ELECTRONIC SUPPORTING INFORMATION

Azaborahelicene Fluorophores Derived from Four-Coordinate *N,C*-Boron Chelates: Synthesis, Photophysical and Chiroptical Properties

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1. Materials and methods

General information and materials

Anhydrous tetrahydrofuran (THF) and 1,4-dioxane were obtained by distillation over Na/benzophenone. Other solvents such as *n*-hexane, ethyl acetate (EtOAc), methanol, dichloromethane (DCM), chloroform, dimethoxyethane (DME), cyclohexane, toluene, and isopropanol were purchased in chromatographic purity and used as received. Pinacolborane (HBpin), Bis(pinacolate)diboron (B_2pin_2), and $(Mes)_2BF$ were supplied by Aldrich, Frontier Scientific, and TCI, respectively, and used as received. *n*-BuLi (1.6 M in hexane), Ir(μ-OMe)(cod)]$_2$, [$Pd(PPh_3)_4$], and $CuBr_2$ were provided by Aldrich. The pyridino-hydrazone ligand, used in the Ir(I)-catalyzd borylation reaction, was synthesized according to previously described methodology.[1] The arylboronic acids **2a**–**f** are either commercially available (**2a** from Aldrich, **2d** and **2e** from BLDpharma) or were prepared according to published procedures (**2b**, **2c**, and **2f**).[2-4]

All synthetic transformations were done in oven-dried Schlenk tubes under inert (Ar) atmosphere. Specific rotations (in deg cm^2 g^{-1}) were measured in a 10 cm thermostated quartz cell on a PerkinElmer Model 341 polarimeter. The ^{1}H- and ^{13}C-NMR spectra were measured on a DRX-400 spectrometer (Bruker) at 400 MHz or 100 MHz, respectively, using the residual solvent signal ($CDCl_3$; 7.26 ppm) as reference. The ^{11}B-NMR spectra were obtained with complete proton decoupling at 160 MHz, employing $BF_3 \times Et_2O$ (0.00 ppm) as standard. Multiplicity of signals: s – singlet, d – doublet, t – triplet, q – quartet, br s – broad signal, m – multiplet. The racemic dyes **5a-f** were separated into their enantiopure forms by CSP-HPLC on Shimadzu LC-2030C Plus 3D RoHS-Prominence-I chromatograph, using chiral Chiralpak IA column. High-resolution mass spectra (ESI) were acquired on a Thermo Fisher Orbitrap Elite with an orbitrap mass analyzer.

Low-temperature diffraction data were collected on a Bruker D8 Quest APEX-III single crystal diffractometer, equipped with a Photon III detector and a IμS 3.0 microfocus X-ray source. Data were collected by means of ω and φ scans using monochromatic radiation λ(Mo Kα1) = 0.71073 Å. The diffraction images collected were processed and scaled using APEX-4 v2021.4-0 software. The structures were solved with SHELXT and was refined against F2 on all data by full-matrix least squares with SHELXL,[5] using Olex2 as graphical interface.[6] All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included in the model at geometrically calculated positions and refined using a riding model, unless otherwise noted. The isotropic displacement parameters of all hydrogen atoms were fixed to 1.2 times the U value of the atoms to which they are linked (1.5 times for methyl groups).

Photophysical measurements

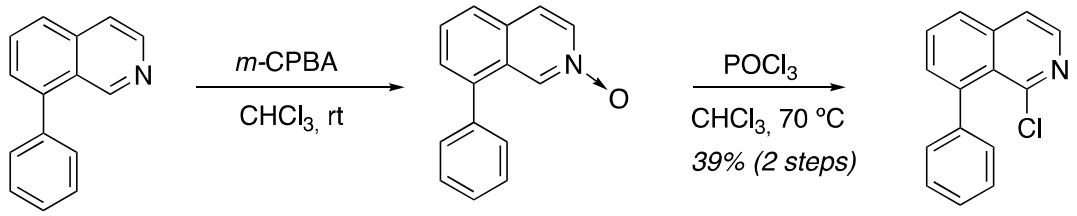
The measurements were performed at room temperature (25ºC) with dye solutions, contained in quartz cuvettes with 1 cm optical pathlength, using spectroscopic-grade solvents. The obtained data refer to air-equilibrated solutions. UV/vis absorption spectra were recorded on a CARY 5000 UV/Vis spectrophotometer (Agilent). The fluorescence emission was characterized with a Varian Eclipse fluorimeter and corrected for the response of the photomultiplier. The fluorescence quantum yields were obtained with 4-amino-*N*-propyl-1,8-naphthalimide (Φ_f = 0.48 in acetonitrile) as reference.[7] This reference was calibrated against quinine sulfate in 0.05 M sulfuric acid (Φ_f = 0.55).[8,9] Time-correlated single-photon-counting (TCSPC) experiments were carried out with an FLS 920 fluorimeter from Edinburgh Instruments. A picosecond pulsed diode laser EPL-445 (output 442.2 nm, pulse width at FWHM: 78 ps) was used as excitation

source. The fluorescence lifetimes were extracted from the decay traces by deconvolution analysis, taking into account the instrument response function.

Electronic circular dichroism (ECD, in $M^{-1}cm^{-1}$) was measured on a Jasco J-1700 Circular Dichroism Spectrometer. The circularly polarized luminescence (CPL) measurements were performed using a JASCO 300 CPL spectrofluoropolarimeter. The following parameters were used: emission slit width ≈ 20 mm, integration time = 4 sec, scan speed = 50 nm/min, accumulations = 8. The concentration of all the samples was *ca*. 10^{-5}–10^{-6} M. Excitation of the samples was performed at 380 nm.

2. Synthetic procedures

Synthesis of chloride 1

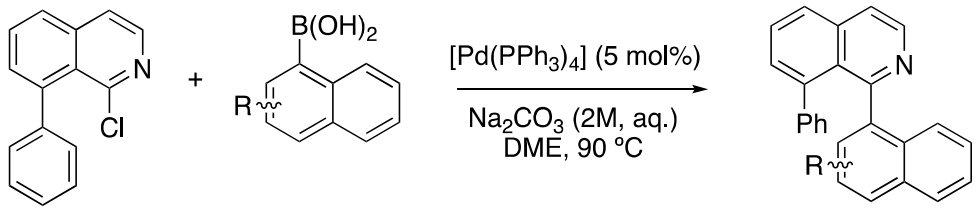


N-oxydation step: Over a cooled solution (0 ºC) of 8-phenylisoquinoline (21 mmol, 4.3 g) in $CHCl_3$ (200 mL), *m*-CPBA (77% purity, 32 mmol, 5.52 g) was added in portions. The reaction was stirred overnight at room temperature, and then, a saturated $NaHCO_3$ solution (60 mL) was poured into the reaction medium and the resulting two phases mixture was stirred for 30 min. The phases were separated, and the aqueous phase was extracted with chloroform (3 × 50 mL). Organic extracts were dried over $MgSO_4$, filtered and concentrated dryness. This reaction crude was used in the next step without purification.

Chlorination step: Over a round-bottom flask containing the previous reaction crude dissolved in $CHCl_3$ (30 mL), $POCl_3$ (50 mmol, 4.7 mL) was dropwise added. Then, the reaction mixture was stirred for 2 hours at 70 °C, cooled to room temperature, and neutralized with NH_3 (30% aqueous solution) until neutral pH. The aqueous phase was extracted with DCM (3 × 100 mL). The combined organic phases were dried with $MgSO_4$ and evaporated under reduced pressure. The raw product was purified by column chromatography on silica gel (cyclohexane/EtOAc 8:1) to afford **1** (1.96 g, 39%) as a yellow-orange viscous oil. **^{1}H-NMR (400 MHz, $CDCl_3$, 298 K):** δ 8.28 (d, 1H, *J* = 5.3 Hz), 7.86 (d, 1H, *J* = 8.2 Hz), 7.71 (t, 1H, *J* = 8.3 Hz), 7.66 (d, 1H, *J* = 5.3 Hz), 7.53 (d, 1H, *J* = 6.7 Hz), 7.45–7.41 (m, 3H), 7.34–7.31 (m, 2H) ppm. **^{13}C-NMR (100 MHz, $CDCl_3$, 298 K):** δ 150.3 (Cq), 142.1 (Cq), 141.0, 140.8 (Cq), 139.3 (Cq),

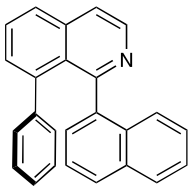
132.2, 129.8, 129.4 (2 × C), 127.6 (2 × C), 127.3, 127.2, 125.0 (Cq), 121.2 ppm. **HRMS (ESI)** calcd. for $C_{15}H_{11}ClN$ ($M + H^+$) 240.0575. Found 240.0573.

Suzuki Coupling general procedure



A Schlenk tube was charged with $[Pd(PPh_3)_4]$ (5 mol%), **1** (0.4 mmol, 96 mg) and the corresponding boronic acid **2a–f**. After three cycles of evacuation/nitrogen flushing, deoxygenized DME (1 mL/mmol) and Na_2CO_3 solution (2 M aqueous solution, 0.4 mL) were added and the reaction was stirred overnight at 90°C. After cooling down to rt, the reaction was quenched with water (10 mL) and extracted with DCM (3 × 20 mL). The combined organic phase was dried over anhydrous $MgSO_4$, filtered, concentrated to dryness, and the crude was purified by column chromatography on silica gel.

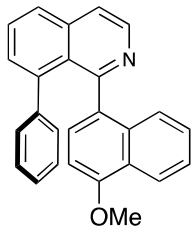
Synthesis of 3a



Following the general procedure, purification by column chromatography on silica gel (toluene/EtOAc 12:1) afforded **3a** (105 mg, 79%) as pale brown solid. **^{1}H-NMR (400 MHz, CD_2Cl_2, 298 K):** δ 8.70 (d, 1H, *J* = 5.4 Hz), 7.99 (d, 1H, *J* = 7.8 Hz), 7.83 (d, 1H, *J* = 5.4 Hz), 7.74 (t, 1H, *J* = 7.5 Hz), 7.65 (d, 1H, *J* = 8.0 Hz), 7.48 (d, 1H, *J* = 6.8 Hz), 7.41–7.26 (m, 3H), 7.28 (t, 1H, *J* = 7.4 Hz), 7.18–7.12 (m, 2H), 6.92 (d, 1H, *J* = 7.5 Hz, br s), 6.84 (t, 1H, *J* = 7.5 Hz, br s), 6.66 (t, 1H, *J* = 7.5 Hz), 6.43 (d, 1H, *J* = 7.6Hz, br s), 6.25 (t, 1H, *J* = 7.6 Hz, br s) ppm. **^{13}C-NMR (100 MHz, CD_2Cl_2, 298 K):** δ 159.9 (Cq), 142.2, 142.1 (Cq), 141.7 (Cq), 140.5 (Cq), 138.5 (Cq), 133.60 (Cq), 132.3 (Cq), 131.8, 129.6, 129.4

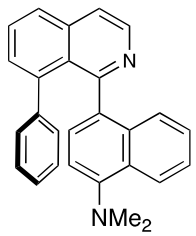
(br s), 128.7, 128.2 (2 × C), 127.4, 126.9, 126.2 (br s), 126.2 (2 × C), 126.0, 126.0, 125.6, 125.1, 120.7 ppm. **HRMS (ESI)** calcd. for $C_{25}H_{18}N$ ($M + H^+$) 332.1434. Found 332.1434.

Synthesis of 3b



Following the general procedure, purification by column chromatography on silica gel (toluene/EtOAc 12:1) afforded **3b** (121 mg, 84%) as a light-yellow amorphous solid. **^{1}H-NMR (400 MHz, $CDCl_3$, 298 K):** δ 8.71 (d, 1H, *J* = 5.4 Hz), 8.03 (d, 1H, *J* = 8.2 Hz) 7.70 (t, 1H, *J* = 7.4 Hz, H_4), 7.34–7.26 (m, 4H), 7.09 (d, 1H, *J* = 7.8 Hz), 6.87 (d, 1H, *J* = 7.6 Hz, br s), 6.82 (t, 1H, *J* = 7.3 Hz, br s), 6.70 (t, 1H, *J* = 7.3 Hz), 6.49 (d, 1H, *J* = 7.8 Hz), 6.37 (d, 1H, *J* = 7.6Hz, br s), 6.29 (t, 1H, *J* = 7.6 Hz, br s), 3.90 (s, 3H) ppm. **^{13}C-NMR (100 MHz, $CDCl_3$, 298 K):** δ 159.7 (Cq), 155.12 (Cq), 142.0 (Cq), 141.8, 141.3 (Cq), 138.1 (Cq), 132.9 (Cq), 132.5 (Cq), 131.4, 129.2, 128.9, 128.7, 128.1, 127.0, 126.8 (Cq), 126.3, 126.2, 125.7, 125.5, 125.4, 125.1 (Cq), 124.6, 121.7, 120.2, 103.3, 55.6 (OMe) ppm. **HRMS (ESI)** calcd. for $C_{26}H_{20}ON$ ($M + H^+$) 362.1539. Found 362.1538.

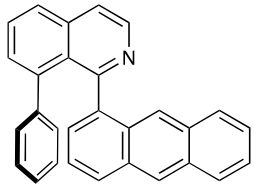
Synthesis of 3c



Following the general procedure, purification by column chromatography on silica gel (cyclohexane/EtOAc 4:1) afforded **3c** (110 mg, 72%) as a dark-green viscous oil. **^{1}H-NMR (400 MHz, $CDCl_3$, 298 K):** δ 8.71 (d, 1H, *J* = 5.5 Hz), 8.02 (d, 1H, *J* = 8.4 Hz), 7.94 (d, 1H, *J* = 8.1 Hz), 7.78 (d, 1H, *J* = 5.5 Hz) 7.70 (t, 1H, *J* = 8.1 Hz), 7.35–7.20 (m, 4H), 7.10 (d, 1H, *J* = 7.7 Hz), 6.88 (d, 1H, *J* = 7.5 Hz, br s), 6.84 (t, 1H, *J* = 7.5 Hz, br

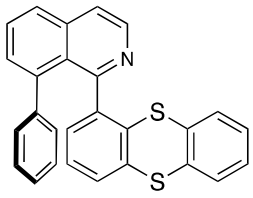
s), 6.76 (d, 1H, *J* = 7.7 Hz), 6.65 (t, 1H, *J* = 7.4 Hz, br s), 6.42 (d, 1H, *J* = 7.5 Hz, br s), 6.29 (t, 1H, *J* = 7.7 Hz, br s), 2.79 (s, 6H) ppm. **^{13}C-NMR (100 MHz, $CDCl_3$, 298 K):** δ 159.9 (Cq), 150.3 (Cq), 141.9 (Cq), 141.8, 141.2 (Cq), 138.0 (Cq), 134.8 (Cq), 133.1 (Cq), 131.2, 130.0, 129.1, 129.0, 128.5 (Cq), 128.4, 128.3, 128.1 (Cq), 126.9, 126.6, 126.1, 125.9, 125.5, 124.5, 123.8, 120.2, 114.2, 44.9 (NMe_2) ppm. **HRMS (ESI)** calcd. for $C_{27}H_{23}N_2$ ($M + H^+$) 375.1856. Found 375.1855.

Synthesis of 3d



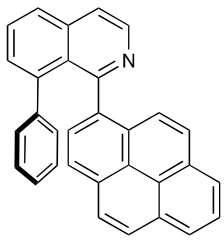
Following the general procedure, purification by column chromatography on silica gel (cyclohexane/EtOAc 5:1) afforded **3d** (121 mg, *ca*. 79%; the product was contaminated with an unidentified product) as a light-yellow foam. **^{1}H-NMR (400 MHz, $CDCl_3$, 298 K):** δ 8.78 (d, 1H, *J* = 5.5 Hz), 8.23 (s, 1H), 8.01 (d, 1H, *J* = 8.4 Hz), 8.00 (s, 1H), 7.96 (d, 1H, *J* = 8.4 Hz), 7.87 (d, 1H, *J* = 5.5 Hz), 7.74–7.72 (m, 2H), 7.64 (m, 1H), 7.41 (d, 1H, *J* = 8.2 Hz), 7.38-7.34 (m, 2H), 7.14–7.11 (m, 2H), 6.95 (d, 1H, *J* = 6.9 Hz, br s), 6.86 (t, 1H, *J* = 7.0 Hz, br s), 6.61 (t, 1H, *J* = 7.4 Hz), 6.22 (d, 1H, *J* = 7.0 Hz, br s), 5.91 (t, 1H, *J* = 7.0 Hz, br s) ppm. **^{13}C-NMR (100 MHz, $CDCl_3$, 298 K):** δ 159.6 (Cq), 141.9, 141.8 (Cq), 141.2 (Cq), 139.6 (Cq), 138.2 (Cq), 131.6, 131.6, 131.4, 131.2 (Cq), 130.5 (Cq), 129.3, 128.8, 128.5, 128.4, 128.2, 128.0, 127.9, 127.1, 126.6 (Cq), 126.4 (Cq), 126.1, 125.9, 125.7 (Cq), 125.1, 124.9, 124.6, 124.3, 120.6 ppm. **HRMS (ESI)** calcd. $C_{29}H_{20}N$ ($M + H^+$) 382.1589. Found 382.1601.

Synthesis of 3e



Following the general procedure, but at 1 mmol scale of **1**, purification by column chromatography on silica gel (cyclohexane/EtOAc 10:1) afforded **3e** (294 mg, 70%) as a yellow viscous oil. **^{1}H-NMR (400 MHz, $CDCl_3$, 298 K):** δ 8.72 (d, 1H, *J* = 5.5 Hz), 7.96 (d, 1H, *J* = 8.0 Hz), 7.81 (d, *J* = 5.6 Hz), 7.74 (t, 1H, *J* = 7.6 Hz), 7.51 (d, 1H, *J* = 7.2 Hz), 7.43 (d, 1H, *J* = 7.2 Hz), 7.36 (d, 1H, *J* = 7.6 Hz), 7.28 (d, 1H, *J* = 6.8 Hz), 7.20 (t, 1H, *J* = 7.6 Hz), 7.12–7.10 (br s, 2H), 6.98 (t, 1H, *J* = 7.2 Hz), 6.79–6.75 (2H, br s), 6.72–6.69 (2H, br s), 5.68 (t, 1H, *J* = 7.2 Hz) ppm. **^{13}C-NMR (100 MHz, $CDCl_3$, 298 K):** δ 158.6 (Cq), 142.7 (Cq), 141.4, 141.3 (Cq), 141.2 (Cq), 138.3 (Cq), 136.7 (Cq), 136.5 (Cq), 134.8 (Cq), 134.6 (Cq), 131.4, 129.9, 129.8, 129.5, 128.8, 128.7, 128.6, 127.8, 127.5, 127.4, 127.3, 127.0, 126.6, 126.1, 125.1 (Cq), 120.7 ppm. **HRMS (ESI)** calcd. $C_{27}H_{18}NS_2$ ($M + H^+$) 420.0874. Found 420.0886.

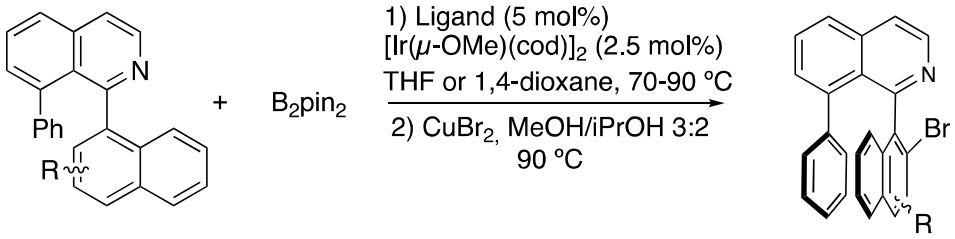
Synthesis of 3f



Following the general procedure, purification by column chromatography on silica gel (toluene/EtOAc 12:1) afforded **3f** (147 mg, 90%) as a yellow viscous oil. **^{1}H-NMR (400 MHz, $CDCl_3$, 298 K):** δ 8.84 (d, 1H, *J* = 5.3 Hz), 8.18 (d, 1H, *J* = 7.4 Hz), 8.14 (d, 1H, *J* = 7.4 Hz), 8.05–7.98 (m, 3H), 7.94-7.89 (m, 4H), 7.81–7.75 (m, 2H), 7.59 (d, 1H, *J* = 9.3 Hz), 7.40 (d, 1H, *J* = 7.2 Hz), 6.77 (d, 1H, *J* = 7.6 Hz), 6.58 (t, 1H, *J* = 7.6 Hz), 6.47 (d, 1H, *J* = 7.6 Hz), 6.14 (t, 1H, *J* = 7.6 Hz), 5.66 (t, 1H, *J* = 7.6 Hz) ppm. **^{13}C-NMR (100 MHz, $CDCl_3$, 298 K):** δ 160.0 (Cq), 141.9, 141.9 (Cq), 140.8 (Cq), 138.1, 137.4 (Cq), 131.6, 131.2 (Cq), 130.8 (Cq), 129.4, 129.2 (Cq), 128.9, 128.1, 127.9, 127.4, 127.2, 127.1, 127.1, 127.0 (Cq), 126.1, 125.6, 125.2, 125.0, 125.0, 124.8, 124.5 (Cq),

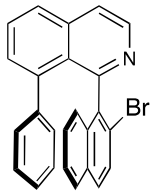
124.3, 120.6 ppm. 2 C signals are not visible. **HRMS (ESI)** calcd. $C_{31}H_{20}N$ ($M + H^+$) 406.1589. Found 406.1601.

General procedure for borylation-bromination



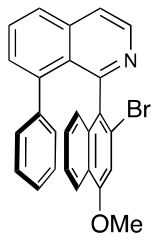
A dried Schlenk tube was charged with [Ir(μ-OMe)(cod)]$_2$ (2.5 mol%), ligand (2-pyridinecarboxaldehyde *N*,*N*-dibenzylhydrazone, 5 mol), B_2pin_2 (1.2 eq), and **3a–f** (1 eq.). After three cycles of vacuum/nitrogen flushing, anhydrous THF or 1,4-dioxane (2.5 mL/mmol substrate) and HBpin (10 mol%) were added and the reaction mixture was stirred overnight at 70°C (THF) or 90°C (1,4-dioxane) (monitoring the consumption of the starting materials by TLC analysis). Then the reaction mixture was cooled to room temperature and concentrated to dryness. The resulting crude was dissolved in an isopropanol/MeOH 2:3 mixture (19 mL/mmol substrate) and treated with a solution of $CuBr_2$ (3 eq.) in H_2O (9.5 mL/mmol substrate). The mixture was stirred overnight at 90°C, subsequently cooled to room temperature, diluted with DCM (40 mL), and finally washed with aqueous NH_3 solution (30%) to remove the copper salts. The organic phase was dried over anhydrous $MgSO_4$, filtered, concentrated to dryness, and the crude product was purified by column chromatography, yielding **4a-f** as racemic mixtures.

Synthesis of *rac*-4a



Following the general procedure, starting from **3a** (0.54 mmol, 180 mg) and carrying out the borylation step at 70ºC, purification by column chromatography on silica gel (cyclohexane/EtOAc 8:1) afforded *rac*-**4a** (208 mg, 79%) as a yellow foam. **^{1}H-NMR (400 MHz, $CDCl_3$, 298 K):** δ 8.75 (d, 1H, *J* = 5.6 Hz), 7.99 (d, 1H, *J* = 8.0 Hz), 7.87 (d, 1H, *J* = 5.6 Hz), 7.71 (t, 1H, *J* = 7.2 Hz), 7.62 (d, 1H, *J* = 8.0 Hz), 7.38 (t, 1H, *J* = 6.8 Hz), 7.32–7.25 (m, 5H), 7.13 (d, 1H, *J* = 8.0 Hz), 6.91 (t, 1H, *J* = 7.2 Hz), 6.70 (t, 1H, *J* = 7.6 Hz), 6.31 (d, 1H, *J* = 7.6 Hz), 6.19 (t, 1H, *J* = 7.2 Hz) ppm. **^{13}C-NMR (100 MHz, $CDCl_3$, 298 K):** δ 158.3 (Cq), 142.1, 141.1 (Cq), 140.3 (Cq), 139.4 (Cq), 137.7 (Cq), 133.8 (Cq), 132.1 (Cq), 131.3, 129.5, 129.3, 129.2, 128.2, 127.7 (2 × C), 127.4, 126.7 (Cq), 126.6, 126.5, 126.4, 126.3, 125.6, 125.2, 122.0 (Cq), 121.3 ppm. **HRMS (ESI)** calcd. $C_{25}H_{17}BrN^+$ ($M + H^+$) 410.0539 (^{79}Br), 412.0518 (^{81}Br). Found 410.0526, 412.0504.

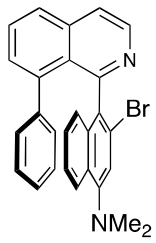
Synthesis of *rac*-4b



Following the general procedure, starting from **3b** (0.78 mmol, 284 mg) and carrying out the borylation step at 70 ºC, purification by column chromatography on silica gel (cyclohexane/EtOAc 10:1) afforded *rac*-**4b** (270 mg, 79%) as a light-yellow foam. **^{1}H-NMR (400 MHz, $CDCl_3$, 298 K):** δ 8.75 (d, 1H, *J* = 5.6 Hz), 8.01 (d, 1H, *J* = 8.0 Hz), 7.97 (d, *J* = 8.0 Hz, 1H, 7.84 (d, 1H, *J* = 5.6 Hz), 7.69 (t, 1H, *J* = 6.8 Hz), 7.37 (t, 1H, *J* = 7.2 Hz), 7.30–7.26 (m, 3H), 7.06 (d, 1H, *J* = 8.4 Hz), 6.93 (t, 1H, *J* = 7.6 Hz), 6.75 (t, 1H, *J* = 6.8 Hz), 6.59 (s, 1H), 6.25–6.20 (m, 2H), 3.88 (s, 3H) ppm. **^{13}C-NMR (100 MHz, $CDCl_3$, 298 K):** δ 158.5 (Cq), 155.1 (Cq), 142.1, 141.3 (Cq), 140.7 (Cq), 137.8 (Cq), 134.4 (Cq), 132.1 (Cq), 131.3, 129.2, 128.1, 127.6, 127.4, 127.2, 127.1 (Cq), 126.3, 126.0, 125.9, 125.2,

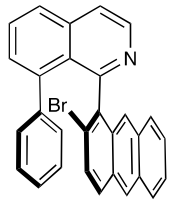
124.9, 124.5 (Cq), 122.1 (Cq), 121.8, 121.2, 108.3, 55.8 ppm. **HRMS (ESI)** calcd. $C_{26}H_{19}BrNO^+$ (M + H^+) 440.0645 (^{79}Br), 442.0624 (^{81}Br). Found 440.0641, 442.0617.

Synthesis of *rac*-4c



Following the general procedure (except for the use of solely 2 eq. $CuBr_2$), starting from **3c** (0.63 mmol, 263 mg) and carrying out the borylation step at 90ºC, purification by column chromatography on silica gel (cyclohexane/EtOAc 10:1) afforded *rac*-**4c** (170 mg, 61%) as a yellow-orange foam. **^{1}H-NMR (400 MHz, $CDCl_3$, 298 K):** δ 8.74 (d, 1H, *J* = 5.6 Hz), 7.99 (d, 1H, *J* = 7.5 Hz), 7.97 (d, 1H, *J* = 8.2 Hz), 7.84 (d, 1H, *J* = 5.6 Hz,), 7.70 (t, 1H, *J* = 7.2 Hz), 7.37 (t, 1H, *J* = 8.3 Hz,), 7.30-7.23 (m, 3H), 7.09 (d, 1H, *J* = 8.1 Hz), 6.94 (t, 1H, *J* = 7.2 Hz), 6.83 (s, 1H), 6.70 (t, 1H, *J* = 7.6 Hz), 6.29 (d, 1H, *J* = 7.6 Hz), 6.23 (t, 1H, *J* = 7.2 Hz), 2.79 (s, 6H) ppm. **^{13}C-NMR (100 MHz, $CDCl_3$, 298 K):** δ 158.7 (Cq), 151.1 (Cq), 142.1, 141.3 (Cq), 140.7 (Cq), 137.7 (Cq), 134.9 (Cq), 134.3 (Cq), 131.3, 129.2, 128.2, 127.8, 127.6 (Cq), 127.4, 127.0 (Cq), 126.8, 126.5, 126.4, 126.3, 125.2, 124.8, 124.0, 122.3 (Cq), 121.1, 118.3, 44.9 ppm. **HRMS (ESI)** calcd. $C_{27}H_{22}BrN_2^+$ (M + H^+) 453.0961 (^{79}Br), 455.0940 (^{81}Br). Found 453.0964, 455.0940.

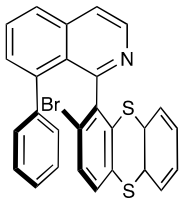
Synthesis of *rac*-4d



Following the general procedure, starting from **3d** (0.76 mmol, 290 mg) and carrying out the borylation step at 70ºC, purification by column chromatography on silica gel (cyclohexane/EtOAc 10:1) afforded *rac*-**4d** (240 mg, 69%) as a light-yellow foam. **^{1}H-NMR (400 MHz, $CDCl_3$, 298 K):** δ 8.81 (d, 1H, *J* = 5.6 Hz), 8.23 (s, 1H), 8.03 (d, 1H, *J* = 8.2 Hz), 7.96 (d, *J* = 8.4 Hz, 1H), 7.92 (d, 1H, *J* = 5.6 Hz), 7.75–7.71 (m, 3H), 7.49–7.43 (m, 2H), 7.38 (t, 1H, *J* = 7.2 Hz),

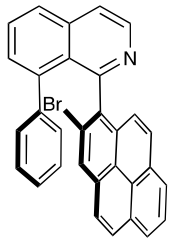
7.32-7.28 (m, 2H), 7.21 (d, 1H, *J* = 9.1 Hz), 6.94 (t, 1H, *J* = 7.6 Hz), 6.65 (t, 1H, *J* = 7.2 Hz), 6.12 (d, 1H, *J* = 7.7 Hz), 5.83 (t, 1H, *J* = 7.6 Hz) ppm. **^{13}C-NMR (100 MHz, $CDCl_3$, 298 K):** δ 158.4 (Cq), 142.2, 141.1 (Cq), 140.3 (Cq), 139.1 (Cq), 137.8 (Cq), 132.2 (Cq), 131.9 (Cq), 131.3, 131.2 (Cq), 130.2 (Cq), 129.6, 129.3, 129.1, 128.5, 128.2, 127.9, 127.7, 127.5, 126.8 (Cq), 126.5, 126.4, 126.3, 125.61, 125.57, 125.1, 125.1, 122.0 (Cq), 121.4 ppm. **HRMS (ESI)** calcd. $C_{29}H_{19}BrN^+$ (M + H^+) 460.0695 (^{79}Br), 462.0675 (^{81}Br). Found 460.0681, 462.0659.

Synthesis of *rac*-4e



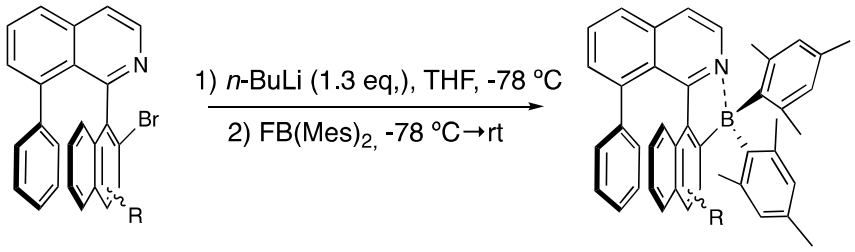
Following the general procedure, starting from **3e** (0.38 mmol, 162 mg) and carrying out the borylation step at 90ºC for 48 h, purification by column chromatography on silica gel (cyclohexane/EtOAc 10:1) afforded *rac*-**4e** (40 mg, 21%) as a light-brown foam. **^{1}H-NMR (400 MHz, $CDCl_3$, 298 K):** δ 8.72 (d, 1H, *J* = 5.6 Hz), 7.98 (d, 1H, *J* = 8.3 Hz), 7.86 (d, 1H, *J* = 5.6 Hz), 7.73 (t, 1H, *J* = 7.2 Hz), 7.52 (d, 1H, *J* = 7.6 Hz), 7.40–7.20 (m, 5H), 7.03–6.89 (m, 3H), 6.78–6.76 (m, 2H), 5.65 (t, 1H, *J* = 7.6 Hz) ppm. **^{13}C-NMR (100 MHz, $CDCl_3$, 298 K):** δ 157.6 (Cq), 142.2 (Cq), 141.8, 140.9 (Cq), 140.5 (Cq), 137.8 (Cq), 137.4 (Cq), 136.2 (Cq), 135.6 (Cq), 134.3 (Cq), 131.3, 130.8, 129.7, 129.4, 129.0, 128.7, 128.4, 127.9, 127.7, 127.6, 127.4, 127.2, 127.1, 126.1, 125.4 (Cq), 123.1 (Cq), 121.7 ppm. **HRMS (ESI)** calcd. $C_{27}H_{17}BrNS_2^+$ (M + H^+) 497.9980 (^{79}Br), 499.9960 (^{81}Br). Found 497.9983, 499.9959.

Synthesis of *rac*-4f



Following the general procedure, starting from **3f** (0.63 mmol, 254 mg) and carrying out the borylation step at 70ºC, purification by two column chromatographies on silica gel (first with cyclohexane/EtOAc 10:1 and then with toluene/EtOAc 50:1) afforded *rac*-**4f** (137 mg, 45%) as a light-yellow foam. **^{1}H-NMR (400 MHz, $CDCl_3$, 298 K):** δ 8.83 (d, 1H, *J* = 5.6 Hz), 8.18 (d, 1H, *J* = 7.6 Hz), 8.14 (d, 1H, *J* = 7.6 Hz), 8.04–8.01 (m, 4H), 7.93 (d, 1H, *J* = 5.6 Hz), 7.90 (d, 1H, *J* = 9.3 Hz), 7.73 (t, 1H, *J* = 8.2 Hz), 7.36 (d, 1H, *J* = 8.9 Hz), 7.29 (d, 1H, *J* = 7.2 Hz), 7.19 (d, 1H, *J* = 7.6 Hz), 6.66 (t, 1H, *J* = 7.6 Hz), 6.30 (d, 1H, *J* = 7.6 Hz), 6.12 (t, 1H, *J* = 7.6 Hz), 5.50 (t, 1H, *J* = 7.6 Hz) ppm. **^{13}C-NMR (100 MHz, $CDCl_3$, 298 K):** δ 158.6 (Cq), 142.0, 141.2 (Cq), 140.3 (Cq), 137.7 (Cq), 136.7 (Cq), 131.9 (Cq), 131.4 (Cq), 131.3, 130.8 (Cq), 130.3 (Cq), 129.3, 128.3, 128.2, 127.84, 127.80, 127.6, 127.4, 127.2 (Cq), 126.2, 126.0, 125.9, 125.6, 125.5 (2 × C), 125.3, 124.7, 124.0 (Cq), 123.3 (Cq), 122.0 (Cq), 121.4 ppm. **HRMS (ESI)** calcd. $C_{31}H_{19}BrN^+$ ($M + H^+$) 484.0695 (^{79}Br), 486.0675 (^{81}Br). Found 484.0691, 486.0671.

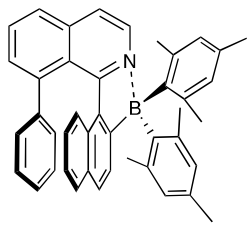
General procedure for lithiation-borylation. Synthesis of boranes 5a-f



A dried Schlenk tube was charged with **4a–f** (1 eq.), and after three cycles of vacuum/argon flushing, anhydrous THF (2 mL/0.1 mmol substrate) was added. The reaction mixture was cooled to –78 °C, then *n*-BuLi (1.6 M in hexane, 1.3 eq.) was added dropwise, and the resulting solution was stirred at this temperature for one hour.

Then, Mes_2BF (1.3 eq.) was added at –78 °C under Schlenk conditions, and the resulting mixture was stirred at this temperature for 15 minutes and then at room temperature overnight. The reaction was quenched with water and the mixture was extracted with DCM. The combined organic phase was dried over anhydrous $MgSO_4$, filtered, concentrated to dryness, and the crude product was purified by column chromatography yielding the target dyes **5a**–**f**.

Synthesis of *rac*-5a

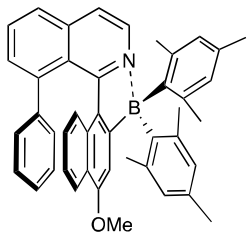


Following the general procedure, starting from **4a** (0.2 mmol, 81.8 mg), purification by column chromatography on silica gel (cyclohexane/EtOAc 30:1) afforded *rac*-**5a** (111 mg, 96%) as a yellow foam. **^{1}H-NMR (400 MHz, $CDCl_3$, 298 K):** δ 8.64 (d, 1H, *J* = 6.4 Hz), 7.91–7.85 (m, 2H), 7.81 (d, 1H, *J* = 8.2 Hz), 7.72 (d, 1H, *J* = 6.6 Hz), 7.71 (d, 1H, *J* = 6.4 Hz), 7.60 (d, 1H, *J* = 6.8 Hz), 7.44 (d, 1H, *J* = 8.3 Hz), 7.40 (d, 1H, *J* = 7.60 Hz), 7.16–7.09 (m, 2H), 6.90 (br s, 1H, H_{Mes}), 6.81–6.78 (m, 3H), 6.76–6.49 (br s, 4H), 6.25 (s, 1H, H_{Mes}), 2.39 (s, 1H, CH_{3Mes}), 2.30 (s, 1H, CH_{3Mes}), 2.28 (s, 1H, CH_{3Mes}), 2.24 (s, 1H, CH_{3Mes}), 2.08 (s, 1H, CH_{3Mes}), 1.18 (s, 1H, CH_{3Mes}) ppm. **^{13}C-NMR (100 MHz, $CDCl_3$, 298 K):** δ 160.9 (Cq), 144.0 (Cq), 142.4 (Cq), 141.6 (Cq), 140.8 (Cq), 140.3 (Cq), 139.7 (Cq), 137.7 (Cq), 136.5, 134.7 (Cq), 133.3 (Cq), 132.2 (Cq), 132.1, 131.8 (2xC), 131.5, 130.31, 130.25, 129.6 (br s), 129.5 (2xC), 129.0, 128.4, 127.7, 127.3, 126.3 (br s), 125.7, 125.2, 123.9, 123.5, 122.8 (Cq), 119.3, 28.0, 25.6, 25.5, 21.8, 20.9, 20.7 ppm, (*C*–B were not observed). **^{11}B-NMR (128 MHz, $CDCl_3$, 298 K):** δ 5.5 (br s) ppm. **HRMS (ESI)** calcd. $C_{43}H_{38}BNNa^+$ (M + Na^+) 602.2990. Found 602.2986.

The enantiomers of the title compound were separated by semipreparative CSP- HPLC (IA column, *n*-hexane:isopropanol 99:1, T = 303 K, F = 12 mL/min), affording the first

enantiomer *M*-**5a** with a retention time of 8.24 min and $[\alpha]^{20}_{D}$ –577 (c 0.25, $CHCl_3$) for er 99:1, and the second enantiomer *P*-**5a** with a retention time of 10.13 min and $[\alpha]^{20}_{D}$ +565 (c 0.25, $CHCl_3$) for er 98:2. The absolute configuration of the reported chiral emitters was assigned by comparison of the experimental ECD spectra with our previous results,[10] and further confirmed by the computed ones (see below).

Synthesis of *rac*-5b

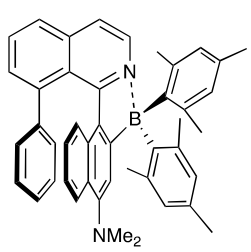


Following the general procedure, starting from **4b** (0.2 mmol, 88 mg), purification by column chromatography on silica gel (cyclohexane/EtOAc 30:1) afforded *rac*-**5b** (101 mg, 83%) as a yellow foam. **^{1}H-NMR (400 MHz, $CDCl_3$, 298 K):** δ 8.50 (d, 1H, *J* = 6.5 Hz), 7.88–7.78 (m, 3H), 7.69–7.66 (m, 2H), 7.49 (d, 1H, *J* = 6.4 Hz), 7.19 (s, 1H), 7.14–7.08 (m, 3H), 6.88 (s, 1H, H_{Mes}), 6.82–6.78 (m, 3H), 6.75–6.59 (br s, 3H), 6.26 (s, 1H, H_{Mes}), 3.86 (s, 3H, OMe), 2.39 (s, 3H, CH_{3Mes}), 2.26 (s, 3H, CH_{3Mes}), 2.24 (s, 3H, CH_{3Mes}), 2.23 (s, 3H, CH_{3Mes}), 2.08 (s, 3H, CH_{3Mes}), 1.21 (s, 3H, CH_{3Mes}) ppm. **^{13}C-NMR (100 MHz, $CDCl_3$, 298 K):** δ 160.8 (Cq), 157.8 (Cq), 144.1 (Cq), 142.5 (Cq), 141.5 (Cq), 140.7 (Cq), 140.3 (Cq), 139.9 (Cq), 137.9 (Cq), 136.4, 134.6 (Cq), 133.2 (Cq), 131.8, 131.5, 130.6 (Cq), 130.3, 130.2, 129.7 (br s), 129.5, 128.9, 127.2, 126.3 (br s), 126.2 (Cq), 125.7, 125.6, 124.4 (Cq), 123.5, 123.2, 122.2 (Cq), 121.9, 117.9, 106.1, 55.2, 27.6, 25.5, 25.3, 21.7, 20.8, 20.6 ppm, (*C*–B were not observed). **^{11}B-NMR (128 MHz, $CDCl_3$, 298 K):** δ 5.4 (br s) ppm. **HRMS (ESI)** calcd. $C_{44}H_{40}BNNaO^+$ ($M + Na^+$) 632.3095. Found 632.3095.

The enantiomers of the title compound were separated by semipreparative CSP- HPLC (IA column, *n*-hexane:isopropanol 99:1, T = 303 K, F = 9 mL/min), affording the first enantiomer *M*-**5b** with a retention time of 10.69 min and $[\alpha]^{20}_{D}$ –522 (c 0.15, $CHCl_3$)

for er >99:1, and the second enantiomer *P*-**5b** with a retention time of 12.44 min and $[\alpha]^{20}_{D}$ +410 (c 0.1, $CHCl_3$) for er >99:1. The absolute configuration of the reported chiral emitters was assigned by comparison of the experimental ECD spectra with our previous results,[10] and further confirmed by the computed ones (see below).

Synthesis of *rac*-5c

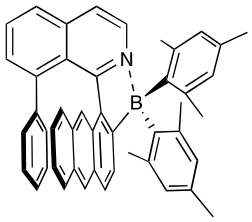


Following the general procedure, starting from **4c** (0.2 mmol, 91 mg), purification by column chromatography on silica gel (toluene/EtOAc 2:1) afforded *rac*-**5c** (66 mg, 53%) as an orange foam. **^{1}H-NMR (400 MHz, $CDCl_3$, 298 K):** δ 8.41 (d, 1H, *J* = 6.4 Hz), 7.87–7.80 (m, 2H), 7.65 (dd, 1H, *J* = 6.3, 2.1 Hz), 7.63–7.61 (m, 2H), 7.44 (d, 1H, *J* = 6.4 Hz), 7.29–7.25 (m, 2H), 7.07 (t, *J* = 8.2 Hz, 1H), 7.02 (t, 1H, *J* = 6.7 Hz), 6.88 (br s, 1H, H_{Mes}), 6.78 (s, 1H, H_{Mes}), 6.74–6.49 (m + br s, 5H), 6.24 (s, 1H, H_{Mes}), 2.79 (s, 6H, NMe_2), 2.38 (s, 3H, CH_{3Mes}), 2.28 (s, 3H, CH_{3mes}), 2.22 (s, 3H, CH_{3mes}), 2.18 (s, 3H, CH_{3Mes}), 2.06 (s, 3H, CH_{3Mes}), 1.27 (s, 3H, CH_{3mes}) ppm. **^{13}C-NMR (100 MHz, $CDCl_3$, 298 K):** δ 160.8 (Cq), 153.1 (Cq), 143.8 (Cq), 142.5 (Cq), 141.6 (Cq), 141.1 (Cq), 140.5 (Cq), 139.7 (Cq), 137.9 (Cq), 136.5, 134.6 (Cq), 133.0 (Cq), 131.6, 131.5 (Cq), 131.3, 130.1, 129.9, 129.5 (br s), 129.4 (br s), 129.3, 128.7, 126.9 (Cq), 126.7, 126.5 (Cq), 125.6, 124.8 (2 × C), 123.4, 123.1, 121.8 (Cq), 117.2, 112.7, 43.7, 27.1, 25.4, 25.1, 21.7, 20.8, 20.6 ppm, *C*–B were not observed. **^{11}B-NMR (128 MHz, $CDCl_3$, 298 K):** δ 5.5 (br s) ppm. **HRMS(ESI)** calcd. $C_{45}H_{44}BN_2^+$ ($M + H^+$) 623.3592. Found 623.3592.

The enantiomers of the title compound were separated by semipreparative CSP- HPLC (IA column, *n*-hexane:isopropanol 99:1, T = 303 K, F = 9 mL/min), affording the first enantiomer *M*-**5c** with a retention time of 6.67 min and $[\alpha]^{20}_{D}$ −522 (c 0.1, $CHCl_3$) for er >99:1, and the second enantiomer *P*-**5c** with a retention time of 8.46 min and $[\alpha]^{20}_{D}$

+570 (c 0.1, $CHCl_3$) for er >99:1. The absolute configuration of the reported chiral emitters was assigned by comparison of the experimental ECD spectra with our previous results,[10] and further confirmed by the computed ones (see below).

