Supporting Information

for

Planar chiral [2.2]paracyclophanyl-based boron fluoride complexes: synthesis, crystal structure and photophysical properties

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1. Experimental section

Materials and measurements

All the solvents were of analytical grade. Column flash chromatography was carried out on silica gel (200–400 *mesh*). Thin-layer chromatography (TLC) was performed on *silica gel GF254.* The fluorescence spectra were measured on a *F-4600 spectrofluorimeter (Hitachi, Japan)* luminescence spectrophotometer (the pathlength of the quartz cell is 1 cm) with a xenon arc lamp as the light source. Absorbance spectra measurements were performed on a *T9CS UV–vis spectrophotometer (Persee Instrument Co., Ltd. Beijing, China)*. ^{1}H and ^{13}C NMR spectra were recorded on a *Varian Mercury-plus 400MHz spectrometer* and a Bruker AVANCE NEO 500 MHz spectrometer and referenced to the residual proton signals of the solvent. HRMS spectra were recorded on an *Agilent 100 ABI-API4000 spectrometer*. X-ray data were collected on *Bruker Smart APEX II CCD* diffractometer. Ground-state geometry optimizations were performed by DFT by using the B3LYP functional and 6-31G(d) basis sets of the Gaussian 09 software package. The polarized continuum model (PCM) was used to provide an THF solvation environment.

Synthesis procedures

Complexes (R_p, *R*)/(S_p, *R*)-**3a**; (R_p)/(S_p)-**3b**; (R_p, *S*)/(S_p, *S*)-**3c** and (R_p)/(S_p)-**3d** were readily prepared according to Scheme 1.

The resolution of (R_p)/(S_p)-**1**.[1-2]

Compound **1**[3] (3.75 mmol) was dissolved in dry toluene (10 mL), and (*R*)-α-phenylethylamine (4 mmol) was added at room temperature and refluxed at 150 ° C for 16 hours. After cooling to temperature, the reaction solvent was removed by rotary evaporation. The crude material was resolution by column chromatography on silica gel (eluent: from petroleum ether/CH_2Cl_2 = 1:3 to CH_2Cl_2/ethyl acetate = 20:1) to give compounds (R_p, *R*)-**2a** (yield: 37%) *and* (S_p, *R*)-**2a** (yield: 32%).

(R_p, *R*)-**2a:** ^{1}H NMR (400 MHz, $CDCl_3$) δ 15.98 (s, 1H), 7.58 – 7.52 (m, 1H), 7.47 (t, *J* = 7.7 Hz, 1H), 7.41 – 7.32 (m, 2H), 7.27 (dt, *J* = 5.7, 2.8 Hz, 1H), 7.06 (ddd, *J* = 18.7, 7.7, 1.9 Hz, 1H), 6.62 (ddd, *J* = 21.8, 7.9, 2.0 Hz, 1H), 6.55 – 6.40 (m, 3H), 6.21 (dd, *J* = 7.5, 5.8 Hz, 1H), 4.90 (dq, *J* = 8.5, 6.6 Hz, 1H), 3.54 – 3.35 (m, 1H), 3.32 – 2.80 (m, 5H), 2.71 – 2.50 (m, 2H), 2.29 (d, *J* = 3.8 Hz, 3H), 1.74 (dd, *J* = 28.2, 6.6 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 170.33, 163.31, 143.72, 140.77, 140.05, 137.59, 136.13, 132.74, 131.43, 129.66, 129.56, 128.83, 127.17, 127.14, 126.25, 125.60, 122.20, 58.17, 37.36, 35.46, 33.89, 30.46, 25.43, 20.46; HRMS(ESI): calcd: $[M+H]^+$ = 370.2171, found: $[M+H]^+$ = 370.2161.

(S_p, *R*)-**2a:** ^{1}H NMR (400 MHz, $CDCl_3$) δ 15.93 (s, 1H), 7.59 – 7.52 (m, 2H), 7.47 (td, *J* = 7.7, 1.8 Hz, 2H), 7.35 (tt, *J* = 7.3, 1.5 Hz, 1H), 7.02 (dt, *J* = 7.8, 2.3 Hz, 1H), 6.59 (dt, *J* = 7.8, 1.9 Hz, 1H), 6.54 – 6.39 (m, 2H), 6.25 – 6.06 (m, 2H), 4.88 (d, *J* = 6.6 Hz, 1H), 3.45 (ddt, *J* = 12.8, 10.2, 2.4 Hz, 1H), 3.33 – 3.13 (m, 2H), 3.11 – 2.92 (m, 2H), 2.85 (ddd, *J* = 13.9, 9.6, 7.1 Hz, 1H), 2.56 (ddtd, *J* = 12.9, 10.7, 6.3, 5.2, 1.8 Hz, 1H), 2.40 (ddd, *J* = 12.5, 9.0, 6.9 Hz, 1H), 2.29 (s, 3H), 1.70 (dd, *J* = 6.6, 1.6 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 170.10, 163.22, 144.55, 140.85, 139.92, 137.61, 136.24, 132.63, 131.44, 130.18, 129.44, 128.83, 127.30, 127.04, 126.46, 125.60, 122.22, 58.08, 37.21, 35.36, 33.88, 30.47, 24.96, 20.38; HRMS(ESI): calcd: $[M+H]^+$ = 370.2171, found: $[M+H]^+$ = 370.2163.

Then (R_p, *R*)-**2a** or (S_p, *R*)-**2a** was dissolved in tetrahydrofuran (15 mL), hydrochloric acid (1 mol/L, 24 mmol) was added dropwise at 0 °C, and the reaction was refluxed for 15 h. After cooling to temperature, the reaction solvent was removed by rotary evaporation. Then the reaction mixture was dissolved in CH_2Cl_2 (15 mL) and washed three times with water (3 × 10 mL). The organic layer was separated, dried over $MgSO_4$ and evaporated in vacuo. The residue was purified by column chromatography on silica gel (petroleum ether/CH_2Cl_2 = 3:1) to give the product (R_p)-**1** (yield: 70 %) or (S_p)-**1** (yield: 68%) as a yellow powder.

Compound **1:** ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.88 (s, 1H), 6.97 (dd, *J* = 7.8, 1.5 Hz, 1H), 6.62 (d, *J* = 7.9 Hz, 1H), 6.54 (t, *J* = 7.5 Hz, 1H), 6.47 (dd, *J* = 19.7, 7.0 Hz, 2H), 6.31 (d, *J* = 7.5 Hz, 1H), 3.64 (dd, *J* = 14.0, 9.5 Hz, 1H), 3.42 (ddd, *J* = 13.1, 10.4, 2.8 Hz, 1H), 3.27 – 2.89 (m, 5H), 2.79 – 2.64 (m, 1H), 2.57 (s, 3H).

The synthesis of (R_p, *R*)/(S_p, *R*)-**3a**; (R_p)/(S_p)-**3b**; (R_p, *S*)/(S_p, *S*)-**3c** and (R_p)/(S_p)-**3d.**

The synthesis method of (R_p)/(S_p)-**2b** *and* (R_p)/(S_p)-**2d** follows the same procedure of (R_p, *R*)/(S_p, *R*)-**2a** with the compound (R_p)-**1** *or* (S_p)-**1** with benzylamine and ethanolamine**.**

(R_p)-**2b**: Yield: 65%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (d, *J* = 6.7 Hz, 4H), 7.35 (t, *J* = 6.5 Hz, 1H), 6.99 (d, *J* = 7.7 Hz, 1H), 6.63 (d, *J* = 7.8 Hz, 1H), 6.48 (dd, *J* = 23.0, 7.7 Hz, 2H), 6.35 (d, *J* = 7.7 Hz, 1H), 6.23 (d, *J* = 7.5 Hz, 1H), 4.87 – 4.71 (m, 2H), 3.49 – 3.32 (m, 2H), 3.22 – 2.86 (m, 4H), 2.73 – 2.48 (m, 2H), 2.38 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.20, 162.42, 140.81, 140.08, 138.70, 137.65, 136.30, 132.65, 131.60, 129.98, 129.35, 128.85, 127.51, 127.26, 127.24, 125.72, 53.21, 37.16, 35.48, 33.90, 30.46, 20.87; HRMS(ESI): calcd: $[M+H]^+$ = 356.2014, found: $[M+H]^+$ = 356.2030.

(S_p)-**2b:** Yield: 65%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 (d, *J* = 6.8 Hz, 4H), 7.38 – 7.32 (m, 1H), 6.98 (dd, *J* = 7.7, 1.6 Hz, 1H), 6.63 (dd, *J* = 7.9, 1.7 Hz, 1H), 6.50 (dd, *J* = 7.8, 1.5 Hz, 2H), 6.45 (d, *J* = 7.5 Hz, 1H), 6.34 (dd, *J* = 7.8, 1.7 Hz, 1H), 4.78 (d, *J* = 4.7 Hz, 2H), 3.48 – 3.33 (m, 2H), 3.21 – 2.90 (m, 4H), 2.64 (ddd, *J* = 14.1, 10.0, 7.5 Hz, 2H), 2.39 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.18, 162.42, 140.80, 140.07, 138.70, 137.65, 136.29, 132.65, 131.60, 129.97, 129.34, 128.85, 127.50, 127.26, 127.24, 125.71, 122.60, 53.21, 37.15, 35.48, 33.90, 30.46, 20.86; HRMS(ESI): calcd: $[M+H]^+$ = 356.2014, found: $[M+H]^+$ = 356.2015.

(R_p)-**2d:** Yield: 89%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.95 (dd, *J* = 7.8, 1.9 Hz, 1H), 6.60 (dd, *J* = 7.8, 2.0 Hz, 1H), 6.47 (dd, *J* = 7.8, 1.9 Hz, 1H), 6.41 (d, *J* = 7.5 Hz, 1H), 6.33 (dd, *J* = 7.8, 2.0 Hz, 1H), 6.19 (d, *J* = 7.5 Hz, 1H), 4.05 (t, *J* = 5.4 Hz, 2H), 3.67 (q, *J* = 5.6 Hz, 2H), 3.36 (dddd, *J* = 14.6, 11.9, 9.9, 2.7 Hz, 2H), 3.20 – 2.85 (m, 4H), 2.64 (ddd, *J* = 13.1, 9.4, 7.0 Hz, 1H), 2.51 (ddd, *J* = 12.9, 10.6, 5.2 Hz, 1H), 2.30 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 13C NMR (126 MHz, $CDCl_3$) δ 172.05, 161.43, 139.79, 138.99, 136.66, 135.33, 131.62, 130.61, 128.81, 128.30, 126.14, 124.69, 121.38, 61.44, 50.27, 36.08, 34.39, 32.86, 29.40, 19.84; HRMS (ESI): calcd: $[M+H]^+$ = 310.1807, found: $[M+H]^+$ = 310.1799

(S_p)-**2d:** Yield: 89%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.13 – 7.02 (m, 1H), 6.69 – 6.52 (m, 3H), 6.39 – 6.17 (m, 2H), 4.34 – 4.16 (m, 1H), 4.09 – 3.87 (m, 3H), 3.56 (dddd, *J* = 23.9, 13.6, 10.4, 3.8 Hz, 1H), 3.36 – 3.11 (m, 3H), 3.11 – 2.89 (m, 3H), 2.63 (s, 3H), 2.43 (s, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.05, 161.42, 139.79, 138.99, 136.66, 135.33, 131.62, 130.61, 128.81, 128.29, 126.14, 124.69, 121.38, 61.44, 50.28, 36.08, 34.39, 32.86, 29.40, 19.84; HRMS(ESI): calcd: $[M+H]^+$ = 310.1807, found: $[M+H]^+$ = 310.1797.

The synthesis method of (R_p, *S*)/(S_p, *S*)-**2c.**[4-5]

Compound **1** was dissolved in dry toluene (10 mL), and (*S*)-*tert*-Leucinol (4 mmol) was added at room temperature and refluxed for 36 h. After cooling to temperature, the reaction solvent was removed by rotary evaporation. The residue was purified by column chromatography on silica gel (CH_2Cl_2 to CH_2Cl_2/ ethyl acetate = 5:1) to give the products (R_p, *S*)-**2c** (yield: 42 %) and (S_p, *S*)-**2c** (yield: 45 %) as brownish yellow solid.

(R_p, *S*)-**2c:** Yield: 42%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.95 (dd, *J* = 7.8, 1.9 Hz, 1H), 6.64 (dd, *J* = 7.9, 2.0 Hz, 1H), 6.51 (dd, *J* = 7.9, 1.9 Hz, 1H), 6.42 – 6.34 (m, 2H), 6.17 (dt, *J* = 5.5, 2.7 Hz, 1H), 3.97 – 3.92 (m, 1H), 3.82 – 3.75 (m, 1H), 3.66 (dd, *J* = 7.3, 5.1 Hz, 1H), 3.35 (dddd, *J* = 26.2, 12.6, 9.5, 4.9 Hz, 2H), 3.15 (ddd, *J* = 12.9, 10.2, 5.3 Hz, 1H), 3.10 – 2.87 (m, 4H), 2.77 – 2.65 (m, 1H), 2.56 – 2.44 (m, 1H), 2.35 (d, *J* = 2.0 Hz, 3H), 1.15 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.49, 164.58, 141.10, 140.19, 137.75, 136.73, 132.63, 131.76, 130.53, 129.58, 127.11, 125.34, 122.18, 68.68, 63.42, 37.29, 35.58, 34.09, 33.93, 30.49, 27.14, 20.63; HRMS(ESI): calcd: $[M+H]^+$ = 366.2433, found: $[M+H]^+$ = 366.2423.

(S_p, S)-**2c:** Yield: 45%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.97 (dd, J = 7.8, 1.9 Hz, 1H), 6.61 (dd, J = 7.9, 1.9 Hz, 1H), 6.47 (dd, J = 7.9, 1.9 Hz, 1H), 6.44 – 6.40 (m, 2H), 6.21 (d, J = 7.5 Hz, 1H), 4.14 (dd, J = 10.2, 2.9 Hz, 1H), 3.89 – 3.84 (m, 1H), 3.65 (dd, J = 9.2, 2.9 Hz, 1H), 3.45 – 3.38 (m, 2H), 3.19 – 2.83 (m, 5H), 2.67 (ddd, J = 13.2, 9.3, 7.6 Hz, 1H), 2.51 (ddd, J = 13.0, 10.7, 5.0 Hz, 1H), 2.34 (s, 3H), 1.03 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.16, 162.37, 141.01, 139.93, 137.92, 135.93, 132.75, 131.43, 129.99, 129.28, 127.02, 125.73, 122.54, 69.19, 63.95, 37.60, 35.24, 33.92, 33.85, 30.27, 27.08, 20.89;HRMS(ESI): calcd: $[M+H]^+$ = 366.2433, found: $[M+H]^+$ = 366.2428.

The synthesis of (R_p, R)/(S_p, R)-**3a**; (R_p)/(S_p)-**3b**; (R_p, S)/(S_p, S)-**3c** and (R_p)/(S_p)-**3d.**

Compound (R_p, R) -**2a** or (S_p, R)-**2a** or (R_p)-**2b** or (S_p)-**2b** or (R_p, S) -**2c** or (S_p, S)-**2c** or (R_p)-**2d** or (S_p)-**2d** (1.0 mmol) in was dissolved in dry toluene (15 mL), and Et_3N (0.3 mL) was added. After the mixture was stirred for 15 min, $BF_3 \cdot Et_2O$ (1.28 mL) was added dropwise, and further stirred at room temperature for 3 h. The reaction solvent was removed by rotary evaporation. The residue was dissolved in CH_2Cl_2 (15 mL) and washed three times with water (3 × 10 mL). The organic layer was separated, dried over $MgSO_4$ and evaporated in vacuo. The residue was purified by column chromatography on silica gel (petroleum ether/CH_2Cl_2 = 3:1 to CH_2Cl_2/ ethyl acetate = 5:1) to give the corresponding product as yellow solid compound.

(R_p, R)-**3a:** Yield: 43%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.33 (ddd, J = 25.4, 16.3, 7.8 Hz, 5H), 7.14 (dd, J = 14.7, 7.7 Hz, 1H), 6.65 (d, J = 7.8 Hz, 1H), 6.62 – 6.55 (m, 2H), 6.42 – 6.38 (m, 1H), 6.24 (dd, J = 14.3, 7.4 Hz, 1H), 3.58 (ddt, J = 15.1, 9.1, 4.4 Hz, 1H), 3.36 – 3.27 (m, 1H), 3.19 (ddt, J = 21.3, 14.0, 8.4 Hz, 2H), 2.99 (dtd, J = 27.7, 13.0, 11.2, 5.4 Hz, 3H), 2.76 (ddd, J = 12.7, 9.0, 6.9 Hz, 1H), 2.67 – 2.56 (m, 1H), 2.36 (s, 1H), 2.25 (s, 2H), 2.01 – 1.94 (m, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ δ171.82, 158.87, 158.83, 142.28, 140.91, 140.43, 139.79, 137.38, 132.80, 132.03, 131.76, 130.30, 129.78, 129.73, 129.28, 128.79, 127.59, 126.54, 126.53, 56.48, 38.12, 36.03, 34.28, 29.12, 22.71, 18.87; HRMS (ESI): calcd: $[M+Na]^+$ = 440.1973, found: $[M+Na]^+$ = 440.1981.

(S_p, R)-**3a:** Yield: 39%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.47 – 7.30 (m, 5H), 7.14 (dd, J = 15.3, 7.8 Hz, 1H), 6.69 – 6.53 (m, 3H), 6.32 (d, J = 7.7 Hz, 1H), 6.24 (dd, J = 14.2, 7.4 Hz, 1H), 3.64 – 3.49 (m, 1H), 3.40 – 2.88 (m, 6H), 2.76 (dt, J = 14.1, 7.9 Hz, 1H), 2.69 – 2.55 (m, 1H), 2.36 (s, 3H), 1.99 (d, J = 7.2 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.57, 158.84, 158.78, 142.28, 141.17, 140.84, 140.48, 137.49, 133.26, 131.95, 131.73, 130.02, 129.97, 129.26, 128.88, 127.48, 126.33, 46.30, 37.65, 37.64, 36.05, 34.44, 29.01, 23.34; HRMS (ESI): calcd: $[M+Na]^+$ = 440.1973, found: $[M+Na]^+$ = 440.1982.

