Supplementary Information (SI) for Organic Chemistry Frontiers.

Supporting information

Cross-Shaped Organic Framework; a Multi-Functional Template Arranging Chromophores

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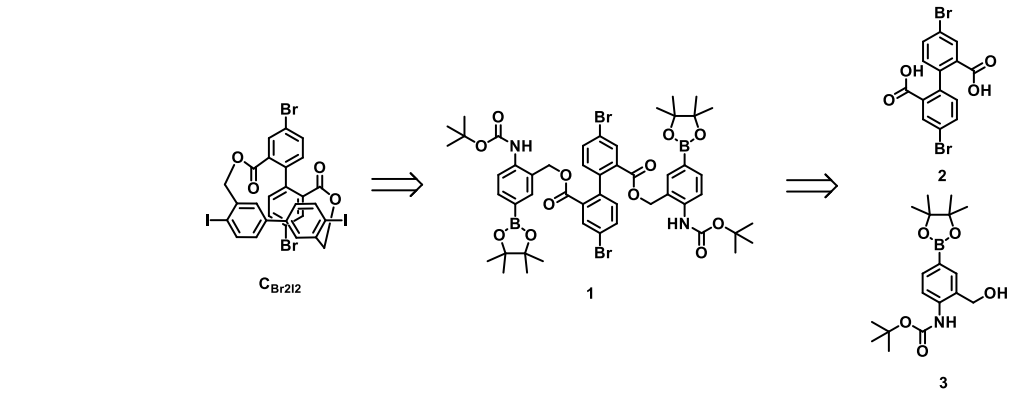
General

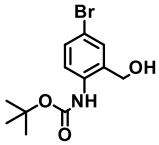
All chemicals and solvents were purchased from SigmaAldrich, Acros, Apollo Scientific, Alfa Aesar and Fluorochem and used as received. NMR solvents were obtained from CIL Cambridge Isotope Laboratories, Inc., Acros, Sigma-Aldrich, or Apollo Scientific. Dry solvents were used as crown capped and purchased from Acros and Sigma-Aldrich. Column chromatography was performed manually or on a Biotage Isolera using SilicaFlashR P60 from Silicycle with particle size of 40-63 µm (230-400 mesh) as stationary phase. TLC was performed with silica gel 60 F254 glass plates purchased from Merck. Recycling size-exclusion chromatography (SEC or GPC) was performed with a Shimadzu Prominence System equipped with SDV preparative columns from Polymer Standards Service (two Shodex columns in series, 20×600 mm each, exclusion limit: 30 000 g mol^{-1}) with chloroform as solvent. NMR experiments were performed on Bruker Avance III NMR spectrometers operating at 250, 400 or 500 MHz proton frequencies. The instruments were equipped with a direct-observe 5 mm BBFO smart probe (250, 400 MHz), or an indirect-detection 5 mm BBI probe (500, 600 MHz). All probes were equipped with actively shielded z-gradients (10 A). The chemical shifts are reported in ppm relative to TMS or referenced to residual solvent peak and the J values are given in Hz. Infrared spectra were recorded neat with an ATR equipped Schimadzu IRTacer-100. High-resolution mass spectra (HR-MS) were measured with a Bruker Maxis 4G ESI-TOF instrument. CD measurements were performed on a JASCO J-1500 CD Spectrophotometer in a 1 cm quartz glass cuvette. Quantum yields were recorded on an Absolute PL Quantum Yield Spectrometer: Hamamatsu Quantaurus QY - C11347. Fluorescence lifetime measurements were performed on a Compact Fluorescence Lifetime Spectrometer: Hamamatsu Quantaurus Tau – 11367. For analytical HPLC, a Shimadzu LC-20AT HPLC was used, equipped with a diode-array UV/Vis detector (SPD-M20 A VP from Shimadzu, λ=200–600 nm) and a column oven Shimadzu CTO-20AC. For preparative HPLC, a Shimadzu LC-20AP HPLC was used equipped with a diode-array UV/Vis detector (SPD-M20 A VP from Shimadzu, λ=200–600 nm). The used column for analytical separation on chiral stationary phase was a Chiralpak IG, IA, IC or IBN-5; 5 µm, 4.6×250 mm, Daicel Chemical Industries Ltd and for preparative separation, Chiralpak IG, 5 µm, 30×250 mm, Daicel Chemical Industries Ltd. DFT calculations[1]; Geometries were optimized either using Gausian 09 or Gaussian 16 and stationary points were analyzed by subsequent frequency analysis. C_{Br2I2} was optimized at the B3LYP/3-21G level of theory while all other structures were optimized at the B3LYP/6-31G(d,p) level of theory. The initial guess was obtained from the crystallographic data and the *P* isomer was optimized. From the resulting geometry all initial guesses were modeled. CD spectra were simulated by calculation of rotary strengths at the TD-cam-B3LYP/6-31G(p,d) level of theory of the 50 lowest singlet transitions except for (*P*)-C_{Br2I2} where we used the 3-21G basis set.[2] The simulated spectrum was fitted using SpecDis.[3]

Synthesis



Scheme S1: Molecular design and retro-synthetic analysis of universal cross-shaped building block $\mathbf{C_{Br2I2}}$.

Experimental procedure C_{Br2I2}



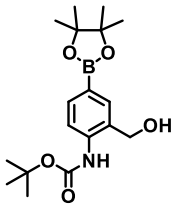
Compound 5: To a stirred solution of (2-amino-5-bromophenyl)methanol **4** (5.01 gr, 1 equiv.) in dry THF (82.5 mL) was added DIPEA (6 mL, 1.5 equiv.) at 0°C. A solution of di-tert-butyl dicarbonate (5.9 mL, 1.1 equiv.) in dry THF was added dropwise after which the reaction was allowed to warm to room temperature and where it was stirred for 18 hours. The mixture was diluted with EtOAc and washed with 0.1 M HCl 3 times. The organic phase was collected, dried with sodium sulfate and concentrated in vacuo. The crude was purified by column chromatography (SiO_2, cyclohexane:ethyl acetate 8:2 v/v) obtaining the boc-protected amine as a white solid (5.00 gr, 66 %).

TLC: R_f = 0.15 (SiO_2, cyclohexane: ethyl acetate 8:2 v/v)

^{1}H-NMR: (500 MHz, CD_2Cl_2): δ 7.85 (d, *J* = 8.7 Hz, 1H), 7.67 (s, 1H), 7.40 (dd, *J* = 8.8, 2.4 Hz, 1H), 7.31 (d, *J* = 2.4 Hz, 1H), 4.64 (d, *J* = 5.7 Hz, 2H), 2.32 – 2.27 (m, 1H), 1.50 (s, 9H).

^{13}C-NMR {1H}: (126 MHz, CD_2Cl_2): δ 153.31, 137.89, 131.96, 131.80, 131.29, 122.63, 115.42, 80.94, 63.95, 28.42.

HR-ESI-MS: *m/z* calculated for $C_{12}H_{16}BrNNaO_3$ $[M+Na]^+$; 324.0206 found 324.0203.



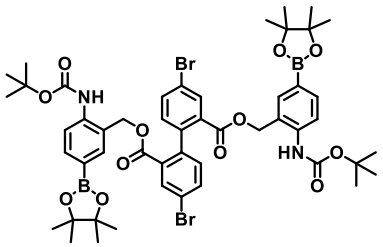
Compound 3: Protected amine **5** (2.0 gr, 1 equiv.)**,** B_2Pin_2 (1.94 mg, 1.15 equiv.) and KOAc (1.30 gr, 2 equiv.) were added to a 100 mL *Schlenk* tube and cycled between vacuum and argon 3 times. 40 mL dry dioxane was added and the mixture was degassed for 15 min. Pd(ddpf)Cl_2 (5 mol%) was added, the tube was sealed and heated to 90°C. After 16 hours the reaction was cooled, filtered over silica and flushed down with EtOAc. The volatiles were removed under reduced pressure and the crude is subjected to column chromatography (SiO_2, cyclohexane: ethyl acetate 9:1 to 3:1 v/v) obtaining the product in the as a white fluffy solid (2.27 gr, 98 %).

TLC: R_f = 0.15 (SiO_2, cyclohexane: ethyl acetate 6:4 (v/v)).

^{1}H-NMR: (500 MHz, CD_2Cl_2) δ 8.00 (d, *J* = 8.2 Hz, 1H), 7.89 (s, 1H), 7.68 (dd, *J* = 8.1, 1.6 Hz, 1H), 7.55 (d, *J* = 1.5 Hz, 1H), 4.71 (s, 2H), 2.00 (s, 1H), 1.51 (s, 9H), 1.31 (s, 12H).

^{13}C-NMR {1H}: (126 MHz, CD_2Cl_2) δ 153.15, 141.71, 136.10, 135.67, 127.66, 119.37, 84.13, 80.76, 64.77, 28.45, 25.07.

HR-ESI-MS: *m/z* calculated for $C_{18}H_{29}BNO_5$ $[M+H]^+$; 350.2137 found 350.2132.

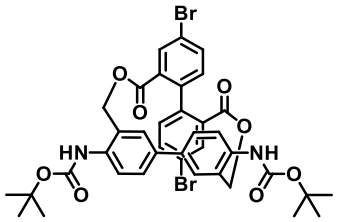


Compound 1: To a solution of **3** (2.0 gr, 2.05 equiv.) and Diacid **2** (1.11 gr, 1 equiv.) in dry DCM/DMF (23:4.4 mL) were added, *N,N'*-dicyclohexylcarbodiimide (1.27 gr, 2.2 equiv.) and finally 4-(dimethylamino)pyridine (35 mg, 0.1 equiv.) at room temperature under inert atmosphere. The reaction mixture was stirred at room temperature for 4 hours before it was filtered through a pad of celite and flushed down with DCM. The organic phase was washed with water (3 times), dried over sodium sulfate and solvents were removed under vacuum. The crude was purified by flash column chromatography on silica gel (cyclohexane : ethyl acetate 9:1→8:2 v/v) obtaining the product as a white fluffy solid (2.87 gr, 97 %), which was used in the next step without further purification. **TLC:** R_f = 0.27 (SiO_2, cyclohexane: ethyl acetate 6:4 (v/v)).

^{1}H-NMR: (500 MHz, CD_2Cl_2) δ 7.96 (d, *J* = 2.1 Hz, 2H), 7.88 (d, *J* = 8.2 Hz, 2H), 7.73 (dd, *J* = 8.3, 1.6 Hz, 2H), 7.51 (d, *J* = 1.5 Hz, 2H), 7.45 (dd, *J* = 8.2, 2.2 Hz, 2H), 7.05 (s, 2H), 6.87 (d, *J* = 8.1 Hz, 2H), 5.02 (d, *J* = 1.3 Hz, 4H), 1.50 (s, 18H), 1.33 (d, *J* = 3.6 Hz, 24H).

^{13}C-NMR {1H}: (126 MHz, CD_2Cl_2) δ 165.63, 152.47, 140.65, 140.32, 137.85, 136.45, 134.64, 132.91, 131.51, 130.39, 122.88, 121.36, 120.13, 83.80, 80.62, 64.39, 28.05, 24.71.

HR-ESI-MS: *m/z* calculated for $C_{50}H_{61}B_2Br_2N_2O_{12}$ $[M+Na]^+$; 1061.2774 found 1061.2778.

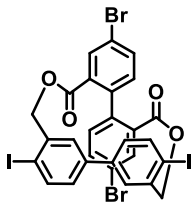


Compound $C_{Br_2NBoc_2}$: 1 (3.44 gr, 1 equiv.), $PdCl_2PPh_3$ (459 mg, 20 mol %) and boric acid (1.20 gr, 6 equiv.) were dissolved a 600 mL toluene/150 mL MeOH mixture. The solution was stirred vigorously for 15 minutes, followed by the addition of 150 mL H_2O and KF (1.88 gr, 10 equiv.). The reaction mixture was allowed to stir at room temperature for 7 hours open to the air. The mixture was portioned between toluene and water, followed by subsequent extraction of the aqueous phase with toluene. The combined organic layers were dried over sodium sulfate and concentrated in vacuo. The crude reaction mixture was purified by column chromatography (SiO_2, cyclohexane: ethyl acetate 9:1→8:2→1:1 v/v) obtaining the product as an off-white powder (1.69 gr, 61 %). **TLC:** R_f = 0.17 (SiO_2, cyclohexane: ethyl acetate 6:4 (v/v)).

^{1}H-NMR: (500 MHz, CD_2Cl_2): δ 8.44 – 8.41 (m, 2H), 7.77 – 7.73 (m, 2H), 7.43 (s, 4H), 7.21 – 7.18 (m, 2H), 6.94 (s, 2H), 6.22 (s, 2H), 5.67 (d, *J* = 14.2 Hz, 2H), 5.04 (d, *J* = 14.3 Hz, 2H), 1.50 (s, 18H).

^{13}C-NMR {1H}: (126 MHz, CD_2Cl_2) δ 164.66, 153.60, 143.45, 137.50, 135.42, 134.19, 133.41, 132.99, 130.24, 128.64, 125.51, 125.31, 124.82, 121.63, 81.07, 62.80, 28.40.

HR-ESI-MS: *m/z* calculated for $C_{38}H_{36}Br_2N_2NaO_8$ $[M+Na]^+$; 829.0731 found 829.0725.



Compound $C_{Br_2I_2}$: To a solution of p-TsOH*H2O (579 mg, 6 equiv.) in 2.5 mL toluene and 2.5 mL ACN was added **$C_{Br_2Nboc_2}$** (400 mg, 0.495 mmol, 1 equiv.). The mixture was stirred for 4 hours, until full deprotection was observed (LC-MS). The white suspension was cooled to -15°C before a solution of $NaNO_2$ (137 mg, 4 equiv.) and KI (411 mg, 5 equiv.) in 0.75 mL water was added dropwise. The mixture was stirred on ice for 10 minutes before it was warmed to room temperature. After stirring 1 hour the reaction mixture was diluted with water, sat $NaHCO_3$ and 40% aq. $NaHSO_3$, followed by extraction with toluene. The organics were collected, combined, dried with Na_2SO_4 and concentrated. The resulting crude was purified by column chromatography (Cyclohexane:CH_2Cl_2 9:1 --> 1:1) obtaining the product in the 1st fraction as a white solid (256 mg, 62 %).

TLC: R_f = 0.18 (SiO_2, cyclohexane: dichloromethane 9:1).

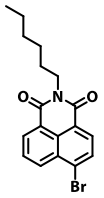
^{1}H-NMR: (500 MHz, CD_2Cl_2) δ 8.44 (d, *J* = 2.1 Hz, 2H), 7.84 (d, *J* = 8.1 Hz, 2H), 7.76 (dd, *J* = 8.3, 2.1 Hz, 2H), 7.20 (d, *J* = 8.2 Hz, 2H), 7.18 – 7.15 (m, 2H), 6.77 – 6.76 (m, 2H), 5.49 (dt, *J* = 14.8, 1.0 Hz, 2H), 4.98 (dt, *J* = 14.7, 0.8 Hz, 2H).

^{13}C-NMR {1H}: (126 MHz, CD_2Cl_2) δ 164.31, 143.48, 140.60, 139.71, 138.61, 135.64, 134.24, 132.95, 128.34, 126.80, 126.09, 121.69, 93.35, 70.45.

HR-ESI-MS: *m/z* calculated for $C_{28}H_{16}Br_2I_2NaO_4$ $[M+Na]^+$; 850.7397 found 850.7389.

FT-IR (ATR) ṽ [cm^{-1}]: 3070 (w), 2906 (w), 1729 (s), 1583 (m), 1551 (m), 1462 (w), 1438 (w), 1424 (w), 1369 (m), 1274 (m), 1229 (s), 1140 (m), 1090 (m), 1073 (s), 1011 (w), 1003 (m), 984 (w), 964 (w), 897 (w), 872 (w), 826 (s), 810 (s), 786 (s), 724 (s), 704 (m), 694 (m), 670 (w), 654 (w), 581 (w), 565 (w), 546 (m), 531 (m), 497 (m), 418 (m).

Experimental procedures Chromophore library



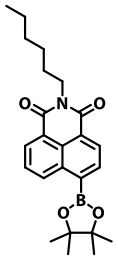
NI-Br: 4-bromo-1,8-naphthalicanhydride (1.07 g, 1 equiv.) was treated with n-hexylamine (0.35 mL, 4.83 mmol, 1.25 equiv.) in ethanol (25 mL). The mixture was heated at reflux for 16 hours before cooled down to room temperature. Hydrochloric acid (2M, 10 mL) was added and the mixture was diluted with EtOAc. Phases were separated and the organic phase was collected, dried and concentrated. The crude was purified by silica column chromatography (cyclohexane:CH2Cl2 7:3 → 1:1 v/v) obtaining the product as a yellow solid (1.3 gr, 93 %).

TLC: R_f = 0.20 (SiO_2, cyclohexane: dichloromethane 7:3)

^{1}H-NMR: (400 MHz, CD_2Cl_2) δ 8.61 (dd, *J* = 7.3, 1.1 Hz, 1H), 8.56 (dd, *J* = 8.5, 1.1 Hz, 1H), 8.37 (d, *J* = 7.9 Hz, 1H), 8.04 (d, *J* = 7.9 Hz, 1H), 7.85 (dd, *J* = 8.5, 7.3 Hz, 1H), 4.15 – 4.09 (m, 2H), 1.70 (p, *J* = 7.4 Hz, 2H), 1.45 – 1.27 (m, 6H), 0.92 – 0.86 (m, 3H).

^{13}C-NMR {1H}: (101 MHz, CD_2Cl_2) δ 163.83, 163.80, 133.37, 132.10, 131.49, 131.32, 130.99, 130.27, 129.37, 128.47, 123.71, 122.89, 40.84, 31.96, 28.36, 27.18, 22.99, 14.22.

HR-ESI-MS: *m/z* calculated for $C_{18}H_{18}BrNNaO_2$ $[M+Na]^+$; 382.0413 found 382.0412.

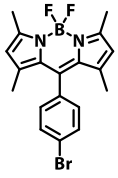


NI-BPin: NI-Br (768 mg, 1 equiv.), B_2Pin_2 (650 mg, 1.2 equiv.) and KOAc (418 mg, 2 equiv.) were added to a 25 mL *Schlenk* tube and cycled between vacuum and argon 3 times. The solids were dispersed in 12 mL dry dioxane followed by degassing with argon for 15 minutes. $PdCl_2$(dppf) (78 mg, 5 mol %) was added, the tube sealed and heated to 85 °C for 4 hours. The reaction mixture was cooled down, filtered over a celite pad and the filtrate was concentrated under reduced pressure. The crude was plugged over silica with dichloromethane, obtaining the product as a white-greenish solid (900 mg, 99 %).

^{1}H-NMR: (500 MHz, CD_2Cl_2) δ 9.12 (dd, *J* = 8.5, 1.1 Hz, 1H), 8.61 – 8.49 (m, 2H), 8.27 (d, *J* = 7.3 Hz, 1H), 7.83 – 7.74 (m, 1H), 4.17 – 4.09 (m, 2H), 1.70 (p, *J* = 7.4 Hz, 2H), 1.44 (s, 12H), 1.43 – 1.28 (m, 6H), 0.95 – 0.86 (m, 3H).

^{13}C-NMR {1H}: (101 MHz, CD_2Cl_2) δ 164.48, 164.46, 135.97, 135.64, 135.14, 130.91, 129.80, 128.24, 127.37, 125.32, 123.26, 85.01, 40.73, 31.99, 28.40, 27.22, 25.15, 23.00, 14.23.

HR-ESI-MS: *m/z* calculated for $C_{24}H_{31}BNO_4$ $[M+H]^+$; 408.2345 found 408.2341.



BY-Br: At room temperature, a solution of TFA (22 µL) in 2 mL of dry-DCM was added to a degassed mixture of 2,4-dimethylpyrrole (0.45 mL, 2.25 equiv.) and 3,5-dibromobenzaldehyde (359 mg, 1 equiv.) in 97 mL dry-DCM under argon atmosphere. The mixture was stirred for 3 hours before it was cooled to 0 °C and a mixture of DDQ (460 mg, 1 equiv.) in 28 mL dry-DCM was added dropwise. After full addition the mixture was heated to room temperature and was stirred for one hour. Et_3N (3.9 mL, 14 equiv.) was added and the mixture was cooled on ice before $BF_3{\cdot}Et_2O$ (3.9 mL) was added slowly. The reaction was stirred for an additional 2 hours at room temperature. The mixture was washed with sat. Na_2CO_3 (twice) and the organics were collected, dried over Na_2SO_4 and evaporated to dryness. The crude product was subjected to silica column chromatography (cyclohexane:CH_2Cl_2 6:4) obtaining the product as a red-solid (230 mg, 29 %).

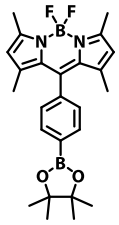
^{1}H-NMR: (400 MHz, CD_2Cl_2) δ 7.67 (d, *J* = 8.4 Hz, 2H), 7.21 (d, *J* = 8.4 Hz, 2H), 6.03 (s, 2H), 2.51 (s, 6H), 1.43 (s, 6H).

^{13}C-NMR {1H}: (101 MHz, CD_2Cl_2) δ 156.19, 143.61, 140.73, 134.30, 132.88, 131.58, 130.39, 123.63, 121.76, 14.81, 14.73.

^{19}F-NMR {1H}: (376 MHz, CD_2Cl_2, not referenced) δ -146.27 (dd, *J* = 65.8, 33.0 Hz).

^{11}B NMR: (128 MHz, CD_2Cl_2, not referenced) δ 0.69 (t, *J* = 32.9 Hz).

HR-ESI-MS: *m/z* calculated for $C_{19}H_{18}B_2F_2N_2Na$ $[M+H]^+$; 425.0610 found 425.0604.



BY-Bpin: BY-Br (160 mg, 1 equiv.), B_2Pin_2 (170 mg, 1.5 equiv.) and KOAc (85 mg, 2 equiv.) were added to a 5 mL *Schlenk* tube and cycled between vacuum and argon 3 times. The solids were dispersed in 2.5 mL dry dioxane followed by degassing for 15 minutes. $PdCl_2$(dppf) (25 mg, 7 mol %) was added, the tube sealed and heated to 85 °C for 20 hours. The reaction mixture was cooled down, filtered over a silica pad and the filtrate was concentrated under reduced pressure. The obtained crude was plugged over silica with dichloromethane and the obtained solid was washed with heptane, yielding the product as a red-solid (150 mg, 83 %).

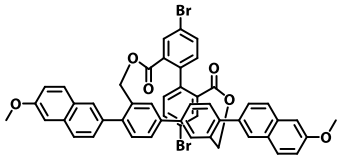
^{1}H-NMR: (400 MHz, CD_2Cl_2) δ 7.88 (d, *J* = 7.8 Hz, 2H), 7.31 (d, *J* = 7.9 Hz, 2H), 6.01 (s, 2H), 2.50 (s, 6H), 1.38 (s, 6H), 1.36 (s, 12H).

^{13}C-NMR {1H}: (101 MHz, CD_2Cl_2) δ 143.80, 139.08, 138.04, 135.69, 127.77, 121.49, 84.50, 25.25, 14.70, 14.64.

^{19}F-NMR {1H}: (376 MHz, CD_2Cl_2, not referenced) δ -δ -146.28 (dd, *J* = 65.9, 33.1 Hz).

^{11}B NMR: (128 MHz, CD_2Cl_2, not referenced) δ 30.38, 0.71 (t, *J* = 32.9 Hz).

HR-ESI-MS: *m/z* calculated for $C_{25}H_{30}B_2F_2N_2NaO_2$ $[M+Na]^+$; 473.2362 found 473.2357.



Compound $C_{Br_2Naph_2}$: $C_{Br_2I_2}$ (30.2 mg, 1. equiv.), 6-Methoxy-naphtalene boric acid (16.4 mg, 2.2 equiv) and K_2CO_3 (25.0 mg, 5 equiv.) were added to a 10 mL *Schlenk* tube and dispersed in 4 mL of a 4:1:4 mixture of toluene:EtoH:H_2O. The mixture was degassed with argon for 15 minutes, before $PdCl_2$(dppf) (10 mol%) was added. The tube was sealed and heated at 60 °C for 17 hours. The reaction was cooled to r.t. and extracted with CH_2Cl_2. Organic phases were dried with Na_2SO_2, filtered and concentrated under reduced pressure. The crude was purified by column chromatography (SiO_2, cyclohexane:CH_2Cl_2 8:2 → 1:1) obtaining the product (21.3 mg, 62 %) as a white solid.

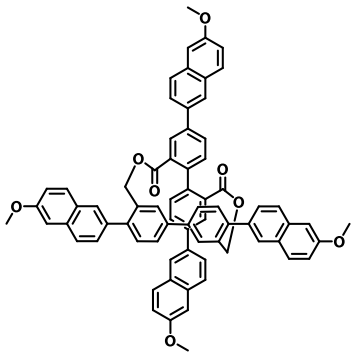
TLC: R_f = 0.24 (SiO_2, cyclohexane: dichloromethane 1:1).

^{1}H-NMR: (500 MHz, CD_2Cl_2): δ 8.39 (d, J = 2.1 Hz, 2H), 7.85 (d, J = 8.4 Hz, 2H), 7.80 (d, J = 8.9 Hz, 2H), 7.75 (d, J = 2.0 Hz, 3H), 7.73 (d, J = 2.1 Hz, 1H), 7.67 (dd, J = 7.9, 2.0 Hz, 2H), 7.47 (dd, J = 8.3, 1.8 Hz, 2H), 7.43 (d, J = 7.8 Hz, 2H), 7.32 (d, J = 1.9 Hz, 2H), 7.25 – 7.16 (m, 6H), 5.90 (d, J = 14.0 Hz, 2H), 4.96 (d, J = 14.0 Hz, 2H), 3.95 (s, 6H).

^{13}C-NMR {1H}: (126 MHz, CD_2Cl_2): (126 MHz, CD_2Cl_2) δ 165.00, 158.50, 143.66, 139.65, 139.54, 135.41, 135.18, 134.77, 134.25, 134.14, 132.80, 131.00, 129.91, 129.13, 128.94, 128.14, 128.08, 127.31, 125.93, 125.09, 121.53, 119.71, 106.00, 64.46, 55.76.

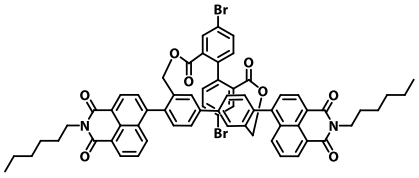
HR-ESI-MS: *m/z* calculated for $C_{50}H_{34}Br_2NaO_6$ $[M+Na]^+$; 911.0614 found 911.0605.

FT-IR (ATR) $\tilde{\nu}$ [cm^{-1}]: 3060 (w), 2967 (m), 2902 (m), 2837 (w), 1725 (s), 1633 (w), 1605 (m), 1554 (w), 1495 (m), 1463 (w), 1388 (m), 1372 (m), 1269 (m), 1232 (s), 1204 (s), 1145 (m), 1082 (m), 1070 (s), 1031 (m), 1003 (m), 916 (w), 892 (w), 856 (w), 830 (m), 806 (m), 787 (m), 716 (w), 675 (w), 654 (w), 569 (w), 548 (w), 522 (w), 476 (m).



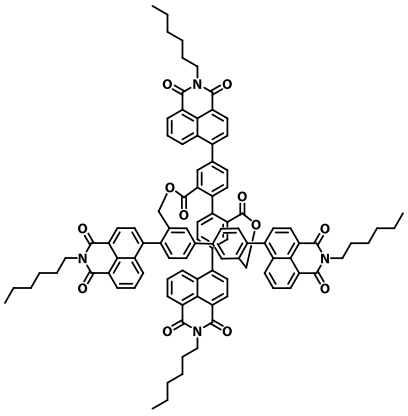
Compound C_{Naph_4}: Route 1 (two-fold *Suzuki*): A 5 ml *Schlenk* tube was charged with **$C_{Br_2Naph_2}$** (21.3 mg, 1 equiv.), Methoxy-naphtalene boric acid (11.6 mg, 2.4 equiv.) and K_2CO_3 (16.4 mg, 5 equiv.) in 2.5 mL of a mixture of toluene:EtOH:H_2O (4/1/4 v/v/v). The mixture was degassed for 15 min with argon and $PdCl_2$(dppf) (10 mol %) was added. The reaction mixture was heated at 85 °C for 24 hours. After completion the mixture was cooled down and extracted with CH_2Cl_2. The combined organic layers were dried over Na_2SO_4 and evaporated under reduced pressure. The crude product was purified by a column chromatography (SiO_2, cyclohexane:DCM; 1:1 v/v) collecting the 2nd peak. After concentration the solid was triturated with diethylether yielding the product as a white solid (13.2 mg, 47 %).

Route 2 (four-fold *Suzuki*): A 10 mL *Schlenk* tube was charged with $\mathbf{C_{Br_2I_2}}$ (29.8 mg, 1 equiv.), 6-methoxy naphtalene boric acid (40.2 mg, 5.5 equiv.) and K_2CO_3 (40 mg, 8 equiv.). The solids were dispersed in a 6 mL mixture of toluene/Etoh/H_2O v/v/v 4:1:1 and the solution was degassed with Argon for 15 minutes. PdCl2(dppf) 20 mol% was added, the tube sealed and the mixture was heated to 85°C for 16 hours. After completion the mixture was cooled to r.t. diluted with toluene and washed with water. Organics were concentrated in vacuo and the crude was purified by silica column chromatography (cyclohexane:DCM; 1:1 v/v) obtaining the product as a white solid (21 mg, 56 %).
TLC: R_f = 0.19 (SiO_2, cyclohexane:dichloromethane 4:6).
^{1}H-NMR: (500 MHz, THF-d8) δ 8.64 (d, *J* = 2.0 Hz, 2H), 8.15 (s, 2H), 8.02 (dd, *J* = 8.0, 2.0 Hz, 2H), 7.87 – 7.79 (m, 12H), 7.68 (dd, *J* = 7.9, 1.7 Hz, 2H), 7.49 (d, *J* = 8.4 Hz, 4H), 7.45 (d, *J* = 8.0 Hz, 2H), 7.40 (d, *J* = 7.8 Hz, 2H), 7.29 (d, *J* = 2.4 Hz, 2H), 7.24 (d, *J* = 2.4 Hz, 2H), 7.19 – 7.11 (m, 4H), 5.96 (d, *J* = 14.4 Hz, 2H), 5.01 (d, *J* = 14.3 Hz, 2H), 3.92 (s, 6H), 3.90 (s, 6H).
^{13}C-NMR {1H}: (126 MHz, THF-d8) δ 166.32, 159.38, 159.32, 145.36, 141.13, 140.32, 140.22, 136.11, 136.04, 135.43, 135.19, 132.98, 131.33, 131.17, 130.64, 130.51, 130.45, 130.09, 128.76, 128.72, 128.56, 128.38, 127.89, 126.57, 126.51, 126.44, 125.28, 120.25, 120.16, 106.47, 55.70, 55.67.
HR-ESI-MS: *m/z* calculated for $C_{72}H_{52}NaO_8$ $[M+Na]^+$; 1067.3554 found 1067.3553.
FT-IR (ATR) $\tilde{\nu}$ [cm^{-1}]: 3065 (w), 2996(w), 2955 (m), 2935 (m), 2842 (w), 1724 (s), 1632 (w), 1604 (m), 1495 (s), 1465 (w), 1452 (w), 1391 (w), 1375 (w), 1304 (w), 1271 (w), 1251 (m), 1225 (s), 1203 (s), 1153 (m), 1071 (s), 1033 (m), 1005 (w), 916 (w), 891 (w), 840 (m), 834 (w), 808 (w), 796 (w), 788 (w), 684 (w), 522 (w), 473 (m).



Compound $\mathbf{C_{Br_2NI_2}}$: Racemate synthesis: A 10 mL *Schlenk* tube was charged with $\mathbf{C_{Br_2I_2}}$ (60 mg, 1 equiv.), **NI-Bpin** (63.5 mg, 2.05 equiv.) and K_2CO_3 (50 mg, 5 equiv.). The solids were dispersed in a 5 mL mixture of THF/H_2O 4:1 and the solution was degassed with Argon for 15 minutes. $PdCl_2$(dppf) 10 mol% was added, the tube sealed and the mixture heated to 55°C for 4.5 hours. After completion the mixture was cooled to r.t. diluted with EtOAC and water. The phases were separated and the organics were concentrated in vacuo. The crude was purified by silica column chromatography (cyclohexane:CH_2Cl_2 4:6) collecting the 1st band. The obtained solid was triturated with DCM/MeOH to obtain the product (50 mg, 61 %) as an ivory white solid.
Enantiopure synthesis (*P*)-$\mathbf{C_{Br_2NI_2}}$: A 5 mL *Schlenk* tube was charged with (*P*)- $\mathbf{C_{Br_2I_2}}$ (28.7 mg, 1 equiv.), **NI-Bpin** (29.6 mg, 2.05 equiv.) and K_2CO_3 (23.9 mg, 5 equiv.). The solids were dispersed in a 2.5 mL mixture of THF/H_2O 4:1 and the solution was degassed with Argon for 15 minutes. $PdCl_2$(dppf) 10 mol% was added, the tube sealed and the mixture heated to 55°C for 6 hours. After completion the mixture was cooled to r.t. diluted with EtOAC and water. The phases were separated and the organics were dried over Na_2SO, filtered and concentrated in vacuo. The crude was purified by silica column chromatography (cyclohexane:CH_2Cl_2 4:6) collecting the 3rd band. The obtained solid was subjected to GPC (chloroform) obtaining the product (20 mg, 51 %) as an ivory white solid.
TLC: R_f = 0.18 (SiO_2, Cyclohexane:CH_2Cl_2 4:6)
^{1}H-NMR: (500 MHz, CD_2Cl_2) δ 8.72 – 8.65 (m, 2H), 8.65 – 8.57 (m, 2H), 8.37 (dd, *J* = 8.7, 2.1 Hz, 1H), 8.32 (dd, *J* = 7.5, 2.1 Hz, 1H), 8.05 (ddd, *J* = 8.3, 7.1, 1.1 Hz, 1H), 7.91 – 7.82 (m, 2H), 7.81 – 7.76 (m, 3H), 7.75 – 7.66 (m, 4H), 7.51 – 7.38 (m, 4H), 7.12 (td, *J* = 8.2, 1.7 Hz, 2H), 5.70 (t, *J* = 14.5 Hz, 1H), 5.50 (dd, *J* = 18.4, 14.0 Hz, 1H), 4.57 (dd, *J* = 18.4, 14.2 Hz, 1H), 4.44 (dd, *J* = 14.0, 9.4 Hz, 1H), 4.24 – 4.15 (m, 4H), 1.80 – 1.70 (m, 4H), 1.49 – 1.41 (m, 4H), 1.41 – 1.31 (m, 8H), 0.91 (t, *J* = 7.0 Hz, 6H).
^{13}C-NMR {1H}: (151 MHz, CD_2Cl_2) δ 164.90, 164.83, 164.78, 164.73, 164.38, 164.33, 164.19, 144.16, 143.92, 143.67, 143.56, 141.02, 140.84, 140.72, 140.55, 135.97, 135.94, 135.90, 135.84, 135.62, 135.58, 134.07, 132.84, 132.70, 132.45, 132.40, 132.24, 131.58, 131.44, 131.18, 131.09, 130.90, 130.79, 130.71, 128.90, 128.69, 128.61, 128.55, 128.23, 128.21, 127.80, 127.73, 127.09, 126.47, 126.44, 125.84, 125.47, 125.25, 123.63, 123.16, 121.53, 63.96, 63.92, 63.84, 63.80, 40.79, 32.00, 28.43, 27.21, 23.01, 14.24.
HR-ESI-MS: *m/z* calculated for $C_{64}H_{53}Br_2N_2O_8$ $[M+H]^+$; 135.2163 found 1135.2164.

FT-IR (ATR) ṽ [cm^{-1}]: 3065 (w), 2958 (m), 2927 (m), 2853 (m), 1729 (m), 1699 (s), 1657 (s), 1616 (w), 1589 (m), 1464 (w), 1386 (w), 1353 (s), 1293 (w), 1274 (w), 1228 (s), 1176 (w), 1147 (w), 1092 (m), 1069 (m), 1002 (w), 822 (m), 784 (s), 759 (m).



Compound C_{NI_4}: Racemate synthesis: $C_{Br_2I_2}$ (19 mg, 1 equiv.), **NI-Bpin** (60 mg, 6 equiv.) and K_2CO_3 (30 mg, 10 equiv.) were added to a 10 mL *Schlenk*. 4 mL of a 4:1:1 mixture of toluene/EtOH/H_2O was added the solution was degassed with Argon for 15 minutes. $PdCl_2$(dppf) 20 mol% was added, the tube sealed and the mixture heated to 85 °C for 18 hours. After completion the mixture was cooled to r.t. diluted with toluene and water. The phases were separated and the organics were concentrated in vacuo. The crude was subjected to silica column chromatography (cyclohexane:CH_2Cl_2 4:6 → 0:10) collecting the band. The obtained solid after concentration was purified by GPC with chloroform as mobile phase obtaining the product (10 mg, 27 %) as a white solid.

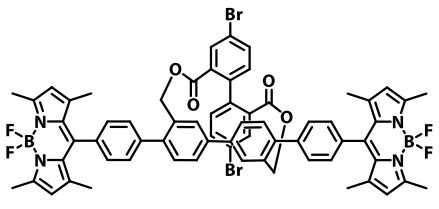
Enantiopure synthesis (*P*)-C_{NI_4}: (*P*)-$C_{Br_2NI_2}$ (15 mg, 1 equiv.), **NI-Bpin** (17 mg, 3 equiv.) and K_2CO_3 (10 mg, 5 equiv.) were added to a 5 mL *Schlenk* flask. 1.25 mL of a 4:1 mixture of dioxane/H_2O was added followed by degassing with Argon for 15 minutes. $PdCl_2$(dppf) 10 mol% was added, the tube sealed and the mixture heated to 85 °C for 16 hours. After completion the mixture was cooled to r.t. diluted with EtOac and water. The phases were separated and the organics were concentrated in vacuo. The crude was subjected to silica column chromatography (CH_2Cl_2 isocratic). The obtained solid after concentration was purified by GPC with chloroform as mobile phase obtaining the product (2.5 mg, 12 %) as a white solid. **TLC:** R_f = 0.15 (SiO_2, CH_2Cl_2).

^{1}H-NMR: (500 MHz, CD_2Cl_2) δ 8.69 – 8.59 (m, 6H), 8.50 – 8.42 (m, 3H), 8.34 (dd, *J* = 8.4, 5.5 Hz, 2H), 7.95 (ddd, *J* = 8.3, 6.2, 1.1 Hz, 1H), 7.92 – 7.64 (m, 13H), 7.63 – 7.54 (m, 4H), 7.49 (ddd, *J* = 9.8, 8.4, 7.3 Hz, 1H), 7.45 – 7.39 (m, 2H), 5.77 (dd, *J* = 14.4, 7.8 Hz, 1H), 5.57 (dd, *J* = 14.6, 9.3 Hz, 1H), 4.60 (t, *J* = 14.0 Hz, 1H), 4.48 (dd, *J* = 14.4, 4.7 Hz, 1H), 4.17 (q, *J* = 7.0 Hz, 8H), 1.73 (p, *J* = 7.4 Hz, 8H), 1.43 (t, *J* = 6.7 Hz, 8H), 1.41 – 1.31 (m, 16H), 0.94 – 0.88 (m, 12H).

^{13}C-NMR {1H}: (151 MHz, CD_2Cl_2) δ 165.93, 165.87, 165.83, 165.77, 164.37, 164.36, 164.29, 164.25, 164.18, 164.13, 145.63, 145.59, 145.47, 145.44, 145.35, 145.31, 144.14, 143.84, 140.87, 140.73, 140.61, 140.46, 138.58, 138.54, 135.98, 135.96, 135.92, 135.90, 135.84, 135.81, 135.78, 133.99, 132.69, 132.64, 132.35, 132.21, 131.89, 131.76, 131.43, 131.37, 131.22, 131.10, 131.05, 131.02, 130.86, 130.67, 130.23, 129.07, 128.86, 128.71, 128.65, 128.51, 128.18, 127.79, 127.56, 127.53, 127.50, 127.45, 126.81, 126.46, 126.41, 126.04, 125.36, 125.32, 125.19, 123.65, 123.63, 123.60, 123.52, 123.13, 123.12, 122.90, 122.87, 122.83, 63.90, 63.82, 40.77, 31.98, 28.41, 27.22, 27.19, 23.00, 14.23.

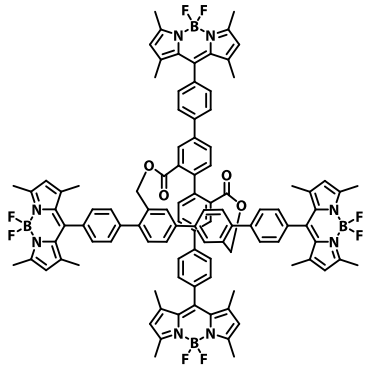
HR-ESI-MS: *m/z* calculated for $C_{200}H_{176}N_8Na_2O_{24}$ $[2M+2Na]^{2+}$; 1559.6291 found 1559.6321.

FT-IR (ATR) ṽ [cm^{-1}]: 3072 (w), 2954 (m), 2928 (m), 2858 (m), 1725 (m), 1700 (s), 1657 (s), 1616 (w), 1589 (m), 1441 (w), 1386 (w), 1349 (s), 1300 (w), 1228 (s), 1179 (w), 1153 (w), 1095 (w), 1069 (m), 1003 (w), 843(w), 824 (w), 782 (s), 757 (m), 651 (w) 586 (w).

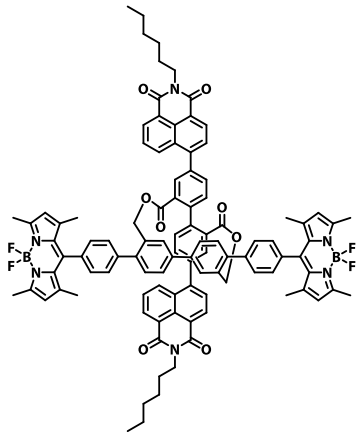


Compound $C_{Br_2BY_2}$: A 10 mL *Schlenk* tube was charged with $C_{Br_2I_2}$ (63 mg, 1 equiv.), **BY-Bpin** (71 mg, 2.05 equiv.) and K_2CO_3 (70 mg, 7 equiv.). The solids were dispersed in a 5 mL mixture of THF/H_2O 4:1 and the solution was degassed with Argon for 15 minutes. $PdCl_2$(dppf) 12 mol% was added, the tube sealed and the mixture heated to 55°C for 4 hours. The mixture was cooled to r.t. and the orange precipitate was filtered and washed with water and methanol, yielding the product (85 mg, 90 %).

^{1}H-NMR: (500 MHz, CD_2Cl_2) δ 8.42 (d, *J* = 2.1 Hz, 2H), 7.76 (dd, *J* = 8.3, 2.1 Hz, 2H), 7.68 (dd, *J* = 7.9, 1.8 Hz, 2H), 7.51 (d, *J* = 8.3 Hz, 4H), 7.42 (dd, *J* = 8.1, 4.8 Hz, 6H), 7.26 (d, *J* = 1.3 Hz, 2H), 7.19 (d, *J* = 8.3 Hz, 2H), 6.06 (s, 4H), 5.83 (d, *J* = 14.2 Hz, 2H), 4.88 (d, *J* = 14.1 Hz, 2H), 2.53 (s, 12H), 1.51 (s, 12H).
^{13}C-NMR {1H}: (151 MHz, CD_2Cl_2) δ 164.89, 155.92, 143.64, 141.82, 140.78, 139.81, 138.66, 135.53, 134.65, 134.28, 134.15, 132.80, 131.76, 130.76, 130.19, 128.73, 128.68, 125.50, 125.08, 121.64, 121.57, 64.26, 14.73, 14.69.
^{19}F-NMR {1H}: (376 MHz, CD_2Cl_2, not referenced) -146.24 (dd, *J* = 66.3, 32.7 Hz)
^{11}B NMR: (128 MHz, CD_2Cl_2, not referenced) 0.75 (t, *J* = 33.0 Hz)
HR-ESI-MS: *m/z* calculated for $C_{132}H_{105}B_4Br_4F_8N_8O_8$ $[2M+H]^+$; 2441.5087 found 2441.5071.
FT-IR (ATR) ṽ [cm^{-1}]: 2980 (m), 2920 (m), 1729 (s), 1545 (s), 1513 (s), 1468 (m), 1437 (w), 1409 (m), 1373 (w), 1307 (w), 1234 (m), 1192 (s), 1154 (m), 1077 (s), 1053 (m), 1003 (w), 976 (s), 899 (w), 822 (m), 787 (m), 773 (w), 718 (s), 643 (w), 582 (w), 478 (s).