Synthesis of *rac*-5d

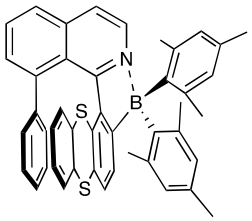


Following the general procedure, starting from **4d** (0.2 mmol, 91.8 mg), purification by column chromatography on silica gel (cyclohexane/EtOAc 30:1) afforded *rac*-**5d** (80 mg, 64%) as a orange foam. **^{1}H-NMR (400 MHz, $CDCl_3$, 298 K):** δ 8.64 (d, 1H, *J* = 6.4 Hz), 8.23 (s, 1H), 7.96–7.88 (m, 3H), 7.82 (d, 1H, *J* = 10.2 Hz), 7.80 (d, 1H, *J* = 8.5 Hz), 7.63–7.54 (m, 2H), 7.60 (d, 1H, *J* = 6.4 Hz), 7.57 (d, 1H, *J* = 8.4 Hz), 7.43 (t, 1H, *J* = 6.8 Hz), 7.38 (d, 1H, *J* = 8.0 Hz), 7.05-7.30 (br s, 2H), 6.90 (s, 1H, H_{Mes}), 6.79 (s, 1H, H_{Mes}), 6.71 (s, 1H, H_{Mes}), 6.60 (t, 1H, *J* = 7.6 Hz,), 6.51–6.27 (br s, 2H), 6.22 (s, 1H, H_{Mes}), 2.42 (s, 3H, CH_{3Mes}), 2.30 (s, 3H, CH_{3Mes}), 2.27 (s, 3H, CH_{3Mes}), 2.24 (s, 3H, CH_{3Mes}), 2.06 (s, 3H, CH_{3Mes}), 1.22 (s, 3H, CH_{3Mes}). **^{13}C-NMR (100 MHz, $CDCl_3$, 298 K):** δ 161.0 (Cq), 144.1 (Cq), 142.4 (Cq), 141.5 (Cq), 141.1 (Cq), 140.7 (Cq), 139.9 (Cq), 138.0 (Cq), 136.5, 134.7 (Cq), 133.5 (Cq), 132.1, 131.7, 131.5 (2xC), 131.3 (Cq), 130.7 (Cq), 130.5 (Cq), 130.3 (2xC), 129.6, 129.0, 128.7 (br s), 128.5, 128.0, 127.9, 127.4 (Cq), 127.3, 126.1 (br s), 125.9, 125.8, 125.5, 124.5, 122.7 (Cq), 121.4, 119.0, 27.6, 25.5 (2 × C), 21.9, 20.9, 20.6 ppm, *C*–B were not observed and 2 C are not observable. **^{11}B-NMR (128 MHz, $CDCl_3$, 298 K):** δ 5.3 (br s) ppm. **HRMS(ESI)** calcd. $C_{47}H_{41}BN^+$ ($M + H^+$) 630.3327. Found 630.3321.

The enantiomers of the title compound were separated by semipreparative CSP- HPLC (IA column, *n*-hexane:isopropanol 99:1, T = 303 K, F = 18 mL/min), affording the first enantiomer *M*-**5d** with a retention time of 5.96 min and $[\alpha]^{20}_D$ –390 (c 0.1, $CHCl_3$) for

er >99:1, and the second enantiomer *P*-**5d** with a retention time of 8.81 min and $[\alpha]^{20}_{D}$ +404 (c 0.1, $CHCl_3$) for er >99:1. The absolute configuration of the reported chiral emitters was assigned by comparison of the experimental ECD spectra with our previous results,[10] and further confirmed by the computed ones (see below).

Synthesis of *rac*-5e

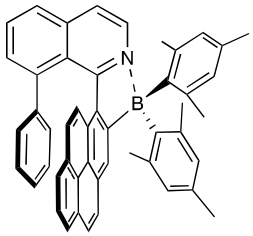


Following the general procedure, starting from **4e** (0.054 mmol, 36 mg), purification by column chromatography on silica gel (toluene/cyclohexane 1:1) afforded *rac*-**5e** (14 mg, 39%) as an orange foam. **^{1}H-NMR (400 MHz, $CDCl_3$, 298 K):** 8.62 (d, 1H, *J* = 6.4 Hz), 7.96 (t, 1H, *J* = 8.2 Hz), 7.94–7.87 (m, 2H), 7.70 (d, 1H, *J* = 6.4 Hz), 7.55 (d, 1H, *J* = 7.8 Hz), 7.52–7.30 (br s, 2H), 7.27–7.24 (m, 1H), 7.19–7.12 (m, 3H), 7.10–7.01 (m, 2H), 7.01–6.95 (m, 2H), 6.83 (s, 1H, H_{Mes}), 6.73 (s, 1H, H_{Mes}), 6.66 (s, 1H, H_{mMs}), 6.23 (s, 1H, H_{Mes}), 2.34 (s, 3H, CH_{3Mes}), 2.22 (s, 3H, CH_{3Mes}), 2.18 (s, 3H, CH_{3Mes}), 2.11 (s, 3H, CH_{3Mes}), 2.06 (s, 3H, CH_{3mes}), 1.00 (s, 3H, CH_{3Mes}) ppm. **^{13}C-NMR (100 MHz, $CDCl_3$, 298 K):** 159.5 (Cq), 143.4 (Cq), 142.0 (Cq), 141.6 (Cq), 140.5 (Cq), 139.3 (Cq), 138.9 (Cq), 138.8 (Cq), 137.5 (Cq), 135.9, 135.8 (Cq), 135.2 (Cq), 134.8 (Cq), 133.6 (Cq), 133.0, 132.5, 132.4, 130.8 (Cq), 130.4, 130.0, 129.5, 129.3, 129.1, 128.5, 128.4 (Cq), 128.2, 128.3, 128.2, 127.6, 127.3, 127.0, 126.8, 125.6, 123.5 (Cq), 120.7, 28.1, 25.5, 25.2, 21.2, 20.8, 20.7 ppm, *C*–B were not observed. **^{11}B-NMR (128 MHz, $CDCl_3$, 298 K):** δ 5.9 (br s) ppm. **HRMS (ESI)** calcd. $C_{45}H_{38}BNNaS_2^+$ ($M + Na^+$) 690.2431. Found 690.2407.

The enantiomers of the title compound were separated by semipreparative CSP- HPLC (IA column, *n*-hexane:isopropanol 97:3, T = 303 K, F = 18 mL/min), affording the first enantiomer *M*-**5e** with a retention time of 6.04 min and $[\alpha]^{20}_{D}$ −79 (c 0.1, $CHCl_3$) for er

>99:1, and the second enantiomer *P*-**5e** with a retention time of 11.77 min and and $[\alpha]^{20}_{D}$ +70 (c 0.1, $CHCl_3$) for er >99:1. The absolute configuration of the reported chiral emitters was assigned by comparison of the experimental ECD spectra with our previous results,[10] and further confirmed by the computed ones (see below).

Synthesis of *rac*-5f



Following the general procedure, starting from **4f** (0.11 mmol, 72.6 mg), purification by column chromatography on silica gel (toluene/cyclohexane 1:1) afforded *rac*-**5f** (48 mg, 65%) as a yellow-orange foam. **^{1}H-NMR (400 MHz, $CDCl_3$, 298 K):** δ 8.71 (d, 1H, *J* = 6.4 Hz), 8.41 (s, 1H), 8.04–8.00 (m, 3H), 7.95–7.89 (m, 2H), 7.87–7.83 (m, 2H), 7.80–7.74 (m, 3H), 7.67 (d, 1H, *J* = 6.4 Hz), 7.20–6.90 (br s, 1H), 6.92 (br s, 1H, H_{Mes}), 6.83–6.80 (m, 2H), 6.69 (br s, 1H, H_{Mes}), 6.33 (t, 2H, *J* = 7.5 Hz), 6.24 (t, 1H, *J* = 7.2 Hz), 6.16 (br s, 1H, H_{Mes}), 2.42 (s, 3H, CH_{3Mes}), 2.37 (s, 3H, CH_{3Mes}), 2.29 (br s, 8H, CH_{3Mes} overlapped), 2.01 (s, 3H, CH_{3Mes}), 1.19 (s, 3H, CH_{3Mes}) ppm. **^{13}C-NMR (100 MHz, $CDCl_3$, 298 K):** δ 160.9 (Cq), 144.1 (Cq), 142.4 (Cq), 142.0 (Cq), 140.6 (Cq), 139.8 (Cq), 139.7 (Cq), 138.9 (Cq), 136.8, 134.7 (Cq), 133.3 (Cq), 133.1 (Cq), 132.2 (2xC), 131.6 (Cq), 130.5 (Cq), 130.4 (br s), 130.2 (br s), 130.1 (Cq), 129.8 (br s), 129.3 (br s), 129.1 (br s), 128.4, 128.3, 128.0, 127.4 (Cq), 127.0, 126.90, 126.85, 125.9, 125.8, 125.4, 125.0, 124.8, 124.3 (Cq), 124.0, 123.3 (Cq), 123.0 (Cq), 119.9, 28.6, 25.7, 25.6, 21.9, 20.9, 20.6 ppm, *C*–B were not observed. **^{11}B-NMR (128 MHz, $CDCl_3$, 298 K):** δ 5.9 (br s) ppm. **HRMS (ESI)** calcd. $C_{49}H_{40}BNNa^+$ ($M + Na^+$) 676.3138. Found 676.3157.

The enantiomers of the title compound were separated by semipreparative CSP- HPLC (IA column, *n*-hexane:isopropanol 97:3, T = 303 K, F = 18 mL/min), affording the first

enantiomer *M*-**5f** with a retention time of 6.14 min and $[\alpha]^{20}_{D}$ –95 (c 0.1, $CHCl_3$) for er >99:1, and the second enantiomer *P*-**5f** with a retention time of 9.15 min and $[\alpha]^{20}_{D}$ +96 (c 0.1, $CHCl_3$) for er >99:1. The absolute configuration of the reported chiral emitters was assigned by comparison of the experimental ECD spectra with our previous results,[10] and further confirmed by the computed ones (see below).

3. NMR spectra, HRMS, HPLC chromatograms

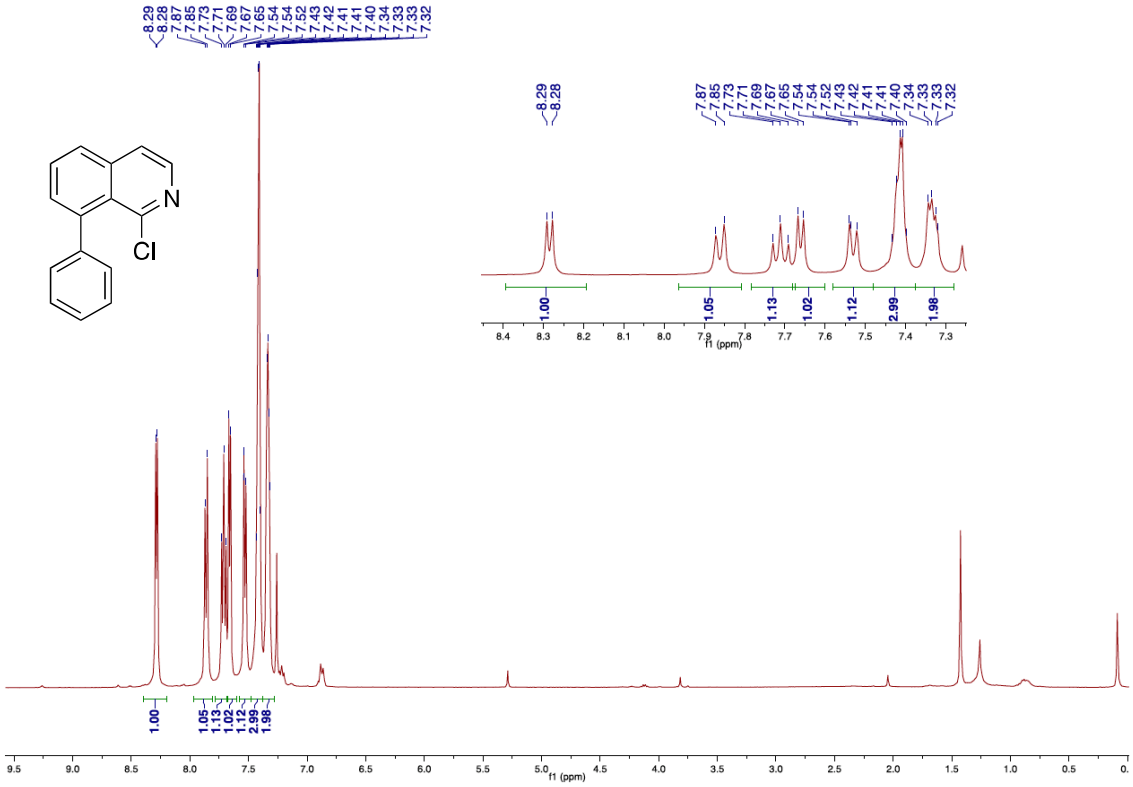


Figure S1. ^{1}H-NMR (400 MHz, $CDCl_3$, 298 K) for **1**.

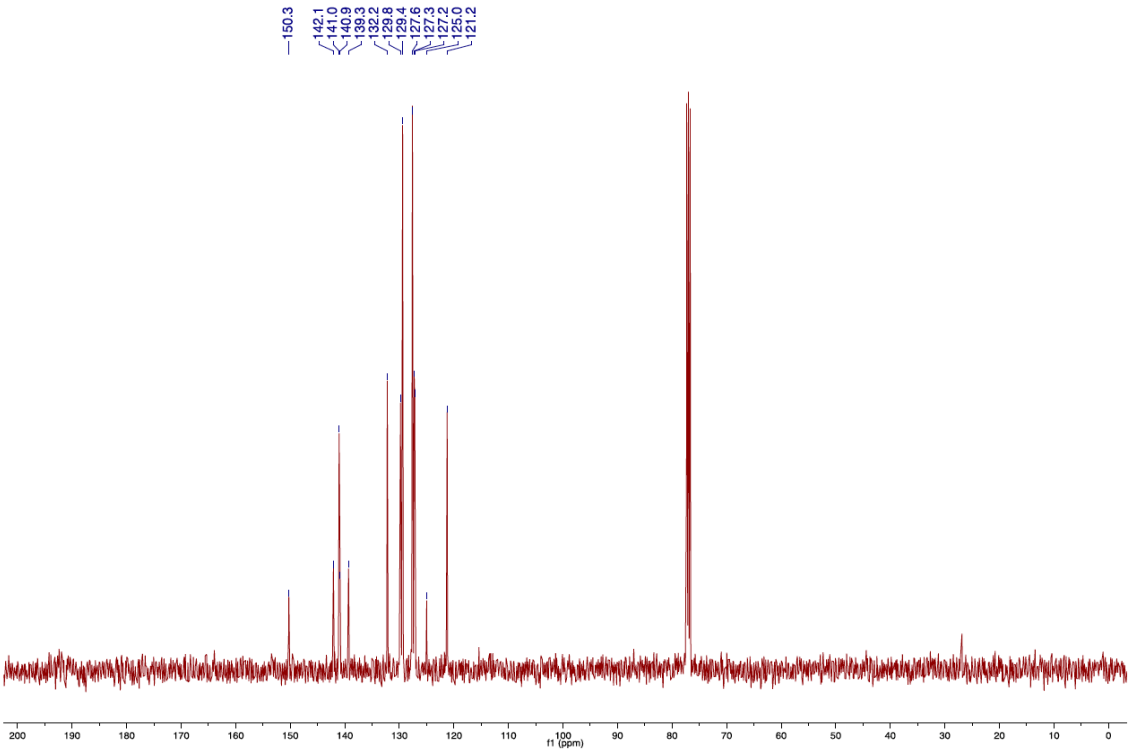


Figure S2. ^{13}C-NMR (100 MHz, $CDCl_3$, 298 K) for **1**.

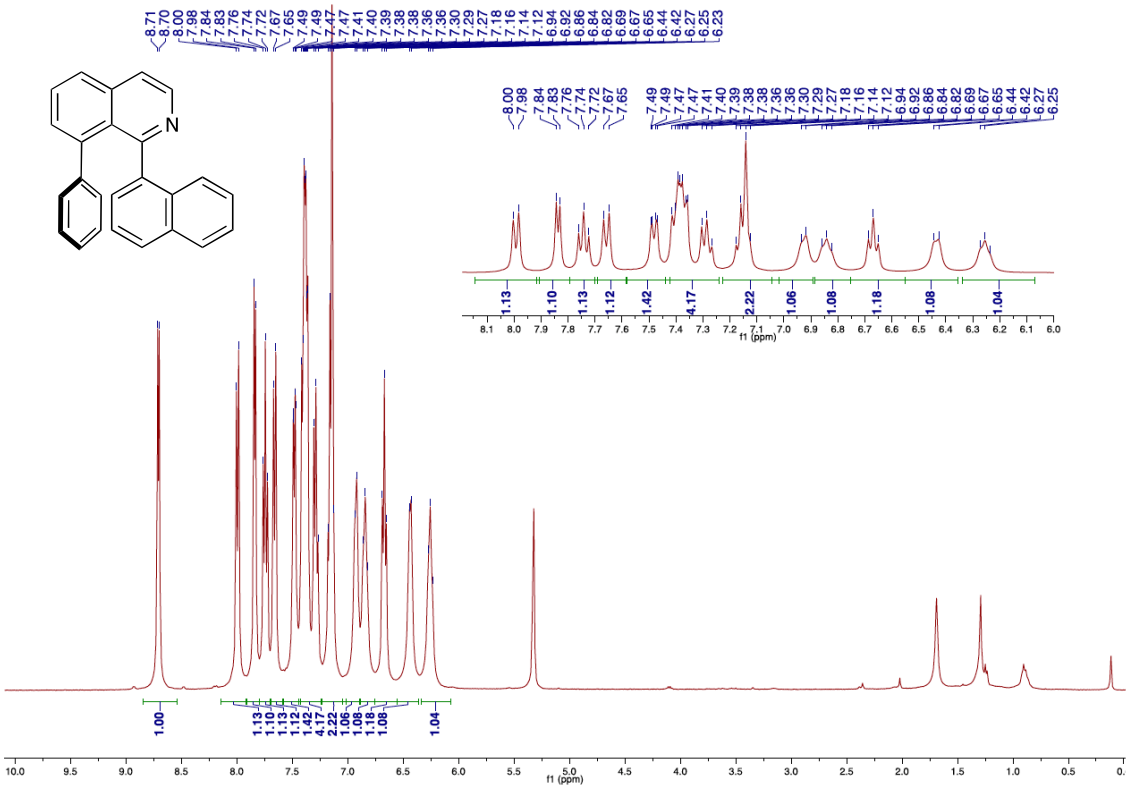


Figure S3. ^{1}H-NMR (400 MHz, CD_2Cl_2, 298 K) for **3a**.

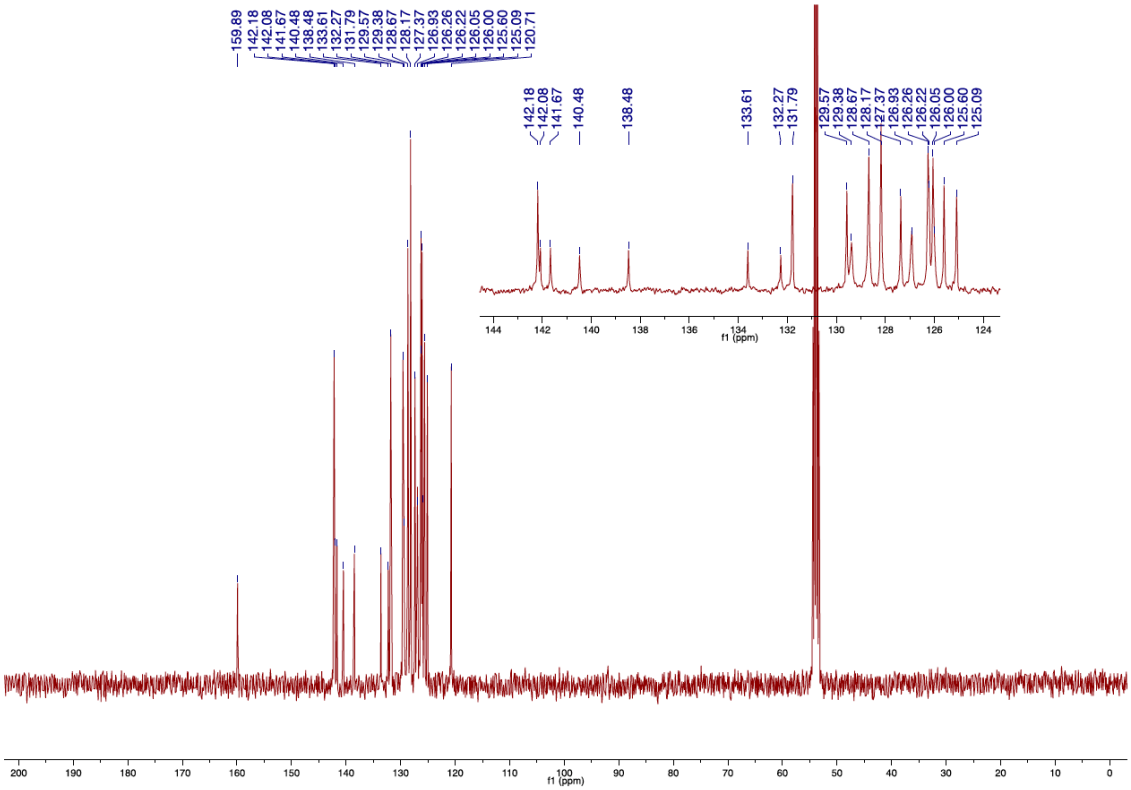


Figure S4. ^{13}C-NMR (100 MHz, CD_2Cl_2, 298 K) for **3a.**

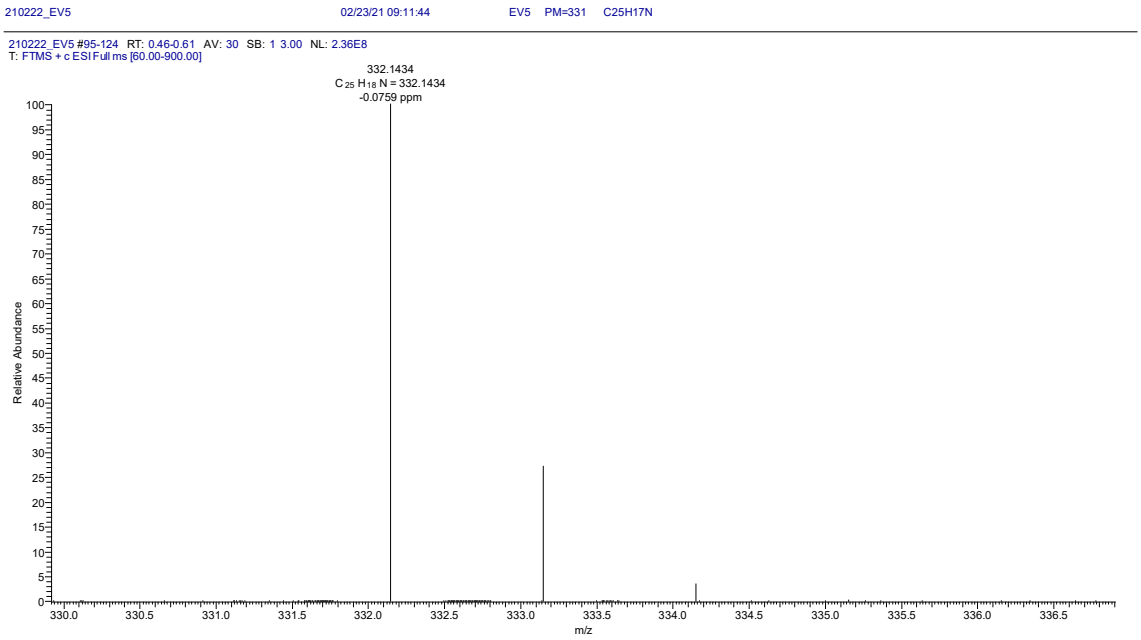


Figure S5. HRMS-ESI for **3a.**

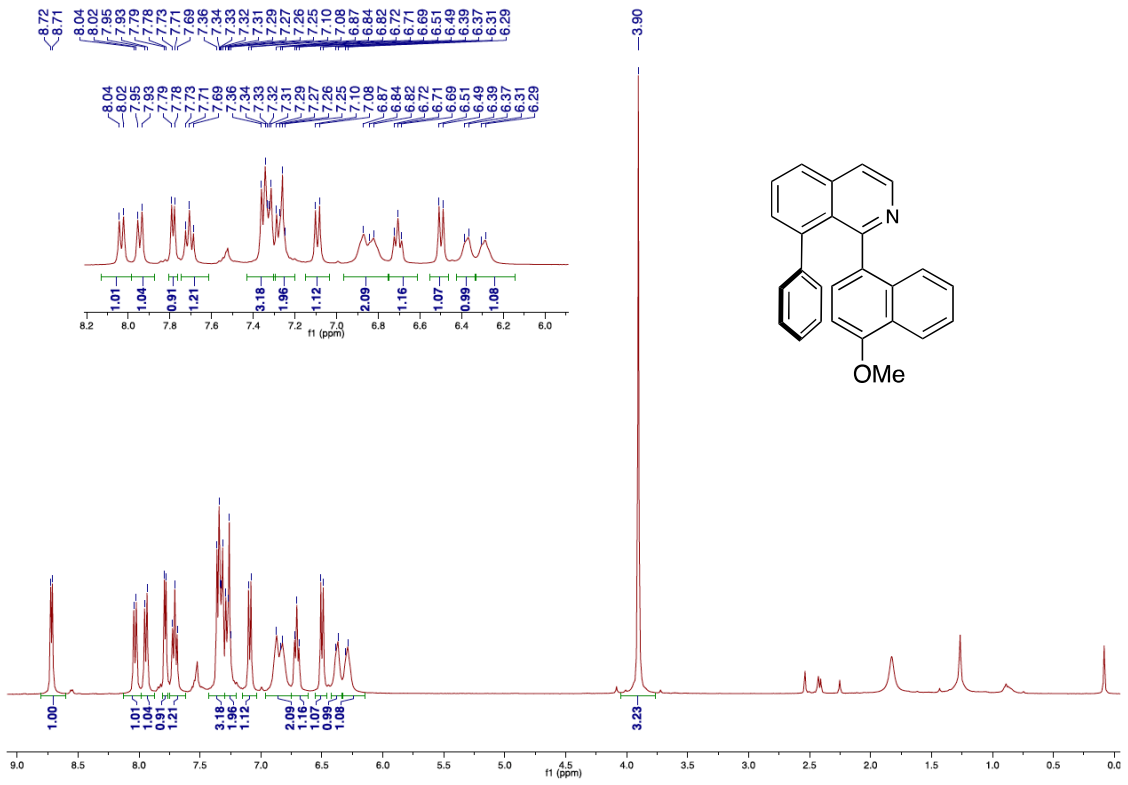


Figure S6. ^{1}H-NMR (400 MHz, $CDCl_3$, 298 K) for **3b**.

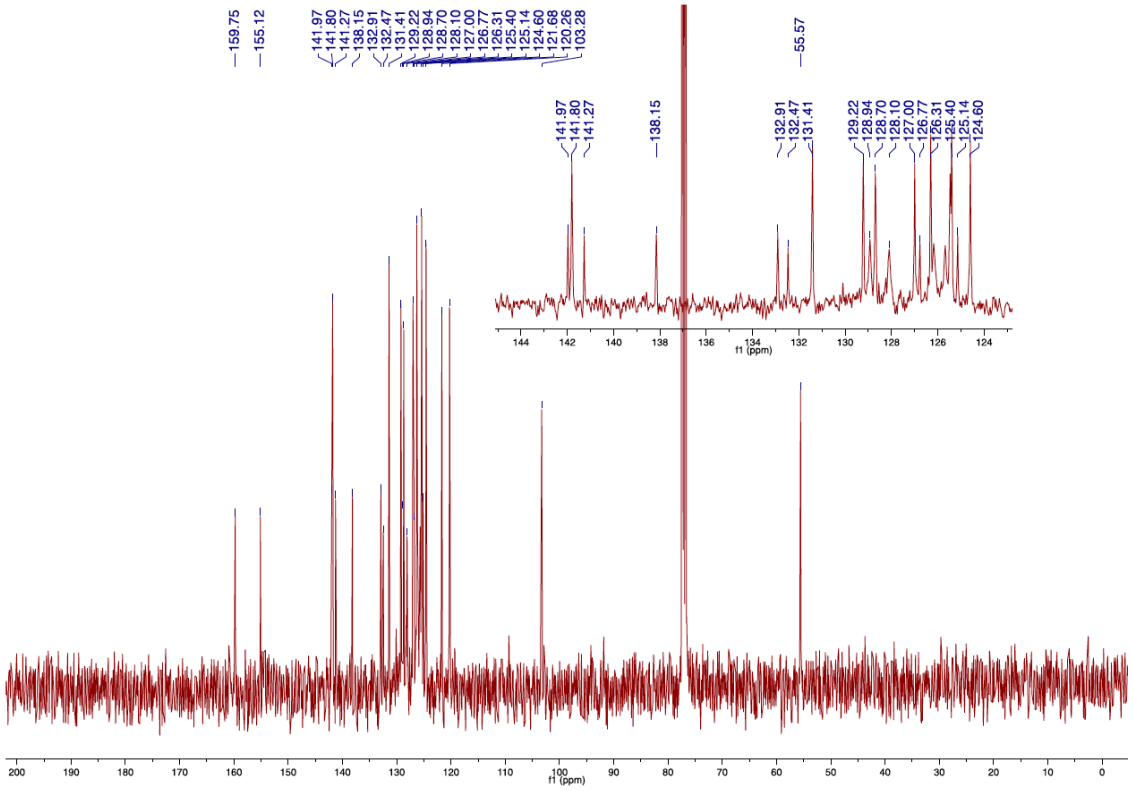


Figure S7. ^{13}C-NMR (100 MHz, $CDCl_3$, 298 K) for **3b**.

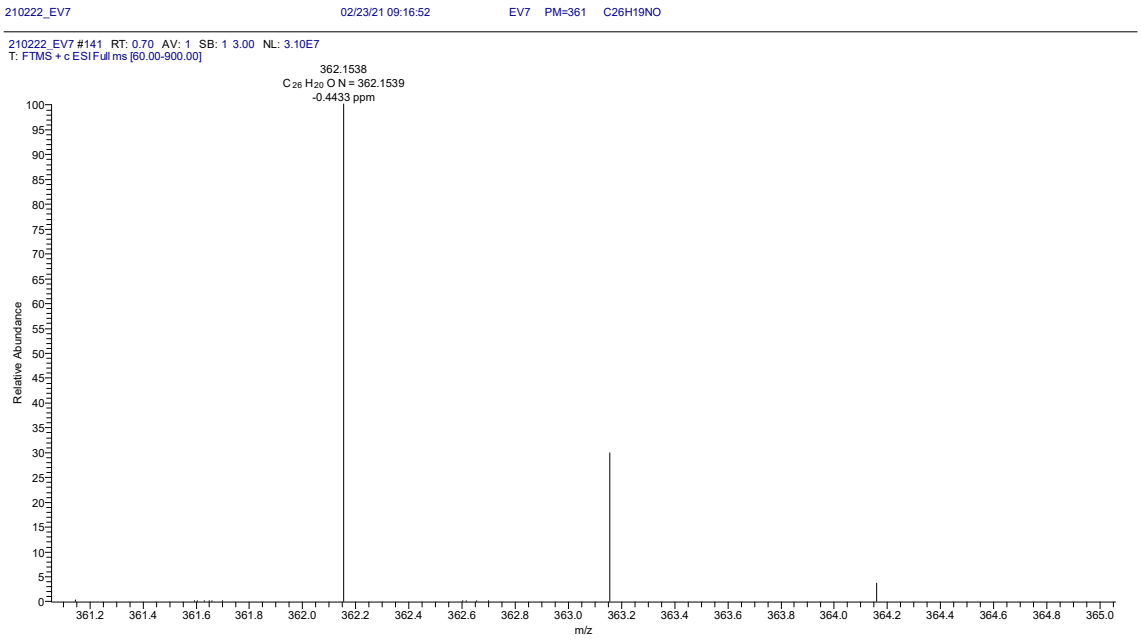


Figure S8. HRMS-ESI for **3b.**

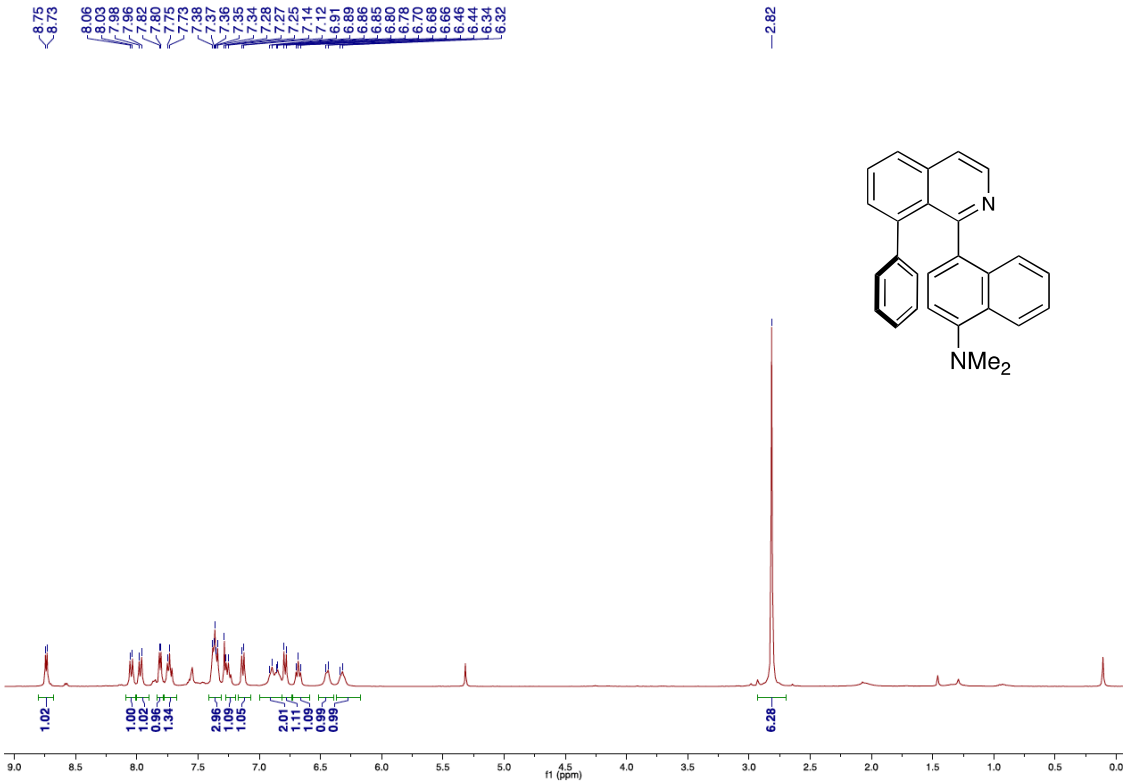


Figure S9. ^{1}H-NMR (400 MHz, $CDCl_3$, 298 K) for **3c**.

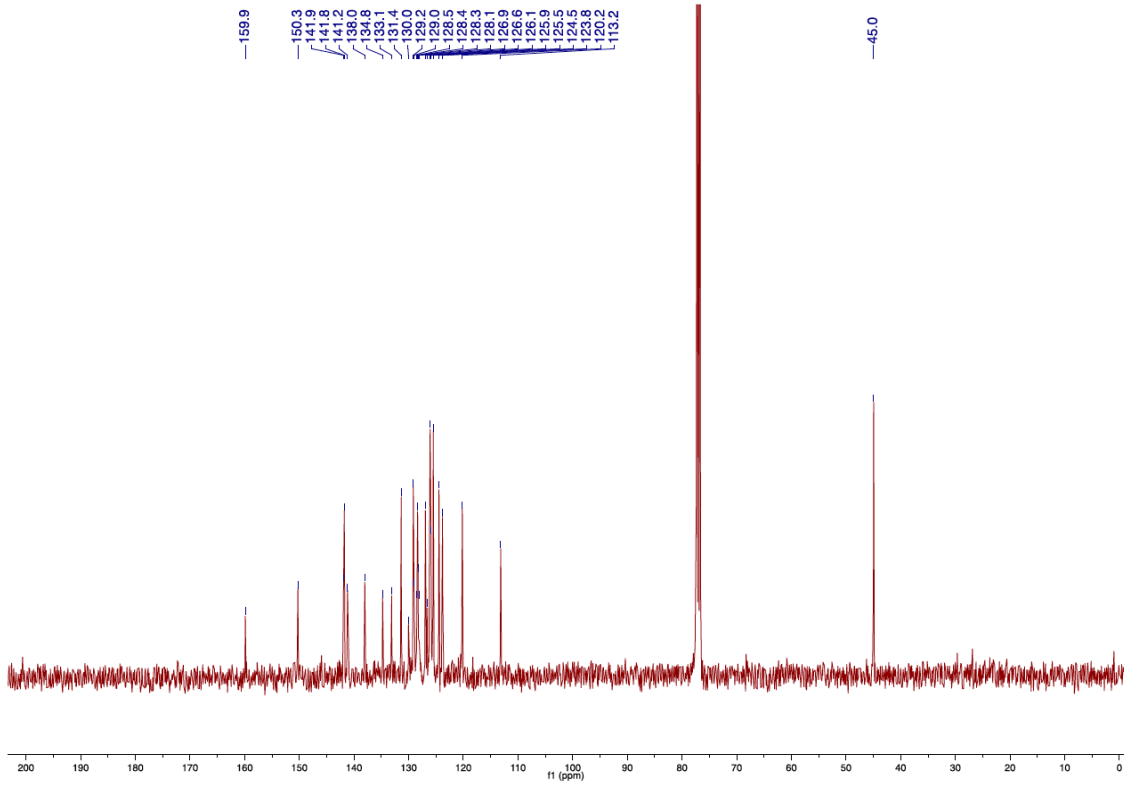


Figure S10. ^{13}C-NMR (100 MHz, $CDCl_3$, 298 K) for **3c**.

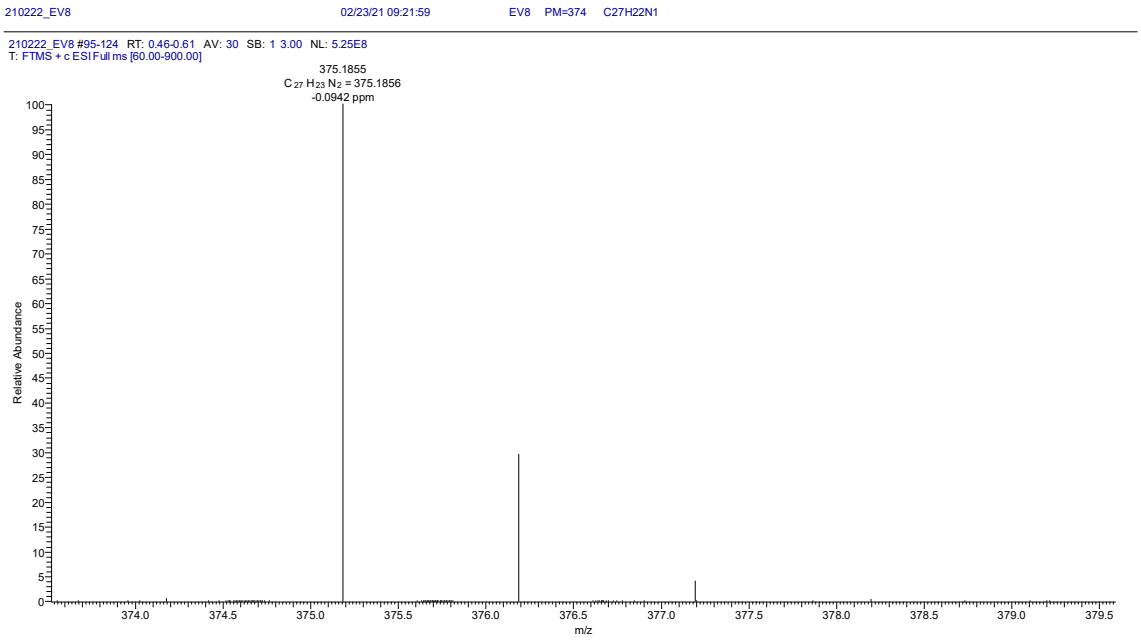


Figure S11. HRMS-ESI for **3c.**

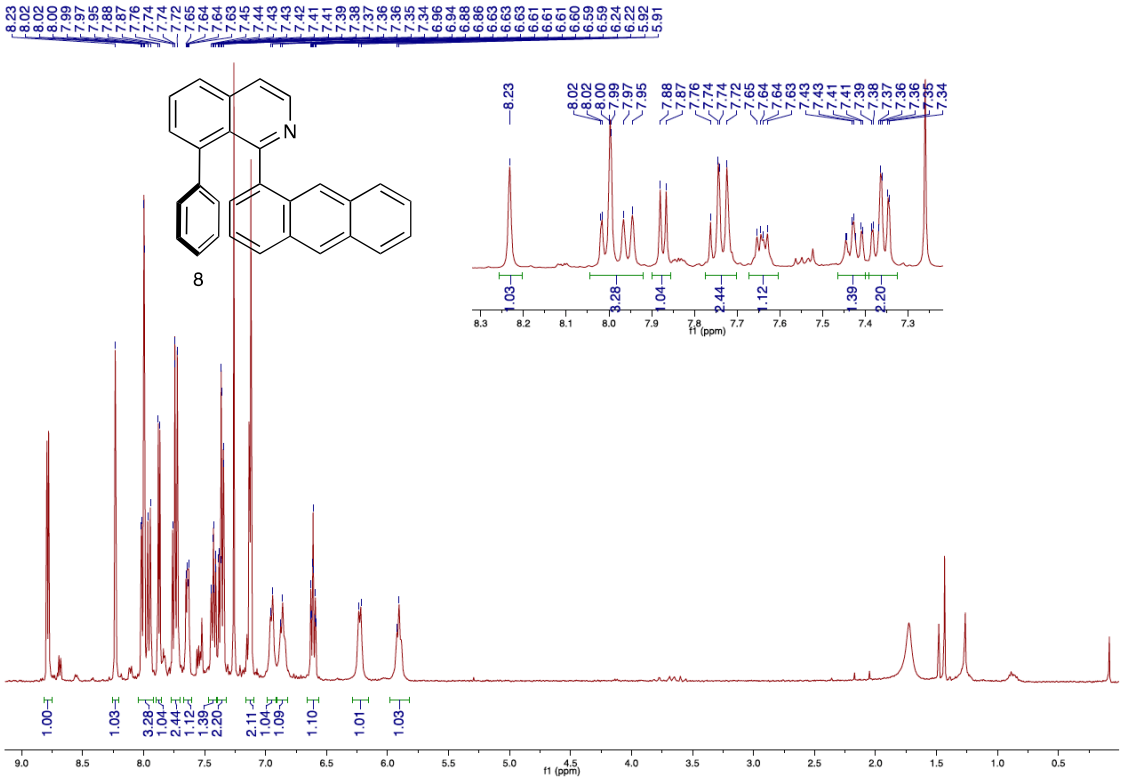


Figure S12. ^{1}H-NMR (400 MHz, $CDCl_3$, 298 K) for **3d**.

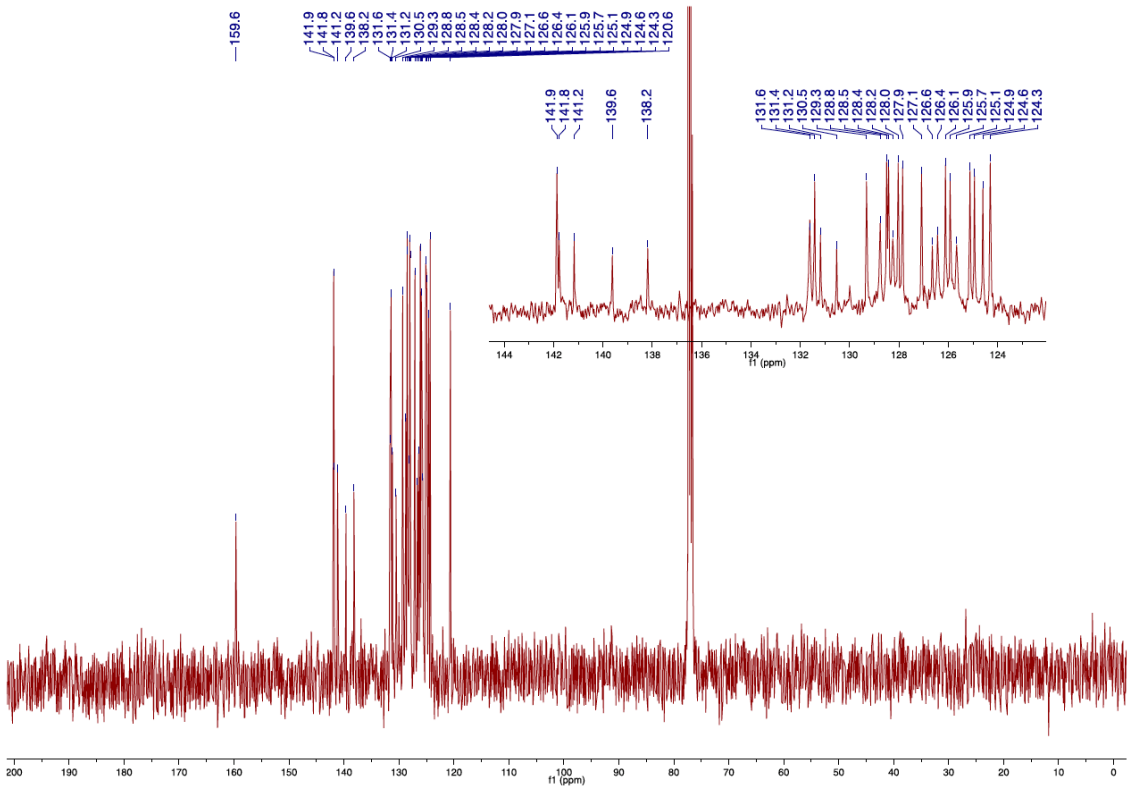


Figure S13. ^{13}C-NMR (100 MHz, $CDCl_3$, 298 K) for **3d**.