(R_p)-**3b:** Yield: 40%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.38 (d, J = 4.4 Hz, 4H), 7.31 (dq, J = 8.7, 4.1 Hz, 1H), 7.15 (dd, J = 7.8, 1.5 Hz, 1H), 6.68 – 6.55 (m, 3H), 6.34 (dd, J = 7.8, 1.7 Hz, 1H), 6.26 (d, J = 7.4 Hz, 1H), 5.11 (d, J = 15.3 Hz, 1H), 4.87 (d, J = 15.5 Hz, 1H), 3.59 (ddd, J = 13.6, 10.4, 3.8 Hz, 1H), 3.30 (ddd, J = 14.6, 10.5, 4.3 Hz, 1H), 3.22 (ddd, J = 12.6, 9.3, 3.2 Hz, 1H), 3.10 – 2.94 (m, 3H), 2.72 (ddd, J = 13.2, 9.3, 5.7 Hz, 1H), 2.62 (ddd, J = 14.7, 10.7, 4.3 Hz, 1H), 2.38 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.58, 159.02, 142.56, 141.55, 140.56, 137.45, 135.98, 133.01, 132.07, 131.81, 130.27, 129.88, 129.84, 129.16, 129.06, 127.78, 127.21, 51.18, 37.48, 36.02, 34.35, 29.26, 22.15; HRMS (ESI): calcd: $[M+ Na]^+$ = 426.1817, found: $[M+ Na]^+$ = 426.1813

(S_p)-**3b:** Yield: 41%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.38 (d, J = 4.3 Hz, 5H), 7.14 (d, J = 7.5 Hz, 1H), 6.67 – 6.56 (m, 3H), 6.34-6.26 (m, 2H), 5.11 (d, J = 15.4 Hz, 1H), 4.87 (d, J = 15.6 Hz, 1H), 3.59 (ddd, J = 13.6, 10.6, 3.7 Hz, 1H), 3.30 (td, J = 11.9, 10.6, 4.1 Hz, 1H), 3.20 (td, J = 8.2, 7.6, 4.5 Hz, 1H), 3.12 – 2.93 (m, 3H), 2.72 (ddd, J = 13.5, 9.3, 5.7 Hz, 1H), 2.62 (td, J = 12.3, 10.9, 4.1 Hz, 1H), 2.38 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.53, 158.19, 141.51, 140.50, 139.51, 136.40, 131.96, 131.02, 130.76, 129.21, 128.83, 128.78, 128.11, 128.01, 126.74, 126.16, 50.14, 46.03, 36.44, 34.98, 33.30, 28.21; HRMS(ESI): calcd: $[M+ Na]^+$ = 426.1817 , found: $[M+Na]^+$ = 426.1810

(R_p, S)-**3c:** Yield: 42%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.76 (dd, J = 7.8, 1.6 Hz, 1H), 6.70 (d, J = 7.9 Hz, 1H), 6.65 – 6.57 (m, 2H), 6.22 – 6.13 (m, 2H), 4.27 (d, J = 8.9 Hz, 1H), 4.13 – 3.97 (m, 2H), 3.71 – 3.57 (m, 2H), 3.28 – 2.96 (m, 6H), 2.83 (s, 3H), 1.14 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.06, 159.27, 141.69, 141.04, 140.48, 137.10, 132.71, 131.71, 130.55, 128.86, 128.20, 120.18, 119.13, 70.01, 65.52, 37.31, 36.63, 35.09, 33.73, 29.33, 27.75, 22.14; HRMS(ESI): calcd: $[M+ Na]^+$ = 416.2173, found: $[M+ Na]^+$ = 416.2167

(S_p, S)-**3c:** Yield: 42%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.19 – 7.10 (m, 1H), 6.67 (qd, J = 7.8, 1.5 Hz, 2H), 6.57 (d, J = 7.4 Hz, 1H), 6.40 (d, J = 7.7 Hz, 1H), 6.21 (d, J = 7.4 Hz, 1H), 4.15 (d, J = 9.1 Hz, 1H), 3.78 (ddd, J = 9.4, 6.0, 3.4 Hz, 1H), 3.72 – 3.52 (m, 2H), 3.38 – 3.11 (m, 3H), 3.05 (q, J = 7.1 Hz, 2H), 2.92 (ddd, J = 12.9, 10.5, 4.5 Hz, 1H), 2.66 (ddd, J = 13.7, 10.6, 3.6 Hz, 1H), 2.53 (s, 3H), 1.24 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.13, 154.17, 137.17, 136.48, 135.88, 132.62, 129.04, 127.33, 126.52, 126.43, 126.33, 125.15, 124.11, 72.58, 72.26, 71.94, 65.10, 59.65, 31.74, 31.42, 31.34, 30.05, 24.47, 22.98, 22.96, 19.31; HRMS(ESI): calcd: $[M+ Na]^+$ = 416.2173, found: $[M+ Na]^+$ = 416.2185.

(R_p)-**3d:** Yield: 38%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.05 (dd, J = 7.8, 1.9 Hz, 1H), 6.66 (dd, J = 7.9, 2.0 Hz, 1H), 6.60 (d, J = 7.8 Hz, 2H), 6.31 (dd, J = 7.9, 2.0 Hz, 1H), 6.27 (d, J = 7.4 Hz, 1H), 4.20 (ddd, J = 11.6, 7.6, 4.3 Hz, 1H), 4.06 – 3.91 (m, 3H), 3.62 – 3.48 (m, 1H), 3.27 (dddd, J = 18.5, 16.0, 9.6, 4.9 Hz, 2H), 3.16 (ddd, J = 14.3, 9.3, 5.9 Hz, 1H), 3.07 – 2.86 (m, 3H), 2.63 (s, 3H), 2.61 (d, J = 6.1 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.55, 165.58, 141.16, 140.18, 137.72, 136.87, 132.60, 131.71, 130.54, 129.82, 127.09, 125.24, 121.90, 68.49, 63.17, 37.35, 35.58, 35.46, 34.04, 33.92, 30.50, 27.13; HRMS(ESI): calcd: $[M+ Na]^+$ = 360.1547 , found: $[M+ Na]^+$ = 360.1538

(S_p)-**3d:** Yield: 39%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.05 (d, J = 7.6 Hz, 1H), 6.63 (dd, J = 30.3, 7.6 Hz, 3H), 6.29 (dd, J = 20.8, 7.5 Hz, 2H), 4.19 (s, 1H), 4.06 – 3.92 (m, 3H), 3.53 (t, J = 11.7 Hz, 1H), 3.34 – 2.88 (m, 7H), 2.63 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.15, 154.19, 137.19, 136.49, 135.89, 132.63, 129.05, 129.04, 127.34, 126.53, 126.44, 126.35, 125.17, 124.13, 65.11, 59.66, 31.74, 31.43, 31.35, 30.06, 24.47, 22.98, 22.96; HRMS(ESI): calcd: $[M+ Na]^+$ = 360.1547 , found: $[M+ Na]^+$ = 360.1575.

References

[1] (a) D. Y. Antonov, Y. N. Belokon, N. S. Ikonnikov, S. A. Orlova, A. P. Pisarevsky, N. I. Raevski, V. I. Rozenberg, E. V. Sergeeva, Y. T. Struchkov, V. I. Tararov, E. V. Vorontsov, *J. Chem. Soc. Perkin. Trans.* 1995, **1**, 1873-1879.

[2] M. Cakici, Z. G. Gu, M. Nieger, J. Bürck, L. Heinke, S. Bräse, *Chem. Commun*. 2015, **51**, 4796-4798.

[3] C. J. Friedmann, S. Ay, S. Bräse, *J. Org. Chem.* 2010, **75**, 4612-4614.

[4] D. Y. Xin, Y. D. Ma, F. Y. He, *Tetrahedron: Asymmetry*, 2010, **21**, 333-338.

[5] F. Y. He, Y. D. Ma, L. Zhao, W. Z. Duan, J. Q. Chen, Z. X. Zhao, *Tetrahedron: Asymmetry*, 2012, **23**, 809-817.

2. Spectroscopic Properties

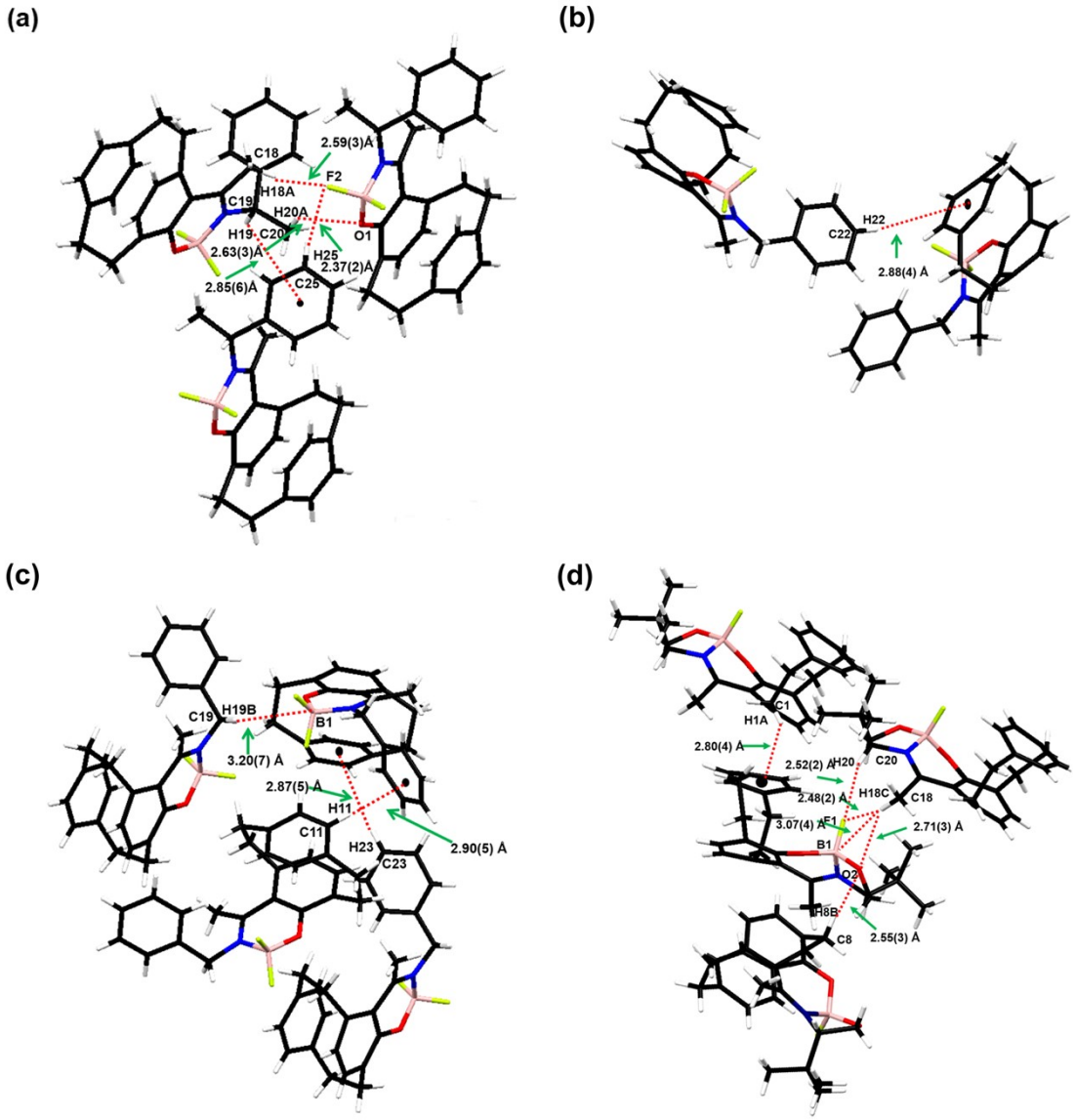


Figure S1. Crystal packing structures of (S_p, *R*)-**3a** (a), (R_p)-**3b** (b), (S_p)-**3b** (c) and (R_p, *S*)-**3c** (d).

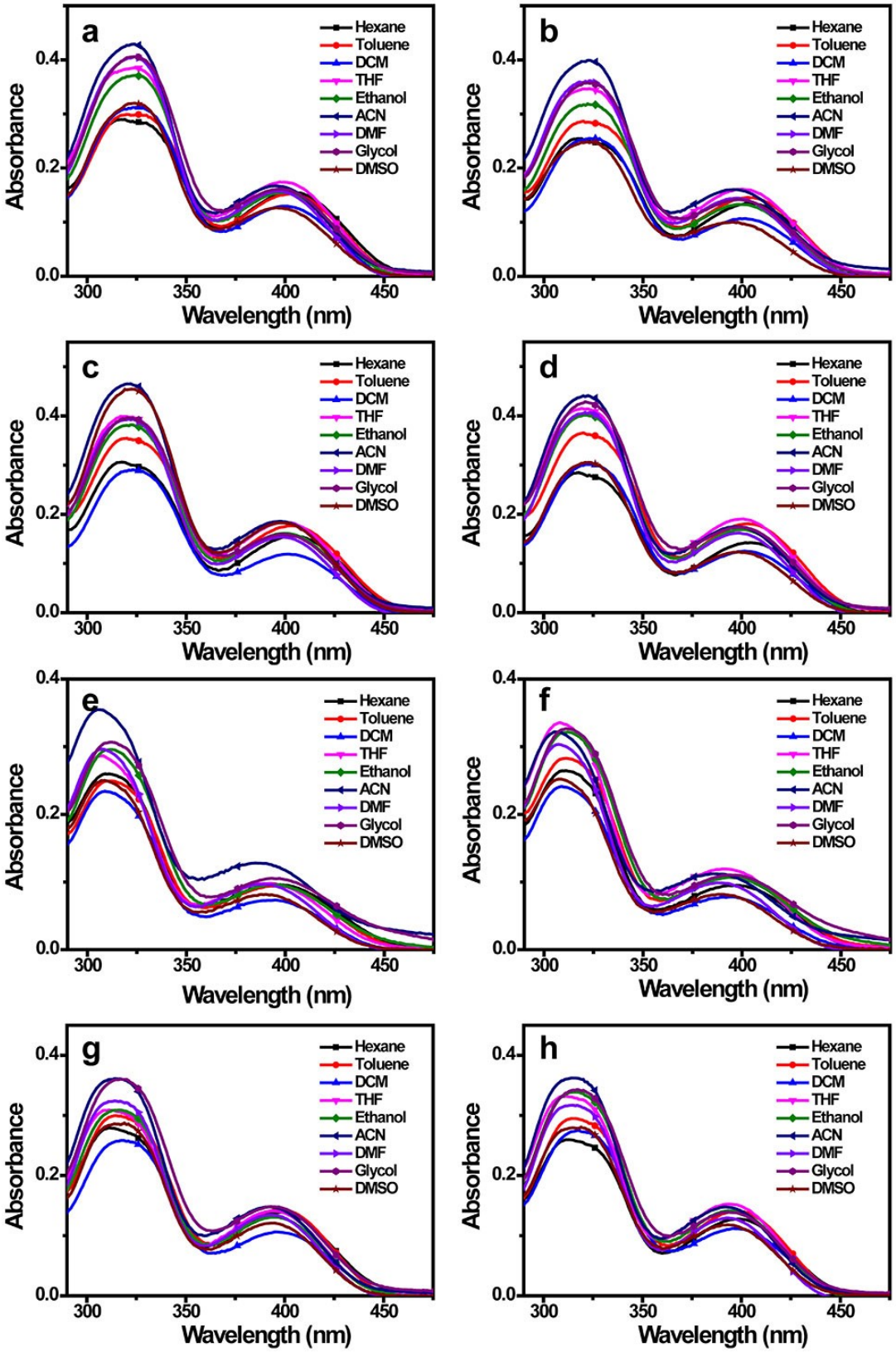


Figure **S2**. Absorption spectra of compounds (R_p, R)-**3a** (a), (S_p, R)-**3a** (b), (R_p)-**3b** (c), (S_p)-**3b** (d), (R_p, S)-**3c** (e), (S_p, S)-**3c** (f), (R_p)-**3d** (g) and (S_p)-**3d**(h) in various solvents (50 μM) such as hexane, toluene, dichloromethane (DCM), tetrahydrofuran (THF), ethanol, acetonitrile (ACN), dimethylformamide (DMF), ethylene glycol (Glycol) and dimethyl sulfoxide (DMSO), respectively.