Compound C_{BY_4}: To a 5 mL *Schlenk* tube was added $C_{Br_2BY_2}$ (21 mg, 1 equiv.), **BY-Bpin** (19 mg, 2.5 equiv.), K_2CO_3 (20 mg, 10 equiv.) and 2.5 mL dioxane/H_2O (4/1). The suspension was degassed with Argon, followed by the addition of $PdCl_2$(dppf) (10 mol%). The tube was sealed and heated at 90 °C for 24 hours. The mixture was cooled and partioned between CH_2Cl_2 and water. The organics were collected, dried over sodium sulphate and concentrated. The crude was purified by silica column chromatography (cyclohexane:CH_2Cl_2 2:8 → 0:10) obtaining the product (6 mg, 21 %) as a red solid.
TLC: R_f = 0.15 (SiO_2, dichloromethane 100 %)
^{1}H-NMR: (500 MHz, CD_2Cl_2) δ 8.66 (d, *J* = 1.9 Hz, 2H), 8.01 (dd, *J* = 8.0, 2.0 Hz, 2H), 7.92 – 7.87 (m, 4H), 7.67 (dd, *J* = 7.9, 1.7 Hz, 2H), 7.53 – 7.49 (m, 6H), 7.45 – 7.39 (m, 10H), 7.34 (s, 2H), 6.04 (d, *J* = 13.9 Hz, 8H), 5.87 (d, *J* = 14.6 Hz, 2H), 4.96 (d, *J* = 14.4 Hz, 2H), 2.53 (s, 12H), 2.52 (s, 12H), 1.51 (s, 12H), 1.46 (s, 12H).
^{13}C-NMR {1H}: (151 MHz, CD_2Cl_2) δ 165.93, 155.93, 155.87, 145.04, 143.70, 143.62, 141.83, 141.79, 140.84, 140.63, 139.82, 139.61, 138.46, 134.82, 134.65, 134.40, 132.16, 131.75, 131.72, 130.85, 130.74, 130.13, 129.74, 129.15, 128.73, 128.05, 127.60, 125.19, 124.95, 121.65, 121.57, 64.18, 14.75, 14.73, 14.71, 14.69.
^{19}F-NMR {1H}: (376 MHz, CD_2Cl_2, not referenced) δ -146.25 (dd, *J* = 65.7, 32.1 Hz)
^{11}B NMR: (128 MHz, CD_2Cl_2, not referenced) δ 0.73 (t, *J* = 32.9 Hz)
HR-ESI-MS: *m/z* calculated for $C_{208}H_{176}B_8F_{16}N_{16}Na_2O_8$ $[2M+2Na]^{2+}$; 1731.7104 found 1731.7131.
FT-IR (ATR) ṽ [cm^{-1}]: 2972 (m), 2924 (m), 1719 (s), 1543 (s), 1511 (s), 1473 (m), 1442 (w), 1409 (m), 1372 (w), 1304 (s), 1229 (w), 1193 (m), 1158 (m), 1121 (w), 1076 (s), 1054 (m), 1006 (w), 976 (s), 821 (m), 797 (w), 770 (w), 715 (m), 643 (w), 582 (w), 479 (s).



Compound $C_{NI_2BY_2}$: A 5 mL *Schlenk* tube was charged with $C_{Br_2BY_2}$ (16 mg, 1 equiv.), **NI-Bpin** (17 mg, 2.5 equiv.) and K_2CO_3 (14 mg, 6 equiv.). The solids were dispersed in a mixture of dioxane (1.8 mL, DMF (0.2 mL) and H_2O (0.5 mL) and the solution was degassed with argon. $PdCl_2$(dppf) 10 mol% was added, the tube sealed and the mixture heated to 90°C for 16 hours. The mixture was cooled to r.t. diluted with EtOAC and water. The phases were separated and the organics were washed with brine two times, before dried over sodium sulphate and concentrated in vacuo. The crude was purified by silica column chromatography (cyclohexane:CH_2Cl_2:EtOAc 2:8:0 → 0:9:1) obtaining the product as an orange solid (13 mg, 61 %).
TLC: R_f = 0.38 (SiO_2, dichloromethane 100 %)
^{1}H-NMR: (500 MHz, CD_2Cl_2) δ 8.65 (d, J = 7.5 Hz, 2H), 8.63 (dd, J = 7.3, 1.0 Hz, 2H), 8.52 (d, J = 1.9 Hz, 2H), 8.38 (dd, J = 8.5, 1.0 Hz, 2H), 7.88 – 7.85 (m, 4H), 7.77 (dd, J = 8.5,

7.3 Hz, 2H), 7.69 (dd, J = 7.9, 1.6 Hz, 2H), 7.63 (d, J = 7.9 Hz, 2H), 7.50 (d, J = 8.1 Hz, 4H), 7.43 – 7.38 (m, 8H), 6.04 (s, 4H), 5.89 (d, J = 14.5 Hz, 2H), 4.92 (d, J = 14.4 Hz, 2H), 4.20 – 4.13 (m, 4H), 2.52 (s, 12H), 1.73 (p, J = 7.5 Hz, 4H), 1.48 (s, 12H), 1.46 – 1.31 (m, 12H), 0.93 – 0.86 (m, 6H).
^{13}C-NMR {1H}: (101 MHz, CD_2Cl_2) δ 165.93, 164.42, 164.22, 145.55, 145.48, 143.62, 141.78, 140.77, 139.84, 139.81, 139.73, 138.64, 134.70, 134.43, 133.91, 132.72, 132.47, 131.88, 131.76, 131.37, 130.89, 130.82, 130.34, 130.14, 129.10, 128.76, 128.56, 127.61, 127.57, 125.51, 125.07, 123.63, 122.86, 121.67, 64.20, 40.79, 32.00, 28.42, 27.22, 23.00, 14.73, 14.68, 14.23.
^{19}F-NMR {1H}: (376 MHz, CD_2Cl_2, not referenced) δ -146.26 (dd, *J* = 65.6, 30.5 Hz)
^{11}B NMR: (128 MHz, CD_2Cl_2, not referenced) δ 0.73 (t, *J* = 33.0 Hz)
HR-ESI-MS: *m/z* calculated for $C_{204}H_{176}B_4F_8N_{12}Na_2O_{16}$ $[2M+2Na]^{2+}$; 1645.6713 found 1645.6731.
FT-IR (ATR) ṽ [cm^{-1}]: 3037 (w), 2958 (m), 2928 (m), 2858 (m) 1734 (m), 1704 (s), 1663 (s), 1592 (m), 1546 (s), 1514 (s), 1477 (m), 1442 (w), 1410 (w), 1388 (w), 1360 (m), 1308 (m), 1236 (m), 1187 (s), 1158 (s), 1121 (w), 1077 (m), 1052 (w), 975 (s), 837 (w), 819 (w), 786 (s), 772 (m), 760 (m), 718 (m), 643 (w), 586 (w), 479 (s).

Procedure template cleavage

Chromophore **$C_{Chromophore_4}$** was dissolved in a THF/MeOH (5/1) mixture [c~10^{-6}]. To the solution 2M LiOH (20 vol %) solution was added and stirred at room temperature overnight. CH_2Cl_2 and conc. HCl were added and the phases were separated. The organics were collected, dried over sodium sulphate, and concentrated under reduced pressure. The obtained solids were taken up in CH_2Cl_2 and fluorescence spectra were recorded.

Physico-Chemical analysis

Characterization $C_{Br_2I_2}$

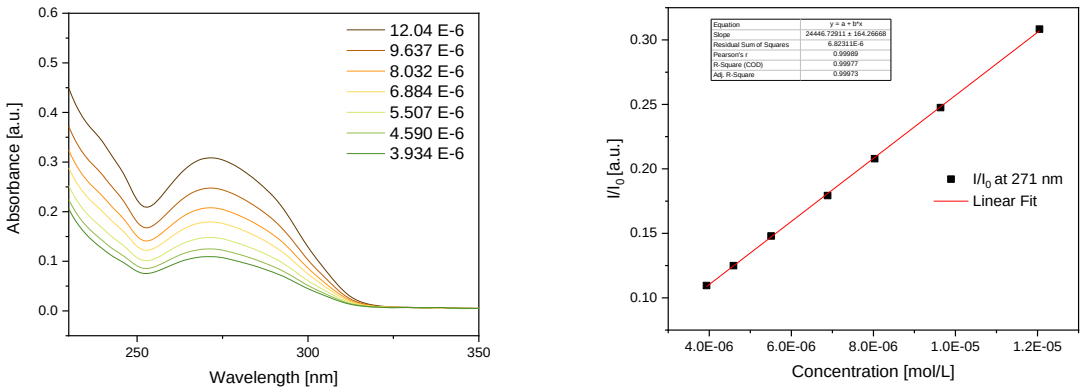


Figure S1: Dilution series of the absorption (left) and linear regression (right) of the absorption at 271 nm versus concentration of $\mathbf{C_{Br_2I_2}}$ in CH_2Cl_2.

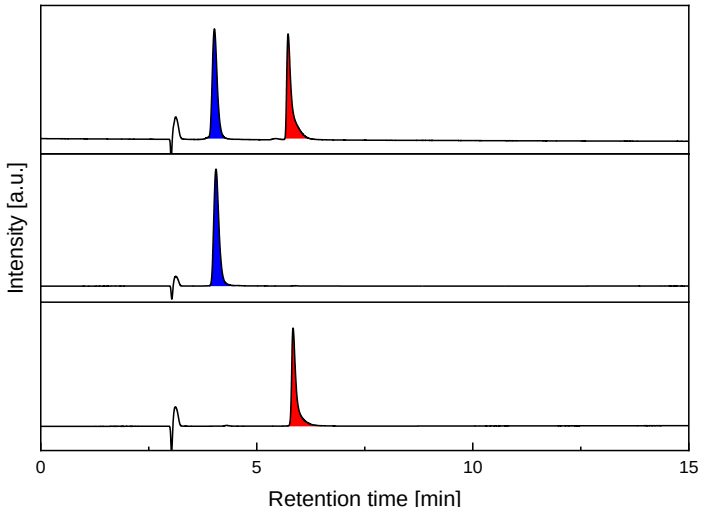


Figure S2: HPLC chromatogram of rac-$\mathbf{C_{Br_2I_2}}$ (top) and its respective preparative isolated enantiomers (E1, middle and E2, bottom). IG-column, CH_2Cl_2/heptane 1/1, 20 °C.

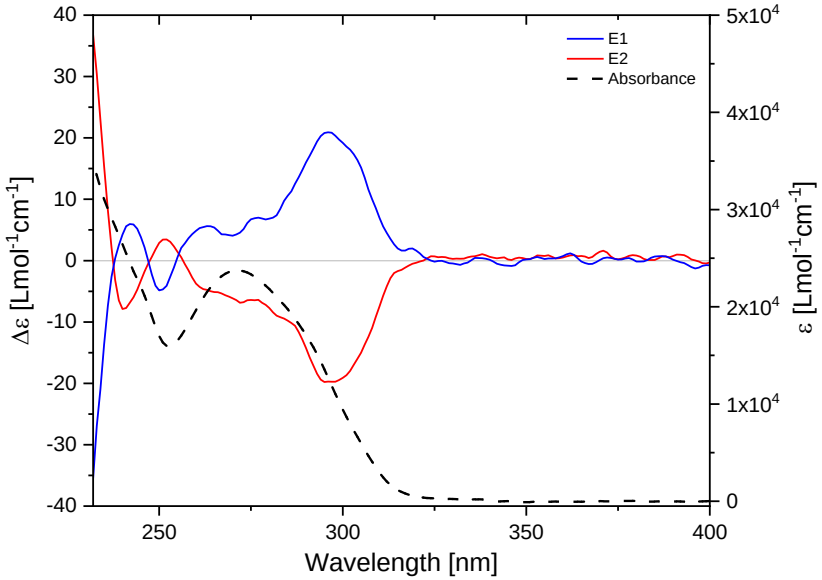


Figure S3: Absorptivity and CD-spectra of the first eluting E1 and second eluting E2 enantiomer of $\mathbf{C_{Br_2I_2}}$, in CH_2Cl_2.

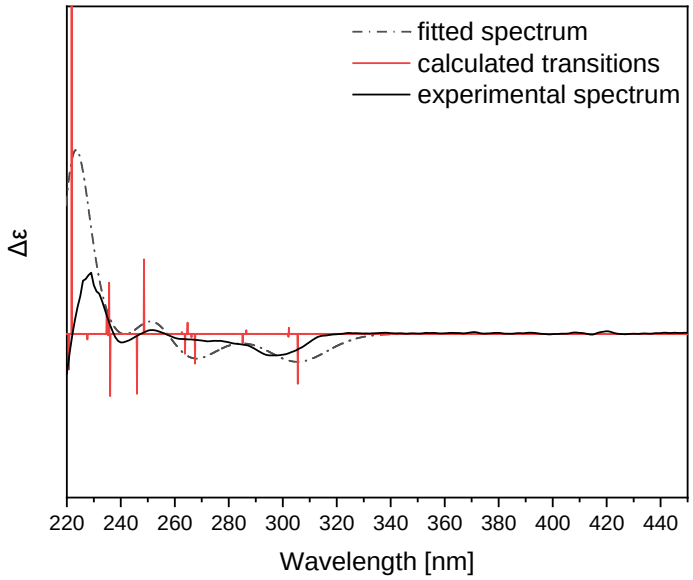


Figure S4. Calculated (dash-dot line, fitted with σ = 0.2 eV, shifted by 0.7 eV) and experimental (black solid line) spectrum of E2/(*P*)- $\mathbf{C_{Br_2I_2}}$. The computed transitions are indicated as bars (red).

Characterization chromophores

Table S1. Overview of the (chiro)-optical properties of the library of compounds, measured in CH_2Cl_2 at 20 °C.

Compound	λ_{abs} [nm]	ε [$L*mol^{-1}*cm^{-1}$]	λ_{em}[nm]	ϕ_F*	τ_F [ns]	g_{abs}
$C_{Br_2I_2}$	271	24446	/	/	/	$1.5*10^{-3}$ (305 nm)
$C_{Br_2Naph_2}$	275; 302	42094; 36304	378	2.7 % (300 nm)	0.36; 4.63	$1.1*10^{-4}$ (305 nm)
C_{Naph_4}	264; 303	101009; 60934	432	43.3 % (300 nm)	1.76	$3.49*10^{-4}$ (326 nm)
$C_{Br_2NI_2}$	344; 357	36368; 38971	441	51.8 % (357 nm)	1.74	$8.59*10^{-4}$ (296 nm)
C_{NI_4}	346; 357	75211; 80821	438	54.9 % (357 nm)	1.74	$7.31*10^{-4}$ (250 nm) $1.8*10^{-4}$ (372 nm)
$C_{Br_2BY_2}$	280 ; 502	50455; 168551	513	56.5 % (280 nm)	3.96 (470 nm) 4.12 (280 nm)	$1.9*10^{-4}$ (508 nm)
C_{BY_4}	273; 502	66799; 208635	513	42.5 % (280 nm)	3.61 (280 nm) 3.70 (470 nm)	$4.7*10^{-5}$ (508 nm)
$C_{NI_2BY_2}$	276; 357; 502	49435; 51053; 148036	513	57.5 % (280 nm)	3.73 (280 nm) 3.70 (365 nm) 3.76 (470 nm)	$5.7*10^{-5}$ (508 nm)

Optical analysis

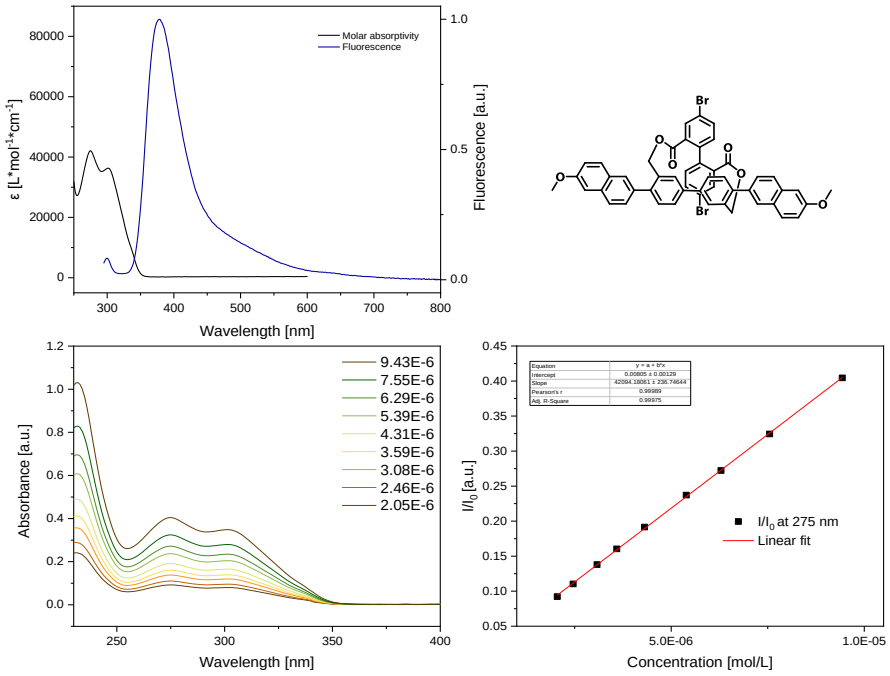


Figure S5: Top) Absorptivity (c ~ $5*10^{-6}$) and normalized fluorescence (c ~ $1*10^{-6}$, 300 nm) plot in CH_2Cl_2 of $C_{Br_2Naph_2}$. Bottom) Dilution series of the absorption and linear regression of the absorption value of $C_{Br_2Naph_2}$ at 275 nm in CH_2Cl_2 versus concentration.

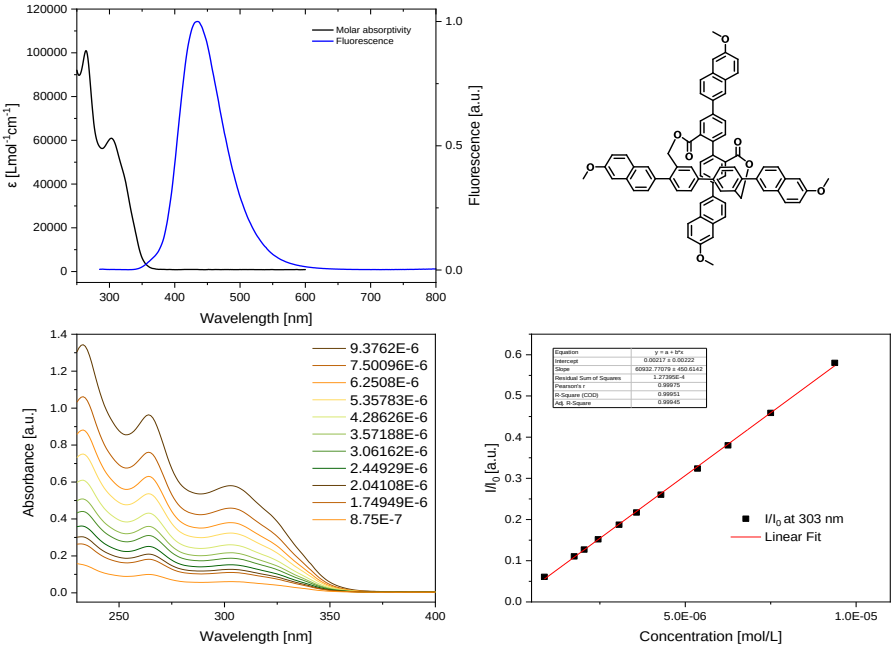


Figure S6: Top) Absorptivity (c ~ 5*10^{-6}) and normalized fluorescence (c ~ 1*10^{-6}, 303 nm) plot in CH_2Cl_2 of $\mathbf{C_{Naph_4}}$. Bottom) Dilution series of the absorption and linear regression of the absorption value of $\mathbf{C_{Naph_4}}$ at 303 nm in CH_2Cl_2 versus concentration.

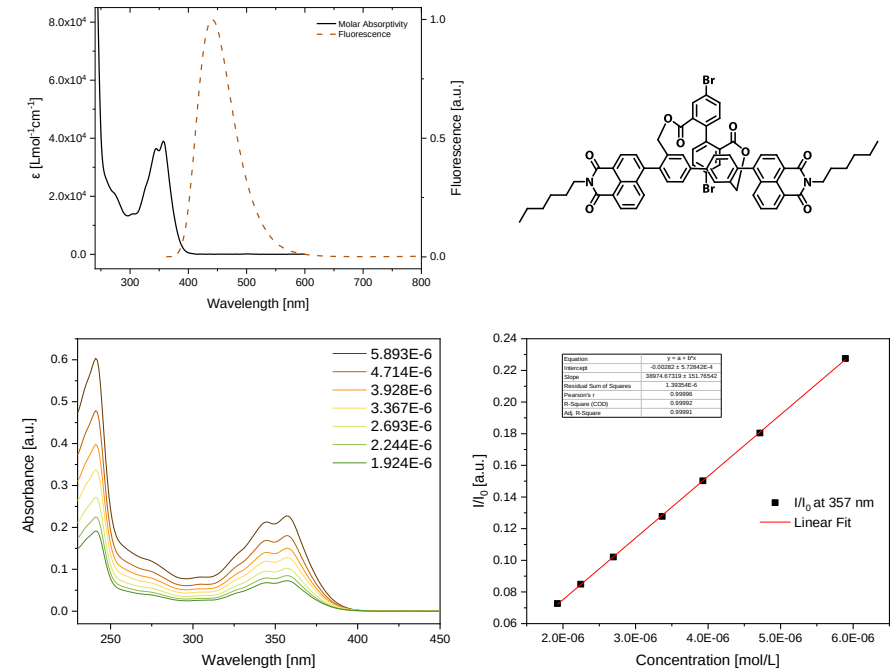


Figure S7: Top) Absorptivity (c ~ 5*10^{-6}) and normalized fluorescence (c ~ 1*10^{-6}, 358 nm) plot in CH_2Cl_2 of $\mathbf{C_{Br_2NI_2}}$. Bottom) Dilution series of the absorption and linear regression of the absorption value of $\mathbf{C_{Br_2NI_2}}$ at 357 nm in CH_2Cl_2 versus concentration.

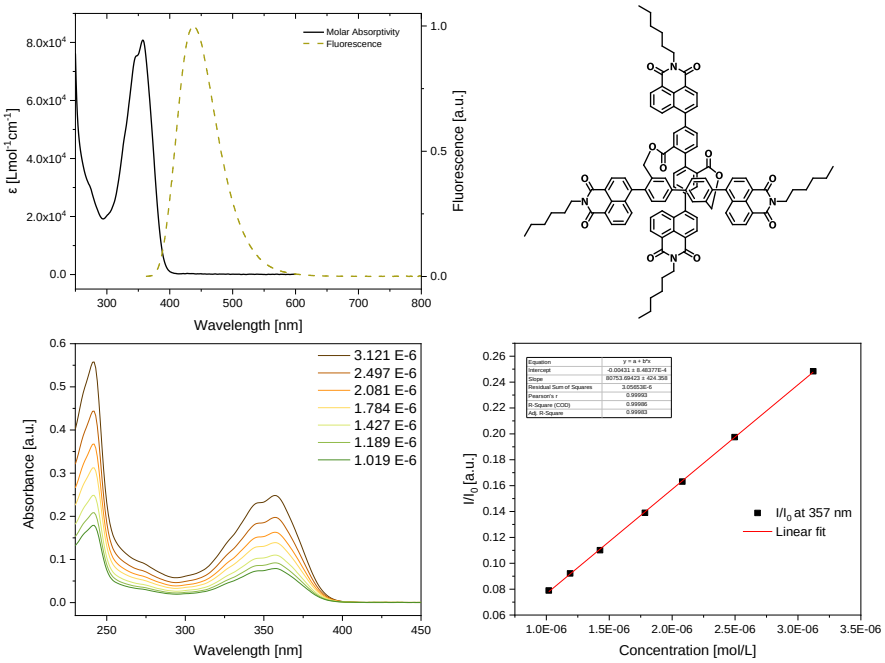


Figure S8: Absorptivity (c ~ 5*10^{-6}) and normalized fluorescence (c ~ 1*10^{-6}, 357 nm) plot in CH_2Cl_2 of $\mathbf{C_{NI_4}}$. Bottom) Dilution series of the absorption and linear regression of the absorption value of $\mathbf{C_{NI_4}}$ at 357 nm in CH_2Cl_2 versus concentration.

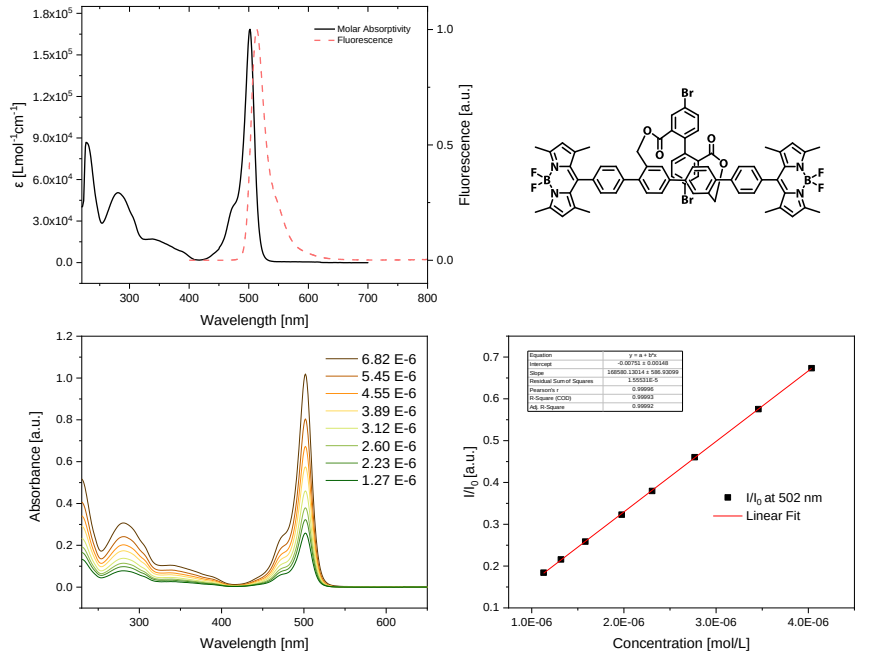


Figure S9: Top) Absorptivity (c ~ 5*10^{-6}) and normalized fluorescence (c ~ 0.5*10^{-6}, 280 nm) plot in CH_2Cl_2 of $\mathbf{C_{Br_2BY_2}}$. Bottom) Dilution series of the absorption and linear regression of the absorption value of $\mathbf{C_{Br_2BY_2}}$ at 502 nm in CH_2Cl_2 versus concentration.

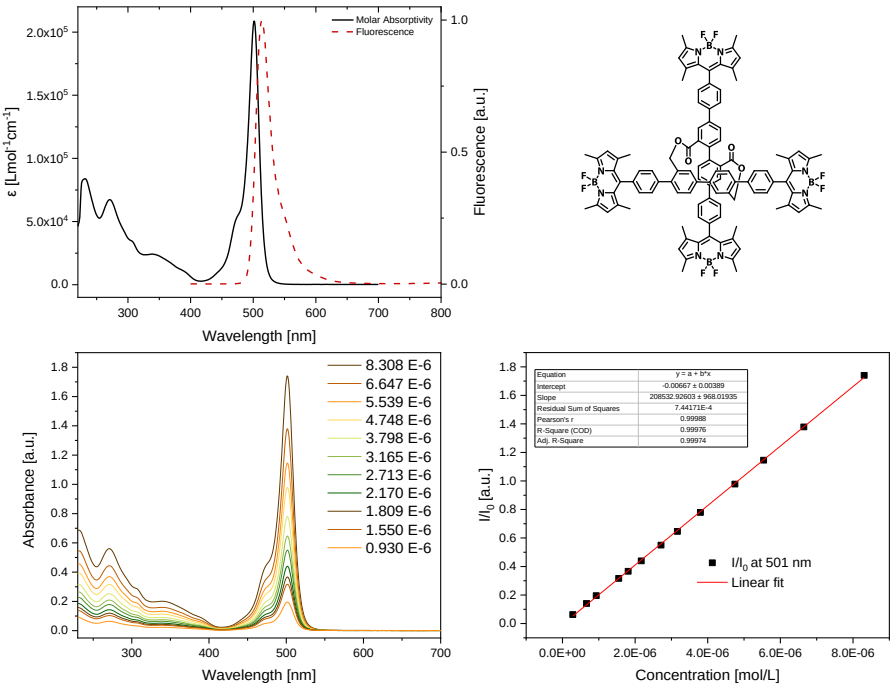


Figure S10: Top) Absorptivity (c ~ 3*10^{-6}) and normalized fluorescence (c ~ 0.5*10^{-6}, 280 nm) plot in CH_2Cl_2 of $\mathbf{C_{BY_4}}$. Bottom) Dilution series of the absorption and linear regression of the absorption value of $\mathbf{C_{BY_4}}$ at 501 nm in CH_2Cl_2 versus concentration.

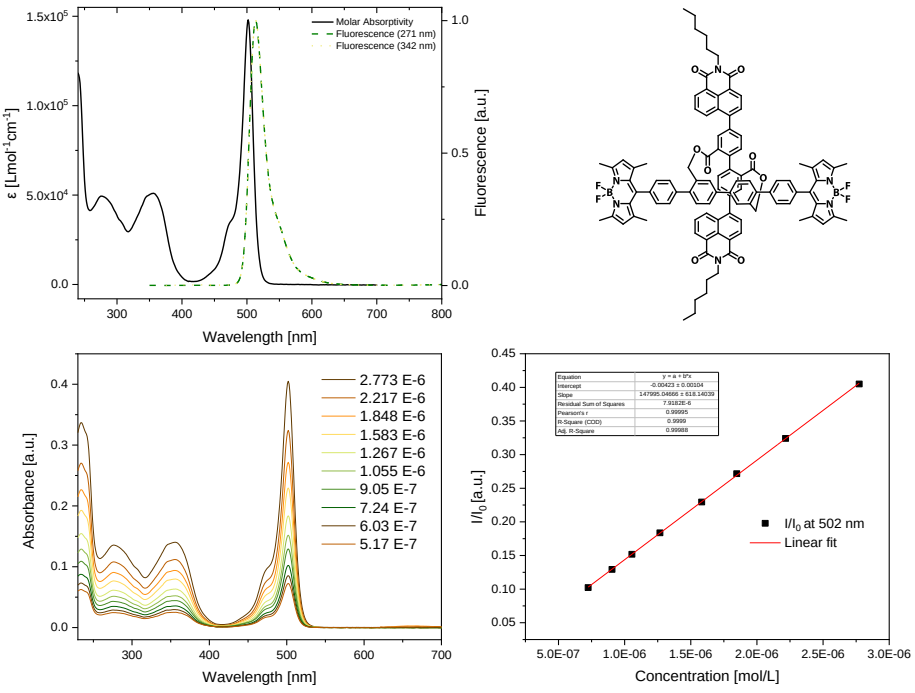


Figure S11: Top) Absorptivity (c ~ 5*10^{-6}) and normalized fluorescence (c ~ 0.5*10^{-6}, 280 nm and 342 nm) plot in CH_2Cl_2 of $\mathbf{C_{NI_2BY_2}}$. Bottom) Dilution series of the absorption and linear regression of the absorption value of $\mathbf{C_{NI_2BY_2}}$ at 502 nm in CH_2Cl_2 versus concentration.

Chiral-analysis

Naph-series

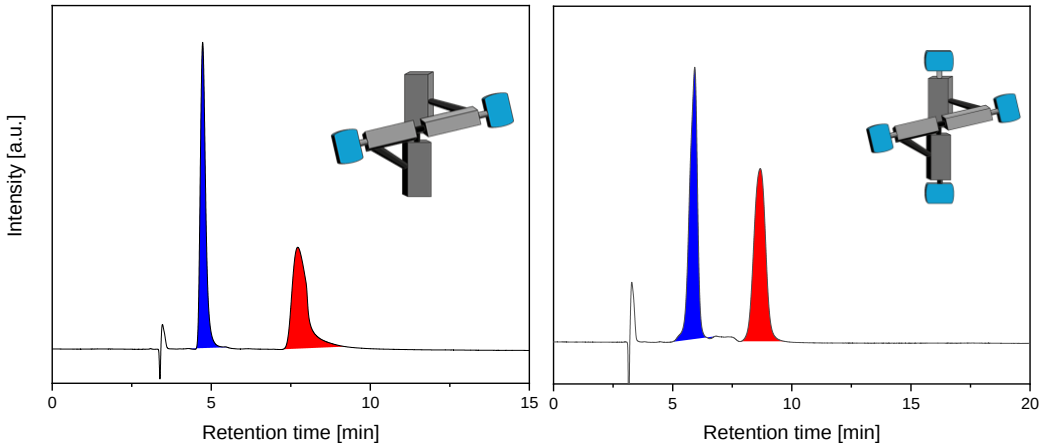


Figure S12: HPLC chromatogram of (left) rac-$\mathbf{C_{Br_2Naph_2}}$, IC-column CH_2Cl_2/heptane/EtOH (49/49/2) and (right) rac-$\mathbf{C_{Naph_4}}$, IA-column CH_2Cl_2/heptane (4/6). First eluting (E1) and second eluting (E2) enantiomer are depicted in blue and red respectively.

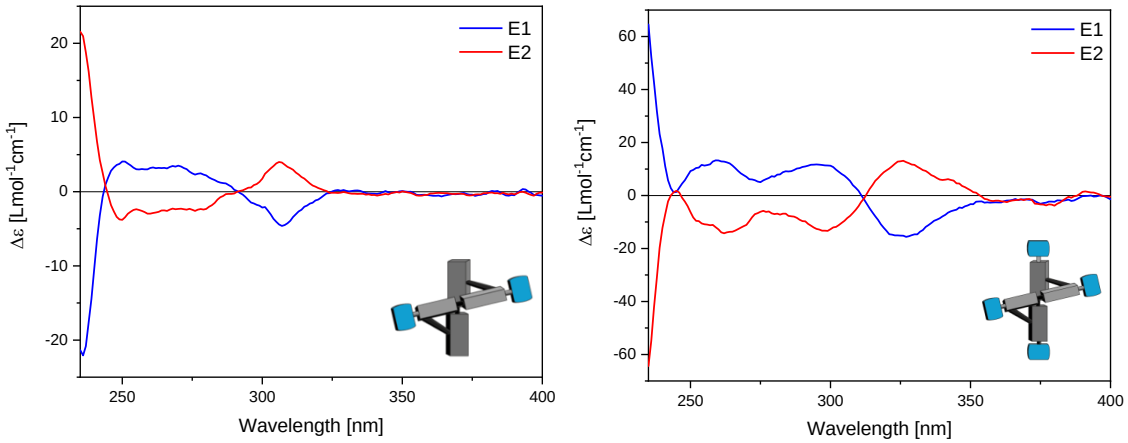


Figure S13: CD-spectra of the first eluting E1 (blue) and second eluting E2 (red) enantiomer of left) $\mathbf{C_{Br_2Naph_2}}$ and right) $\mathbf{C_{Naph_4}}$, in CH_2Cl_2.

Assignment of CD-spectra

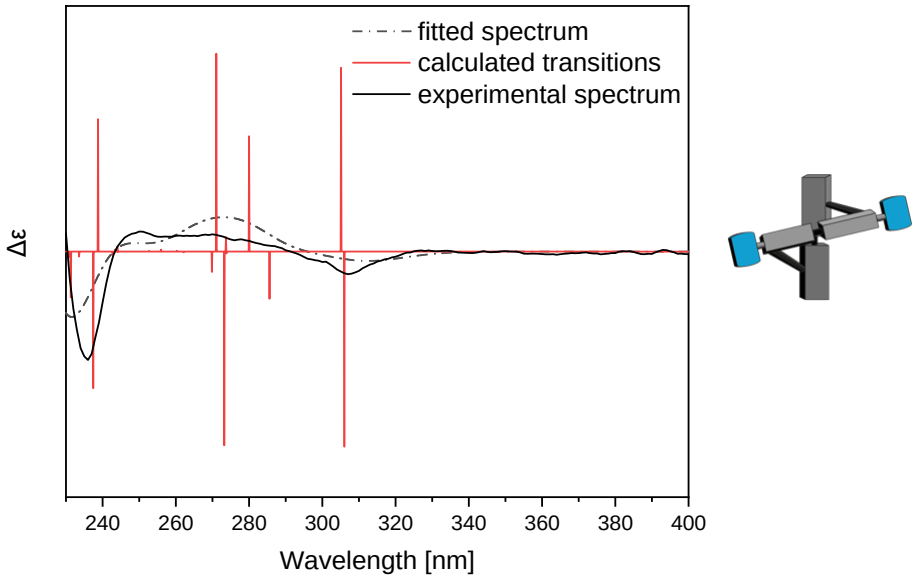


Figure S14: Calculated (dash-dot line, fitted with σ = 0.2 eV, shifted by 0.2 eV) and experimental (black solid line) spectrum of E1/*(P)*- $\mathbf{C_{Br_2Naph_2}}$. The computed transitions are indicated as bars (red).

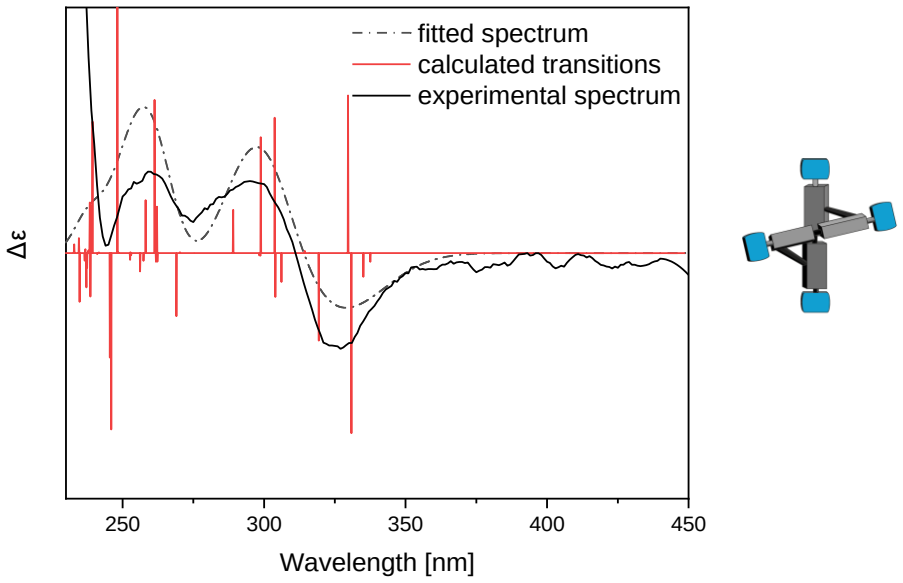


Figure S15: Calculated (dash-dot line, fitted with σ = 0.2 eV, shifted by 0.5 eV) and experimental (black solid line) spectrum of E1/*(P)*- $\mathbf{C_{Naph_4}}$. The computed transitions are indicated as bars (red).

NI-series

^{1}H-NMR full assignment of $\mathbf{C_{Br_2NI_2}}$

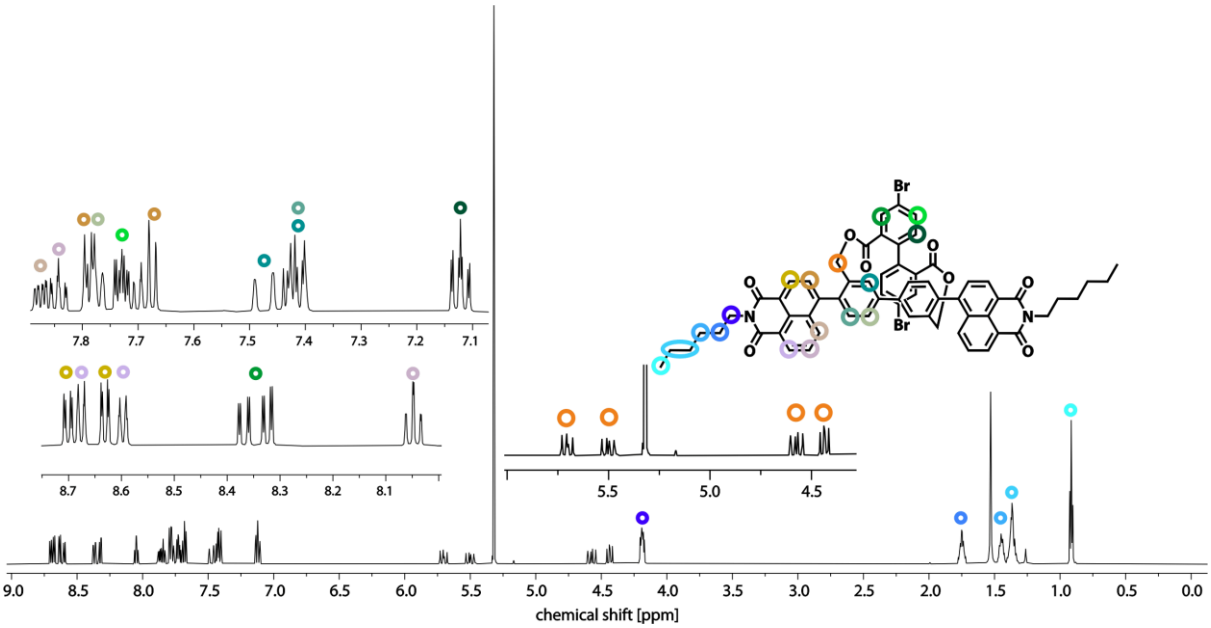


Figure S16: Full assignment of ^{1}H-NMR of $\mathbf{C_{Br_2NI_2}}$ in CD_2Cl_2 at 20 °C, 600 MHz. Zoom in on the diastereotopic CH_2 ester protons reveals a set of 8 doublets. While in the aromatic region several signals of the **NI** split in two distinct regions.

Conformer analysis of $\mathbf{C_{Br_2NI_2}}$

CREST was used to preliminary identify possible conformers of $\mathbf{C_{Br_2NI_2}}$. Three isomers were identified as (S_a, *P* ,S_a)-, (S_a, *P*, R_a)-, and (R_a, *P*, R_a)- $\mathbf{C_{Br_2NI_2}}$ further optimized by DFT calculations. We calculated the Boltzmann distribution where (S_a, *P* ,S_a)- $\mathbf{C_{Br_2NI_2}}$ is significantly more stable than (R_a, *P*, R_a)-$\mathbf{C_{Br_2NI_2}}$. The geometries of $\mathbf{C_{Br_2NI_2}}$ were used to model the initial guesses of $\mathbf{C_{NI_4}}$ and optimized the corresponding (S_a, *P* ,S_a)-, (S_a, *P*, R_a)-, and (R_a, *P*, R_a) configurations and calculated their Boltzmann distribution. Interestingly, the (R_a, *P*, R_a)- $\mathbf{C_{NI_4}}$ is dramatically less stable then the other configurations. All conformers are displayed in the 'Geometry optimized structures' section.

Table S2: Boltzmann distribution of (*P*)-$\mathbf{C_{Br_2NI_2}}$

Conformer	*SP E [Hartree]*	*ZPC [Hartree]*	*corr E [Hartree]*	*Thermal corrections [Hartree]*	*G [Hartree]*	$p_i = e^{\frac{G_i - G_1}{kT}}$	$\frac{p_i}{p_{tot}}$	$\frac{p_i}{p_{tot}} * 100$
(R_a, *P*, R_a)	-7932.0942	0.731457	-7931.362743	0.78471	-7931.30949	0.319267592	0.171357475	17.13575
(S_a, *P*, R_a)	-7932.0948	0.731665	-7931.363135	0.784807	-7931.309993	0.543899403	0.291921982	29.1922
(S_a, *P*, S_a)	-7932.0954	0.731721	-7931.363679	0.784832	-7931.310568	1	0.536720542	53.67205

Table S3: Boltzmann distribution of (*P*)-$\mathbf{C_{NI_4}}$

Conformer	*SP E [Hartree]*	*ZPC [Hartree]*	*corr E [Hartree]*	*Thermal corrections [Hartree]*	*G [Hartree]*	$p_i = e^{\frac{G_i - G_1}{kT}}$	$\frac{p_i}{p_{tot}}$	$\frac{p_i}{p_{tot}} * 100$
(R_a, *P*, R_a)	-4199.4675	0.603688	-4198.863812	0.648764	-4198.818736	2.49008E-06	1.54992E-06	0.000155
(S_a, *P*, R_a)	-4199.4674	0.592	-4198.8754	0.636953	-4198.830447	0.606590009	0.377563078	37.75631
(S_a, *P*, S_a)	-4199.4679	0.592037	-4198.875863	0.636981	-4198.830919	1	0.622435372	62.24354

VT-NMR of $C_{Br_2NI_2}$

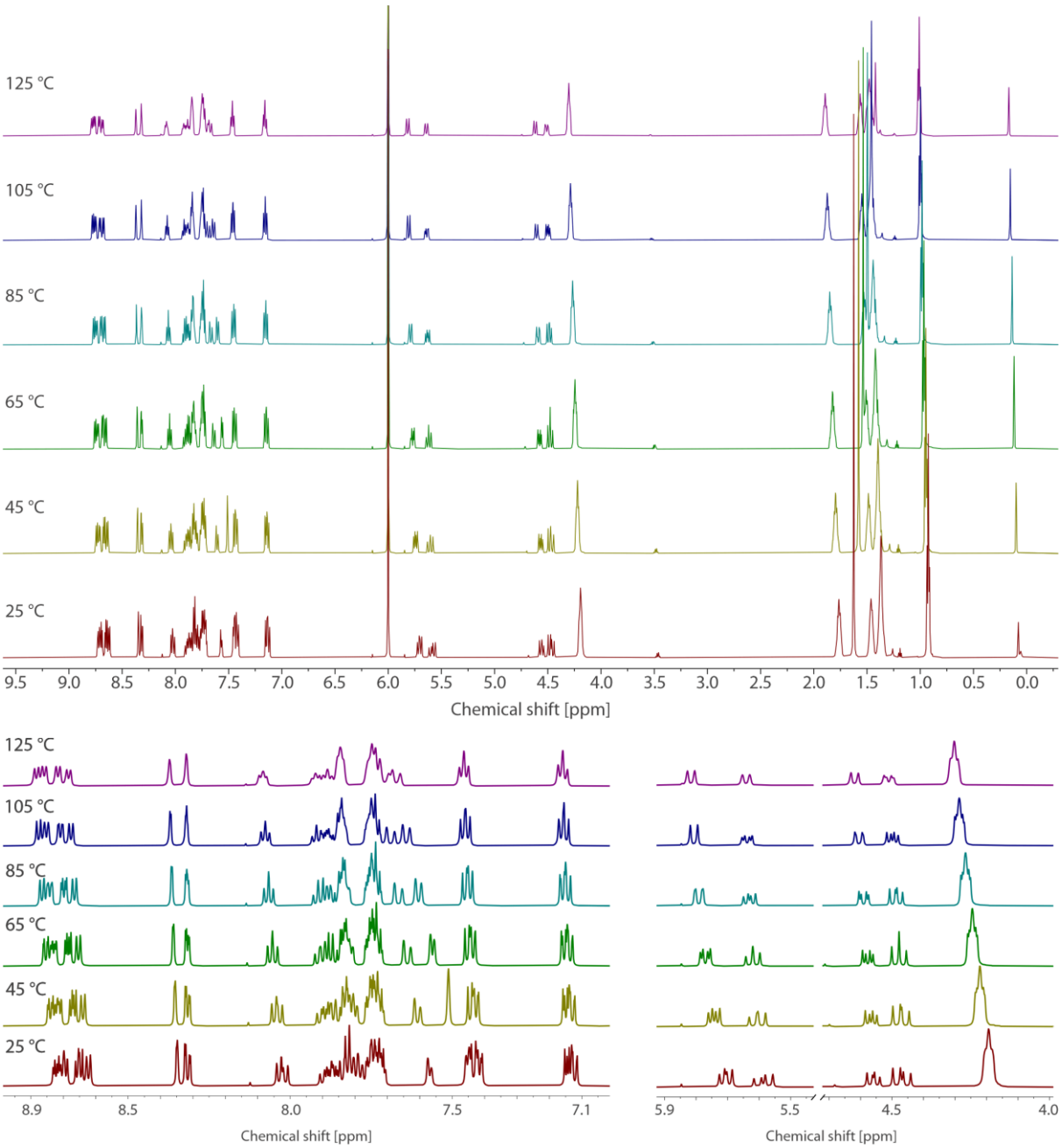


Figure S17: Stacked ^{1}H-NMR of $\mathbf{C_{Br_2NI_2}}$ in $TCED_2$ (600 MHz) at variable temperatures between 25 °C and 125 °C. Bottom is the zoom in on the aromatic (left) and ester (right) region respectively.