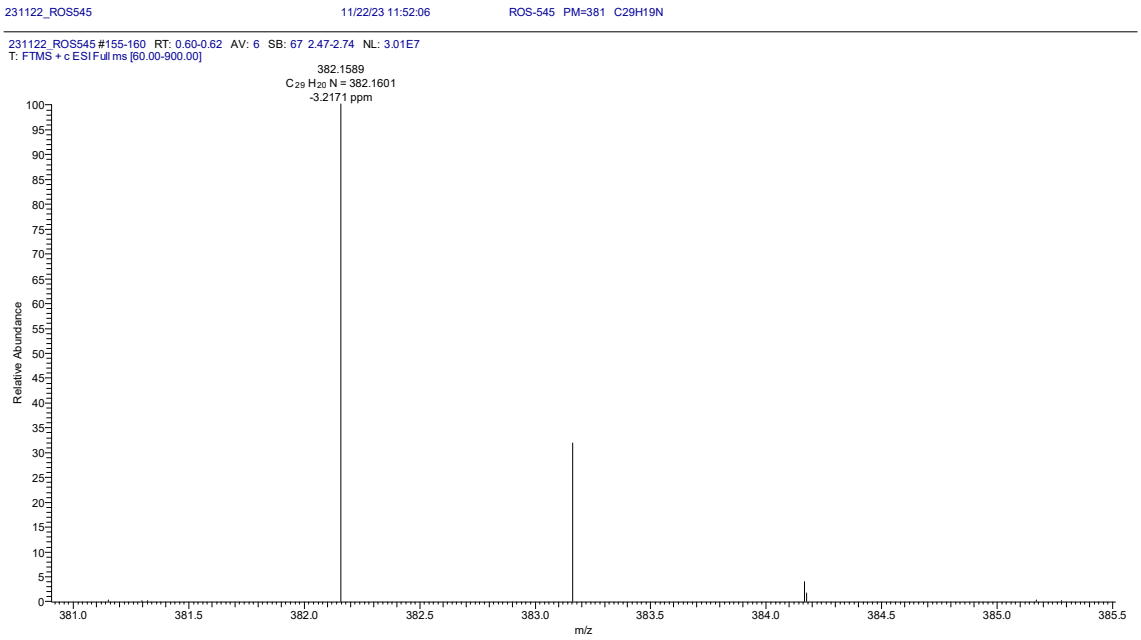


Figure S14. HRM-ESI for **3d.**

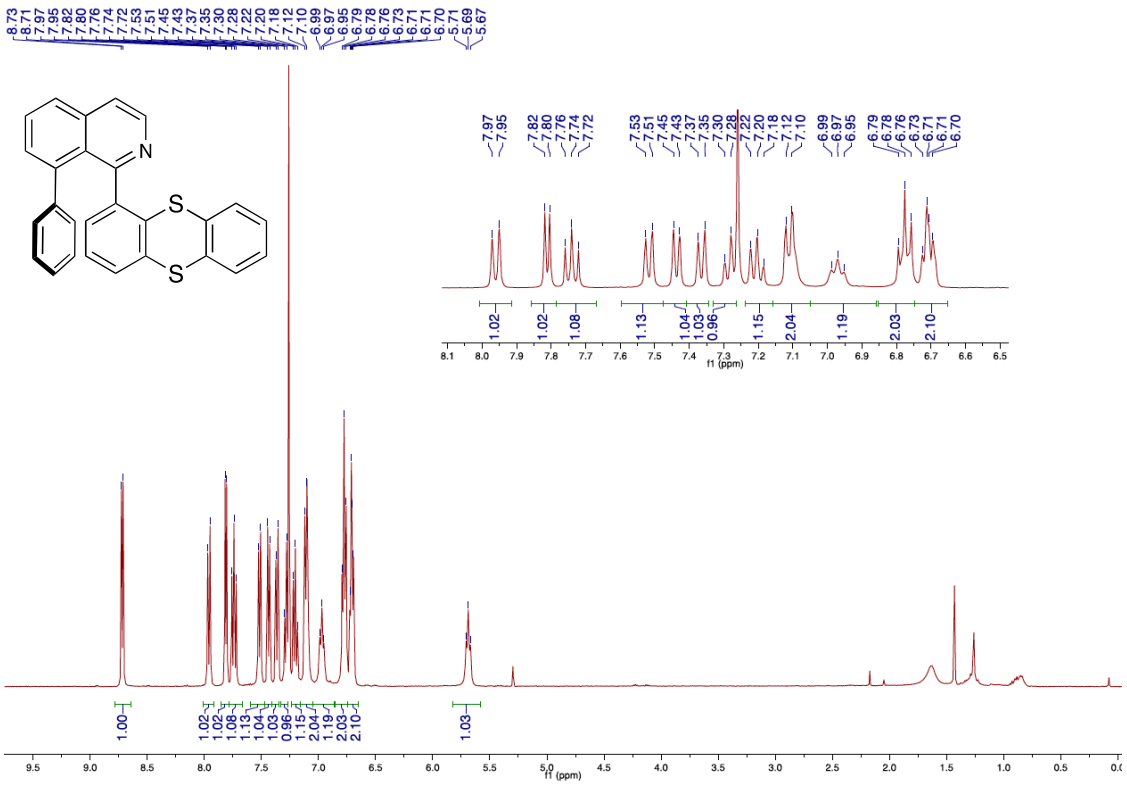


Figure S15. ^{1}H-NMR (400 MHz, $CDCl_3$, 298 K) for **3e**.

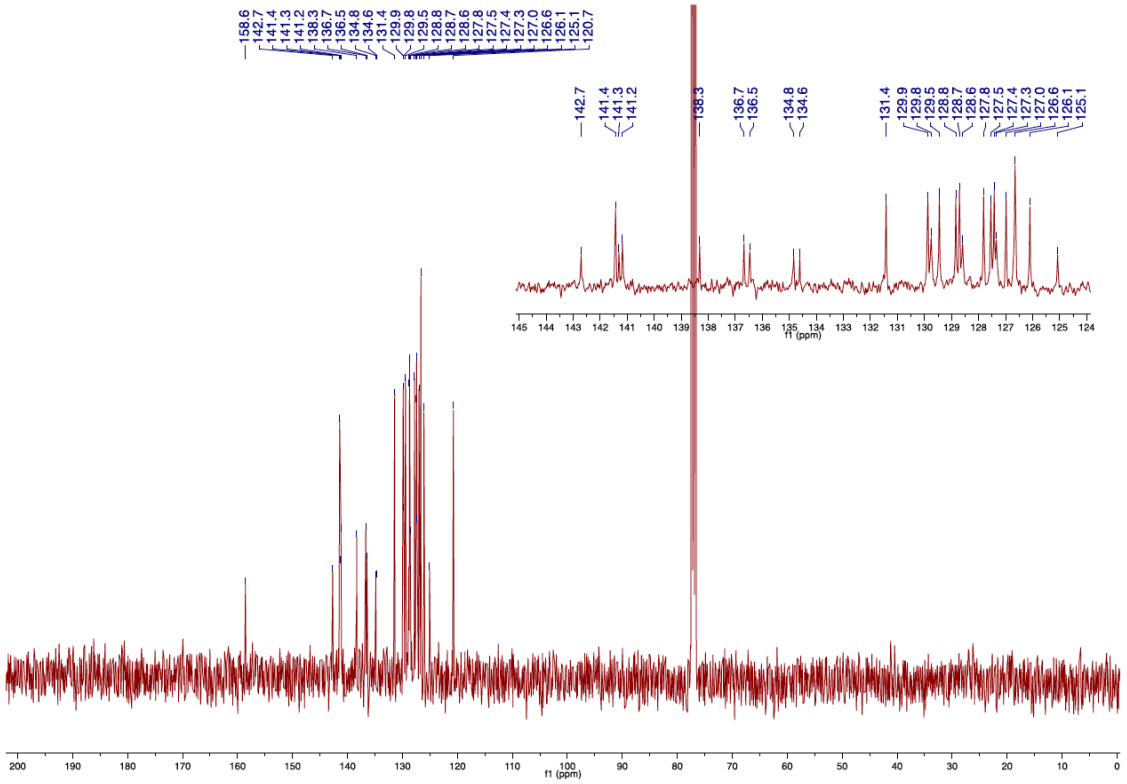


Figure S16. ^{13}C-NMR (100 MHz, $CDCl_3$, 298 K) for **3e**.

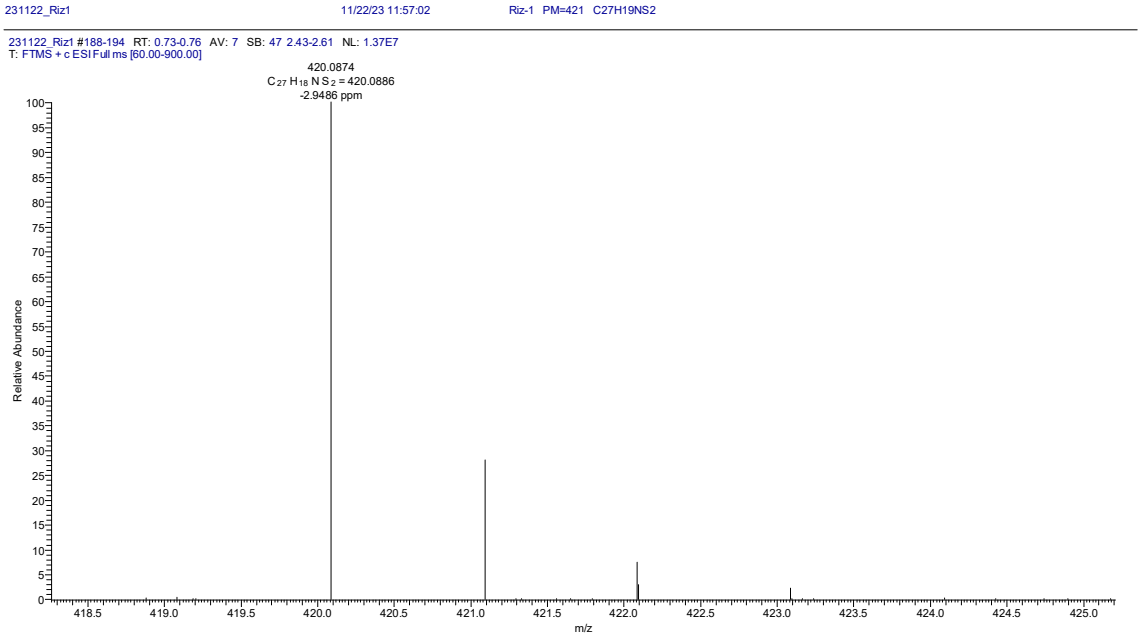


Figure S17. HRM-ESI for **3e.**

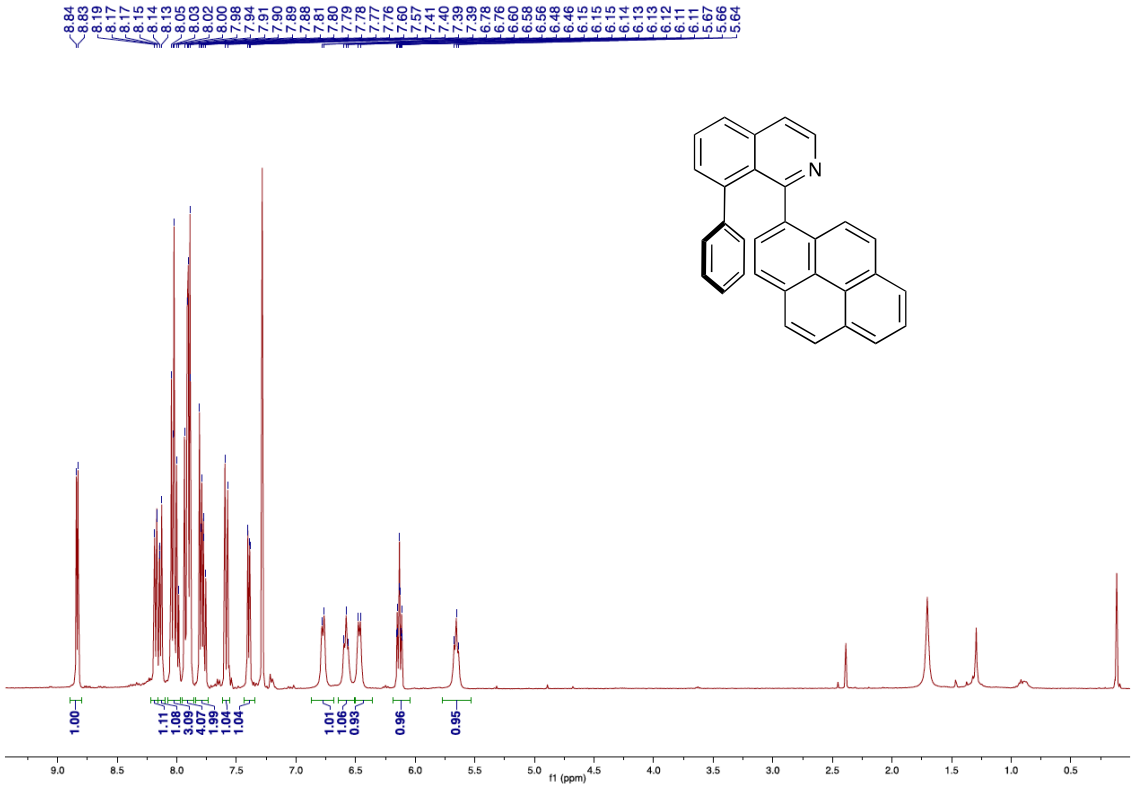


Figure S18. ^{1}H-NMR (400 MHz, $CDCl_3$, 298 K) for **3f**.

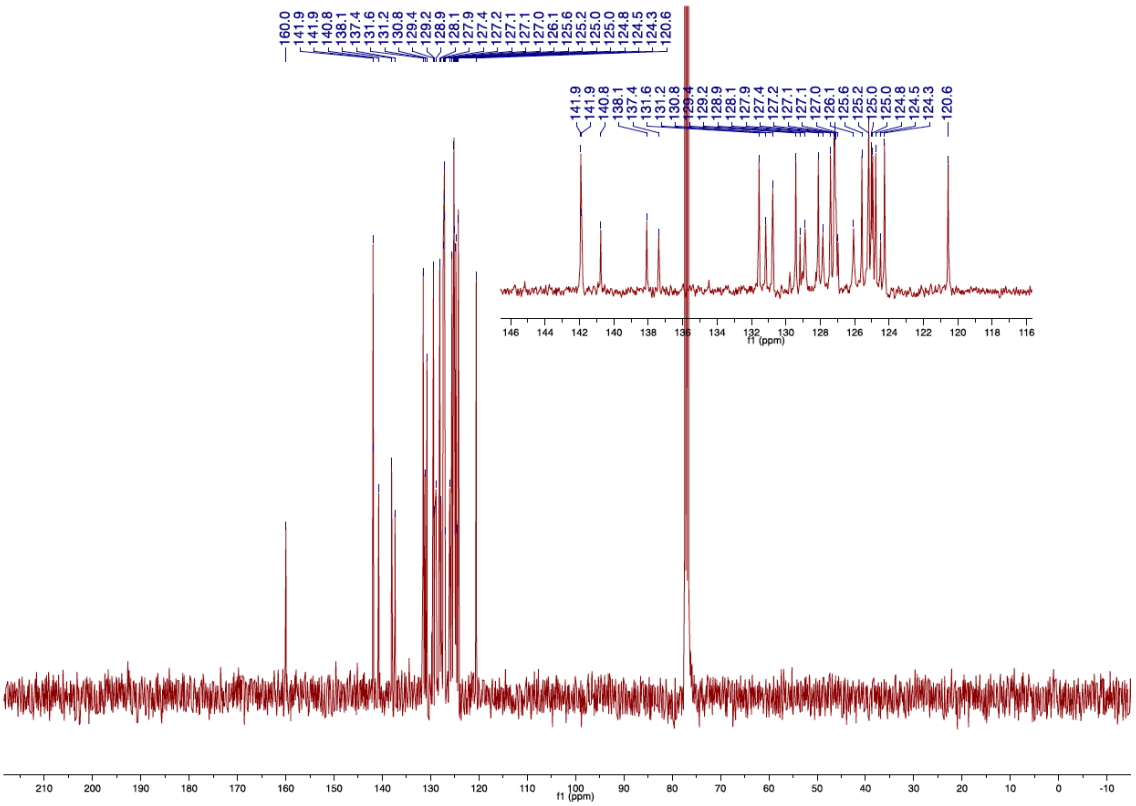


Figure S19. ^{13}C-NMR (100 MHz, $CDCl_3$, 298 K) for **3f**.

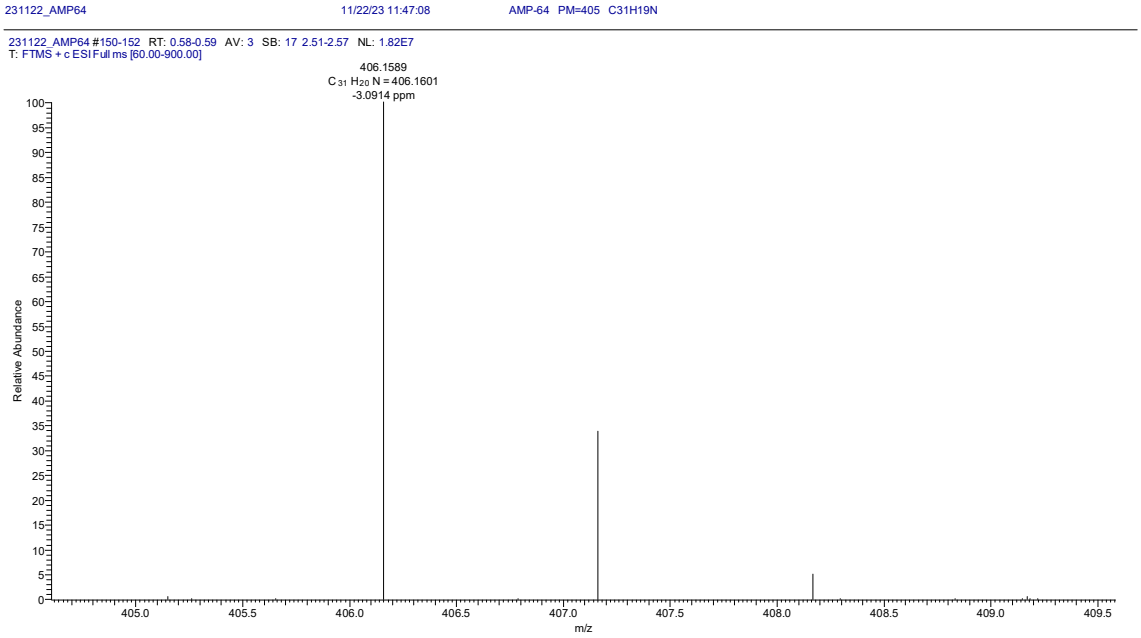


Figure S20. HRM-ESI for **3f.**

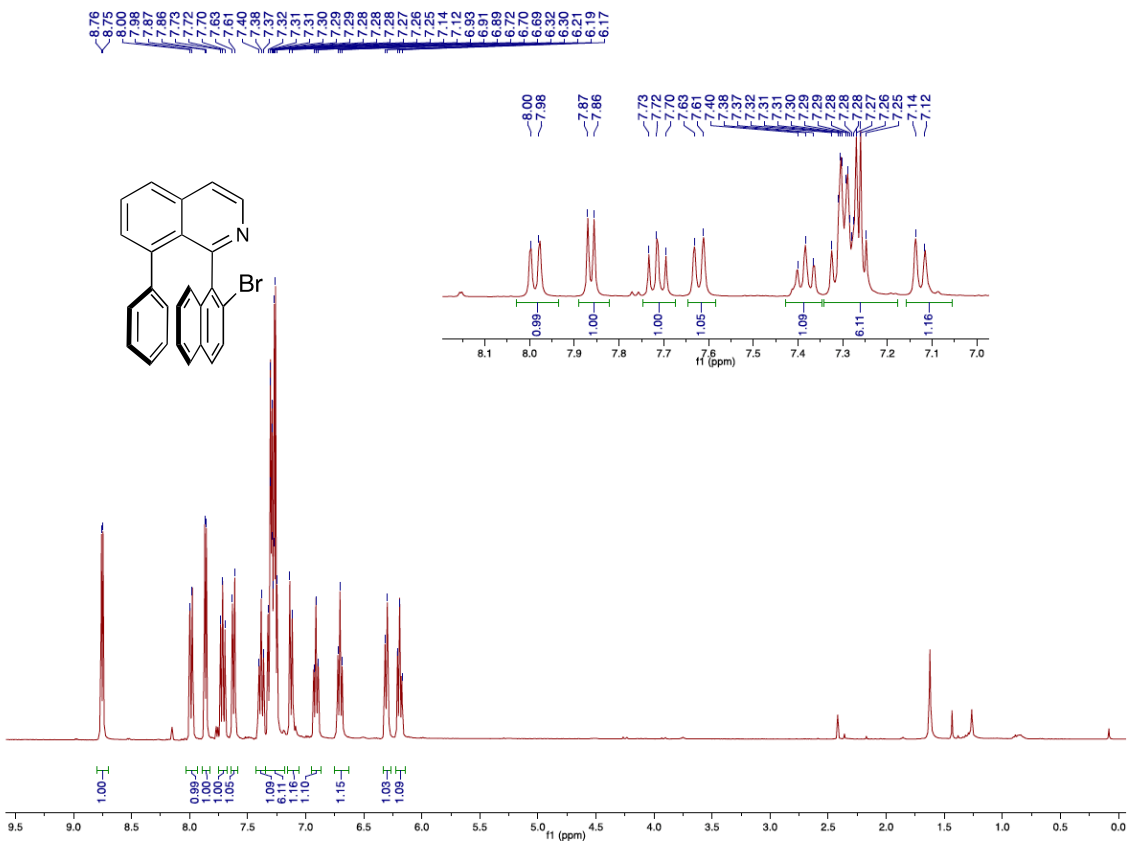


Figure S21. ^{1}H-NMR (400 MHz, $CDCl_3$, 298 K) for *rac*-**4a**.

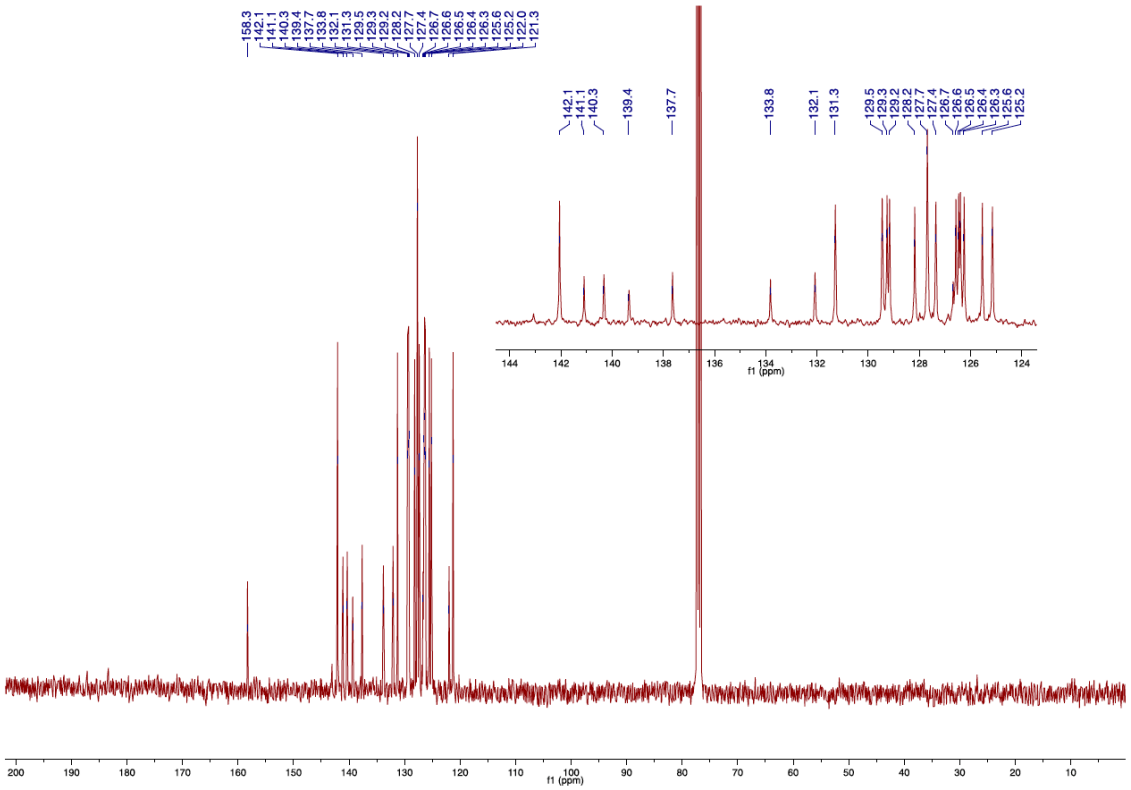


Figure S22. ^{13}C-NMR (100 MHz, $CDCl_3$, 298 K) for *rac*-**4a**.

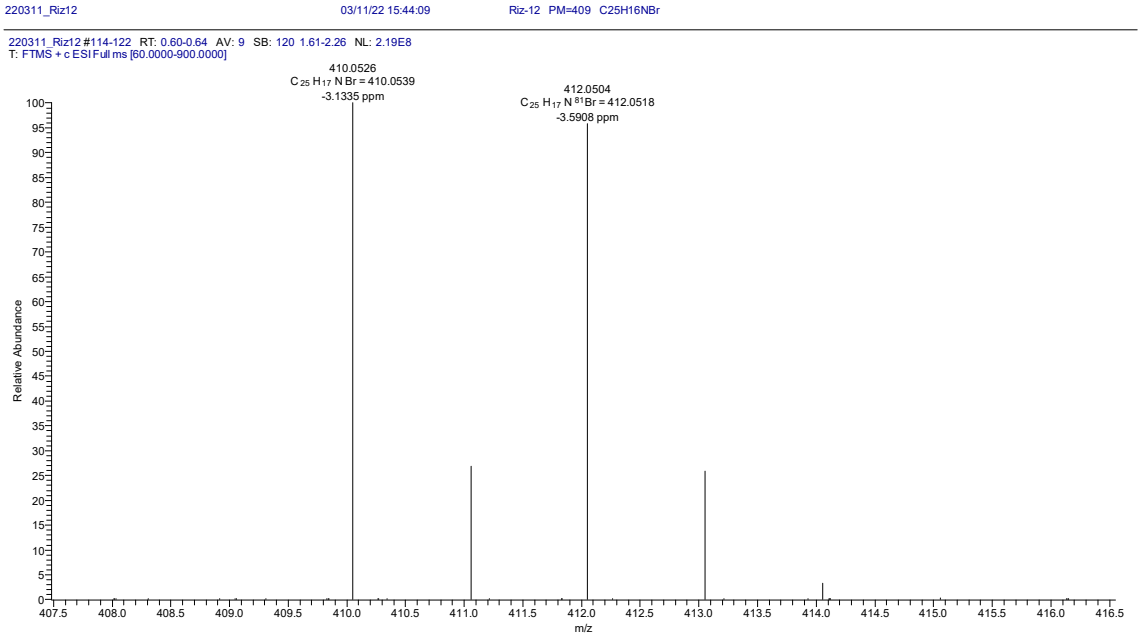


Figure S23. HRM-ESI for *rac*-**4a**.

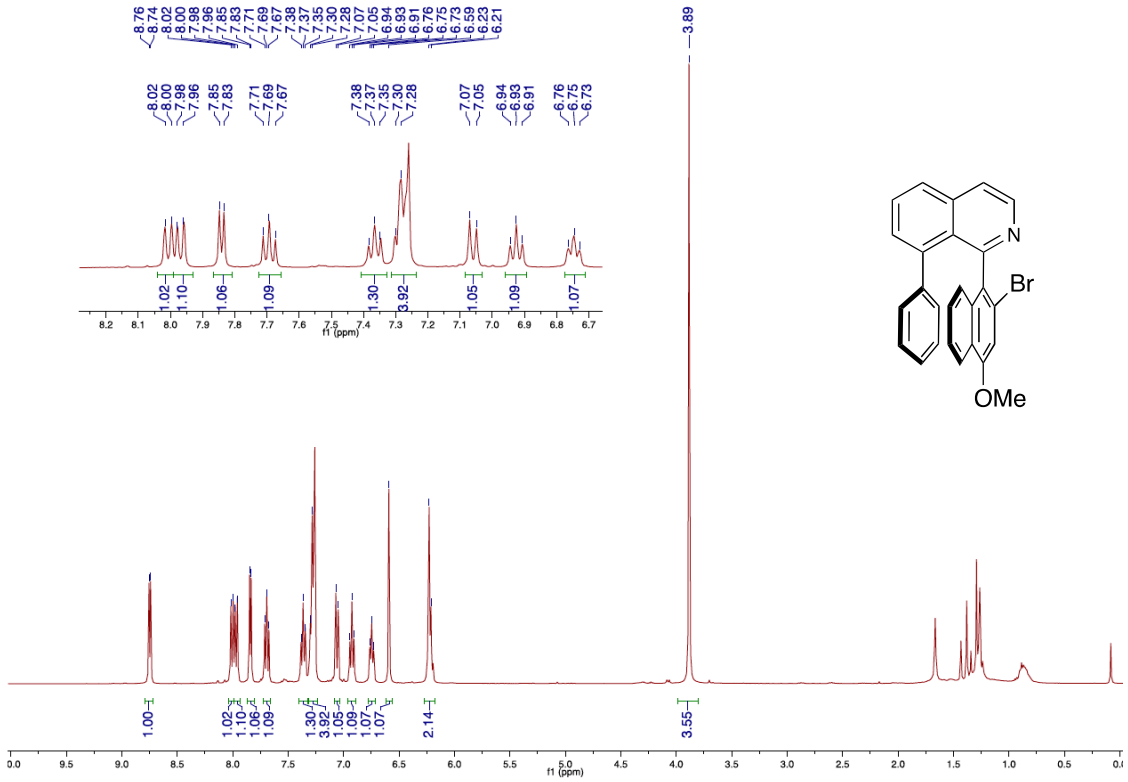


Figure S24. ^{1}H-NMR (400 MHz, $CDCl_3$, 298 K) for *rac*-**4b**.

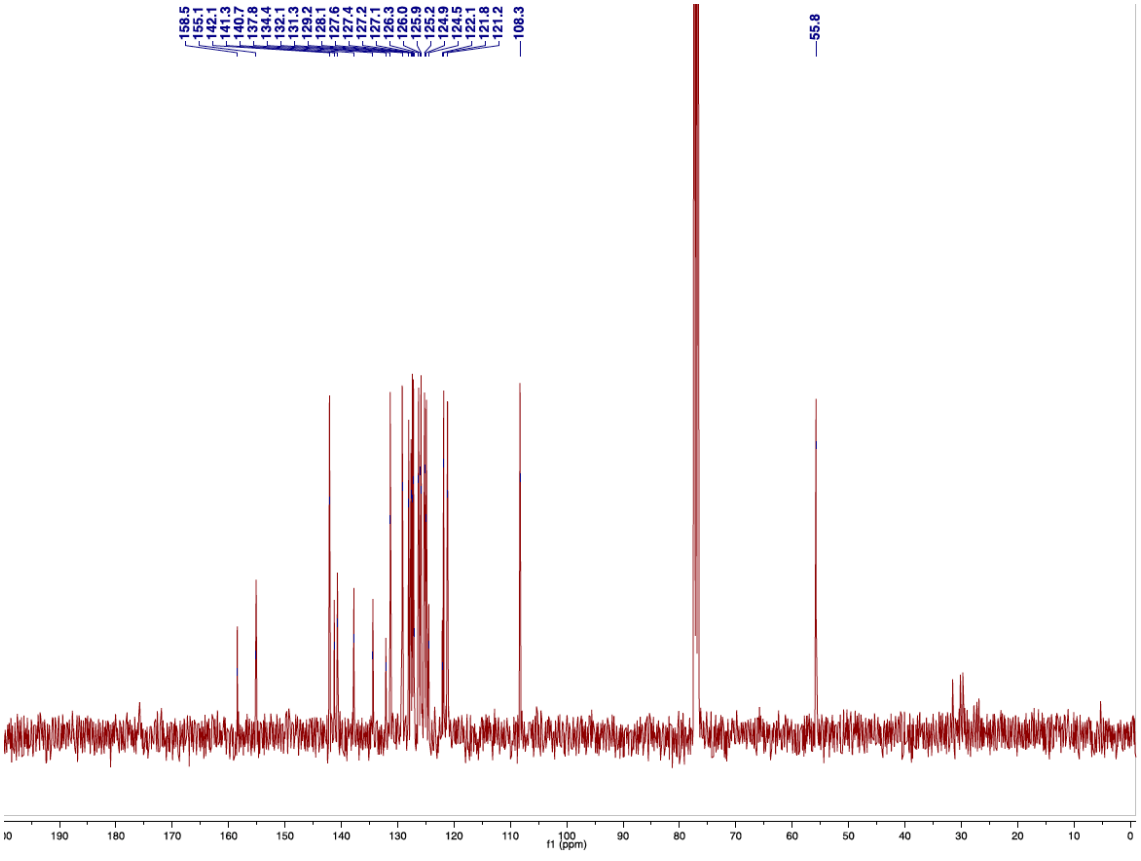


Figure S25. ^{13}C-NMR (100 MHz, $CDCl_3$, 298 K) for *rac*-**4b**.

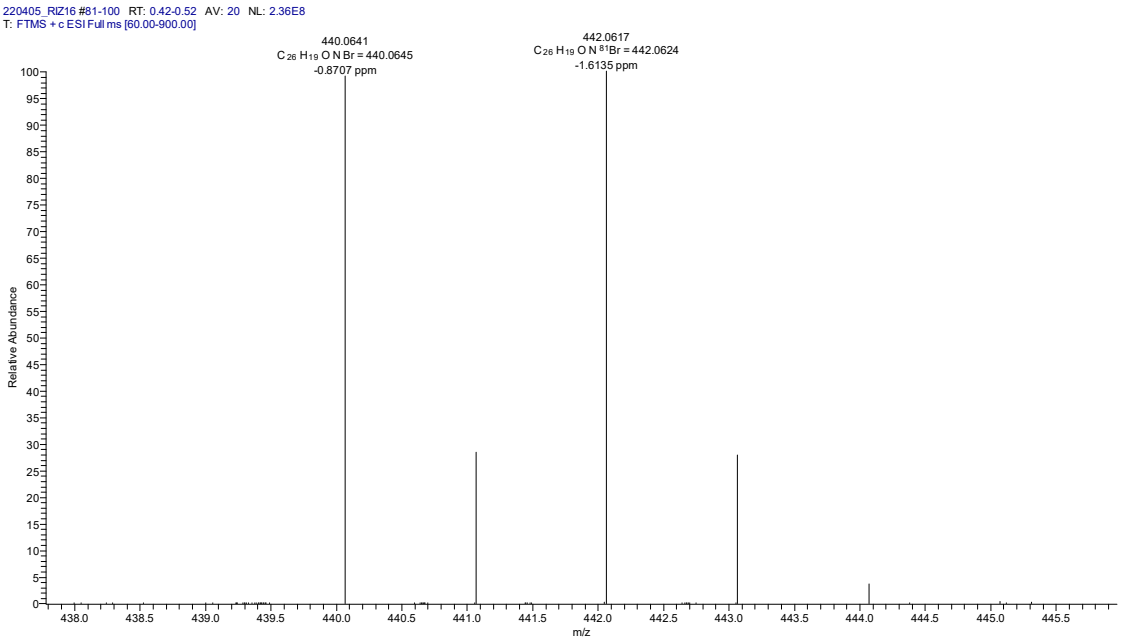


Figure S26. HRM-ESI for *rac*-**4b**.

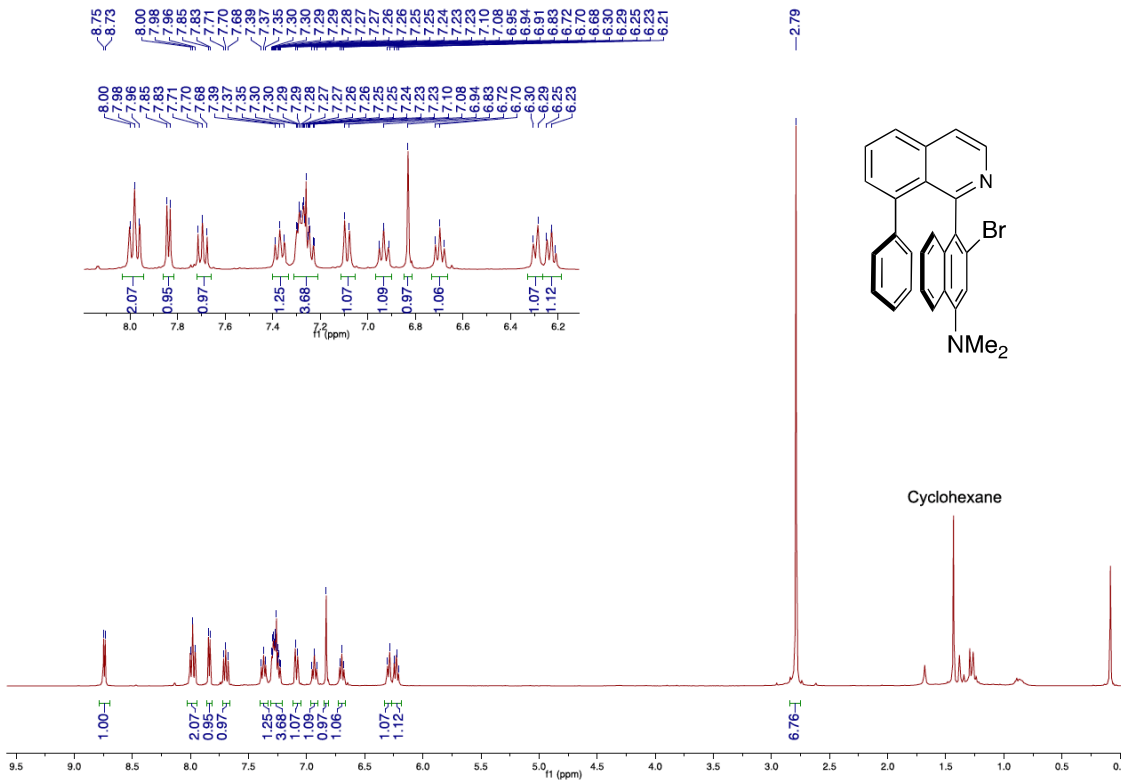


Figure S27. ^{1}H-NMR (400 MHz, $CDCl_3$, 298 K) for *rac*-**4c**.

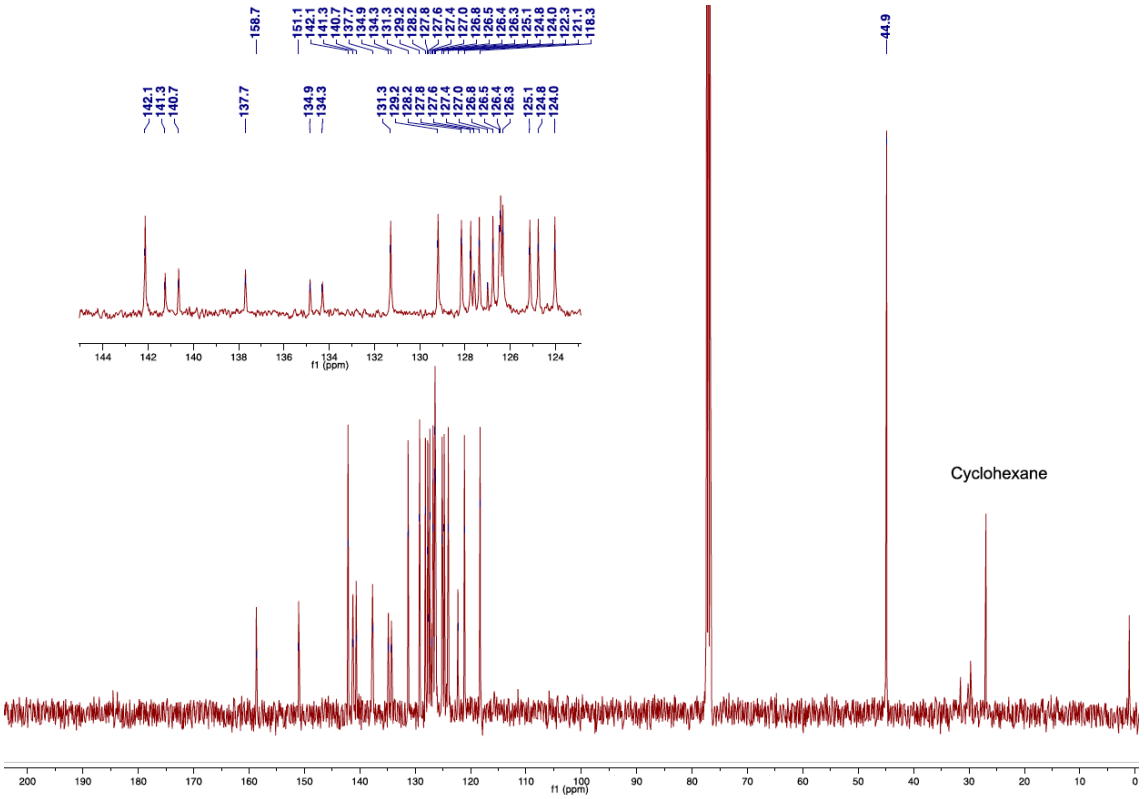


Figure S28. ^{13}C-NMR (100 MHz, $CDCl_3$, 298 K) for *rac*-**4c**.

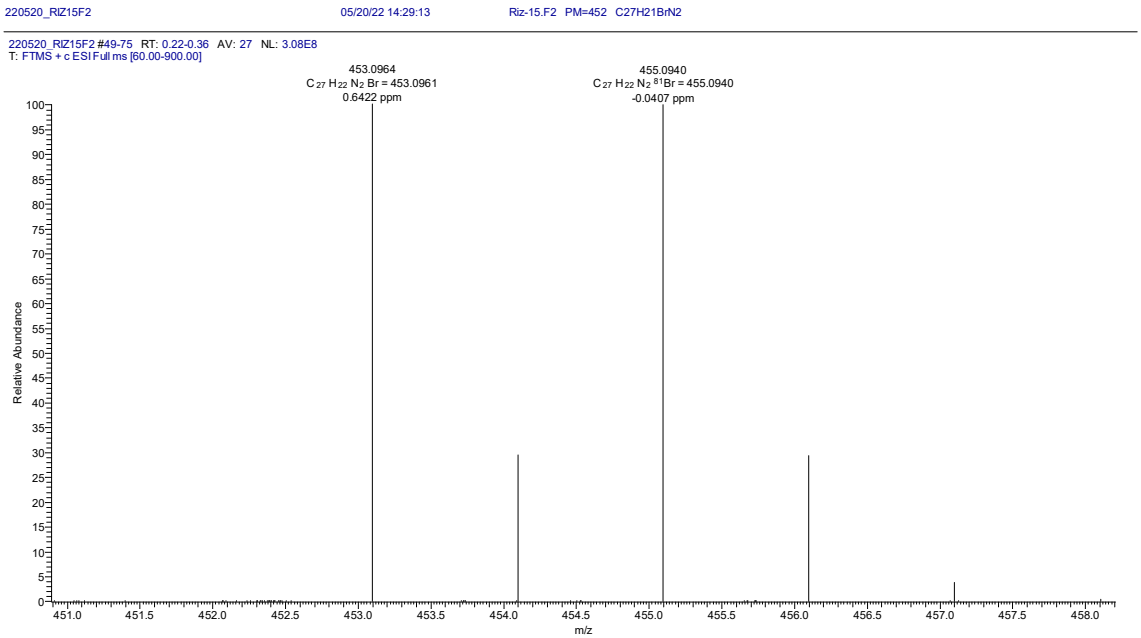


Figure S29. HRM-ESI for *rac*-**4c**.