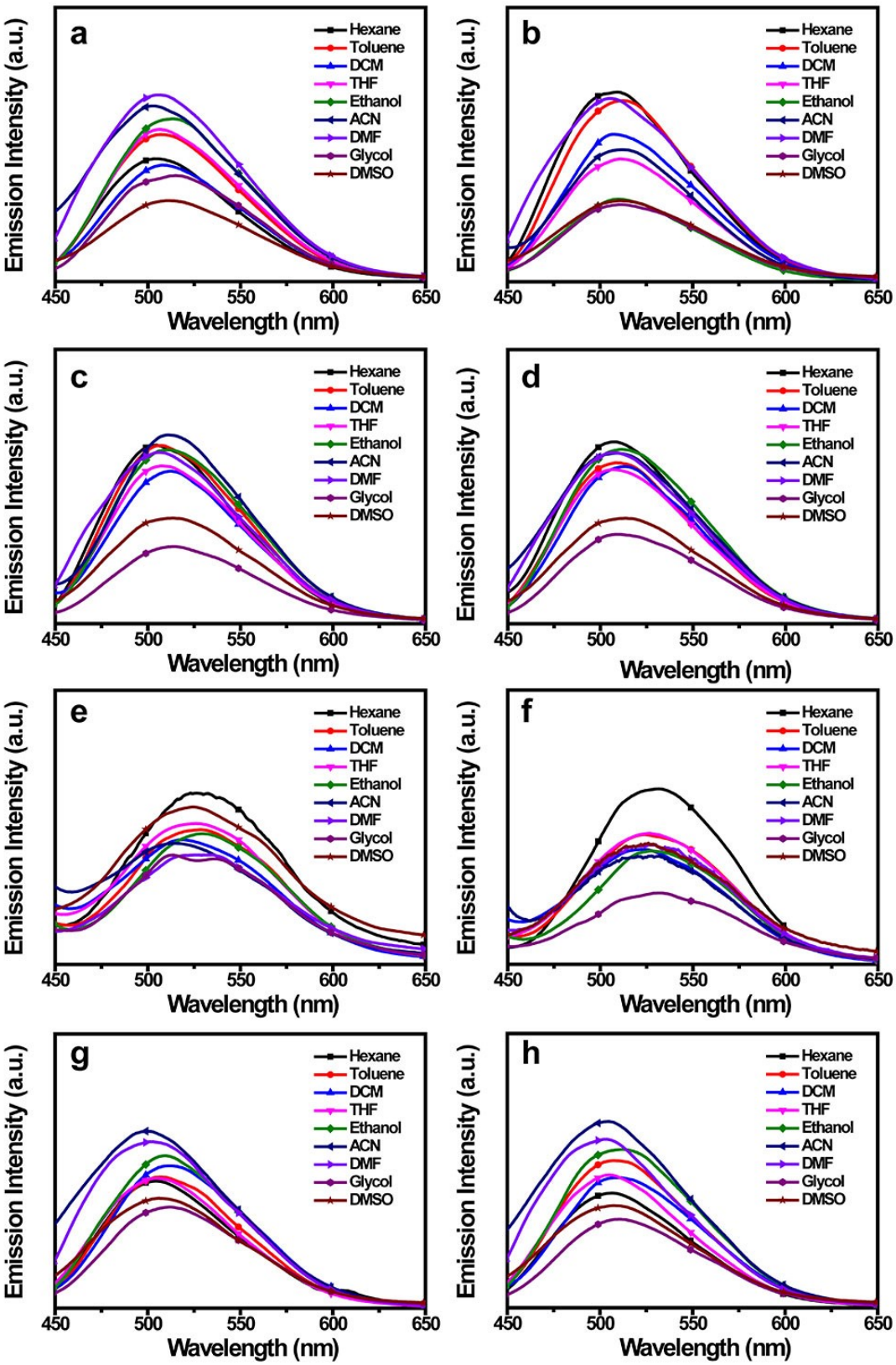


Figure S3. Emission spectra of compounds (R_p, *R*)-**3a** (a), (S_p, *R*)-**3a** (b), (R_p)-**3b** (c), (S_p)-**3b** (d), (R_p, *S*)-**3c** (e), (S_p, *S*)-**3c** (f), (R_p)-**3d** (g) and (S_p)-**3d**(h) in various solvents (50 μM) such as hexane, toluene, dichloromethane (DCM), tetrahydrofuran (THF), ethanol, acetonitrile (ACN), dimethylformamide (DMF), ethylene glycol (Glycol) and dimethyl sulfoxide (DMSO) respectively.

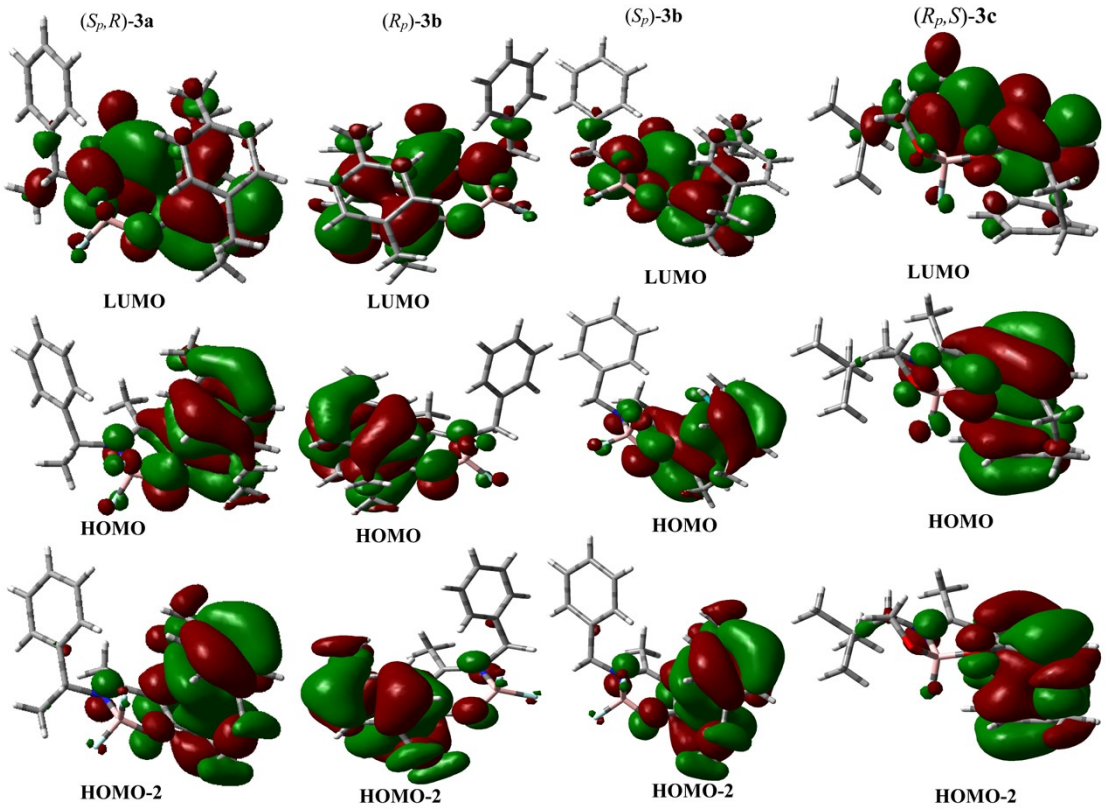


Figure S4. The angular nodal patterns of the LUMO, HOMO and HOMO-2 of (S_p, *R*)**-3a** (a), (R_p)**-3b** (b), (S_p)**-3b** (c) and (R_p, *S*)**-3c** (d), calculated by using B3LYP/6-31G(d) basis set with the G09 program package.

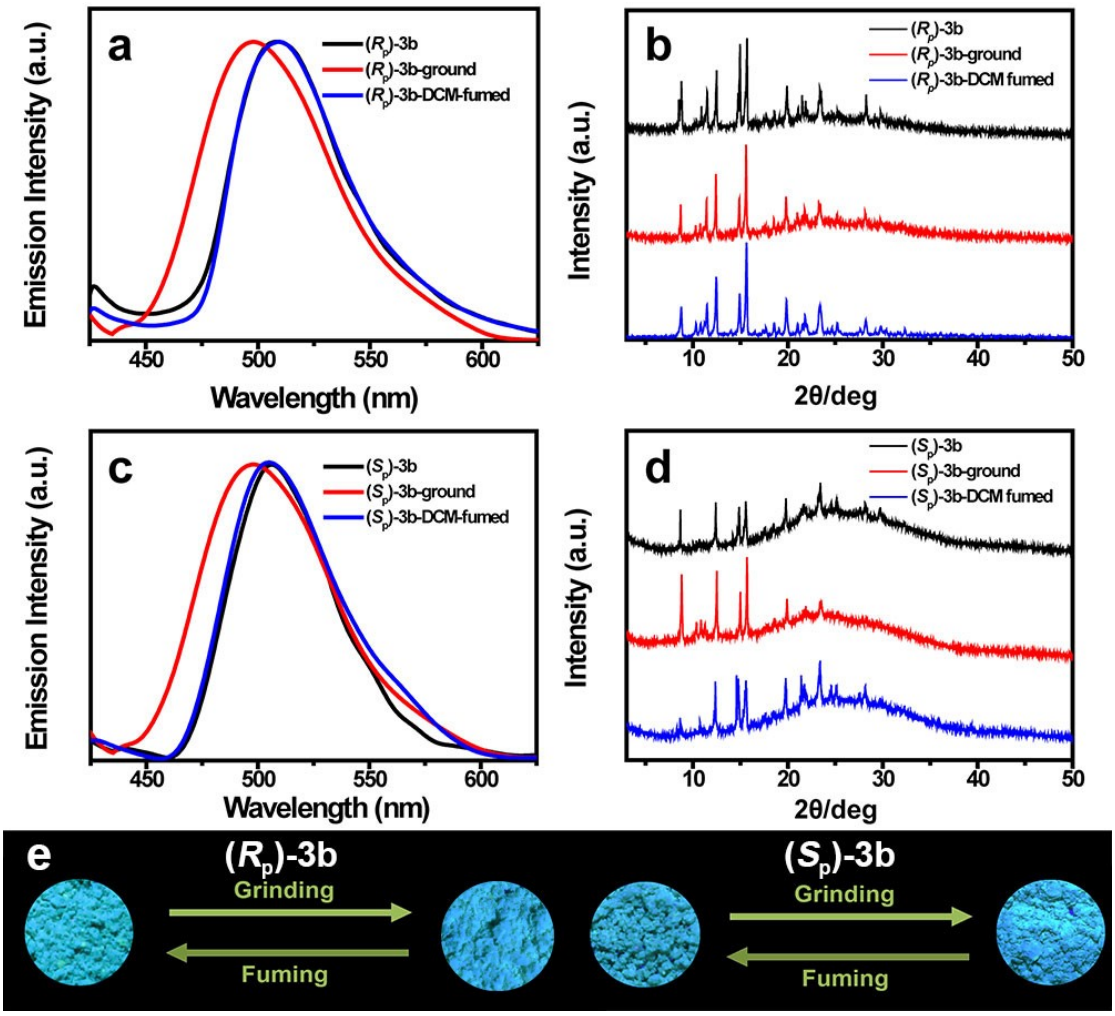


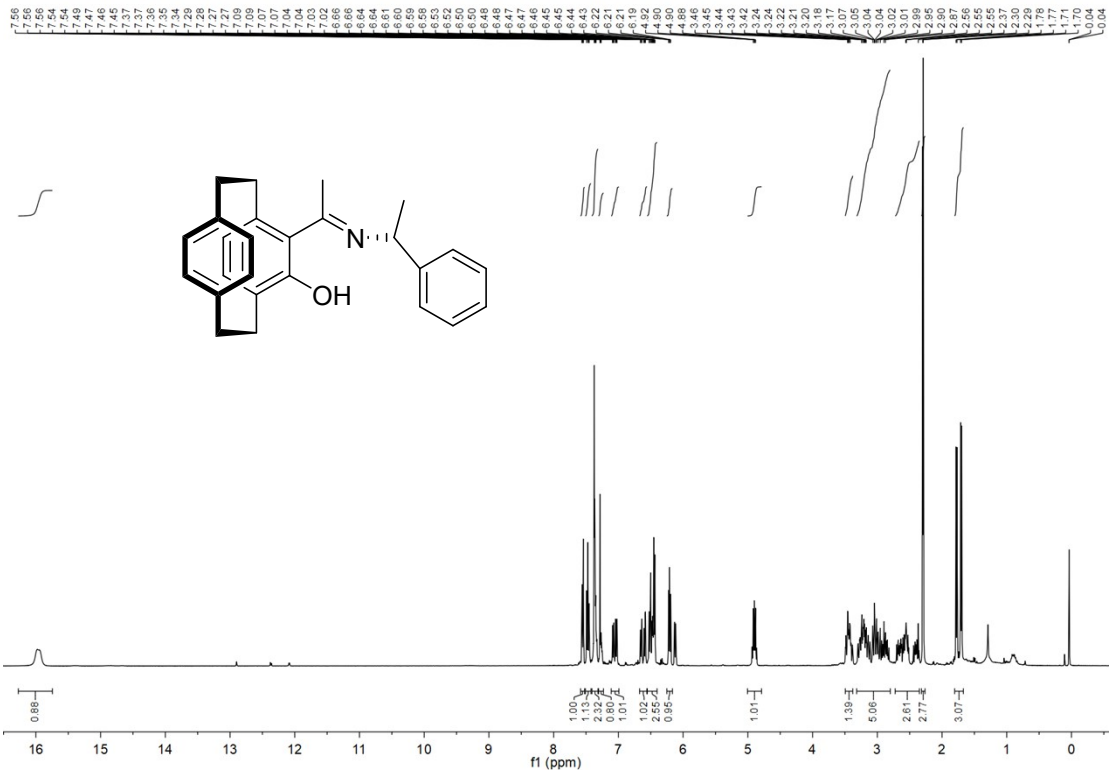
Figure S5. (1) Normalized fluorescence spectra of (R_p)-**3b** (a), (S_p)-**3b** (c) in solid-state, after being ground and DCM (dichloromethane) fumed; (2) Powder XRD patterns of (R_p)-**3b** (b), (S_p)-**3b** (d) in solid-state; (3) Photographs of (R_p)/(S_P)-**3b** upon grinding and fuming with DCM at 365 nm UV irradiation.

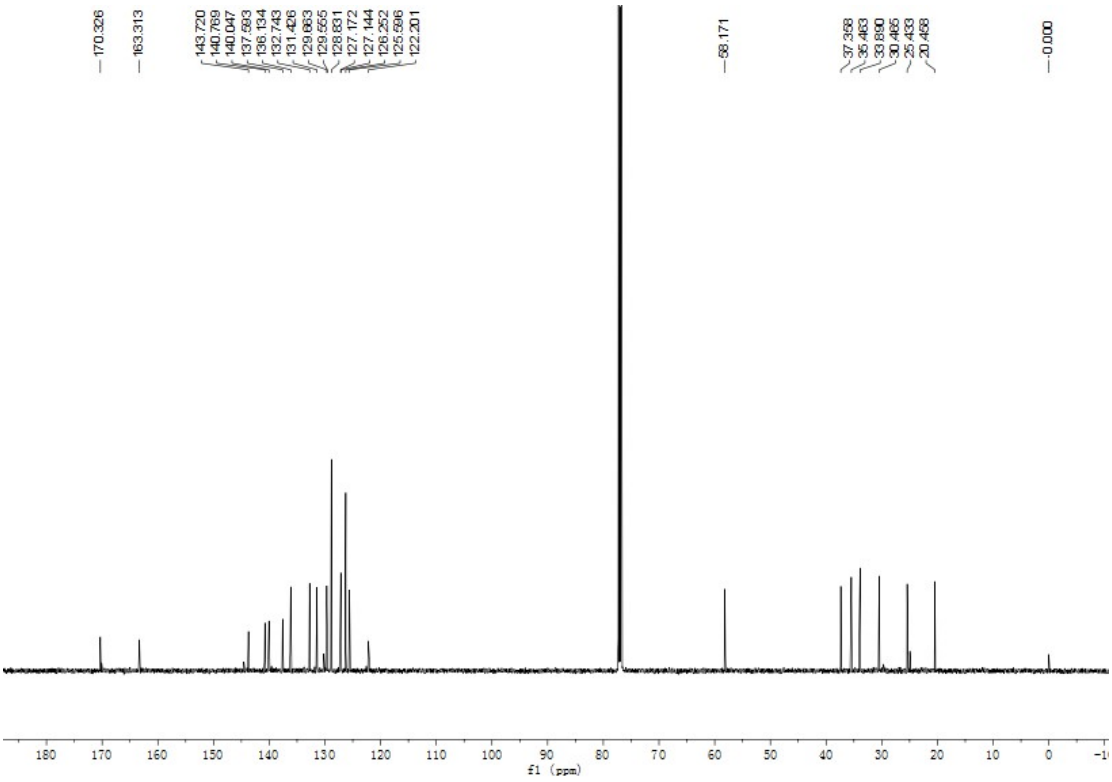
Table S1. Calculated excited wavelength (λ) and oscillator strengths (f) and related wave functions

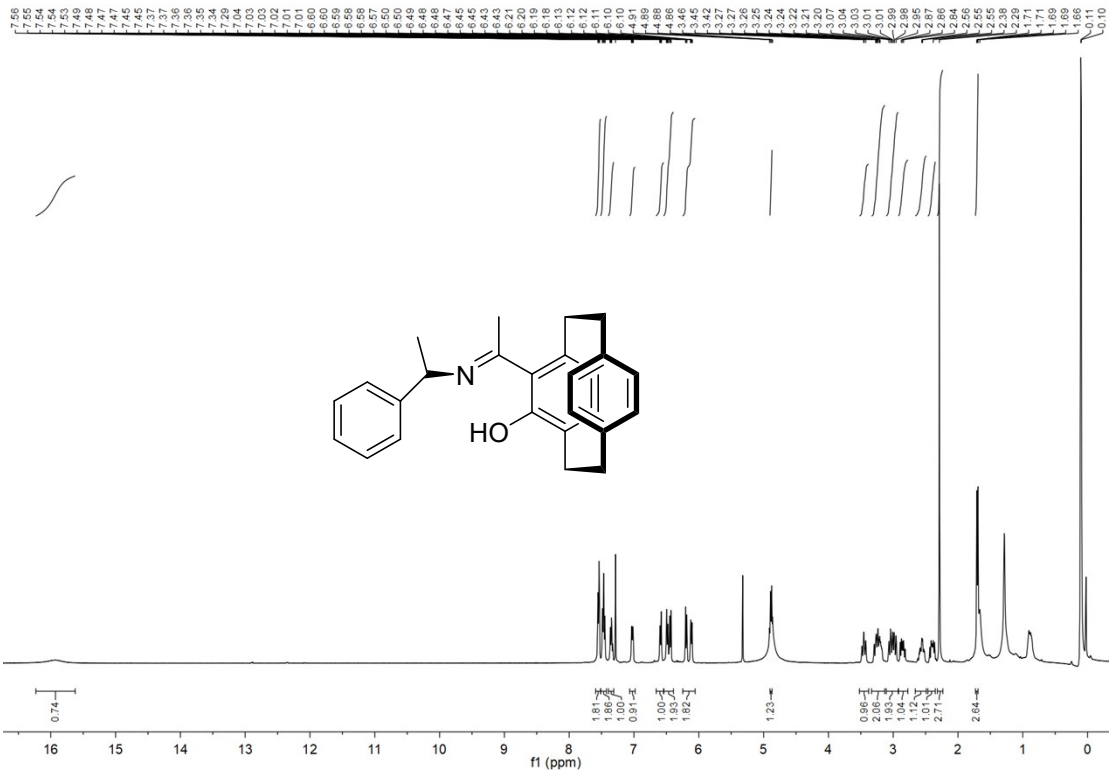
Compound	State	Energy [eV]	λ [nm]	f[b]	Orbitals (coefficient)[c]
(S_p,R)-**3a**	S_1	3.1110	398.54	0.0444	H>L (69.2%)
	S_3	3.7142	333.81	0.0616	H-2>L(68.9%)
(R_p)-**3b**	S_1	3.0884	401.46	0.0414	H>L (69.2%)
	S_3	3.7414	331.39	0.0569	H-2>L (68.8%)
(S_p)-**3b**	S_1	3.0896	401.29	0.0399	H>L (69.3%)
	S_3	3.7316	332.26	0.0603	H-2>L (68.7%)
(R_p,S)-**3c**	S_1	3.0748	403.22	0.0460	H>L (69.9%)
	S_3	3.8436	322.57	0.0932	H-2>L (68.7%)

[a]Excited state; [b]Oscillator strength; [c]MOs involved in the transitions, H = HOMO, L = LUMO.