Chiral-separation

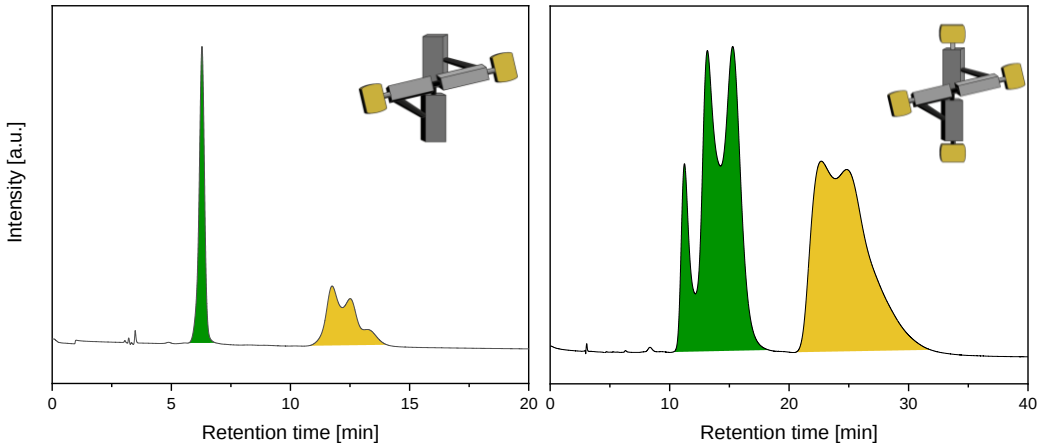


Figure S18: HPLC chromatogram of (left) rac-$\mathbf{C_{Br_2NI_2}}$, IA-column heptane/EtOAc (50/50) and (right) rac-$\mathbf{C_{NI_4}}$, IG-column CH_2Cl_2/heptane/EtOH (49/49/2). First eluting (E1) and second eluting (E2) enantiomer set are depicted in green and yellow respectively.

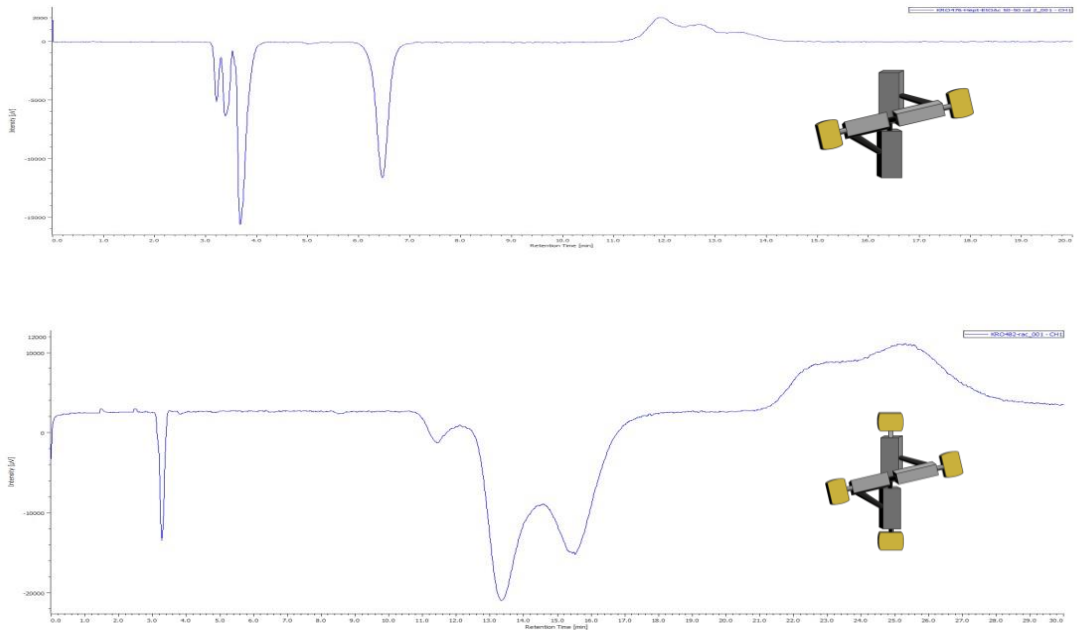


Figure S19: Screen shot of in-line CD-detection chromatogram corresponding to HPLC traces shown in Figure SX of (top) rac-$\mathbf{C_{Br_2NI_2}}$, 300 nm and (bottom) rac-$\mathbf{C_{NI_4}}$, 250 nm. Excluding the injection peak signal (3-4 minutes) in both cases the first set of conformers show a negative polarity at the corresponding wavelength while the second eluting set of conformers show a positive polarity.

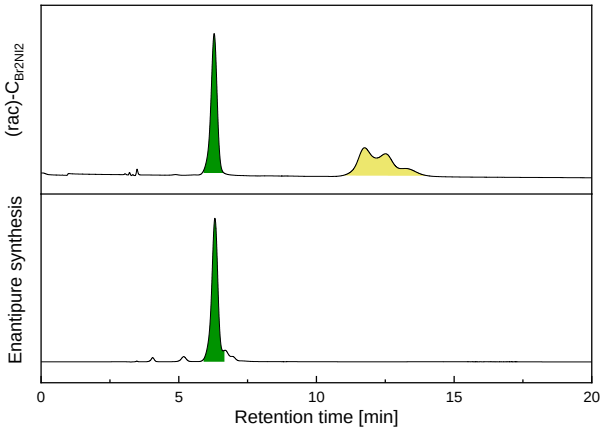


Figure S20: HPLC chromatogram of (top) rac- $\mathbf{C_{Br_2NI_2}}$ and (bottom) enantiopure synthesis product (*P*)- $\mathbf{C_{Br_2NI_2}}$, IA-column heptane/EtOAc (50/50).

CD-spectra

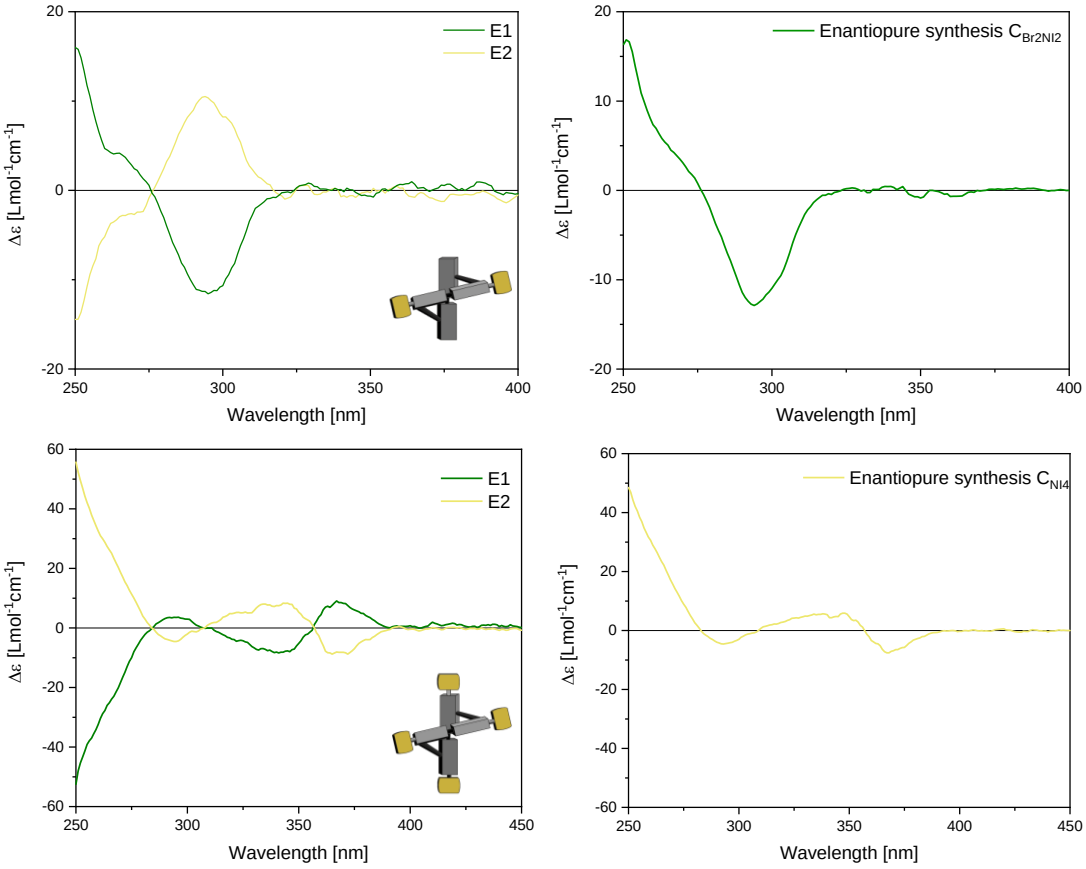


Figure S21: CD-spectra in CH_2Cl_2 of left) the first eluting E1(green) and second eluting E2 (yellow) enantiomer of $\mathbf{C_{Br_2NI_2}}$ (top) and $\mathbf{C_{NI_4}}$ (bottom) and right) the corresponding enantiopure synthesis product of (*P*)- $\mathbf{C_{Br_2NI_2}}$ and (*P*)- $\mathbf{C_{NI_4}}$ respectively.

Assignment of CD-spectra

For *(P)*- $\mathbf{C}_{Br_2NI_2}$ and *(P)*- $\mathbf{C}_{NI_4}$ we assumed Boltzmann distribution as presented above, neglecting kinetic contributions to the distribution during the Suzuki coupling.

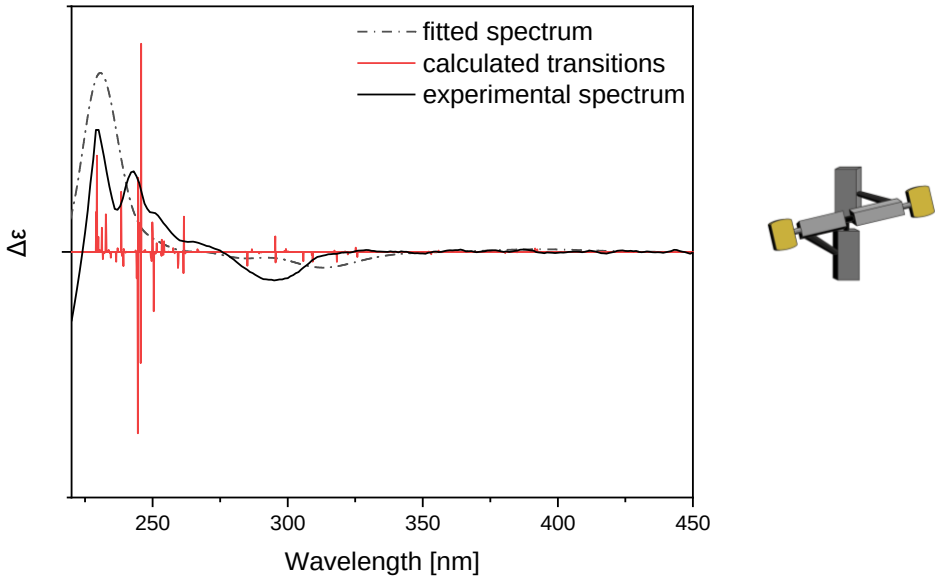


Figure S22: Calculated (dash-dot line, fitted with σ = 0.2 eV, shifted by 0.8 eV) and experimental (black solid line) spectrum of E1/*(P)*- $\mathbf{C}_{Br_2NI_2}$. The computed transitions are indicated as bars (red).

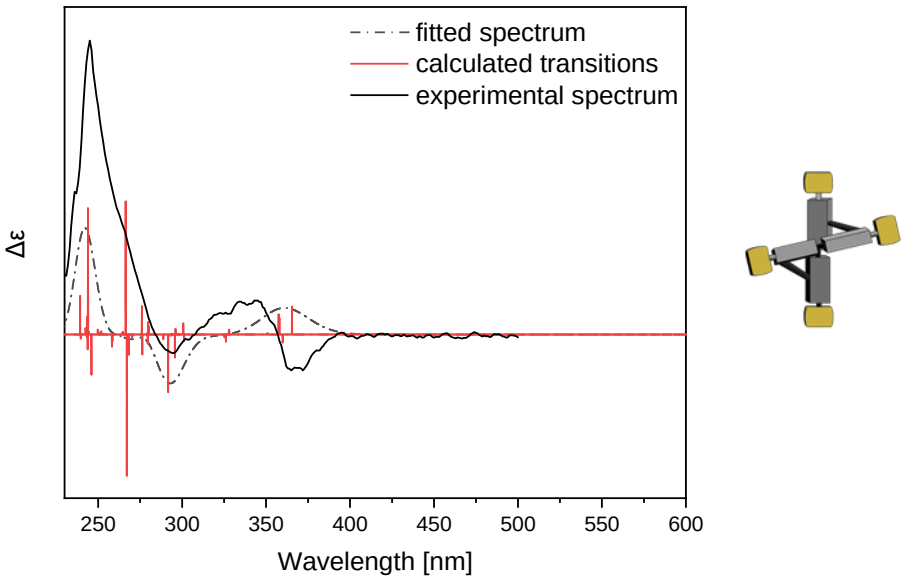


Figure S23: Calculated (dash-dot line, fitted with σ = 0.2 eV, shifted by 0.5 eV) and experimental (black solid line) spectrum of E2/*(P)*-$\mathbf{C}_{NI_4}$. The computed transitions are indicated as bars (red).

BY-series

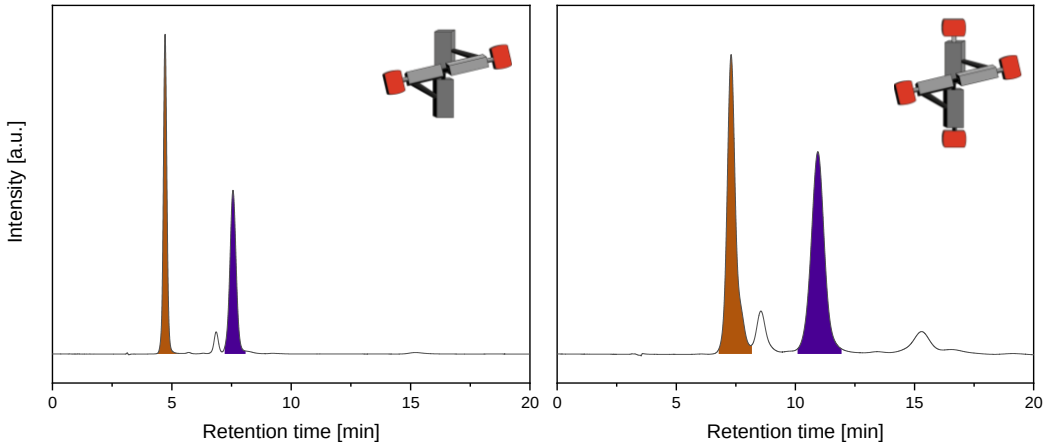


Figure S24: HPLC chromatogram of (left) rac-$\mathbf{C_{Br_2BY_2}}$, IA-column CH_2Cl_2/heptane (40/60) and (right) rac-$\mathbf{C_{BY_4}}$, IA-column heptane/EtOAc (60/40). First eluting (E1) and second eluting (E2) enantiomer set are depicted in orange and purple respectively.

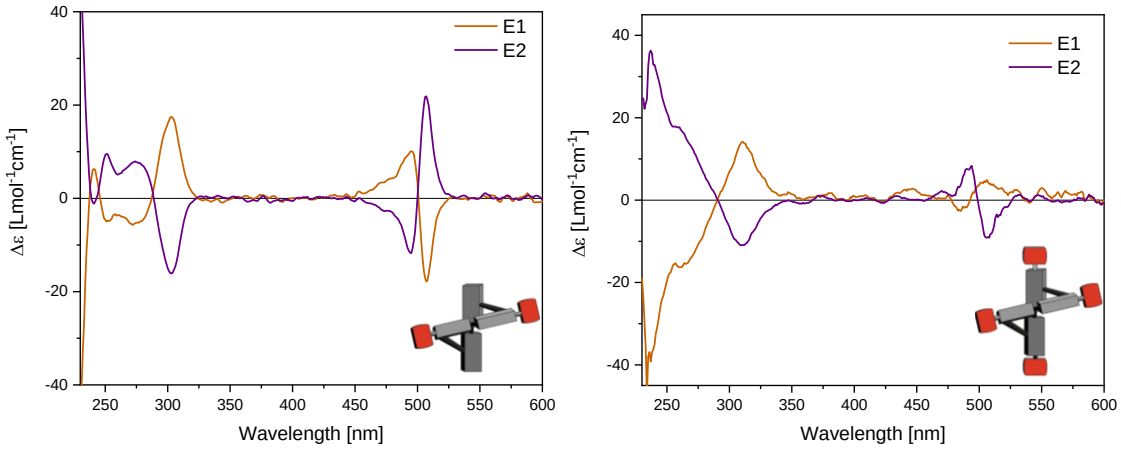


Figure S25: CD-spectra of the first eluting E1 (orange) and second eluting E2 (purple) enantiomer of left) $\mathbf{C_{Br_2BY_2}}$ and right) $\mathbf{C_{BY_4}}$, in CH_2Cl_2.

Assignment of CD-spectra

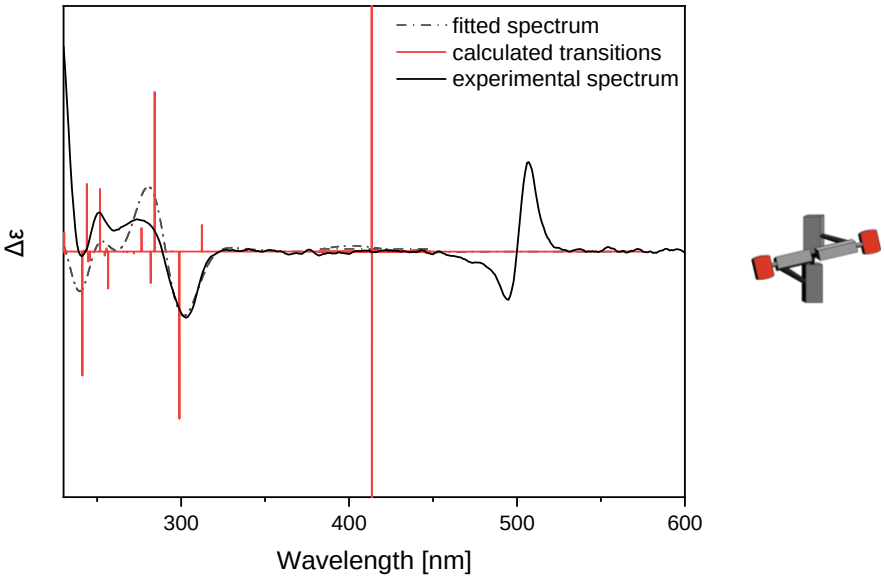


Figure S26: Calculated (dash-dot line, fitted with σ = 0.2 eV, shifted by 0.5 eV) and experimental (black solid line) spectrum of E2/*(P)*- $\mathbf{C}_{\mathbf{Br_2BY_2}}$. The computed transitions are indicated as bars (red).

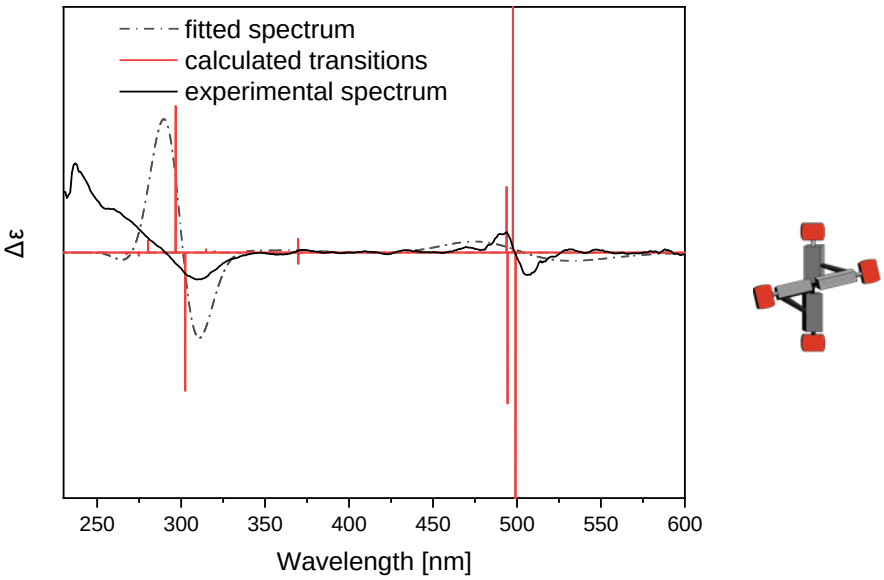


Figure S27: Calculated (dash-dot line, fitted with σ = 0.2 eV, shifted by 0.5 eV) and experimental (black solid line) spectrum of E2/*(P)*-$\mathbf{C}_{\mathbf{BY_4}}$. The computed transitions are indicated as bars (red).

NI/BY chromophore

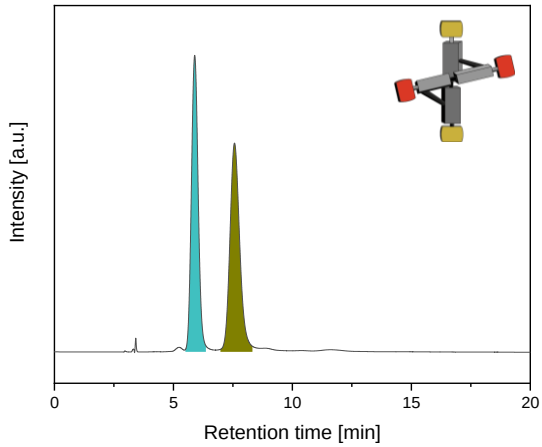


Figure S28: HPLC chromatogram of rac-$\mathbf{C_{NI_2BY_2}}$, IBN-5-column heptane/EtOAc (50/50) First eluting (E1) and second eluting (E2) enantiomer set are depicted in cyan and dark-yellow respectively.

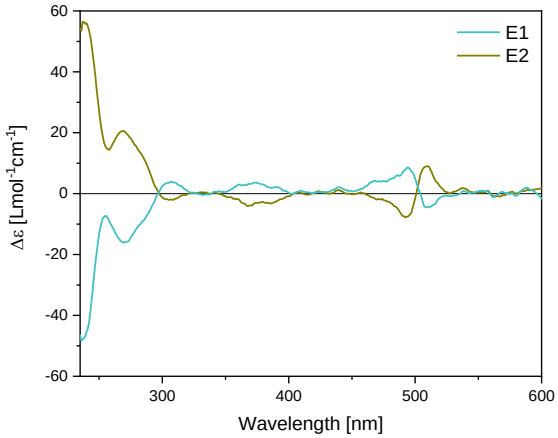


Figure S29: CD-spectra of the first eluting E1 (cyan) and second eluting E2 (dark-yellow) enantiomer of left) $\mathbf{C_{NI_2BY_2}}$ in CH_2Cl_2.

Assignment of CD-spectra

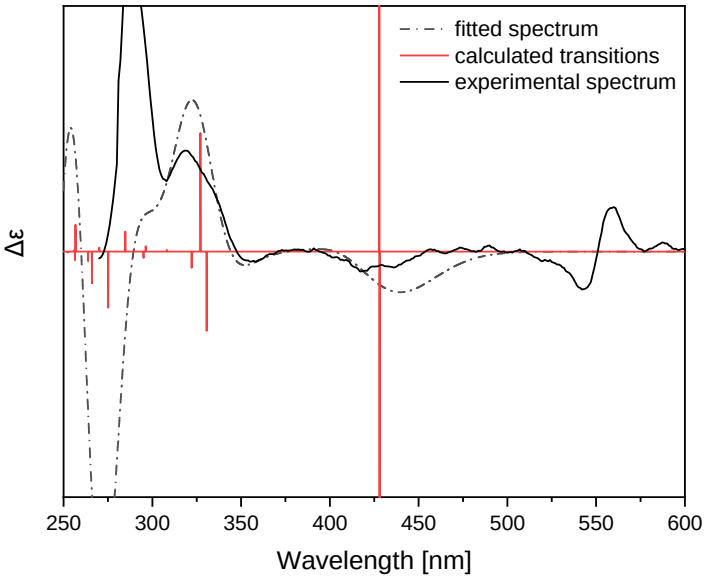


Figure S30: Calculated (dash-dot line, fitted with σ = 0.2 eV, shifted by 0.1 eV) and experimental (black solid line) spectrum of E2/*(P)*- $\mathbf{C_{NI_2BY_2}}$. The computed transitions are indicated as bars (red).

Comparison CD-spectra *(P)*-$\mathbf{C_{Naph_4}}$, *(P)*-$\mathbf{C_{NI_4}}$ and *(P)*-$\mathbf{C_{BY_4}}$

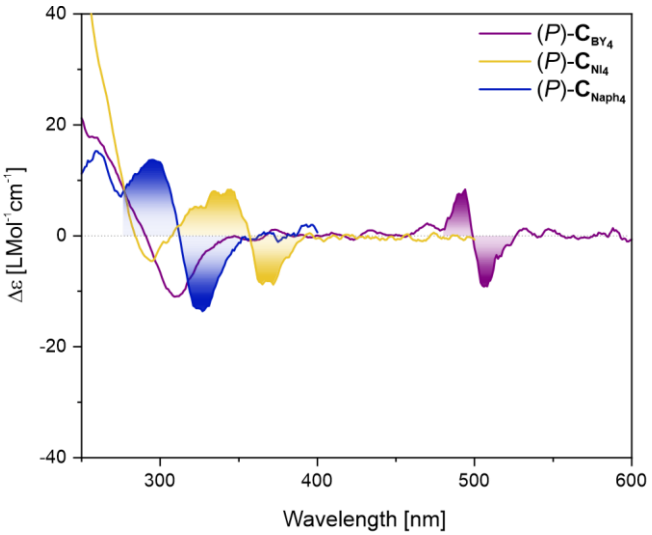


Figure S31: ECD-spectra of (P)-enantiomer of in blue $\mathbf{C_{Naph_4}}$, yellow $\mathbf{C_{NI_4}}$ and in purple $\mathbf{C_{BY_4}}$ bisignate signals are following a negative couplet indicated by integrated signals under the respective plots.

Geometry analysis $C_{Br_2BY_2}$

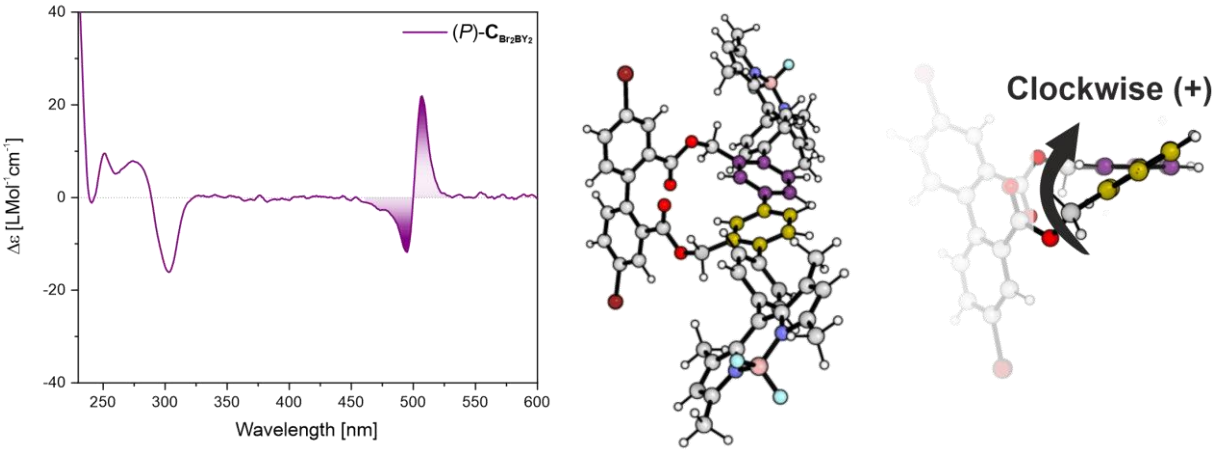


Figure S32: ECD-spectrum of *(P)*- $\mathbf{C_{Br_2BY_2}}$ and geometry optimized structure (side view). The center 'twist' between the biphenyls colored in yellow and purple follow a R configuration, which results in that on average the **BY** motives will be oriented in R configuration. This results in a clockwise and therefore positive couplet, hence explains the CD signal.

FRET-System

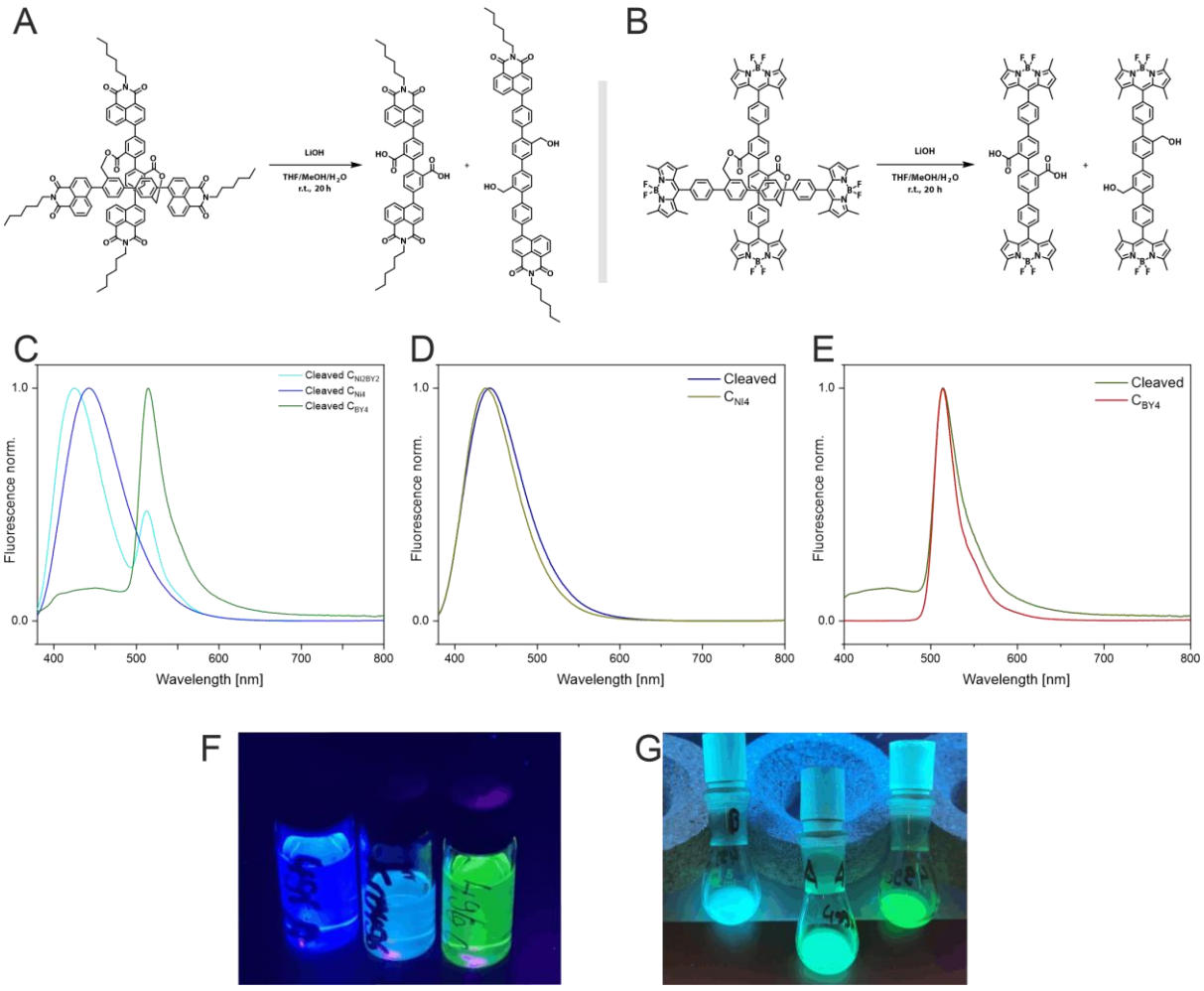


Figure S33: Template removal and resulting fluorescence spectra. A,B) Scheme of template removal ($\mathbf{C_{NI_4}}$ and $\mathbf{C_{BY_4}}$ respectively). Fluorescence spectra of C) comparison of cleaved products of $\mathbf{C_{NI2BY2}}$, $\mathbf{C_{NI4}}$ and $\mathbf{C_{BY4}}$ D,E) comparison of $\mathbf{C_{NI_4}}$ and $\mathbf{C_{BY_4}}$ and their cleaved products respectively, in CH_2Cl_2 at 20 °C with λ_{em} = 360 nm. F) Picture of a solution of the cleaved products of $\mathbf{C_{NI_4}}$, $\mathbf{C_{NI_2BY_2}}$ and $\mathbf{C_{BY_4}}$ (from left to right respectively) in a CH_2Cl_2 upon irradiation with λ_{em} = 366. G) Picture taken of the reaction mixtures from left to right $\mathbf{C_{NI_4}}$, $\mathbf{C_{NI_2BY_2}}$ and $\mathbf{C_{BY_4}}$ upon irradiation with λ_{em} = 366.

Crystallographic data

(rac)-$C_{Br_2I_2}$ (CCDC – 2378892)

Table S4. Crystal data and structure refinement for **(rac)-$C_{Br_2I_2}$**

Identification code	(rac)-$C_{Br_2I_2}$
Empirical formula	$C_{29.17}H_{17}Br_2I_2O_4$
Formula weight	845.05
Temperature/K	150
Crystal system	triclinic
Space group	P-1
a/Å	12.6865(2)
b/Å	14.4512(2)
c/Å	23.5383(4)
α/°	78.8510(10)
β/°	80.2510(10)
γ/°	81.8160(10)
Volume/Å^3	4145.92(11)
Z	6
ρ_{calc}g/cm^3	2.031
μ/mm^{-1}	14.710
F(000)	2400.0
Crystal size/mm^3	0.16 × 0.117 × 0.04
Radiation	GaKα (λ = 1.34143)
2Θ range for data collection/°	5.458 to 111.432
Index ranges	$-15 \leq h \leq 15$, $-17 \leq k \leq 16$, $-28 \leq l \leq 22$
Reflections collected	68037
Independent reflections	15876 [R_{int} = 0.0204, R_{sigma} = 0.0158]
Data/restraints/parameters	15876/7/1022
Goodness-of-fit on F^2	1.027
Final R indexes [I>=2σ (I)]	R_1 = 0.0333, wR_2 = 0.0917
Final R indexes [all data]	R_1 = 0.0362, wR_2 = 0.0935
Largest diff. peak/hole / e Å^{-3}	1.61/-2.00

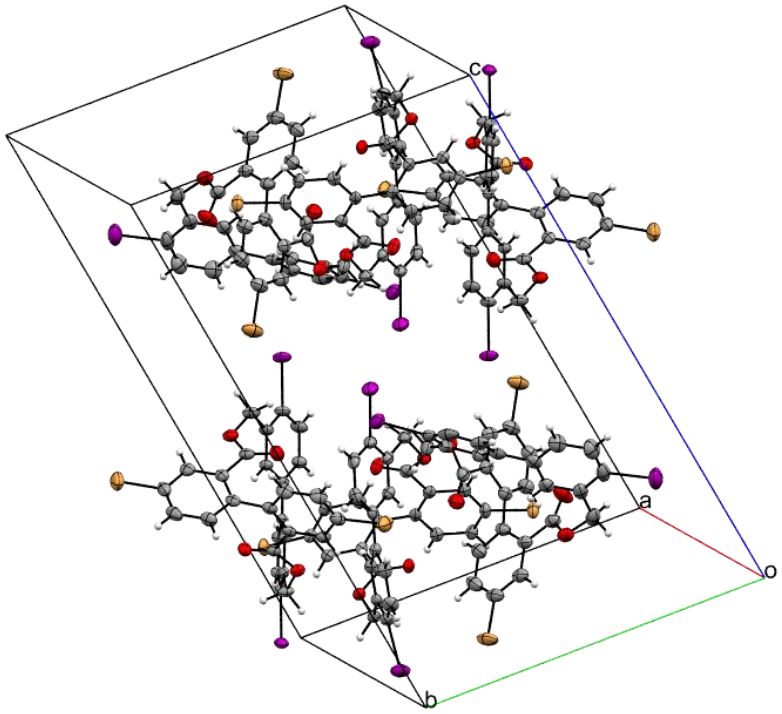


Figure S34. Unit-cell of the solid-state structure of (rac)-$\mathbf{C_{Br_2I_2}}$. Visualized as ORTEP representation with 50 % probability.

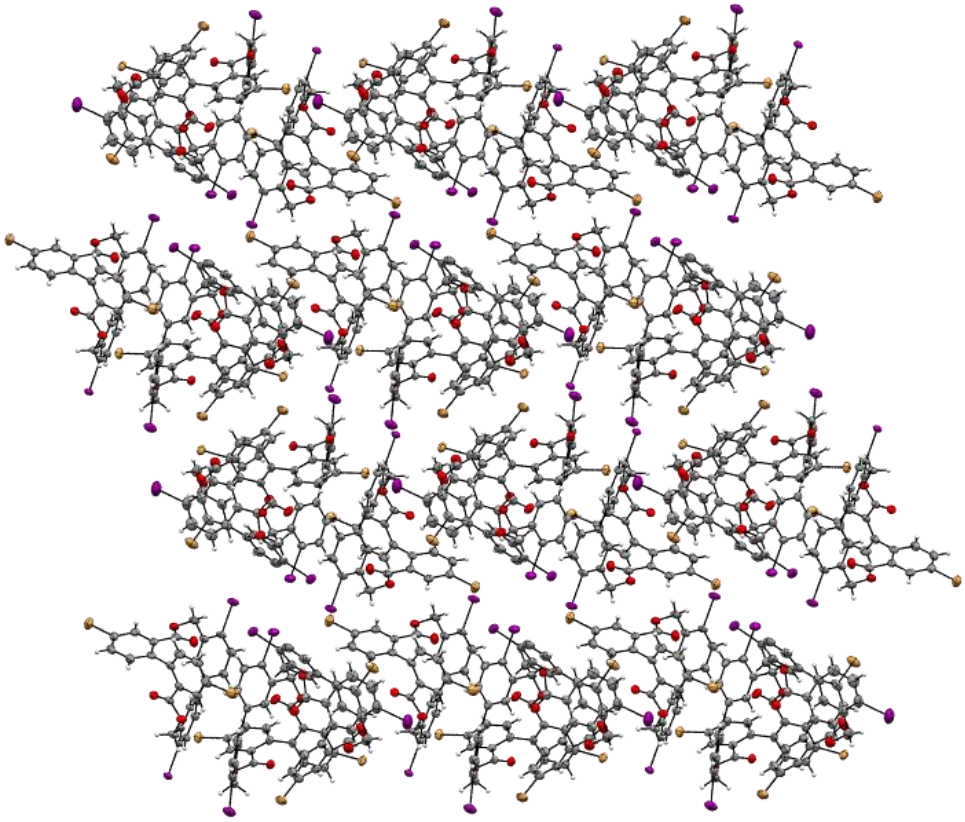


Figure S35. Enantiopure layer packing of **(rac)-$\mathbf{C_{Br_2I_2}}$**, visualized as ORTEP representation with 50 % probability. Top to bottom the horizontal layers contain only P, M, P, M enantiomers respectively.

(P)-C_{Br2I2} (CCDC – 2378893)

Table S5. Crystal data and structure refinement for **(P)-$C_{Br_2I_2}$**

Identification code	(*P*)- $C_{Br_2I_2}$
Empirical formula	$C_{32.15}H_{20.3}Br_2I_2O_4$
Formula weight	884.14
Temperature/K	150
Crystal system	monoclinic
Space group	I2
a/Å	37.2339(2)
b/Å	18.2754(2)
c/Å	28.1115(2)
α/°	90
β/°	90.1840(10)
γ/°	90
Volume/Å^3	19128.8(3)
Z	24
ρ_{calc}g/cm^3	1.842
μ/mm^{-1}	18.709
F(000)	10108.0
Crystal size/mm^3	0.3 × 0.243 × 0.2
Radiation	Cu Kα (λ = 1.54186)
2Θ range for data collection/°	9.726 to 140.562
Index ranges	$-44 \leq h \leq 29$, $-21 \leq k \leq 22$, $-33 \leq l \leq 34$
Reflections collected	227119
Independent reflections	35522 [R_{int} = 0.0348, R_{sigma} = 0.0205]
Data/restraints/parameters	35522/823/2001
Goodness-of-fit on F^2	1.036
Final R indexes [I>=2σ (I)]	R_1 = 0.0845, wR_2 = 0.2270
Final R indexes [all data]	R_1 = 0.0882, wR_2 = 0.2324
Largest diff. peak/hole / e Å^{-3}	6.78/-3.01
Flack parameter	0.026(6)

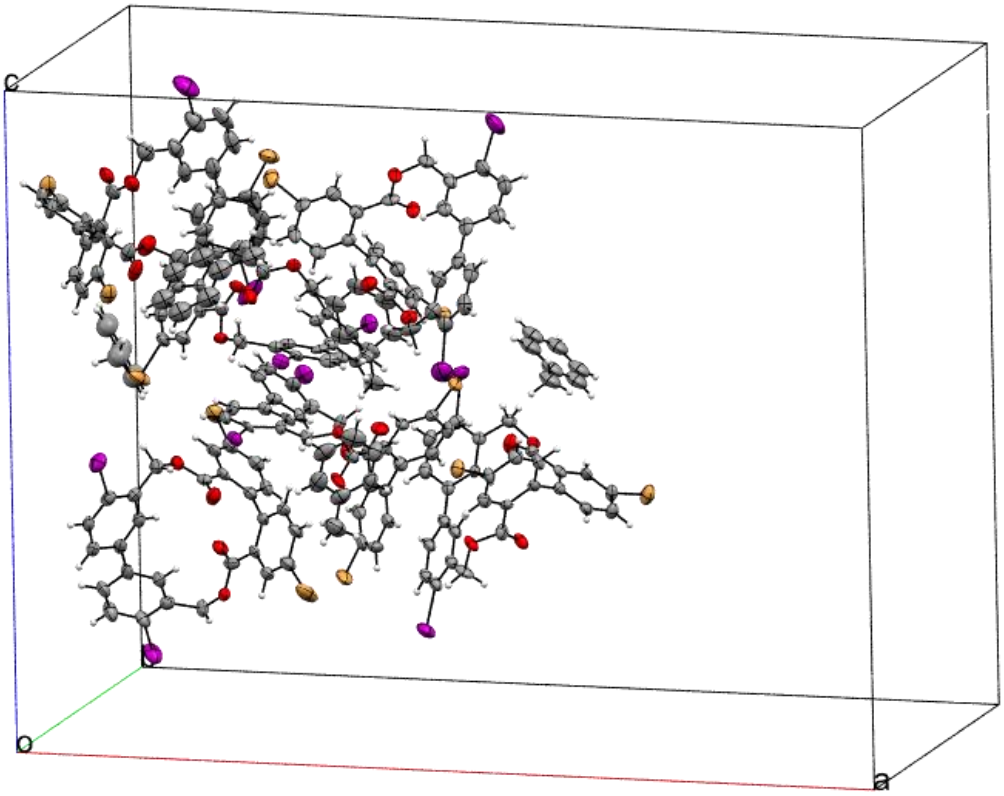


Figure S36. Unit-cell of the solid-state structure of (*P*)-$\mathbf{C_{Br_2I_2}}$. Visualized as ORTEP representation with 50 % probability.