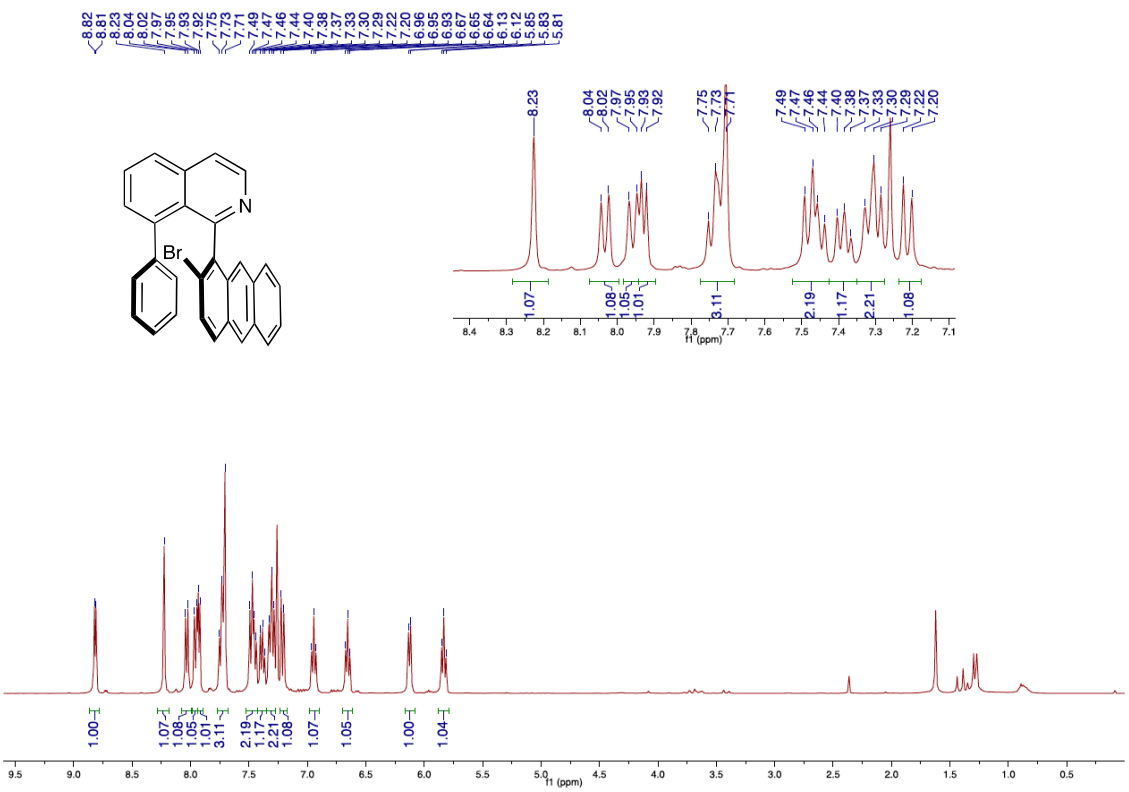


Figure S30. ^{1}H-NMR (400 MHz, $CDCl_3$, 298 K) for *rac*-**4d**.

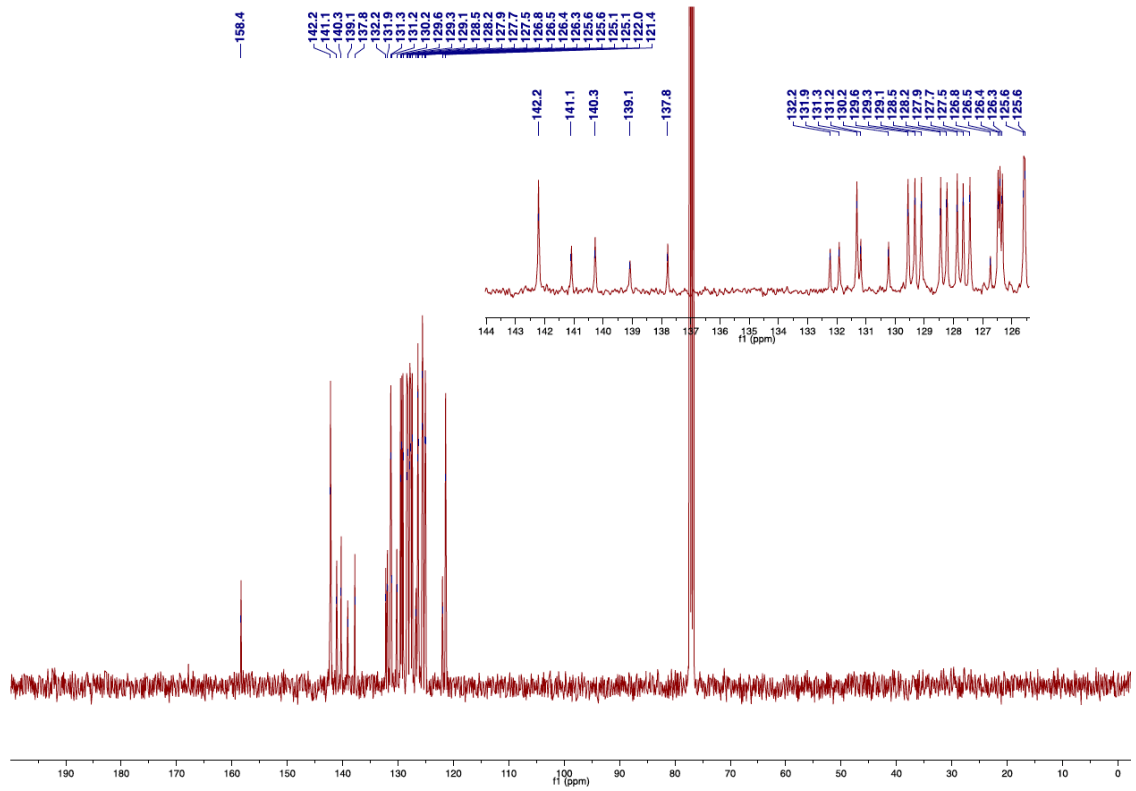


Figure S31. ^{13}C-NMR (100 MHz, $CDCl_3$, 298 K) for *rac*-**4d**.

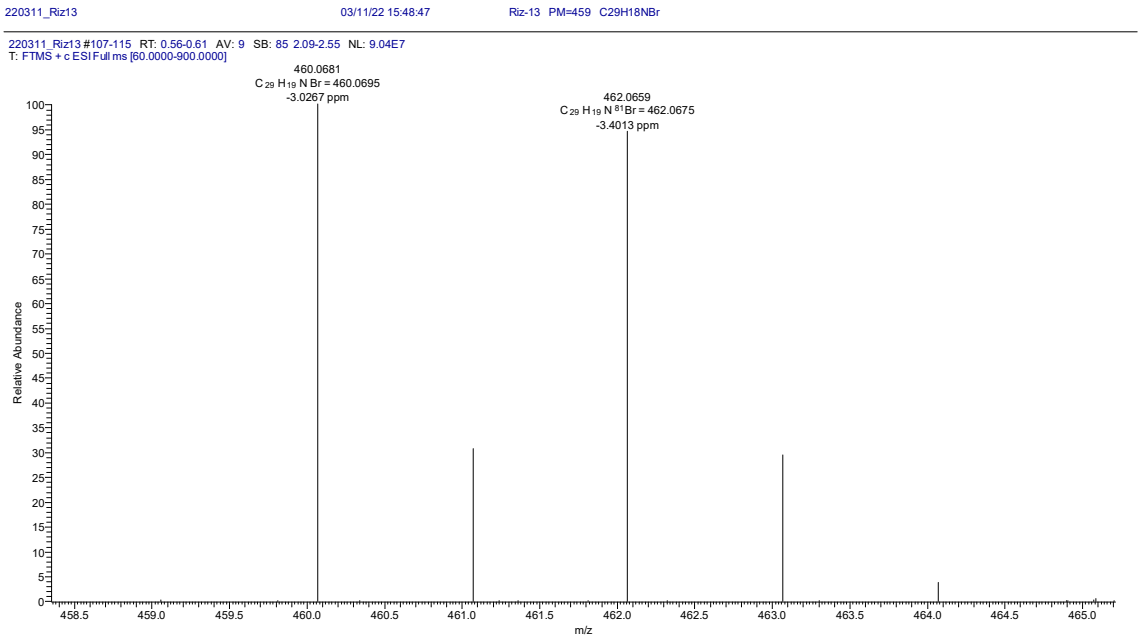


Figure S32. HRM-ESI for *rac*-**4d**.

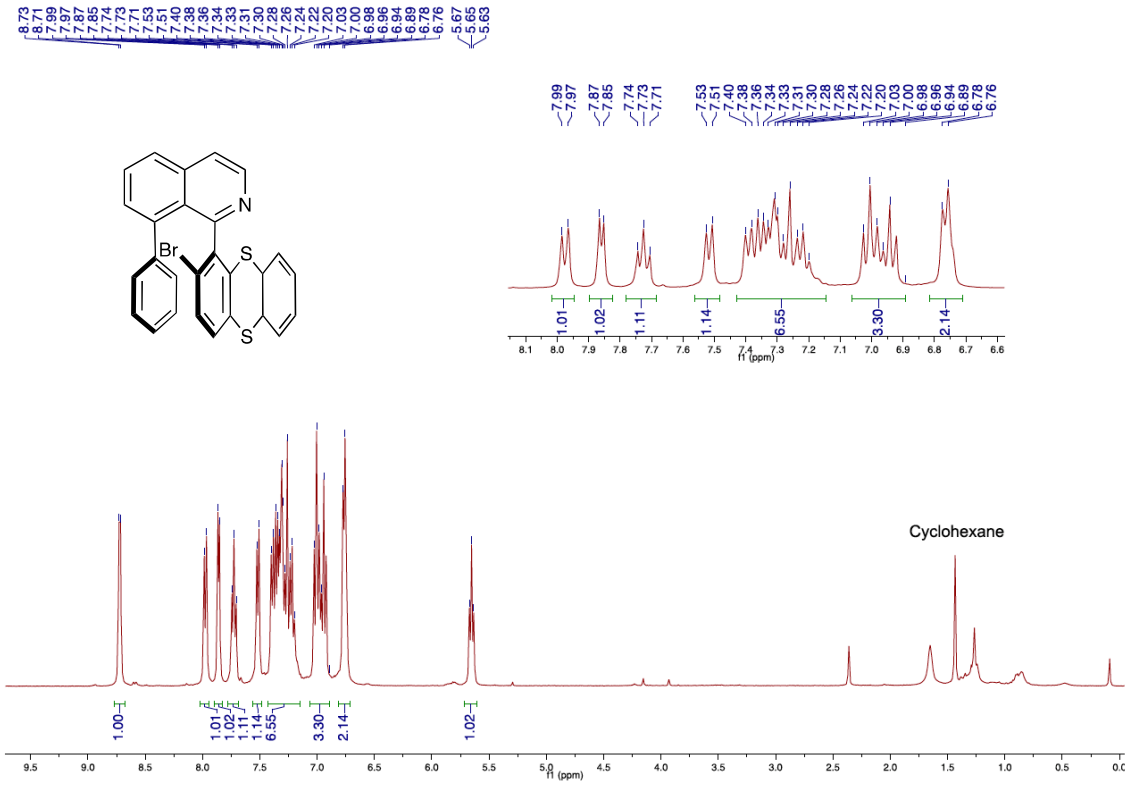


Figure S33. ^{1}H-NMR (400 MHz, $CDCl_3$, 298 K) for *rac*-**4e**.

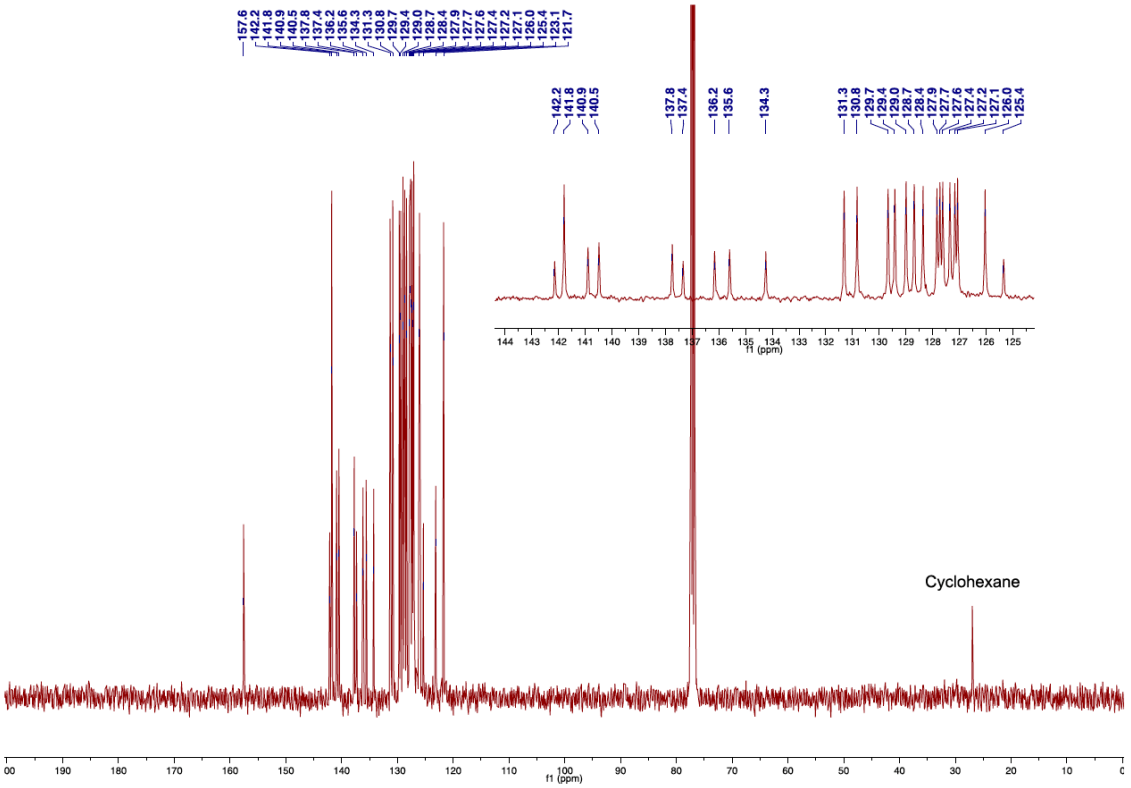


Figure S34. ^{13}C-NMR (100 MHz, $CDCl_3$, 298 K) for *rac*-**4e**.

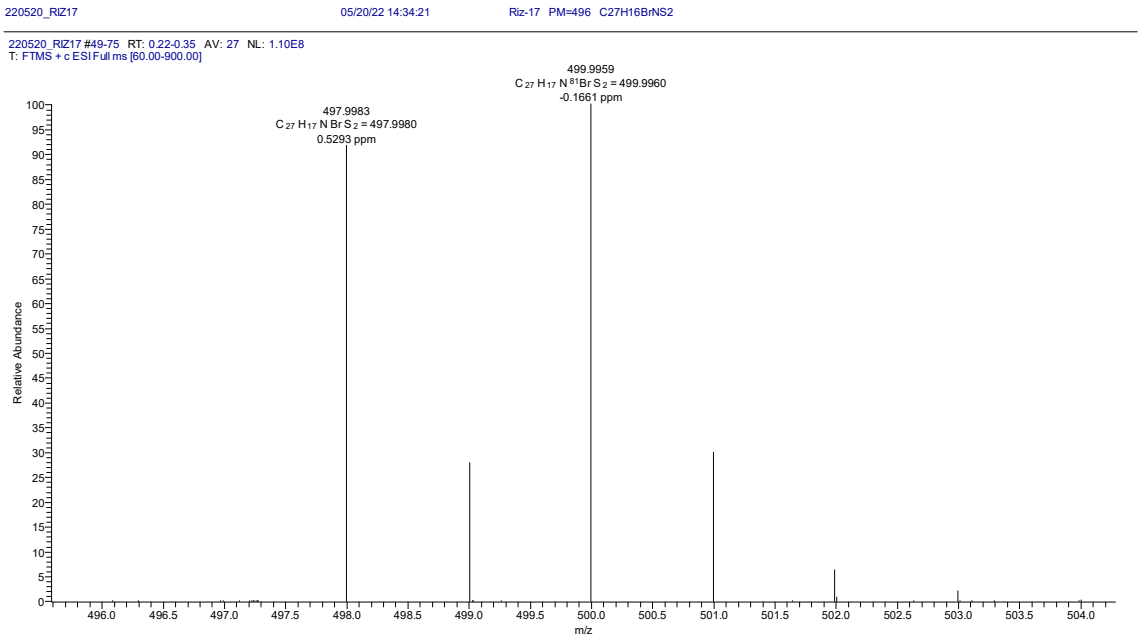


Figure S35. HRM-ESI for *rac*-**4e**.

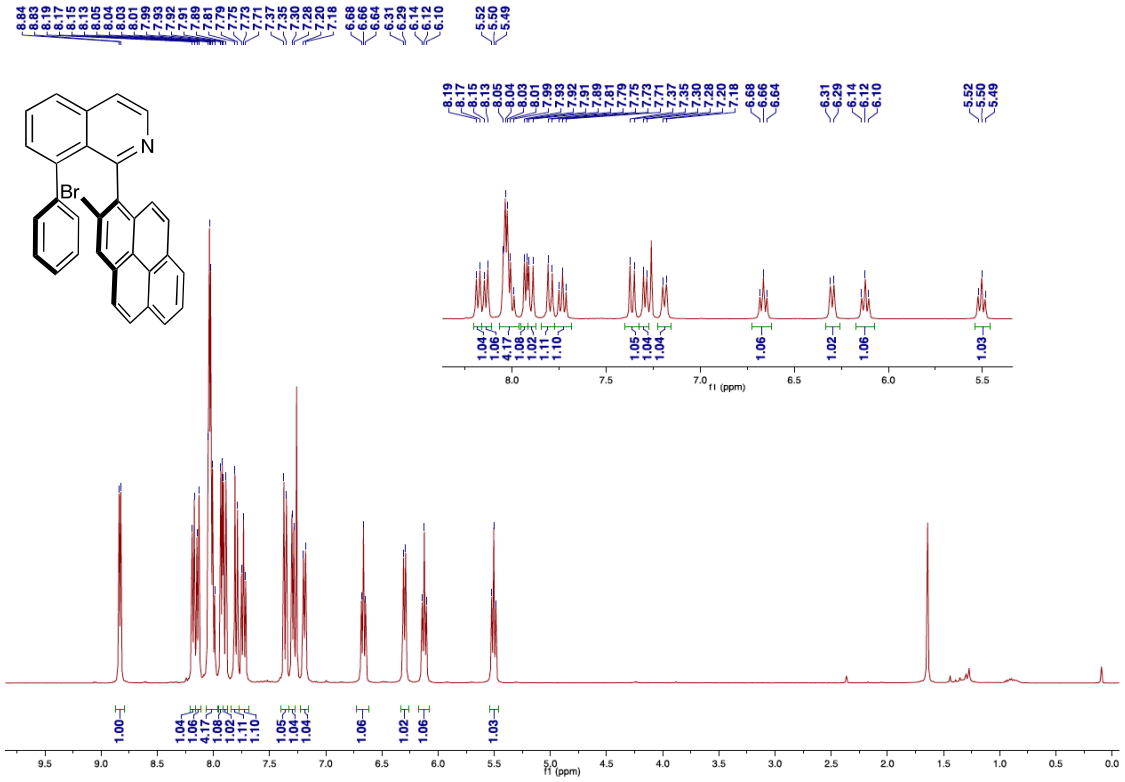


Figure S36. ^{1}H-NMR (400 MHz, $CDCl_3$, 298 K) for *rac*-**4f**.

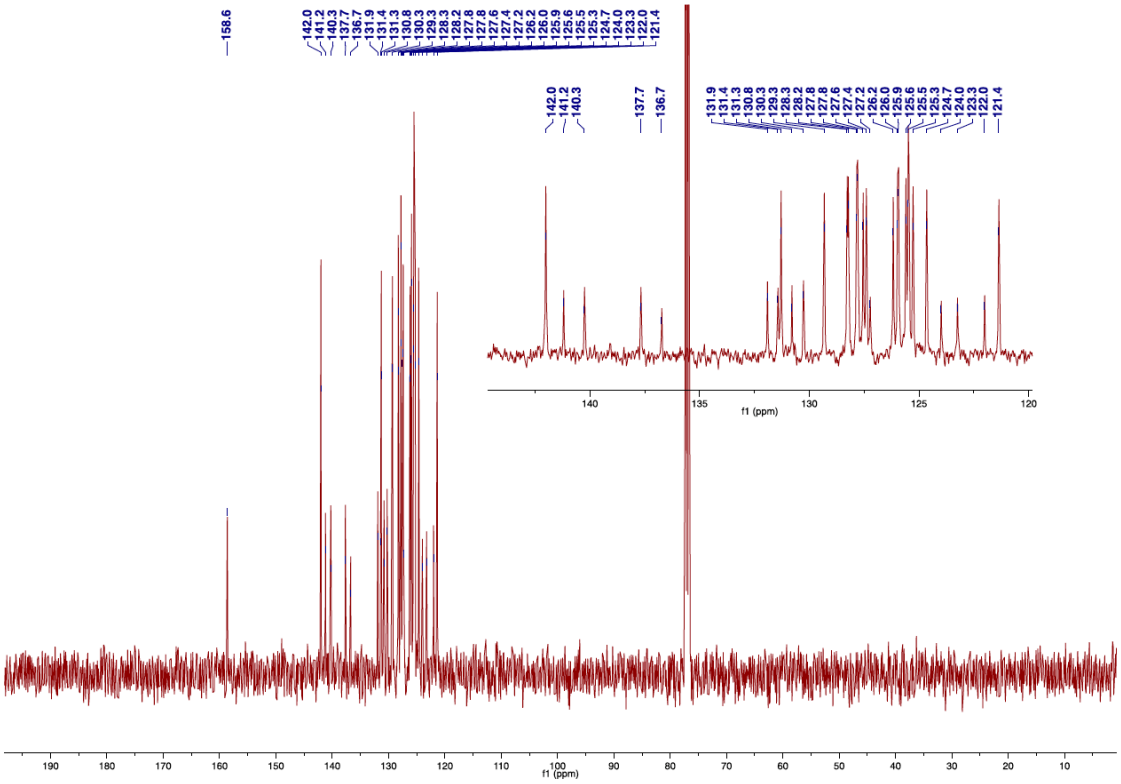


Figure S37. ^{13}C-NMR (100 MHz, $CDCl_3$, 298 K) for *rac*-**4f**.

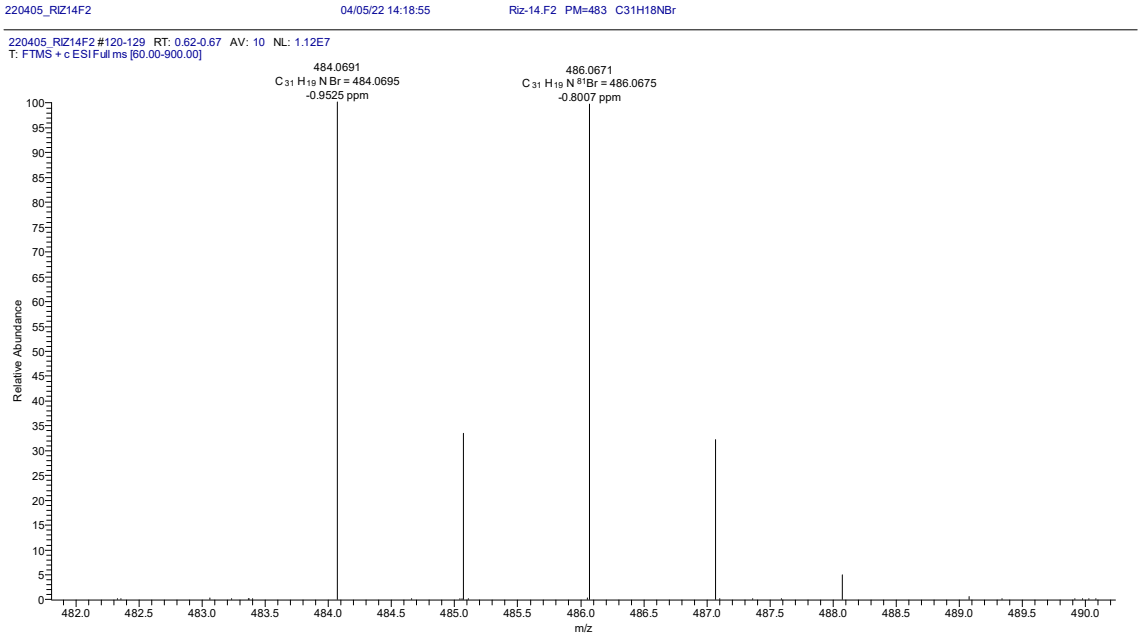


Figure S38. HRM-ESI for *rac*-**4f**.

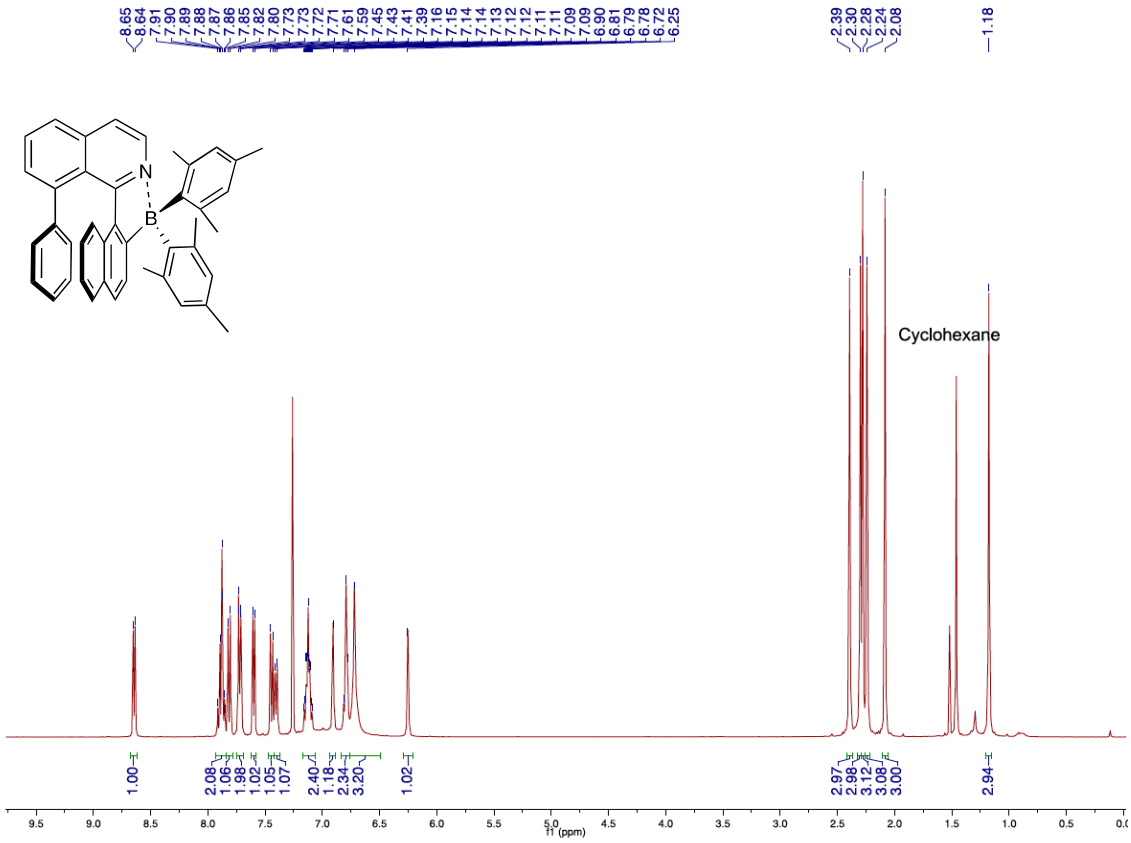


Figure S39. ^{1}H-NMR (400 MHz, $CDCl_3$, 298 K) for *rac*-**5a**.

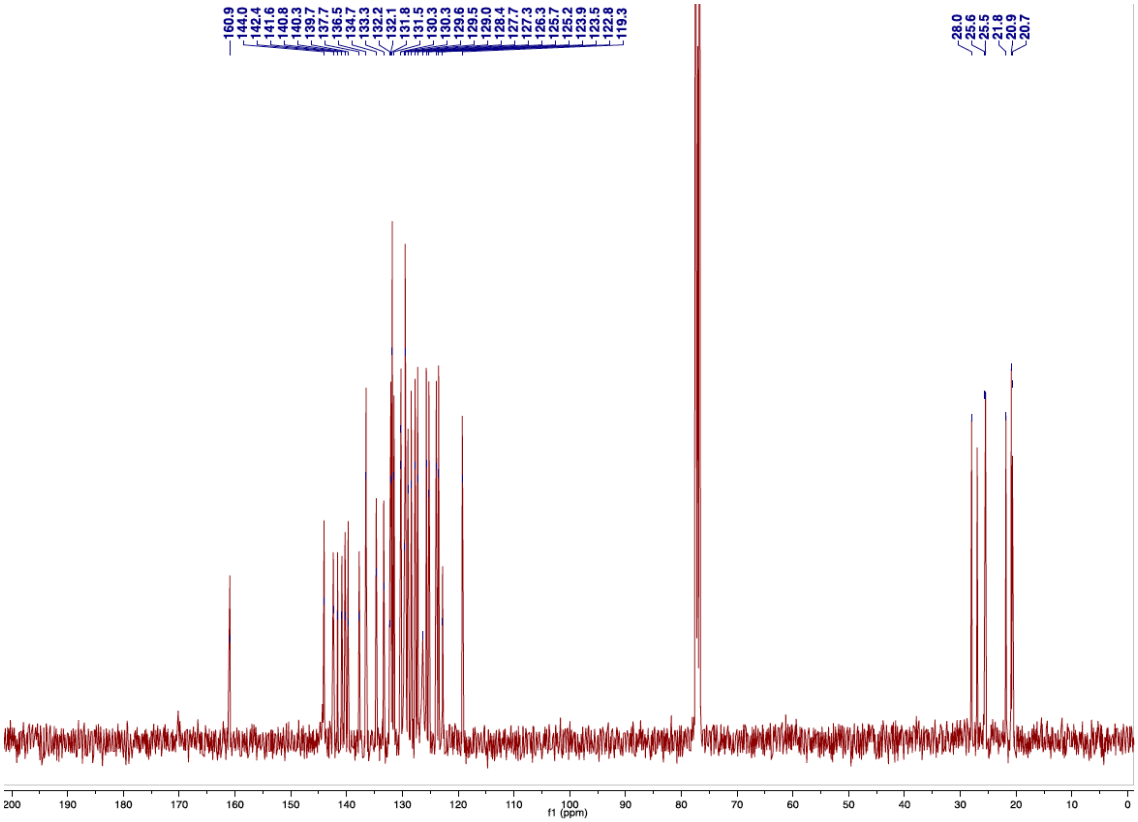


Figure S40. ^{13}C-NMR (100 MHz, $CDCl_3$, 298 K) for *rac*-**5a**.

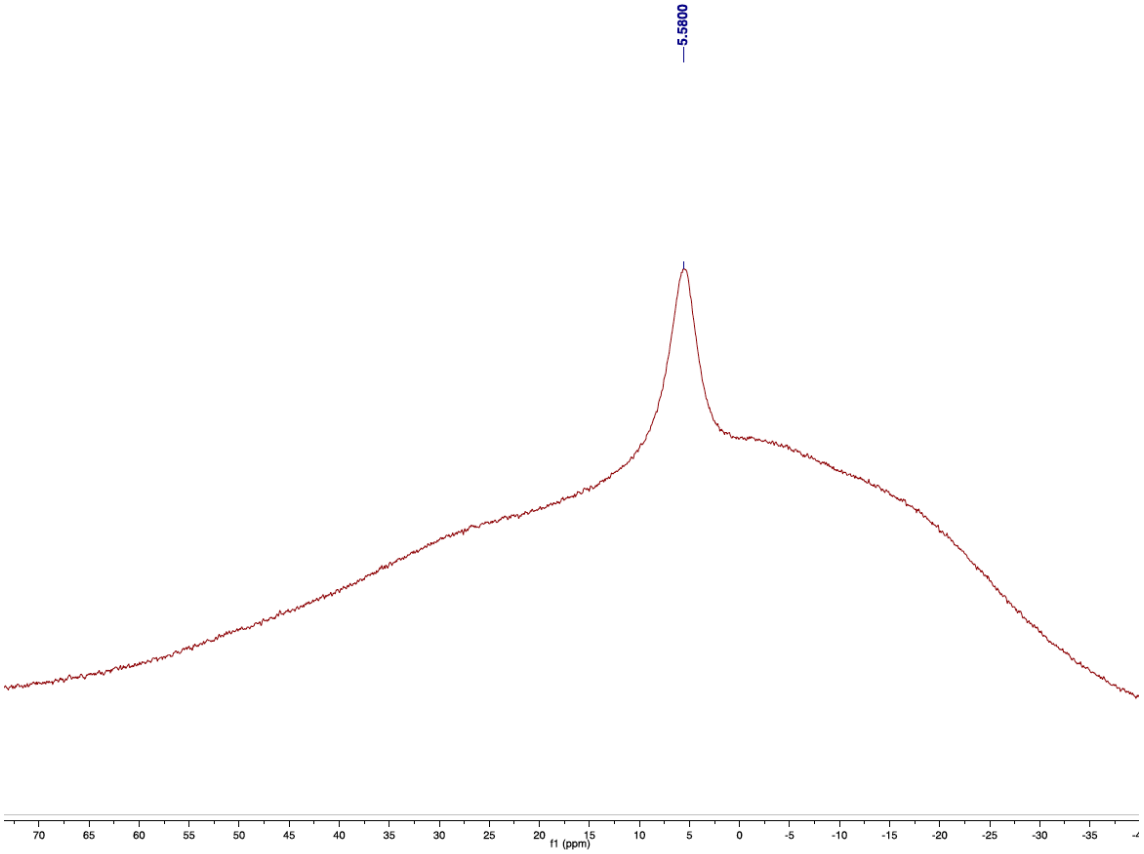


Figure S41. ^{11}B-NMR (128 MHz, $CDCl_3$, 298 K) for *rac*-**5a**.

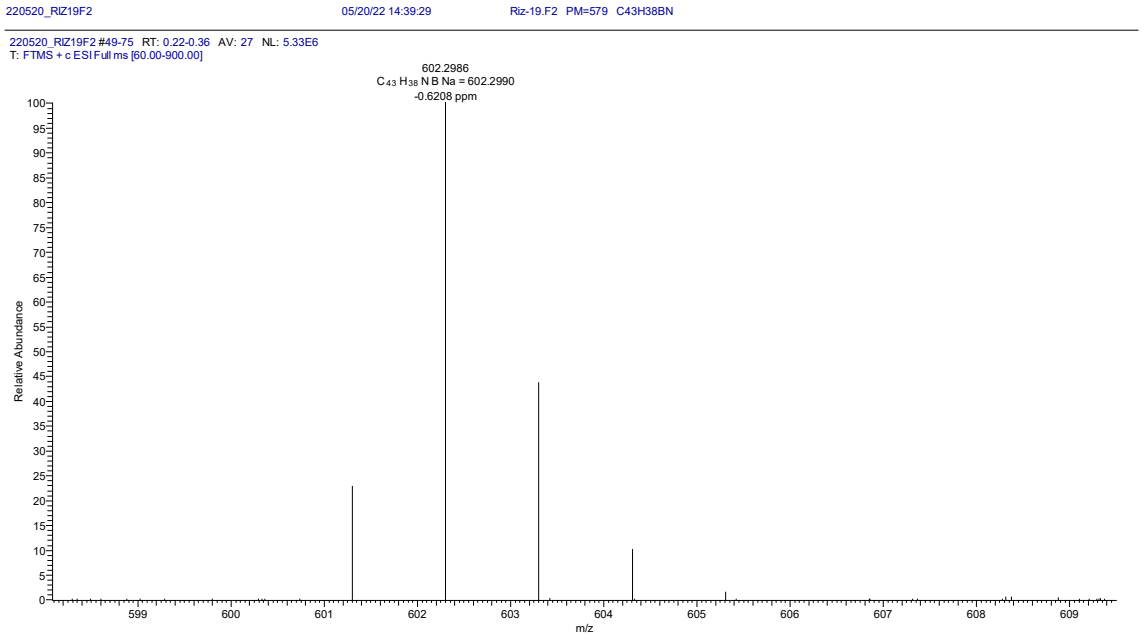


Figure S42. HRM-ESI for *rac*-**5a**.

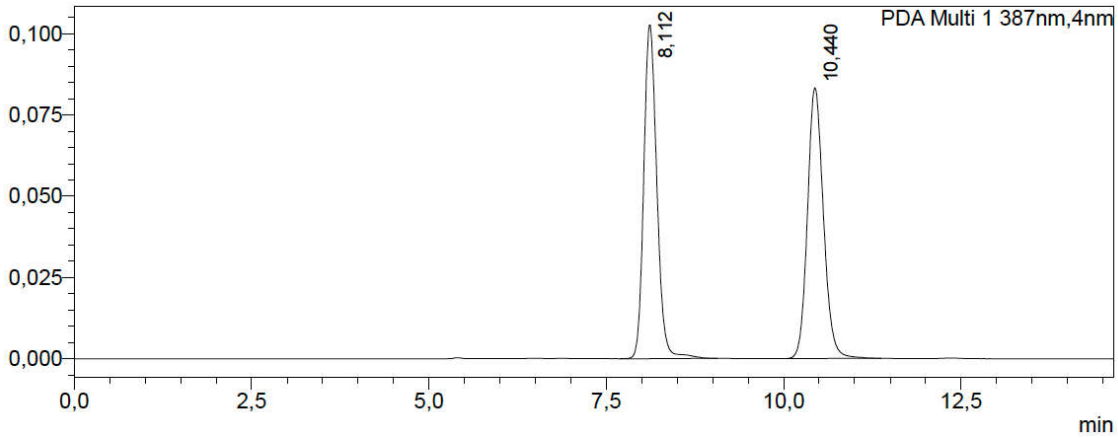


Figure S43. Chiral HPLC chromatogram for *rac*-**5a**: IA column, *n*-hexane:isopropanol 99:1, T = 303 K, F = 0.7 mL/min.

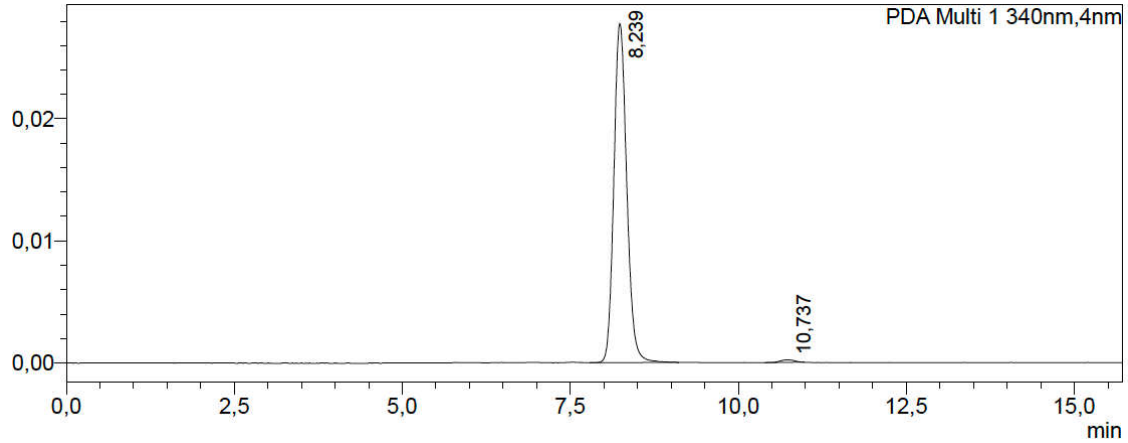


Figure S44. Chiral HPLC chromatogram for *M*-**5a**: er 99:1; *n*-hexane:isopropanol 99:1, T = 303 K, F = 0.7 mL/min.

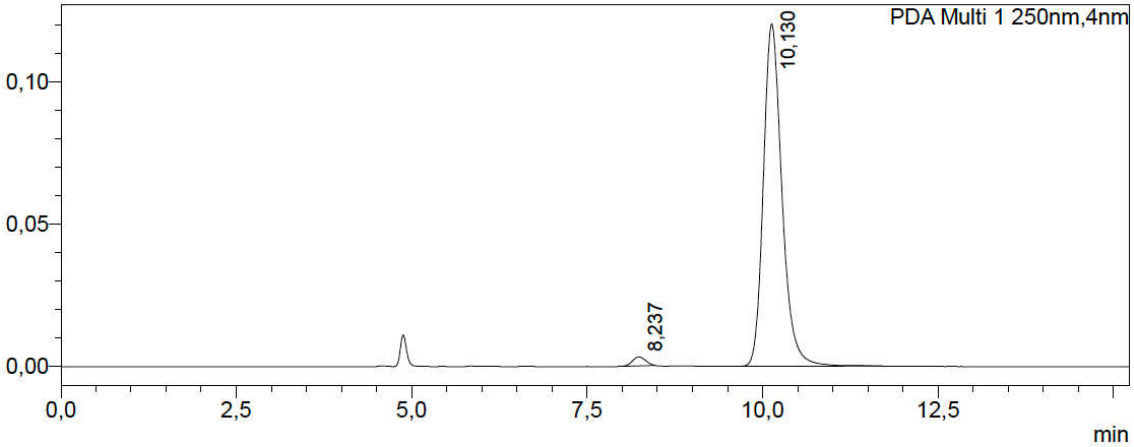


Figure S45. Chiral HPLC chromatogram for *P*-**5a:** er 2:98; *n*-hexane:isopropanol 99:1, T = 303 K, F = 0.7 mL/min.

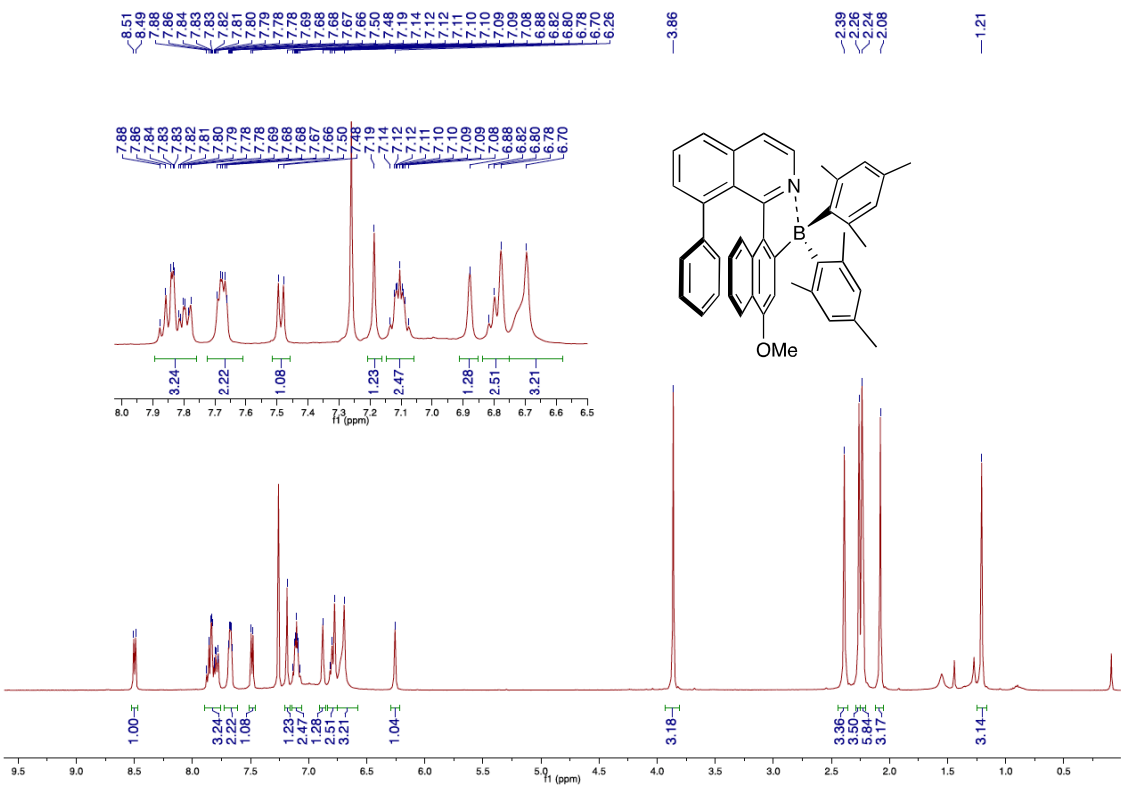


Figure S46. ^{1}H-NMR (400 MHz, $CDCl_3$, 298 K) for *rac*-**5b**.