3. **NMR spectra**



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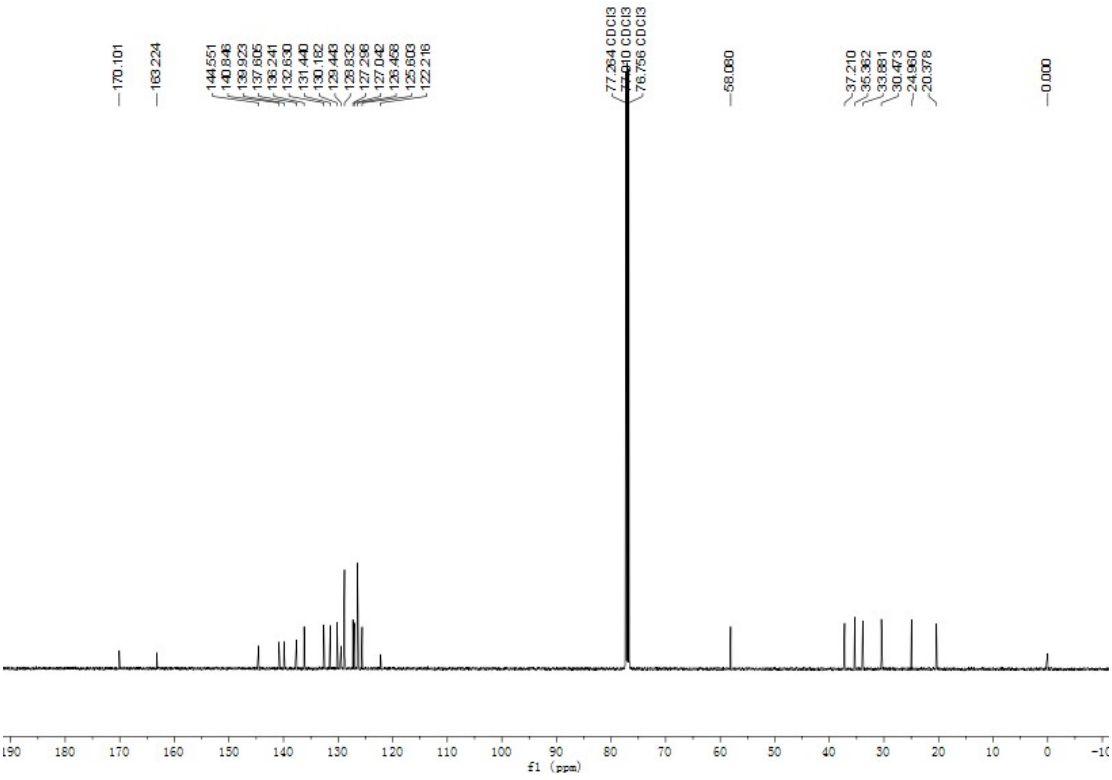
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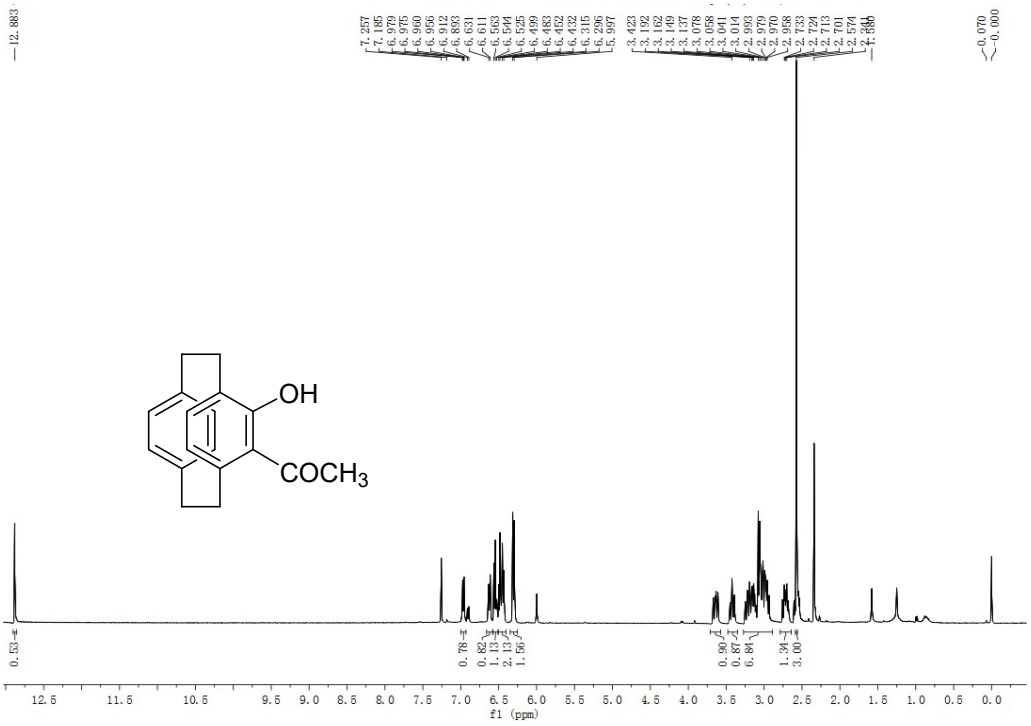
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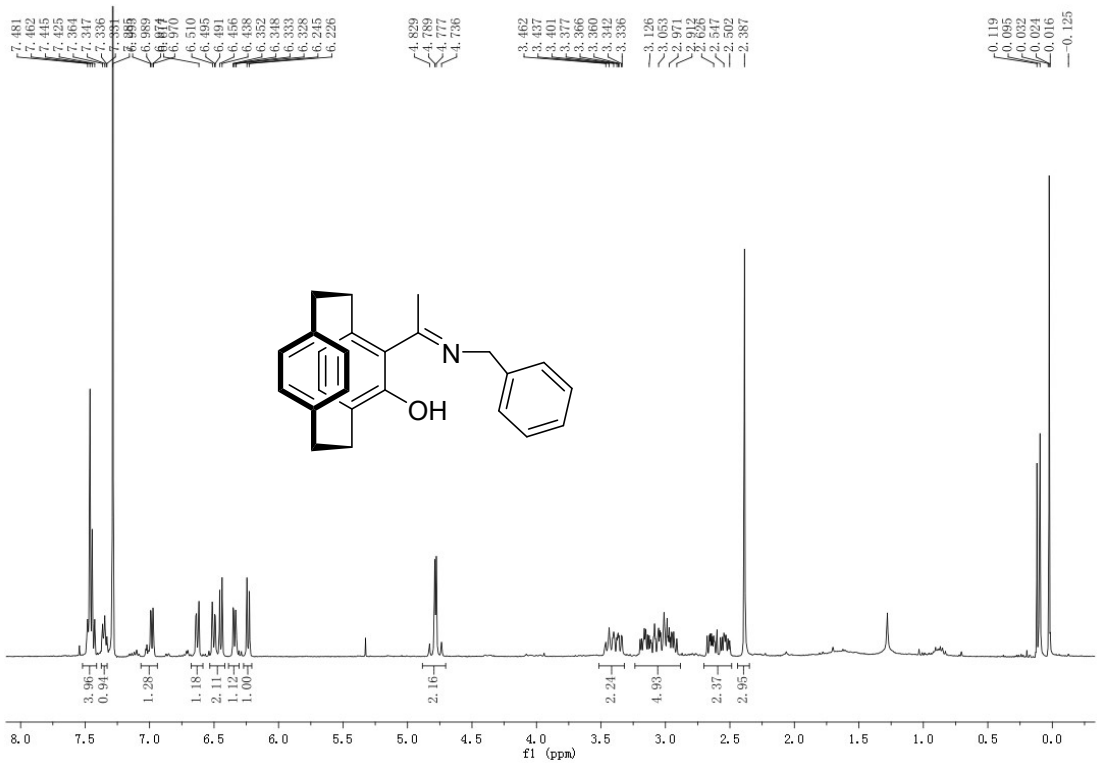
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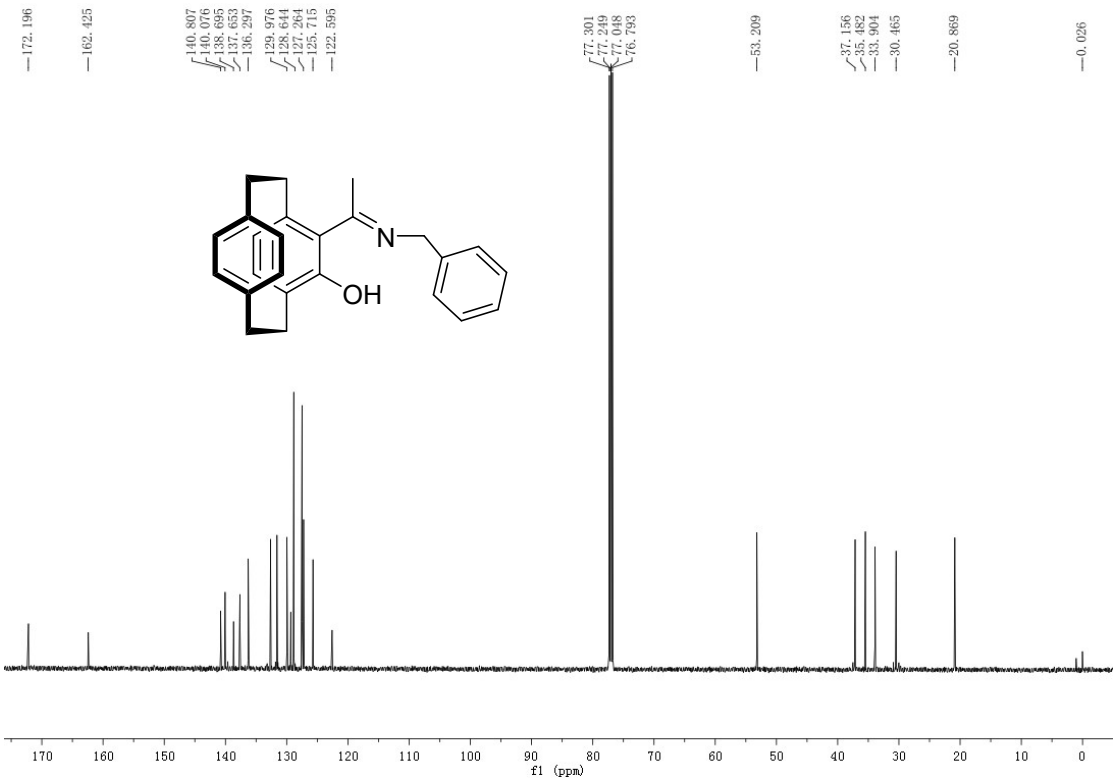
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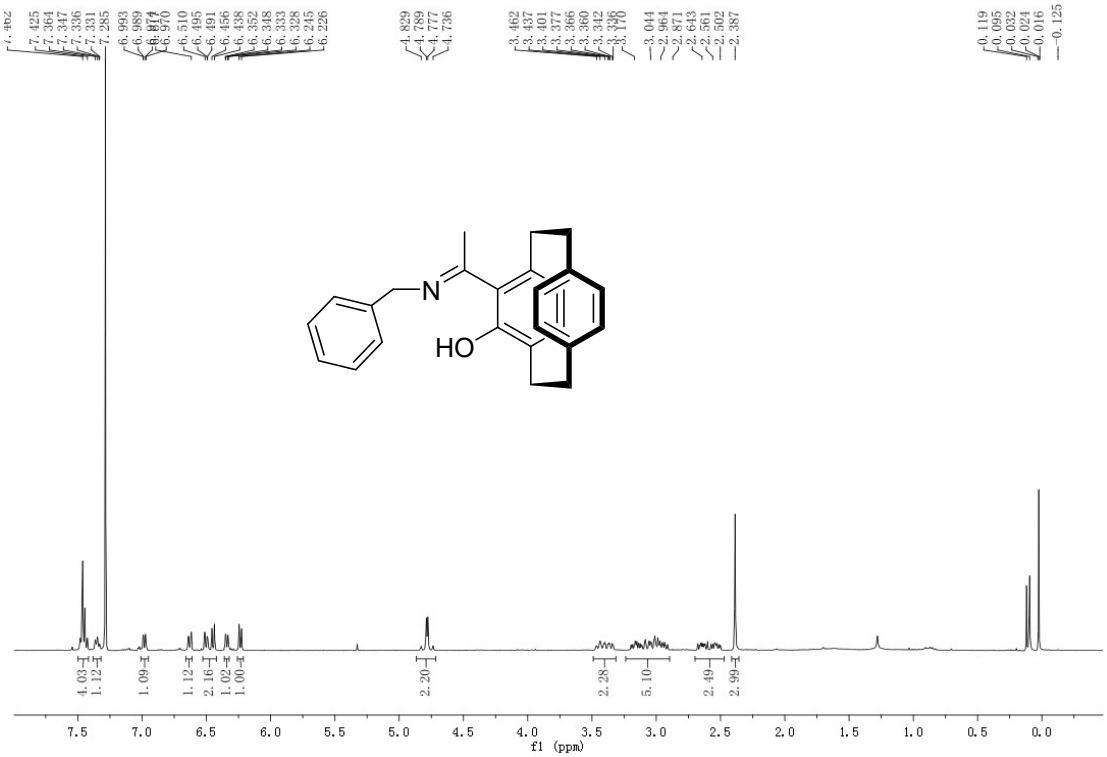
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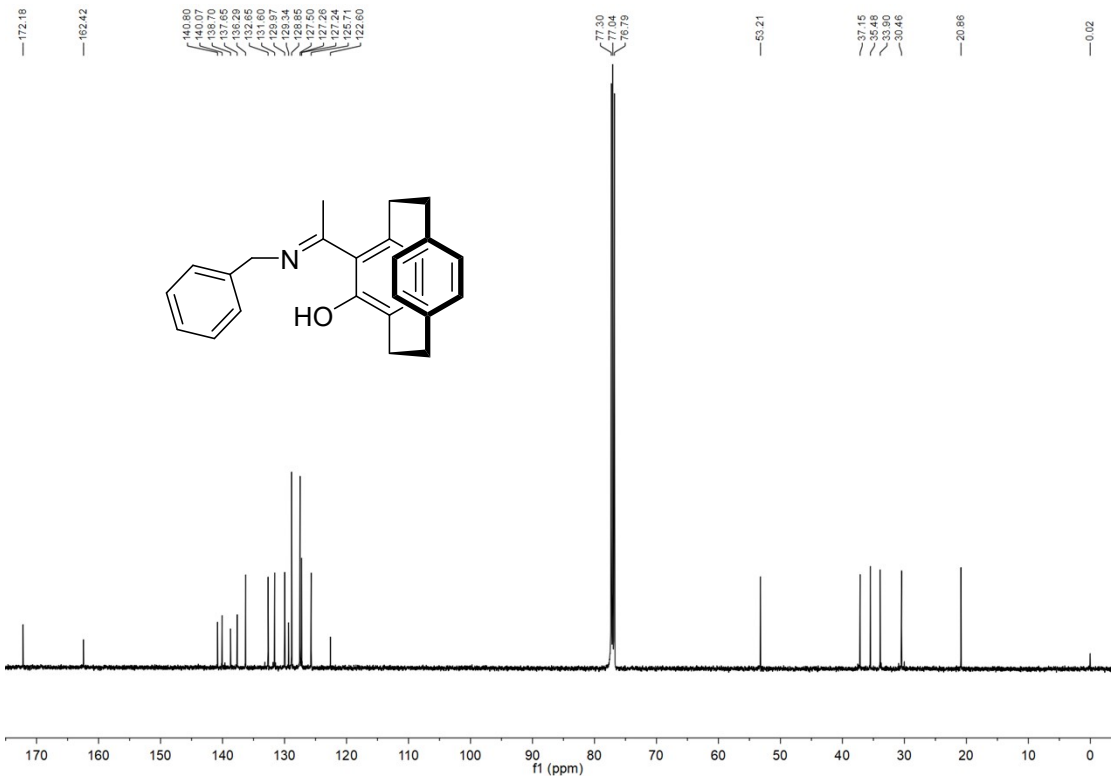
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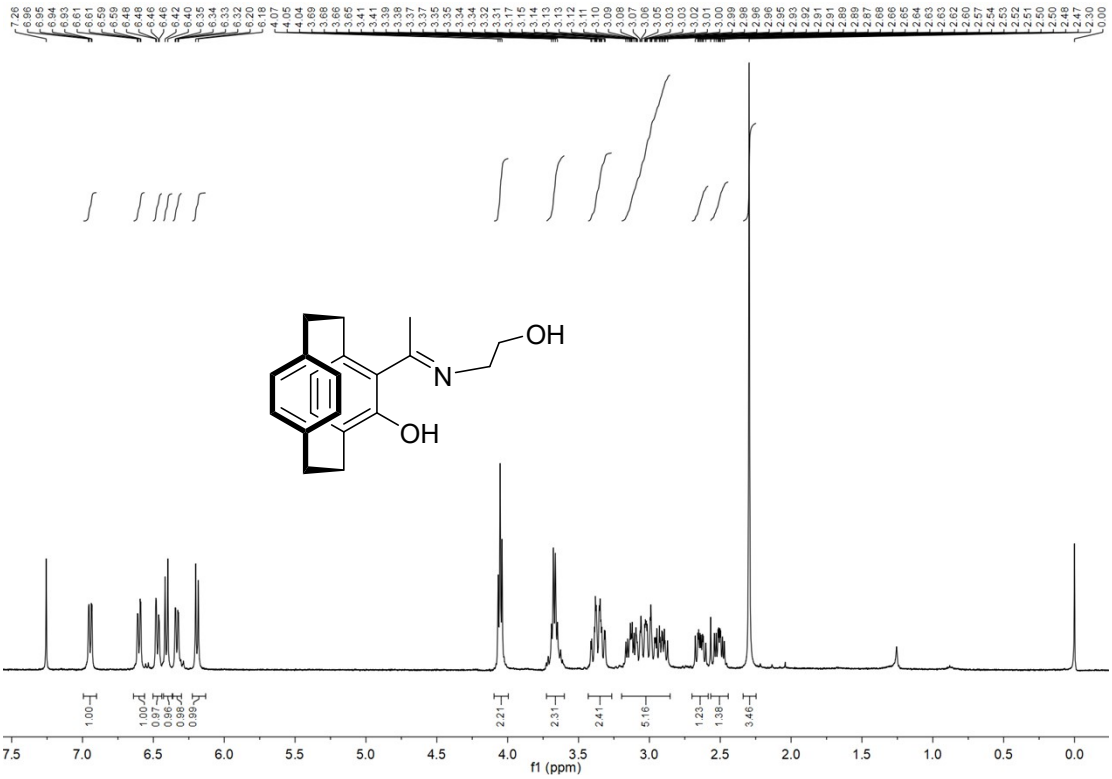
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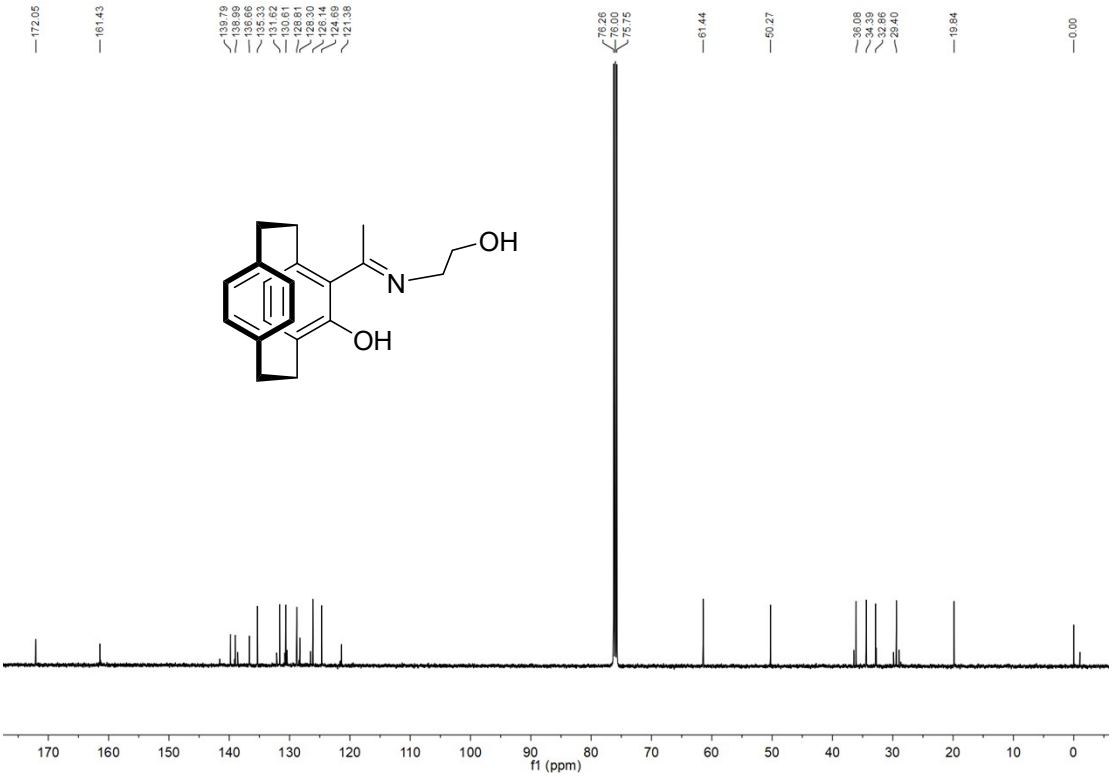
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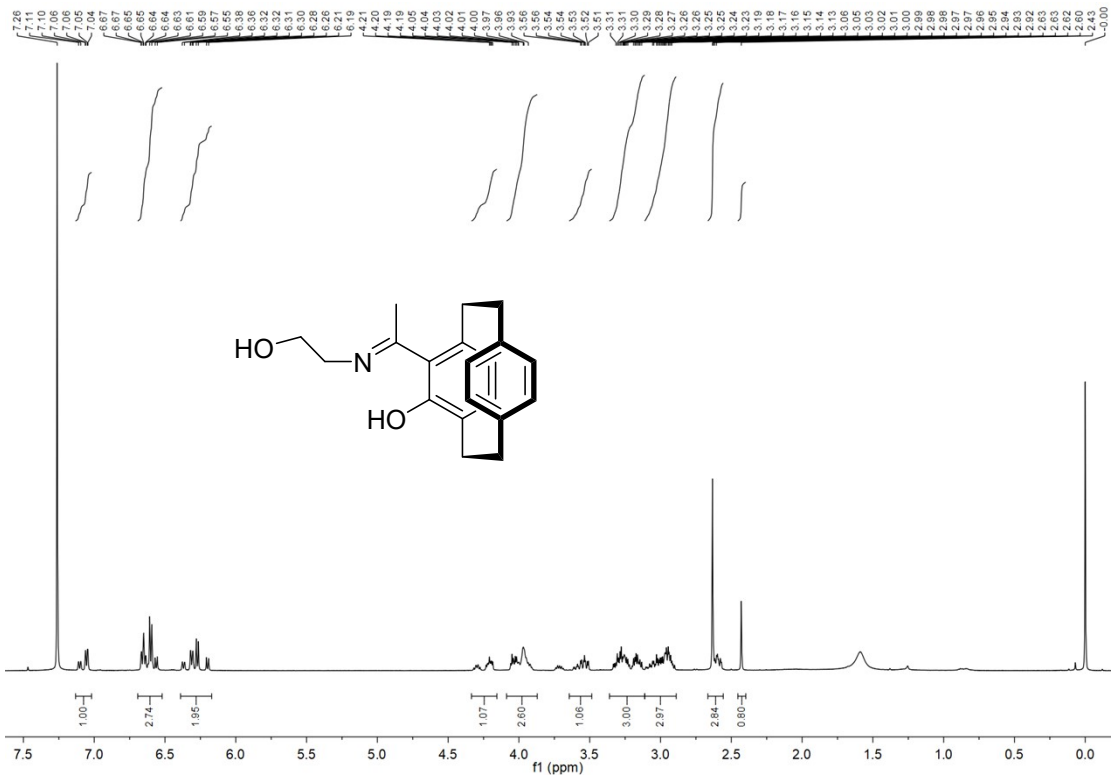
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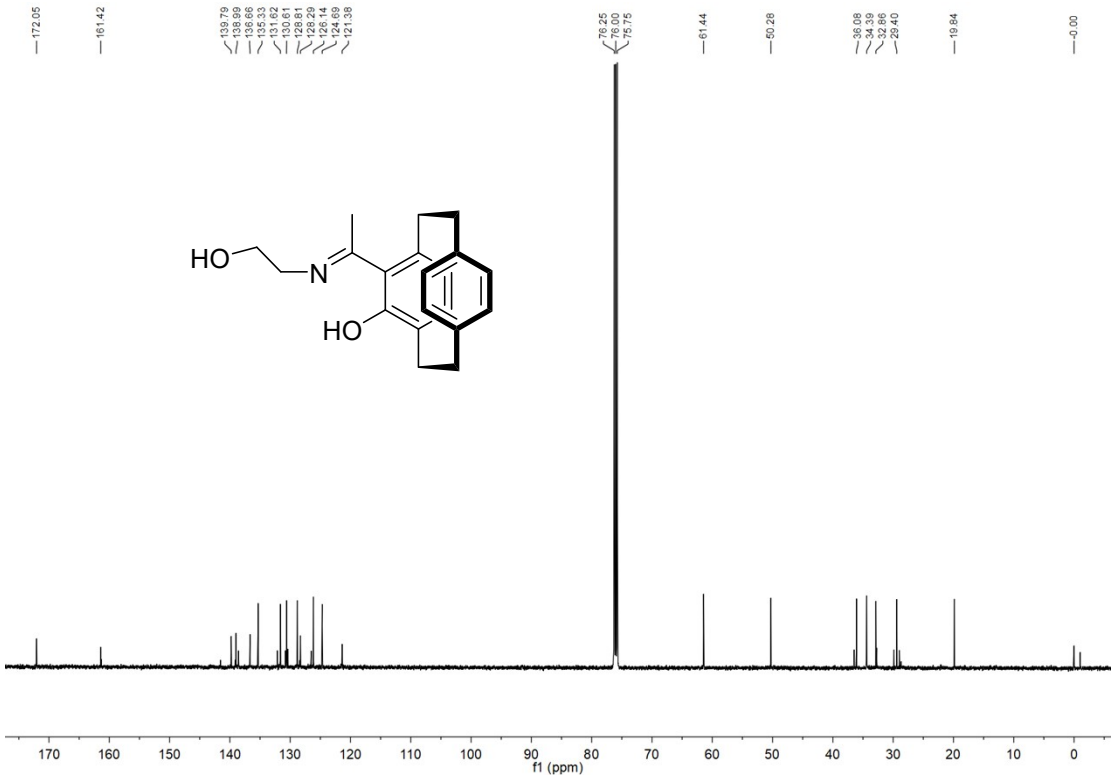
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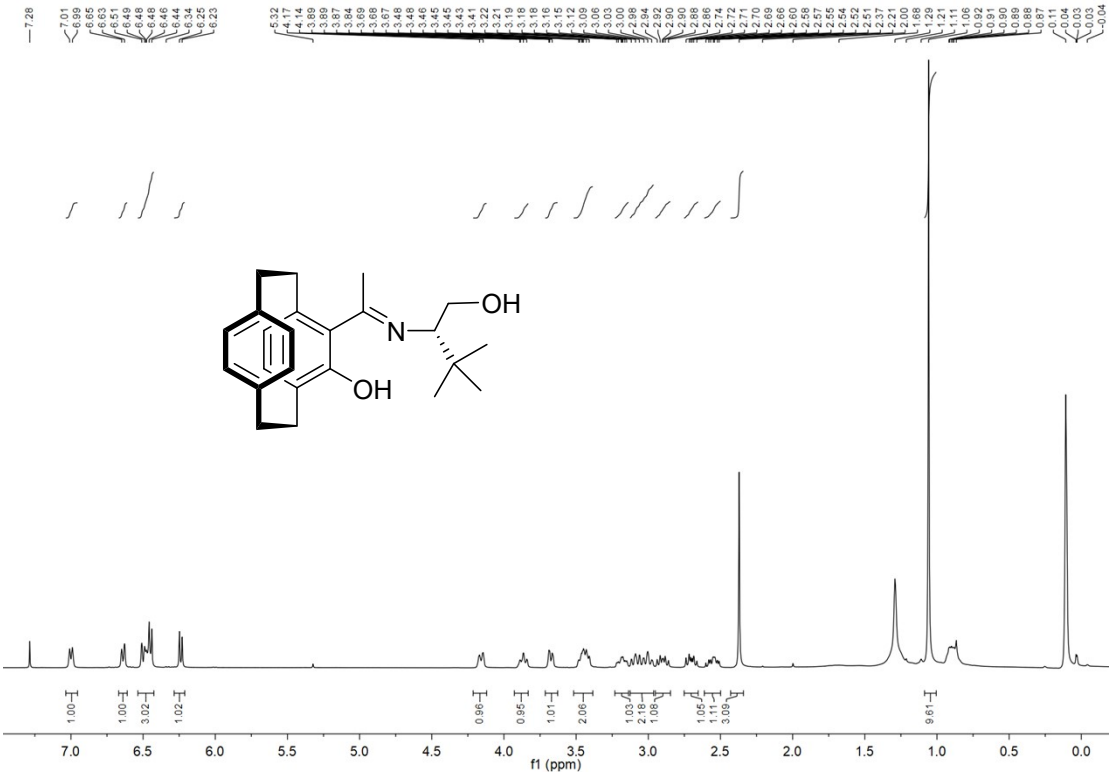
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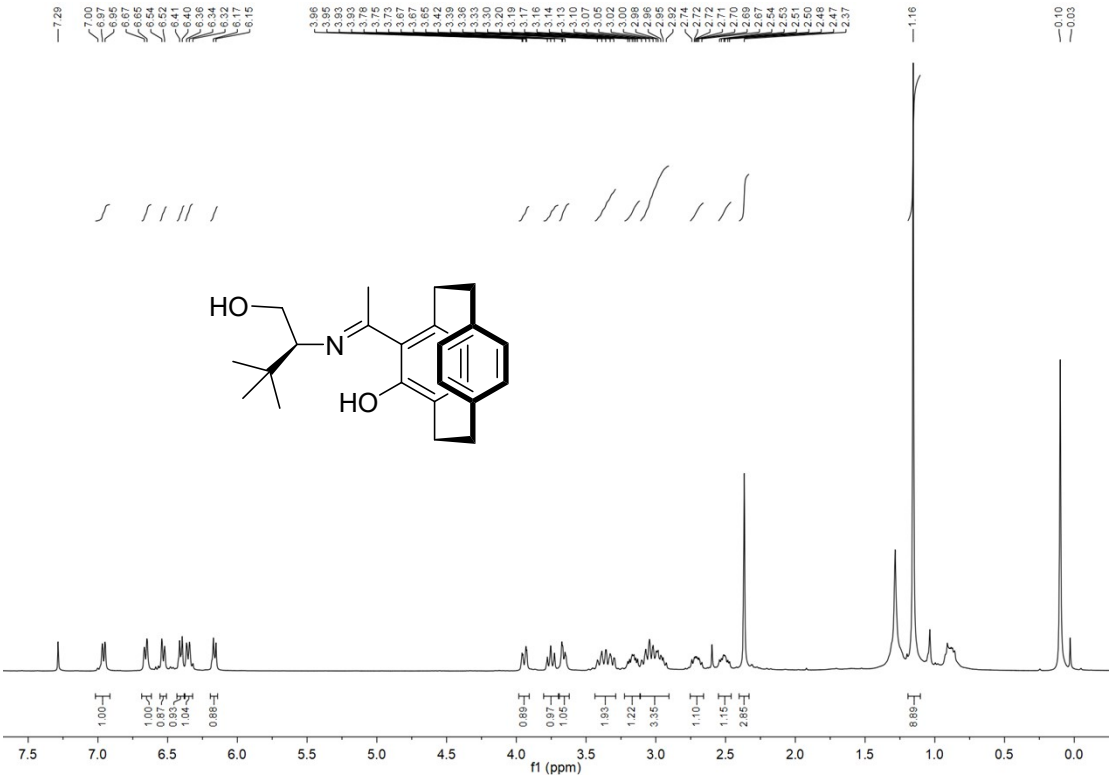
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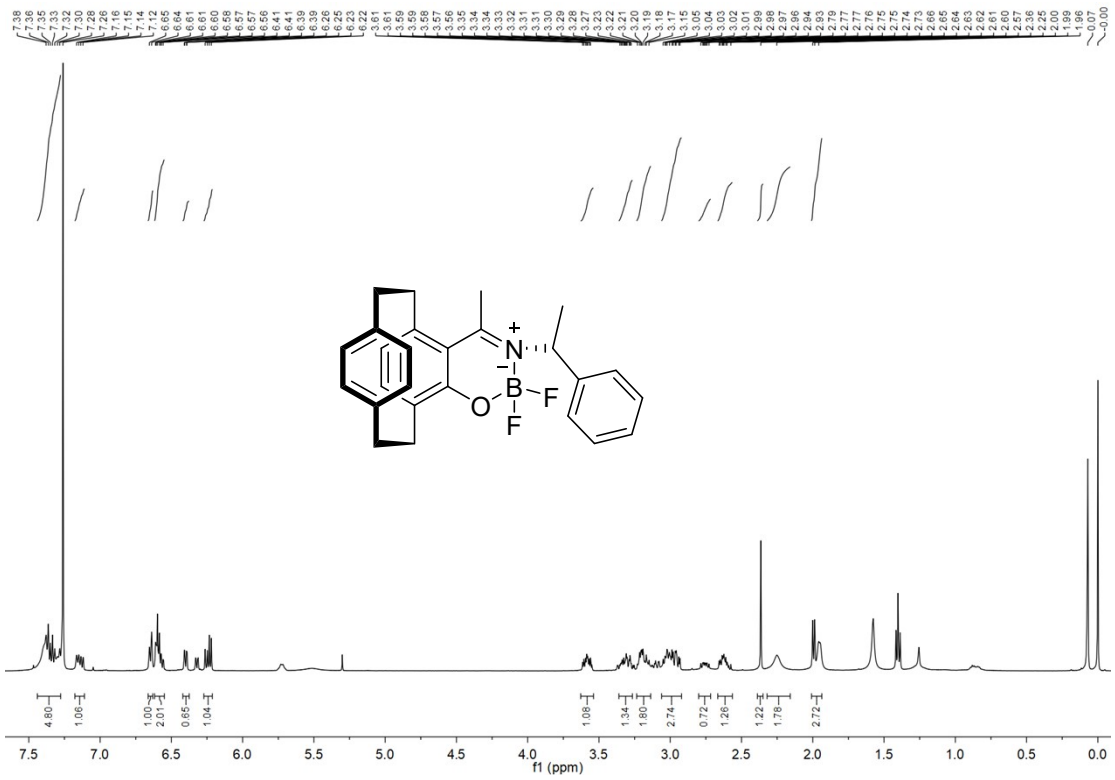
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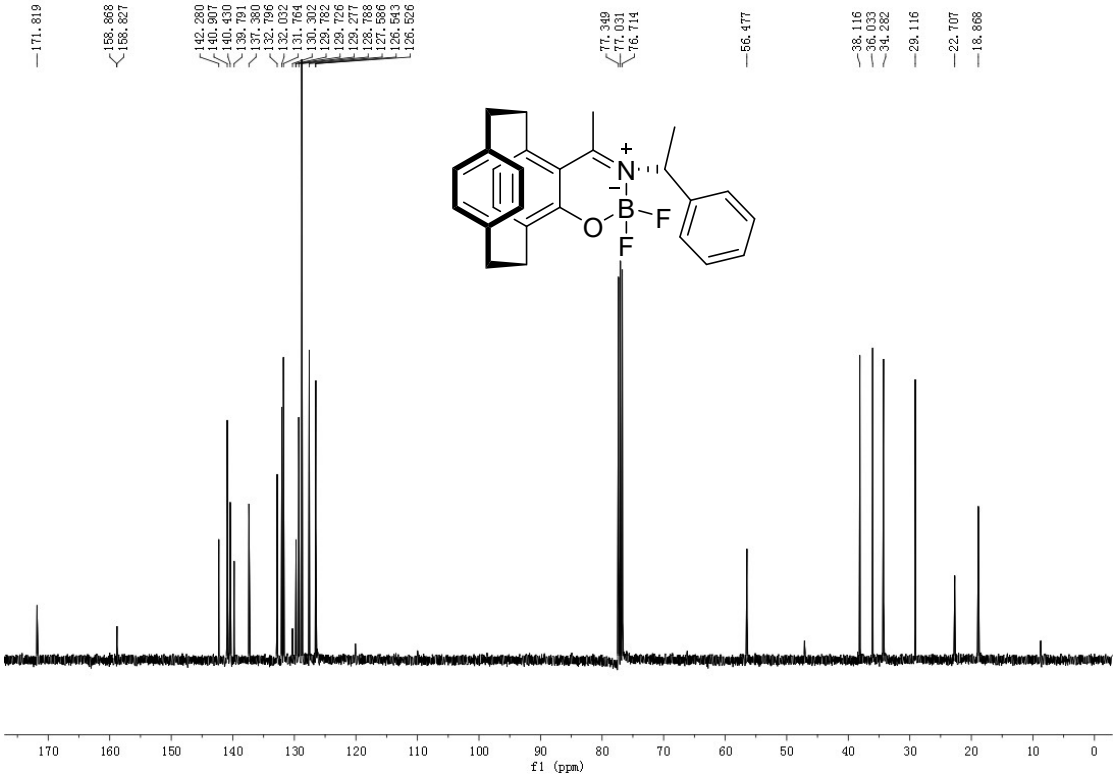