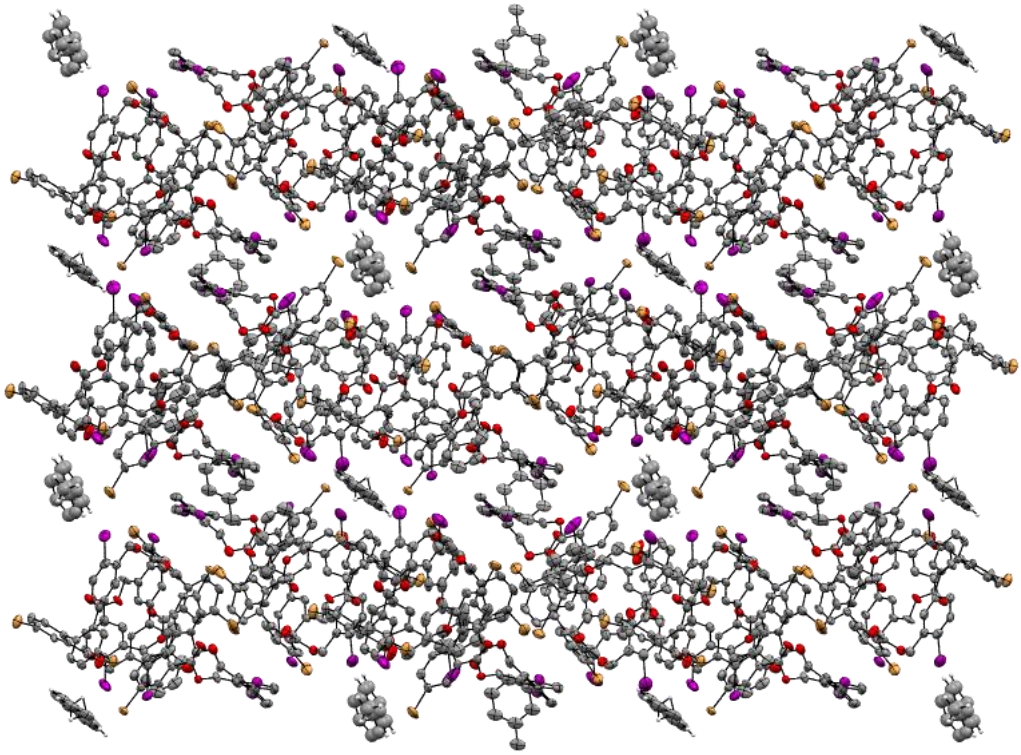


Figure S37. Layered packing of *(P)*-$\mathbf{C_{Br_2I_2}}$, visualized as ORTEP representation with 50 % probability. Horizontal layers of (*P*)-$\mathbf{C_{BR2I2}}$ with toluene molecules positioned in between the layers.

(rac)-$C_{Br_2BY_2}$ (CCDC – 2378894)

Table S6. Crystal data and structure refinement for **(rac)-$C_{Br_2BY_2}$**

Identification code	(rac)-$C_{Br_2BY_2}$
Empirical formula	$C_{74.4}H_{71.2}B_2Br_2F_4N_4O_4$
Formula weight	1342.79
Temperature/K	150
Crystal system	monoclinic
Space group	I2/a
a/Å	13.8303(3)
b/Å	16.4157(3)
c/Å	28.8295(6)
α/°	90
β/°	103.133(2)
γ/°	90
Volume/Å^3	6374.1(2)
Z	4
ρ_{calc}g/cm^3	1.399
μ/mm^{-1}	2.154
F(000)	2774.0
Crystal size/mm^3	0.25 × 0.123 × 0.05
Radiation	Cu Kα (λ = 1.54186)
2Θ range for data collection/°	6.238 to 140.046
Index ranges	$-16 \leq h \leq 11$, $-19 \leq k \leq 19$, $-31 \leq l \leq 35$
Reflections collected	54522
Independent reflections	5955 [R_{int} = 0.0362, R_{sigma} = 0.0177]
Data/restraints/parameters	5955/0/374
Goodness-of-fit on F^2	1.034
Final R indexes [I>=2σ (I)]	R_1 = 0.0428, wR_2 = 0.1089
Final R indexes [all data]	R_1 = 0.0584, wR_2 = 0.1190
Largest diff. peak/hole / e Å^{-3}	0.49/-0.58

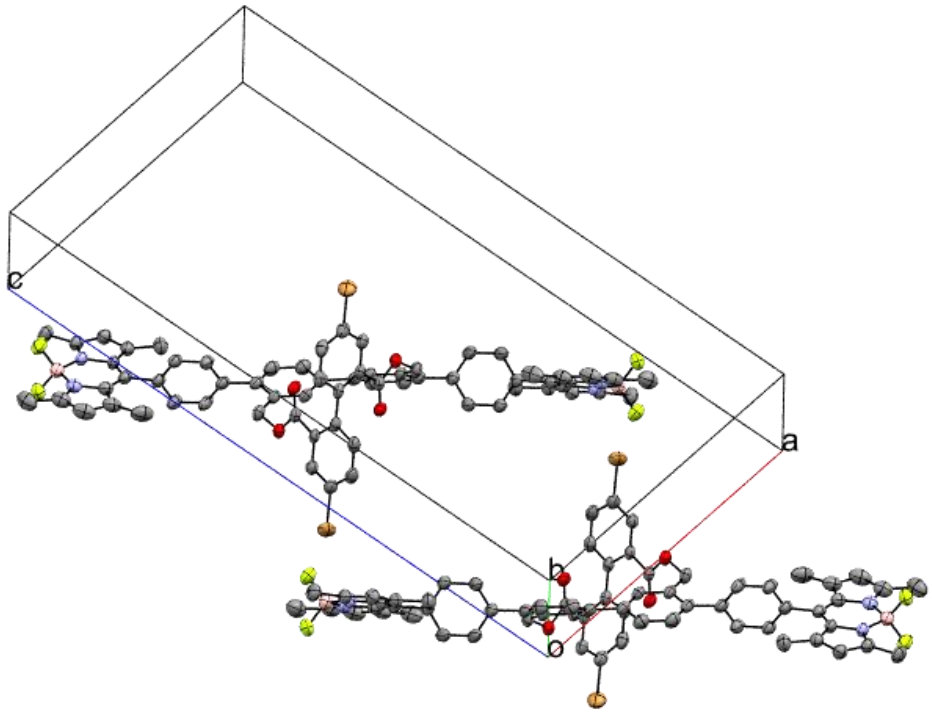


Figure S38. Unit-cell of the solid-state structure of (rac)-$\mathbf{C_{Br_2BY_2}}$. Visualized as ORTEP representation with 50 % probability.

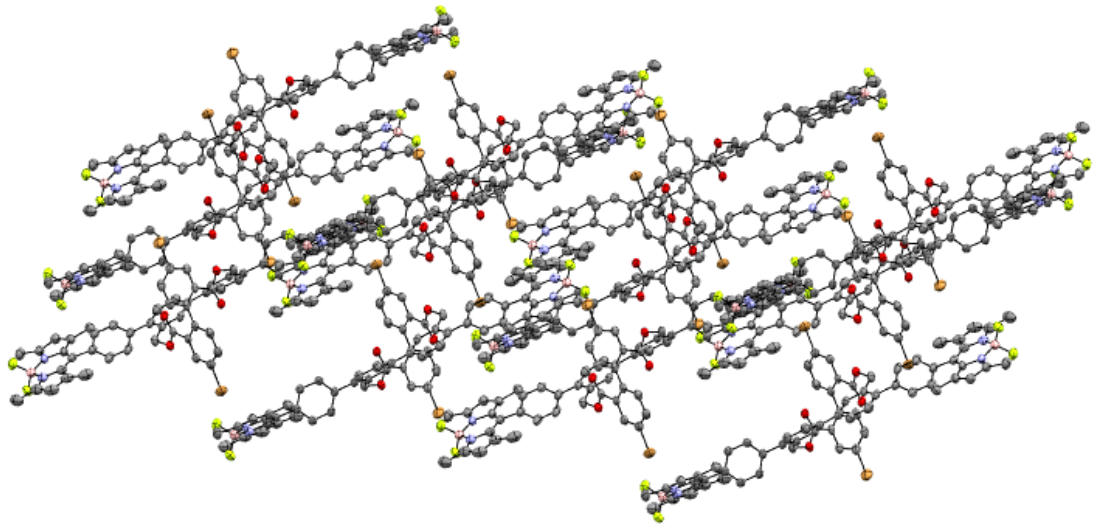


Figure S39. Packing of (rac)-$\mathbf{C_{Br_2BY_2}}$, visualized as ORTEP representation with 50 % probability.

Geometry optimized structures

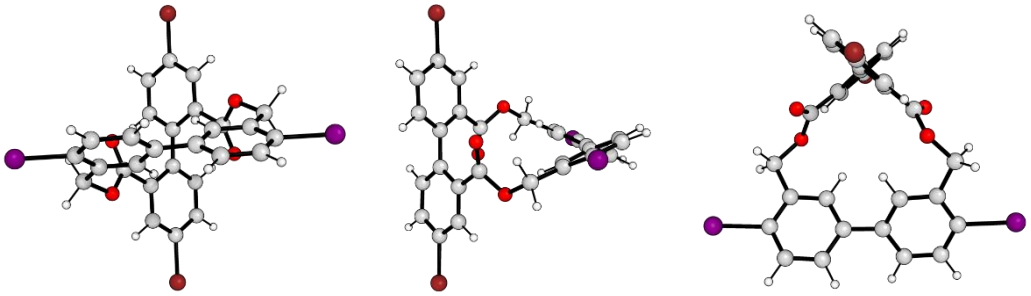


Figure S40. Geometry optimized structure of *(P)*-$\mathbf{C}_{\mathbf{Br_2I_2}}$, displayed in front, side and top view.

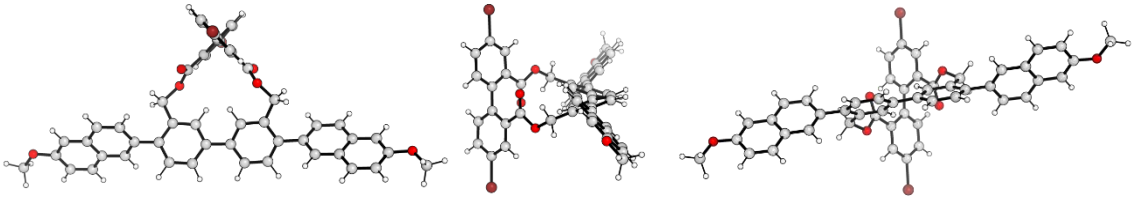


Figure S41. Geometry optimized structure of *(P)*-$\mathbf{C}_{\mathbf{Br_2Naph_2}}$, displayed in front, side and top view.

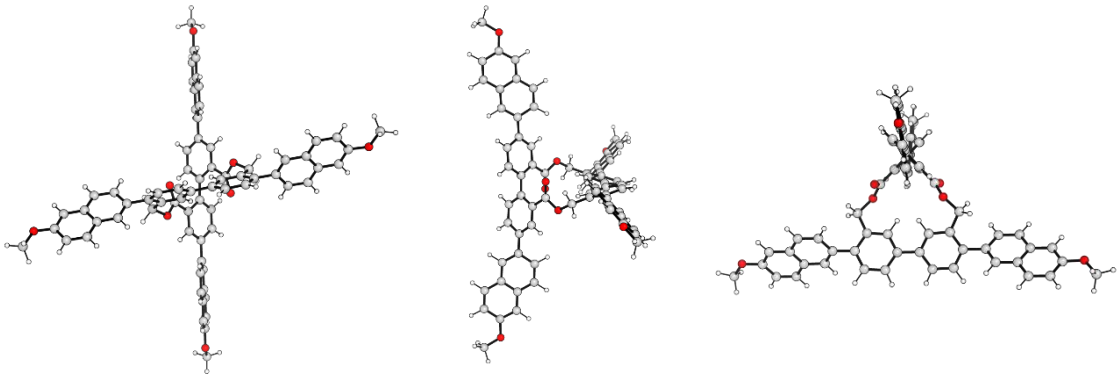


Figure S42. Geometry optimized structure of *(P)*-$\mathbf{C}_{\mathbf{Naph_4}}$, displayed in front, side and top view.

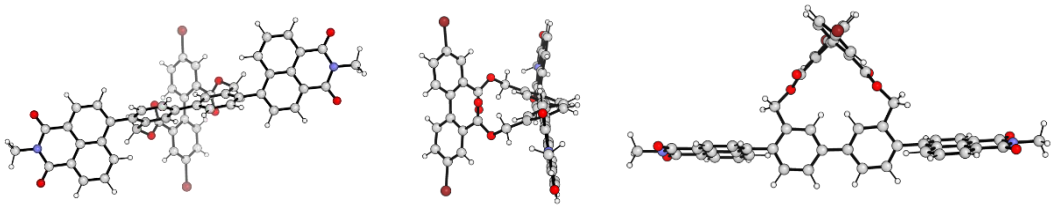


Figure S43. Geometry optimized structure of *(P)*-$\mathbf{C}_{\mathbf{Br_2NI_2}}$ configuration 1, displayed in front, side and top view.

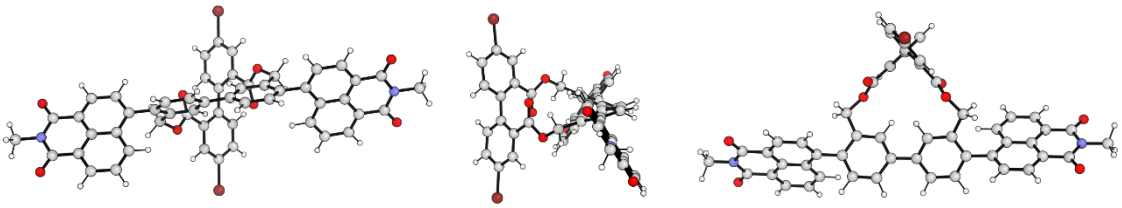


Figure S44. Geometry optimized structure of *(P)*-$\mathbf{C}_{\mathbf{Br_2NI_2}}$ configuration 2, displayed in front, side and top view.

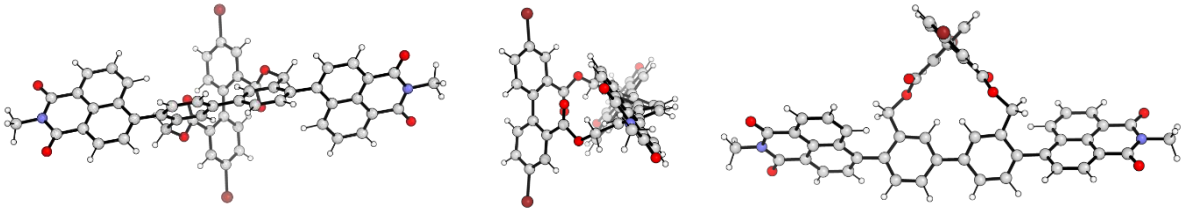


Figure S45. Geometry optimized structure of *(P)*-$\mathbf{C}_{\mathbf{Br_2NI_2}}$ configuration 3, displayed in front, side and top view.

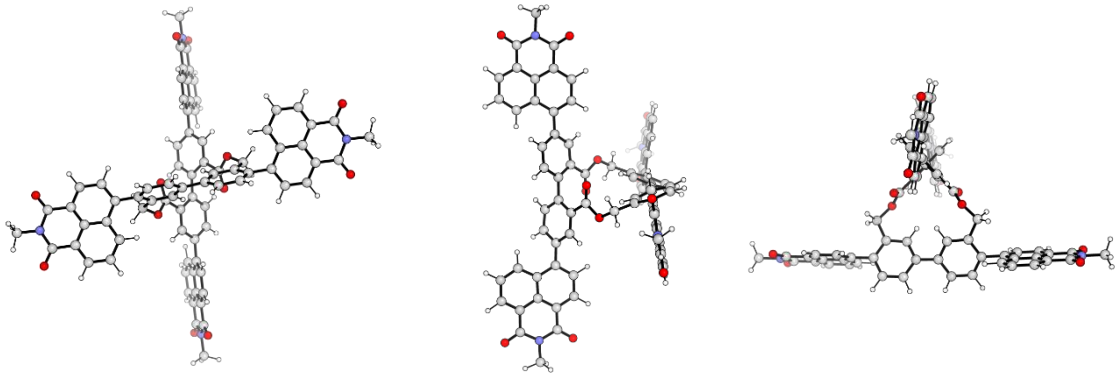


Figure S46. Geometry optimized structure of *(P)*-$\mathbf{C}_{\mathbf{NI_4}}$, displayed in front, side and top view.

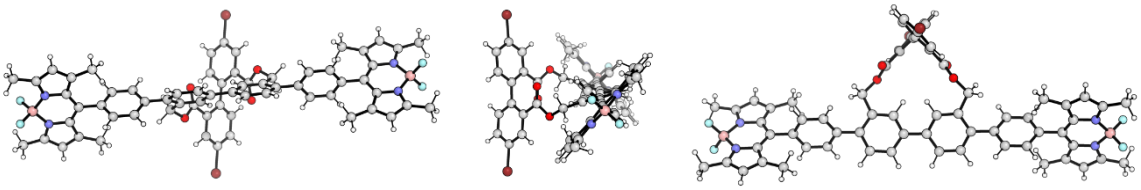


Figure S47. Geometry optimized structure of *(P)*-$\mathbf{C}_{\mathbf{Br_2BY_2}}$, displayed in front, side and top view.

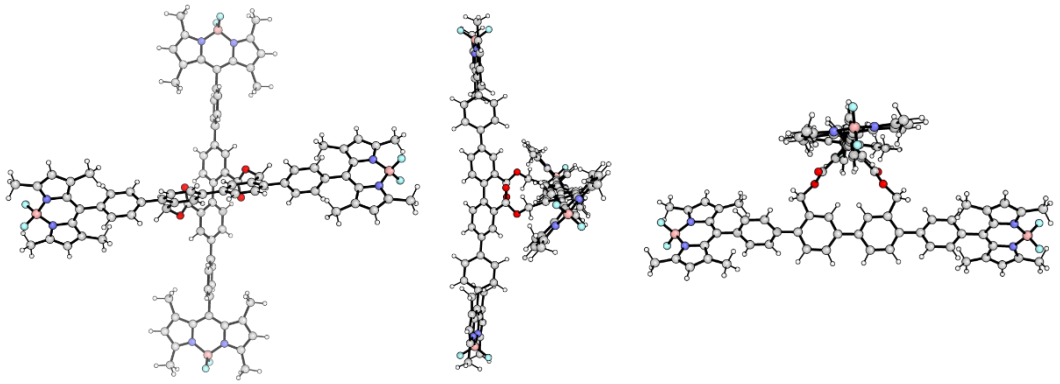


Figure S48. Geometry optimized structure of *(P)*-$\mathbf{C}_{\mathbf{BY_4}}$, displayed in front, side and top view.

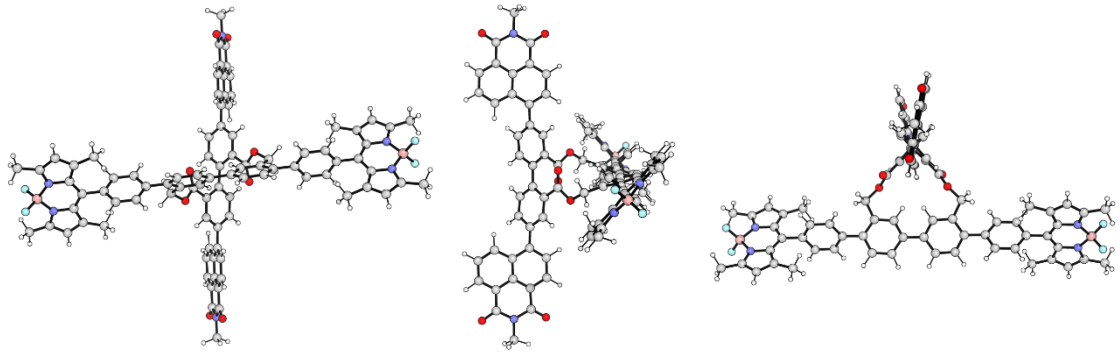


Figure S49. Geometry optimized structure of *(P)*-$\mathbf{C}_{\mathbf{NI_2BY_2}}$, displayed in front, side and top view.

Coordinates (energies in kcal)

52

$\mathbf{C}_{\mathbf{Br_2I_2}}$ Energy: -12722570.5715545

I	-5.64864	-2.73140	0.72209
I	5.64854	-2.73176	-0.72133
Br	-0.91807	3.20280	-5.40396
Br	0.91808	3.20439	5.40313
O	-2.67036	0.50009	-1.25895
O	-2.30339	1.60267	0.72950
O	2.67026	0.50018	1.25903
O	2.30364	1.60238	-0.72972
C	-1.38565	2.35270	-2.69462
H	-2.16287	1.73643	-3.11822
C	1.38570	2.35339	2.69408
H	2.16279	1.73713	3.11794
C	-0.73968	-2.91357	0.07360
C	1.17869	2.32914	1.30628
C	-2.07691	1.49073	-0.46877
C	2.84642	-1.69816	0.15820
C	-1.17856	2.32885	-1.30681
C	-2.84652	-1.69804	-0.15774
C	0.14770	3.09987	0.73485
C	-0.41053	3.93326	2.94967
H	-1.02304	4.55258	3.59060
C	-1.46494	-1.78687	-0.33430
H	-0.95317	-0.96790	-0.81970
C	-0.60462	3.15806	-3.50232
C	0.73953	-2.91360	-0.07309
C	0.60476	3.15916	3.50147
C	-1.43315	-3.99528	0.63178
H	-0.89187	-4.87224	0.96672
C	3.51499	-2.78675	-0.41047
C	1.46482	-1.78690	0.33471
H	0.95309	-0.96784	0.81998
C	-0.14741	3.09961	-0.73569
C	-0.64223	3.88954	1.57870
H	-1.45446	4.46371	1.15252
C	1.43297	-3.99541	-0.63113
H	0.89167	-4.87238	-0.96601
C	2.07702	1.49071	0.46854
C	-3.51512	-2.78653	0.41109
C	-3.58027	-0.43171	-0.56731
H	-4.37414	-0.64280	-1.28572
H	-3.98314	0.06566	0.31983
C	3.58022	-0.43183	0.56768
H	4.37393	-0.64286	1.28629
H	3.98329	0.06537	-0.31946
C	0.41088	3.93212	-2.95084
H	1.02348	4.55110	-3.59201
C	0.64265	3.88882	-1.57987

H	1.45504	4.46294	-1.15393
C	2.81681	-3.93138	-0.79420
H	3.34769	-4.76400	-1.23661
C	-2.81698	-3.93116	0.79490
H	-3.34789	-4.76371	1.23743

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$C_{Br_2Naph_2}$ Energy: -4718790.1902745

Br	1.22778	3.89719	5.36038
Br	-1.22779	3.89728	-5.36033
O	2.70271	1.09596	1.12809
O	1.97917	2.01511	-0.84209
O	-2.70271	1.09596	-1.12810
O	-1.97920	2.01508	0.84210
C	1.48067	2.97507	2.64002
H	2.23149	2.31021	3.04343
C	-1.48068	2.97511	-2.63999
H	-2.23150	2.31025	-3.04341
C	0.74030	-2.43279	-0.05937
C	-1.19531	2.93643	-1.26173
C	1.96506	2.00517	0.39711
C	-2.83628	-1.15780	-0.07662
C	1.19529	2.93641	1.26175
C	2.83628	-1.15779	0.07658
C	-0.19634	3.78532	-0.72376
C	0.14787	4.74309	-2.94644
H	0.65719	5.44256	-3.59856
C	1.45272	-1.25476	0.23493
H	0.90969	-0.40604	0.62826
C	0.80602	3.86669	3.45969
C	-0.74029	-2.43280	0.05932
C	-0.80604	3.86674	-3.45965
C	1.47218	-3.55796	-0.47644
H	0.95825	-4.48050	-0.72858
C	-3.56672	-2.29026	0.36188
C	-1.45272	-1.25477	-0.23497
H	-0.90969	-0.40605	-0.62831
C	0.19632	3.78531	0.72381
C	0.44613	4.69133	-1.58328
H	1.21089	5.34664	-1.17990
C	-1.47217	-3.55797	0.47639
H	-0.95823	-4.48050	0.72853
C	-1.96508	2.00517	-0.39711
C	3.56673	-2.29025	-0.36192
C	3.55750	0.14143	0.39205
H	4.40441	-0.02246	1.06072
H	3.90190	0.64172	-0.51629
C	-3.55750	0.14141	-0.39209
H	-4.40440	-0.02248	-1.06078
H	-3.90192	0.64169	0.51626
C	-0.14789	4.74303	2.94650
H	-0.65721	5.44250	3.59863
C	-0.44615	4.69130	1.58334
H	-1.21092	5.34662	1.17997
C	-2.86130	-3.48245	0.61399
H	-3.41474	-4.35081	0.95947
C	2.86132	-3.48244	-0.61403
H	3.41476	-4.35079	-0.95951
C	5.04725	-2.25298	-0.55921
C	5.88512	-3.07743	0.17759
C	5.62801	-1.39005	-1.54296
C	7.29678	-3.07114	-0.01224
H	5.46251	-3.73909	0.92989
C	6.99034	-1.36256	-1.75500
H	4.97487	-0.76883	-2.14923
C	8.16908	-3.90266	0.74241
C	7.87014	-2.19332	-0.99744
H	7.41147	-0.70911	-2.51413
C	9.53830	-3.87950	0.54345
H	7.74496	-4.56777	1.48981
C	9.27492	-2.18361	-1.18774
C	10.09222	-3.00894	-0.43351
H	10.17674	-4.52524	1.13413
H	9.72511	-1.52932	-1.92668
C	-5.04724	-2.25300	0.55919
C	-5.88511	-3.07743	-0.17763
C	-5.62799	-1.39008	1.54295
C	-7.29677	-3.07115	0.01221
H	-5.46251	-3.73908	-0.92994
C	-6.99031	-1.36261	1.75500
H	-4.97485	-0.76888	2.14923
C	-8.16908	-3.90265	-0.74245
C	-7.87013	-2.19335	0.99743
H	-7.41144	-0.70916	2.51415
C	-9.53829	-3.87950	-0.54348
H	-7.74496	-4.56775	-1.48986
C	-9.27490	-2.18364	1.18774
C	-10.09220	-3.00896	0.43351
H	-10.17673	-4.52522	-1.13416
H	-9.72509	-1.52937	1.92670
O	11.45985	-2.92468	-0.69602
O	-11.45984	-2.92470	0.69603
C	12.38690	-3.75909	0.05442
H	12.18588	-4.82354	-0.11408
H	13.37040	-3.50290	-0.33775
H	12.34405	-3.53235	1.12615
C	-12.38689	-3.75910	-0.05443
H	-12.18587	-4.82355	0.11405
H	-13.37039	-3.50291	0.33776
H	-12.34405	-3.53233	-1.12615

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C_{Naph_4} Energy: -2118523.8924662

O	-2.85642	0.63854	-0.10930

O	-1.11354	1.82208	-1.01041
O	2.85642	-0.63854	-0.10929
O	1.11354	-1.82208	-1.01041
C	-2.77482	-1.25067	-2.05625
H	-3.63035	-1.10743	-1.40902
C	2.77483	1.25067	-2.05625
H	3.63035	1.10743	-1.40902
C	-0.57801	0.46659	3.42912
C	1.72049	0.32237	-1.97582
C	-1.83039	0.81073	-1.02395
C	2.37646	-1.55722	2.15605
C	-1.72049	-0.32237	-1.97582
C	-2.37646	1.55722	2.15605
C	0.58749	0.46685	-2.81538
C	1.63638	2.43888	-3.81023
H	1.57509	3.26802	-4.50825
C	-1.32015	0.64847	2.24673
H	-1.08336	0.03875	1.38565
C	-2.75798	-2.31778	-2.96661
C	0.57800	-0.46659	3.42912
C	2.75798	2.31779	-2.96661
C	-0.96232	1.20108	4.56482
H	-0.40502	1.10566	5.49160
C	2.75231	-2.30176	3.30219
C	1.32015	-0.64847	2.24673
H	1.08336	-0.03874	1.38565
C	-0.58749	-0.46684	-2.81538
C	0.58135	1.53087	-3.73270
H	-0.28665	1.66231	-4.37097
C	0.96231	-1.20109	4.56482
H	0.40502	-1.10566	5.49160
C	1.83039	-0.81073	-1.02395
C	-2.75232	2.30176	3.30219
C	-3.12506	1.73134	0.84563
H	-4.20582	1.69481	0.99424
H	-2.85662	2.67008	0.35414
C	3.12506	-1.73134	0.84563
H	4.20582	-1.69481	0.99424
H	2.85662	-2.67008	0.35414
C	-1.63637	-2.43887	-3.81023
H	-1.57508	-3.26802	-4.50825
C	-0.58135	-1.53087	-3.73270
H	0.28666	-1.66230	-4.37097
C	2.03708	-2.09173	4.49720
H	2.31189	-2.66851	5.37561
C	-2.03709	2.09173	4.49720
H	-2.31190	2.66850	5.37561
C	-3.87636	3.28549	3.28416
C	-4.96834	3.12975	4.12619
C	-3.83251	4.43190	2.42784
C	-6.03954	4.06813	4.14505
H	-5.02139	2.26425	4.78219
C	-4.85097	5.36172	2.42392
H	-2.96456	4.58130	1.79243
C	-7.16921	3.91576	4.99514
C	-5.98803	5.21193	3.27388
H	-4.79366	6.23095	1.77439
C	-8.20019	4.83886	4.99664
H	-7.21753	3.05384	5.65520
C	-7.05311	6.14753	3.28964
C	-8.13647	5.96519	4.13272
H	-9.04741	4.69521	5.65622
H	-7.03097	7.01663	2.64079
C	3.87635	-3.28549	3.28416
C	4.96834	-3.12975	4.12619
C	3.83251	-4.43190	2.42784
C	6.03954	-4.06814	4.14505
H	5.02139	-2.26426	4.78220
C	4.85097	-5.36172	2.42391
H	2.96456	-4.58130	1.79243
C	7.16920	-3.91576	4.99514
C	5.98802	-5.21193	3.27388
H	4.79366	-6.23095	1.77439
C	8.20018	-4.83887	4.99664
H	7.21752	-3.05385	5.65520
C	7.05310	-6.14753	3.28964
C	8.13646	-5.96519	4.13273
H	9.04741	-4.69522	5.65623
H	7.03096	-7.01663	2.64079
O	-9.13229	6.94126	4.07305
O	9.13228	-6.94126	4.07306
C	-10.30473	6.82190	4.92701
H	-10.02567	6.84277	5.98704
H	-10.91188	7.69436	4.68828
H	-10.86562	5.90692	4.70306
C	10.30472	-6.82191	4.92701
H	10.02567	-6.84278	5.98704
H	10.91187	-7.69437	4.68828
H	10.86562	-5.90692	4.70307
C	-3.88812	-3.28064	-3.03783
C	-4.31932	-3.80079	-4.25099
C	-4.56042	-3.69443	-1.84332
C	-5.39920	-4.72402	-4.32936
H	-3.84579	-3.48379	-5.17665
C	-5.60967	-4.58705	-1.88405
H	-4.21563	-3.31421	-0.88686
C	-5.85412	-5.25869	-5.56631
C	-6.06701	-5.13125	-3.12189
H	-6.09788	-4.89655	-0.96404
C	-6.90801	-6.15379	-5.62141
H	-5.35807	-4.95479	-6.48425
C	-7.14430	-6.04929	-3.19753
C	-7.55654	-6.55041	-4.42099
H	-7.22995	-6.54454	-6.57911
H	-7.65842	-6.36869	-2.29724
O	-8.62606	-7.44702	-4.38894

C	-9.12156	-8.01547	-5.63345
H	-8.34498	-8.60340	-6.13676
H	-9.94135	-8.66745	-5.33390
H	-9.49564	-7.23313	-6.30432
C	3.88812	3.28064	-3.03782
C	4.31932	3.80079	-4.25099
C	4.56042	3.69443	-1.84331
C	5.39921	4.72402	-4.32936
H	3.84580	3.48379	-5.17665
C	5.60967	4.58705	-1.88404
H	4.21563	3.31422	-0.88686
C	5.85413	5.25869	-5.56631
C	6.06702	5.13126	-3.12188
H	6.09788	4.89656	-0.96403
C	6.90802	6.15379	-5.62141
H	5.35808	4.95478	-6.48424
C	7.14430	6.04930	-3.19752
C	7.55655	6.55041	-4.42098
H	7.22996	6.54454	-6.57911
H	7.65842	6.36869	-2.29724
O	8.62606	7.44702	-4.38894
C	9.12157	8.01547	-5.63345
H	8.34499	8.60340	-6.13675
H	9.94136	8.66745	-5.33389
H	9.49565	7.23313	-6.30431

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C$_{Br_2Ni_2}$ (conf1) Energy: -4977464.1927304

Br	1.74071	4.13930	5.16027
Br	-1.74072	4.13934	-5.16024
O	2.80448	1.16756	0.94952
O	1.86608	1.97189	-0.94231
O	-2.80448	1.16757	-0.94951
O	-1.86608	1.97188	0.94232
C	1.73799	3.08856	2.50599
H	2.54395	2.45636	2.85711
C	-1.73800	3.08858	-2.50596
H	-2.54395	2.45638	-2.85709
C	0.73428	-2.34668	-0.10474
C	-1.30887	2.98372	-1.17266
C	1.99492	2.01709	0.26014
C	-2.83337	-1.08732	0.05224
C	1.30887	2.98372	1.17269
C	2.83337	-1.08731	-0.05225
C	-0.25221	3.79712	-0.70643
C	-0.10489	4.82434	-2.91639
H	0.35879	5.53944	-3.58870
C	1.46475	-1.18428	0.18675
H	0.94382	-0.34036	0.62420
C	1.13865	4.00250	3.36292
C	-0.73428	-2.34668	0.10471
C	-1.13865	4.00253	-3.36289
C	1.42591	-3.45383	-0.61345
H	0.88757	-4.36410	-0.86573
C	-3.52110	-2.20529	0.57043
C	-1.46475	-1.18429	-0.18676
H	-0.94382	-0.34036	-0.62421
C	0.25221	3.79712	0.70646
C	0.32477	4.71171	-1.59718
H	1.13755	5.34245	-1.24720
C	-1.42590	-3.45384	0.61341
H	-0.88756	-4.36411	0.86568
C	-1.99492	2.01709	-0.26013
C	3.52110	-2.20528	-0.57046
C	3.56890	0.22061	0.18182
H	4.48176	0.06296	0.76258
H	3.83635	0.67334	-0.77961
C	-3.56890	0.22061	-0.18182
H	-4.48176	0.06296	-0.76259
H	-3.83636	0.67332	0.77962
C	0.10488	4.82432	2.91643
H	-0.35880	5.53940	3.58875
C	-0.32477	4.71170	1.59723
H	-1.13756	5.34244	1.24724
C	-2.79980	-3.37804	0.83692
H	-3.32907	-4.23834	1.24010
C	2.79980	-3.37803	-0.83696
H	3.32908	-4.23833	-1.24014
C	4.98687	-2.16091	-0.87390
C	5.96550	-2.33066	0.16080
C	5.41028	-1.97322	-2.18181
C	5.62210	-2.55376	1.52217
C	7.35236	-2.28495	-0.18605
C	6.77882	-1.93301	-2.51543
H	4.66603	-1.84914	-2.96447
C	6.59927	-2.70890	2.48589
H	4.57208	-2.60669	1.79642
C	8.33836	-2.44821	0.82116
C	7.74108	-2.08251	-1.53437
H	7.10088	-1.78204	-3.54172
C	7.96393	-2.65462	2.13755
H	6.31632	-2.87851	3.52152
H	8.74245	-2.77577	2.88493
C	-4.98686	-2.16093	0.87388
C	-5.96549	-2.33065	-0.16082
C	-5.41027	-1.97327	2.18180
C	-5.62210	-2.55372	-1.52220
C	-7.35236	-2.28495	0.18603
C	-6.77881	-1.93307	2.51542
H	-4.66602	-1.84921	2.96445
C	-6.59927	-2.70884	-2.48592
H	-4.57208	-2.60664	-1.79645
C	-8.33836	-2.44818	-0.82118
C	-7.74107	-2.08254	1.53436
H	-7.10087	-1.78213	3.54171
C	-7.96393	-2.65456	-2.13758

H	-6.31632	-2.87842	-3.52156
H	-8.74245	-2.77570	-2.88496
C	9.17733	-2.03304	-1.90627
C	9.78595	-2.40207	0.48259
C	-9.17732	-2.03308	1.90626
C	-9.78595	-2.40205	-0.48261
O	-9.56009	-1.86093	3.05211
O	9.56010	-1.86085	-3.05211
O	10.65669	-2.53562	1.32672
O	-10.65669	-2.53559	-1.32674
N	-10.10750	-2.19508	0.86969
N	10.10750	-2.19506	-0.86970
C	11.52228	-2.14226	-1.25528
H	12.11818	-2.28044	-0.35503
H	11.73756	-2.92878	-1.98406
H	11.74400	-1.17733	-1.71976
C	-11.52227	-2.14229	1.25528
H	-12.11817	-2.28043	0.35502
H	-11.73756	-2.92883	1.98402
H	-11.74399	-1.17737	1.71979

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$C_{Br_2Ni_2}$ (conf2) Energy: -4977464.6192172

Br	-1.38226	5.68136	-4.13310
Br	0.44049	2.16234	6.01336
O	-2.72593	1.33932	-1.47774
O	-2.24148	1.48800	0.72351
O	2.48539	0.98533	1.30757
O	1.74896	2.35972	-0.32788
C	-1.67290	3.75225	-2.04923
H	-2.33462	3.24534	-2.74043
C	0.96944	2.14577	3.20807
H	1.78366	1.47830	3.46131
C	-0.50152	-2.21952	-1.19145
C	0.76341	2.50564	1.86596
C	-2.15979	1.94062	-0.39647
C	2.89969	-0.77807	-0.36293
C	-1.44934	3.20075	-0.77685
C	-2.68833	-1.11614	-1.19931
C	-0.30193	3.36756	1.52260
C	-0.90655	3.51461	3.88335
H	-1.55025	3.90909	4.66337
C	-1.29764	-1.06408	-1.24014
H	-0.80929	-0.10095	-1.33437
C	-1.05755	4.94317	-2.41255
C	0.97371	-2.07773	-1.13885
C	0.14009	2.65013	4.20128
C	-1.14372	-3.46420	-1.16353
H	-0.55878	-4.37935	-1.11576
C	3.77067	-1.65585	-1.04195
C	1.52803	-1.01502	-0.40938
H	0.86159	-0.37461	0.15621
C	-0.58040	3.84866	0.12911
C	-1.11471	3.86125	2.55150
H	-1.93608	4.52574	2.29717
C	1.84686	-2.95295	-1.79902
H	1.45188	-3.77834	-2.38610
C	1.69147	1.97643	0.81873
C	-3.32722	-2.37436	-1.14447
C	-3.51138	0.16022	-1.22706
H	-4.24097	0.13199	-2.04245
H	-4.04836	0.28899	-0.28189
C	3.44864	0.41382	0.40297
H	4.29120	0.11824	1.03493
H	3.78501	1.19205	-0.28976
C	-0.21007	5.60531	-1.52554
H	0.26621	6.53770	-1.81218
C	0.01821	5.05105	-0.26929
H	0.68762	5.55706	0.42121
C	3.22332	-2.74346	-1.74018
H	3.89331	-3.41838	-2.26792
C	-2.53568	-3.53251	-1.14958
H	-3.02747	-4.50168	-1.11088
C	-4.81622	-2.51358	-1.11319
C	-5.57378	-2.20034	0.06427
C	-5.47966	-2.98568	-2.23764
C	-4.97685	-1.75353	1.27540
C	-6.99498	-2.36092	0.03315
C	-6.87909	-3.14332	-2.25811
H	-4.90230	-3.22897	-3.12610
C	-5.74764	-1.46303	2.38406
H	-3.89713	-1.64203	1.32265
C	-7.76484	-2.05636	1.18539
C	-7.63375	-2.83155	-1.14225
H	-7.38857	-3.50629	-3.14593
C	-7.14861	-1.61123	2.34156
H	-5.27048	-1.12023	3.29831
H	-7.76734	-1.38683	3.20551
C	5.25041	-1.43619	-1.05673
C	6.13522	-2.28862	-0.31659
C	5.78429	-0.40253	-1.81452
C	5.67883	-3.35453	0.50667
C	7.54470	-2.05287	-0.39281
C	7.17252	-0.17644	-1.88133
H	5.11380	0.23487	-2.38600
C	6.56922	-4.14850	1.20237
H	4.61130	-3.53776	0.58390
C	8.43924	-2.88444	0.32911
C	8.04754	-0.98921	-1.18402
H	7.57952	0.63039	-2.48372
C	7.95671	-3.91764	1.11271
H	6.19911	-4.95743	1.82692
H	8.66879	-4.53479	1.65281
C	-9.10921	-3.00263	-1.19467
C	-9.24154	-2.21407	1.16583
C	9.50802	-0.72993	-1.27757

C	9.90475	-2.65463	0.25514
O	9.96685	0.17876	-1.95040
O	-9.68373	-3.40379	-2.19375
O	-9.94814	-1.96026	2.12780
O	10.71462	-3.34391	0.85360
N	10.34342	-1.59058	-0.54607
N	-9.81769	-2.67682	-0.02628
C	-11.27728	-2.82632	-0.02481
H	-11.74835	-1.86300	0.18991
H	-11.57578	-3.18881	-1.00675
H	-11.57692	-3.53323	0.75401
C	11.79424	-1.37971	-0.60542
H	12.28372	-2.27796	-0.99211
H	11.98061	-0.52973	-1.25924
H	12.18224	-1.18557	0.39849

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$C_{Br_2Ni_2}$ (conf3) Energy: -4977464.9633058

Br	0.18211	3.76322	5.44320
Br	-0.18207	3.76286	-5.44340
O	2.41887	0.80161	1.71145
O	2.07875	1.61990	-0.36645
O	-2.41887	0.80153	-1.71145
O	-2.07873	1.61994	0.36640
C	0.94795	2.71979	2.89880
H	1.62156	2.08956	3.46594
C	-0.94793	2.71961	-2.89893
H	-1.62155	2.08935	-3.46603
C	0.73563	-2.69241	0.09279
C	-0.92101	2.61707	-1.49818
C	1.84709	1.65672	0.82126
C	-2.74337	-1.42362	-0.69266
C	0.92104	2.61716	1.49806
C	2.74335	-1.42360	0.69277
C	-0.03901	3.42738	-0.74917
C	0.74147	4.44853	-2.82489
H	1.38146	5.16057	-3.33653
C	1.36068	-1.52836	0.56677
H	0.73831	-0.69348	0.86733
C	0.12361	3.62927	3.54848
C	-0.73565	-2.69241	-0.09262
C	-0.12357	3.62903	-3.54867
C	1.53940	-3.80005	-0.20601
H	1.08964	-4.71483	-0.58400
C	-3.54845	-2.53645	-0.36427
C	-1.36069	-1.52838	-0.56664
H	-0.73832	-0.69352	-0.86724
C	0.03905	3.42743	0.74899
C	0.77370	4.33742	-1.43783
H	1.45462	4.96567	-0.86988
C	-1.53942	-3.80004	0.20622
H	-1.08967	-4.71481	0.58424
C	-1.84707	1.65669	-0.82132
C	3.54843	-2.53644	0.36442
C	3.37770	-0.13547	1.18860
H	4.05838	-0.33521	2.02189
H	3.94114	0.34857	0.38440
C	-3.37771	-0.13551	-1.18854
H	-4.05841	-0.33528	-2.02181
H	-3.94112	0.34858	-0.38435
C	-0.74142	4.44872	2.82464
H	-1.38141	5.16081	3.33624
C	-0.77366	4.33753	1.43759
H	-1.45457	4.96575	0.86960
C	-2.92334	-3.71780	0.06241
H	-3.54306	-4.57590	0.31195
C	2.92332	-3.71781	-0.06221
H	3.54304	-4.57591	-0.31173
C	5.03874	-2.50732	0.48815
C	5.85344	-1.77478	-0.43838
C	5.65154	-3.22724	1.50494
C	5.31767	-1.04855	-1.53737
C	7.27375	-1.78737	-0.26775
C	7.05110	-3.23708	1.66311
H	5.03167	-3.78686	2.20098
C	6.14231	-0.35675	-2.40272
H	4.24260	-1.04475	-1.69447
C	8.10078	-1.06883	-1.16989
C	7.85603	-2.52348	0.79484
H	7.52057	-3.79715	2.46665
C	7.53965	-0.36190	-2.21910
H	5.71153	0.19373	-3.23486
H	8.19936	0.17782	-2.89202
C	-5.03876	-2.50733	-0.48802
C	-5.85346	-1.77476	0.43848
C	-5.65155	-3.22729	-1.50479
C	-5.31770	-1.04849	1.53745
C	-7.27377	-1.78735	0.26784
C	-7.05111	-3.23713	-1.66297
H	-5.03168	-3.78693	-2.20080
C	-6.14234	-0.35665	2.40276
H	-4.24264	-1.04469	1.69456
C	-8.10081	-1.06877	1.16994
C	-7.85604	-2.52349	-0.79473
H	-7.52057	-3.79723	-2.46650
C	-7.53968	-0.36180	2.21913
H	-5.71158	0.19386	3.23488
H	-8.19940	0.17795	2.89202
C	9.32830	-2.54215	0.98324
C	9.57906	-1.06420	-1.00776
C	-9.32831	-2.54216	-0.98315
C	-9.57909	-1.06414	1.00779
O	-9.87363	-3.15956	-1.88371
O	9.87363	-3.15951	1.88382
O	10.31551	-0.45095	-1.76287
O	-10.31554	-0.45086	1.76288