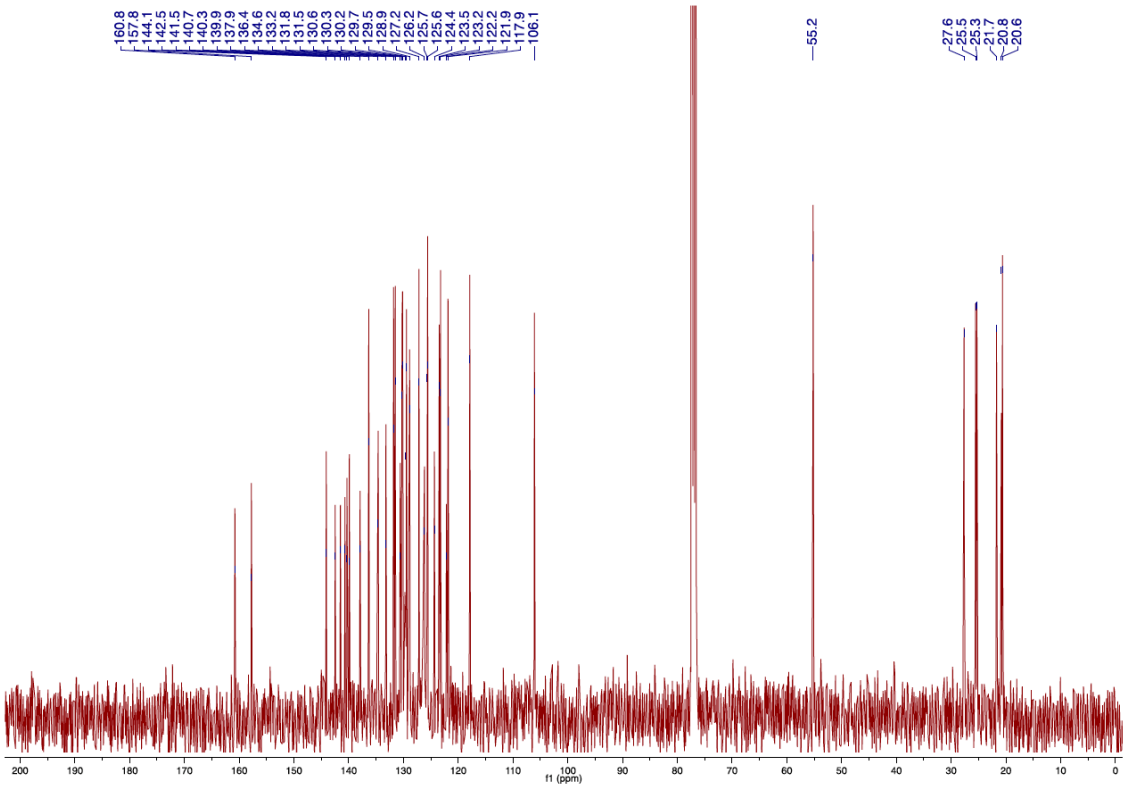


Figure S47. ^{13}C-NMR (100 MHz, $CDCl_3$, 298 K) for *rac*-**5b**.

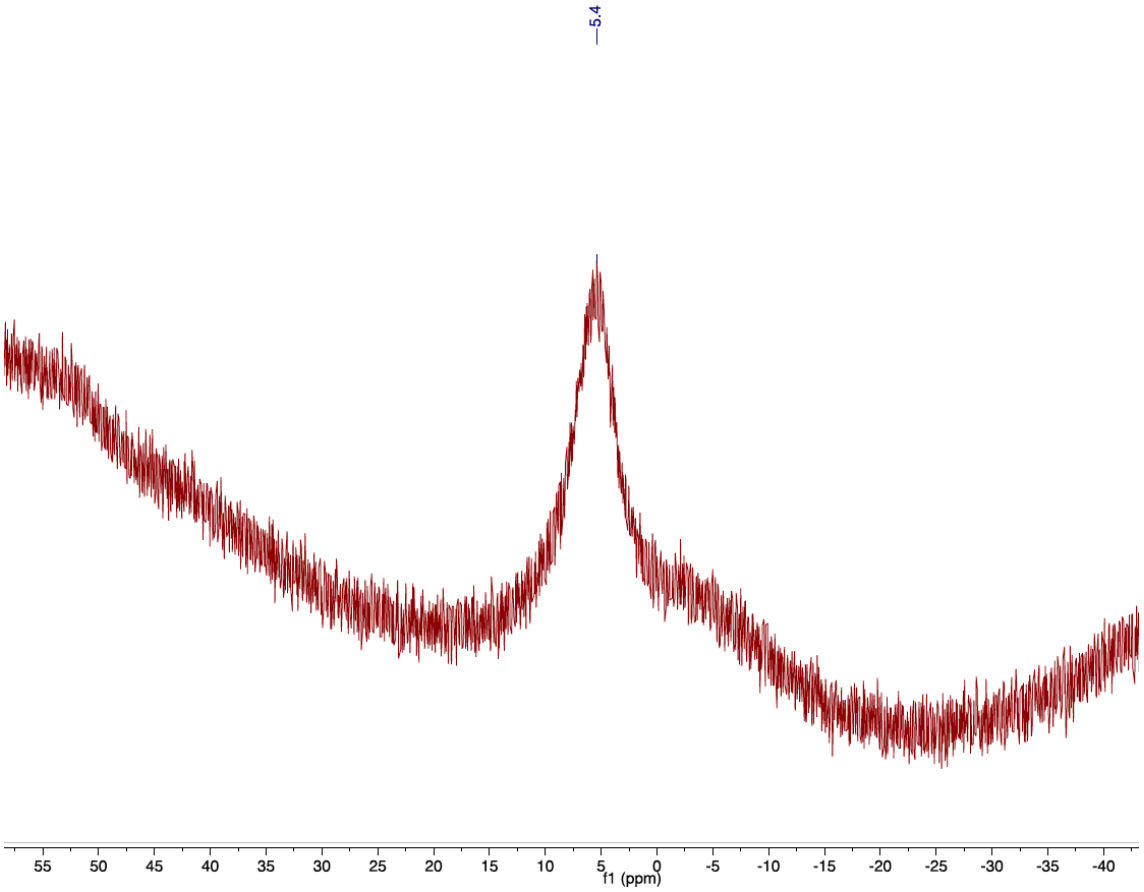


Figure S48. ^{11}B-NMR (128 MHz, $CDCl_3$, 298 K) for *rac*-**5b**.

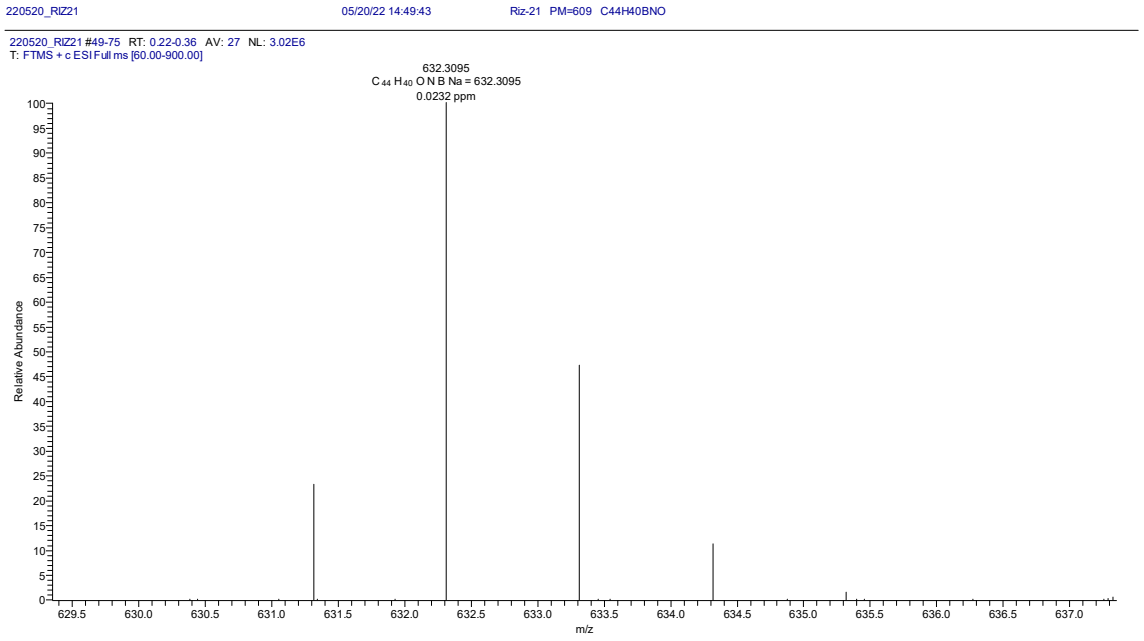


Figure S49. HRM-ESI for *rac*-**5b**.

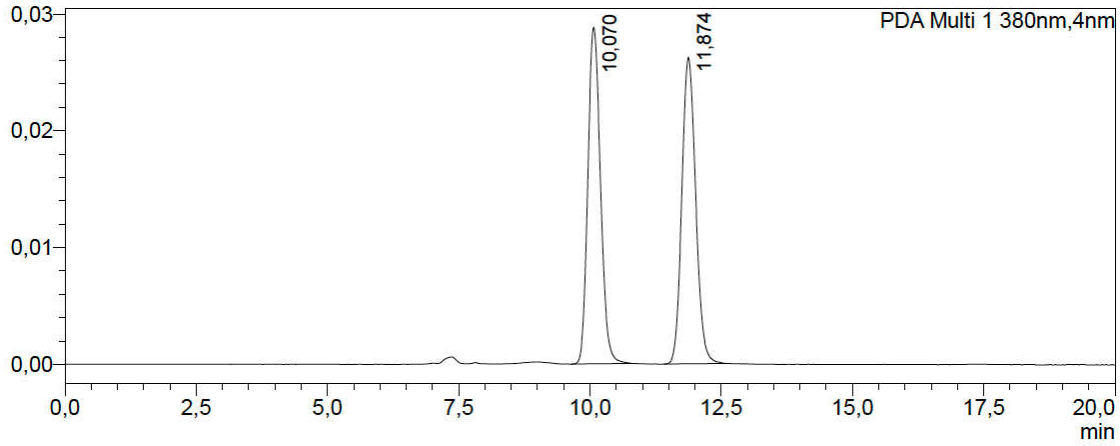


Figure S50. Chiral HPLC chromatogram for *rac*-**5b**: IA column, *n*-hexane:isopropanol 99:1, T = 303 K, F = 0.5 mL/min.

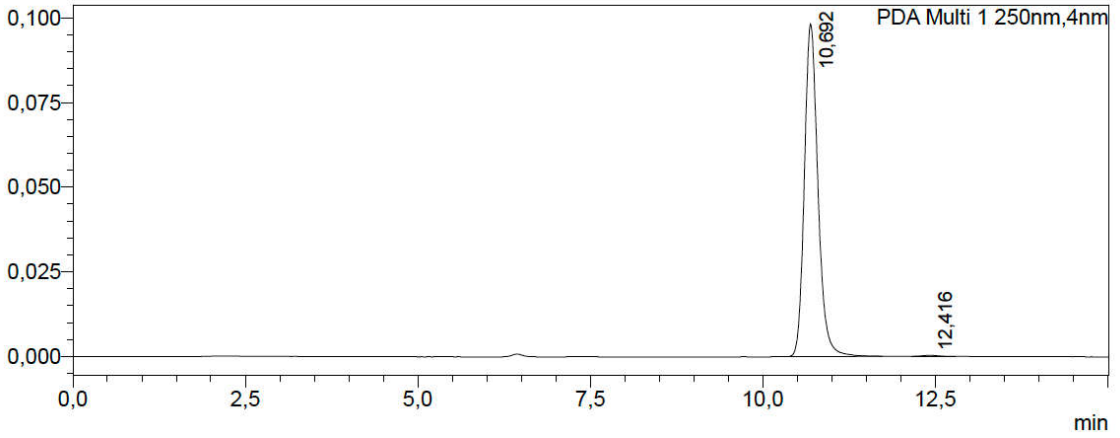


Figure S51. Chiral HPLC chromatogram for *M*-**5b**: er >99:1; IA column, *n*-hexane:isopropanol 99:1, T = 303 K, F = 0.5 mL/min.

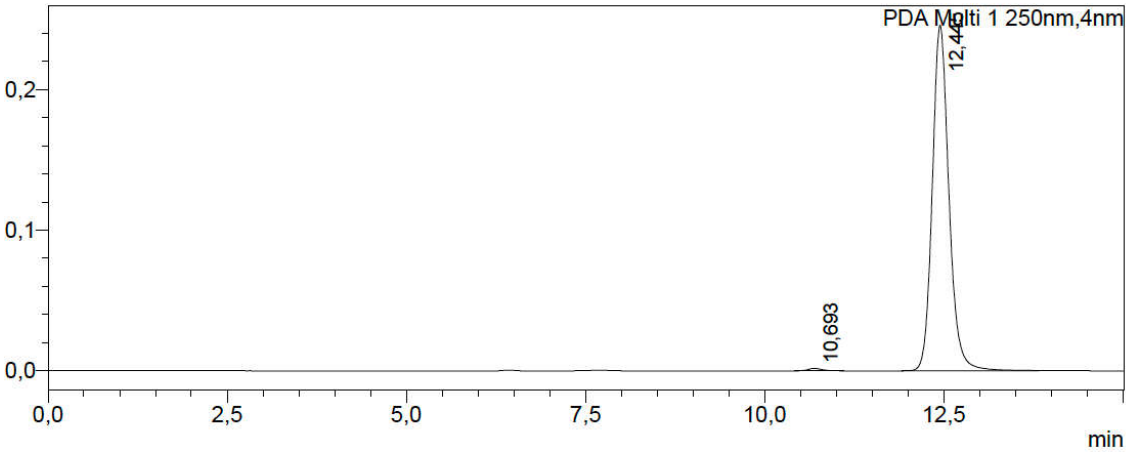


Figure S52. Chiral HPLC chromatogram for *P*-**5b**: er >1:99; IA column, *n*-hexane:isopropanol 99:1, T = 303 K, F = 0.5 mL/min.

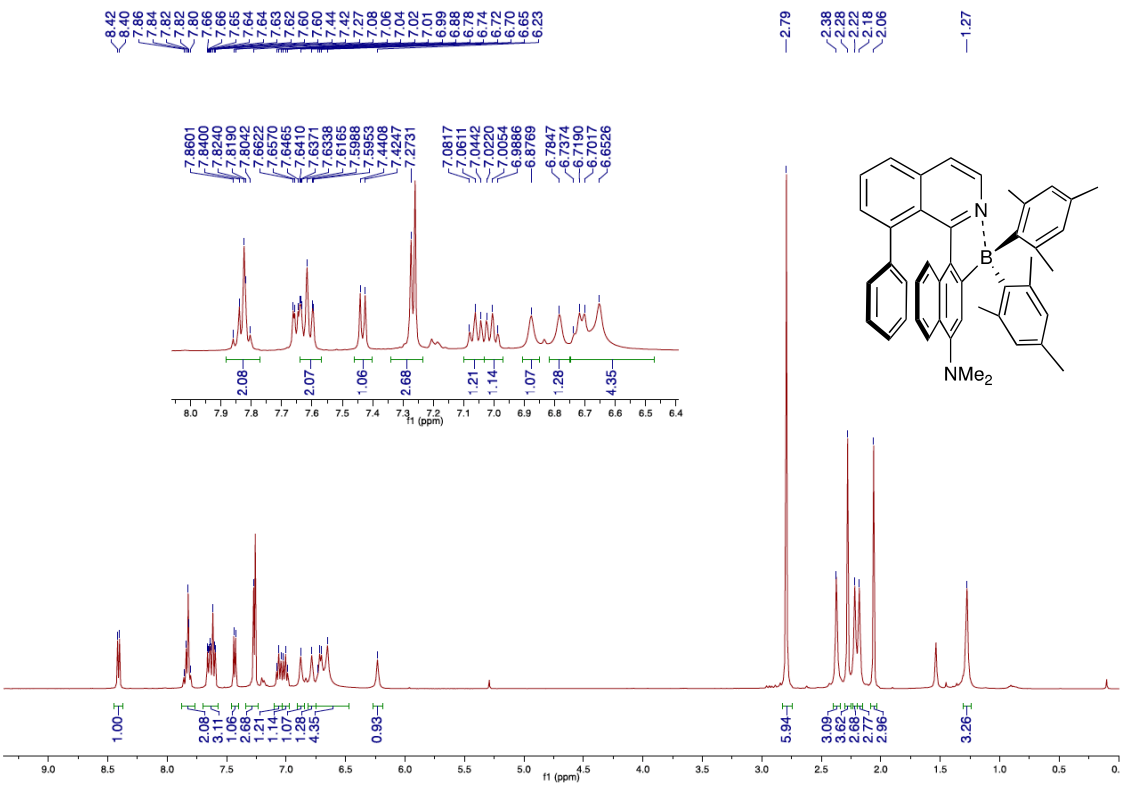


Figure S53. ^{1}H-NMR (400 MHz, $CDCl_3$, 298 K) for *rac*-**5c**.

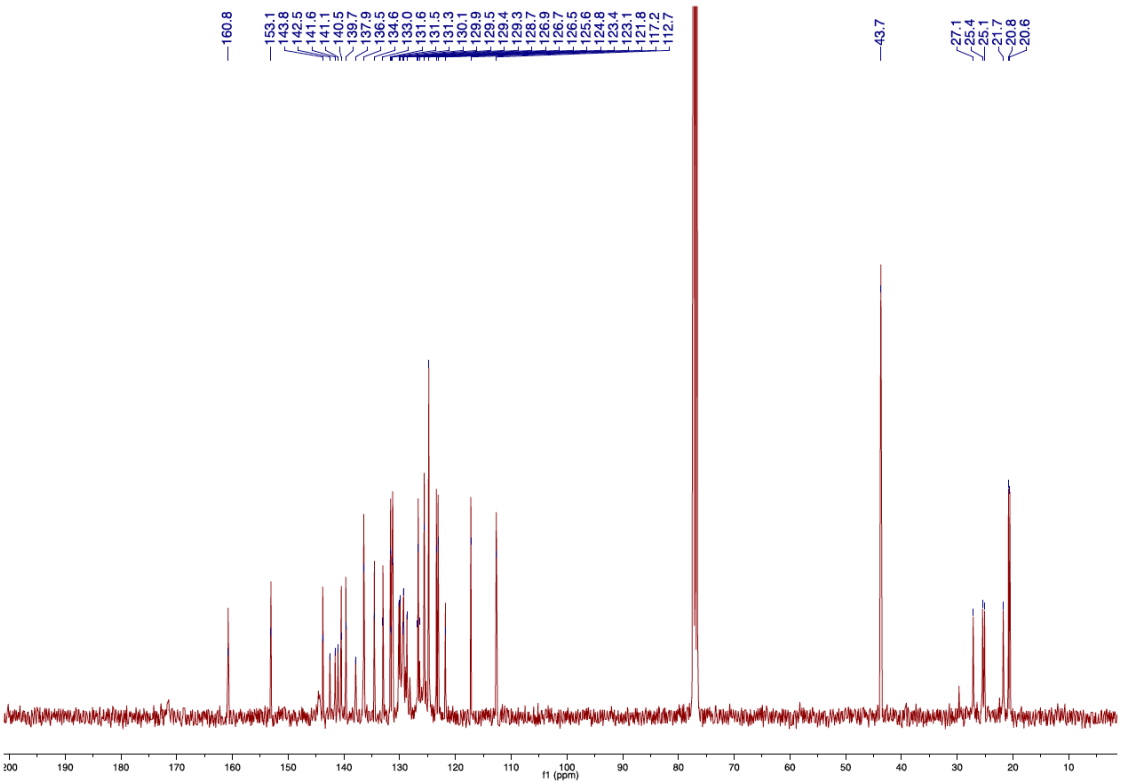


Figure S54. ^{13}C-NMR (100 MHz, $CDCl_3$, 298 K) for *rac*-**5c**.

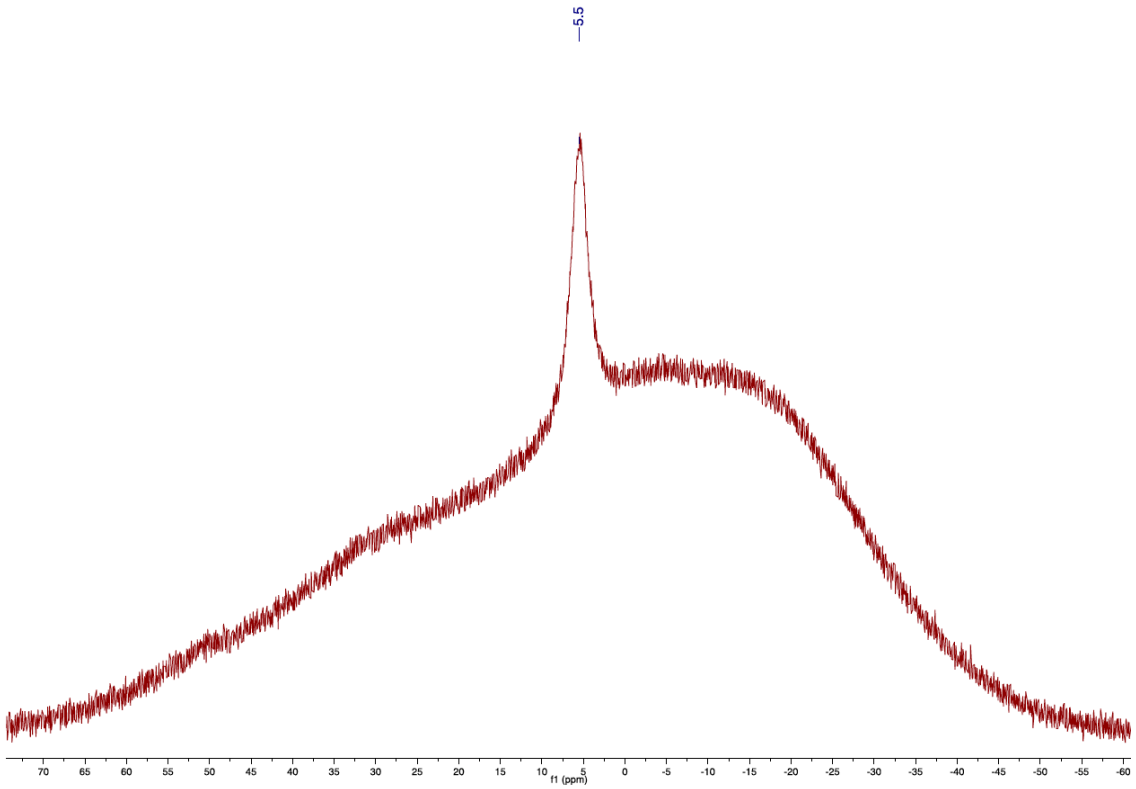


Figure S55. ^{11}B-NMR (128 MHz, $CDCl_3$, 298 K) for *rac*-**5c**.

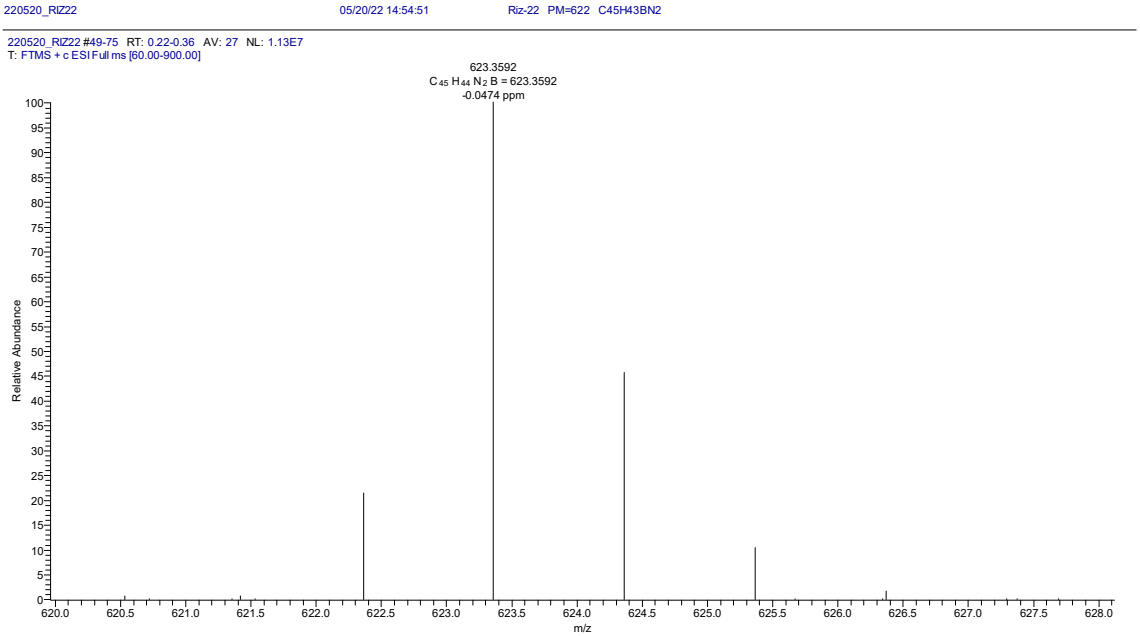


Figure S56. HRM-ESI for *rac*-**5c**.

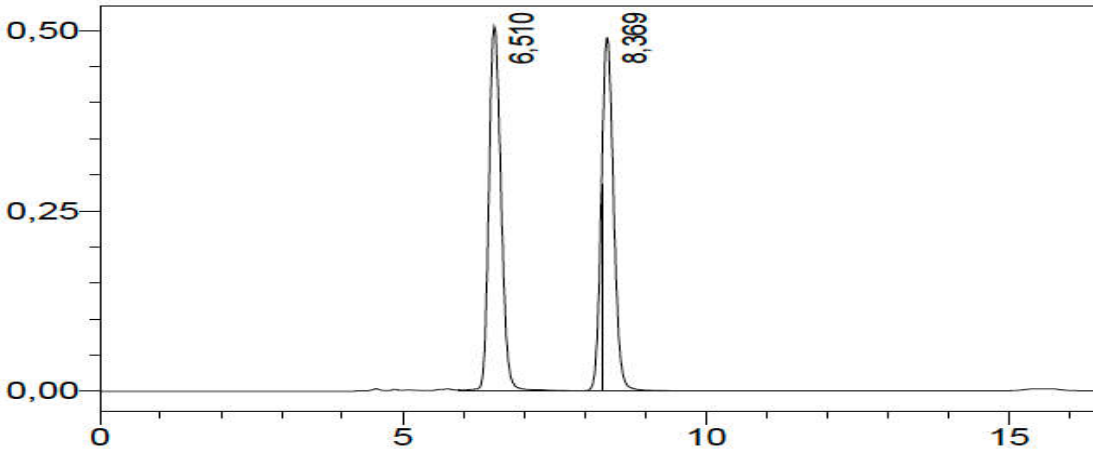


Figure S57. Chiral HPLC chromatogram for *rac*-**5c**: IA column, *n*-hexane:isopropanol 99:1, T = 303 K, F = 0.7 mL/min.

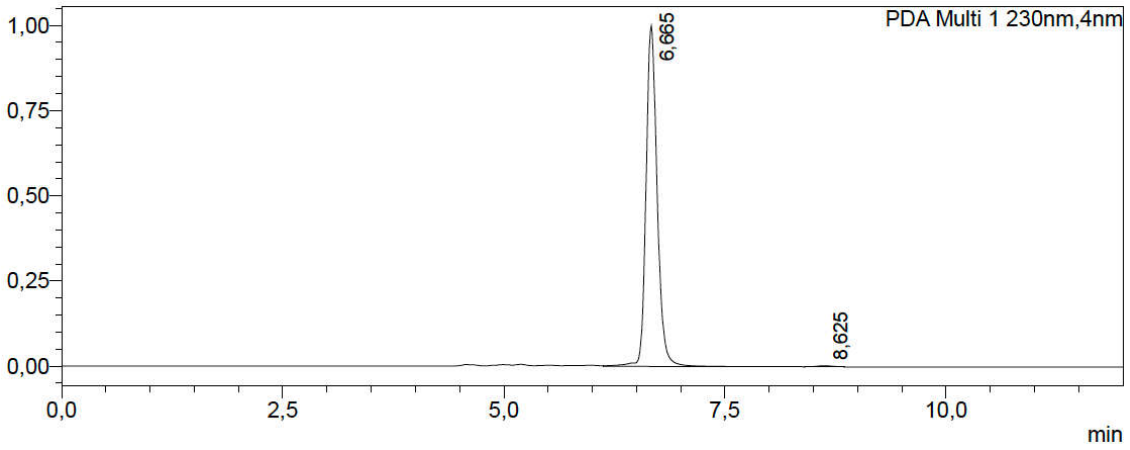


Figure S58. Chiral HPLC chromatogram for *M*-**5c**: er >99:1; IA column, *n*-hexane:isopropanol 99:1, T = 303 K, F = 0.7 mL/min.

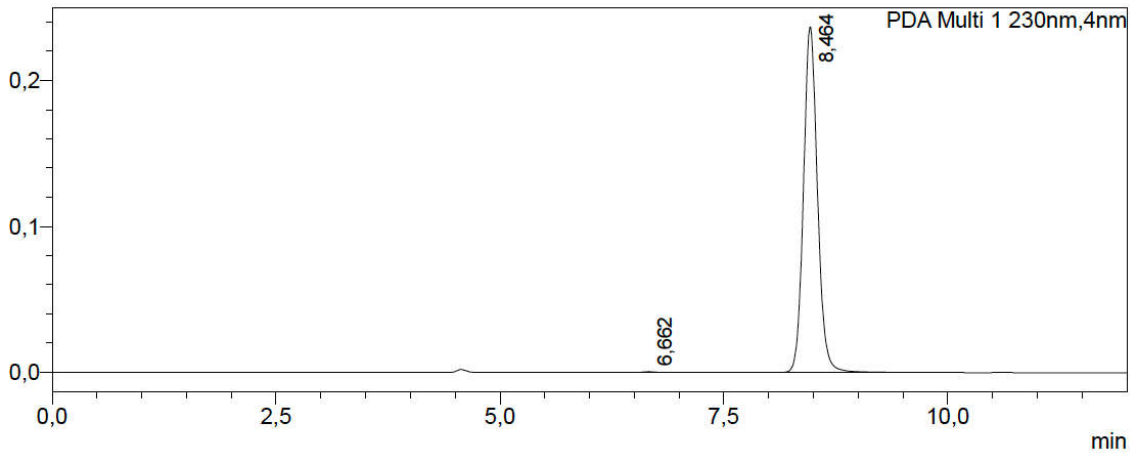


Figure S59. Chiral HPLC chromatogram *P*-**5c**: er >1:99; IA column, *n*-hexane:isopropanol 99:1, T = 303 K, F = 0.7 mL/min.

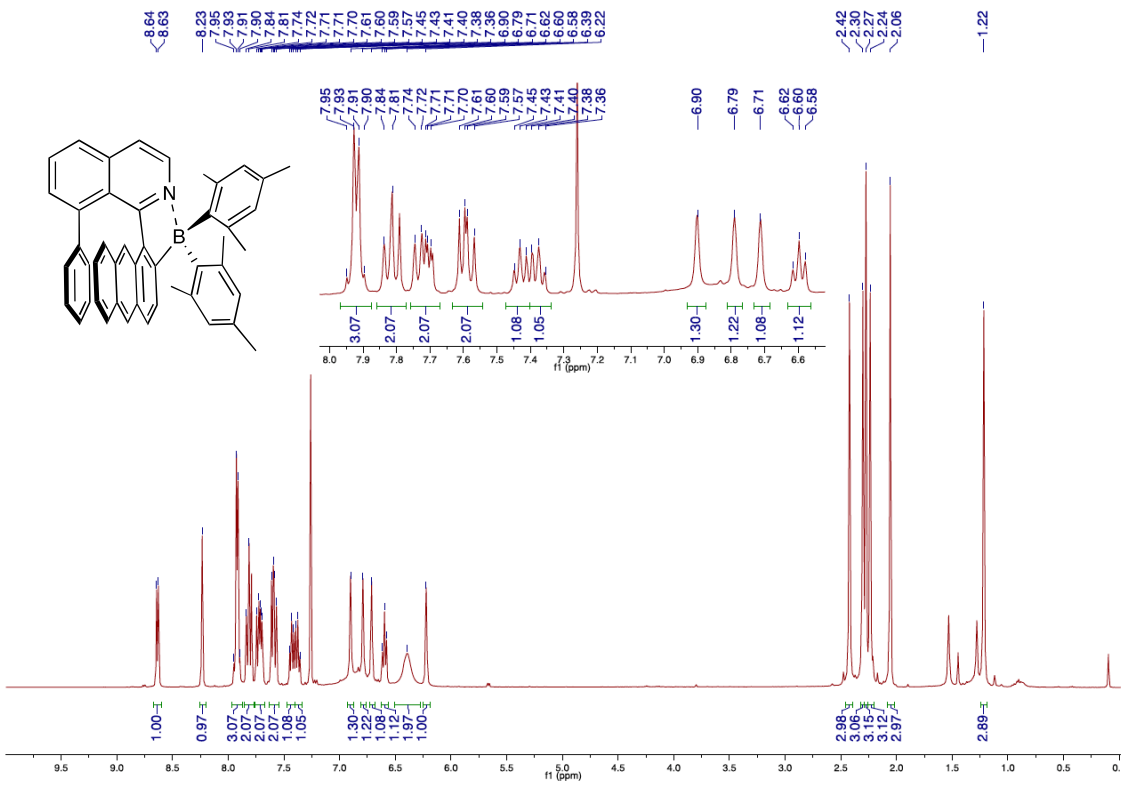


Figure S60. ^{1}H-NMR (400 MHz, $CDCl_3$, 298 K) for *rac*-**5d**.

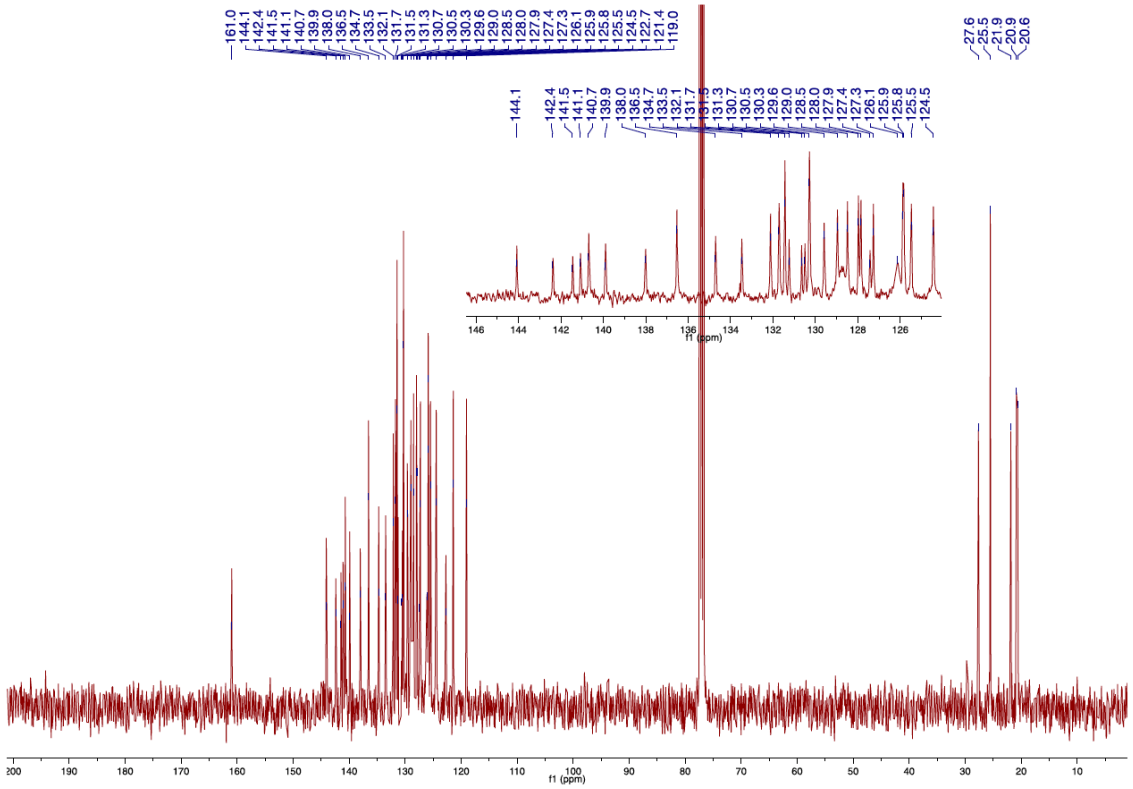


Figure S61. ^{13}C-NMR (100 MHz, $CDCl_3$, 298 K) for *rac*-**5d**.

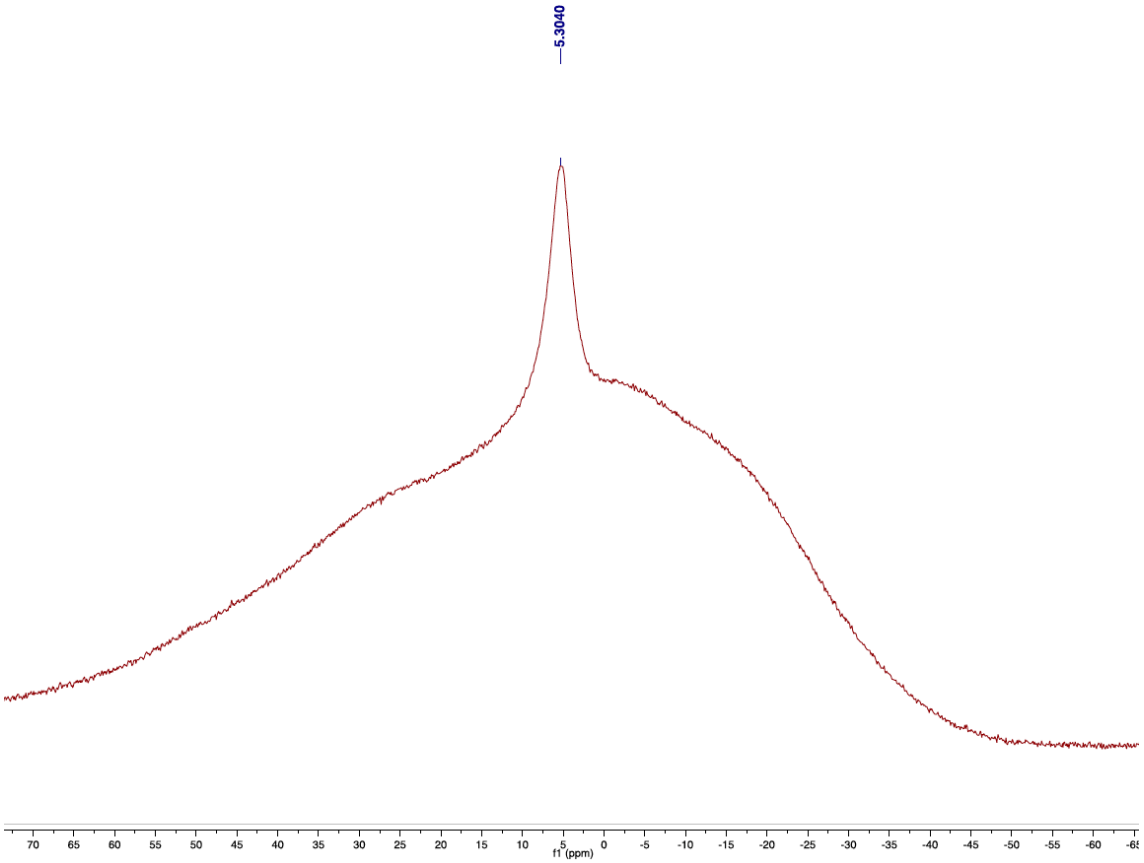


Figure S62. ^{11}B-NMR (128 MHz, $CDCl_3$, 298 K) for *rac*-**5d**.

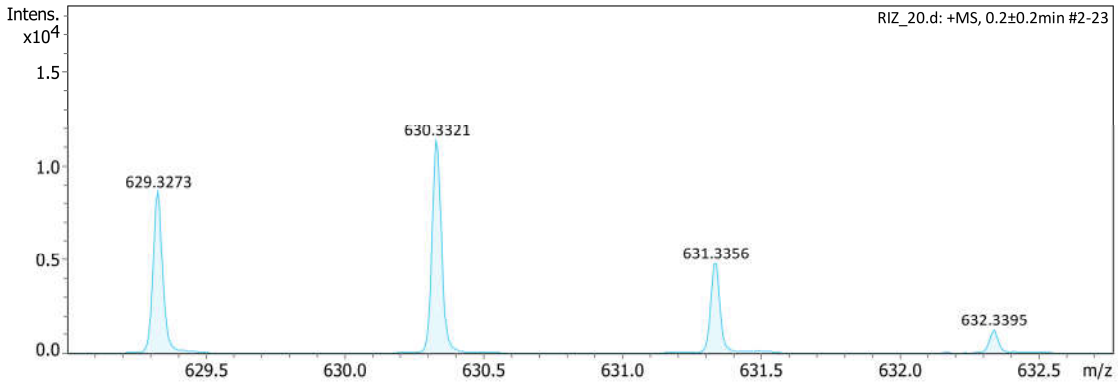


Figure S63. HRM-ESI for *rac*-**5d**.

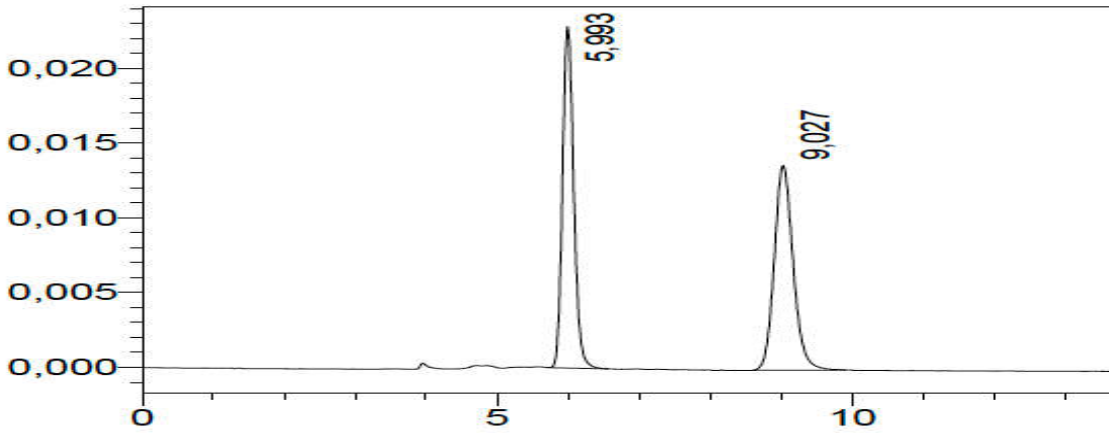


Figure S64. Chiral HPLC chromatogram for *rac*-**5d**: IA column, *n*-hexane:isopropanol 99:1, T = 303 K, F = 1.0 mL/min.

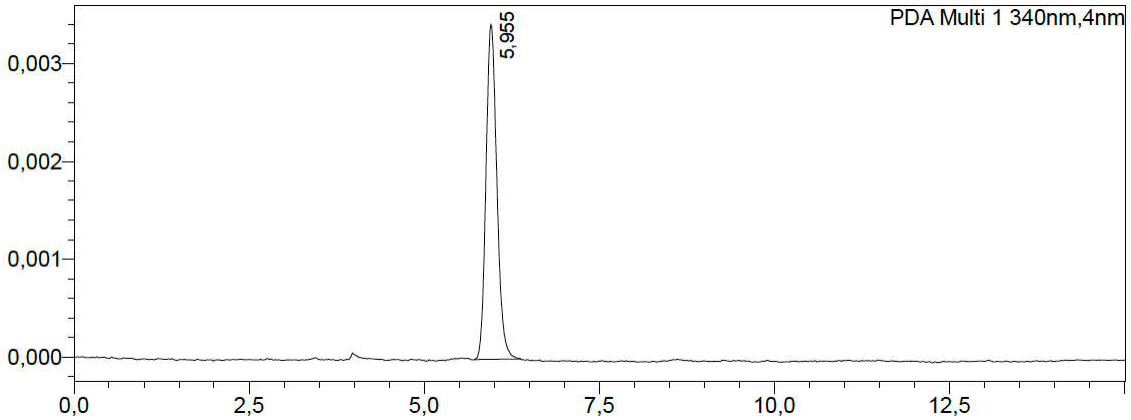


Figure S65. Chiral HPLC chromatogram for *M*-**5d**: er >99:1; IA column, *n*-hexane:isopropanol 99:1, T = 303 K, F = 1.0 mL/min.

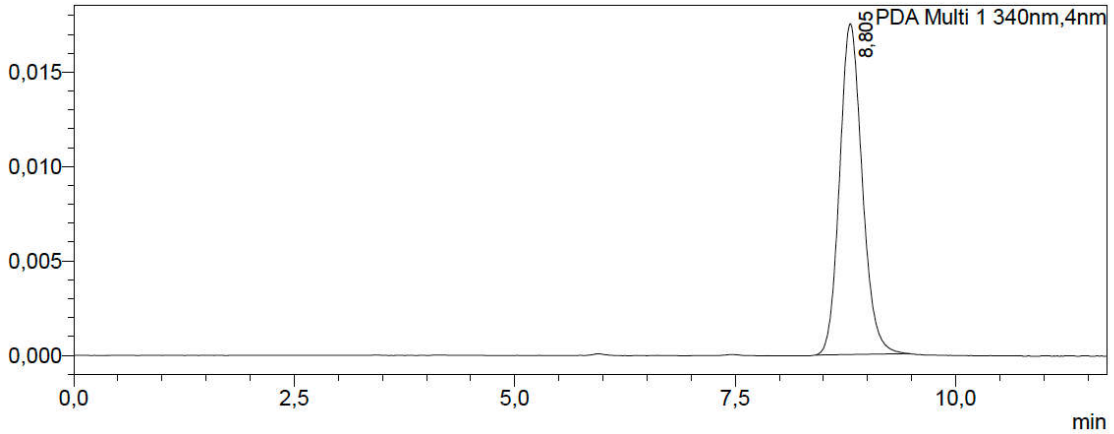


Figure S66. Chiral HPLC chromatogram for *P*-**5d**: er >1:99; IA column, *n*-hexane:isopropanol 99:1, T = 303 K, F = 1.0 mL/min.