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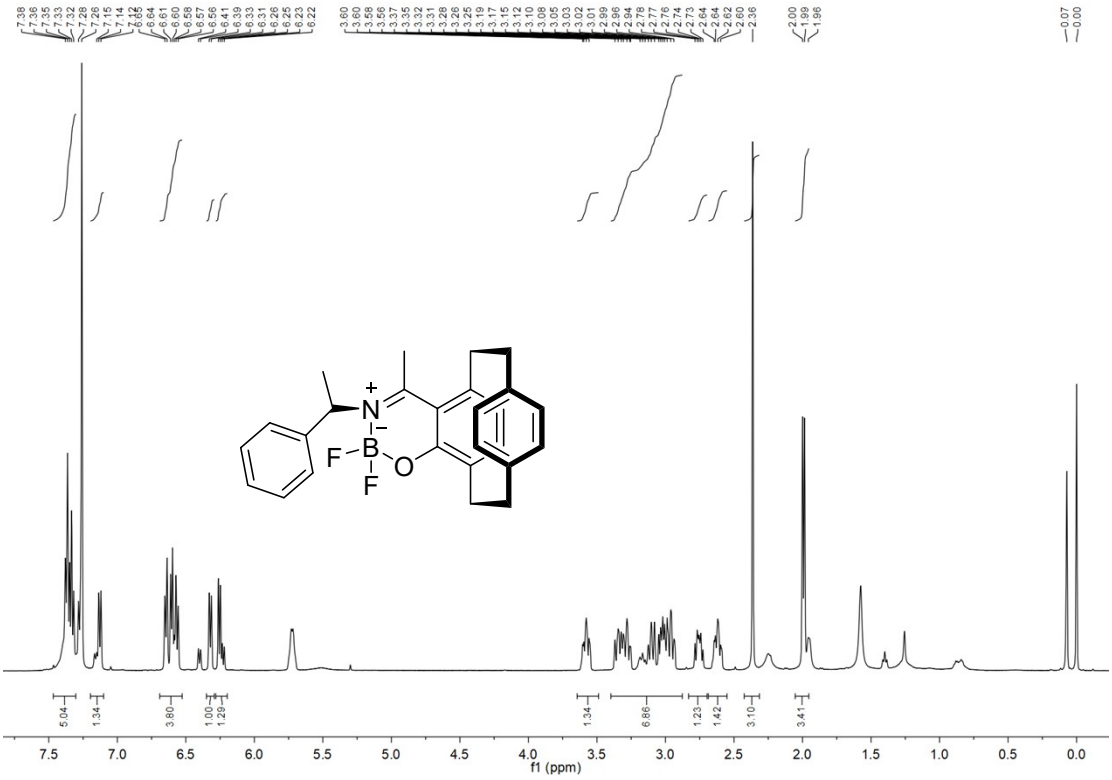
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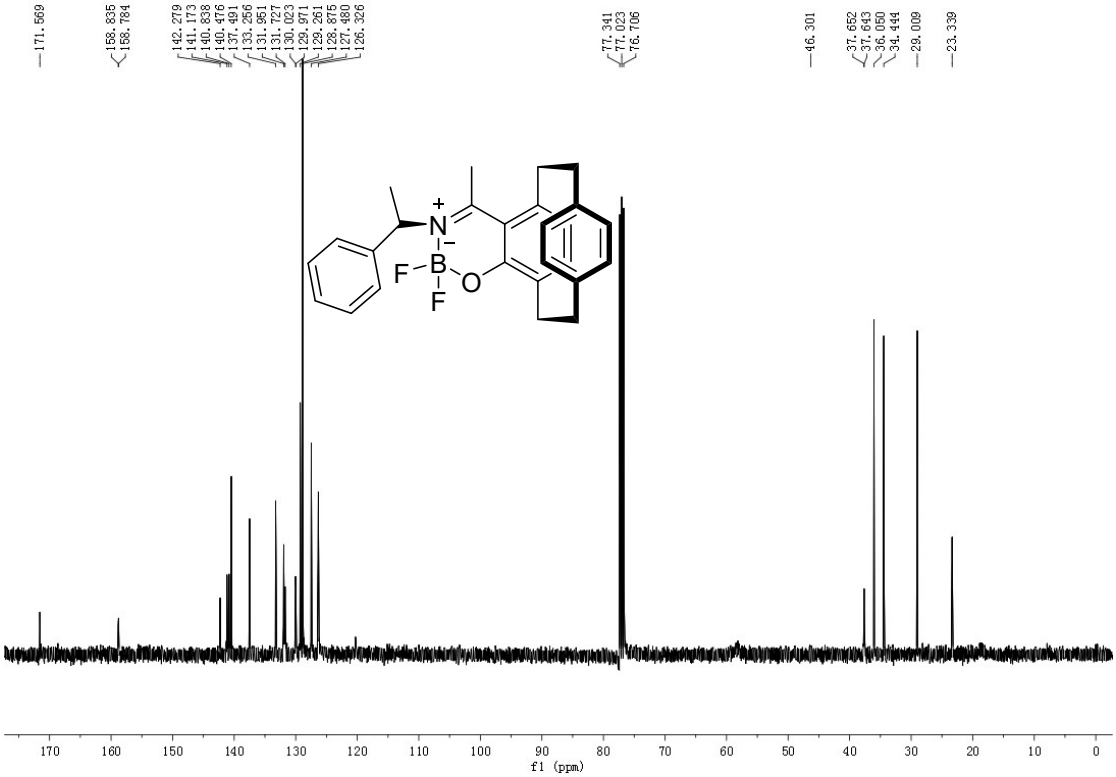
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B
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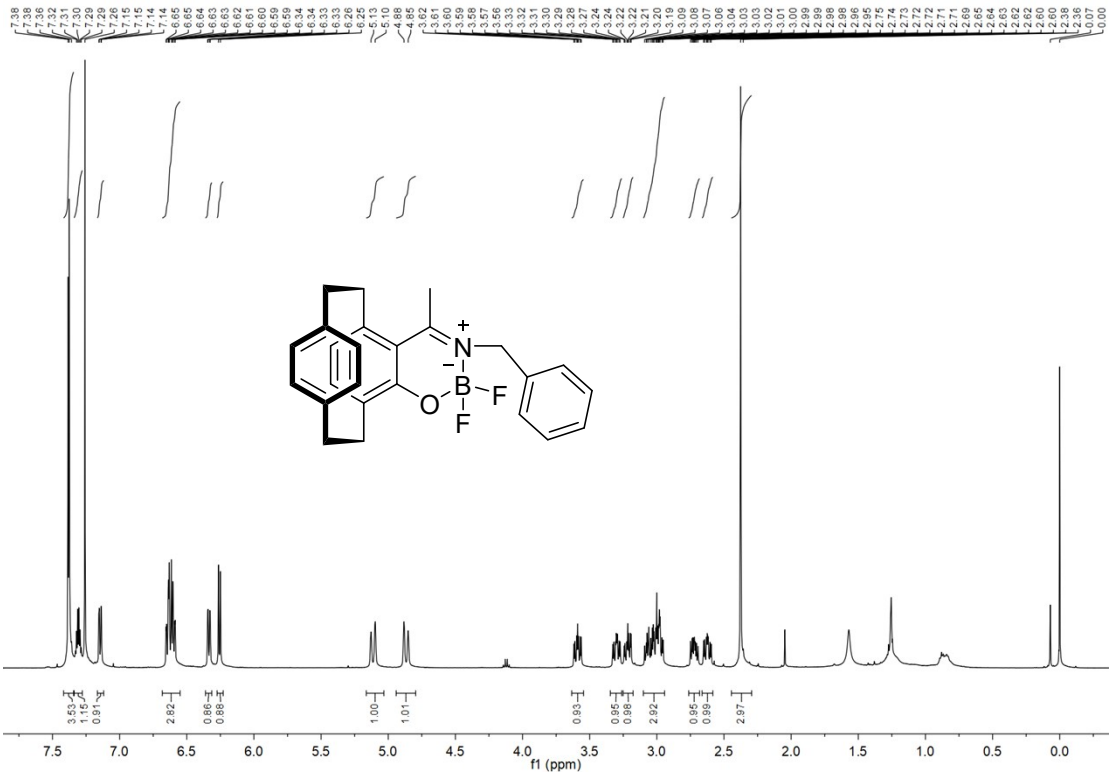
F
O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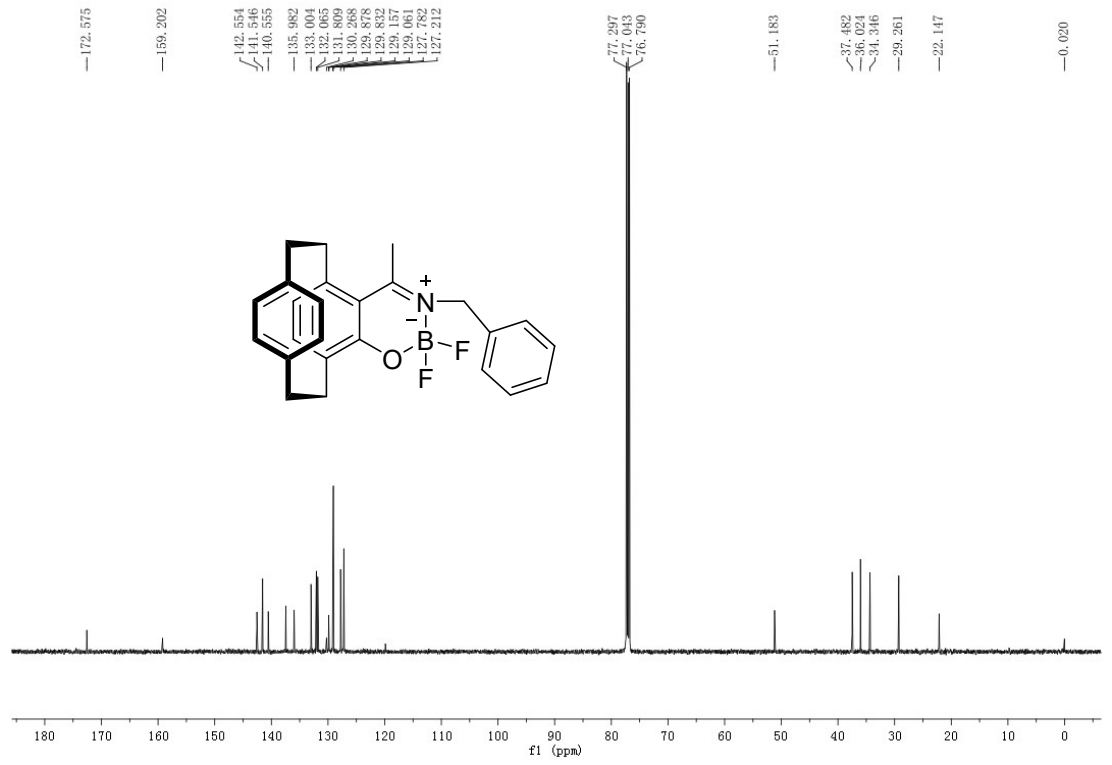
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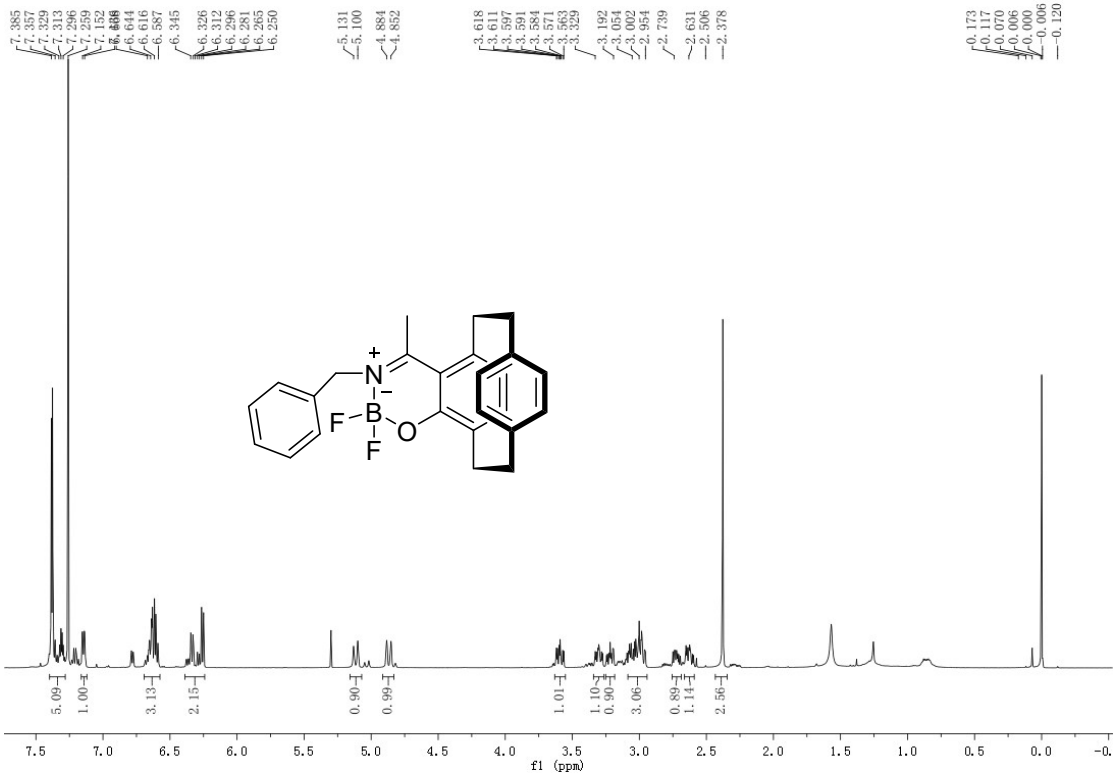
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F
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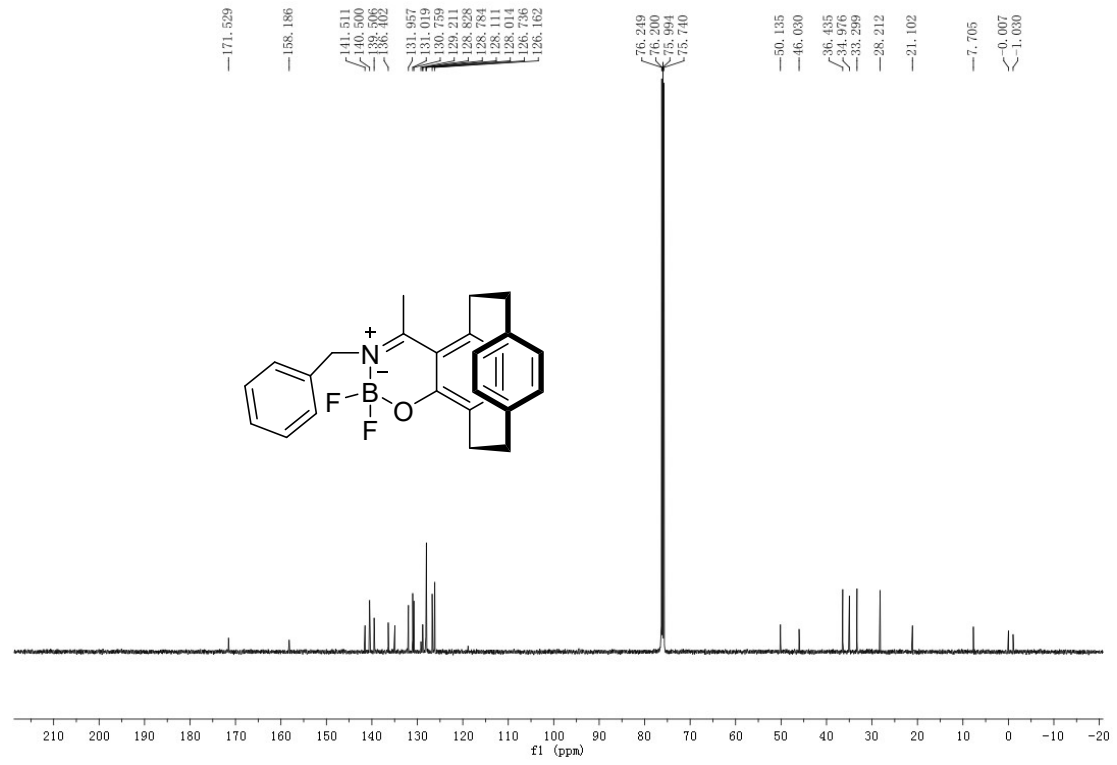
2.56
f1 (ppm)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75.994
75.740
50.135
46.030
36.435
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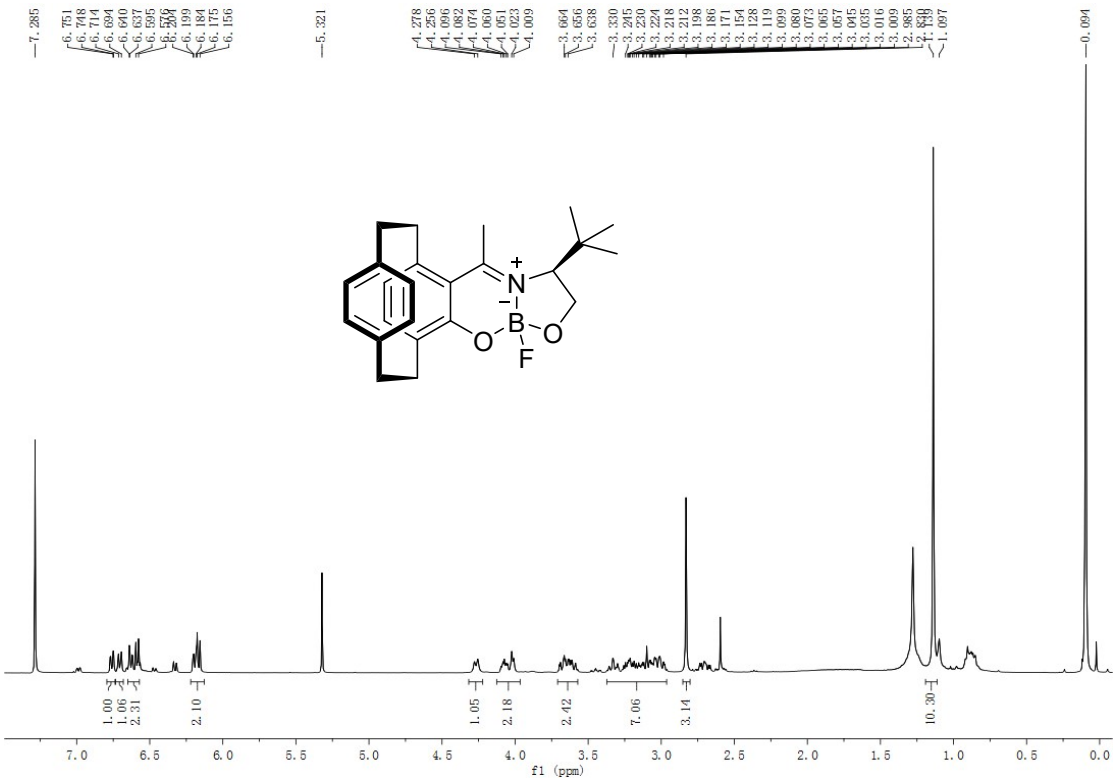
21.102
7.705
-0.007
1.030
N
B
F
F
O
f1 (ppm)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4.051
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4.009
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3.656
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3.245
3.230
3.224
3.218
3.212
3.198
3.186
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3.154
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3.119
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3.080
3.073
3.065
3.057