N	-10.09474	-1.80725	-0.06811
N	10.09472	-1.80727	0.06817
C	11.54771	-1.83551	0.27023
H	12.00388	-1.22552	-0.50725
H	11.79182	-1.44250	1.26118
H	11.91006	-2.86584	0.21352
C	-11.54773	-1.83549	-0.27018
H	-12.00391	-1.22551	0.50729
H	-11.79183	-1.44249	-1.26114
H	-11.91007	-2.86582	-0.21348

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C_{Ni_4} (conf1) Energy: -2635205.1885973

O	-2.85783	-0.76993	-0.13928
O	-1.02743	-1.82049	0.66832
O	2.85783	0.76993	-0.13928
O	1.02743	1.82049	0.66832
C	-2.83067	1.12569	1.78245
H	-3.69474	0.95886	1.14903
C	2.83067	-1.12570	1.78244
H	3.69475	-0.95886	1.14902
C	-0.55176	-0.49569	-3.65256
C	1.73900	-0.25038	1.67587
C	-1.80225	-0.89144	0.71207
C	2.32489	1.62037	-2.39320
C	-1.73899	0.25037	1.67587
C	-2.32489	-1.62038	-2.39319
C	0.60240	-0.44671	2.49147
C	1.71389	-2.36207	3.51209
H	1.68147	-3.18925	4.21659
C	-1.32086	-0.66008	-2.49017
H	-1.13154	-0.00671	-1.64624
C	-2.84270	2.18521	2.69552
C	0.55175	0.49568	-3.65257
C	2.84271	-2.18521	2.69551
C	-0.84323	-1.30325	-4.75972
H	-0.25557	-1.21322	-5.66999
C	2.60783	2.43367	-3.51118
C	1.32085	0.66008	-2.49017
H	1.13154	0.00671	-1.64625
C	-0.60239	0.44670	2.49147
C	0.62135	-1.50785	3.40610
H	-0.25162	-1.67438	4.03164
C	0.84322	1.30325	-4.75972
H	0.25555	1.21322	-5.66998
C	1.80226	0.89143	0.71207
C	-2.60784	-2.43367	-3.51117
C	-3.06580	-1.83449	-1.08488
H	-4.14748	-1.86082	-1.24233
H	-2.75247	-2.78152	-0.63127
C	3.06580	1.83448	-1.08489
H	4.14748	1.86081	-1.24234
H	2.75248	2.78151	-0.63128
C	-1.71388	2.36206	3.51209
H	-1.68146	3.18924	4.21660
C	-0.62134	1.50784	3.40610
H	0.25163	1.67438	4.03164
C	1.86025	2.25362	-4.68392
H	2.07557	2.88316	-5.54422
C	-1.86026	-2.25361	-4.68392
H	-2.07559	-2.88316	-5.54422
C	-3.65671	-3.50157	-3.46680
C	-5.04564	-3.18662	-3.63654
C	-3.28053	-4.82384	-3.27912
C	-5.51805	-1.86446	-3.85963
C	-6.00481	-4.24667	-3.59083
C	-4.23184	-5.86271	-3.23891
H	-2.22661	-5.05985	-3.15504
C	-6.86626	-1.60767	-4.01477
H	-4.79833	-1.05221	-3.91256
C	-7.38456	-3.95866	-3.75408
C	-5.57731	-5.58321	-3.38840
H	-3.92826	-6.89464	-3.08814
C	-7.80614	-2.65660	-3.96049
H	-7.20759	-0.58979	-4.18437
H	-8.86891	-2.46898	-4.08164
C	3.65670	3.50157	-3.46681
C	5.04563	3.18662	-3.63654
C	3.28051	4.82385	-3.27915
C	5.51804	1.86447	-3.85961
C	6.00479	4.24668	-3.59084
C	4.23182	5.86271	-3.23894
H	2.22659	5.05985	-3.15508
C	6.86625	1.60767	-4.01474
H	4.79833	1.05221	-3.91254
C	7.38454	3.95866	-3.75408
C	5.57729	5.58321	-3.38842
H	3.92818	6.89460	-3.08799
C	7.80613	2.65661	-3.96047
H	7.20758	0.58979	-4.18433
H	8.86890	2.46899	-4.08161
C	-6.56356	-6.69155	-3.33894
C	-8.39878	-5.04563	-3.70794
C	6.56354	6.69156	-3.33896
C	8.39876	5.04564	-3.70794
O	6.24380	7.85657	-3.16680
O	-6.24383	-7.85656	-3.16676
O	-9.59200	-4.82895	-3.84150
O	9.59199	4.82897	-3.84148
N	7.91326	6.34809	-3.50096
N	-7.91328	-6.34808	-3.50095
C	-8.87407	-7.45585	-3.44815
H	-9.87019	-7.03958	-3.58633
H	-8.64731	-8.18113	-4.23467
H	-8.79976	-7.96514	-2.48322
C	8.87404	7.45586	-3.44817

H	9.87017	7.03959	-3.58632
H	8.64730	8.18112	-4.23471
H	8.79972	7.96517	-2.48325
C	4.00217	-3.11795	2.74460
C	4.70592	-3.40160	3.96453
C	4.41049	-3.73814	1.56998
C	4.42101	-2.76238	5.20236
C	5.77881	-4.34968	3.93454
C	5.47387	-4.65840	1.54950
H	3.87120	-3.52800	0.65000
C	5.12855	-3.07190	6.34734
H	3.64119	-2.00850	5.24088
C	6.48756	-4.65644	5.12556
C	6.14635	-4.97329	2.71562
H	5.77467	-5.14685	0.62724
C	6.16040	-4.03003	6.31513
H	4.89352	-2.56718	7.28086
C	7.59708	-5.64721	5.11938
C	7.25375	-5.96002	2.67247
H	6.72299	-4.28596	7.20802
O	8.21454	-5.93895	6.13060
N	7.90474	-6.23750	3.88238
O	7.60337	-6.51977	1.64569
C	8.99356	-7.21913	3.82277
H	9.39383	-7.33388	4.82839
H	8.61179	-8.17310	3.44847
H	9.77067	-6.87024	3.13681
C	-4.00216	3.11794	2.74461
C	-4.70590	3.40159	3.96454
C	-4.41048	3.73814	1.56999
C	-4.42099	2.76238	5.20237
C	-5.77879	4.34967	3.93456
C	-5.47386	4.65840	1.54952
H	-3.87119	3.52799	0.65001
C	-5.12853	3.07189	6.34736
H	-3.64118	2.00850	5.24089
C	-6.48754	4.65644	5.12558
C	-6.14633	4.97329	2.71564
H	-5.77466	5.14685	0.62726
C	-6.16038	4.03003	6.31515
H	-4.89350	2.56718	7.28088
C	-7.59706	5.64720	5.11940
C	-7.25374	5.96002	2.67249
H	-6.72297	4.28595	7.20804
O	-8.21451	5.93895	6.13062
N	-7.90472	6.23749	3.88240
O	-7.60336	6.51977	1.64571
C	-8.99354	7.21914	3.82280
H	-9.39381	7.33388	4.82841
H	-8.61177	8.17310	3.44850
H	-9.77066	6.87024	3.13684

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$C_{Br_2BY_2}$ Energy: -5433859.7305435

O	2.60718	1.63600	1.35218
O	2.01021	2.49269	-0.65205
O	-2.60718	1.63601	-1.35218
O	-2.01021	2.49269	0.65205
C	1.32743	3.56305	2.74165
H	2.06518	2.92352	3.21011
C	-1.32744	3.56306	-2.74165
H	-2.06519	2.92353	-3.21011
C	0.74116	-1.87569	0.01394
C	-1.11011	3.46698	-1.35750
C	1.93284	2.50871	0.55598
C	-2.81460	-0.60654	-0.34083
C	1.11011	3.46698	1.35751
C	2.81460	-0.60654	0.34082
C	-0.14223	4.28774	-0.73664
C	0.33789	5.30953	-2.90128
H	0.89508	6.02598	-3.49676
C	1.42526	-0.69926	0.35887
H	0.84753	0.15855	0.68135
C	0.60818	4.47832	3.49921
C	-0.74116	-1.87569	-0.01396
C	-0.60818	4.47833	-3.49920
C	1.50440	-3.00699	-0.30593
H	1.01446	-3.93279	-0.59666
C	-3.57631	-1.74923	-0.00731
C	-1.42526	-0.69926	-0.35888
H	-0.84753	0.15855	-0.68135
C	0.14223	4.28774	0.73665
C	0.55963	5.20360	-1.53113
H	1.30575	5.83979	-1.06261
C	-1.50440	-3.00699	0.30591
H	-1.01446	-3.93280	0.59664
C	-1.93284	2.50871	-0.55598
C	3.57631	-1.74923	0.00730
C	3.49183	0.70706	0.69556
H	4.31102	0.54531	1.40236
H	3.89030	1.19098	-0.20118
C	-3.49183	0.70706	-0.69556
H	-4.31102	0.54532	-1.40236
H	-3.89030	1.19098	0.20118
C	-0.33789	5.30952	2.90129
H	-0.89508	6.02597	3.49677
C	-0.55963	5.20359	1.53114
H	-1.30575	5.83978	1.06262
C	-2.89511	-2.93952	0.29403
H	-3.47680	-3.81931	0.55959
C	2.89511	-2.93952	-0.29405
H	3.47680	-3.81931	-0.55961
C	-5.06770	-1.74642	0.02017
C	-5.79043	-2.65818	-0.76753
C	-5.79139	-0.87539	0.85154

C	-7.18431	-2.69165	-0.73459
H	-5.25038	-3.33899	-1.42132
C	-7.18536	-0.90819	0.88745
H	-5.25841	-0.18474	1.50040
C	-7.89887	-1.81493	0.09245
H	-7.72528	-3.40044	-1.35715
H	-7.72664	-0.23110	1.54405
C	-9.39320	-1.84909	0.12870
C	-10.04356	-2.67724	1.05963
C	-10.12466	-1.05265	-0.76958
N	-11.44143	-2.72184	1.10782
C	-9.54261	-3.57242	2.06541
N	-11.52363	-1.07298	-0.75212
C	-9.71369	-0.13596	-1.79609
B	-12.41539	-1.91950	0.19949
C	-11.81636	-3.58160	2.07343
C	-10.66275	-4.12131	2.68108
C	-8.12480	-3.89868	2.43262
C	-11.98311	-0.23217	-1.69782
C	-10.88564	0.36015	-2.35798
C	-8.33113	0.25620	-2.22792
F	-13.22037	-1.08126	0.97801
F	-13.21510	-2.79571	-0.54186
C	-13.25040	-3.85928	2.38325
H	-10.66250	-4.84167	3.49033
H	-7.56449	-4.31418	1.58756
H	-7.57217	-3.01536	2.77202
H	-8.11339	-4.63583	3.24187
C	-13.44150	-0.02171	-1.93954
H	-10.95669	1.07943	-3.16508
H	-7.75429	0.70020	-1.40865
H	-7.75355	-0.60113	-2.59186
H	-8.39150	0.99125	-3.03691
H	-13.76437	-2.93249	2.66196
H	-13.76236	-4.24498	1.49448
H	-13.33677	-4.58354	3.19739
H	-13.92465	-0.97187	-2.19356
H	-13.92828	0.34204	-1.02766
H	-13.59959	0.69594	-2.74876
C	5.06770	-1.74642	-0.02018
C	5.79043	-2.65818	0.76752
C	5.79139	-0.87539	-0.85155
C	7.18431	-2.69165	0.73458
H	5.25037	-3.33900	1.42131
C	7.18536	-0.90819	-0.88746
H	5.25841	-0.18473	-1.50040
C	7.89887	-1.81493	-0.09246
H	7.72528	-3.40045	1.35714
H	7.72664	-0.23109	-1.54405
C	9.39320	-1.84909	-0.12871
C	10.04357	-2.67724	-1.05963
C	10.12466	-1.05266	0.76958
N	11.44143	-2.72183	-1.10782
C	9.54262	-3.57240	-2.06543
N	11.52363	-1.07298	0.75213
C	9.71368	-0.13597	1.79610
B	12.41539	-1.91950	-0.19949
C	11.81636	-3.58158	-2.07343
C	10.66276	-4.12130	-2.68109
C	8.12481	-3.89867	-2.43264
C	11.98311	-0.23218	1.69784
C	10.88564	0.36014	2.35799
C	8.33113	0.25618	2.22793
F	13.22037	-1.08126	-0.97799
F	13.21510	-2.79571	0.54186
C	13.25041	-3.85927	-2.38326
H	10.66251	-4.84165	-3.49035
H	7.56450	-4.31417	-1.58758
H	7.57217	-3.01534	-2.77203
H	8.11340	-4.63581	-3.24189
C	13.44150	-0.02172	1.93956
H	10.95668	1.07941	3.16509
H	7.75429	0.70020	1.40865
H	7.75355	-0.60114	2.59186
H	8.39149	0.99124	3.03692
H	13.76438	-2.93248	-2.66196
H	13.76236	-4.24497	-1.49448
H	13.33678	-4.58352	-3.19740
H	13.92465	-0.97188	2.19358
H	13.92828	0.34203	1.02768
H	13.59958	0.69593	2.74878
Br	0.92479	4.60503	5.36895
Br	-0.92479	4.60505	-5.36894

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C_{BY_4} Energy: -3547998.6465443

O	-2.88978	-0.51174	0.15369
O	-1.19672	-1.73763	1.01218
O	2.88978	0.51174	0.15369
O	1.19672	1.73763	1.01217
C	-2.71620	1.37324	2.08685
H	-3.58990	1.27157	1.45304
C	2.71620	-1.37324	2.08685
H	3.58991	-1.27157	1.45303
C	-0.59693	-0.43955	-3.35783
C	1.70542	-0.40612	1.98612
C	-1.86950	-0.73093	1.03018
C	2.44036	1.44274	-2.08747
C	-1.70542	0.40612	1.98612
C	-2.44036	-1.44275	-2.08747
C	0.56208	-0.49638	2.81205
C	1.51179	-2.49756	3.83011
H	1.40965	-3.31585	4.53863
C	-1.34816	-0.58381	-2.18063
H	-1.08425	0.02113	-1.32160
C	-2.64278	2.43065	3.00069

C	0.59693	0.43955	-3.35783
C	2.64279	-2.43066	3.00069
C	-1.01016	-1.15573	-4.48976
H	-0.44589	-1.08737	-5.41638
C	2.84426	2.16852	-3.23098
C	1.34815	0.58380	-2.18064
H	1.08425	-0.02114	-1.32160
C	-0.56208	0.49638	2.81205
C	0.49897	-1.54977	3.73319
H	-0.37777	-1.63465	4.36985
C	1.01016	1.15573	-4.48976
H	0.44589	1.08737	-5.41638
C	1.86950	0.73093	1.03018
C	-2.84426	-2.16853	-3.23098
C	-3.18975	-1.57388	-0.77155
H	-4.27069	-1.51819	-0.93142
H	-2.95401	-2.52610	-0.28684
C	3.18975	1.57388	-0.77155
H	4.27069	1.51819	-0.93142
H	2.95401	2.52610	-0.28685
C	-1.51178	2.49756	3.83011
H	-1.40964	3.31585	4.53862
C	-0.49897	1.54977	3.73319
H	0.37777	1.63464	4.36984
C	2.12157	1.99170	-4.42201
H	2.42308	2.55473	-5.30235
C	-2.12158	-1.99170	-4.42200
H	-2.42309	-2.55474	-5.30235
C	4.01173	3.09681	-3.22918
C	5.06047	2.91448	-4.14637
C	4.08502	4.19363	-2.35437
C	6.14687	3.78830	-4.18166
H	5.02632	2.06961	-4.83021
C	5.16968	5.06987	-2.38892
H	3.27075	4.38214	-1.65909
C	6.21532	4.87617	-3.30127
H	6.95159	3.62559	-4.89481
H	5.20331	5.91774	-1.70881
C	7.37919	5.81407	-3.33703
C	7.32586	6.95120	-4.16118
C	8.50920	5.54360	-2.54554
N	8.40553	7.84038	-4.20647
C	6.31327	7.44728	-5.05155
N	9.60846	6.40896	-2.56657
C	8.81137	4.47542	-1.63427
B	9.73351	7.71037	-3.40823
C	8.11256	8.83745	-5.06206
C	6.82556	8.61918	-5.59835
C	4.96390	6.87657	-5.37549
C	10.55185	5.93508	-1.73118
C	10.08510	4.74095	-1.14185
C	7.97884	3.28951	-1.24401
F	9.89954	8.81469	-2.56591
F	10.81681	7.61320	-4.28772
C	9.06086	9.95700	-5.33925
H	6.33063	9.26338	-6.31518
H	5.03270	5.86697	-5.79583
H	4.32204	6.80519	-4.49017
H	4.45941	7.51475	-6.10802
C	11.85684	6.63021	-1.52286
H	10.63560	4.14088	-0.42722
H	7.02438	3.58627	-0.79448
H	7.73839	2.65316	-2.10325
H	8.52244	2.68103	-0.51411
H	9.30261	10.48747	-4.41138
H	10.00650	9.56473	-5.72998
H	8.63123	10.65826	-6.05929
H	12.39143	6.72620	-2.47457
H	11.68935	7.64868	-1.15481
H	12.47740	6.08181	-0.80941
C	-4.01174	-3.09682	-3.22918
C	-5.06048	-2.91448	-4.14637
C	-4.08503	-4.19363	-2.35437
C	-6.14687	-3.78830	-4.18166
H	-5.02632	-2.06961	-4.83022
C	-5.16969	-5.06987	-2.38892
H	-3.27076	-4.38214	-1.65909
C	-6.21533	-4.87617	-3.30126
H	-6.95159	-3.62560	-4.89481
H	-5.20332	-5.91774	-1.70880
C	-7.37920	-5.81407	-3.33703
C	-7.32587	-6.95120	-4.16117
C	-8.50921	-5.54360	-2.54554
N	-8.40554	-7.84038	-4.20647
C	-6.31328	-7.44728	-5.05154
N	-9.60847	-6.40896	-2.56657
C	-8.81138	-4.47541	-1.63428
B	-9.73352	-7.71037	-3.40823
C	-8.11257	-8.83746	-5.06205
C	-6.82557	-8.61919	-5.59834
C	-4.96391	-6.87658	-5.37548
C	-10.55186	-5.93507	-1.73118
C	-10.08511	-4.74094	-1.14186
C	-7.97885	-3.28950	-1.24402
F	-9.89955	-8.81469	-2.56591
F	-10.81681	-7.61319	-4.28773
C	-9.06087	-9.95700	-5.33924
H	-6.33063	-9.26339	-6.31517
H	-5.03270	-5.86697	-5.79582
H	-4.32204	-6.80519	-4.49016
H	-4.45941	-7.51476	-6.10801
C	-11.85685	-6.63020	-1.52287
H	-10.63561	-4.14087	-0.42723
H	-7.02439	-3.58627	-0.79448
H	-7.73840	-2.65315	-2.10326
H	-8.52245	-2.68103	-0.51412

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180

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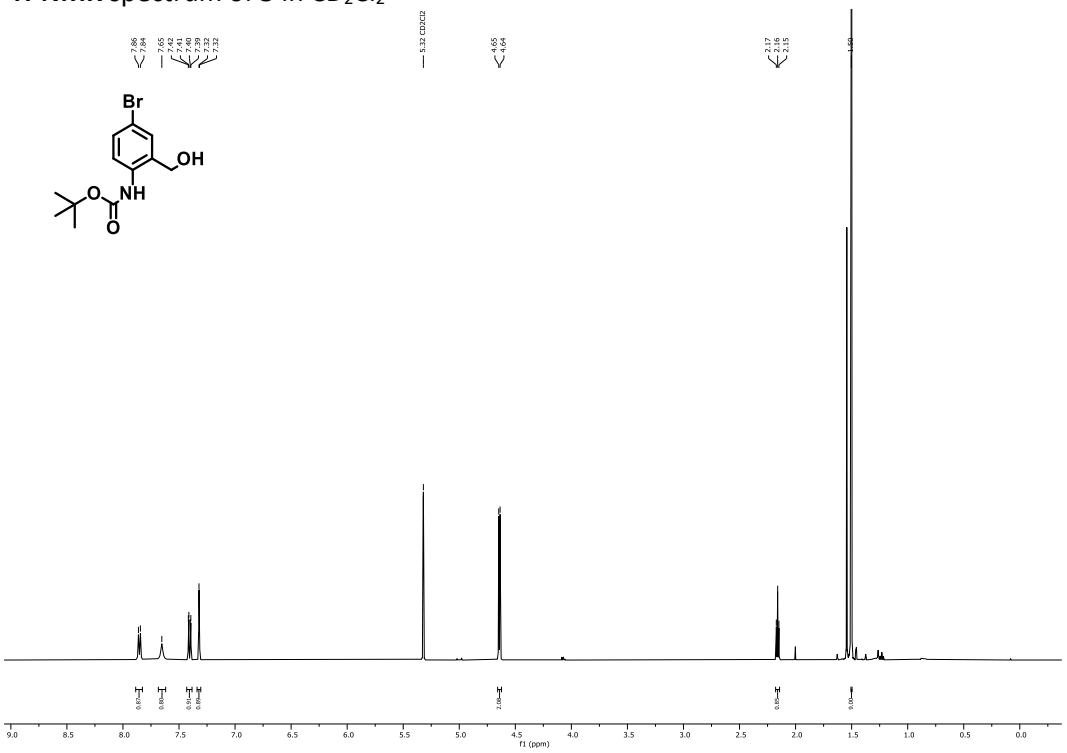
[1] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, **n.d.**

[2] G. Pescitelli, T. Bruhn, *Chirality* **2016**, *28*, 466–474.

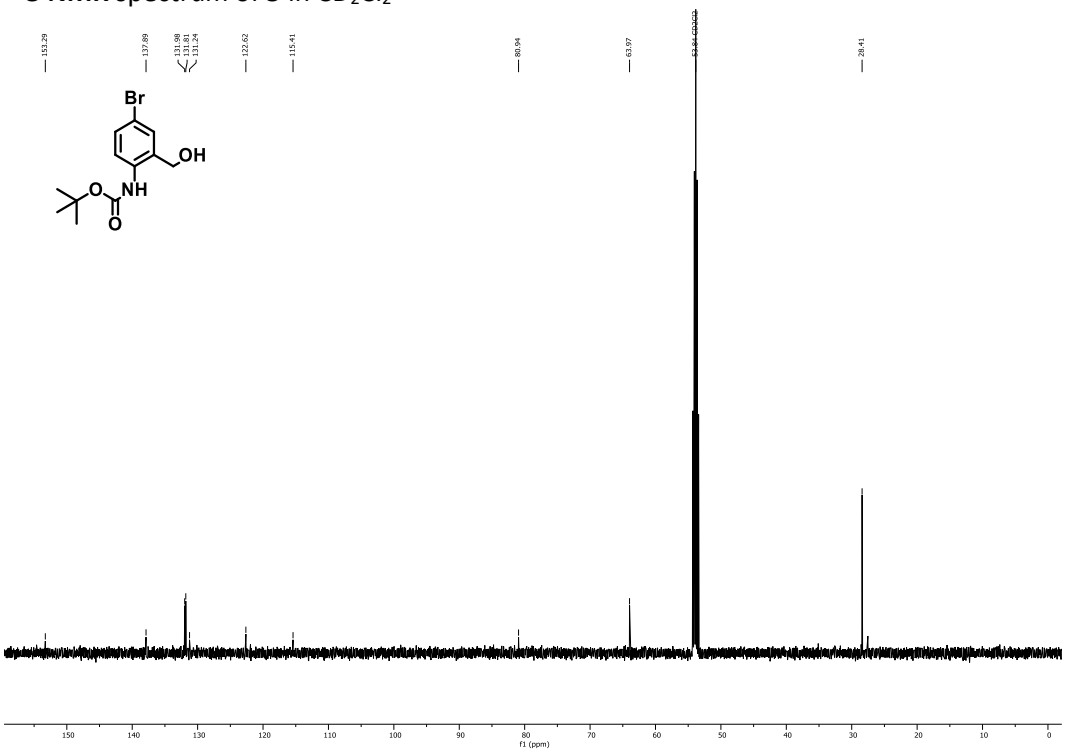
[3] T. Bruhn, A. Schaumlöffel, Y. Hemberger, G. Bringmann, *Chirality* **2013**, *25*, 243–249.

NMR, IR and HR-ESI-MS spectra

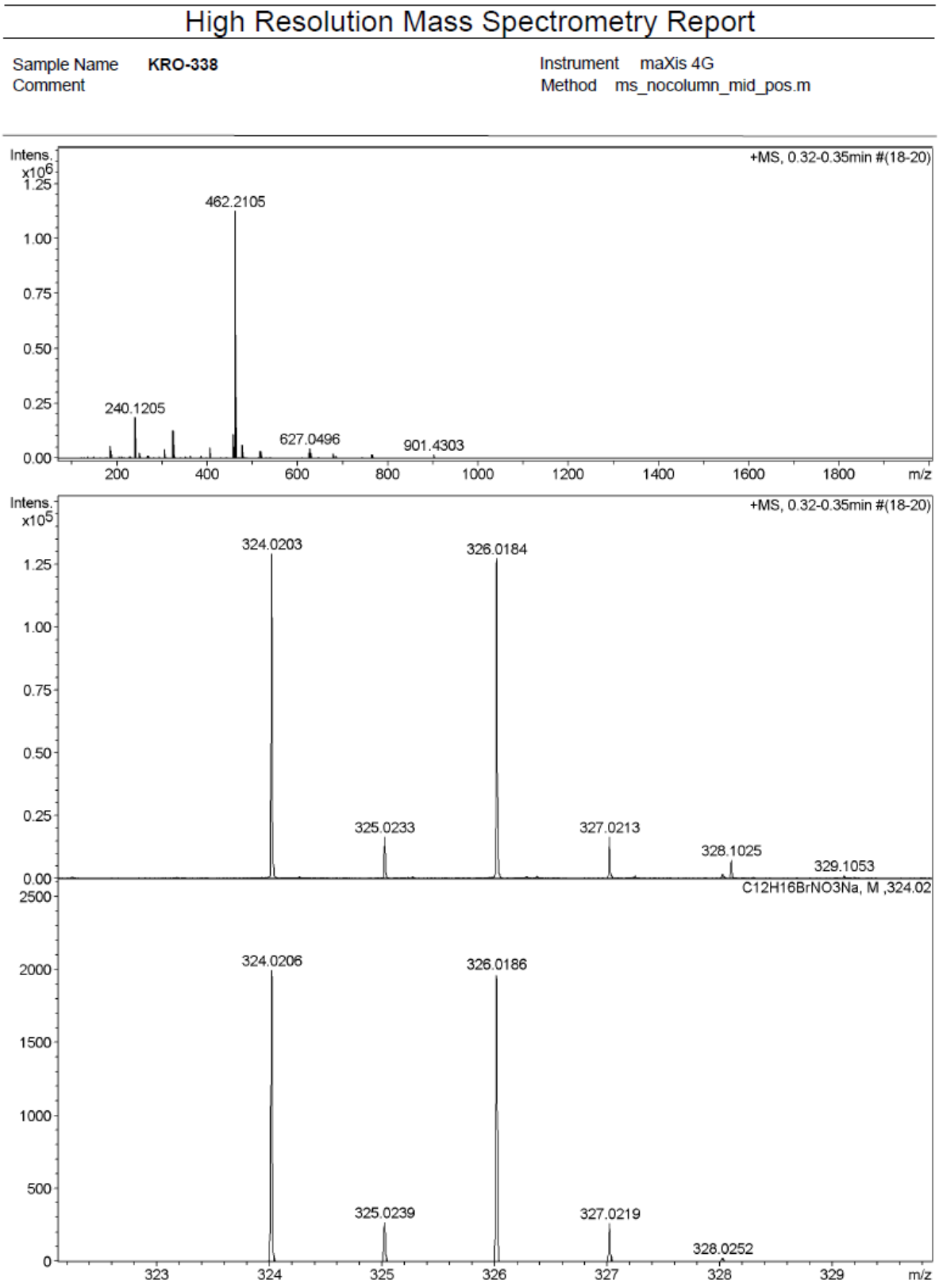
^{1}H-NMR spectrum of **5** in CD_2Cl_2



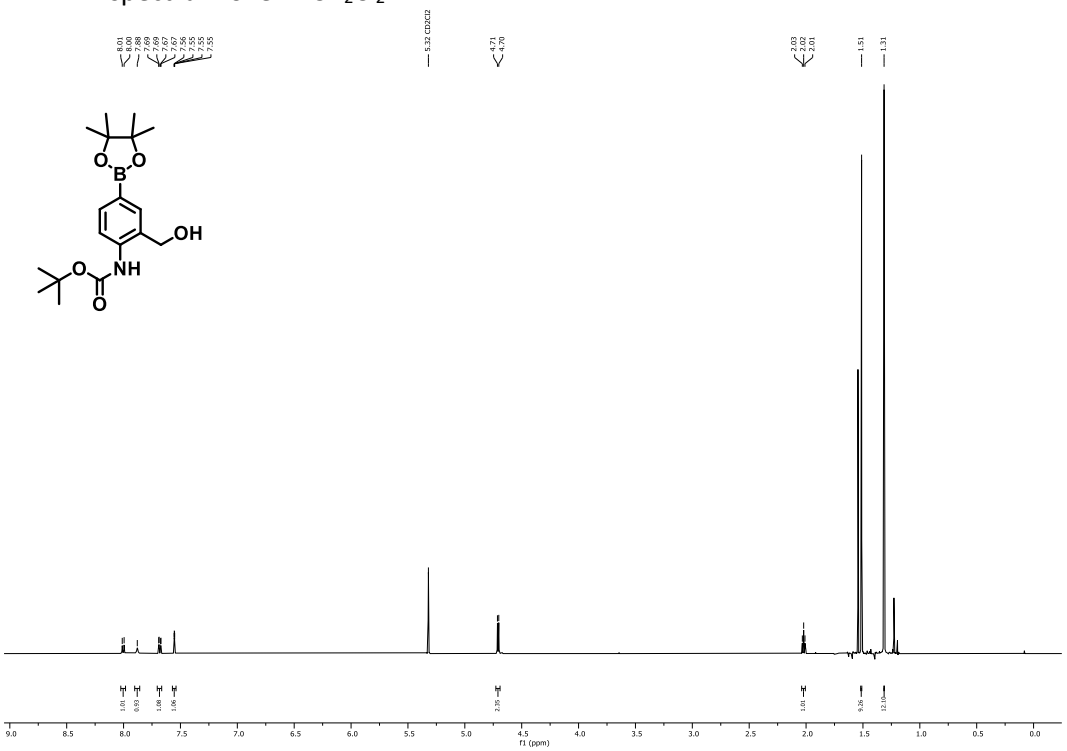
^{13}C-NMR spectrum of **5** in CD_2Cl_2



HR-ESI-MS spectrum of **5**



^{1}H-NMR spectrum of **3** in CD_2Cl_2



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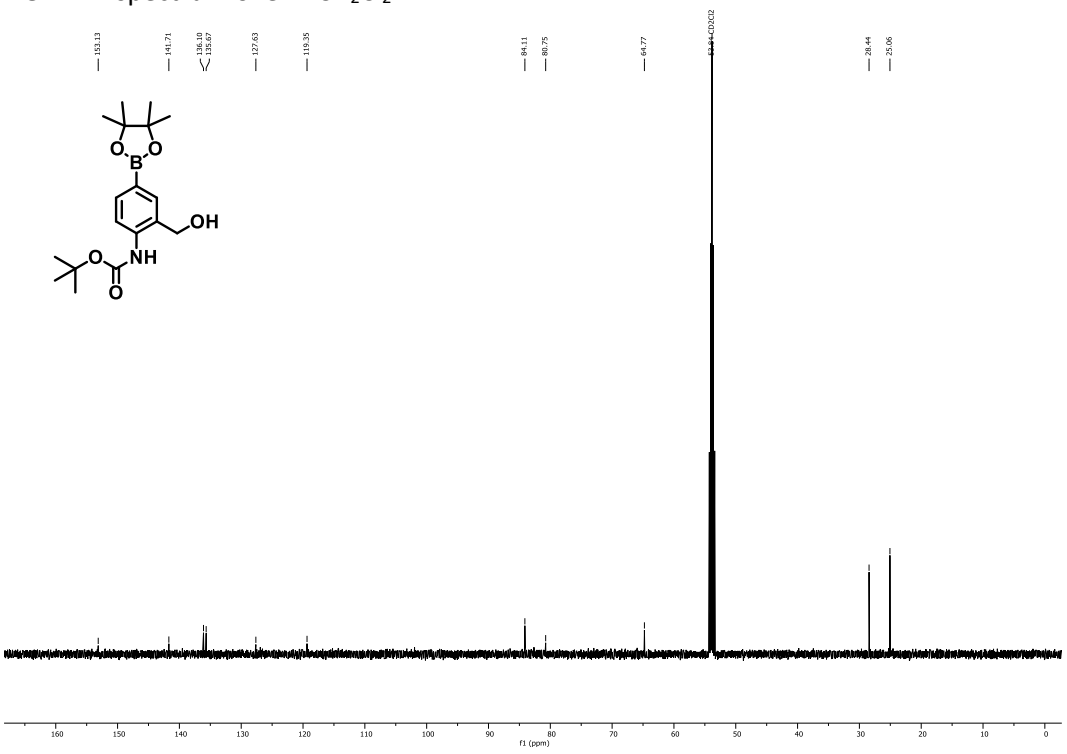
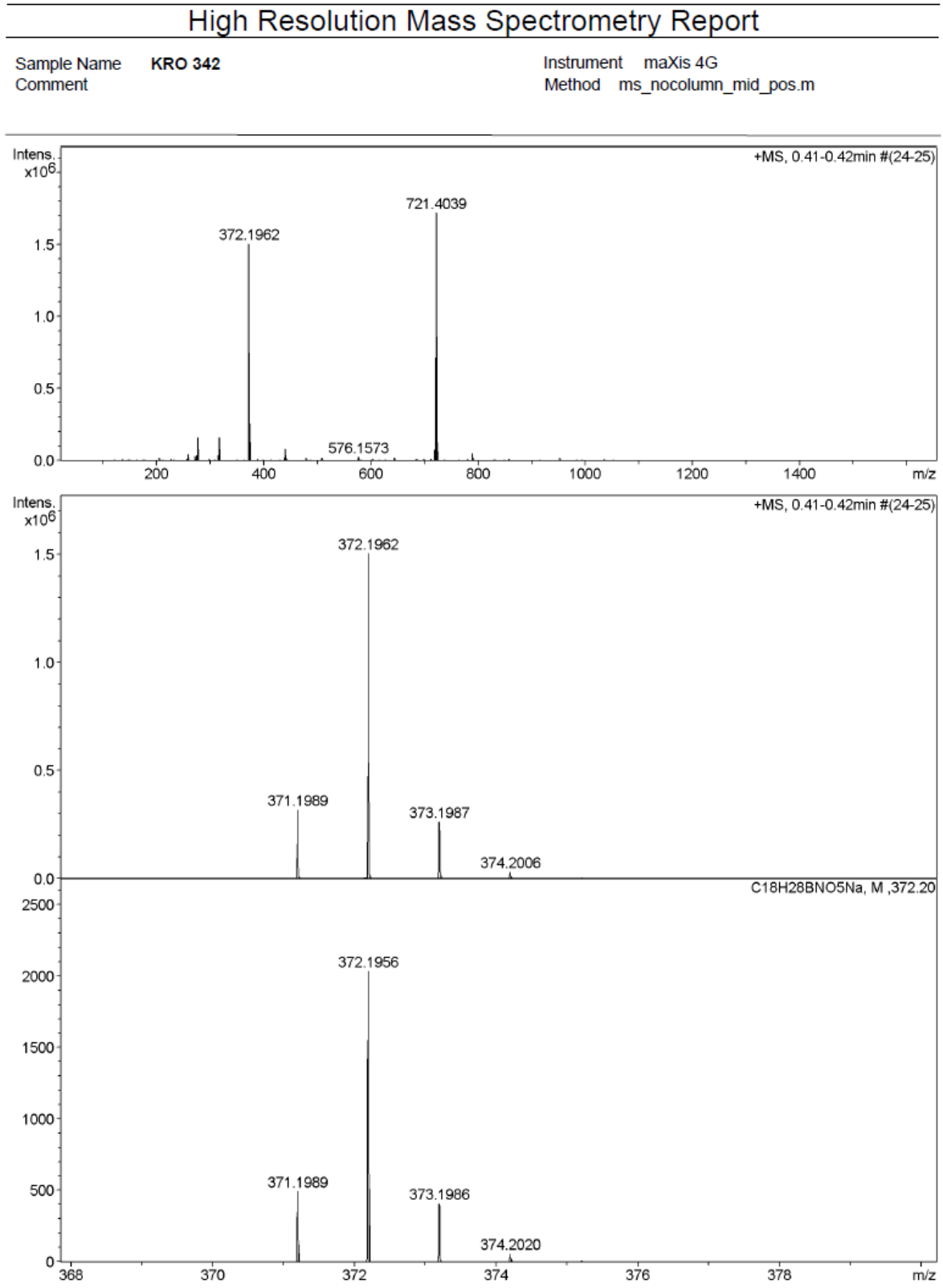
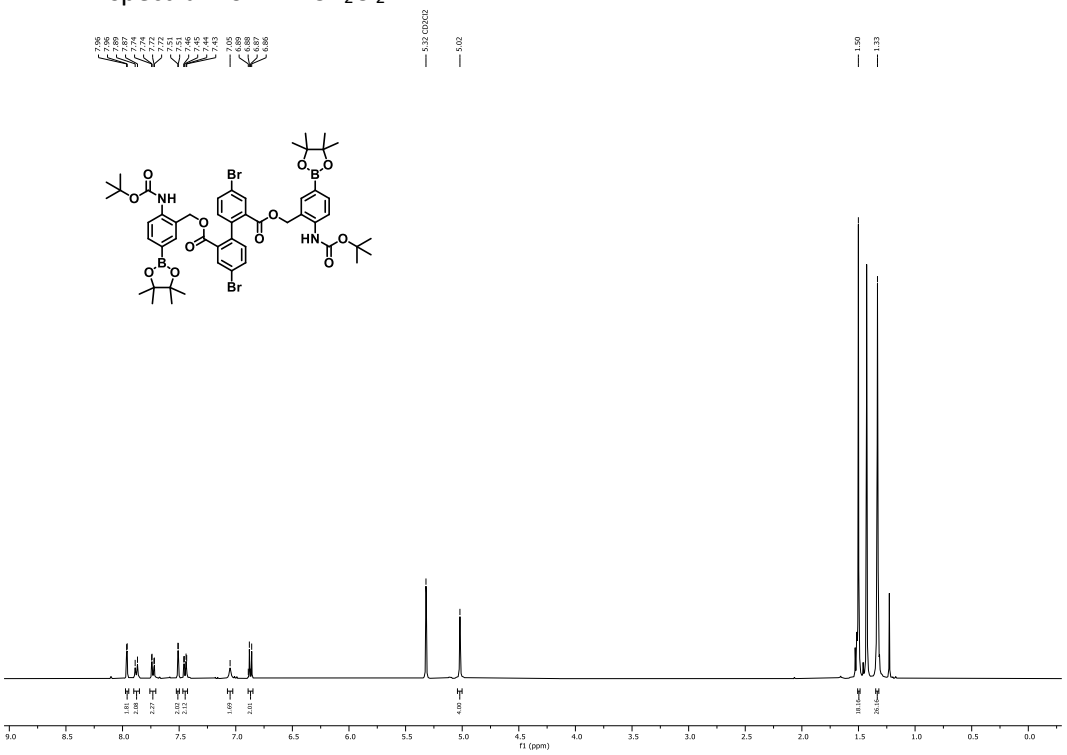


HR-ESI-MS spectrum of 3



^{1}H-NMR spectrum of **1** in CD_2Cl_2



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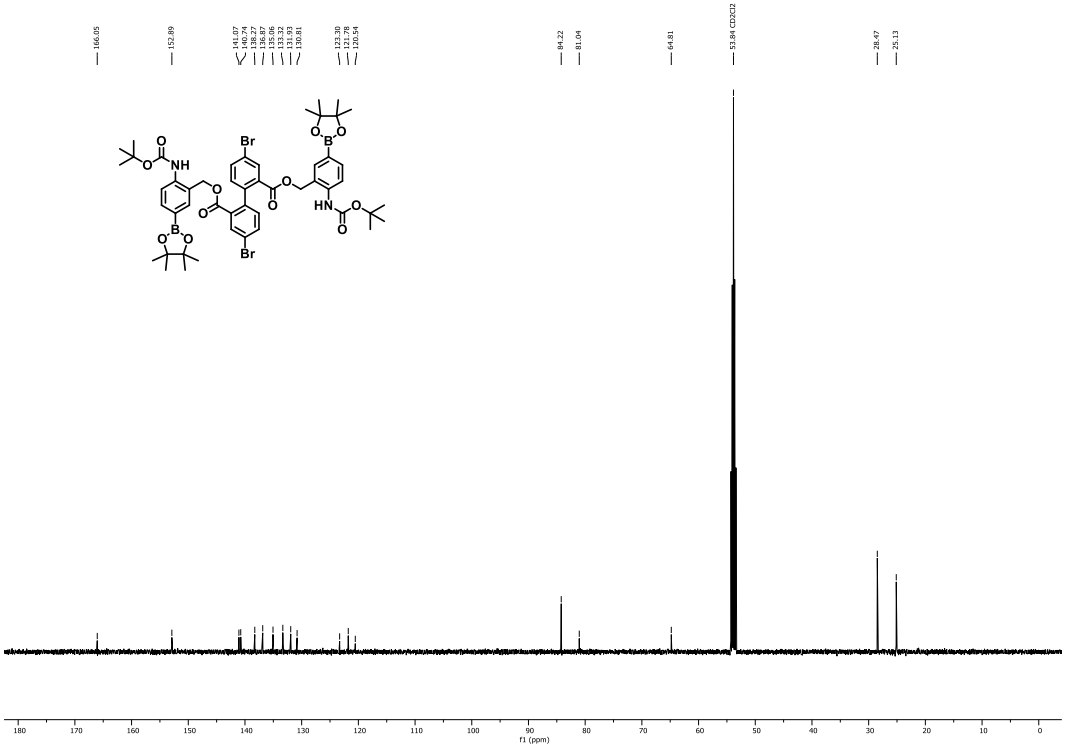