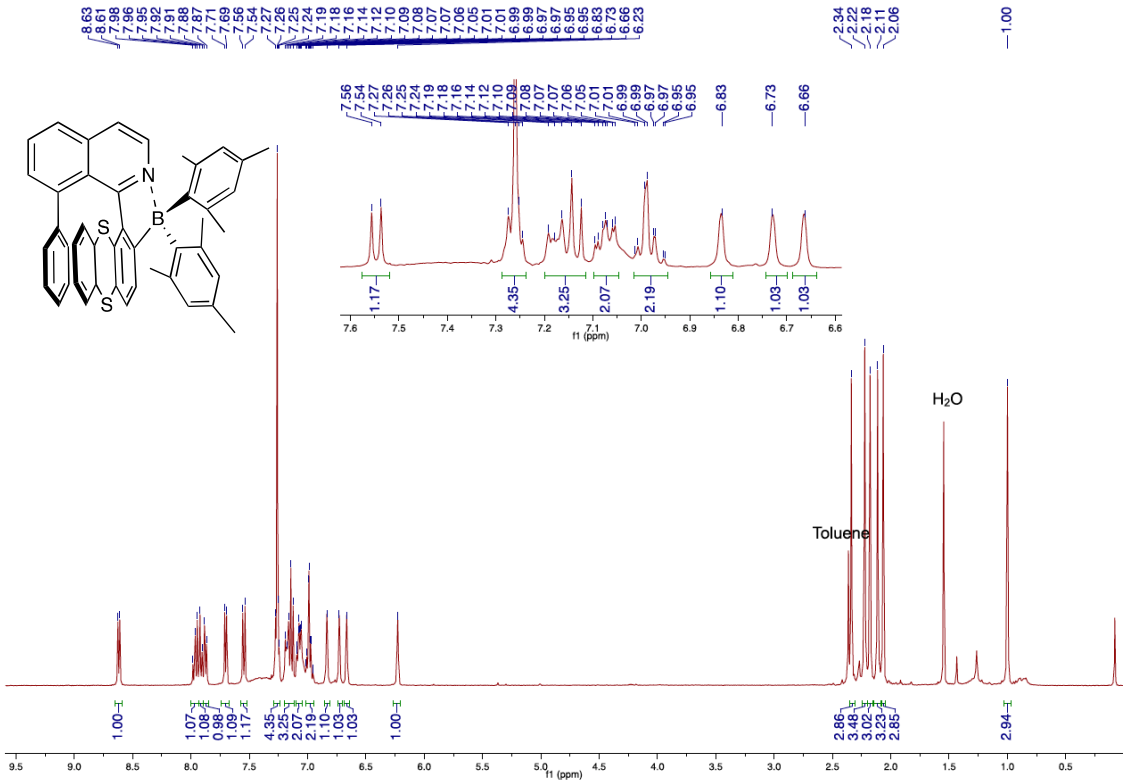


Figure S67. ^{1}H-NMR (400 MHz, $CDCl_3$, 298 K) for *rac*-**5e**.

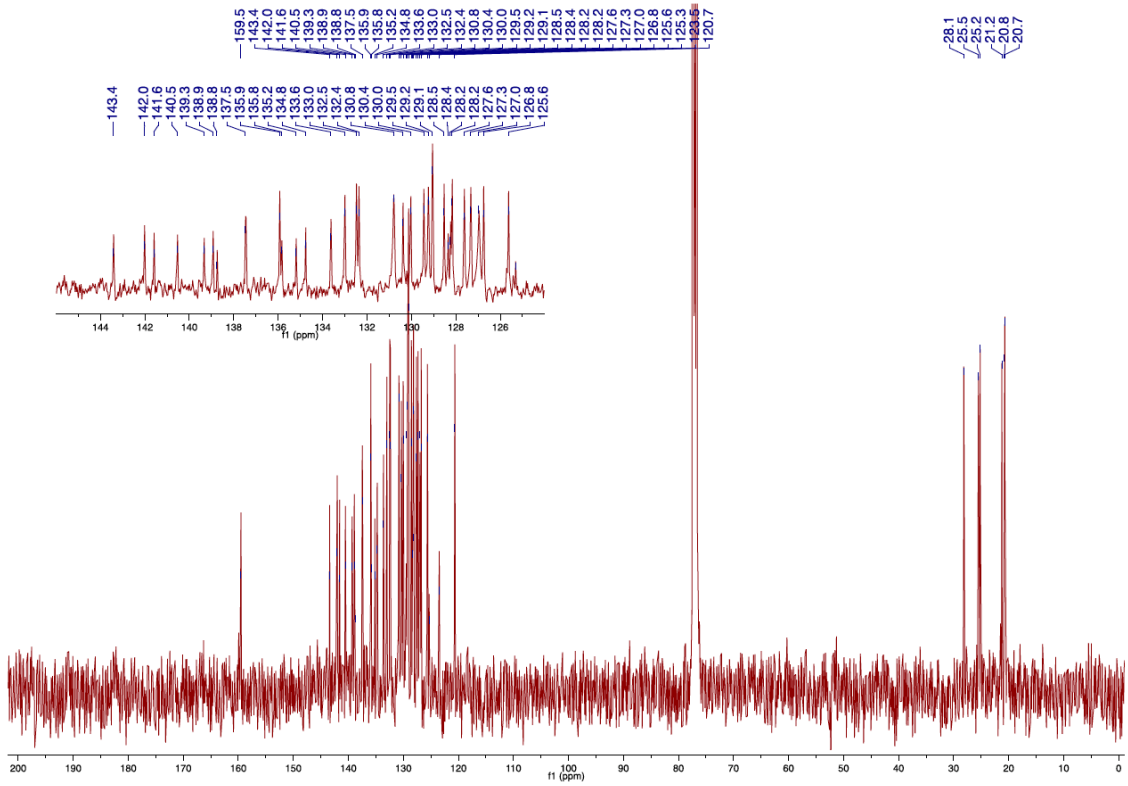


Figure S68. ^{13}C-NMR (100 MHz, $CDCl_3$, 298 K) for *rac*-**5e.**

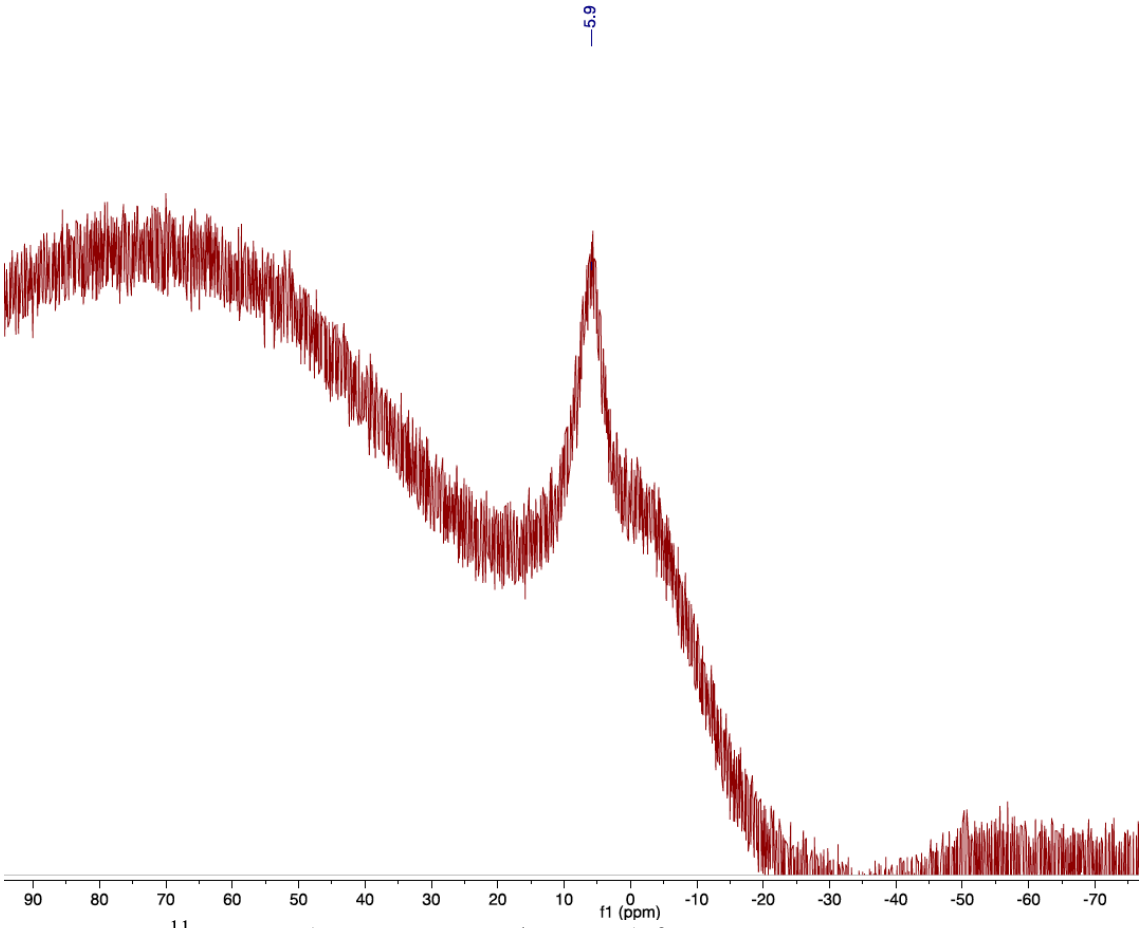


Figure S69. ^{11}B-NMR (128 MHz, $CDCl_3$, 298 K) for *rac*-**5e**.

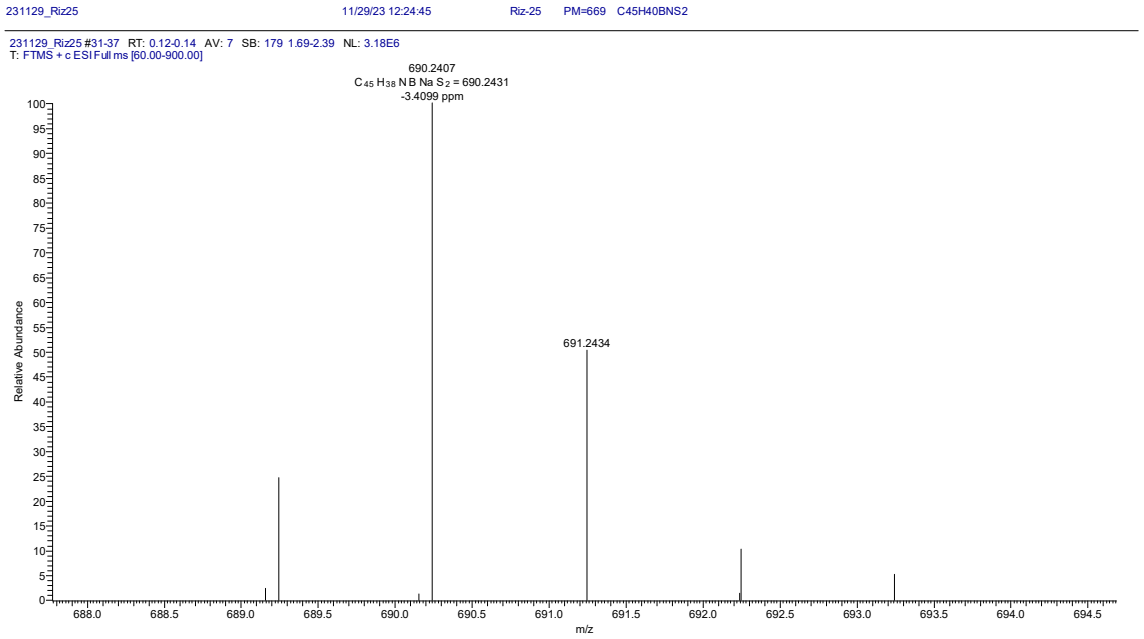


Figure S70. HRM-ESI for *rac*-**5e**.

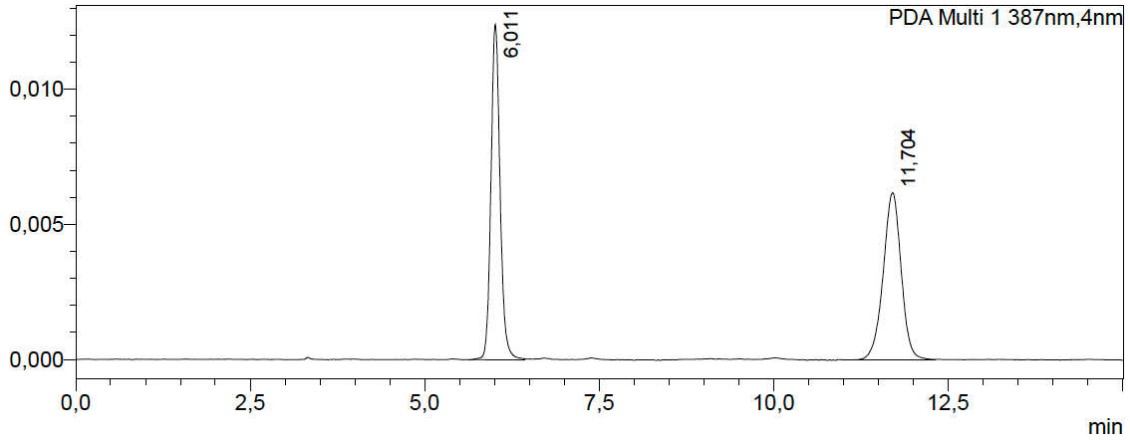


Figure S71. Chiral HPLC chromatogram for *rac*-**5e**: IA column, *n*-hexane:isopropanol 97:3, T = 303 K, F = 1.0 mL/min.

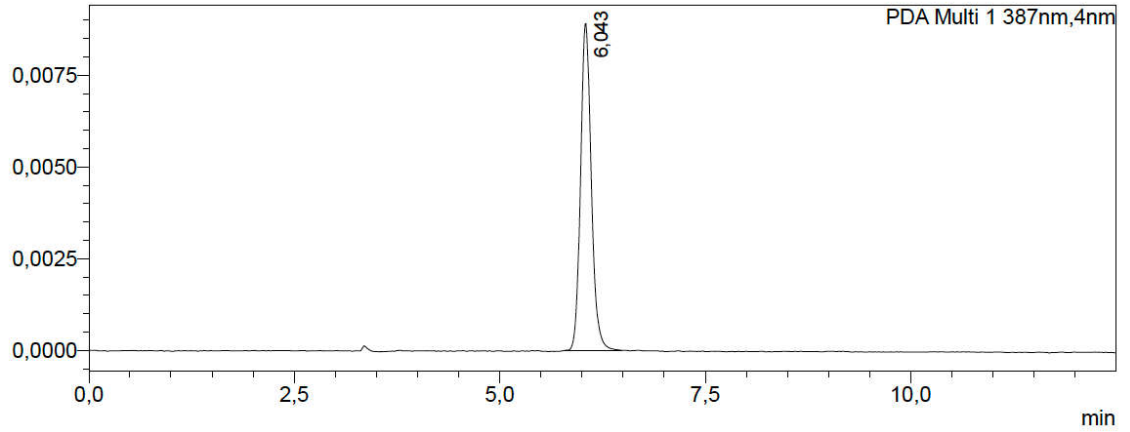


Figure S72. Chiral HPLC chromatogram for *M*-**5e**: er >99:1; IA column, *n*-hexane:isopropanol 97:3, T = 303 K, F = 1.0 mL/min.

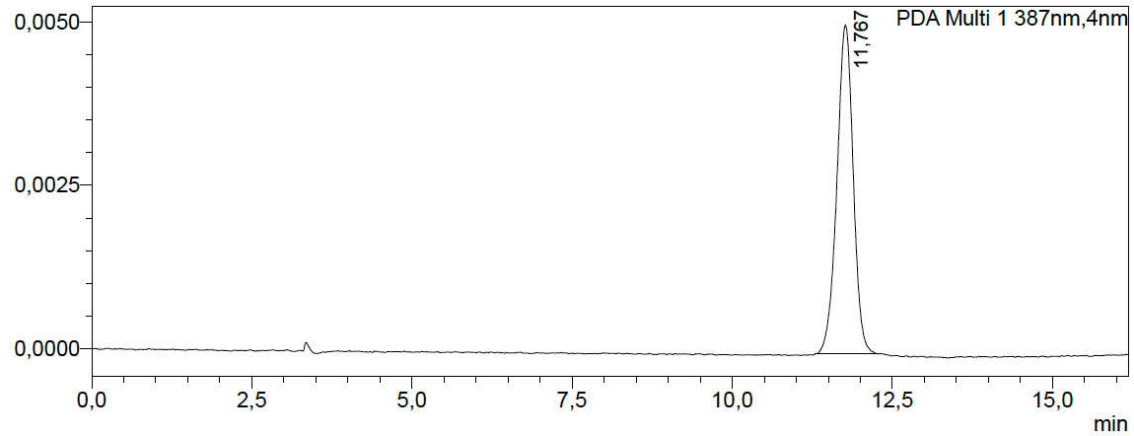


Figure S73. Chiral HPLC chromatogram for *P*-**5e**: er >1:99; IA column, *n*-hexane:isopropanol 97:3, T = 303 K, F = 1.0 mL/min.

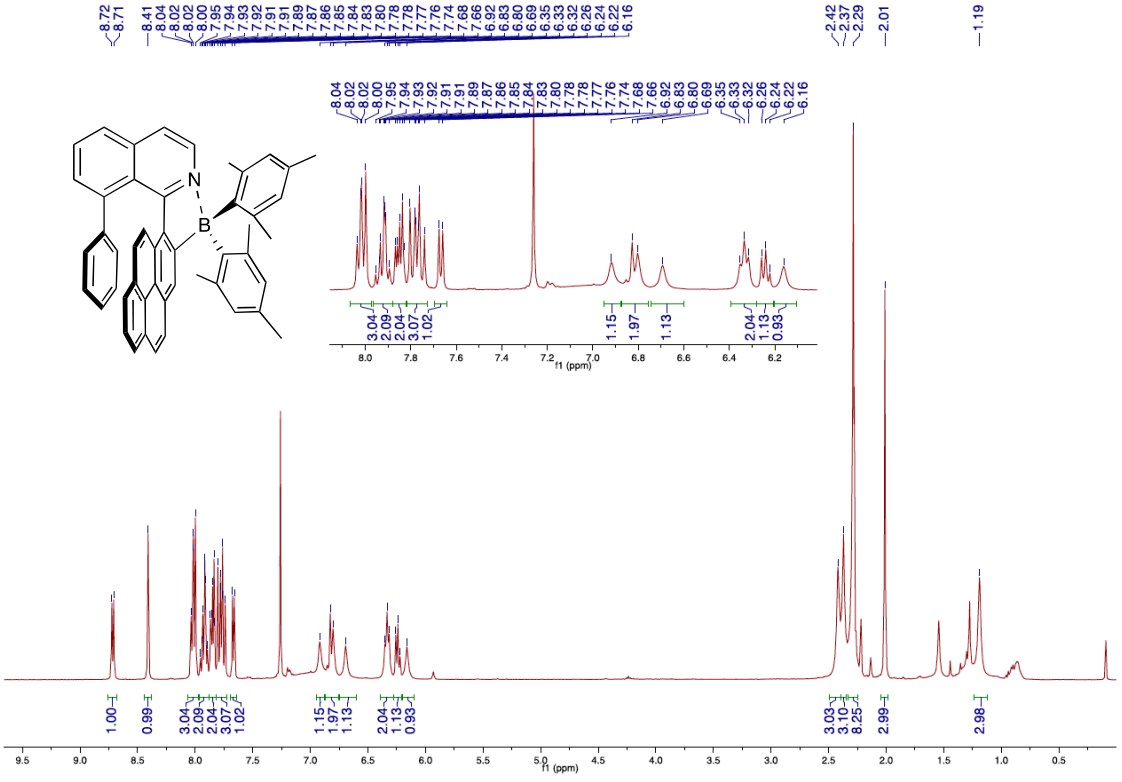


Figure S74. ^{1}H-NMR (400 MHz, $CDCl_3$, 298 K) for *rac*-**5f**.

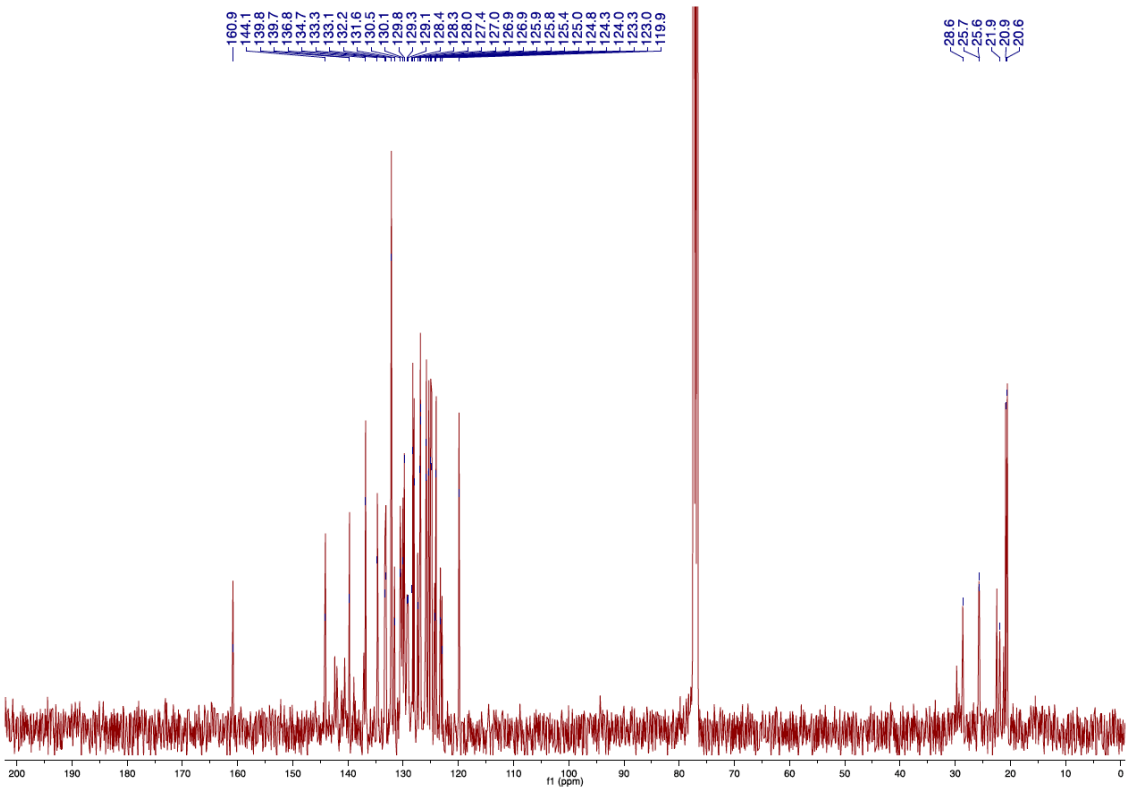


Figure S75. ^{13}C-NMR (100 MHz, $CDCl_3$, 298 K) for *rac*-**5f**.

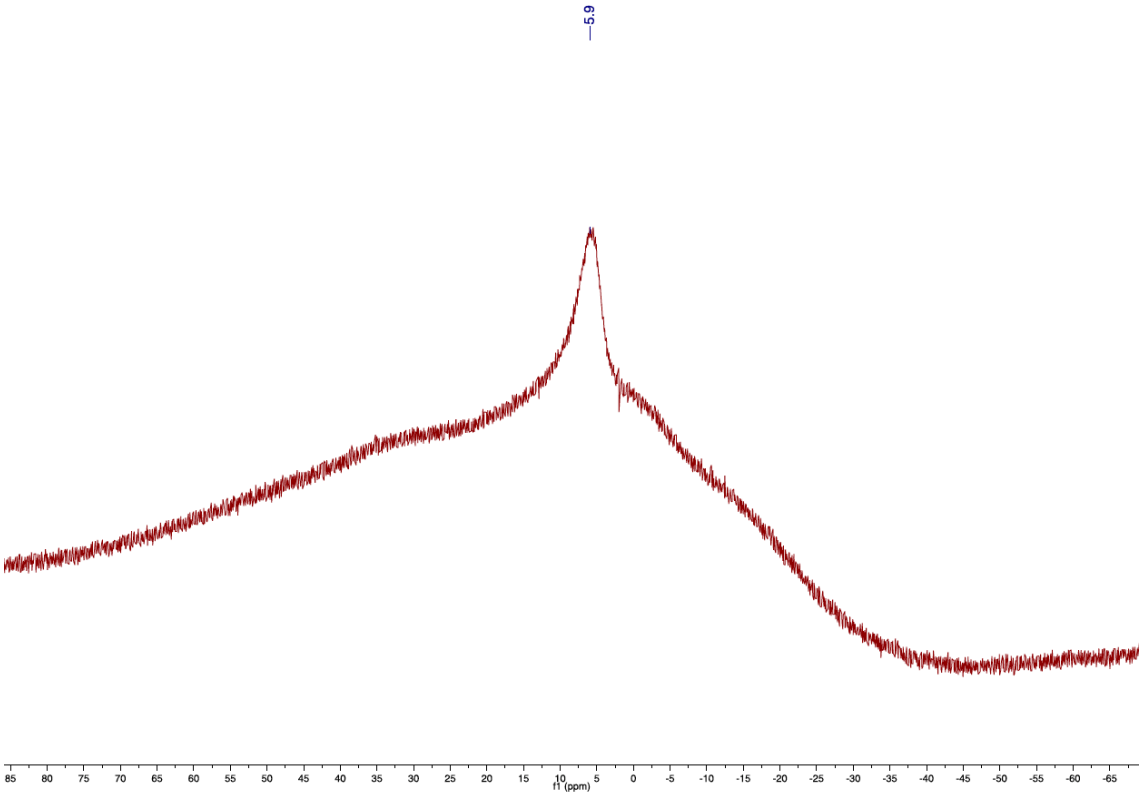


Figure S76. ^{11}B-NMR (128 MHz, $CDCl_3$, 298 K) for *rac*-**5f**.

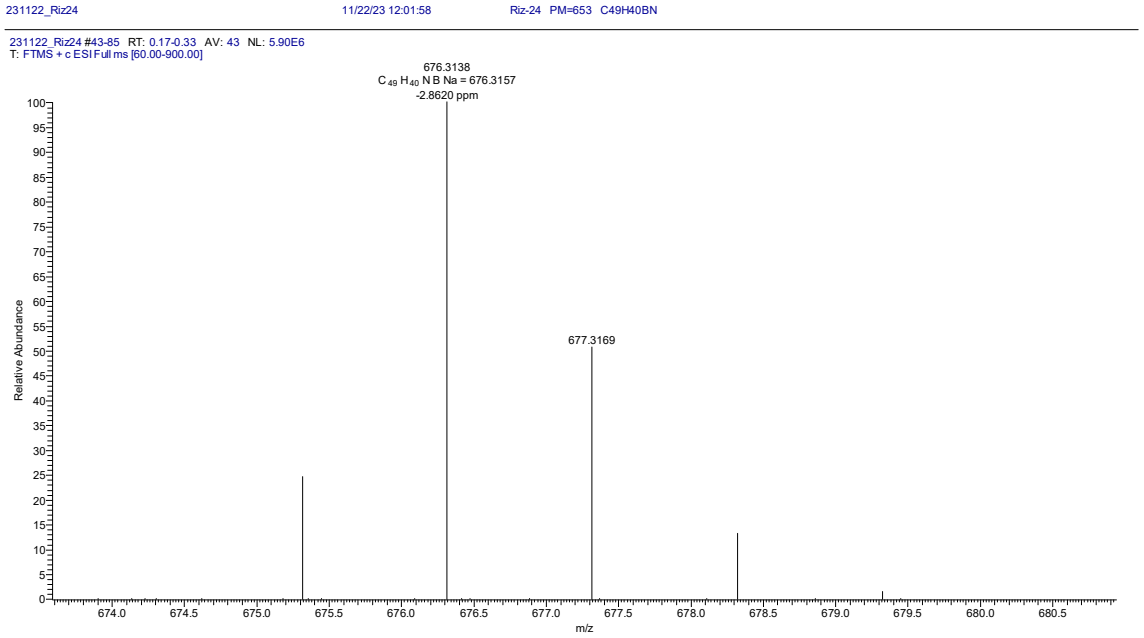


Figure S77. HRM-ESI for *rac*-**5f**.

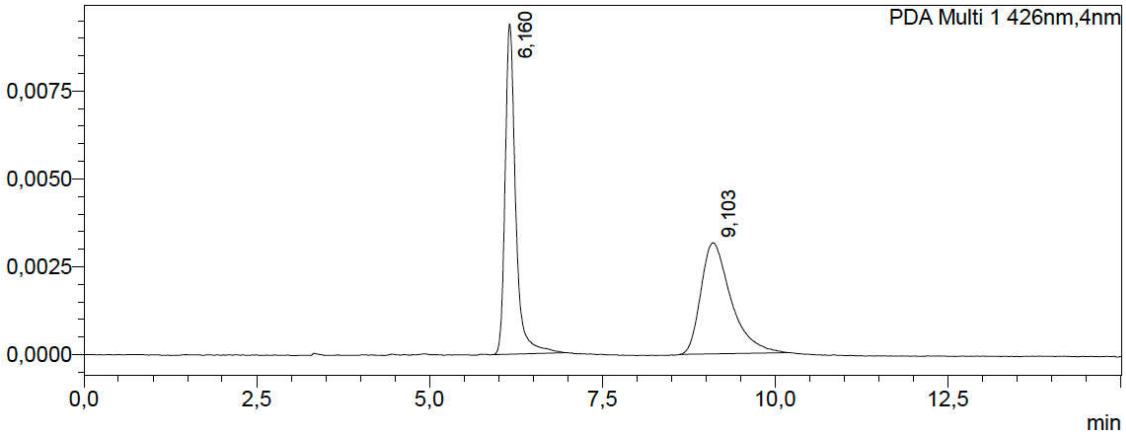


Figure S78. Chiral HPLC chromatogram for *rac*-**5f**: IA column, *n*-hexane:isopropanol 97:3, T = 303 K, F = 1.0 mL/min.

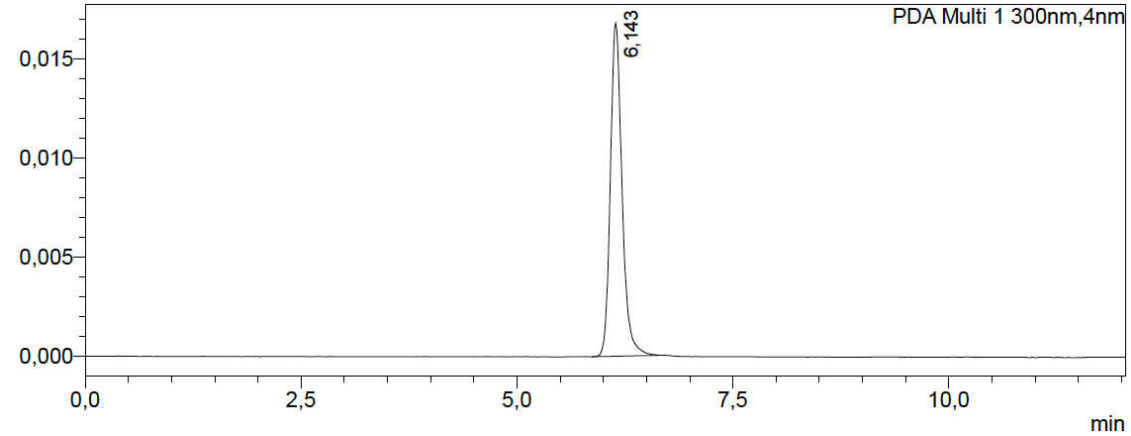


Figure S79. Chiral HPLC chromatogram for *M*-**5f**: er >99:1; IA column, *n*-hexane:isopropanol 97:3, T = 303 K, F = 1.0 mL/min.

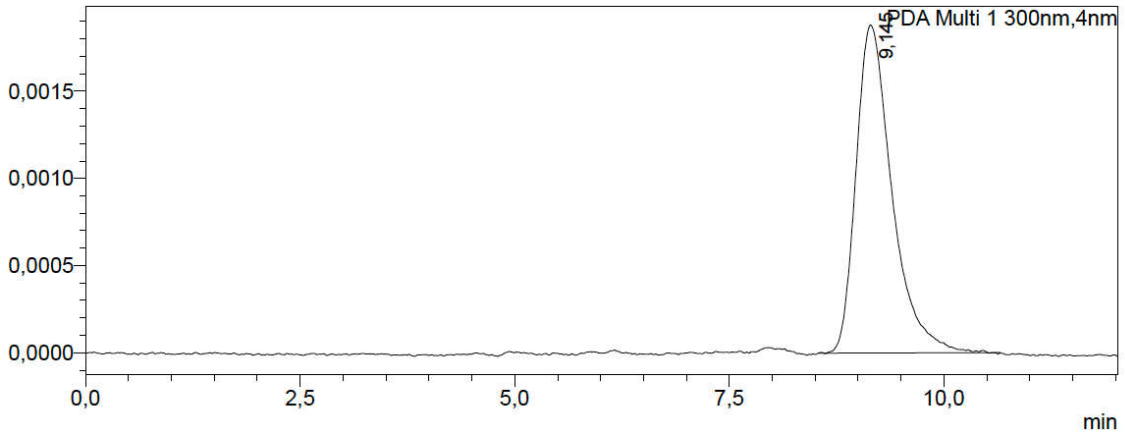


Figure S80. Chiral HPLC chromatogram for *P*-**5f**: er >1:99; IA column, *n*-hexane:isopropanol 97:3, T = 303 K, F = 1.0 mL/min.

4. X-ray crystallographic data

Table S1. Crystal data for **5e**.

Empirical formula	$C_{45}H_{38}BNS_2$	
Formula weight	667.69	
Temperature	193(0) K	
Wavelength	0.56086 Å	
Crystal system	monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 15.9459(13) Å	α= 90°
	b = 12.9259(12) Å	β= 90°
	c = 17.7067(18) Å	γ = 90°
Volume	3570.2(6) $Å^3$	
Z	4	
Density (calculated)	1.242 Mg/m^3	
Absorption coefficient	0.183 mm^{-1}	
F(000)	1408.0	
Crystal size	0.1 × 0.06 × 0.06 mm^3	
2Θ range for data collection	3.86 to 51.46°.	
Index ranges	$-19 \leq h \leq 18$, $-15 \leq k \leq 15$, $-21 \leq l \leq 21$	
Reflections collected	64188	
Independent reflections	6792 [R_{int} = 0.1272, R_{sigma} = 0.0559]	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6792/0/448	
Goodness-of-fit on F^2	1.063	
Final R indices [I>2sigma(I)]	R_1 = 0.0579, wR_2 = 0.1184	
R indices (all data)	R_1 = 0.0917, wR_2 = 0.1318	
Absolute structure parameter	0.020(3)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.25 and –0.39 e×$Å^{-3}$	

5. Additional UV/vis-absorption/emission spectra and photophysical data

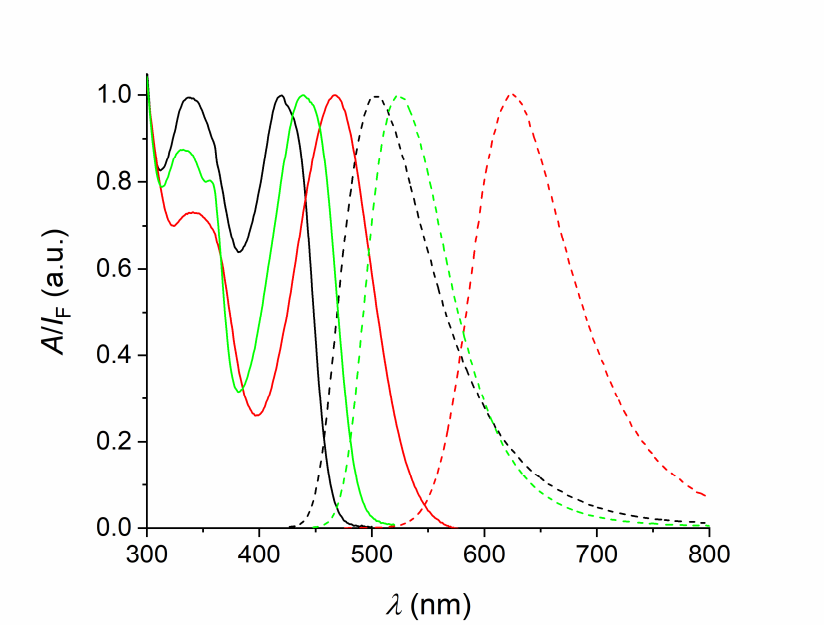


Figure 81. UV/vis absorption (full lines) and fluorescence spectra (dashed lines) of **5a** (black), **5b** (green), and **5c** (red) in air-equilibrated acetonitrile (dye concentration 20 µM).

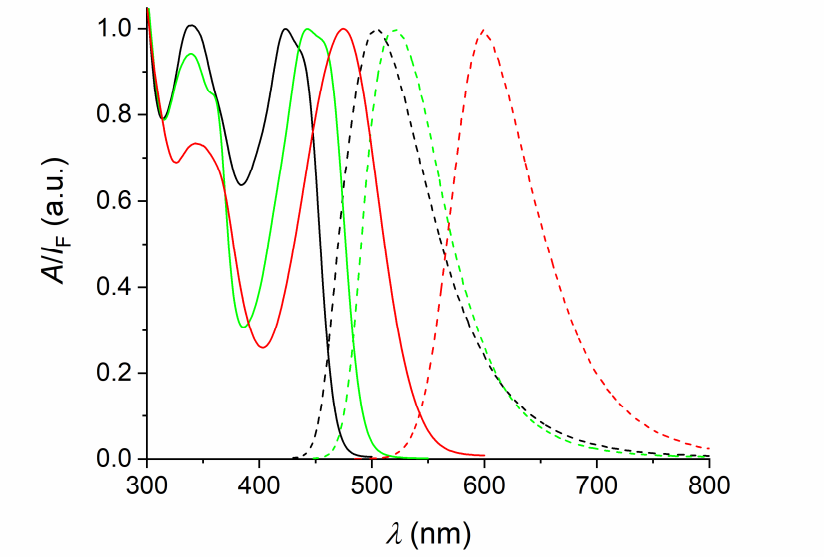


Figure 82. UV/vis absorption (full lines) and fluorescence spectra (dashed lines) of **5a** (black), **5b** (green), and **5c** (red) in air-equilibrated dichloromethane (dye concentration 20 µM).

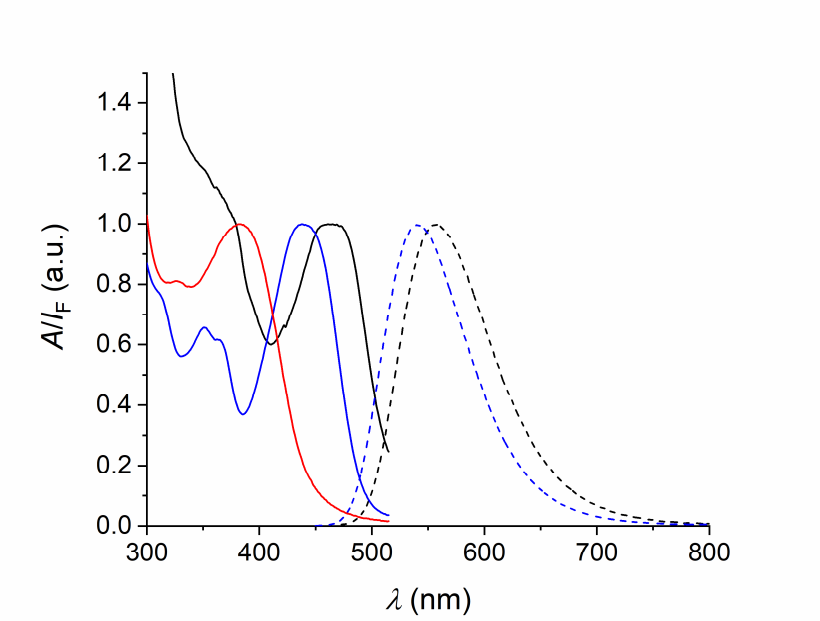


Figure S83. UV/vis absorption (full lines) and fluorescence spectra (dashed lines) of **5d** (black), **5e** (red), and **5f** (blue) in air-equilibrated acetonitrile (dye concentration 20 µM).

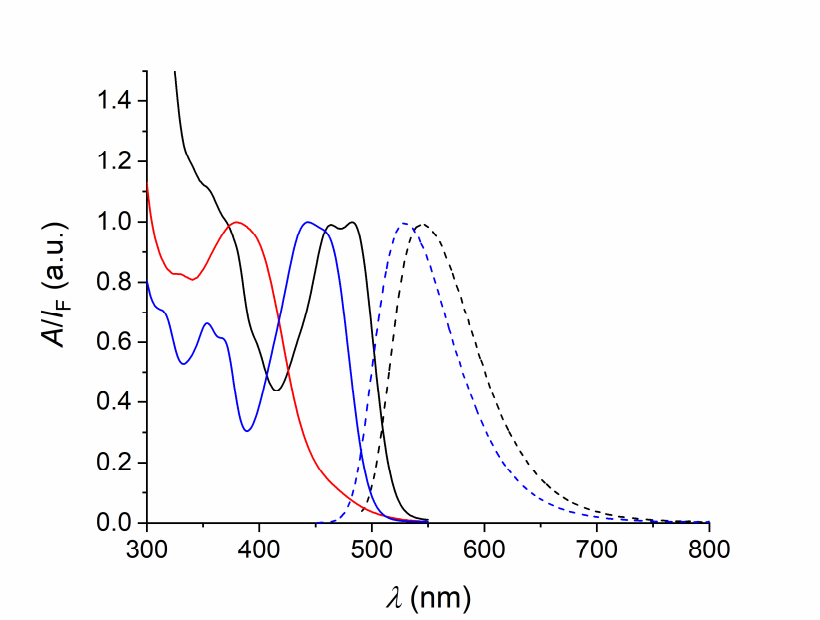


Figure S84. UV/vis absorption (full lines) and fluorescence spectra (dashed lines) of **5d** (black), **5e** (red), and **5f** (blue) in air-equilibrated dichloromethane (dye concentration 20 µM).

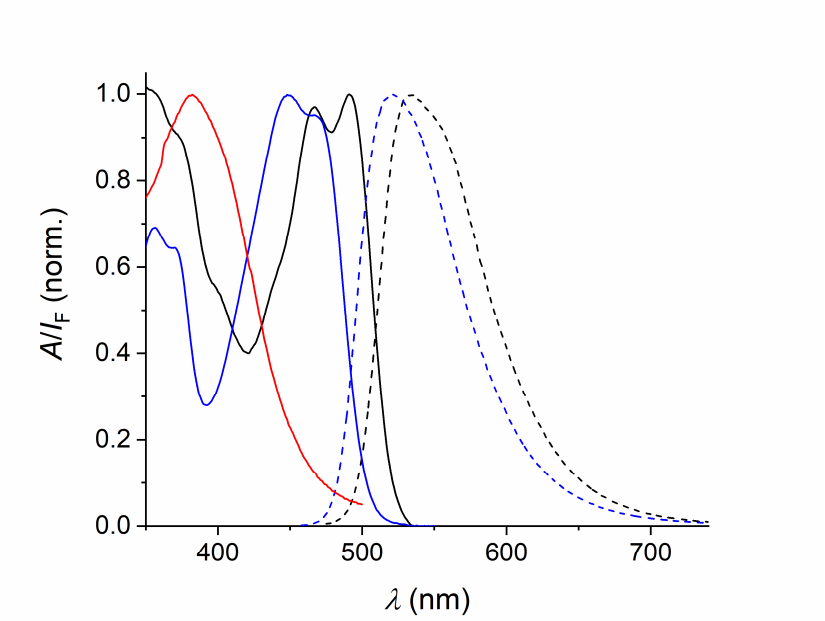


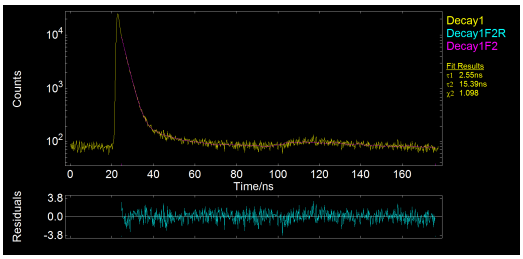
Figure S85. UV/vis absorption (full lines) and fluorescence spectra (dashed lines) of **5d** (black), **5e** (red), and **5f** (blue) in air-equilibrated toluene (dye concentration 20 µM).

Table S1. Radiative and non-radiative decay constants of **5a**–**d** and **5f** in various solvents.