3.045
3.035
3.016
3.009
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2.42
7.06
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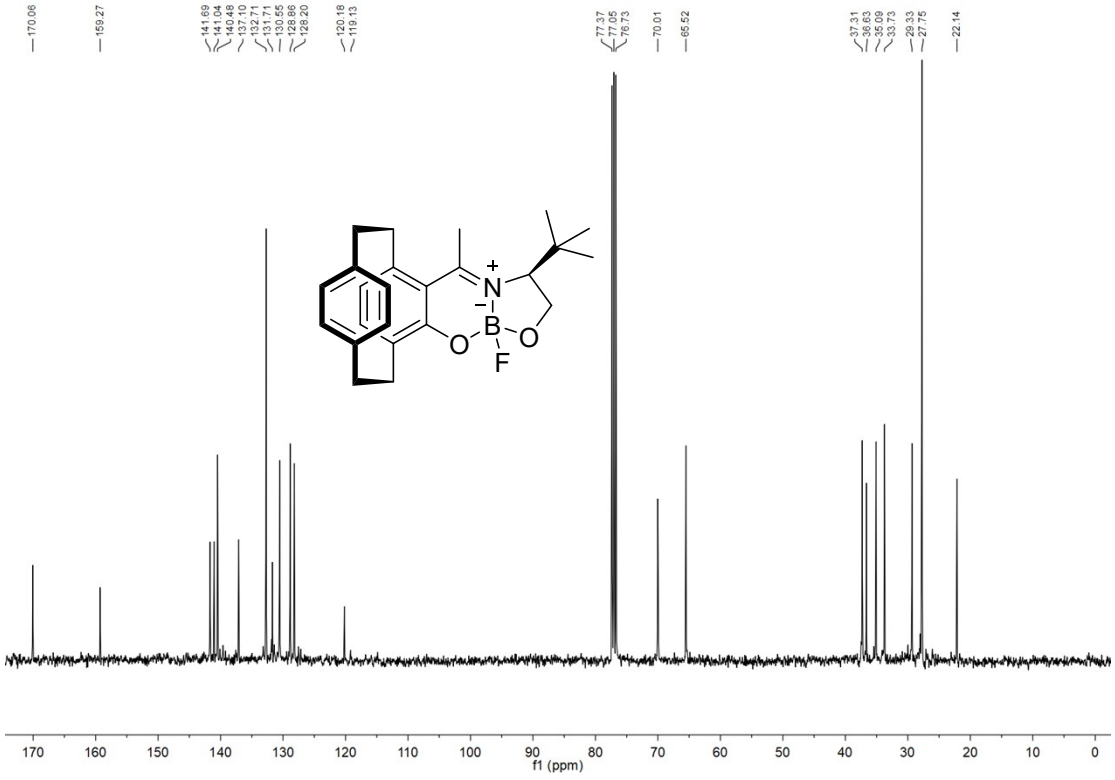
10.30
f1 (ppm)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120.18
119.13
77.37
77.05
76.73
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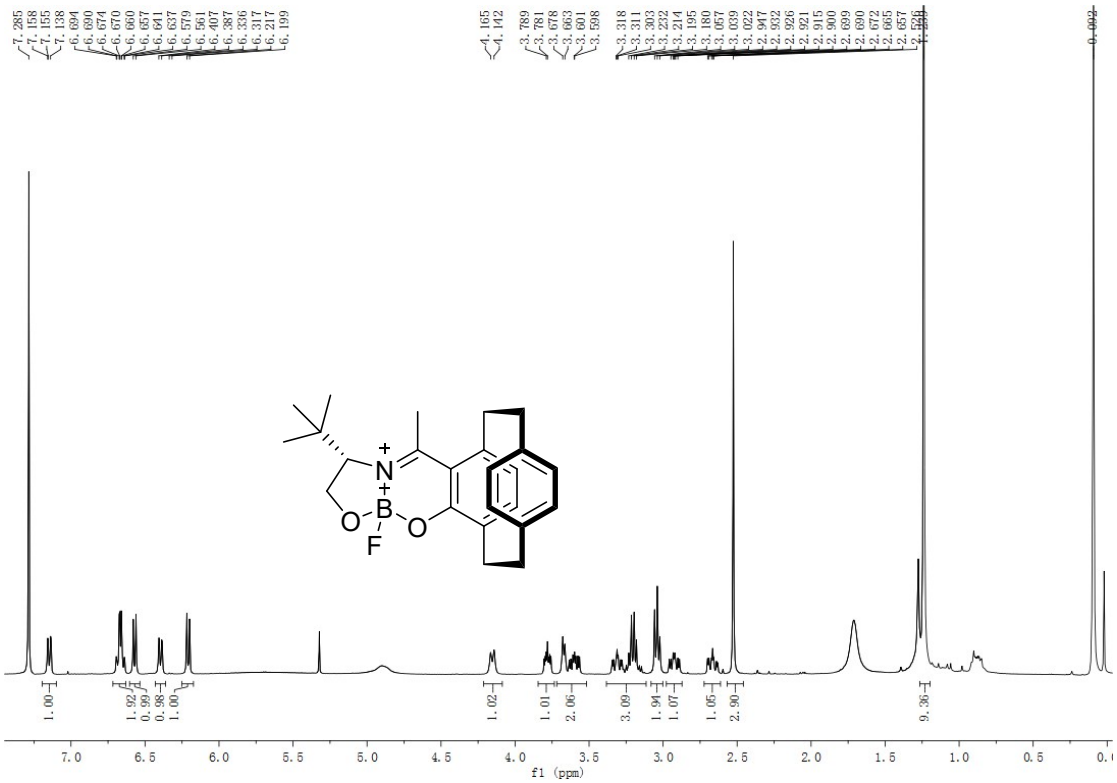
37.31
36.63
35.09
33.73
29.33
27.75
22.14
f1 (ppm)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6.217
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3.789
3.781
3.678
3.663
3.601
3.598
3.318
3.311
3.303
3.232
3.214
3.195
3.180
3.057
3.039
3.022
2.947
2.932
2.926
2.921
2.915
2.900
2.699
2.690
2.672
2.665
2.657
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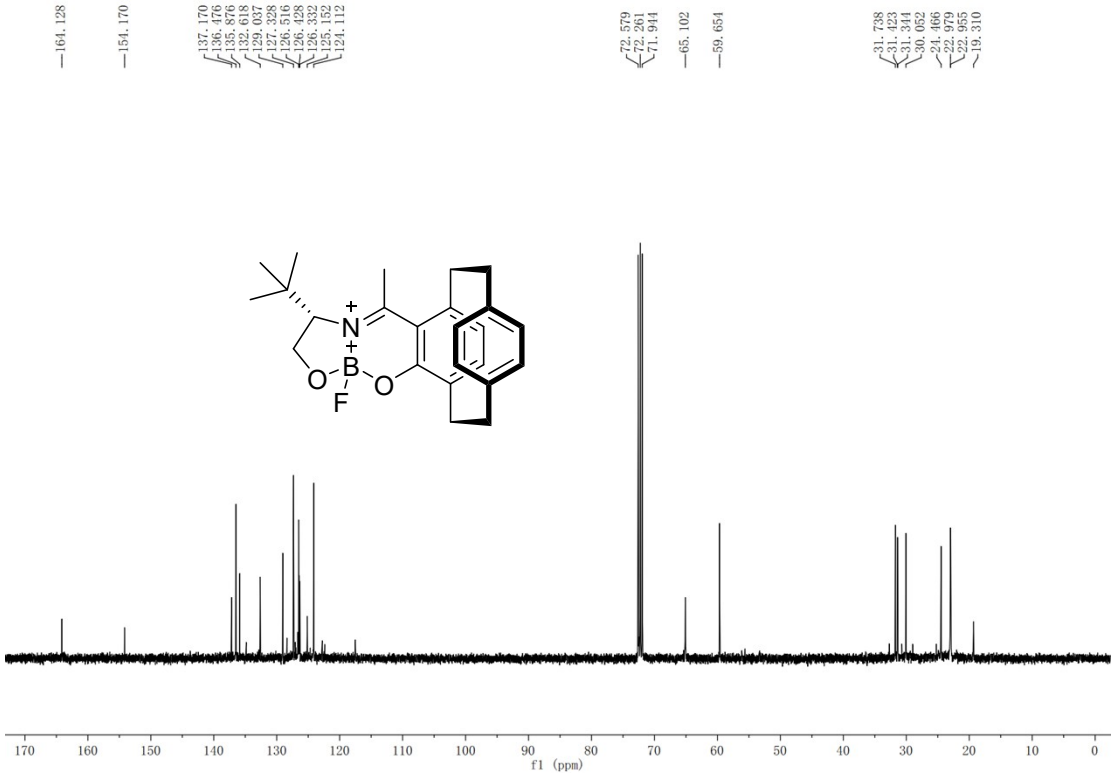
1.92
0.99
0.98
1.00
1.02
1.01
2.06
3.09
1.94
1.07
1.05
2.90
9.36
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)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126.332
125.152
124.112
72.579
72.261
71.944
65.102
59.654
31.738
31.423
31.344
30.052
24.466
22.979
22.955
19.310
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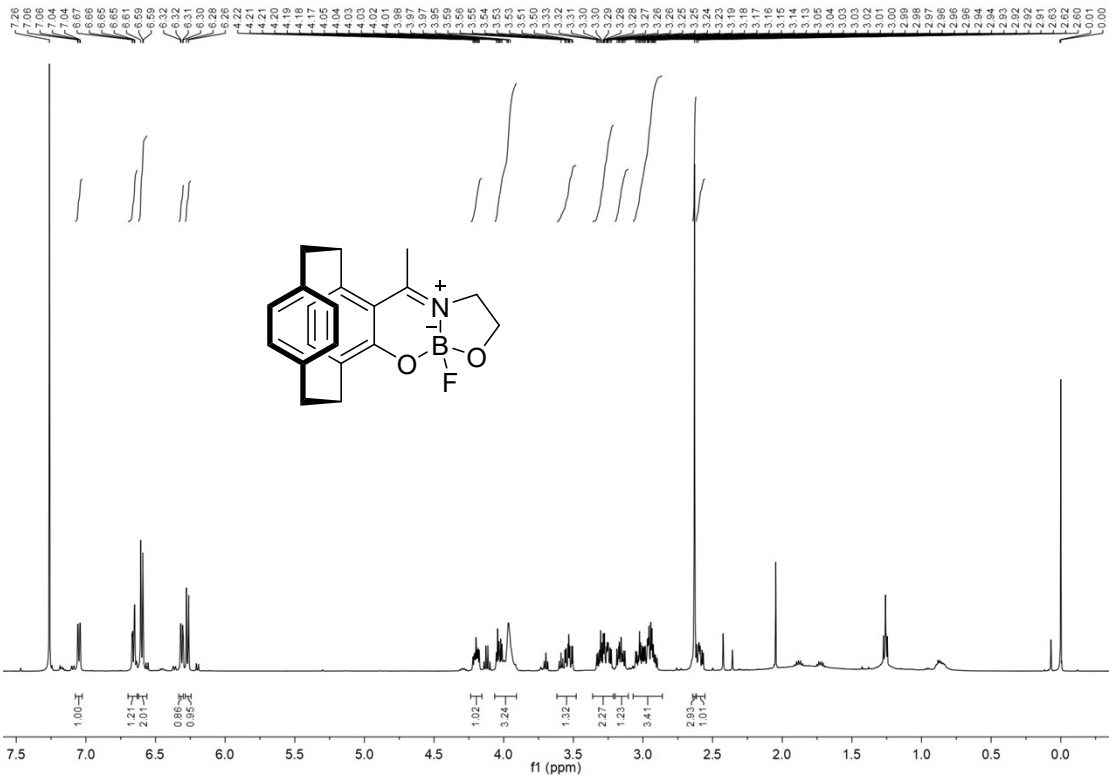
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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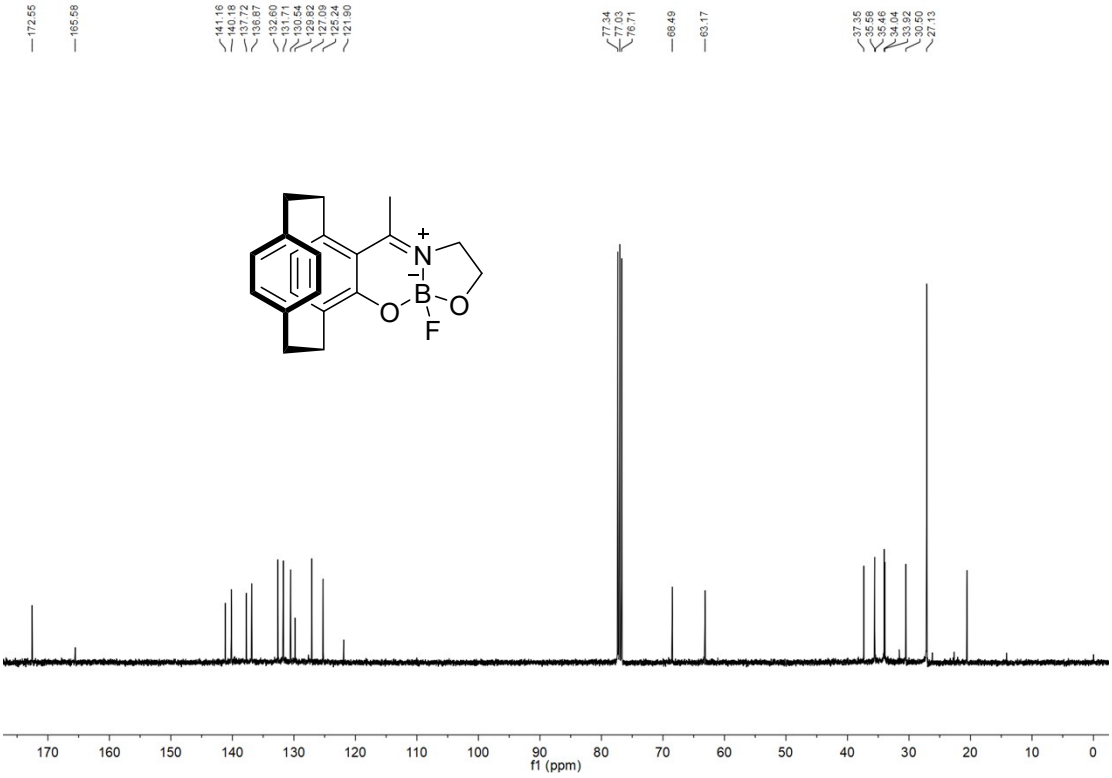
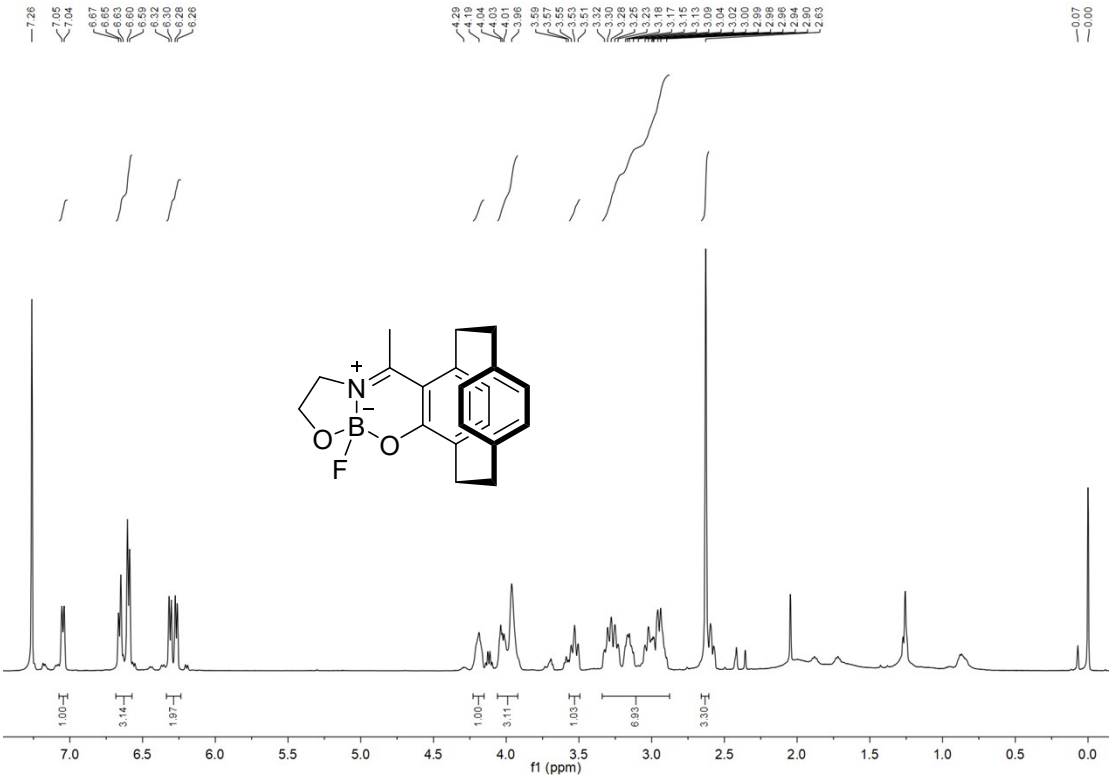