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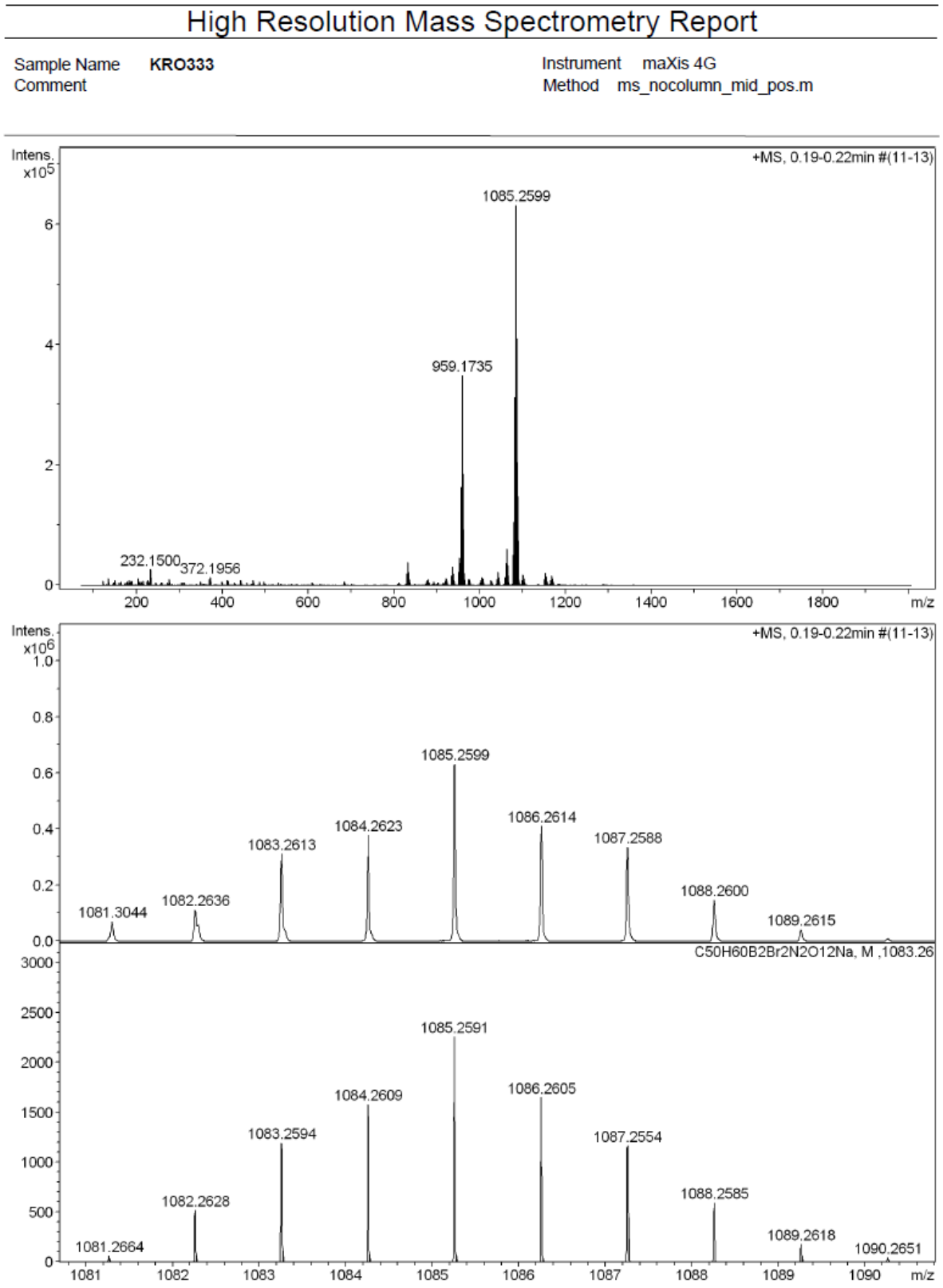
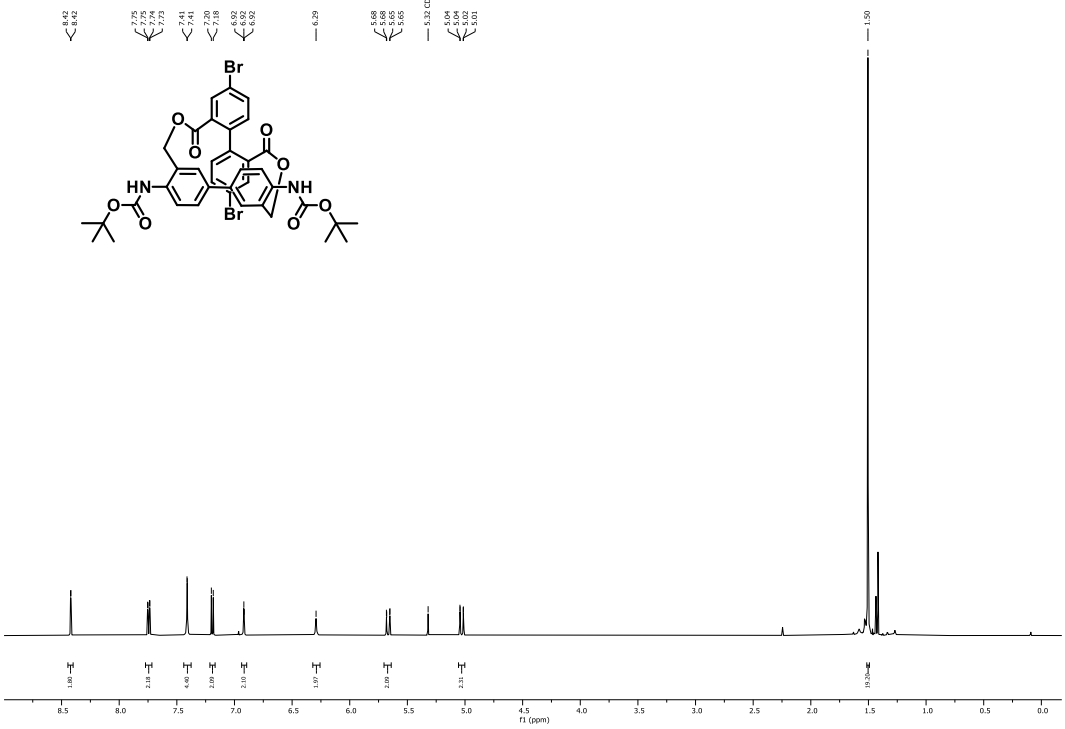


^{1}H-NMR spectrum of **$C_{Br2Boc2}$** in CD_2Cl_2



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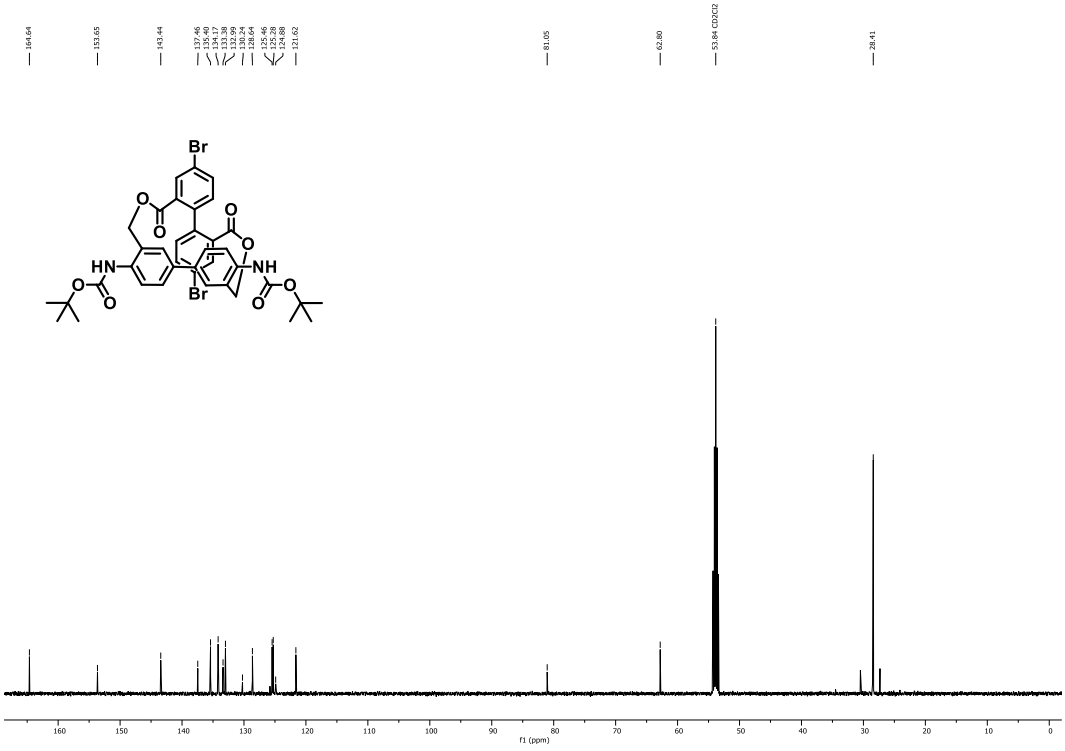
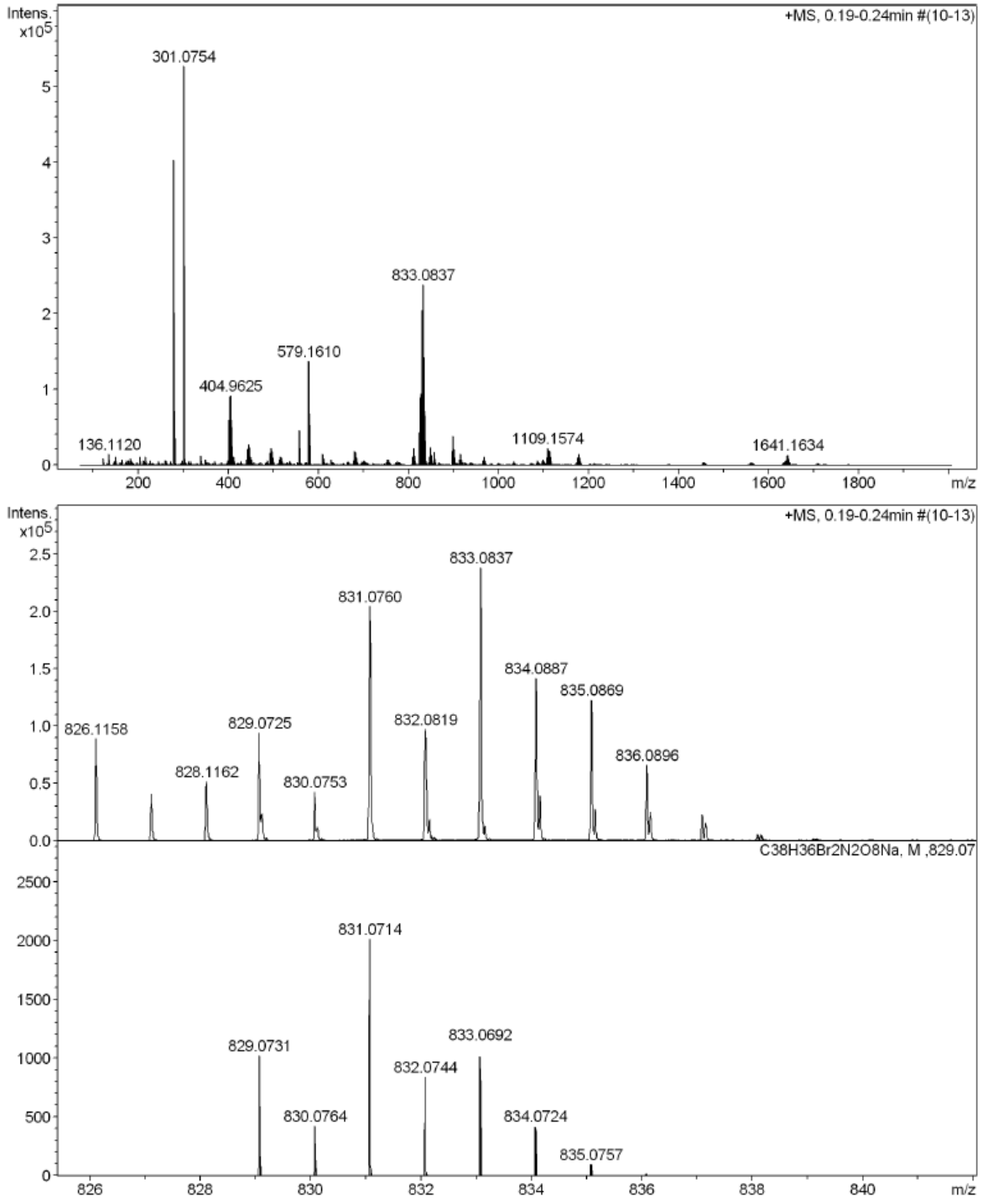


HR-ESI-MS spectrum of $C_{Br2Boc2}$

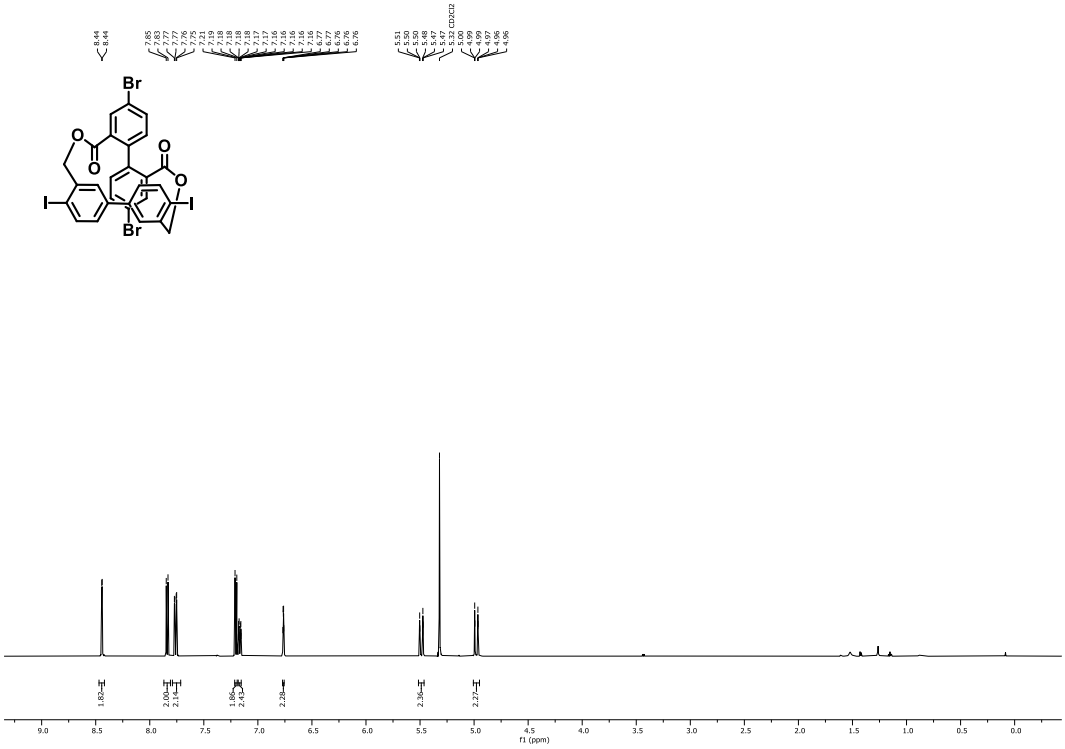
High Resolution Mass Spectrometry Report

Sample Name **KRO335**
Comment

Instrument maXis 4G
Method ms_nocolumn_mid_pos.m



[1]H-NMR spectrum of **C_{Br2I2}** in CD_2Cl_2



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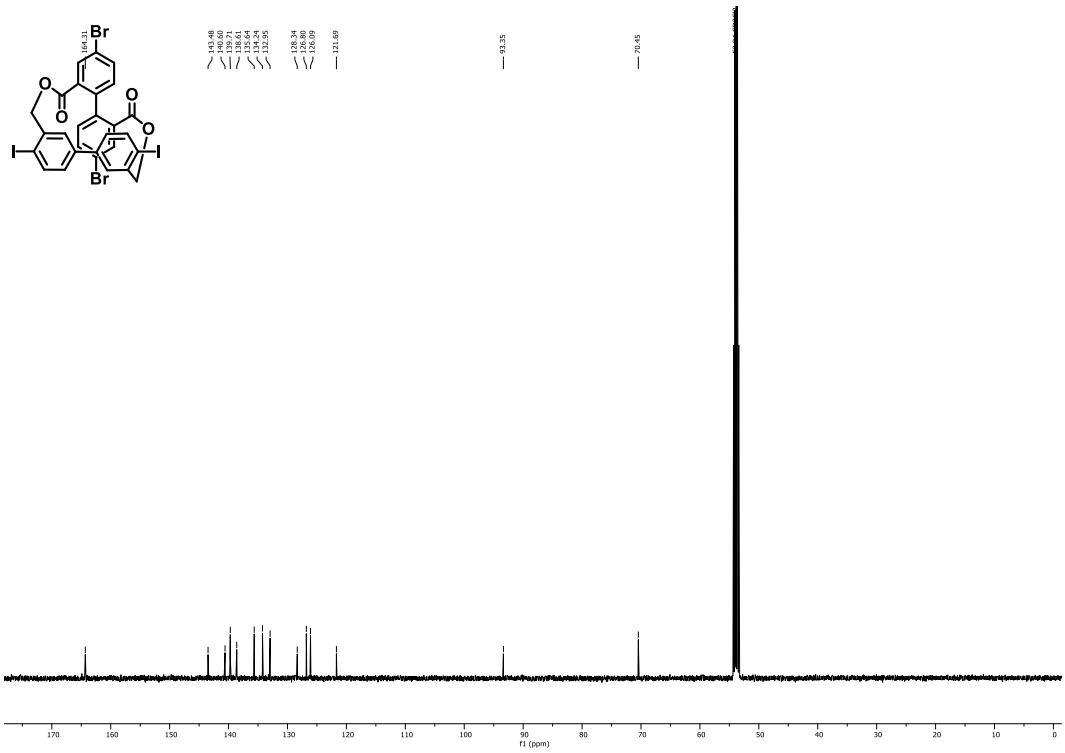
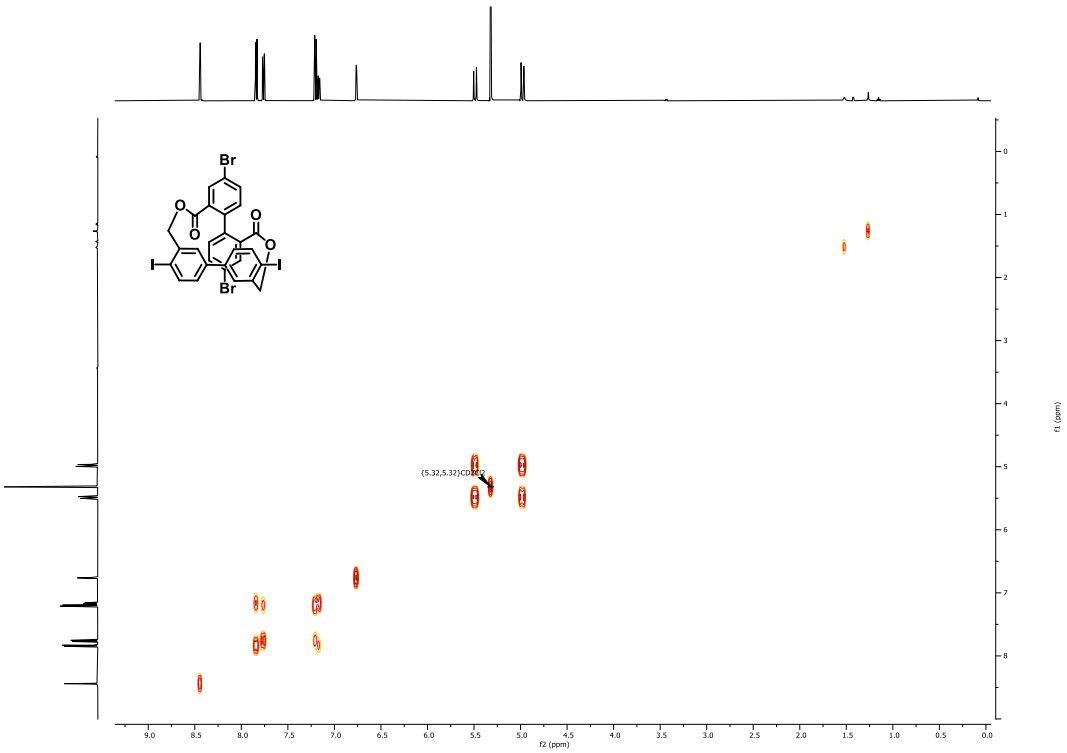
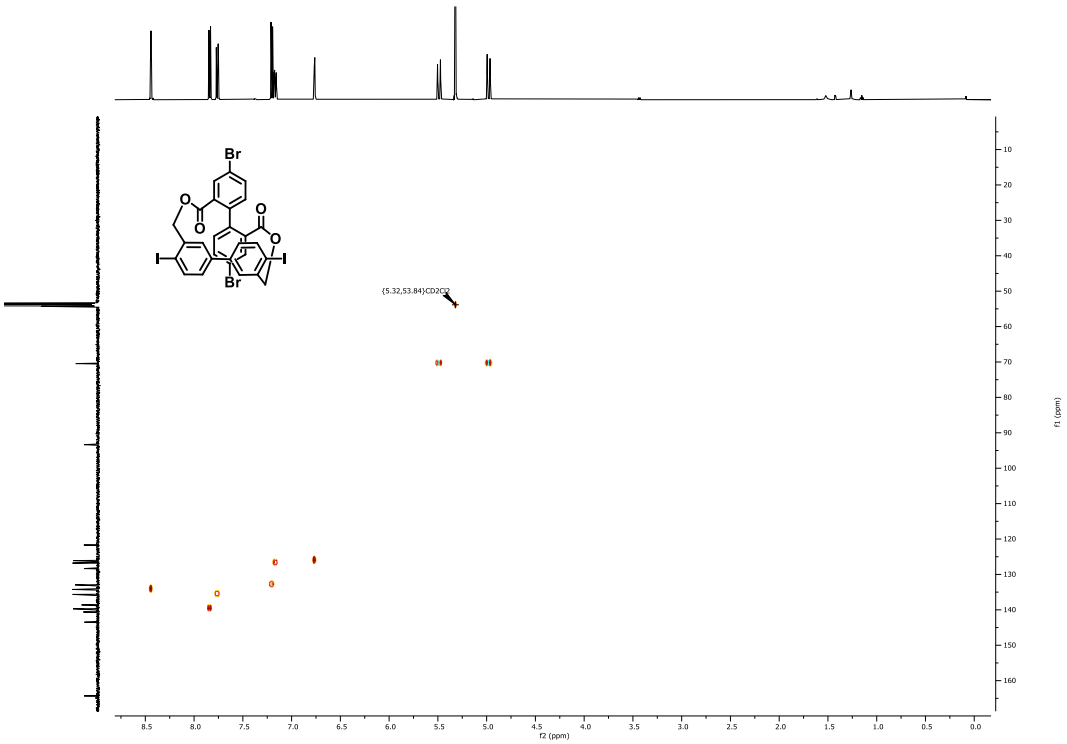


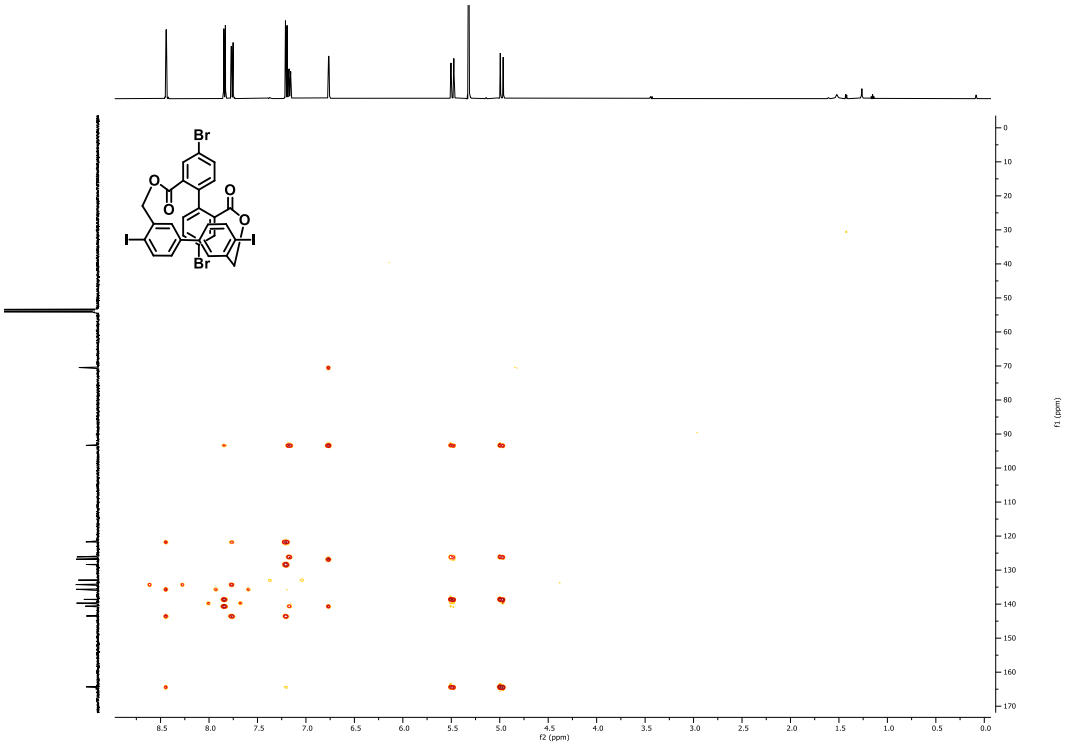
COSY spectrum of $\mathbf{C_{Br2I2}}$ in CD_2Cl_2



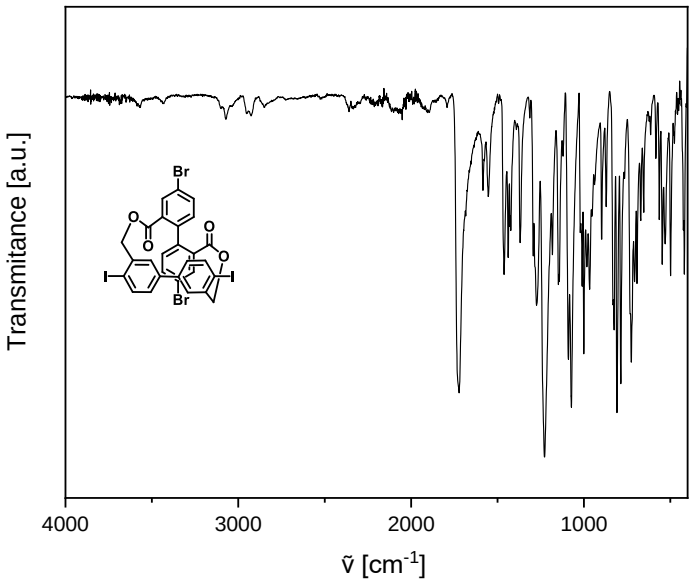
HMQC spectrum of $\mathbf{C_{Br2I2}}$ in CD_2Cl_2



HMBC spectrum of $\mathbf{C_{Br2I2}}$ in CD_2Cl_2



FT-IR spectrum of $\mathbf{C_{Br2I2}}$ (neat)

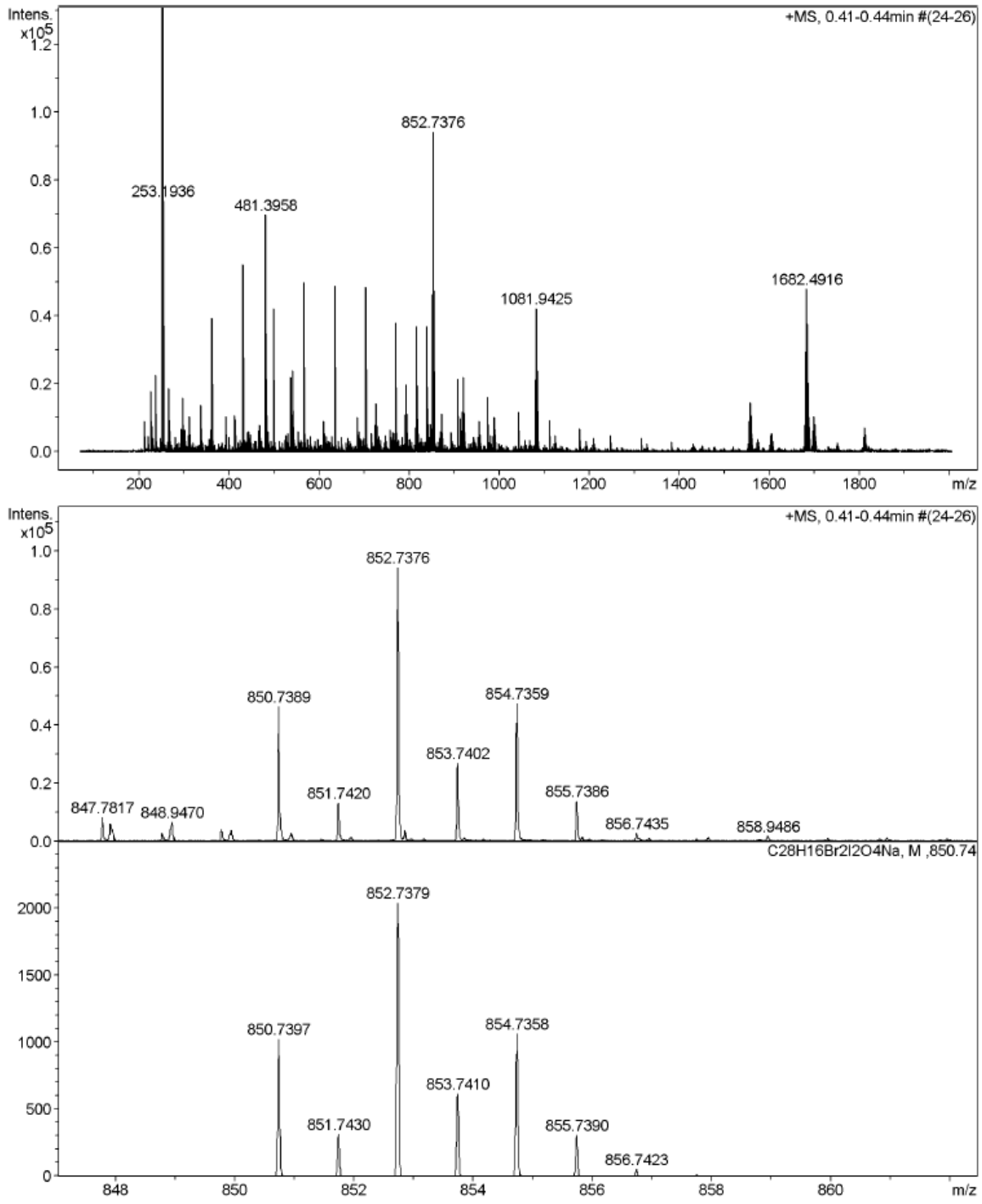


HR-ESI-MS spectrum of $\mathbf{C_{Br2I2}}$

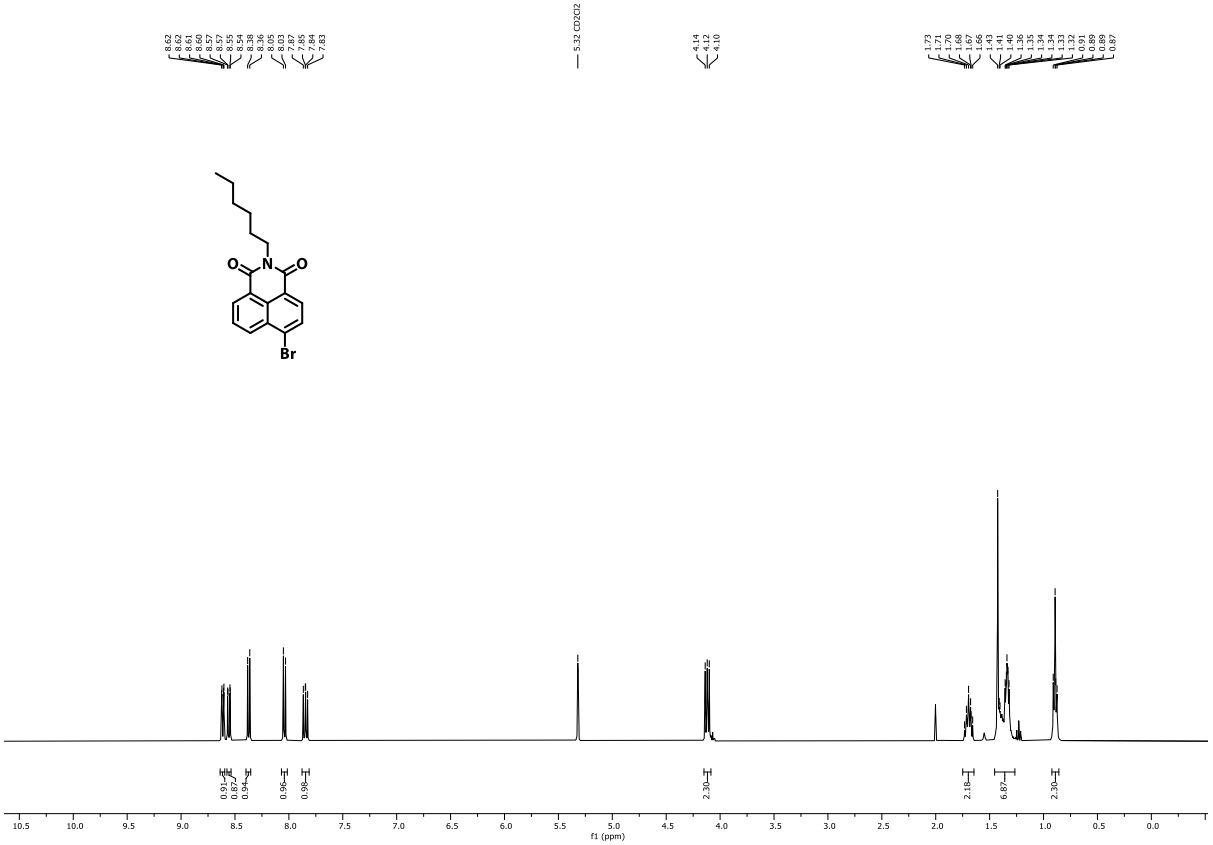
High Resolution Mass Spectrometry Report

Sample Name **KRO337**
Comment

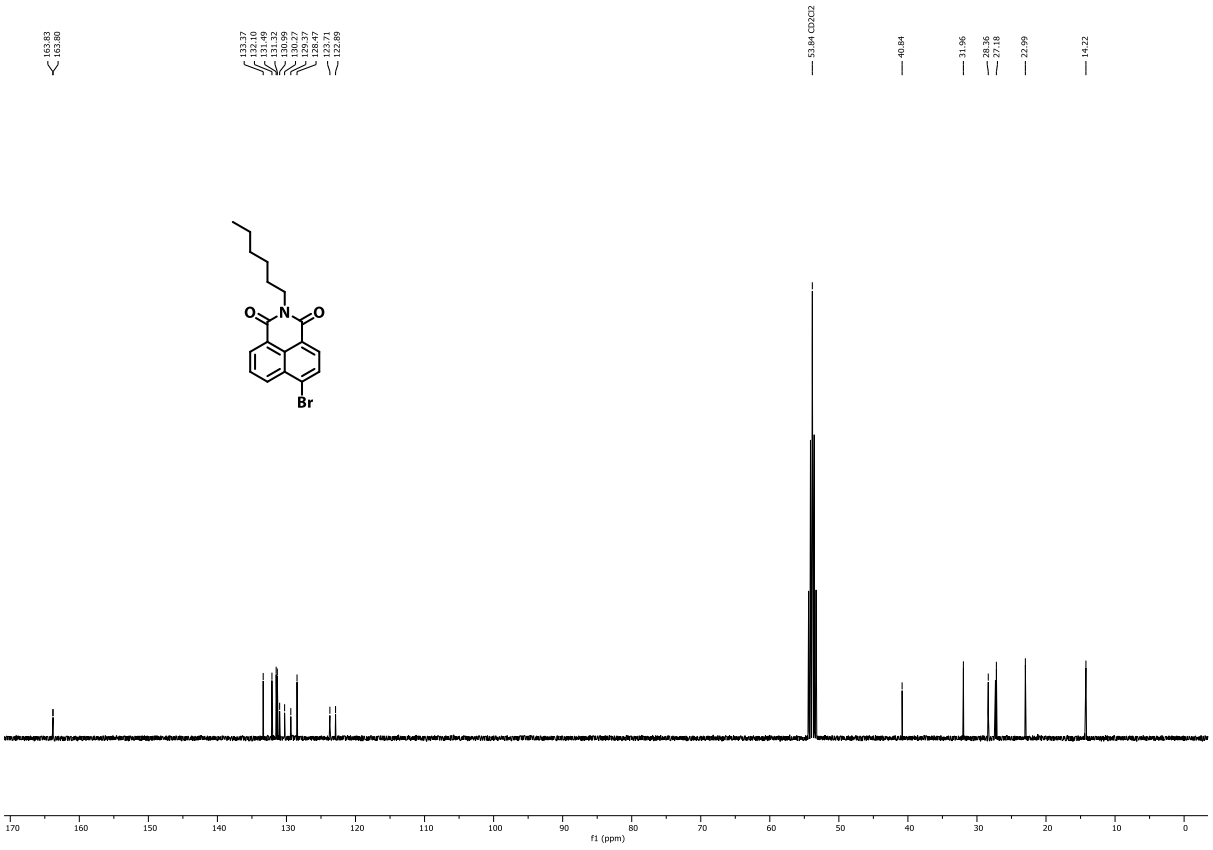
Instrument maXis 4G
Method ms_nocolumn_higher_pos.m



^{1}H-NMR spectrum of **NI-Br** in CD_2Cl_2



^{13}C-NMR spectrum of **NI-Br** in CD_2Cl_2

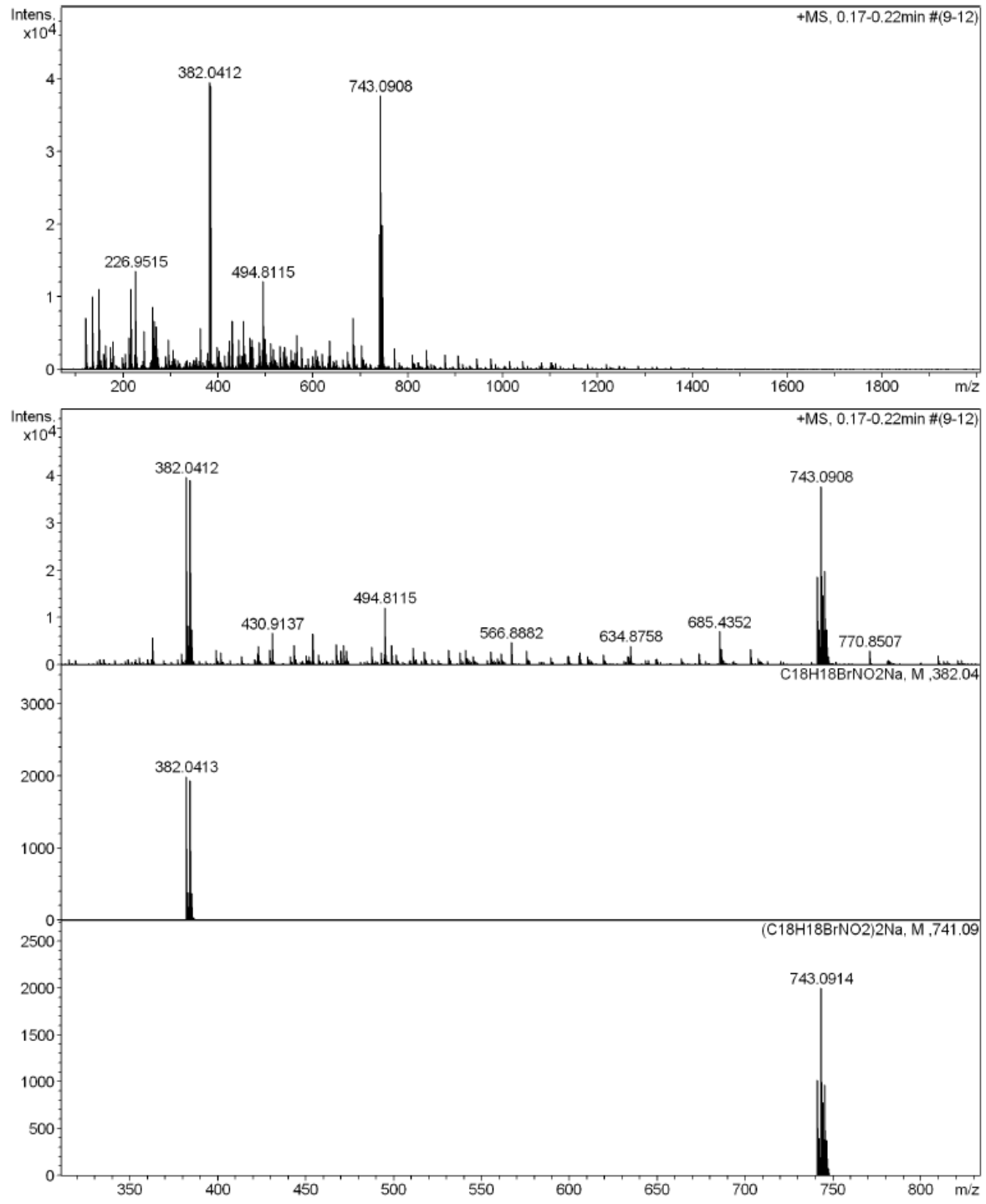


HR-ESI-MS spectrum of **NI-Br**

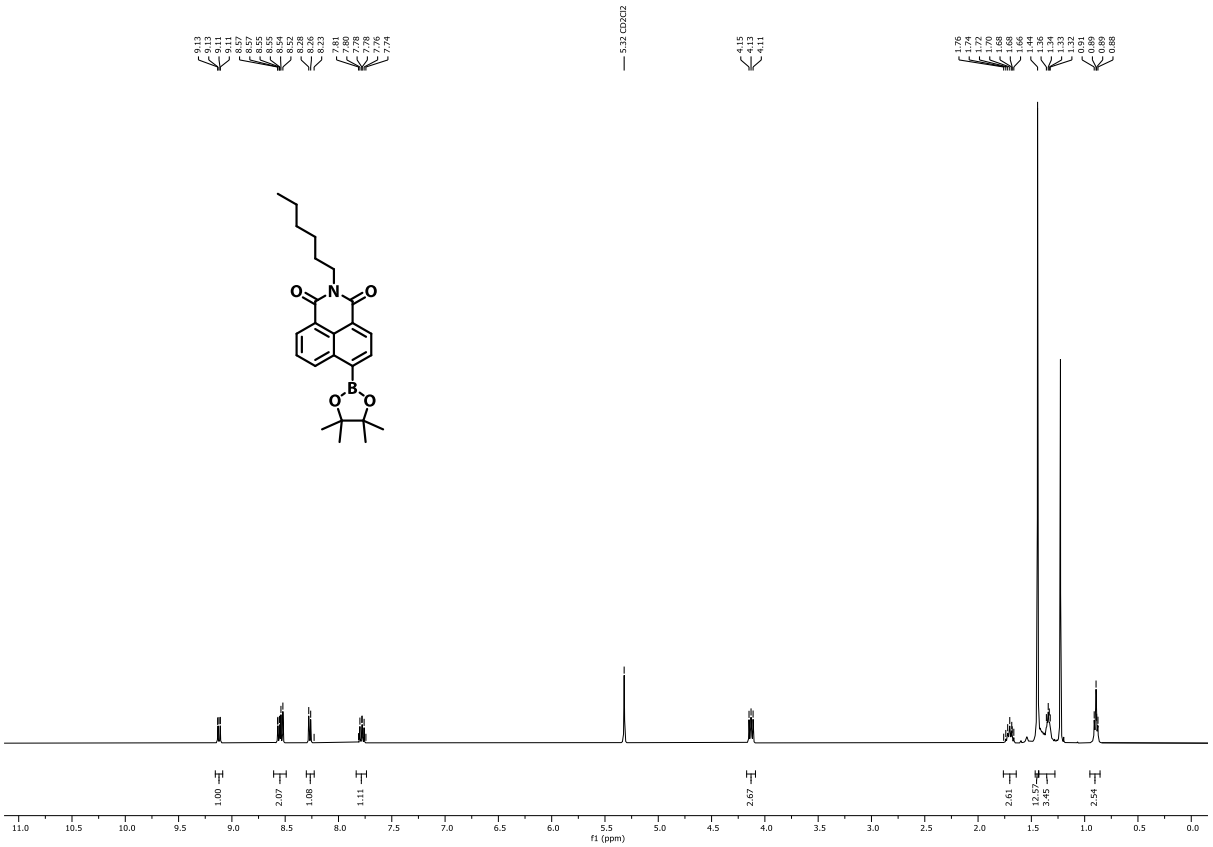
High Resolution Mass Spectrometry Report

Sample Name **KRO472**
Comment

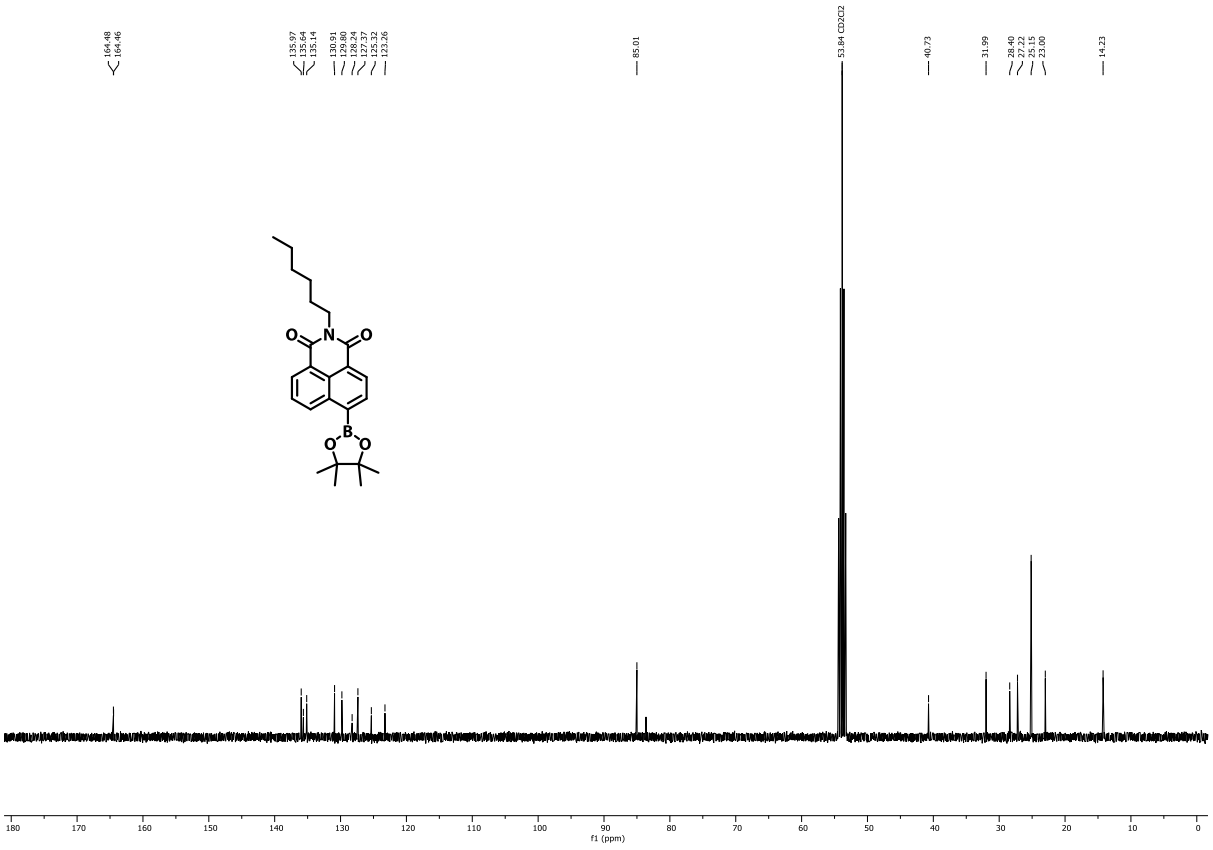
Instrument maXis 4G
Method ms_nocolumn_mid_pos.m