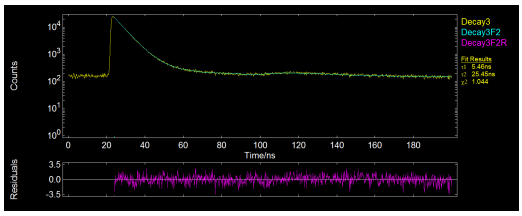
	Toluene		Dichloromethane		Acetonitrile	
	k_r/ (10^7 s^{-1})	k_{nr}/ (10^8 s^{-1})	k_r/ (10^7 s^{-1})	k_{nr}/ (10^8 s^{-1})	k_r/ (10^7 s^{-1})	k_{nr}/ (10^8 s^{-1})
5a	4.2	4.3	5.1	3.1	2.7	3.6
5b	6.0	1.9	5.1	1.3	4.8	1.4
5c	4.8	7.1	4.0	6.3	3.0	1.4
5d	4.6	4.1	4.4	4.5	1.8	3.4
5f	7.1	2.5	6.3	2.4	4.2	2.1

Acetonitrile

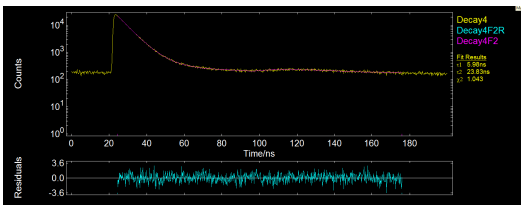
5a



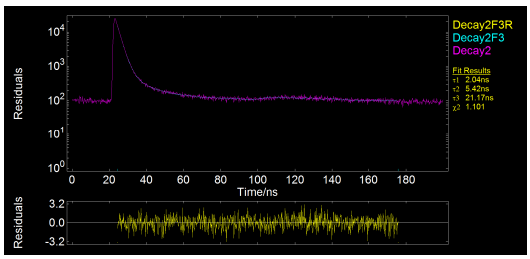
5b



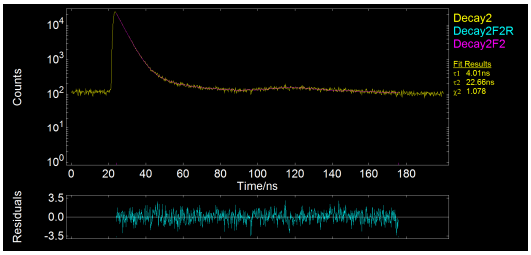
5c



5d

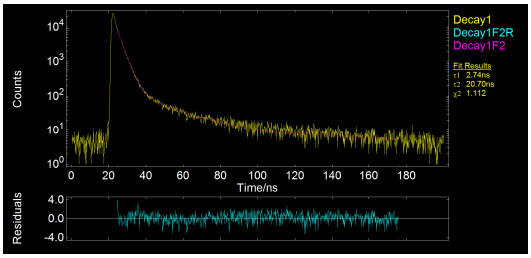


5f

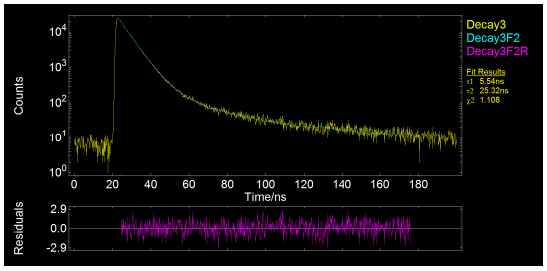


Dichloromethane

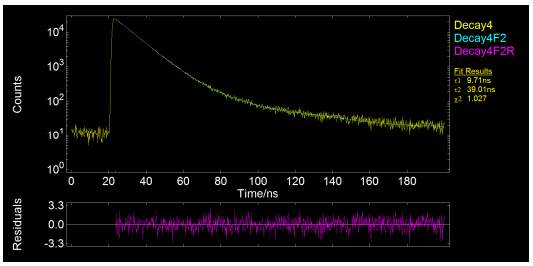
5a



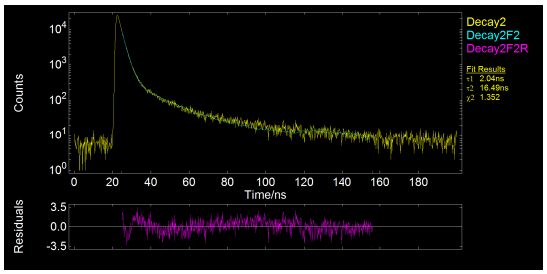
5b



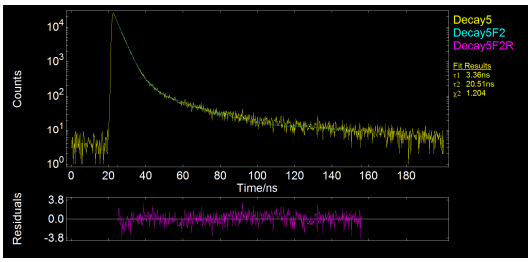
5c



5d



5f



Toluene

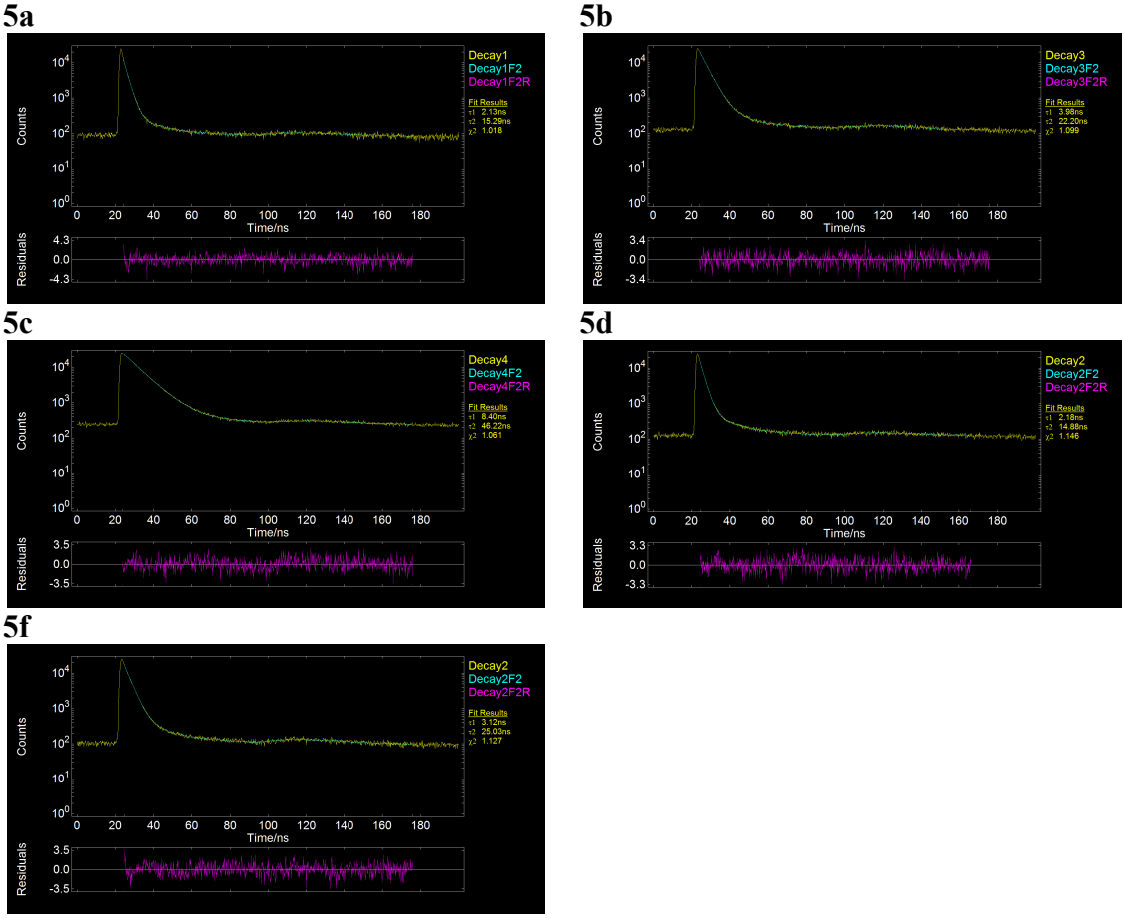


Figure S86. Decay traces and fitting results for the dyes **5a**–**d** and **5f** in various solvents.

Table S2. Detailed fitting data of the dyes **5a**–**d** and **5f** in various solvents.

	τ_F (ns), toluene	τ_F (ns), dichloromethane	τ_F (ns), acetonitrile
5a	2.13 (94.9%), 15.29 (5.1%) χ^2 = 1.018	2.74 (96.2%), 20.70 (3.8%) χ^2 = 1.112	2.55 (96.0%), 15.39 (4.0%) χ^2 = 1.098
5b	3.98 (95.7%), 22.20 (4.3%) χ^2 = 1.099	5.54 (95.4%), 25.32 (4.6%) χ^2 = 1.108	5.46 (94.9%), 25.45 (5.1%) χ^2 = 1.044
5c	8.40 (95.2%), 46.22 (4.8%) χ^2 = 1.061	9.71 (94.9%), 39.01 (5.1%) χ^2 = 1.027	5.98 (94.2%), 23.83 (5.8%) χ^2 = 1.043
5d	2.18 (93.6%), 14.88 (6.4%) χ^2 = 1.146	2.04 (95.7%), 16.49 (4.3%) χ^2 = 1.352	2.04 (85.1%), 5.42 (9.6%) 21.17 (5.3%) χ^2 = 1.101
5f	3.12 (97.5%), 25.03 (2.5%) χ^2 = 1.127	3.36 (96.0%), 20.51 (4.0%) χ^2 = 1.204	4.01 (97.1%), 22.66 (2.9%) χ^2 = 1.078

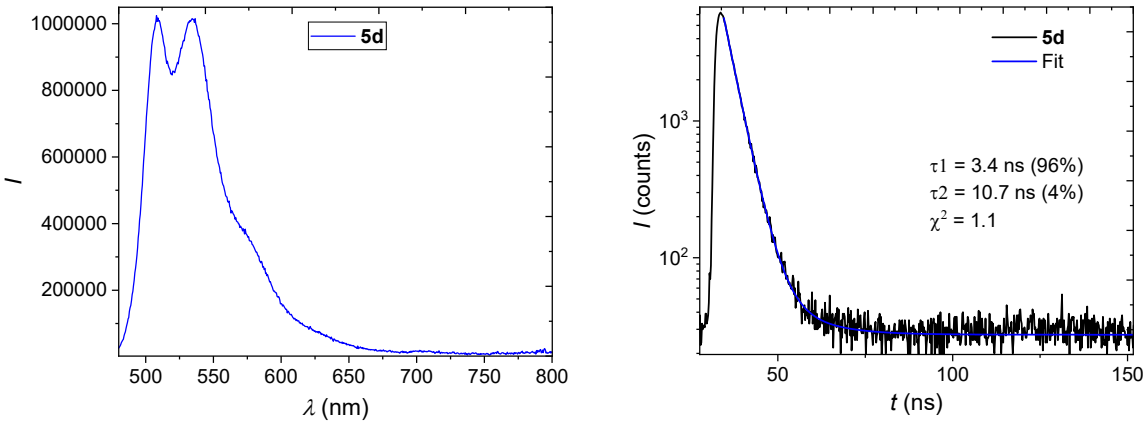


Figure S87. Left: Luminescence spectrum of compound **5d** in 2-methyltetrahydrofuran at 77 K. Right: Corresponding decay recorded at 77 K (frozen glass), monitored at 510 nm.

6. Additional chiroptical data

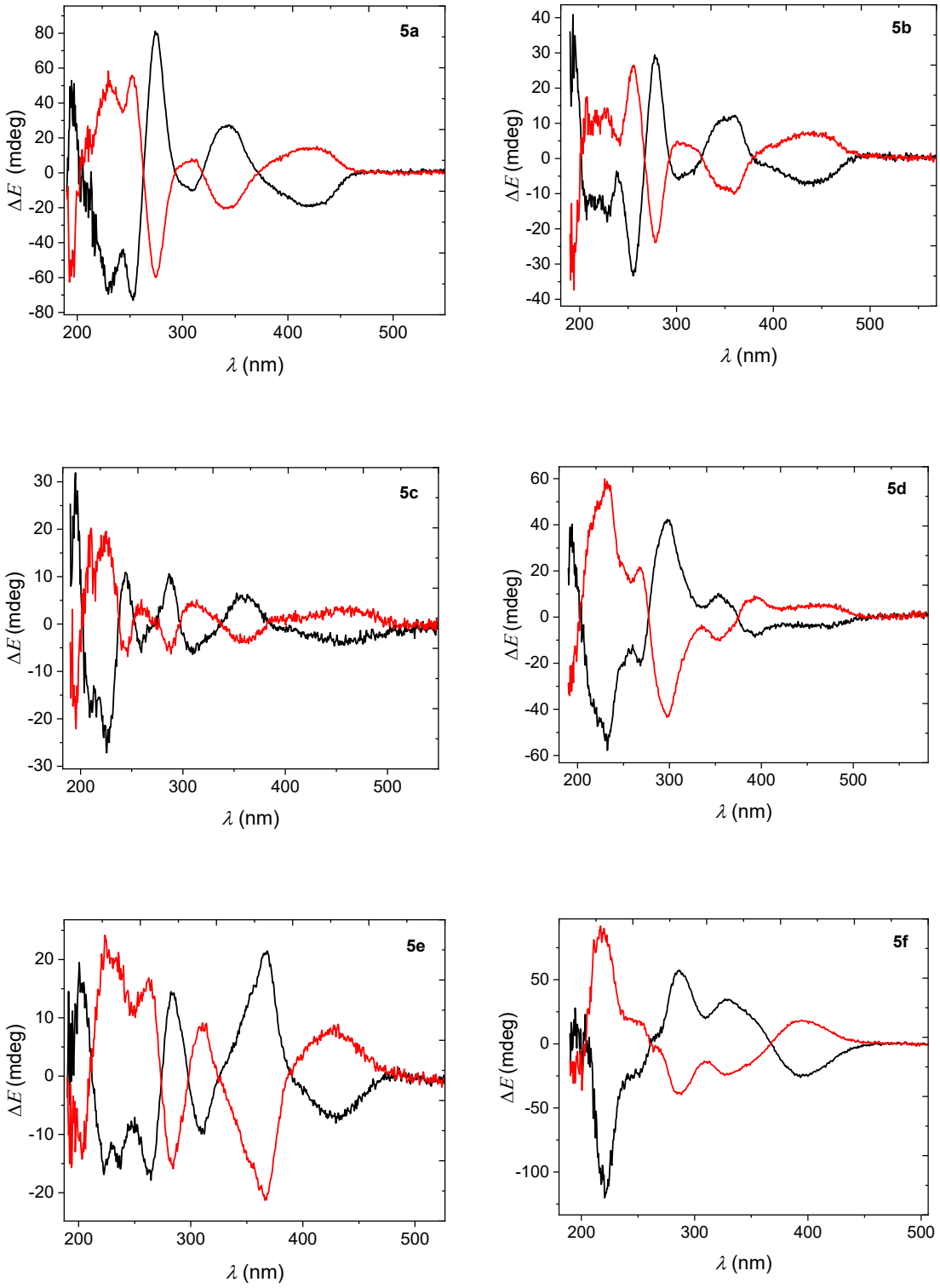


Figure S88. ECD spectra (in mdeg) of the dyes **5a**–**f** in acetonitrile (dye concentration *ca*. 1 μM; air-equilibrated solutions). The black spectra correspond to the *M*-enantiomers and the red spectra to the *P*-enantiomers.

7. Electrochemical data

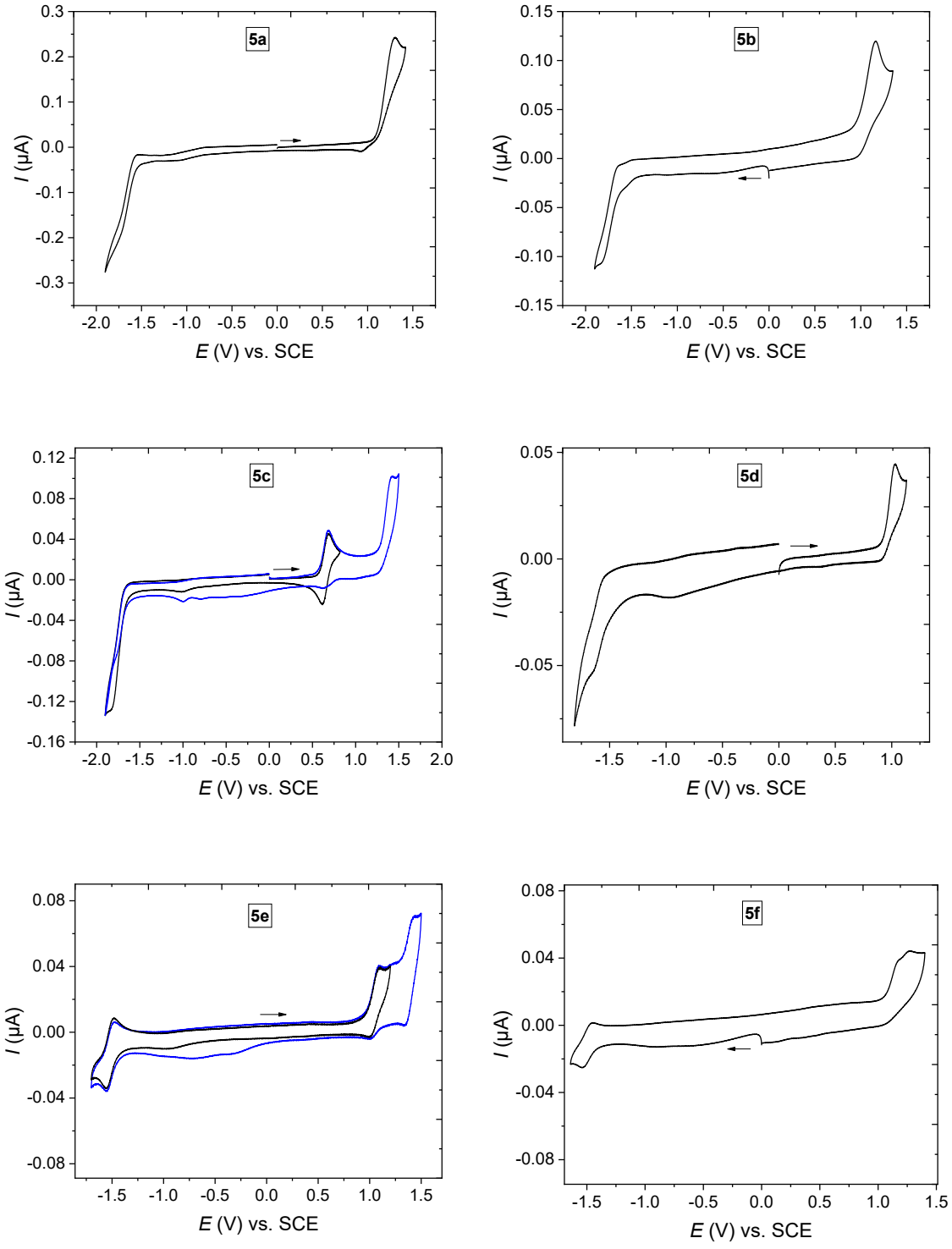


Figure S89. Cyclic voltammograms of **5a**–**f** *versus* saturated calomel electrode (SCE) as the reference and 0.2 M Bu_4NPF_6 in dichloromethane with a scan rate of 200 mV/s.

Table S2. Redox potentials of **5a**, **5b**, **5c**, **5d**, **5e**, and **5f** in dichloromethane, estimated from the corresponding onset of their respective anodic and cathodic peaks, and recorded *versus* saturated calomel electrode (SCE).

	E_{ox} (V)	E_{red} (V)
5a	+1.10	–1.56
5b	+0.94	–1.59
5c	+0.56, +1.27	–1.64
5d	+0.91	–1.46
5e	+0.97, +1.24	–1.44
5f	+1.05	–1.42

8. Theoretical calculations

To model the investigated compounds, we have relied on Time-Dependent Density Functional Theory (TD-DFT) and a wavefunction coupled-cluster (CC) approach. We have used exact dye structures. We have optimized and computed the vibrational frequencies of the dyes in their ground electronic state, and likewise for their first excited state using TD-DFT for the latter. The optimization and vibrational calculations were performed with the M06-2X functional[11] and the 6-31G(d) atomic basis set, including solvent effects (DCM was used) using the Polarizable Continuum Model (PCM), using the standard linear-response (LR) version of PCM for the TD-DFT part.[12] For the modelling of the absorption/ECD spectra, we computed 50 excited-states at the M06-2X/6-31+G(d,p) level on the optimal ground-state geometry, modeling the solvent effects using the LR-PCM approach in its non-equilibrium limit. Next, the obtained "stick" transitions were convoluted.

To obtain more accurate description of the lowest the vertical absorption as well as emission wavelengths, additional TD-DFT and CC calculations were performed on the optimal ground and excited state geometries. The TD-DFT calculations were done both in gas phase and in solution at the TD-M06-2X/6-311+G(2d,p) level, using the cLR model[12,13] for the solution calculation, so as to accounts for both *linear-response* and *state-specific* solvent effects. All DFT and TD-DFT calculations were performed with Gaussian 16, using default algorithms but improved convergence thresholds for both ground state energies and residual forces.[14]

We also computed the transition energies in gas-phase at the second-order coupled-cluster level, CC2,[15] with the *aug*-cc-pVDZ atomic basis set. These latter calculations were performed with the Turbomole package,[16] applying the RI approximation and

freezing the core electrons. It was then possible to obtain corrected vertical fluorescence energies, we simply use

$$\Delta E^{\text{fluo}} = \Delta E^{\text{CC2}}_{\text{Gas}} + \left(\Delta E^{\text{TD-DFT}}_{\text{cLR}^2\text{-PCM}} - \Delta E^{\text{TD-DFT}}_{\text{Gas}}\right)$$

and similarly for the absorption. On that basis, one can further determine 0-0 energies using a similar composite scheme which accounts for the difference of ZPVE between the two states.[17]

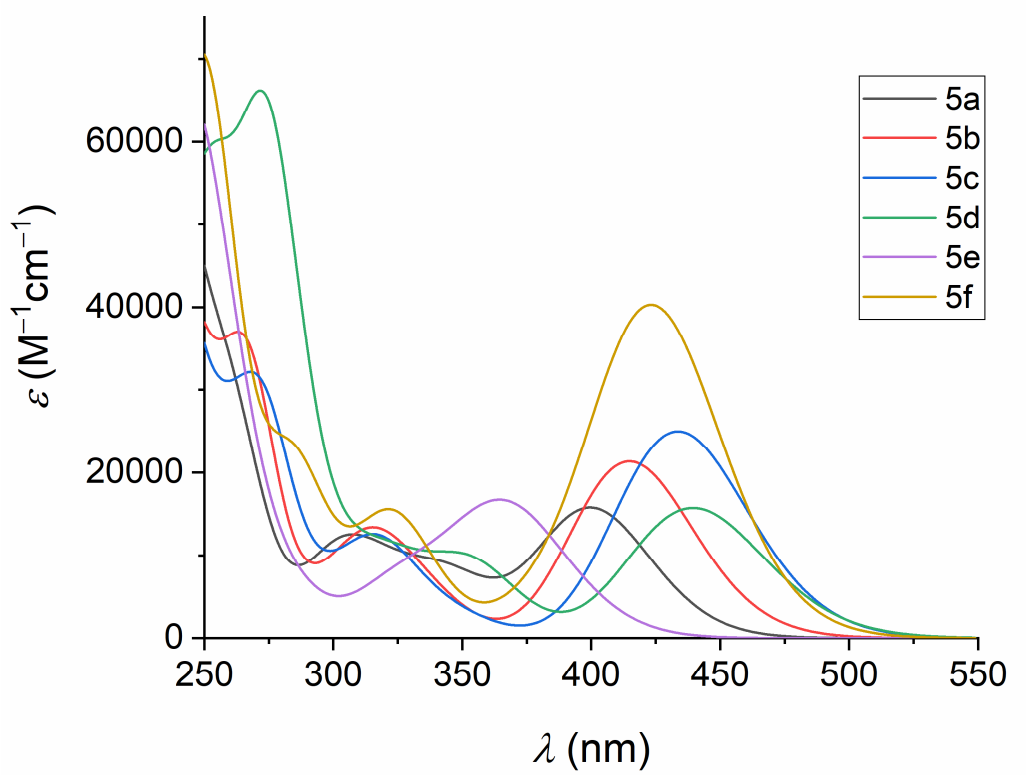


Figure S90. Simulated UV/vis-absorption spectra at the LR(neq)-PCM(DCM)-M06-2X/6-31+G(d,p) level. To obtain this Figure the "stick" vertical transitions were simply convoluted using a Gaussian broadening function with FWHM of 0.4 eV. Note that for **5e**, two quasi-energetic conformers exist (< 1 kcal mol^{-1} difference) and the calculated UV/vis spectrum is the average of the results obtained for the two conformers

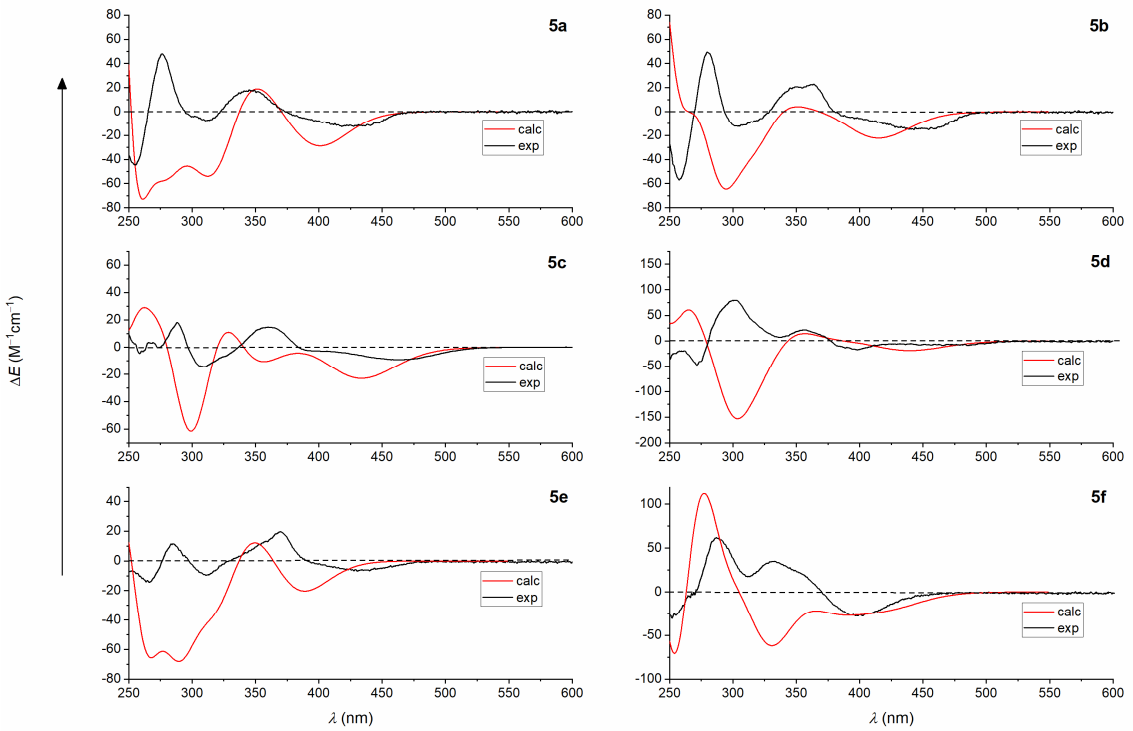


Figure S91. Simulated ECD spectra of the *M*-enantiomer; see caption of Figure S66 for details, and comparison with corresponding experimental spectra in dichloromethane. Note that for **5e**, two quasi-energetic conformers exist (< 1 kcal mol^{-1} difference) and the calculated ECD spectrum is the average of the results obtained for the two conformers

9. Atomic coordinates

Below we list the Cartesian coordinates (in Å), as obtained by DFT/TD-DFT.

5a (ground-state)

C	-1.9682990	-0.5779510	-2.8494360
C	-0.8754550	0.2097610	-3.3120400
C	0.2251530	0.4325290	-2.5264480
C	0.2730520	-0.0422650	-1.1874270
C	-0.8972470	-0.5831790	-0.6625250
C	-1.9832490	-1.0135310	-1.4958750
H	-0.9030120	0.5787380	-4.3346260
H	1.0624800	0.9777820	-2.9465690
C	1.0221880	-1.1953780	2.2884790
C	0.1695210	-1.7117530	3.2154910
C	-1.2326210	-1.5648870	3.0242240
C	-1.7114000	-0.9734390	1.8178560
C	-0.7396120	-0.7788940	0.7778220
H	2.0988240	-1.1762800	2.4122260
H	0.5505660	-2.1608570	4.1253600
N	0.5597030	-0.7069800	1.1077460
B	1.4504620	-0.0105830	-0.0498470
C	2.7917550	-0.9479050	-0.1939880
C	3.9860450	-0.6405880	0.5044430
C	2.7914470	-2.1453480	-0.9538440
C	5.1220420	-1.4490980	0.3698290
C	3.9453910	-2.9238470	-1.0701750
C	5.1353070	-2.5838450	-0.4320500
H	6.0236800	-1.1814030	0.9188910
H	3.9083560	-3.8336290	-1.6676640
C	1.7092440	1.6045340	0.1823210
C	1.1695410	2.4268180	1.2018630
C	2.4620110	2.2589370	-0.8273750
C	1.3150160	3.8184900	1.1464330
C	2.5863970	3.6506730	-0.8466610
C	1.9996740	4.4599510	0.1201700
H	0.8854490	4.4203150	1.9458000
H	3.1704950	4.1132850	-1.6415800
C	6.3797810	-3.4181210	-0.5992650
H	6.9174140	-3.1432030	-1.5138980
H	7.0664980	-3.2787230	0.2402870
H	6.1373260	-4.4824430	-0.6724160
C	4.1398360	0.5422910	1.4436580
H	4.3144240	1.4783690	0.9023590
H	3.2573270	0.7086360	2.0666340
H	4.9932370	0.3758610	2.1075870
C	1.5544670	-2.6737460	-1.6493890
H	0.7038100	-2.7410050	-0.9640540
H	1.2400170	-2.0381760	-2.4830800
H	1.7448630	-3.6752040	-2.0452760
C	0.5088400	1.8996050	2.4629430
H	-0.3923930	1.3068810	2.2887200
H	1.1974000	1.2703200	3.0377380
H	0.2233710	2.7343920	3.1083070
C	2.1012260	5.9627850	0.0582350

H	1.2886180	6.3890950	-0.5412410
H	2.0389650	6.4060250	1.0562290
H	3.0436000	6.2780740	-0.3991080
C	3.2749570	1.5238930	-1.8789780
H	4.2873600	1.3301630	-1.5012490
H	2.8697260	0.5537180	-2.1612660
H	3.3725730	2.1372580	-2.7804920
C	-3.0061070	-0.9799940	-3.7271790
C	-3.9831350	-1.8489350	-3.3074420
H	-2.9922590	-0.6129240	-4.7501730
H	-4.7636770	-2.1692120	-3.9902160
C	-2.9850040	-1.9367260	-1.1019620
C	-3.9503130	-2.3524810	-1.9884140
H	-2.9761020	-2.3408450	-0.0947040
H	-4.6968490	-3.0736280	-1.6694980
C	-3.0781810	-0.5382540	1.7511510
C	-3.9310450	-0.9140380	2.7713350
H	-4.9597030	-0.5678150	2.7467280
C	-2.1517940	-1.9433520	4.0324900
C	-3.4848390	-1.6580260	3.8836040
H	-1.7779970	-2.4297510	4.9280140
H	-4.1940660	-1.9374480	4.6559190
C	-3.5801680	0.4194450	0.7285340
C	-4.8406050	0.2355890	0.1489160
C	-2.8319010	1.5459960	0.3656580
C	-5.3274820	1.1340550	-0.7944270
H	-5.4230620	-0.6440790	0.4091590
C	-3.3183630	2.4462850	-0.5767900
H	-1.8577780	1.7224310	0.8133270
C	-4.5645360	2.2398510	-1.1648740
H	-6.2984790	0.9634170	-1.2487760
H	-2.7202050	3.3100640	-0.8495140
H	-4.9402410	2.9381290	-1.9062240

5a (excited-state)

C	-1.9384840	-0.4638540	-2.8710550
C	-0.8623030	0.3781960	-3.2740700
C	0.2482090	0.5640440	-2.4689670
C	0.3300550	-0.0075250	-1.1897530
C	-0.8659060	-0.6237900	-0.6758610
C	-1.9339590	-1.0164620	-1.5585860
H	-0.8944810	0.8174070	-4.2678940
H	1.0715590	1.1500840	-2.8611000
C	1.0356410	-1.4245260	2.1558060
C	0.1600020	-2.0015450	3.0558850
C	-1.2439570	-1.7920020	2.9221540
C	-1.7200110	-1.0938300	1.7594140
C	-0.7468310	-0.8640430	0.7197190
H	2.1124370	-1.4571860	2.2976190
H	0.5479740	-2.5285850	3.9203530
N	0.6096940	-0.7977240	1.0587240
B	1.4906660	-0.0097250	-0.0238640
C	2.8720710	-0.8705770	-0.2099940
C	4.0452520	-0.5519880	0.5159550
C	2.9279080	-2.0197040	-1.0366790
C	5.2187680	-1.2958560	0.3426390

C	4.1169040	-2.7367120	-1.1915700
C	5.2873000	-2.3785850	-0.5271240
H	6.1038140	-1.0223610	0.9155550
H	4.1246160	-3.6113250	-1.8406720
C	1.6579540	1.6028290	0.2663170
C	1.0481920	2.3335550	1.3206020
C	2.3768390	2.3606910	-0.7003400
C	1.0855960	3.7334580	1.3293730
C	2.3914040	3.7537770	-0.6557750
C	1.7267320	4.4696020	0.3396470
H	0.6050480	4.2643030	2.1495660
H	2.9484650	4.2996690	-1.4165190
C	6.5714430	-3.1404210	-0.7363950
H	7.1234390	-2.7513810	-1.5997030
H	7.2271990	-3.0598130	0.1351520
H	6.3781350	-4.2005760	-0.9245870
C	4.1174930	0.5733420	1.5304630
H	4.2258600	1.5538120	1.0541370
H	3.2214010	0.6292090	2.1550570
H	4.9782440	0.4245140	2.1891480
C	1.7133970	-2.5573430	-1.7640380
H	0.8561510	-2.6655170	-1.0908510
H	1.3963440	-1.9054860	-2.5845000
H	1.9313640	-3.5424530	-2.1865420
C	0.4248100	1.6912390	2.5439100
H	-0.4524580	1.0756930	2.3271330
H	1.1376710	1.0416630	3.0652480
H	0.1117980	2.4656530	3.2493490
C	1.7118720	5.9761410	0.3417760
H	0.9410690	6.3627040	-0.3349780
H	1.5009220	6.3692060	1.3401020
H	2.6708190	6.3828600	0.0069250
C	3.2535340	1.7256780	-1.7640380
H	4.2636860	1.5608180	-1.3669720
H	2.9039270	0.7519280	-2.1049490
H	3.3444440	2.3894160	-2.6297790
C	-2.9791790	-0.8060180	-3.7556870
C	-3.9507370	-1.7249960	-3.3870690
H	-2.9972040	-0.3564310	-4.7448840
H	-4.7359250	-1.9928920	-4.0865730
C	-2.9128320	-1.9655790	-1.2168020
C	-3.9041860	-2.3232040	-2.1223940
H	-2.8788870	-2.4398690	-0.2407930
H	-4.6435720	-3.0673660	-1.8448620
C	-3.0621320	-0.6364140	1.7386620
C	-3.9326540	-1.0697190	2.7485340
H	-4.9648030	-0.7326080	2.7219030
C	-2.1538680	-2.1968260	3.9148280
C	-3.4964170	-1.8663360	3.8079880
H	-1.7845100	-2.7553180	4.7698090
H	-4.2001060	-2.1819050	4.5712100
C	-3.5687700	0.3427020	0.7410210
C	-4.8201260	0.1594850	0.1423470
C	-2.8284320	1.4839980	0.4030800
C	-5.3102040	1.0751460	-0.7857670
H	-5.3994510	-0.7287640	0.3816320

C	-3.3163650	2.3992440	-0.5226120
H	-1.8570580	1.6564960	0.8580190
C	-4.5579350	2.1963900	-1.1252630
H	-6.2765120	0.9044350	-1.2504630
H	-2.7239450	3.2743280	-0.7720530
H	-4.9351670	2.9083710	-1.8526970

5b (ground-state)

C	1.9656910	-1.5903540	-2.1517220
C	0.8679410	-2.4623890	-1.8297600
C	-0.2482860	-1.9895000	-1.1750890
C	-0.2910660	-0.6577560	-0.6986360
C	0.8693970	0.1084890	-0.7811370
C	1.9596970	-0.2678440	-1.6374810
H	-1.0946480	-2.6451400	-1.0291730
C	-1.0850640	2.7576730	0.5952640
C	-0.2472450	3.8173350	0.7629710
C	1.1594120	3.5940060	0.7556660
C	1.6536760	2.2884180	0.4680590
C	0.6939690	1.3406270	-0.0322170
H	-2.1625370	2.8264660	0.6950400
H	-0.6409610	4.8035010	0.9799210
N	-0.6088260	1.5357670	0.2400470
B	-1.4743310	0.1845740	0.0643090
C	-2.8413810	0.6234230	-0.7306830
C	-4.0403870	0.9221220	-0.0369860
C	-2.8620480	0.7979000	-2.1377870
C	-5.2003220	1.2814770	-0.7350660
C	-4.0392480	1.1518010	-2.8015130
C	-5.2329630	1.3773420	-2.1211460
H	-6.1051090	1.5013220	-0.1701200
H	-4.0181230	1.2700610	-3.8839900
C	-1.6770450	-0.6596970	1.4721670
C	-1.1232710	-0.3590340	2.7421050
C	-2.3824860	-1.8862830	1.3658530
C	-1.1978720	-1.2854100	3.7894560
C	-2.4398820	-2.7826690	2.4366220
C	-1.8291590	-2.5175740	3.6571940
H	-0.7569070	-1.0234620	4.7500100
H	-2.9895660	-3.7149880	2.3102670
C	-6.5020330	1.7216080	-2.8585540
H	-7.0108500	0.8164130	-3.2091970
H	-7.2008070	2.2625540	-2.2143460
H	-6.2955260	2.3394570	-3.7374650
C	-4.1699000	0.9032170	1.4751020
H	-4.2981080	-0.1115570	1.8664560
H	-3.2938250	1.3191030	1.9793630
H	-5.0420940	1.4905340	1.7770200
C	-1.6235610	0.6541280	-2.9969750
H	-0.7892760	1.2416600	-2.6015870
H	-1.2784460	-0.3825020	-3.0624330
H	-1.8281310	1.0037210	-4.0128020
C	-0.5266360	0.9859710	3.1175550
H	0.3642100	1.2637570	2.5491490
H	-1.2544910	1.7933540	2.9817230
H	-0.2446810	0.9828060	4.1736950

C	-1.8529750	-3.5162310	4.7861790
H	-0.9894570	-4.1895120	4.7362470
H	-1.8215460	-3.0165130	5.7586850
H	-2.7531910	-4.1364210	4.7480130
C	-3.2167120	-2.2761540	0.1573530
H	-4.2559450	-1.9529340	0.3023870
H	-2.8904830	-1.8250440	-0.7777690
H	-3.2277360	-3.3648300	0.0367330
C	3.0028510	-2.0122630	-3.0156990
C	3.9756760	-1.1280140	-3.4199060
H	2.9975180	-3.0346500	-3.3763980
H	4.7603030	-1.4510470	-4.0965520
C	2.9544010	0.6266240	-2.1041470
C	3.9303200	0.2102490	-2.9799510
H	2.9319070	1.6630410	-1.7835750
H	4.6719130	0.9202040	-3.3337130
C	3.0207960	1.9769200	0.7726290
C	3.8645380	3.0168210	1.1154480
H	4.8945250	2.7917760	1.3746570
C	2.0684520	4.6269940	1.0884020
C	3.4045890	4.3456030	1.2225260
H	1.6854000	5.6274450	1.2640630
H	4.1050880	5.1315730	1.4856620
C	3.5298280	0.5830730	0.8925470
C	4.7954470	0.2460720	0.3998800
C	2.7806810	-0.4023910	1.5475820
C	5.2873630	-1.0488910	0.5286590
H	5.3793840	0.9967880	-0.1258360
C	3.2721330	-1.6971380	1.6785110
H	1.8020330	-0.1642760	1.9544970
C	4.5242910	-2.0266630	1.1636940
H	6.2630570	-1.2961540	0.1220940
H	2.6728130	-2.4472770	2.1850600
H	4.9043920	-3.0390000	1.2587710
O	1.0017030	-3.7263090	-2.2830200
C	-0.0556680	-4.6368070	-2.0293040
H	-0.2354030	-4.7357410	-0.9536040
H	-0.9772510	-4.3136680	-2.5249810
H	0.2667330	-5.5925900	-2.4396660

5b (excited-state)

C	1.9872270	-1.4917770	-2.1941410
C	0.9049920	-2.3873020	-1.8771360
C	-0.2368950	-1.9304330	-1.2132640
C	-0.3169690	-0.6282240	-0.7269750
C	0.8717810	0.1774010	-0.7829760
C	1.9520070	-0.1711230	-1.6710690
H	-1.0706310	-2.6077040	-1.0869620
C	-1.0779130	2.7424380	0.5886710
C	-0.2163110	3.7954590	0.8226640
C	1.1908120	3.5693590	0.9042140
C	1.6832550	2.2531840	0.5979780
C	0.7300220	1.3434950	0.0224570
H	-2.1569790	2.8574150	0.6458270
H	-0.6178310	4.7779380	1.0451430
N	-0.6354300	1.5221000	0.2797130

B	-1.5005380	0.1883860	0.0760830
C	-2.8688020	0.6483880	-0.7067070
C	-4.0646310	0.9322130	-0.0022780
C	-2.8918100	0.8665220	-2.1072370
C	-5.2249770	1.3178170	-0.6847810
C	-4.0688350	1.2461860	-2.7575850
C	-5.2600780	1.4557490	-2.0677900
H	-6.1267400	1.5270460	-0.1107990
H	-4.0495620	1.3982360	-3.8360000
C	-1.7102090	-0.7274600	1.4337250
C	-1.1453860	-0.4743230	2.7088540
C	-2.4171280	-1.9501660	1.2857360
C	-1.2170530	-1.4368510	3.7245360
C	-2.4686110	-2.8846730	2.3212970
C	-1.8516810	-2.6612480	3.5500390
H	-0.7683710	-1.2117060	4.6909240
H	-3.0181870	-3.8128970	2.1660430
C	-6.5294040	1.8283610	-2.7910700
H	-7.0528500	0.9359530	-3.1529720
H	-7.2169600	2.3676770	-2.1334490
H	-6.3207220	2.4580210	-3.6610480
C	-4.1779390	0.8739540	1.5094080
H	-4.2940310	-0.1511250	1.8772980
H	-3.2959470	1.2845360	2.0086900
H	-5.0493510	1.4484690	1.8374880
C	-1.6556500	0.7427910	-2.9736750
H	-0.8085590	1.2917880	-2.5489650
H	-1.3344220	-0.2963530	-3.0973900
H	-1.8515280	1.1510850	-3.9693410
C	-0.5279950	0.8515920	3.1112240
H	0.3614890	1.1216080	2.5357280
H	-1.2378070	1.6785510	2.9931560
H	-0.2365980	0.8201260	4.1646950
C	-1.8755800	-3.7018550	4.6404310
H	-1.0914650	-4.4524480	4.4876800
H	-1.7112360	-3.2503400	5.6227990
H	-2.8324040	-4.2321800	4.6622710
C	-3.2493520	-2.2869720	0.0605930
H	-4.2795030	-1.9333380	0.1987920
H	-2.8963990	-1.8223860	-0.8590780
H	-3.2924660	-3.3715400	-0.0868180
C	3.0327730	-1.8764310	-3.0498520
C	3.9920140	-0.9542310	-3.4410500
H	3.0652200	-2.8952760	-3.4195130
H	4.7863950	-1.2557110	-4.1159530
C	2.9209440	0.7501000	-2.1044430
C	3.9220880	0.3674320	-2.9858010
H	2.8708430	1.7765680	-1.7550630
H	4.6544520	1.0964250	-3.3173190
C	3.0288390	1.9330980	0.9206150
C	3.8845470	2.9685720	1.3204270
H	4.9178930	2.7264030	1.5518690
C	2.0853620	4.5703730	1.3157980
C	3.4318050	4.2774780	1.4872210
H	1.7038750	5.5682930	1.5112130
H	4.1241740	5.0520600	1.8003430

C	3.5437280	0.5388700	0.9317230
C	4.8054260	0.2440060	0.4027090
C	2.7995320	-0.5051880	1.4990340
C	5.3015750	-1.0570150	0.4162080
H	5.3876350	1.0385280	-0.0573010
C	3.2926950	-1.8052230	1.5120500
H	1.8211670	-0.3043180	1.9268580
C	4.5443620	-2.0883880	0.9661530
H	6.2759880	-1.2651420	-0.0152580
H	2.6964890	-2.5986030	1.9527590
H	4.9259670	-3.1046490	0.9708650
O	1.0539410	-3.6352020	-2.3290900
C	0.0186810	-4.5817280	-2.0871700
H	-0.1608370	-4.6896450	-1.0132880
H	-0.9049590	-4.2796670	-2.5901110
H	0.3763810	-5.5220640	-2.5020820

5c (ground-state)

