000
C	1.465096000	2.155794000	-0.099216000	H	6.336744000	-0.842018000	-2.899525000
C	1.730935000	3.482349000	0.354621000	H	7.230472000	0.003889000	-1.630599000
C	0.119695000	1.755396000	-0.348788000	H	7.690089000	-1.643109000	-2.080277000
C	-0.913463000	2.685884000	-0.127145000	H	4.904910000	-2.896513000	-2.331654000
C	-0.667465000	3.989915000	0.317161000	H	6.290772000	-3.593030000	-1.487309000
C	0.663238000	4.366320000	0.549721000	H	4.745457000	-3.429939000	-0.647271000
C	-1.798678000	5.009907000	0.553466000	H	-3.913073000	-1.957975000	2.165843000
C	5.865437000	-1.554392000	-0.881415000	H	-5.079196000	-3.224786000	1.771418000
C	-1.625863000	-1.345265000	0.928581000	H	-3.385931000	-3.394032000	1.310268000
C	-2.285177000	-0.880019000	-0.345264000	H	-1.153389000	-4.469031000	-1.845999000
C	-1.682342000	-0.443104000	1.978699000	H	-2.528978000	-3.581414000	-1.190275000
C	-1.531521000	-0.020314000	-1.148882000	H	-1.174730000	-2.703609000	-1.870986000
C	-0.130580000	0.399161000	-0.810244000				
C	0.921410000	-0.455409000	-0.995113000				
C	-1.053225000	-0.680661000	3.216782000				
C	-0.891629000	-2.577743000	1.082023000				
C	-0.234819000	-2.795017000	2.349919000				
C	-0.339021000	-1.837528000	3.392947000				
C	0.530347000	-3.969650000	2.576170000				
C	0.656936000	-4.920256000	1.597468000				
C	0.004787000	-4.728872000	0.362293000				
C	-0.761091000	-3.610102000	0.078231000				
C	-3.654167000	-1.193184000	-0.696501000				
C	-4.169846000	-0.638145000	-1.924532000				
C	-3.353001000	0.195898000	-2.729382000				
C	-2.076966000	0.507931000	-2.348657000				
C	-4.553629000	-2.018479000	0.082042000				
C	-5.839294000	-2.236346000	-0.387632000				
C	-6.324088000	-1.693837000	-1.594054000				
C	-5.497473000	-0.904710000	-2.349321000				
C	4.125364000	2.991921000	0.408606000				
C	3.098057000	3.863949000	0.598416000				
C	-1.779116000	5.467989000	2.031102000				
C	-1.583612000	6.236404000	-0.365056000				
C	-3.191658000	4.425728000	0.252227000				
C	6.611412000	-1.730685000	0.462506000				
C	6.837184000	-0.970615000	-1.934258000				
C	5.416065000	-2.946171000	-1.364719000				
C	-4.207366000	-2.679303000	1.400660000				
C	-1.438949000	-3.580785000	-1.276186000				
H	3.123039000	-1.968860000	-1.266086000				
H	5.938572000	1.048166000	-0.048977000				
H	-1.929627000	2.366273000	-0.315228000				
H	0.890977000	5.371311000	0.894464000				
H	-2.227193000	0.484435000	1.833132000				
H	0.736999000	-1.466007000	-1.345827000				
H	-1.128259000	0.054967000	4.011863000				
H	0.167207000	-2.041375000	4.332628000				
H	1.013058000	-4.094135000	3.541697000				
H	1.244177000	-5.818196000	1.765542000				
H	0.097555000	-5.497382000	-0.400351000				
H	-3.766471000	0.591616000	-3.653202000				
H	-1.460745000	1.160523000	-2.959330000				
H	-6.504822000	-2.855574000	0.207379000				
H	-7.341687000	-1.901512000	-1.911272000				
H	-5.839415000	-0.466445000	-3.282970000				
H	5.150155000	3.300184000	0.599189000				
H	3.294619000	4.876147000	0.942573000				
H	-0.828177000	5.936483000	2.300815000				
H	-2.574511000	6.199229000	2.214361000				
H	-1.935827000	4.619743000	2.705437000				
H	-0.625583000	6.727757000	-0.171886000				
H	-1.601054000	5.942794000	-1.419661000				
H	-2.375897000	6.976448000	-0.205034000				
- Thermochemistry -							

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.							
Zero-point correction=				0.742923 (Hartree/Particle)			
Thermal correction to Energy=				0.782350			
Thermal correction to Enthalpy=				0.783295			
Thermal correction to Gibbs Free Energy=				0.671617			
Sum of electronic and zero-point Energies=				-1777.603968			
Sum of electronic and thermal Energies=				-1777.564541			
Sum of electronic and thermal Enthalpies=				-1777.563596			
Sum of electronic and thermal Free Energies=				-1777.675274			

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