^{1}H-NMR spectrum of **NI-BPin** in CD_2Cl_2



^{13}C-NMR spectrum of **NI-BPin** in CD_2Cl_2

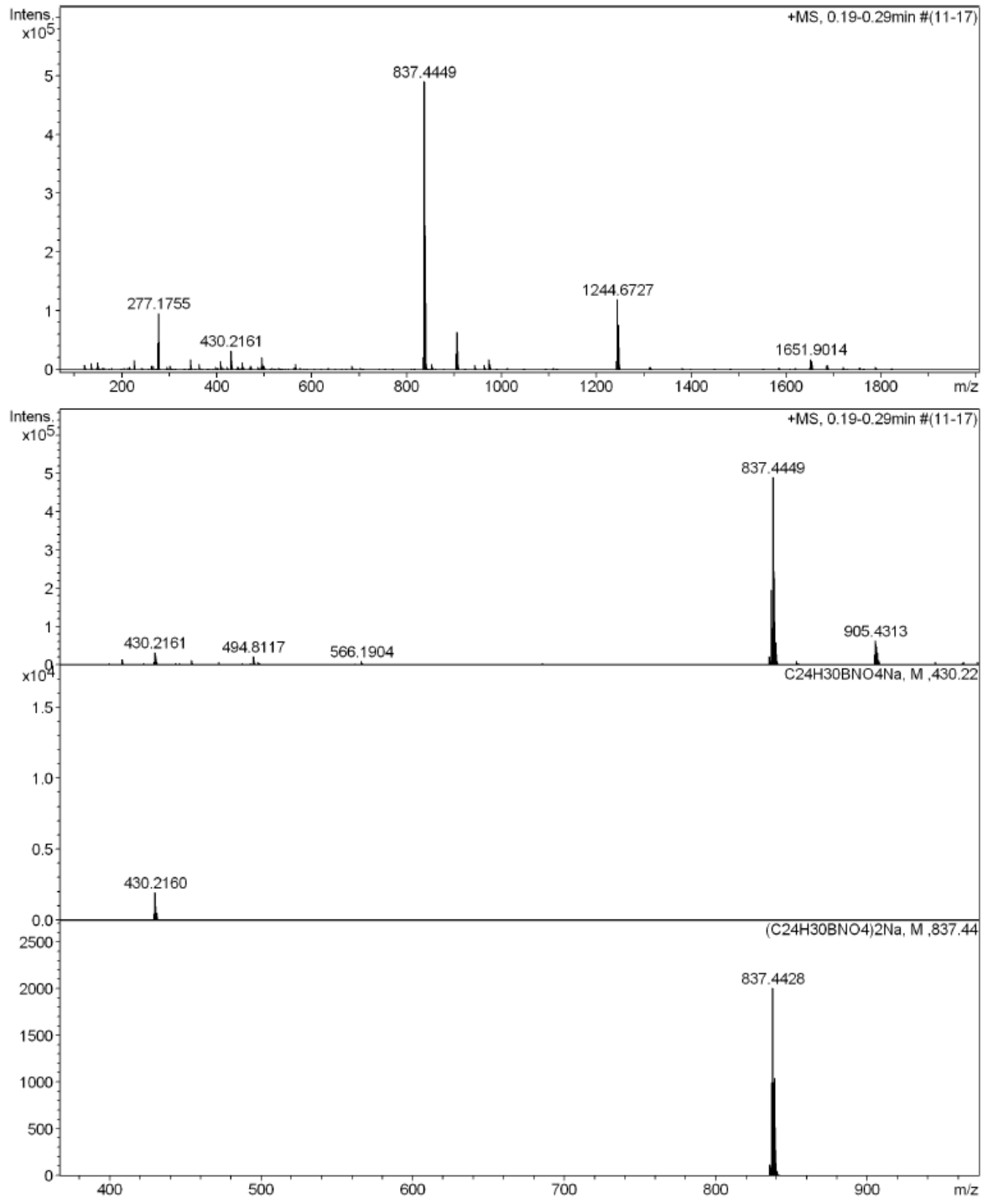


HR-ESI-MS spectrum of **NI-BPIN**

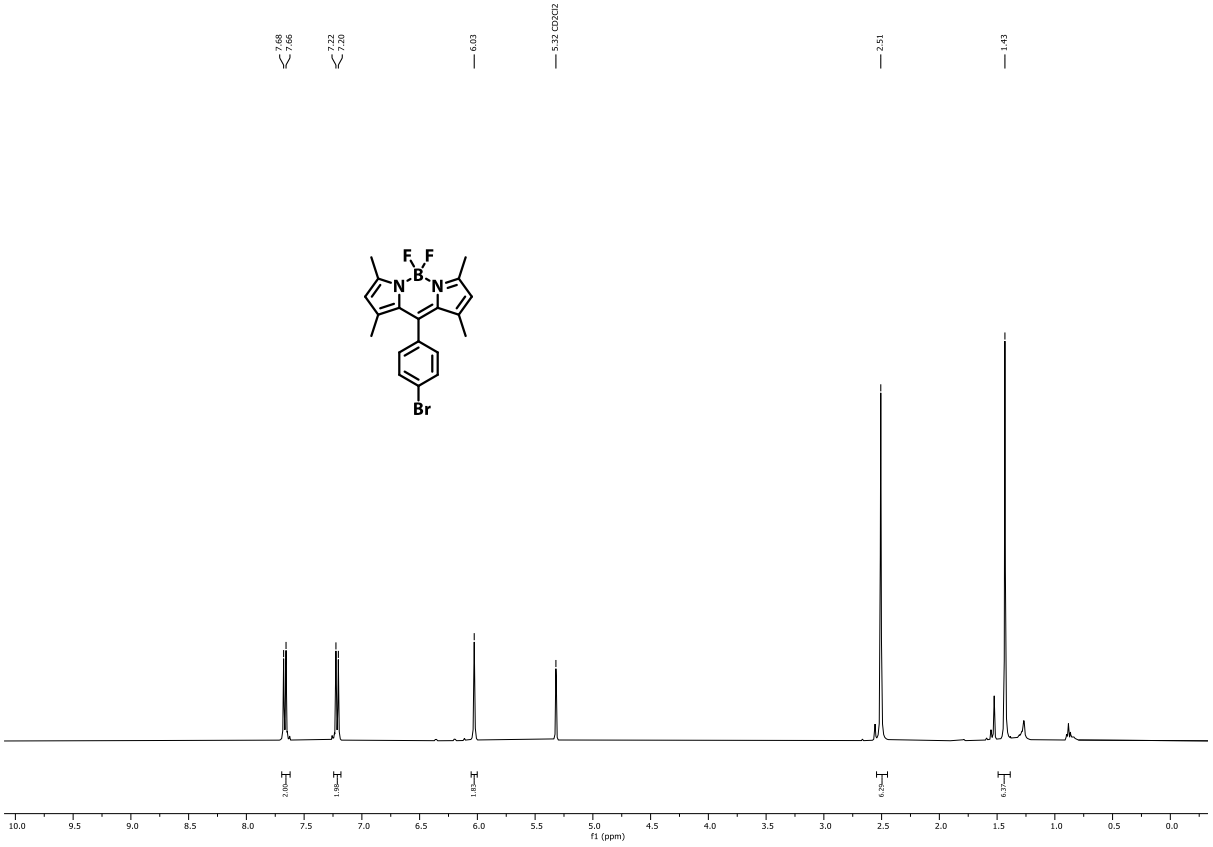
High Resolution Mass Spectrometry Report

Sample Name **KRO475**
Comment

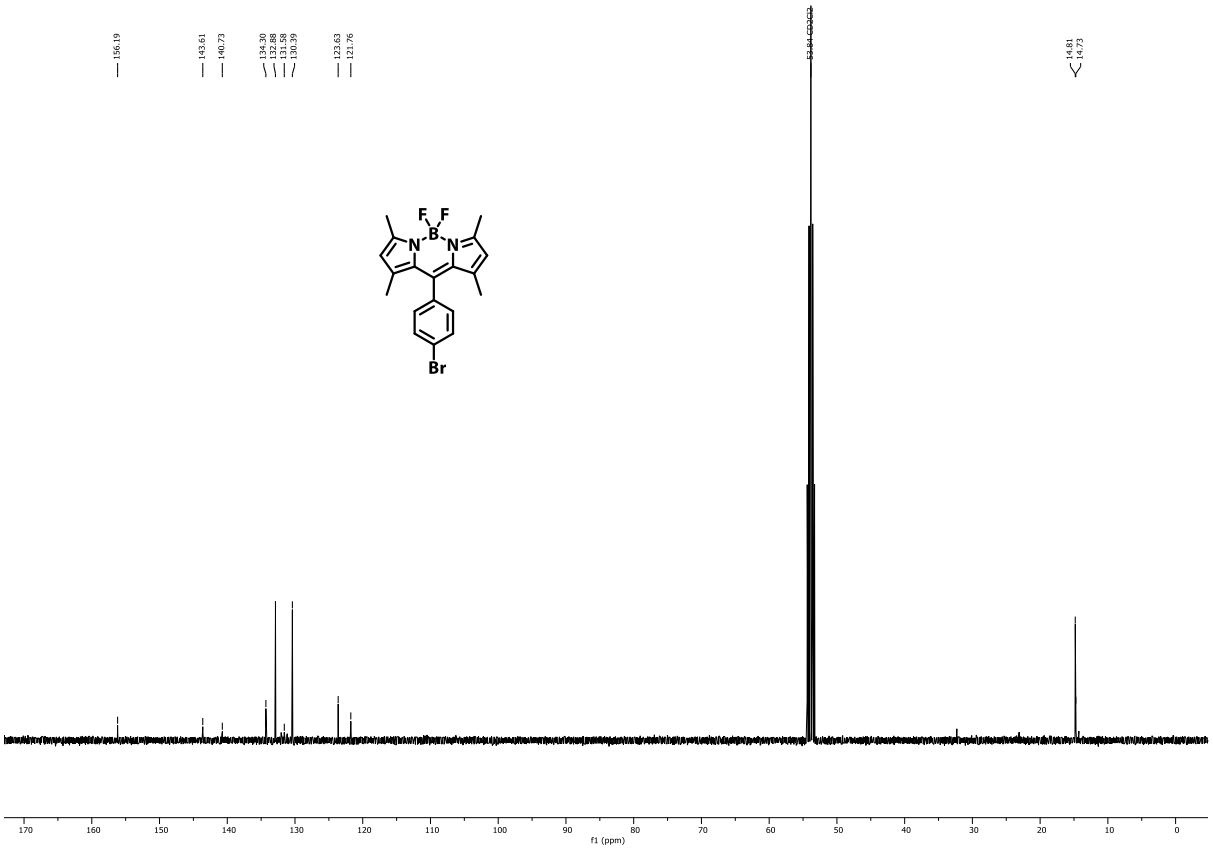
Instrument maXis 4G
Method ms_nocolumn_mid_pos.m



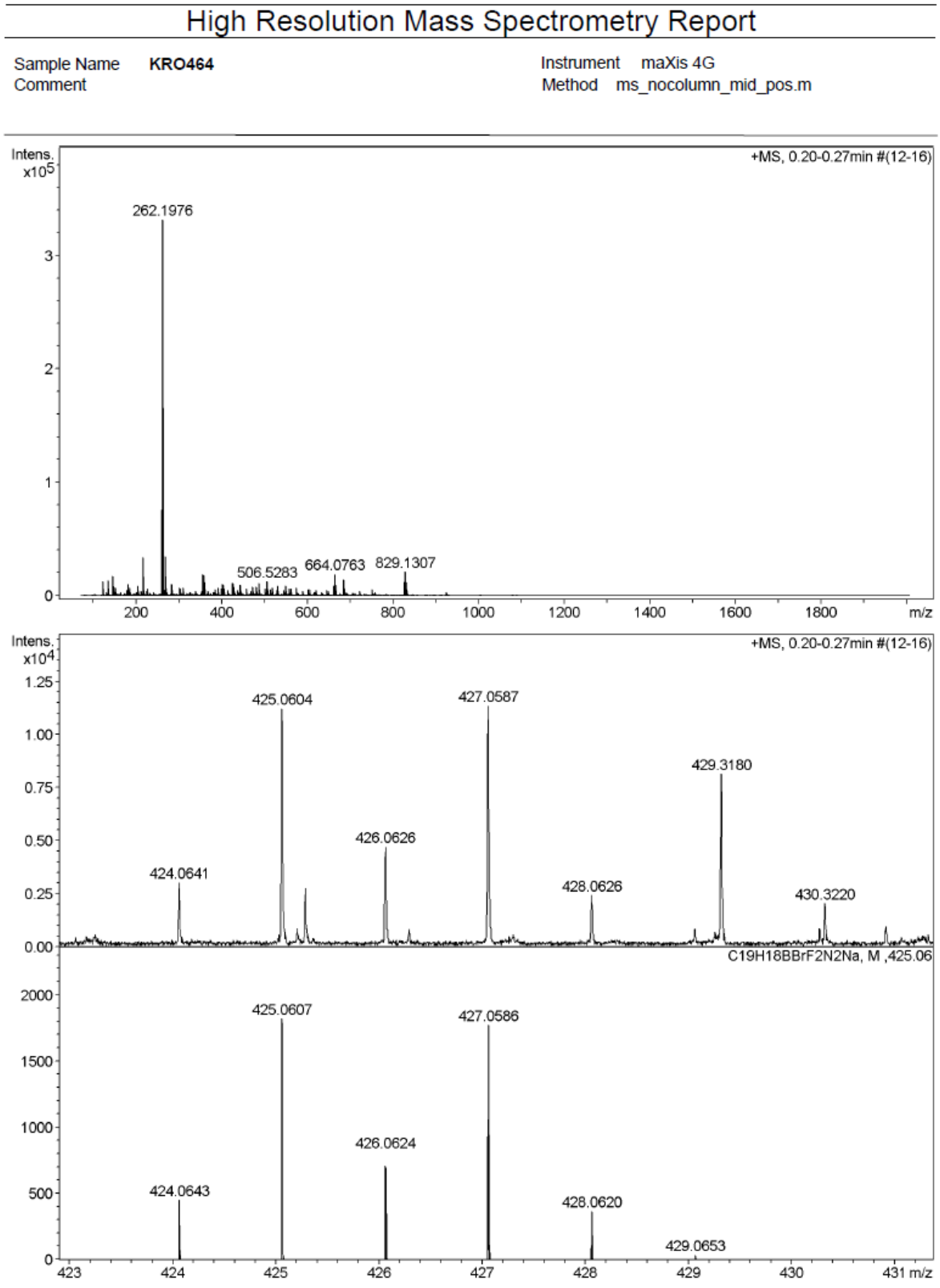
^{1}H-NMR spectrum of **BY-Br** in CD_2Cl_2



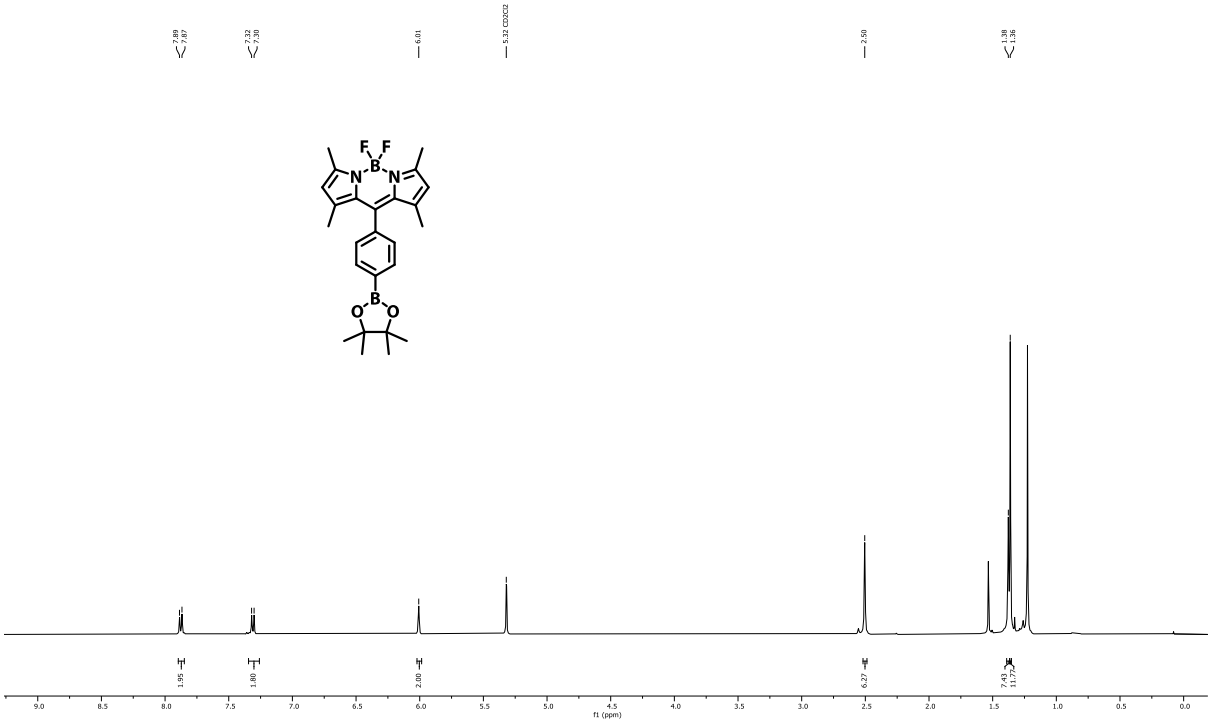
^{13}C-NMR spectrum of **BY-Br** in CD_2Cl_2



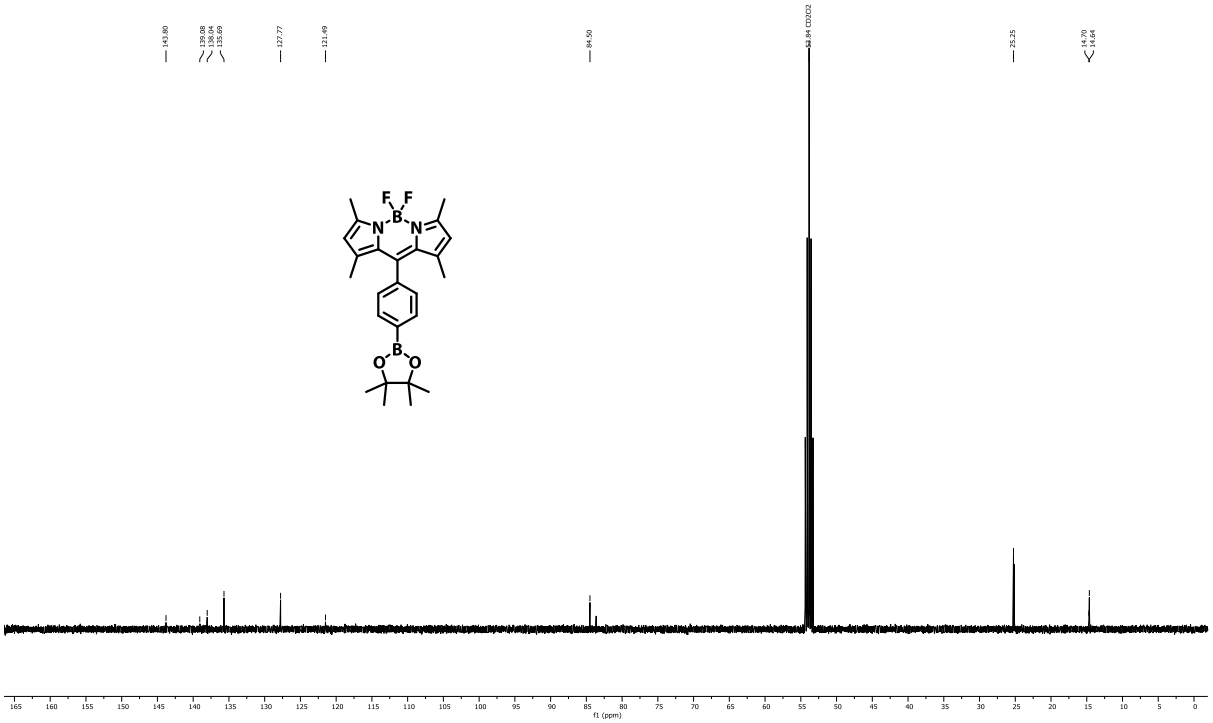
HR-ESI-MS spectrum of **BY-Br**



[1]H-NMR spectrum of **BY-BPin** in CD_2Cl_2



[13]C-NMR spectrum of **BY-BPin** in CD_2Cl_2

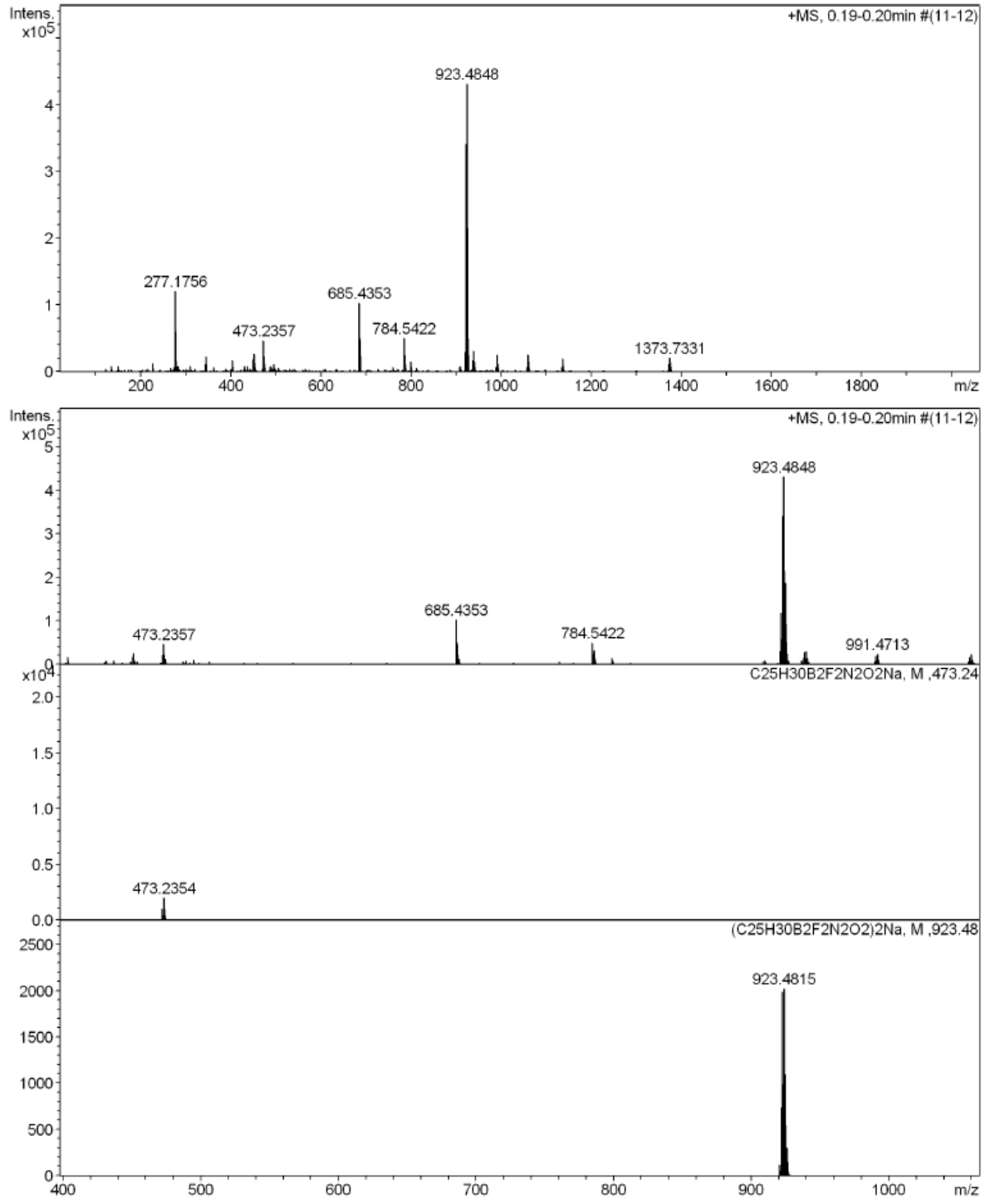


HR-ESI-MS spectrum of **BY-BPin**

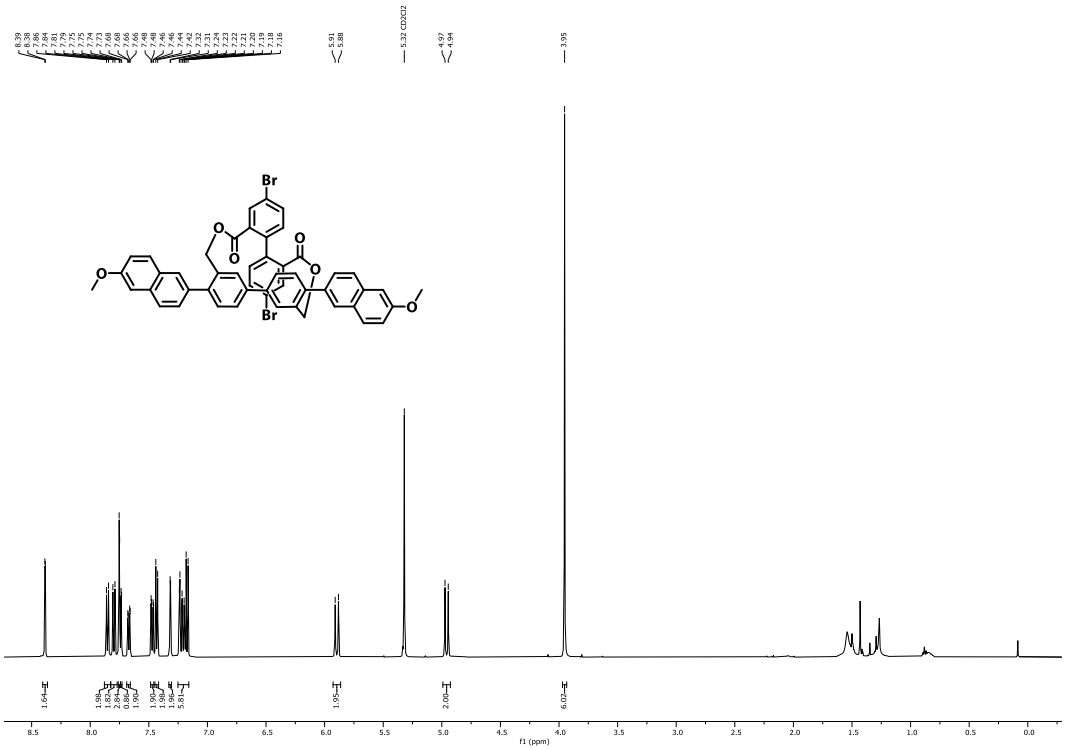
High Resolution Mass Spectrometry Report

Sample Name **KRO468**
Comment

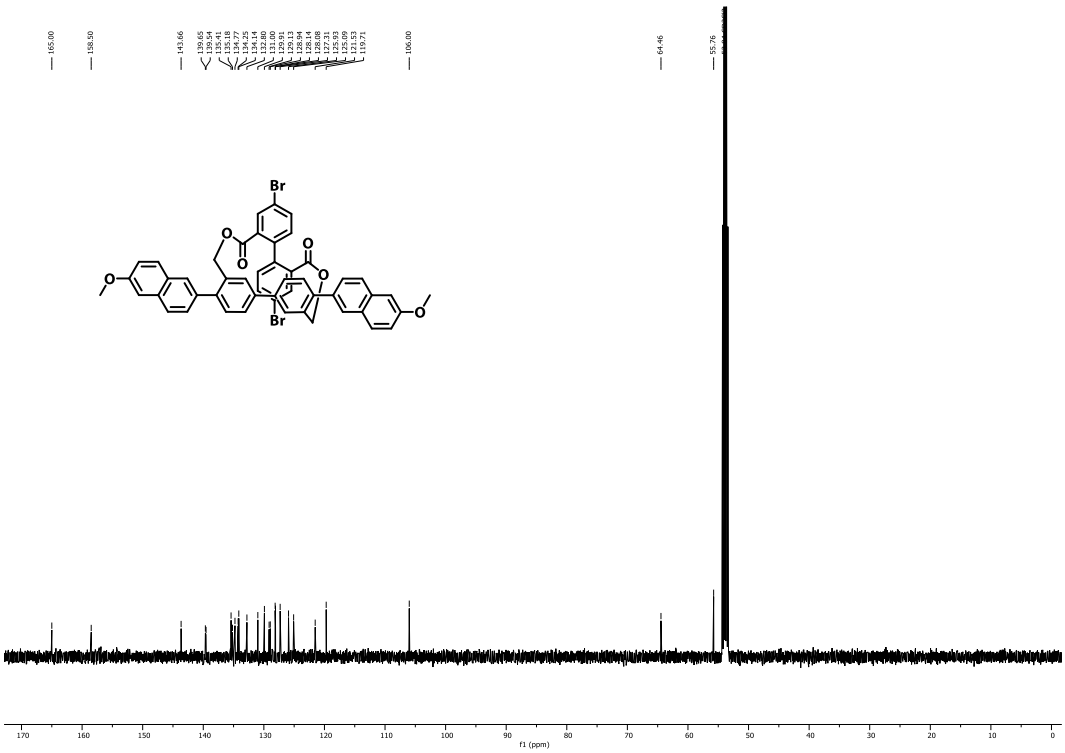
Instrument maXis 4G
Method ms_nocolumn_mid_pos.m



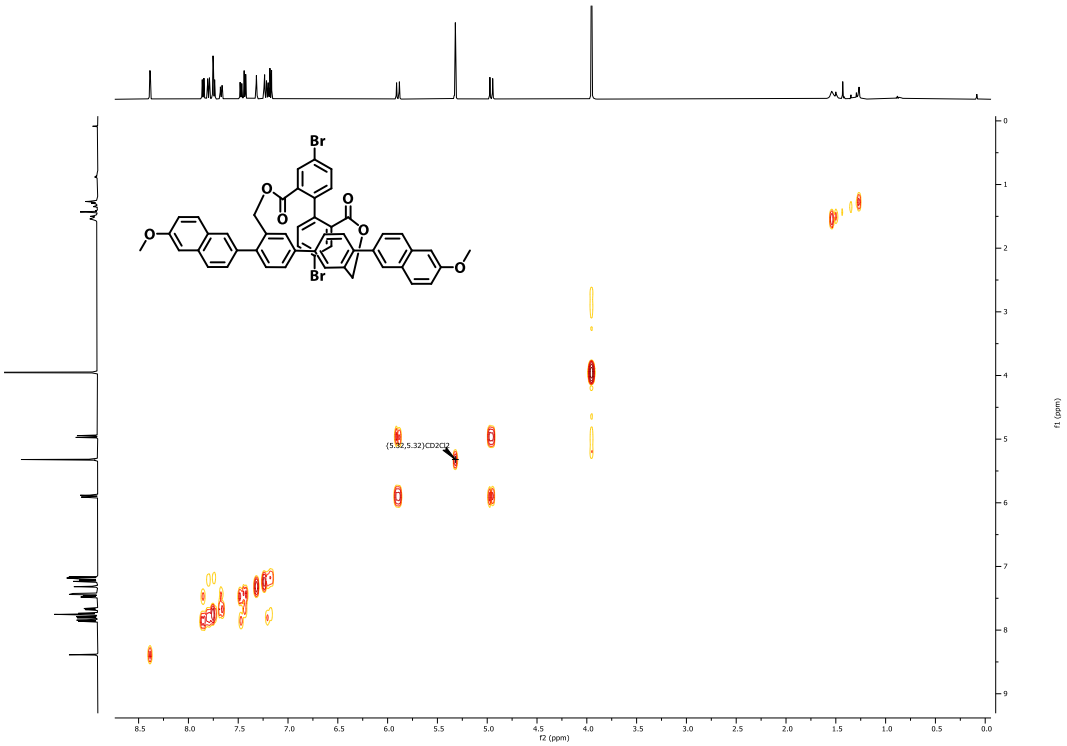
^{1}H-NMR spectrum of $\mathbf{C_{Br2Naph2}}$ in CD_2Cl_2



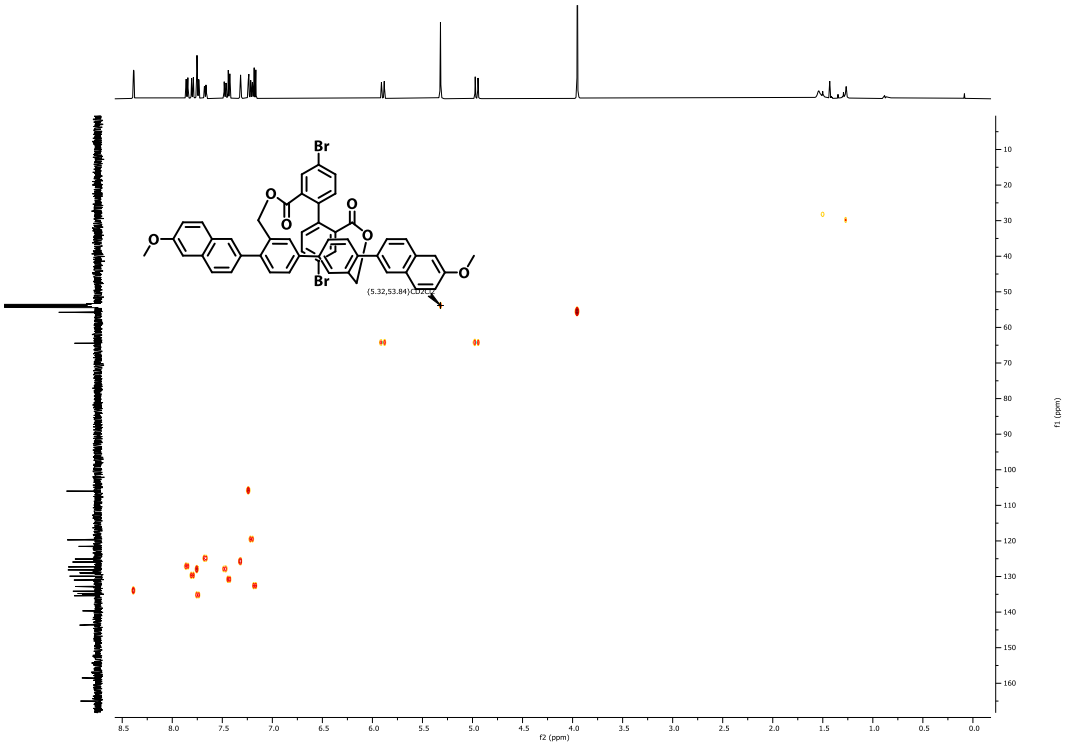
^{13}C-NMR spectrum of $\mathbf{C_{Br2Naph2}}$ in CD_2Cl_2



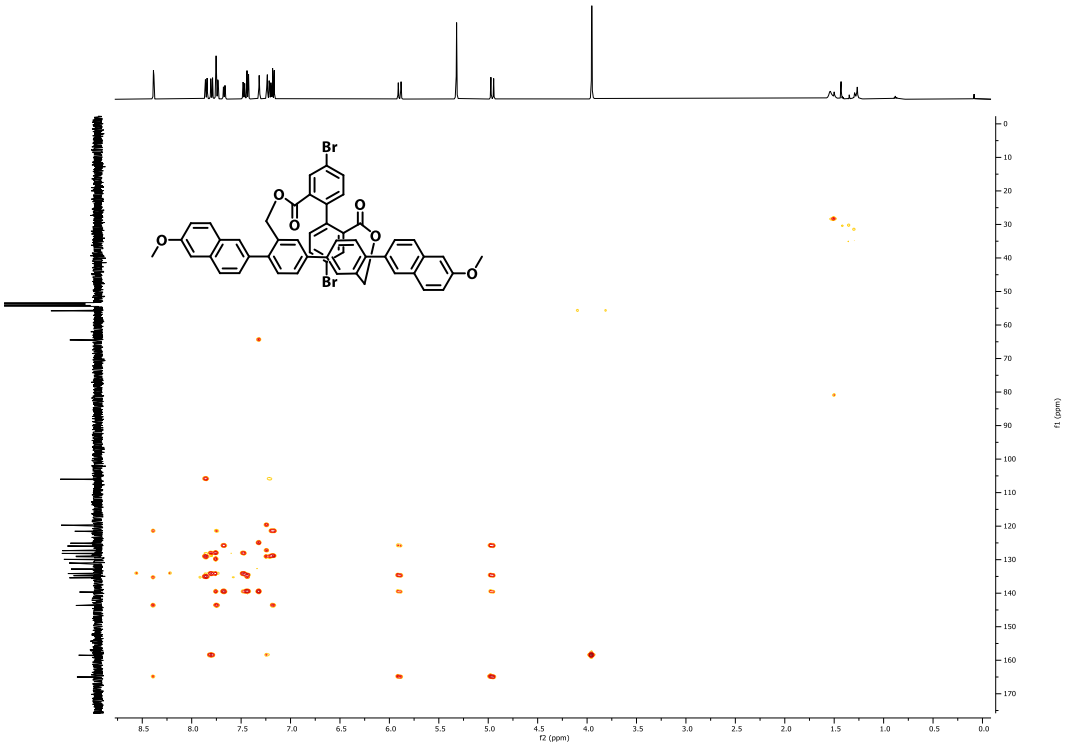
COSY spectrum of $\mathbf{C_{Br2Naph2}}$ in CD_2Cl_2



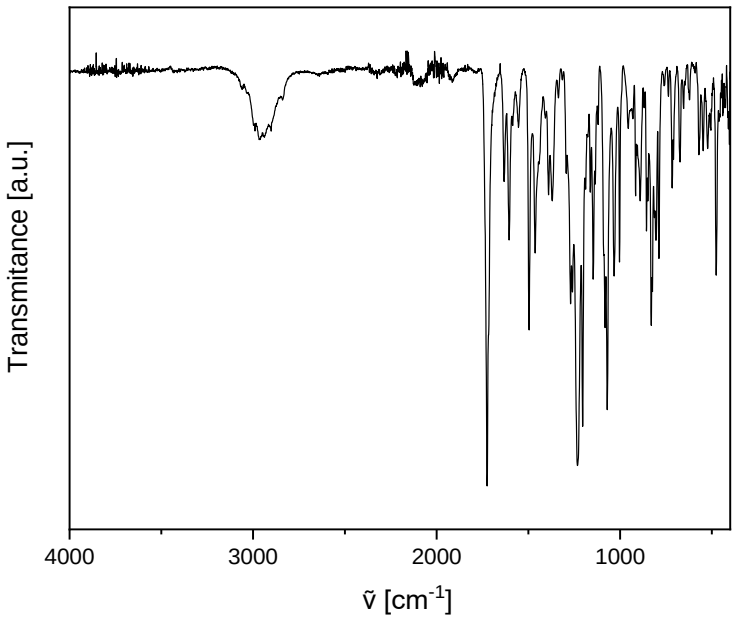
HMQC spectrum of $\mathbf{C_{Br2Naph2}}$ in CD_2Cl_2



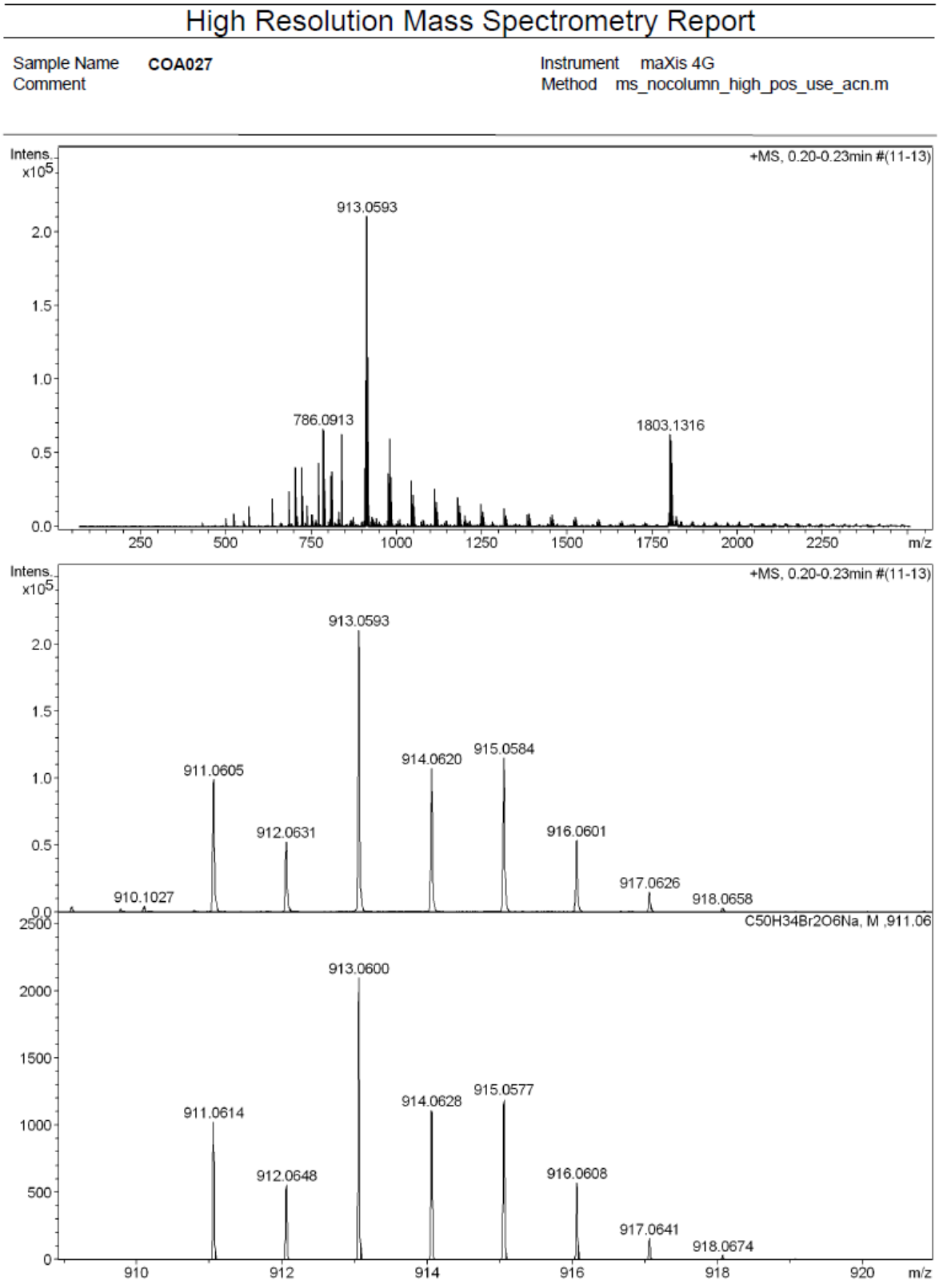
HMBC spectrum of $\mathbf{C_{Br2Naph2}}$ in CD_2Cl_2