f1 (ppm)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6.63
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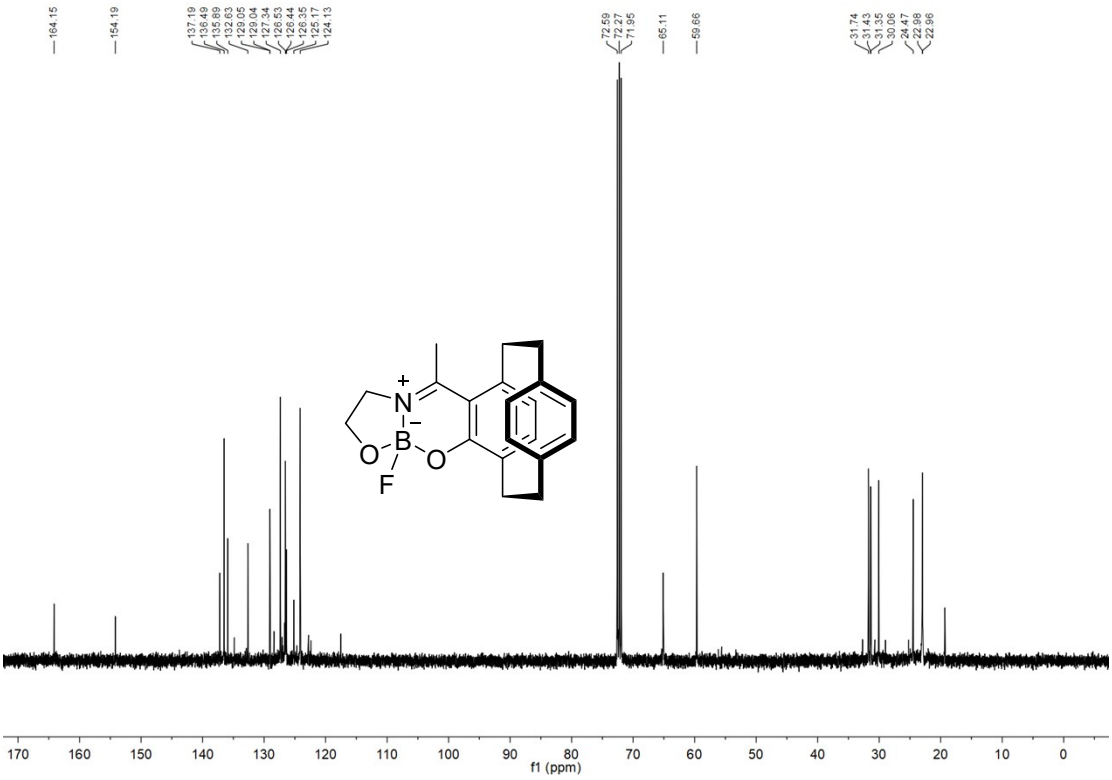
6.30
6.28
6.26
4.29
4.19
4.04
4.03
4.01
3.98
3.59
3.57
3.55
3.53
3.51
3.32
3.30
3.28
3.25
3.23
3.19
3.17
3.15
3.13
3.09
3.04
3.02
3.00
2.99
2.98
2.96
2.94
2.90
2.63
0.07
0.00
1.00
3.14
1.97
1.00
3.11
1.03
6.93
3.30
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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132.63
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129.04
127.74
126.53
126.44
126.35
125.17
124.13
72.59
72.27
71.95
65.11
59.66
31.74
31.43
31.35
30.06
24.47
22.98
22.96
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