C	2.1425840	-1.4295300	-1.8757230
C	1.1854090	-2.4084150	-1.4015120
C	-0.0208380	-1.9712320	-0.8855990
C	-0.2511590	-0.6033450	-0.6020090
C	0.8289160	0.2659100	-0.7158210
C	1.9739830	-0.0688480	-1.5139840
H	-0.7760470	-2.7008500	-0.6265710
C	-1.3736500	2.8093590	0.4656870
C	-0.6227520	3.9341570	0.6250330
C	0.7965760	3.8188020	0.6742690
C	1.3957720	2.5472900	0.4431000
C	0.5251040	1.5126630	-0.0468980
H	-2.4561990	2.8048580	0.5220760
H	-1.0969100	4.8942070	0.7924970
N	-0.7977310	1.6126130	0.1789260
B	-1.5439680	0.1828340	0.0320940
C	-2.8820270	0.4784680	-0.8745760
C	-4.1271920	0.7776790	-0.2684280
C	-2.8379880	0.5279930	-2.2912820
C	-5.2610920	1.0359810	-1.0500140
C	-3.9906360	0.7810440	-3.0383510
C	-5.2243950	1.0210440	-2.4386480
H	-6.2023170	1.2600820	-0.5499480
H	-3.9190030	0.8044890	-4.1248480
C	-1.8000050	-0.6019570	1.4617670
C	-1.3487210	-0.2183140	2.7480570
C	-2.4400210	-1.8656480	1.3649930
C	-1.4743440	-1.0896420	3.8372700
C	-2.5468490	-2.7067650	2.4757170
C	-2.0514500	-2.3495410	3.7255200
H	-1.1147990	-0.7624120	4.8116840
H	-3.0426590	-3.6698450	2.3581800
C	-6.4631660	1.2581210	-3.2645830
H	-6.9055670	0.3101060	-3.5912970
H	-7.2240500	1.7965800	-2.6927690
H	-6.2356410	1.8372160	-4.1645490
C	-4.3459040	0.8463720	1.2323000
H	-4.4711270	-0.1490670	1.6722320

H	-3.5143990	1.3137360	1.7652500
H	-5.2506330	1.4228290	1.4469800
C	-1.5573910	0.3421900	-3.0773830
H	-0.7736450	1.0277700	-2.7405140
H	-1.1535910	-0.6707330	-2.9813170
H	-1.7363250	0.5329940	-4.1392500
C	-0.8042380	1.1582270	3.0834000
H	0.0960470	1.4339800	2.5287900
H	-1.5483660	1.9383570	2.8878200
H	-0.5561000	1.2103650	4.1467710
C	-2.1324540	-3.2877690	4.9028930
H	-1.2667930	-3.9595010	4.9335380
H	-2.1531470	-2.7374470	5.8478960
H	-3.0283550	-3.9133520	4.8506380
C	-3.1364720	-2.3601240	0.1083580
H	-4.1755660	-2.0071430	0.0877720
H	-2.6820140	-2.0137950	-0.8193140
H	-3.1593590	-3.4549320	0.0957600
C	3.1758010	-1.7823580	-2.7765500
C	4.0125620	-0.8252230	-3.3038870
H	3.2623440	-2.8179020	-3.0897050
H	4.7834520	-1.1079570	-4.0137780
C	2.8423430	0.8962410	-2.0791910
C	3.8387240	0.5281690	-2.9537820
H	2.6961440	1.9456970	-1.8416400
H	4.4800630	1.2872910	-3.3913110
C	2.7738800	2.3472300	0.7890810
C	3.5271900	3.4565150	1.1249390
H	4.5644940	3.3175700	1.4139840
C	1.6156110	4.9252260	1.0040430
C	2.9645480	4.7483270	1.1845650
H	1.1545890	5.8987110	1.1395780
H	3.5957050	5.5917720	1.4453720
C	3.3831300	0.9974540	0.9476690
C	4.6711920	0.7405310	0.4666920
C	2.6948320	-0.0305890	1.6050430
C	5.2437220	-0.5207920	0.6038440
H	5.2094180	1.5245440	-0.0592040
C	3.2610940	-1.2941860	1.7345010
H	1.7011130	0.1475260	2.0060520
C	4.5359100	-1.5452220	1.2288020
H	6.2373470	-0.7059730	0.2077170
H	2.7052970	-2.0810790	2.2353010
H	4.9767380	-2.5328740	1.3264860
C	0.3877320	-4.7037550	-1.4367330
H	0.0372900	-4.7874870	-0.3950100
H	-0.4517490	-4.4016440	-2.0671910
H	0.7317440	-5.6891300	-1.7611280
N	1.4853550	-3.7640210	-1.5854010
C	2.6823340	-4.2399020	-0.8877640
H	3.0346520	-5.1620830	-1.3586740
H	3.4753480	-3.4935720	-0.9297450
H	2.4618330	-4.4472430	0.1712750

5c (excited-state)

C	2.2039870	-1.2586240	-1.9246860

C	1.2760570	-2.2857780	-1.4751310
C	0.0005480	-1.8764990	-1.0017800
C	-0.2677210	-0.5636460	-0.6505540
C	0.8372070	0.3425210	-0.6644060
C	1.9782920	0.0784760	-1.5046040
H	-0.7419690	-2.6401210	-0.8095510
C	-1.3779690	2.7583230	0.5966980
C	-0.6152150	3.8695800	0.8767060
C	0.8059910	3.7595320	0.9991980
C	1.4079030	2.4899910	0.6989740
C	0.5515110	1.5092470	0.1041260
H	-2.4638700	2.7883800	0.6075480
H	-1.1019850	4.8142170	1.0932490
N	-0.8282440	1.5755410	0.2932230
B	-1.5733080	0.1745800	0.0407940
C	-2.8998680	0.5383370	-0.8627130
C	-4.1611400	0.7736020	-0.2618440
C	-2.8261410	0.7206450	-2.2670070
C	-5.2819850	1.0862290	-1.0416940
C	-3.9656910	1.0256150	-3.0158570
C	-5.2158060	1.1929110	-2.4259400
H	-6.2356000	1.2597860	-0.5445620
H	-3.8699280	1.1512850	-4.0936360
C	-1.8614810	-0.7427230	1.3826910
C	-1.4329790	-0.4601050	2.7017070
C	-2.4902680	-1.9979580	1.1759920
C	-1.5767070	-1.4117560	3.7196670
C	-2.6138110	-2.9243800	2.2145010
C	-2.1471710	-2.6605490	3.4993680
H	-1.2353800	-1.1605230	4.7230250
H	-3.1000590	-3.8788760	2.0135510
C	-6.4411100	1.4858270	-3.2543090
H	-6.8943080	0.5607650	-3.6289270
H	-7.2013130	2.0086880	-2.6670340
H	-6.1947690	2.1023060	-4.1239200
C	-4.3989760	0.7281150	1.2362940
H	-4.5116960	-0.2975550	1.6042410
H	-3.5775290	1.1711900	1.8054560
H	-5.3144300	1.2748040	1.4821430
C	-1.5235660	0.6332760	-3.0345940
H	-0.7494120	1.2661050	-2.5873580
H	-1.1233240	-0.3851600	-3.0630650
H	-1.6710890	0.9650020	-4.0664490
C	-0.8815240	0.8844590	3.1369450
H	0.0242740	1.1836380	2.6028880
H	-1.6122010	1.6873750	2.9849990
H	-0.6410220	0.8611640	4.2035800
C	-2.2498070	-3.6867710	4.5994440
H	-1.3974950	-4.3759520	4.5801700
H	-2.2639500	-3.2116680	5.5845430
H	-3.1572390	-4.2893850	4.4969030
C	-3.1500180	-2.3906480	-0.1348020
H	-4.1895450	-2.0390310	-0.1573300
H	-2.6696260	-1.9652470	-1.0161860
H	-3.1681430	-3.4808560	-0.2394830
C	3.2190290	-1.5094320	-2.8672370

C	3.9983870	-0.4777360	-3.3662660
H	3.3642560	-2.5137790	-3.2500790
H	4.7636730	-0.6929490	-4.1049430
C	2.7754190	1.1109570	-2.0289530
C	3.7774130	0.8390550	-2.9455270
H	2.5765540	2.1346630	-1.7260560
H	4.3756580	1.6488560	-3.3506990
C	2.7755920	2.2748580	1.0352430
C	3.5407570	3.3717520	1.4445000
H	4.5878620	3.2132970	1.6877750
C	1.6131330	4.8241410	1.4277710
C	2.9782980	4.6386630	1.6112650
H	1.1530890	5.7884230	1.6235420
H	3.6013860	5.4658370	1.9358340
C	3.3821130	0.9187040	1.0532620
C	4.6483570	0.6938050	0.5012670
C	2.7058640	-0.1671830	1.6294810
C	5.2108230	-0.5798750	0.4945170
H	5.1766860	1.5203850	0.0330370
C	3.2635930	-1.4407440	1.6217090
H	1.7258730	-0.0178810	2.0744410
C	4.5181160	-1.6539160	1.0499400
H	6.1867930	-0.7343430	0.0442720
H	2.7177000	-2.2679180	2.0663260
H	4.9551490	-2.6482860	1.0447480
C	0.5622700	-4.6197620	-1.4240410
H	0.2570700	-4.7445680	-0.3758590
H	-0.3115440	-4.3607340	-2.0242650
H	0.9649650	-5.5669360	-1.7869770
N	1.5934820	-3.6028700	-1.5649790
C	2.9489400	-4.1010210	-1.3493210
H	3.3241590	-4.6307510	-2.2314270
H	3.6187290	-3.2796870	-1.0991470
H	2.9295480	-4.8026360	-0.5069760

5d (ground-state)

C	-1.9977050	-0.7663210	-2.1800540
C	-0.8516300	-0.4697710	-2.9890820
C	0.3829010	-0.2969590	-2.4366170
C	0.5654840	-0.3134450	-1.0162960
C	-0.5740080	-0.3392170	-0.2277310
C	-1.8616480	-0.7348360	-0.7498720
H	1.2297040	-0.1336890	-3.0929970
C	1.6704780	-0.4051480	2.5506990
C	0.9083310	-0.3693150	3.6775860
C	-0.4514180	0.0392650	3.5811920
C	-1.0092990	0.3043000	2.2956210
C	-0.2123620	-0.0888250	1.1647920
H	2.7349670	-0.6086900	2.5566430
H	1.3472600	-0.5750090	4.6470070
N	1.1142330	-0.2311330	1.3231360
B	1.9060830	-0.1977740	-0.0848940
C	2.9958540	-1.4237850	-0.0090850
C	4.3258670	-1.2014200	0.4262260
C	2.6369850	-2.7653650	-0.2951850
C	5.2441750	-2.2575470	0.4882770

C	3.5813960	-3.7922890	-0.2287840
C	4.9030300	-3.5594240	0.1426190
H	6.2589900	-2.0503910	0.8248470
H	3.2701620	-4.8096210	-0.4616430
C	2.5077900	1.2888220	-0.4825470
C	2.3198340	2.5078670	0.2147510
C	3.1904100	1.3671780	-1.7243740
C	2.7206230	3.7226480	-0.3543370
C	3.5778180	2.5996970	-2.2574180
C	3.3322410	3.8006070	-1.6007980
H	2.5588450	4.6409040	0.2080580
H	4.0967200	2.6161800	-3.2152670
C	5.9156770	-4.6758060	0.1734160
H	6.3289400	-4.8590730	-0.8249800
H	6.7513820	-4.4351120	0.8363340
H	5.4643020	-5.6120890	0.5148650
C	4.8613670	0.1507460	0.8615490
H	5.1236670	0.7831870	0.0065520
H	4.1441890	0.7218680	1.4564070
H	5.7637020	0.0125610	1.4644130
C	1.2243280	-3.1750450	-0.6542470
H	0.4994410	-2.8143880	0.0821490
H	0.9107830	-2.7823730	-1.6267600
H	1.1471000	-4.2651270	-0.6938860
C	1.7955080	2.6060880	1.6361330
H	0.7789440	2.2294090	1.7716550
H	2.4347460	2.0532900	2.3334620
H	1.7961960	3.6502040	1.9596010
C	3.7108460	5.1255580	-2.2121010
H	2.9061060	5.5107720	-2.8488450
H	3.9061960	5.8766090	-1.4413380
H	4.6045610	5.0335260	-2.8361090
C	3.6538370	0.1510770	-2.5077230
H	4.6548280	-0.1511690	-2.1736050
H	3.0211290	-0.7269710	-2.3889000
H	3.7216540	0.3903470	-3.5738390
C	-3.2127760	-1.1347270	-2.7547860
C	-4.2993290	-1.5377370	-1.9696720
H	-3.3072450	-1.1393670	-3.8386690
C	-2.9236430	-1.1912880	0.0267220
C	-4.1371440	-1.5923210	-0.5478580
H	-2.8269490	-1.2454000	1.1075120
C	-2.2596630	1.0056800	2.2129830
C	-2.9798640	1.1937420	3.3774920
H	-3.9137650	1.7453520	3.3305490
C	-1.2370220	0.2383890	4.7419870
C	-2.4974130	0.7677060	4.6322980
H	-0.8128590	-0.0060940	5.7108030
H	-3.1023010	0.9298730	5.5185030
C	-2.7437550	1.6667230	0.9709660
C	-4.0965520	1.6011610	0.6176030
C	-1.8720760	2.4016490	0.1587930
C	-4.5606040	2.2225210	-0.5369090
H	-4.7800490	1.0165780	1.2281510
C	-2.3358820	3.0265250	-0.9947890
H	-0.8206910	2.4830650	0.4197030

C	-3.6798050	2.9333590	-1.3501740
H	-5.6086560	2.1393770	-0.8075610
H	-1.6429660	3.5864950	-1.6149480
H	-4.0393780	3.4131720	-2.2550600
H	-0.9804430	-0.4446860	-4.0684610
C	-5.5531510	-1.9230770	-2.5377960
C	-6.5834220	-2.3330440	-1.7410150
H	-5.6676940	-1.8815700	-3.6177960
H	-7.5330330	-2.6213300	-2.1806580
C	-5.2364340	-2.0329050	0.2522520
C	-6.4225510	-2.3880040	-0.3243580
H	-5.1091260	-2.0705660	1.3314030
H	-7.2531630	-2.7153870	0.2931220

5d (excited-state)

C	-1.9815280	-0.6407430	-2.2157190
C	-0.8533230	-0.2938920	-2.9976300
C	0.4072360	-0.1618670	-2.4208830
C	0.6054640	-0.2746840	-1.0418860
C	-0.5706400	-0.3466080	-0.2163620
C	-1.8395760	-0.7249560	-0.7811500
H	1.2482950	0.0238520	-3.0799040
C	1.6486420	-0.5558910	2.5051170
C	0.8769410	-0.5681800	3.6422480
C	-0.4732020	-0.1115450	3.5846790
C	-1.0333390	0.2253140	2.3078240
C	-0.2412620	-0.1339700	1.1519910
H	2.7108040	-0.7804420	2.5243370
H	1.3188230	-0.8321230	4.5963140
N	1.1331270	-0.2801510	1.3003010
B	1.9383140	-0.1791260	-0.0863330
C	3.0413780	-1.3968540	-0.0527900
C	4.3707640	-1.1823140	0.3863360
C	2.6887970	-2.7312310	-0.3760710
C	5.2969690	-2.2330020	0.4085710
C	3.6392970	-3.7544570	-0.3495320
C	4.9624310	-3.5246870	0.0193250
H	6.3111490	-2.0315940	0.7510530
H	3.3321970	-4.7663470	-0.6108990
C	2.5307660	1.3178170	-0.4470510
C	2.3175410	2.5083350	0.2923920
C	3.2246860	1.4518750	-1.6793990
C	2.7151860	3.7484710	-0.2228180
C	3.6054710	2.7058850	-2.1600570
C	3.3425110	3.8788100	-1.4567290
H	2.5352080	4.6434090	0.3710360
H	4.1343240	2.7666470	-3.1108730
C	5.9825540	-4.6348170	0.0066090
H	6.3875560	-4.7860100	-1.0005740
H	6.8232390	-4.4085380	0.6684240
H	5.5408760	-5.5840410	0.3244810
C	4.8862460	0.1571150	0.8795310
H	5.1365170	0.8329740	0.0545300
H	4.1566920	0.6846900	1.4999620
H	5.7912190	0.0078180	1.4760900
C	1.2728920	-3.1359820	-0.7286500

H	0.5527460	-2.7611080	0.0063410
H	0.9606580	-2.7529220	-1.7054430
H	1.1874210	-4.2262070	-0.7541600
C	1.7549920	2.5400800	1.7008620
H	0.7394020	2.1441820	1.7825260
H	2.3730860	1.9580240	2.3942530
H	1.7345790	3.5694300	2.0691600
C	3.7188940	5.2286310	-2.0121940
H	2.9428650	5.6085830	-2.6867780
H	3.8477250	5.9642840	-1.2132250
H	4.6498420	5.1766940	-2.5846080
C	3.6947200	0.2660090	-2.5029110
H	4.6893470	-0.0551150	-2.1673340
H	3.0542340	-0.6114890	-2.4229810
H	3.7772250	0.5444840	-3.5585480
C	-3.2145860	-0.9426730	-2.7947650
C	-4.3040320	-1.4086060	-2.0286510
H	-3.3360370	-0.8318430	-3.8702650
C	-2.8878390	-1.2353510	-0.0325980
C	-4.1297300	-1.5904620	-0.6231090
H	-2.7691100	-1.3767380	1.0387550
C	-2.2691180	0.9305280	2.2736200
C	-2.9898520	1.0820090	3.4599390
H	-3.9353230	1.6153790	3.4273740
C	-1.2374510	0.0636140	4.7546460
C	-2.4989980	0.6241240	4.6868230
H	-0.8086050	-0.2301770	5.7081650
H	-3.0884660	0.7588830	5.5879260
C	-2.7995850	1.5843370	1.0484800
C	-4.1511180	1.4542320	0.7109820
C	-1.9745280	2.3560120	0.2199320
C	-4.6610490	2.0459260	-0.4424040
H	-4.8001270	0.8467310	1.3371770
C	-2.4821390	2.9501990	-0.9298930
H	-0.9233810	2.4800620	0.4655950
C	-3.8263010	2.7914890	-1.2698440
H	-5.7076300	1.9102850	-0.6983160
H	-1.8254680	3.5388570	-1.5631280
H	-4.2179760	3.2480830	-2.1734870
H	-0.9735300	-0.2069370	-4.0741310
C	-5.5580300	-1.7196890	-2.6105750
C	-6.5926170	-2.1918450	-1.8319040
H	-5.6897960	-1.5814630	-3.6800460
H	-7.5495700	-2.4261970	-2.2865900
C	-5.2036290	-2.0825400	0.1483230
C	-6.4162140	-2.3758370	-0.4439730
H	-5.0641020	-2.2173950	1.2176370
H	-7.2384970	-2.7487580	0.1576230

5e (ground-state)

C	-1.7479450	-1.1208300	-1.9823230
C	-0.7229950	-0.7258730	-2.8515360
C	0.5347570	-0.4021860	-2.3577780
C	0.7684480	-0.3519410	-0.9801030
C	-0.3586570	-0.4610340	-0.1431760
C	-1.5787450	-0.9969660	-0.6050140

H	1.3297780	-0.2100190	-3.0693020
C	1.9492760	-0.2442670	2.5747390
C	1.2088680	-0.1699110	3.7156700
C	-0.1638930	0.1901560	3.6274180
C	-0.7594500	0.3452570	2.3407640
C	0.0239830	-0.1033100	1.2292250
H	3.0222590	-0.3971090	2.5644310
H	1.6768330	-0.2975660	4.6850510
N	1.3555430	-0.1718630	1.3541400
B	2.1207540	-0.1285040	-0.0788000
C	3.2714660	-1.2969870	0.0105690
C	4.6029810	-0.9930500	0.3901430
C	2.9706070	-2.6662870	-0.2055530
C	5.5758430	-1.9987870	0.4553510
C	3.9688010	-3.6411430	-0.1375520
C	5.2901250	-3.3282480	0.1699730
H	6.5897740	-1.7286720	0.7469870
H	3.7011330	-4.6814620	-0.3164920
C	2.6362640	1.3766070	-0.5213820
C	2.4052290	2.6047030	0.1449350
C	3.2789580	1.4528040	-1.7852240
C	2.7302260	3.8213130	-0.4690120
C	3.5906830	2.6858860	-2.3627520
C	3.3047830	3.8927290	-1.7324670
H	2.5352210	4.7464370	0.0710360
H	4.0809160	2.6996320	-3.3356590
C	6.3600510	-4.3897450	0.2009770
H	6.7651850	-4.5684090	-0.8015860
H	7.1935080	-4.0941730	0.8443110
H	5.9641490	-5.3419640	0.5661060
C	5.0839800	0.3972720	0.7651870
H	5.2916350	1.0131710	-0.1163790
H	4.3570680	0.9527890	1.3629700
H	6.0085200	0.3217260	1.3450550
C	1.5672750	-3.1670510	-0.4778090
H	0.8601230	-2.8147480	0.2801470
H	1.1834690	-2.8377580	-1.4481050
H	1.5500010	-4.2602550	-0.4642150
C	1.9064910	2.7204610	1.5739880
H	0.9157000	2.2914480	1.7435640
H	2.5922280	2.2318070	2.2748870
H	1.8509320	3.7732220	1.8626390
C	3.6030050	5.2154780	-2.3912160
H	2.7800480	5.5251600	-3.0455790
H	3.7459540	6.0051130	-1.6481190
H	4.5047520	5.1571020	-3.0078200
C	3.7728670	0.2375590	-2.5512690
H	4.7958210	-0.0118260	-2.2408180
H	3.1829700	-0.6634050	-2.3907620
H	3.7980580	0.4509750	-3.6246520
C	-4.4748380	-1.4590550	-1.5947520
C	-4.2958400	-1.4681820	-0.2098790
C	-2.0198650	1.0223820	2.2280920
C	-2.7099470	1.2969130	3.3924960
H	-3.6466410	1.8420860	3.3314210
C	-0.9277450	0.4608560	4.7888440

C	-2.1955320	0.9677060	4.6651210
H	-0.4796050	0.2967820	5.7636520
H	-2.7831790	1.1920000	5.5493580
C	-2.5291840	1.5769610	0.9443080
C	-3.8980990	1.5467070	0.6625190
C	-1.6729370	2.1912150	0.0187290
C	-4.3954120	2.0438140	-0.5385030
H	-4.5784760	1.0912800	1.3741990
C	-2.1680340	2.7010320	-1.1762460
H	-0.6084050	2.2691690	0.2225600
C	-3.5290330	2.6143070	-1.4674030
H	-5.4581080	1.9671840	-0.7495370
H	-1.4848470	3.1629900	-1.8821550
H	-3.9109370	2.9965820	-2.4088900
H	-0.8965810	-0.7643260	-3.9232590
C	-5.7371070	-1.1872770	-2.1283420
C	-6.8255330	-0.9876950	-1.2853280
H	-5.8621610	-1.1517130	-3.2062330
H	-7.8054380	-0.7944210	-1.7091680
C	-5.3898420	-1.2594780	0.6323090
C	-6.6542330	-1.0377630	0.0973050
H	-5.2408310	-1.2665920	1.7086990
H	-7.5002080	-0.8893350	0.7602600
S	-2.7100430	-1.7694870	0.5292390
S	-3.1658190	-1.9053670	-2.7041020

5e (ground-state, second conformer)

C	2.0839420	0.4225460	-1.9699720
C	0.9805560	0.5657940	-2.8204320
C	-0.3138920	0.5262030	-2.3190320
C	-0.5462440	0.3020550	-0.9573570
C	0.5671220	-0.0427980	-0.1693860
C	1.8901770	0.1336090	-0.6194350
H	-1.1308540	0.7211700	-3.0037940
C	-1.6453350	0.1407360	2.6220250
C	-0.9237460	-0.2396920	3.7145650
C	0.2940420	-0.9494480	3.5306320
C	0.7809310	-1.1560780	2.2059470
C	0.1217580	-0.4164760	1.1752700
H	-2.6323170	0.5856940	2.6792250
H	-1.3104980	-0.0740800	4.7135750
N	-1.1277590	0.0206590	1.3720090
B	-1.8955790	0.3493620	-0.0212340
C	-2.6758060	1.7696760	0.2337160
C	-4.0459390	1.8109080	0.5951990
C	-1.9951610	3.0131360	0.1819140
C	-4.6983580	3.0349500	0.7865500
C	-2.6808500	4.2153310	0.3741280
C	-4.0441270	4.2540060	0.6529580
H	-5.7527160	3.0298550	1.0591970
H	-2.1268480	5.1512990	0.3193560
C	-2.7973790	-0.9150930	-0.5848160
C	-2.9050810	-2.2159770	-0.0335520
C	-3.4322460	-0.7050060	-1.8367220
C	-3.5240910	-3.2457830	-0.7540920
C	-4.0471780	-1.7560040	-2.5208680

C	-4.0826830	-3.0500270	-2.0118970
H	-3.5829860	-4.2350350	-0.3030740
H	-4.5192770	-1.5506940	-3.4811580
C	-4.7747900	5.5623840	0.8163400
H	-5.1249960	5.9397920	-0.1512120
H	-5.6511310	5.4496570	1.4608220
H	-4.1251600	6.3287040	1.2491260
C	-4.8968570	0.5761170	0.8302270
H	-5.2403280	0.1232500	-0.1055950
H	-4.3610210	-0.2074750	1.3724400
H	-5.7806890	0.8454030	1.4158280
C	-0.4995050	3.1255390	-0.0333320
H	0.0567960	2.4671050	0.6415930
H	-0.1994220	2.8637750	-1.0523760
H	-0.1705200	4.1505360	0.1585880
C	-2.4903230	-2.5849810	1.3800190
H	-1.4224650	-2.4765680	1.5864800
H	-3.0227130	-1.9774220	2.1198530
H	-2.7473550	-3.6285020	1.5792170
C	-4.7015000	-4.1852850	-2.7868340
H	-3.9765700	-4.6342000	-3.4755320
H	-5.0524950	-4.9766940	-2.1185450
H	-5.5494350	-3.8406800	-3.3859950
C	-3.5997570	0.6635830	-2.4736870
H	-4.5602800	1.1001690	-2.1697540
H	-2.8385780	1.3868940	-2.1884820
H	-3.6112330	0.5781770	-3.5650870
C	4.3137510	1.8623440	-1.4696520
C	4.0838430	1.6789220	-0.1025830
C	1.8026750	-2.1392340	1.9772110
C	2.4407520	-2.6729730	3.0789340
H	3.1928170	-3.4413420	2.9291210
C	0.9994640	-1.5056910	4.6260480
C	2.0813920	-2.3162140	4.3973950
H	0.6485040	-1.3070150	5.6337110
H	2.6208950	-2.7544140	5.2306580
C	2.0726930	-2.7292500	0.6356720
C	3.3813110	-3.0403880	0.2469220
C	1.0218890	-3.0494770	-0.2348700
C	3.6365370	-3.6228090	-0.9903660
H	4.2076430	-2.7885670	0.9053040
C	1.2762490	-3.6318680	-1.4717680
H	-0.0067140	-2.8417820	0.0472300
C	2.5851810	-3.9143280	-1.8569190
H	4.6597100	-3.8388270	-1.2809720
H	0.4467590	-3.8648530	-2.1320570
H	2.7846700	-4.3621520	-2.8253590
H	1.1524150	0.7749790	-3.8720670
C	5.0165530	2.9827430	-1.9143700
C	5.5176950	3.8982210	-0.9937620
H	5.1711620	3.1282460	-2.9789650
H	6.0765680	4.7600760	-1.3432960
C	4.5550630	2.6207720	0.8141340
C	5.2852830	3.7186180	0.3688460
H	4.3546490	2.4839690	1.8722470
H	5.6611210	4.4401370	1.0867570

S	3.2789620	0.2125270	0.5021310
S	3.7227280	0.6524800	-2.6295430

5e (excited-state)

C	-1.8471640	-0.0949730	-2.1085160
C	-0.7673990	0.3584470	-2.8752660
C	0.5246100	0.3091780	-2.3460040
C	0.7759360	-0.0700600	-1.0174180
C	-0.3534320	-0.2427170	-0.1847620
C	-1.6318500	-0.4793920	-0.7608860
H	1.3408860	0.6035320	-2.9966870
C	1.9004180	-0.9273270	2.4521430
C	1.1423110	-1.0905730	3.5759400
C	-0.2173160	-0.6208610	3.5927470
C	-0.7749620	-0.1027010	2.3830860
C	0.0109220	-0.2954260	1.1912960
H	2.9617430	-1.1560610	2.4282700
H	1.5862200	-1.4837170	4.4828310
N	1.3759560	-0.4801970	1.2914770
B	2.1372810	-0.1761470	-0.0799670
C	3.2129650	-1.3994290	-0.2834000
C	4.5615330	-1.2806760	0.1307410
C	2.8146180	-2.6608470	-0.7912390
C	5.4611290	-2.3399790	-0.0456300
C	3.7383660	-3.6950530	-0.9595420
C	5.0796810	-3.5501290	-0.6132980
H	6.4920010	-2.2133970	0.2827820
H	3.3957600	-4.6489400	-1.3586860
C	2.7452810	1.3524570	-0.2347090
C	2.5898430	2.4174530	0.6876640
C	3.3946080	1.6618460	-1.4592260
C	3.0057930	3.7118920	0.3554900
C	3.7968950	2.9668670	-1.7544900
C	3.5939770	4.0196040	-0.8677590
H	2.8737440	4.5073900	1.0875400
H	4.2923160	3.1624330	-2.7050920
C	6.0711440	-4.6641550	-0.8358660
H	6.4609630	-4.6465030	-1.8601540
H	6.9251710	-4.5761200	-0.1583680
H	5.6094420	-5.6438790	-0.6809010
C	5.1251490	-0.0424900	0.8025390
H	5.3592650	0.7484400	0.0816230
H	4.4296430	0.3937390	1.5246500
H	6.0480690	-0.2966490	1.3325420
C	1.3748690	-2.9745590	-1.1382870
H	0.7013300	-2.7169560	-0.3134870
H	1.0281070	-2.4217110	-2.0176970
H	1.2593640	-4.0421670	-1.3463110
C	2.0775190	2.2412250	2.1053110
H	1.0580610	1.8532620	2.1639430
H	2.7077310	1.5480750	2.6734540
H	2.0957060	3.2016550	2.6279320
C	3.9883870	5.4317110	-1.2183020
H	3.1782810	5.9491510	-1.7452970
H	4.2185570	6.0136500	-0.3212200
H	4.8650180	5.4481060	-1.8725270

C	3.7960500	0.6084500	-2.4760280
H	4.7898900	0.2103180	-2.2338390
H	3.1291740	-0.2528650	-2.5095800
H	3.8524060	1.0478720	-3.4773480
C	-4.5334880	-0.8309180	-1.8227100
C	-4.2262220	-1.4828600	-0.6166160
C	-2.0173990	0.5975740	2.4340430
C	-2.7534530	0.5674380	3.6213400
H	-3.7007700	1.0970200	3.6626970
C	-0.9903680	-0.6148780	4.7649690
C	-2.2618030	-0.0607020	4.7666830
H	-0.5706470	-1.0383160	5.6729970
H	-2.8555090	-0.0642850	5.6754050
C	-2.5090040	1.4570310	1.3220540
C	-3.8542290	1.4208270	0.9332900
C	-1.6488440	2.3337260	0.6453860
C	-4.3190580	2.2033640	-0.1213270
H	-4.5355090	0.7398230	1.4385770
C	-2.1117700	3.1214880	-0.4036250
H	-0.6011310	2.3856080	0.9276820
C	-3.4472150	3.0539020	-0.7984360
H	-5.3613200	2.1358440	-0.4203010
H	-1.4231990	3.7858260	-0.9168500
H	-3.8052980	3.6585290	-1.6259510
H	-0.9371970	0.7141150	-3.8865890
C	-5.8692760	-0.7975310	-2.2646130
C	-6.8669380	-1.4118560	-1.5348770
H	-6.1061880	-0.2853550	-3.1925370
H	-7.8907930	-1.3761460	-1.8900410
C	-5.2541960	-2.1129550	0.1121790
C	-6.5568520	-2.0803780	-0.3403800
H	-5.0087460	-2.6104580	1.0459000
H	-7.3388430	-2.5635190	0.2344870
S	-2.6573120	-1.5459760	0.1329330
S	-3.3839630	-0.1034960	-2.9127130

5e (excited-state, second conformer)

C	1.9635510	0.4571970	-1.9038410
C	0.8861770	0.3912920	-2.7993830
C	-0.4108780	0.2587920	-2.3082930
C	-0.6419820	0.1548440	-0.9329380
C	0.4708850	-0.0577640	-0.0632250
C	1.7608880	0.2869760	-0.5266910
H	-1.2270920	0.2738060	-3.0197410
C	-1.7574990	0.1113030	2.6871260
C	-1.0354840	-0.2354640	3.7897910
C	0.2330620	-0.9017990	3.6356120
C	0.7562330	-1.0811140	2.3163880
C	0.0656800	-0.3908340	1.2603220
H	-2.7614840	0.5209100	2.7494860
H	-1.4463670	-0.0852650	4.7811290
N	-1.2536270	-0.0126970	1.4370030
B	-2.0081840	0.2461040	0.0825500
C	-2.8995190	1.5872980	0.2195800
C	-4.2732910	1.5056070	0.5423990
C	-2.3242520	2.8757960	0.1328140

C	-5.0362890	2.6685330	0.6914060
C	-3.1165050	4.0167990	0.2780940
C	-4.4828720	3.9368800	0.5394960
H	-6.0918290	2.5789890	0.9436200
H	-2.6492130	4.9973640	0.2003470
C	-2.6296790	-1.0623630	-0.6224130
C	-2.5089090	-2.4122560	-0.1274190
C	-3.2226450	-0.9048560	-1.9337750
C	-2.8089690	-3.4862040	-0.9578490
C	-3.5164430	-2.0108980	-2.7110930
C	-3.2722710	-3.3173270	-2.2651620
H	-2.7090660	-4.4962820	-0.5672310
H	-3.9506990	-1.8662000	-3.6979230
C	-5.3278600	5.1797150	0.6595080
H	-5.6756420	5.5141610	-0.3245620
H	-6.2123990	4.9999350	1.2768030
H	-4.7607980	6.0038240	1.1019060
C	-4.9851020	0.1858280	0.7677350
H	-5.2120610	-0.3324510	-0.1710540
H	-4.3902890	-0.5066320	1.3717550
H	-5.9323040	0.3528770	1.2880600
C	-0.8411380	3.0757680	-0.0883460
H	-0.2489310	2.4865510	0.6204260
H	-0.5290470	2.7709180	-1.0933370
H	-0.5751760	4.1283920	0.0418240
C	-2.2253160	-2.7475450	1.3191730
H	-1.2035750	-2.5325290	1.6404700
H	-2.8860510	-2.1852900	1.9871780
H	-2.4071450	-3.8116800	1.4877270
C	-3.5265300	-4.4944560	-3.1603340
H	-2.6798710	-4.6403290	-3.8419380
H	-3.6522460	-5.4144610	-2.5849250
H	-4.4155590	-4.3372290	-3.7774070
C	-3.6078600	0.4452170	-2.4949200
H	-4.5693290	0.7655590	-2.0756880
H	-2.8983570	1.2381240	-2.2569380
H	-3.7212160	0.3823390	-3.5807150
C	4.1237760	2.0562820	-1.4735480
C	3.8610120	2.0069460	-0.1012150
C	1.8514310	-1.9747420	2.1221630
C	2.5212680	-2.4587070	3.2468440
H	3.3597960	-3.1339260	3.1039380
C	0.9343920	-1.4212650	4.7337690
C	2.0929950	-2.1579240	4.5419770
H	0.5459100	-1.2505850	5.7337750
H	2.6359100	-2.5532960	5.3944660
C	2.2414340	-2.5123010	0.7869260
C	3.5899200	-2.6357970	0.4305420
C	1.2744210	-2.9657540	-0.1215250
C	3.9602050	-3.1612390	-0.8047900
H	4.3544130	-2.2820790	1.1165440
C	1.6404120	-3.4903660	-1.3555290
H	0.2214200	-2.8963200	0.1323170
C	2.9867330	-3.5836460	-1.7068420
H	5.0119790	-3.2296410	-1.0652800
H	0.8692080	-3.8265470	-2.0425120

H	3.2741670	-3.9855480	-2.6734980
H	1.0650260	0.5005700	-3.8632190
C	4.8380340	3.1292150	-2.0104910
C	5.3158160	4.1338680	-1.1757050
H	5.0172490	3.1692880	-3.0804620
H	5.8807040	4.9587030	-1.5971830
C	4.3127220	3.0388320	0.7260000
C	5.0511640	4.0894610	0.1924150
H	4.0879120	3.0063940	1.7876340
H	5.4086830	4.8797640	0.8441360
S	3.0557470	0.6135300	0.6438660
S	3.5820140	0.7570470	-2.5570030

5f (ground-state)

C	2.3252520	-1.5911770	-0.0755520
C	1.4320070	-2.2904780	0.7858100
C	0.0845780	-1.9115440	0.8440040
C	-0.3926260	-0.8087770	0.1384500
C	0.5641620	0.0081460	-0.5008220
C	1.8864810	-0.4234800	-0.7524460
H	-0.5803190	-2.5244390	1.4445310
C	-2.2152710	1.9084450	-1.6854500
C	-1.7024280	2.9802020	-2.3522650
C	-0.3430830	3.3418490	-2.1412630
C	0.4758270	2.5106240	-1.3214000
C	-0.0779240	1.2370540	-0.9596930
H	-3.2640390	1.6353170	-1.7095810
H	-2.3396720	3.5986170	-2.9737890
N	-1.4102010	1.0775070	-0.9739300
B	-1.8949460	-0.1782060	-0.0663540
C	-3.0221200	-0.9603790	-0.9698040
C	-4.4075950	-0.7067680	-0.8091100
C	-2.6594700	-1.8646850	-2.0004110
C	-5.3552620	-1.3938930	-1.5783620
C	-3.6327280	-2.5364740	-2.7441730
C	-4.9942530	-2.3349660	-2.5350720
H	-6.4114220	-1.1764880	-1.4255220
H	-3.3151470	-3.2290360	-3.5223730
C	-2.3494440	0.2442480	1.4644550
C	-2.2774890	1.5233350	2.0679860
C	-2.7417990	-0.8305230	2.3052940
C	-2.5002960	1.6768990	3.4428090
C	-2.9602920	-0.6364840	3.6710530
C	-2.8211810	0.6099240	4.2734700
H	-2.4316000	2.6743150	3.8741770
H	-3.2569740	-1.4894540	4.2806970
C	-6.0295850	-3.0982480	-3.3212980
H	-6.2309410	-4.0732880	-2.8630610
H	-6.9768550	-2.5534200	-3.3636980
H	-5.6930990	-3.2837640	-4.3456000
C	-4.9770440	0.3102430	0.1636100
H	-5.0143100	-0.0743830	1.1883710
H	-4.3922370	1.2327430	0.2036770
H	-5.9971050	0.5714240	-0.1331320
C	-1.2200280	-2.1327880	-2.3867590
H	-0.6667080	-1.2031410	-2.5521050

H	-0.6779510	-2.6911630	-1.6174150
H	-1.1818600	-2.7133020	-3.3127280
C	-2.0751780	2.8194760	1.3034730
H	-1.1284580	2.8845290	0.7615040
H	-2.8738480	2.9761990	0.5700130
H	-2.1056110	3.6655490	1.9949420
C	-3.0108400	0.7925380	5.7578450
H	-2.0933930	0.5494820	6.3060970
H	-3.2737970	1.8262390	5.9995650
H	-3.8006710	0.1392540	6.1404920
C	-3.0631650	-2.2233720	1.7914480
H	-4.1270530	-2.2889360	1.5283830
H	-2.5144210	-2.5071130	0.8951520
H	-2.8710390	-2.9691290	2.5695840
C	3.6583520	-2.0707710	-0.2561660
C	4.5252150	-1.4313550	-1.1810290
C	2.7695070	0.1703270	-1.7219550
C	4.0169660	-0.3195460	-1.9350640
H	2.4153660	1.0068090	-2.3151270
H	4.6599580	0.1314830	-2.6863840
C	1.7301470	3.0194040	-0.8420550
C	2.1984090	4.2020490	-1.3808110
H	3.1312500	4.6137630	-1.0079720
C	0.1921910	4.5373710	-2.6796370
C	1.4591300	4.9333920	-2.3351120
H	-0.4263430	5.1413850	-3.3360230
H	1.8725280	5.8528410	-2.7366330
C	2.4618630	2.4220170	0.3085600
C	3.8567000	2.3156960	0.2822730
C	1.7780460	2.0029950	1.4571190
C	4.5486700	1.7720020	1.3598780
H	4.3973780	2.6219730	-0.6091250
C	2.4686570	1.4608090	2.5356640
H	0.6962440	2.0899800	1.5114980
C	3.8558550	1.3365180	2.4875350
H	5.6289950	1.6771060	1.3123560
H	1.9189550	1.1347330	3.4129990
H	4.3942810	0.9044050	3.3251630
C	1.9276610	-3.4268460	1.5200650
C	3.2068860	-3.8525750	1.3831460
H	1.2420130	-3.9412520	2.1879950
H	3.5677010	-4.7102080	1.9446240
C	4.1175040	-3.1988300	0.4774130
C	5.4304420	-3.6445610	0.2925890
H	5.7826080	-4.5014720	0.8605220
C	6.2785280	-3.0069600	-0.6105320
C	5.8302820	-1.9157200	-1.3459930
H	7.2930600	-3.3685500	-0.7444170
H	6.4893910	-1.4272960	-2.0586930

5f (excited-state)

C	2.3622040	-1.4397810	-0.4206360
C	1.5084260	-2.2785710	0.3528280
C	0.1094570	-1.9646820	0.4445310
C	-0.4274830	-0.8236240	-0.0991380
C	0.5184420	0.1458790	-0.5875370

C	1.8632550	-0.2299330	-0.9565800
H	-0.5141410	-2.6772300	0.9784720
C	-2.2127720	2.2630790	-1.1765110
C	-1.6737920	3.4690590	-1.5703950
C	-0.3137480	3.7743710	-1.2629050
C	0.4962650	2.7490020	-0.6801740
C	-0.0793010	1.4226850	-0.6598030
H	-3.2722590	2.0459630	-1.2748270
H	-2.3102510	4.2246670	-2.0167760
N	-1.4619480	1.2853210	-0.6553620
B	-1.9368920	-0.1474160	-0.0983610
C	-3.0859800	-0.6705780	-1.1529760
C	-4.4619430	-0.4200470	-0.9258340
C	-2.7545750	-1.3143840	-2.3720640
C	-5.4326150	-0.8658630	-1.8321670
C	-3.7489380	-1.7520930	-3.2505400
C	-5.1030830	-1.5575120	-2.9917140
H	-6.4808820	-0.6563860	-1.6231180
H	-3.4543200	-2.2486290	-4.1741610
C	-2.3718140	-0.1678270	1.4917960
C	-2.2826820	0.9058940	2.4096430
C	-2.7748190	-1.4220660	2.0183330
C	-2.5229570	0.6993330	3.7743420
C	-3.0070140	-1.5901950	3.3856490
C	-2.8697920	-0.5432480	4.2926400
H	-2.4442540	1.5472460	4.4533470
H	-3.3131310	-2.5702920	3.7505880
C	-6.1629570	-2.0691280	-3.9340660
H	-6.3957140	-3.1208420	-3.7314000
H	-7.0922350	-1.5016650	-3.8315800
H	-5.8336610	-2.0041890	-4.9753940
C	-4.9920330	0.3415420	0.2750520
H	-5.0429220	-0.2878480	1.1702210
H	-4.3694600	1.2007830	0.5376220
H	-6.0014650	0.7074430	0.0644820
C	-1.3244880	-1.5390870	-2.8155090
H	-0.7385310	-0.6148040	-2.7707550
H	-0.8055950	-2.2737270	-2.1919570
H	-1.3019170	-1.8984090	-3.8482550
C	-2.0222170	2.3452160	2.0058660
H	-1.0703590	2.4959880	1.4896970
H	-2.8035430	2.7227330	1.3361600
H	-2.0174990	2.9853970	2.8923930
C	-3.0802680	-0.7506650	5.7712500
H	-2.1610690	-1.0976310	6.2573720
H	-3.3797550	0.1791180	6.2633620
H	-3.8520390	-1.5026230	5.9606910
C	-3.0757870	-2.6285400	1.1467440
H	-4.1142230	-2.5917620	0.7934210
H	-2.4549980	-2.6922000	0.2526300
H	-2.9542450	-3.5523160	1.7216350
C	3.7023090	-1.8265570	-0.6770170
C	4.5121070	-1.0457790	-1.5469350
C	2.6569910	0.5005510	-1.8666000
C	3.9430900	0.0998030	-2.1636250
H	2.2458280	1.3901110	-2.3348460

H	4.5445790	0.6737590	-2.8630200
C	1.7476360	3.0913350	-0.1032990
C	2.2447600	4.3787870	-0.3127920
H	3.2038360	4.6446300	0.1222280
C	0.2309270	5.0600520	-1.4531200
C	1.5105750	5.3440960	-1.0122380
H	-0.3771470	5.8247490	-1.9272070
H	1.9293950	6.3346300	-1.1582070
C	2.5015300	2.1607550	0.7813050
C	3.8776690	1.9777860	0.6134030
C	1.8520500	1.4517090	1.8010460
C	4.5796330	1.0745940	1.4079080
H	4.3915730	2.5117830	-0.1818810
C	2.5524850	0.5533290	2.5993240
H	0.7861300	1.5872080	1.9619350
C	3.9171950	0.3523470	2.3979760
H	5.6418020	0.9231150	1.2398810
H	2.0270590	0.0043910	3.3748960
H	4.4602900	-0.3628520	3.0080850
C	2.0564670	-3.4394110	0.9444180
C	3.3787490	-3.7808680	0.7631020
H	1.4102030	-4.0736150	1.5450960
H	3.7825590	-4.6732830	1.2328910
C	4.2317760	-2.9973430	-0.0661740
C	5.5739980	-3.3464680	-0.3157210
H	5.9829700	-4.2373080	0.1531680
C	6.3695460	-2.5730640	-1.1597160
C	5.8501100	-1.4430530	-1.7767370
H	7.3994160	-2.8620540	-1.3413200
H	6.4685230	-0.8492500	-2.4440440

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