4. Theoretical calculations

Optimized structure of (S_p,R)-**3a** in the ground state

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

F	0.7867	4.465	9.5908
F	1.8366	3.9971	7.6414
O	2.9758	3.6475	9.6065
N	2.5075	5.9498	8.8377
C	3.9689	4.1277	10.3679
C	1.2549	8.0949	8.515
C	3.537	6.3941	9.4966
C	5.1633	5.9728	11.4229
C	2.8184	3.1846	13.2051
C	3.0907	5.9699	13.3372
C	4.6739	3.1913	11.1609
C	3.6792	3.7742	14.1271
H	4.1739	3.2343	14.6996
C	0.6104	8.0691	9.7452
H	0.4372	7.2522	10.1564
C	5.9757	5.0326	11.9999
H	6.6981	5.3202	12.5108
C	4.2496	5.5094	10.4175
C	2.0597	5.388	12.6229
H	1.4508	5.9326	12.1769
C	1.9137	4.015	12.5561
H	1.208	3.6461	12.077
C	1.4712	9.3275	7.9111
H	1.888	9.3667	7.0801
C	1.6808	6.784	7.8903
H	0.8517	6.2795	7.7536
C	3.8124	5.151	14.2044
H	4.3827	5.5294	14.8337
B	2.0068	4.4755	8.9322
C	5.7639	3.6672	11.8535
H	6.3668	3.0671	12.2282
C	4.981	7.2808	12.1655
H	5.0158	8.0137	11.5291
H	5.7132	7.3945	12.7904
C	4.096	7.7796	9.2621
H	3.947	8.0338	8.3472
H	5.0378	7.7796	9.4458
H	3.6565	8.4045	9.8425
C	0.2186	9.2501	10.3719
H	-0.2073	9.2243	11.198

C	3.6104	7.3468	12.9556
H	3.7337	7.8732	13.7607
H	2.9485	7.7949	12.4052
C	4.099	1.8298	11.4218
H	4.8244	1.2058	11.5861
H	3.6225	1.5307	10.633
C	2.3373	6.8652	6.5116
H	3.1815	7.3162	6.5836
H	1.7655	7.3515	5.9129
H	2.4765	5.9785	6.1726
C	3.1028	1.8087	12.6706
H	2.2677	1.3931	12.4023
H	3.4909	1.2679	13.3754
C	1.0718	10.4999	8.5364
H	1.2171	11.3178	8.1189
C	0.4697	10.4626	9.7549
H	0.2254	11.2557	10.1764

Optimized structure of (R_p)-**3b** in the ground state
Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

F	9.6479	9.9939	8.3205
F	8.3706	8.1386	8.1664
N	10.3446	8.0287	9.5075
O	8.3932	9.3981	10.1312
B	9.1468	8.9029	9.0222
C	5.4422	6.9294	12.6556
H	4.82	7.1715	13.3028
C	6.3175	5.8814	12.9002
H	6.2887	5.4338	13.7152
C	7.2325	5.5019	11.9363
C	7.0687	6.0063	10.662
H	7.553	5.6381	9.9585
C	6.1994	7.0479	10.4133
H	6.0922	7.3669	9.5462
C	5.4879	7.6179	11.4541
C	5.078	9.0693	11.3994
H	4.3149	9.2055	11.9832
H	4.8011	9.2862	10.4954
C	6.2351	10.0441	11.8311
H	6.4584	10.6191	11.0825
H	5.9195	10.6078	12.5541
C	7.4776	9.3227	12.2805
C	7.6423	8.8802	13.5682

H	7.1858	9.3114	14.2537
C	8.464	7.8121	13.8805
H	8.4968	7.5094	14.7599
C	9.2361	7.1866	12.9291
C	9.378	7.8613	11.6784
C	8.4372	8.8629	11.3511
C	9.503	5.7036	13.1152
H	9.4296	5.4842	14.0581
H	10.4111	5.5082	12.8355
C	8.5236	4.8171	12.3131
H	8.9662	4.5208	11.5013
H	8.3161	4.029	12.8387
C	10.4359	7.57	10.7281
C	11.6644	6.8398	11.1714
H	11.593	5.9142	10.9288
H	11.7537	6.9142	12.1255
H	12.4355	7.2244	10.7477
C	11.3945	7.7566	8.5031
H	12.2539	8.0151	8.8718
H	11.2318	8.3102	7.7236
C	11.467	6.314	8.0685
C	10.417	5.4413	8.2083
H	9.6271	5.7314	8.6033
C	10.5202	4.1274	7.7652
H	9.8117	3.5359	7.8853
C	11.6694	3.7074	7.1497
H	11.7438	2.8323	6.8471
C	12.6975	4.5725	6.9829
H	13.4676	4.29	6.5463
C	12.6171	5.8625	7.4503
H	13.3425	6.4363	7.35

Optimized structure of (S_p)-**3b** in the ground state

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

F	3.4033	4.4716	8.1712
F	4.6839	2.6188	8.3231
N	5.3773	4.5789	9.511
O	3.4301	3.2148	10.128
B	4.179	3.6957	9.0148
C	1.349	6.7239	12.9061
H	1.3232	7.1667	13.7228
C	0.4781	5.6779	12.6602
H	-0.1438	5.4344	13.3071
C	0.5227	4.9927	11.4586

C	1.23	5.5643	10.4122
H	1.1179	5.2489	9.5453
C	2.1029	6.609	10.6661
H	2.5899	6.9762	9.9642
C	2.2616	7.1112	11.9341
C	3.56	7.8014	12.3222
H	3.3497	8.5824	12.8575
H	4.0044	8.108	11.5168
C	4.5321	6.9018	13.1147
H	5.4397	7.0986	12.8333
H	4.4617	7.1188	14.0576
C	4.2713	5.4192	12.9319
C	4.4062	4.748	11.6834
C	3.4708	3.7537	11.3486
C	2.5215	3.2906	12.2818
C	2.6762	3.7297	13.5724
H	2.217	3.297	14.2565
C	3.4975	4.7959	13.8829
H	3.5293	5.1013	14.7611
C	1.2707	2.5689	11.837
H	0.9562	2.0087	12.5632
H	1.4899	1.9898	11.0898
C	0.1061	3.548	11.402
H	-0.1686	3.331	10.4963
H	-0.6567	3.413	11.9842
C	5.4725	5.047	10.7356
C	6.7064	5.775	11.1691
H	7.4772	5.3675	10.7664
H	6.7848	5.7309	12.1249
H	6.6499	6.6923	10.8941
C	6.4337	4.8502	8.4989
H	6.267	4.3013	7.7178
H	7.2927	4.5877	8.866
C	6.5081	6.2999	8.0719
C	5.4467	7.173	8.2143
H	4.6561	6.8791	8.6073
C	5.5489	8.4752	7.776
H	4.8386	9.0619	7.9037
C	6.6935	8.918	7.1517
H	6.761	9.7962	6.8541
C	7.7261	8.0449	6.9803
H	8.4929	8.3238	6.5323
C	7.6508	6.7529	7.4574
H	8.3798	6.1838	7.3636

Optimized structure of (R_p,S)-**3c** in the ground state
Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

N	4.9743	8.3511	3.5657
F	4.9428	10.5371	4.6389
O	4.6323	8.6815	5.9776
O	6.7438	9.0686	4.8728
C	3.3556	8.2321	5.8337
B	5.3152	9.228	4.8048
C	3.8224	7.6798	3.5009
C	1.4736	7.5181	4.4682
C	2.5524	8.2598	6.9749
C	1.3341	7.6509	6.8516
H	0.8549	7.4672	7.6261
C	0.7717	7.2951	5.6378
H	-0.0731	6.9069	5.6109
C	2.8494	7.8358	4.5804
C	2.1249	11.0501	5.7689
H	2.9495	11.4567	5.9096
C	1.3026	10.7369	6.8627
C	6.4209	9.0559	1.6453
C	0.4781	10.1361	4.2643
C	0.0011	10.3811	6.5987
H	-0.6153	10.3476	7.2941
C	7.1791	8.1108	3.9324
H	7.2421	7.2385	4.3528
H	8.0565	8.3511	3.5957
C	1.7087	10.7531	4.4808
H	2.252	10.968	3.7569
C	6.1712	8.0657	2.7817
H	6.1206	7.1564	2.4214
C	2.8415	9.1529	8.1634
H	3.7729	9.4256	8.1334
H	2.7088	8.6457	8.979
C	0.6648	7.8115	3.1863
H	1.1845	7.5365	2.415
H	-0.1496	7.2835	3.1974
C	-0.4038	10.0714	5.309
H	-1.2846	9.8173	5.1525
C	3.5884	6.6342	2.4593
H	3.6863	7.0224	1.5869
H	2.7009	6.2806	2.5541
H	4.2274	5.9259	2.5668

C	5.2139	9.1344	0.7318
H	5.0283	8.2633	0.3714
H	5.3961	9.7456	0.0142
H	4.4546	9.4429	1.2312
C	1.9202	10.4608	8.2093
H	1.2171	10.336	8.8652
H	2.4545	11.2222	8.4811
C	6.7831	10.477	2.0784
H	6.9755	11.0096	1.3024
H	7.556	10.4516	2.6474
H	6.0452	10.864	2.5573
C	0.2992	9.2858	3.0394
H	0.8381	9.6624	2.3265
H	-0.6288	9.3436	2.7628
C	7.5863	8.492	0.8156
H	7.3647	7.6082	0.5137
H	8.3771	8.4562	1.3577
H	7.7427	9.0593	0.0569