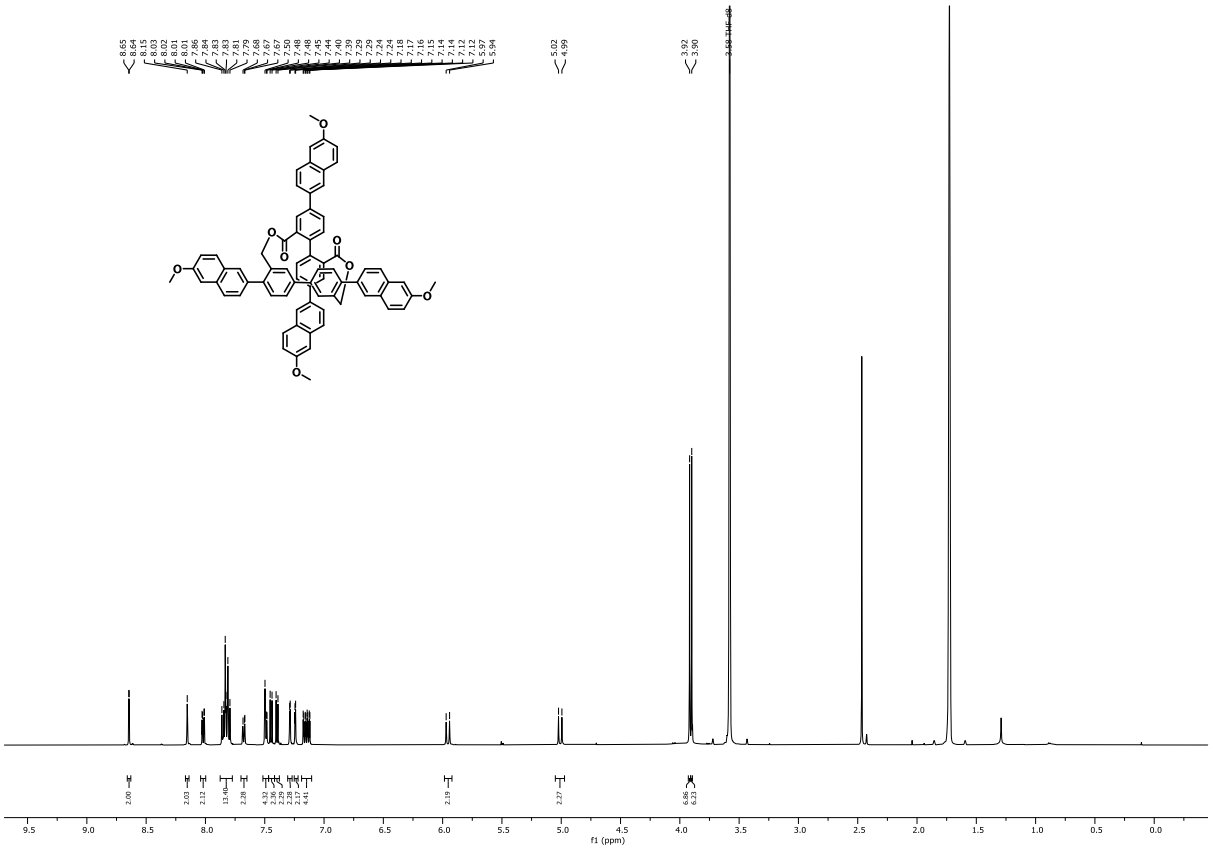
FT-IR spectrum of $\mathbf{C_{Br2Naph2}}$ (neat)



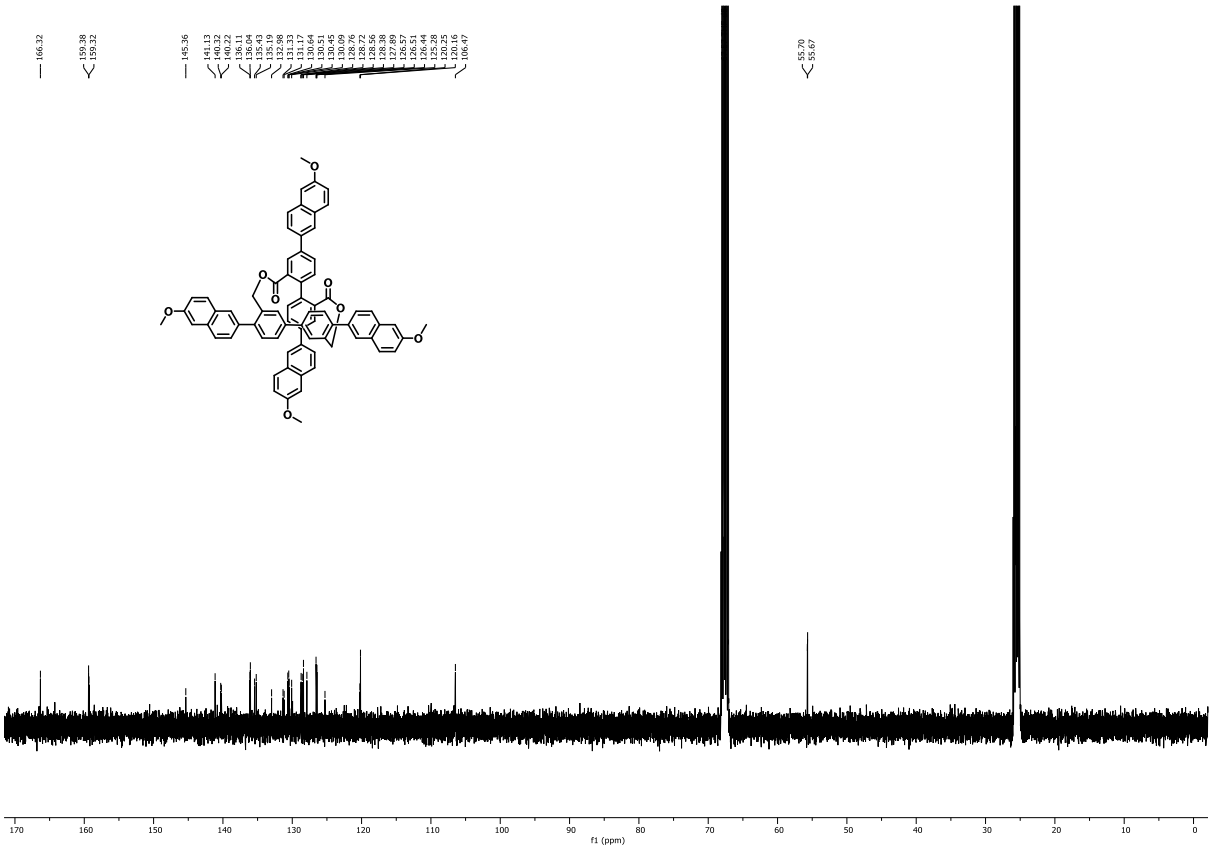
HR-ESI-MS spectrum of $C_{Br2Naph2}$



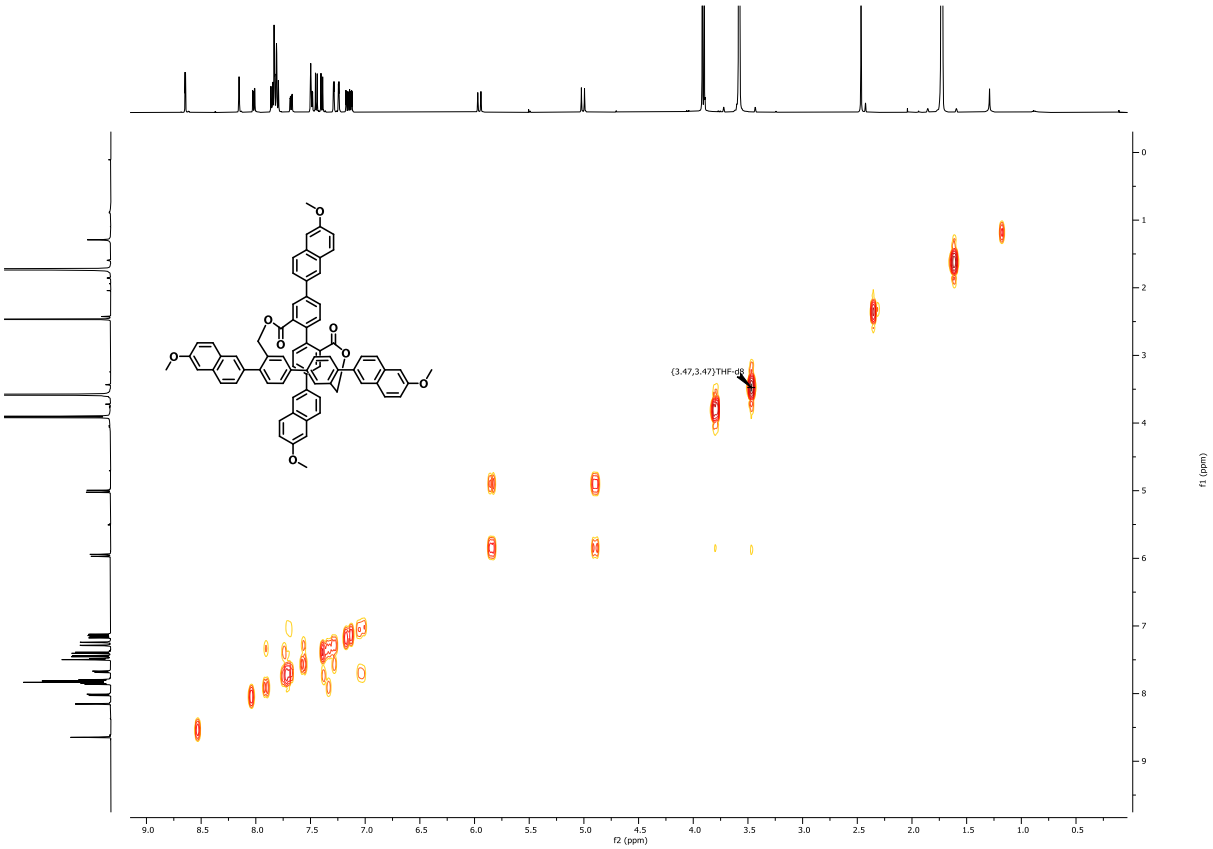
^{1}H-NMR spectrum of **C_{Naph4}** in THF-d8



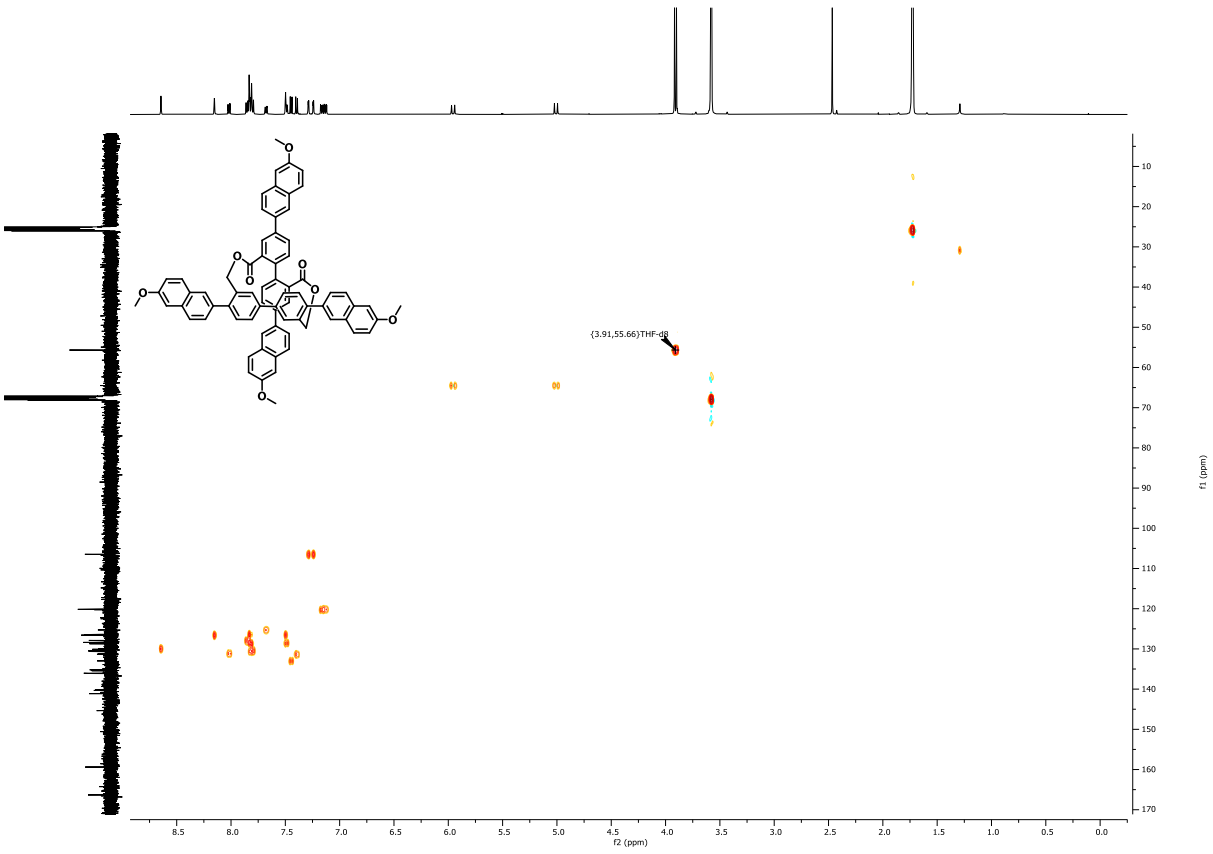
^{13}C-NMR spectrum of **C_{Naph4}** in THF-d8



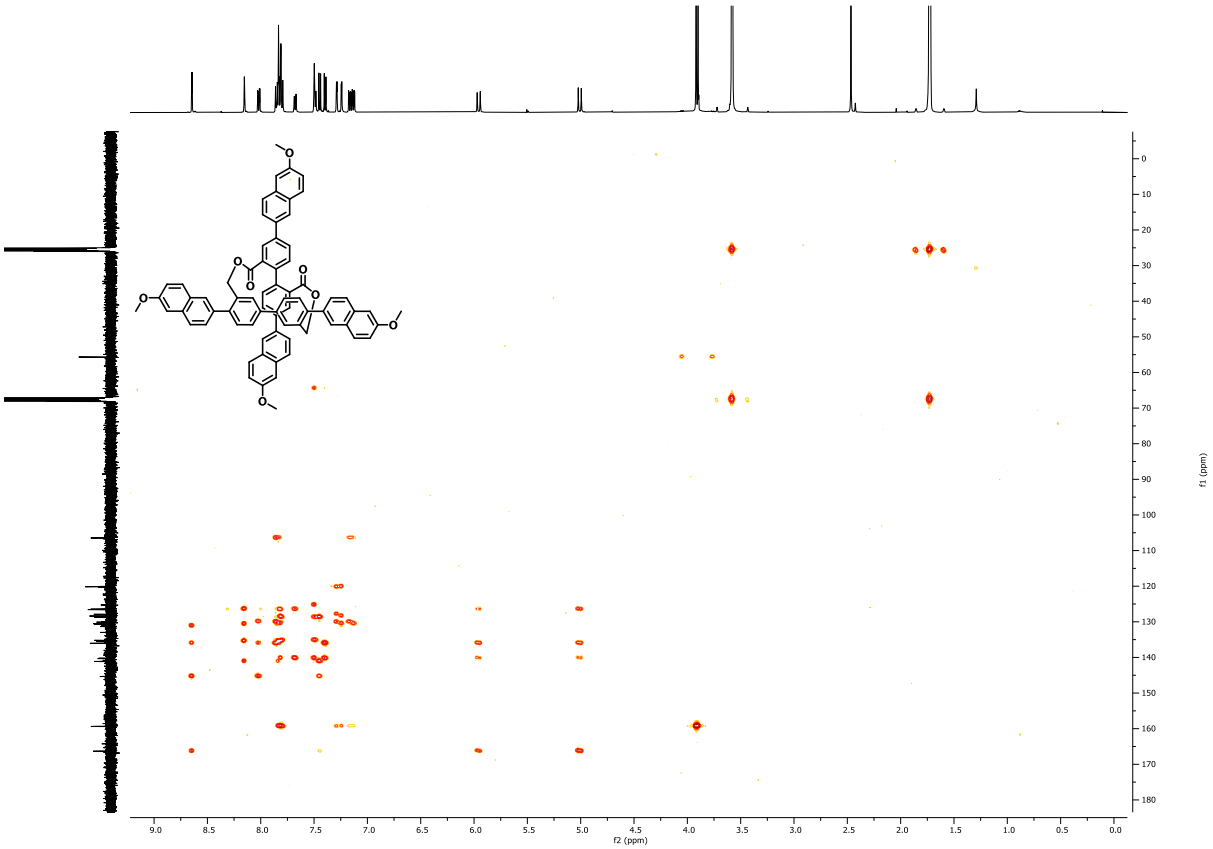
COSY spectrum of $\mathbf{C_{Naph4}}$ in THF-d8



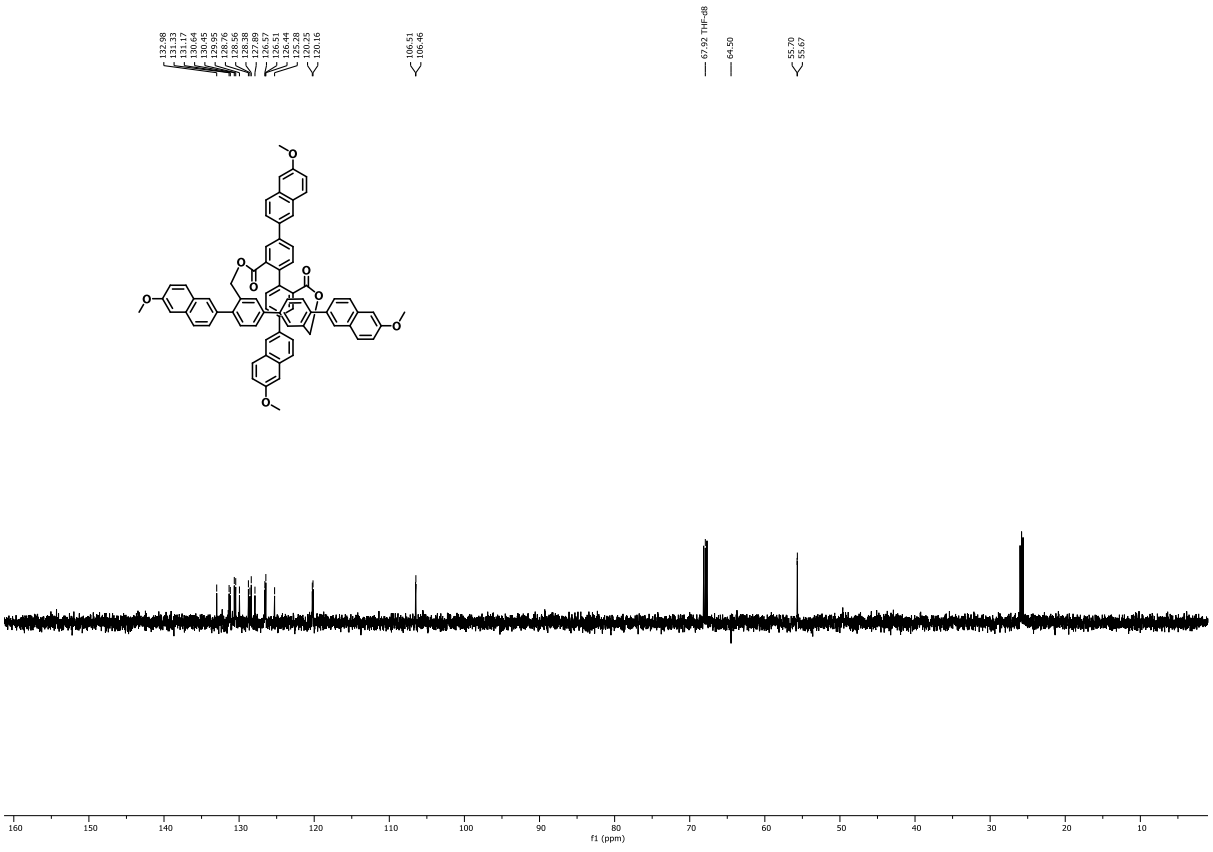
HMQC spectrum of $\mathbf{C_{Naph4}}$ in THF-d8



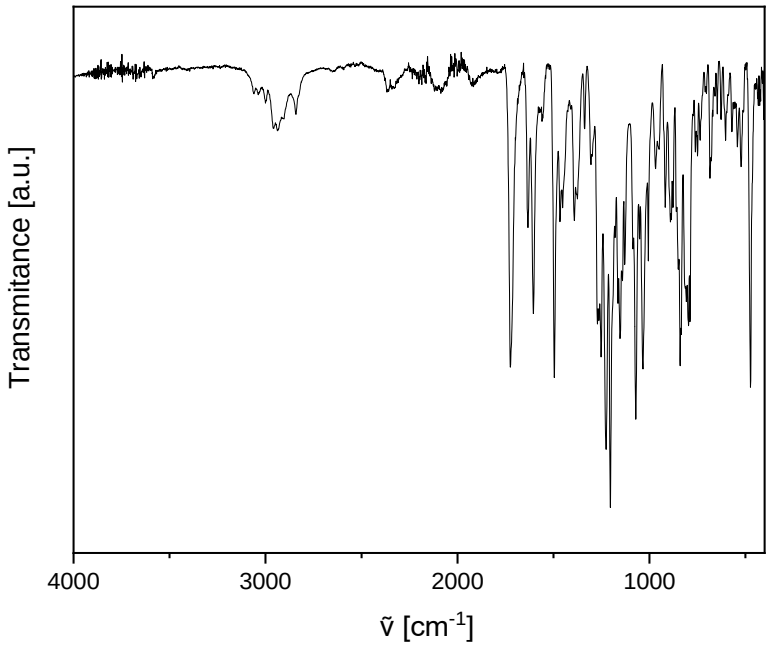
HMBC spectrum of $\mathbf{C_{Naph4}}$ in THF-d8



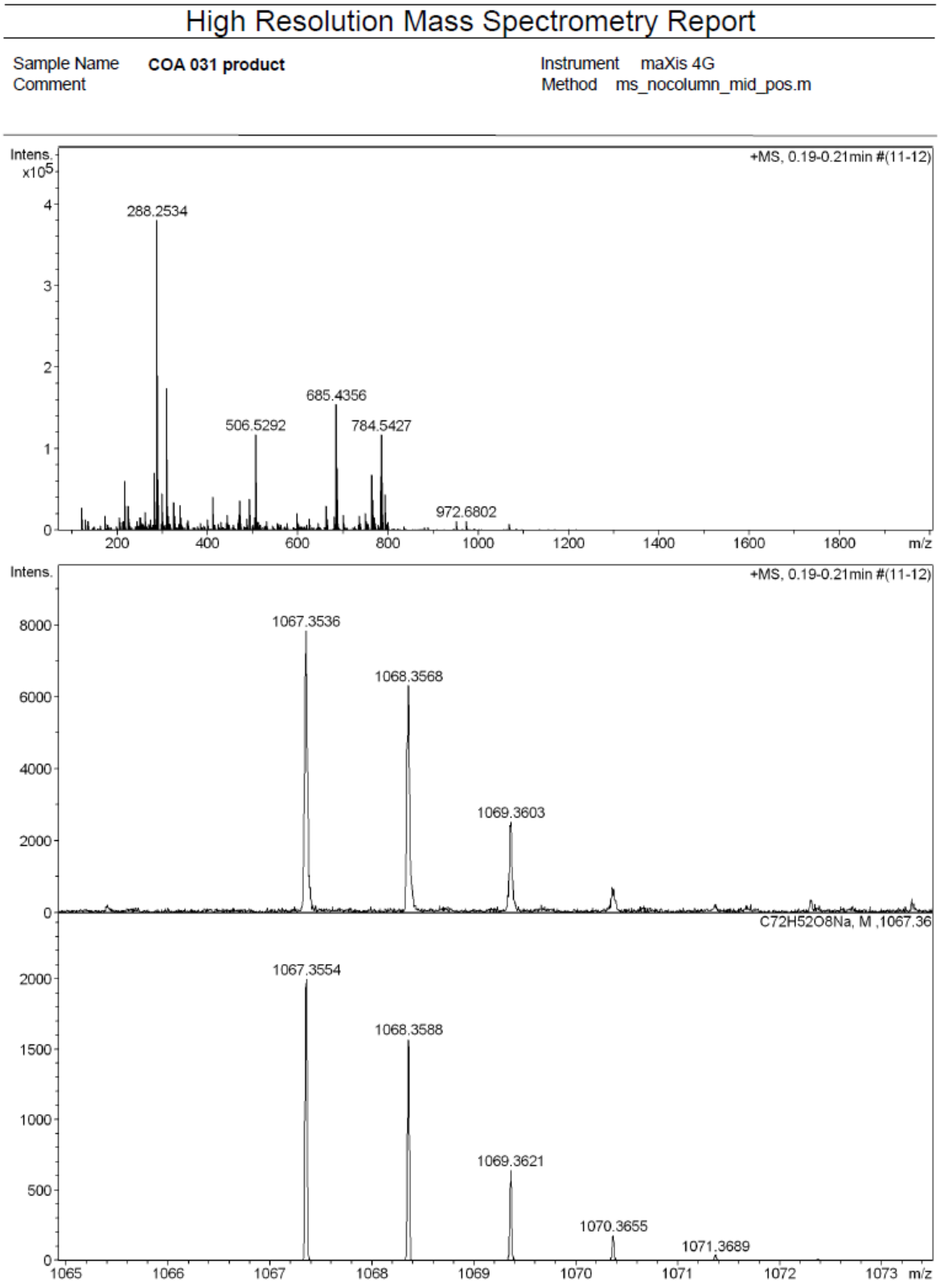
^{13}C-DEPT spectrum of $\mathbf{C_{Naph4}}$ in THF-d8



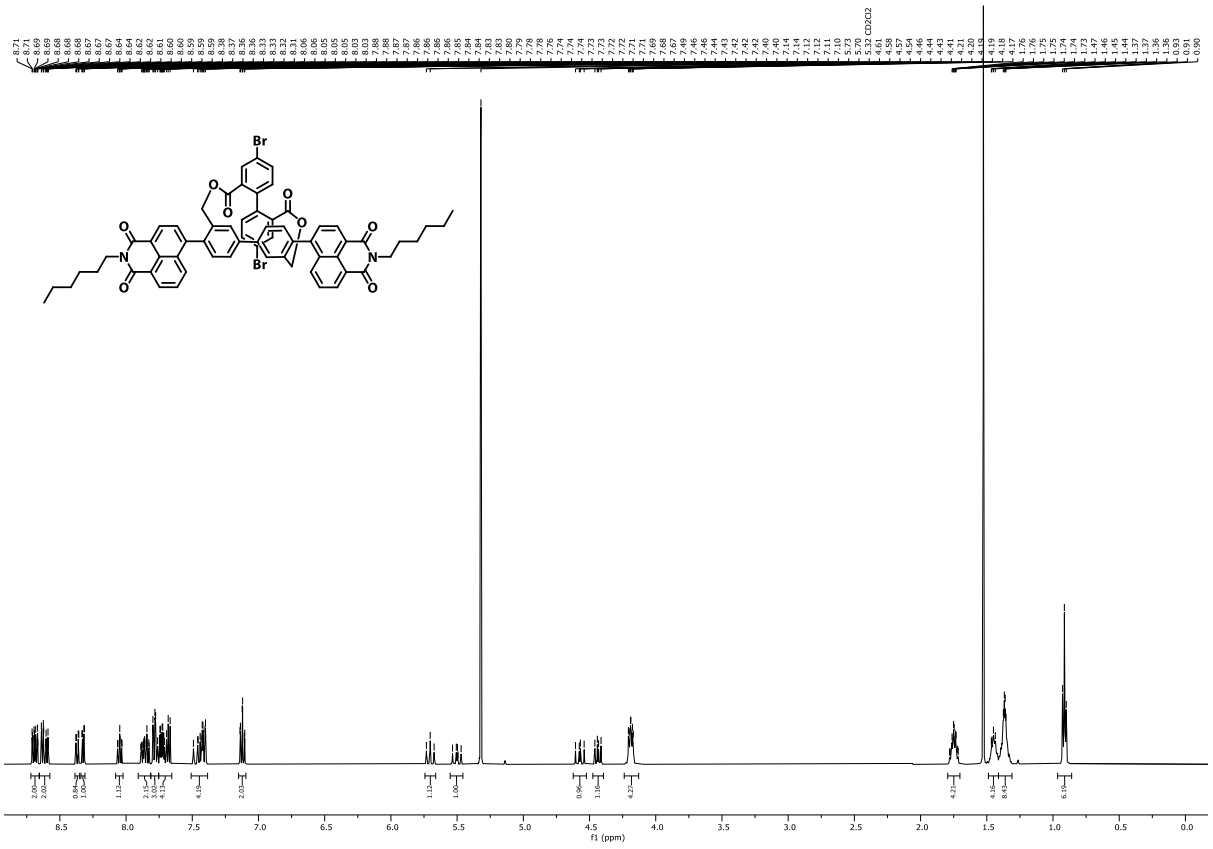
FT-IR spectrum of $\mathbf{C_{Naph4}}$ (neat)



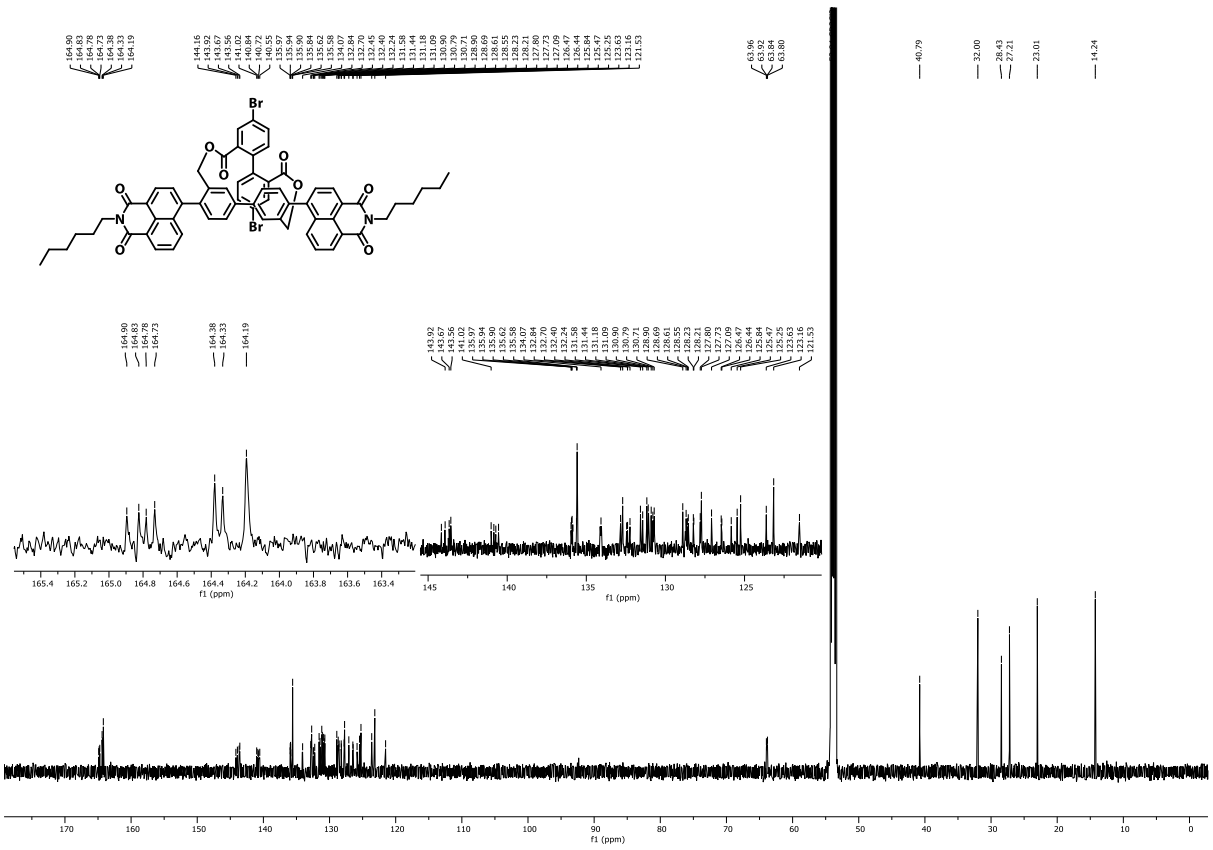
HR-ESI-MS spectrum of C_{Naph4}



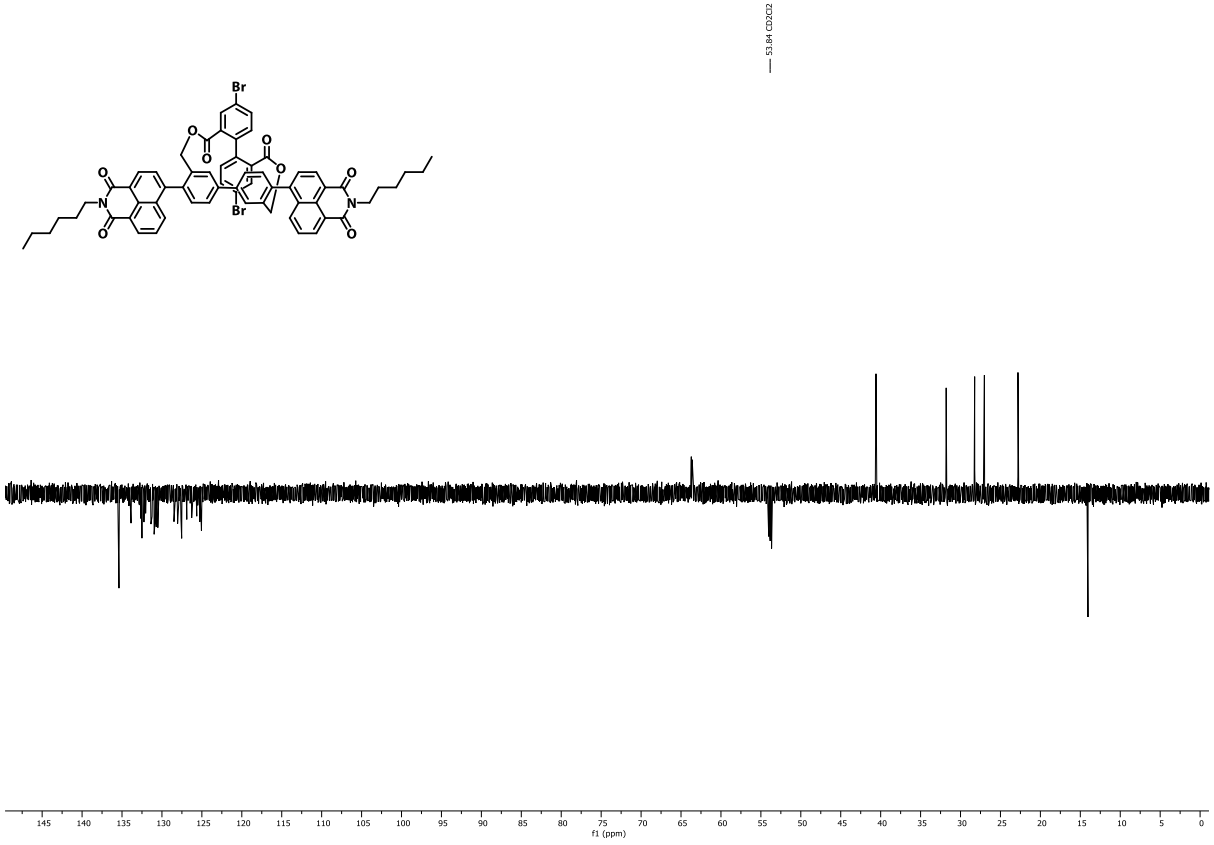
^{1}H-NMR spectrum of $\mathbf{C_{Br2NI2}}$ in CD_2Cl_2



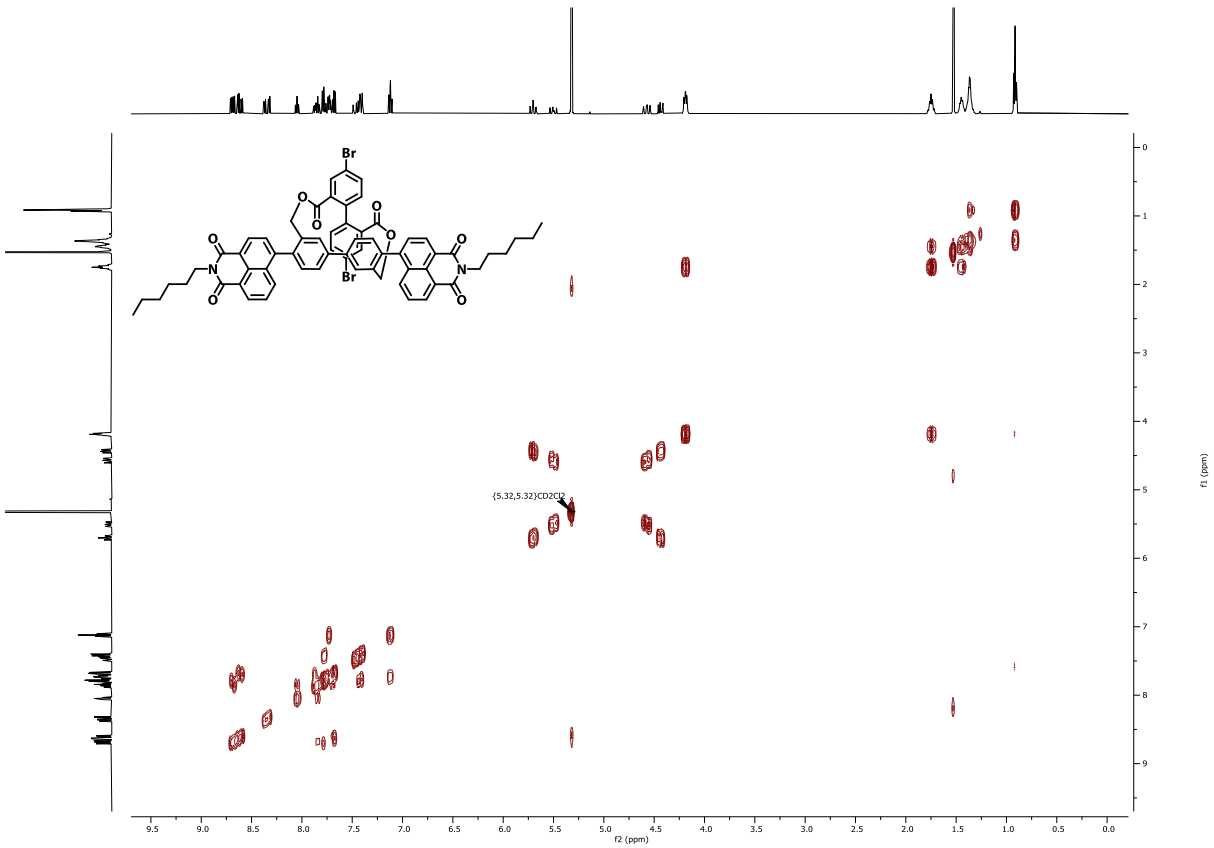
^{13}C-NMR spectrum of $\mathbf{C_{Br2NI2}}$ in CD_2Cl_2



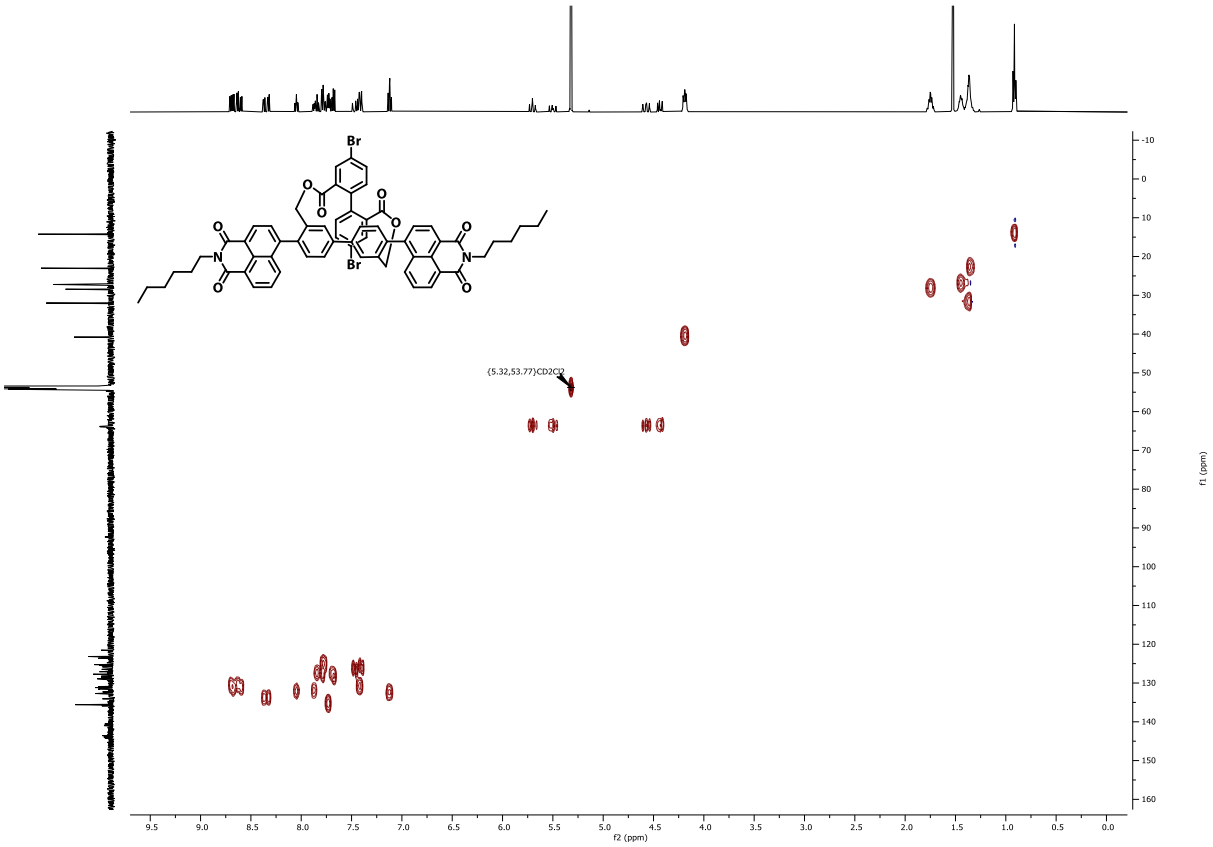
^{13}C-Dept spectrum of $\mathbf{C_{Br2NI2}}$ in CD_2Cl_2



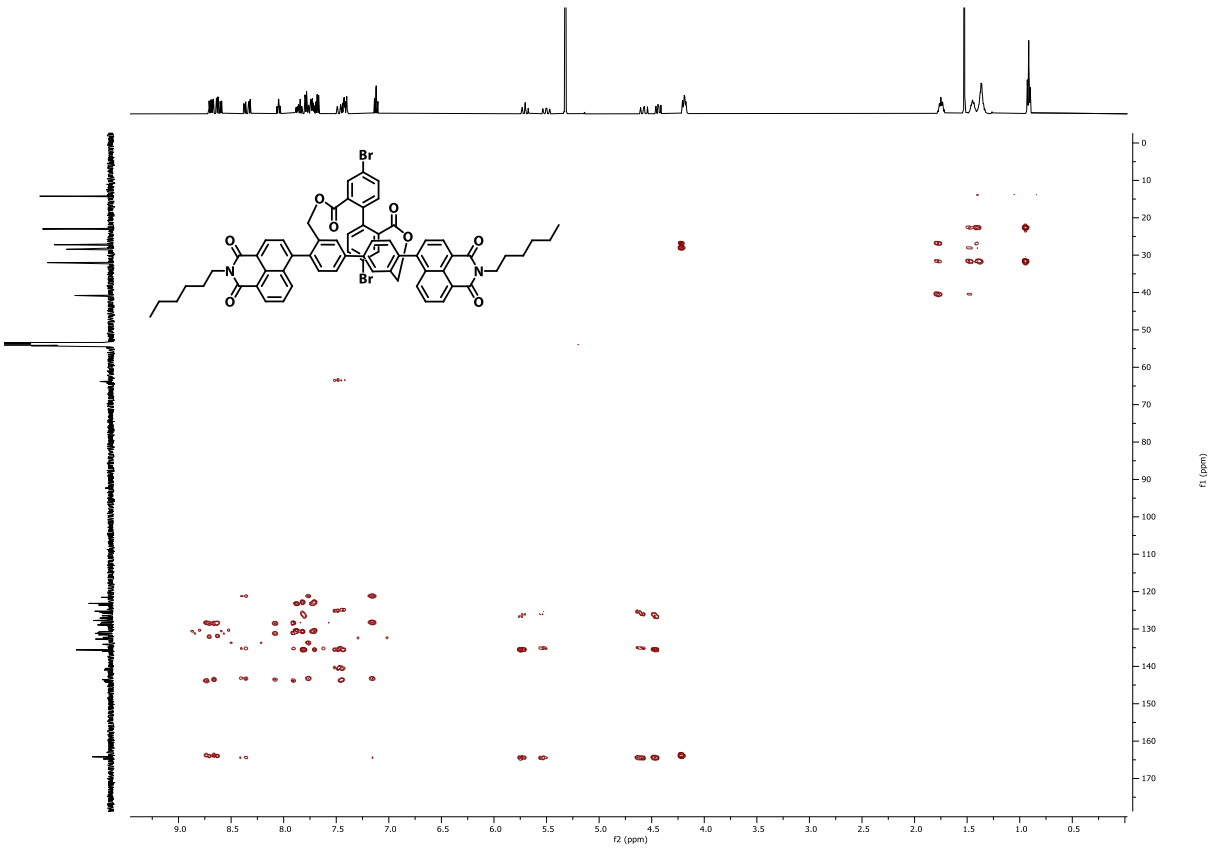
COSY spectrum of $\mathbf{C_{Br2NI2}}$ in CD_2Cl_2



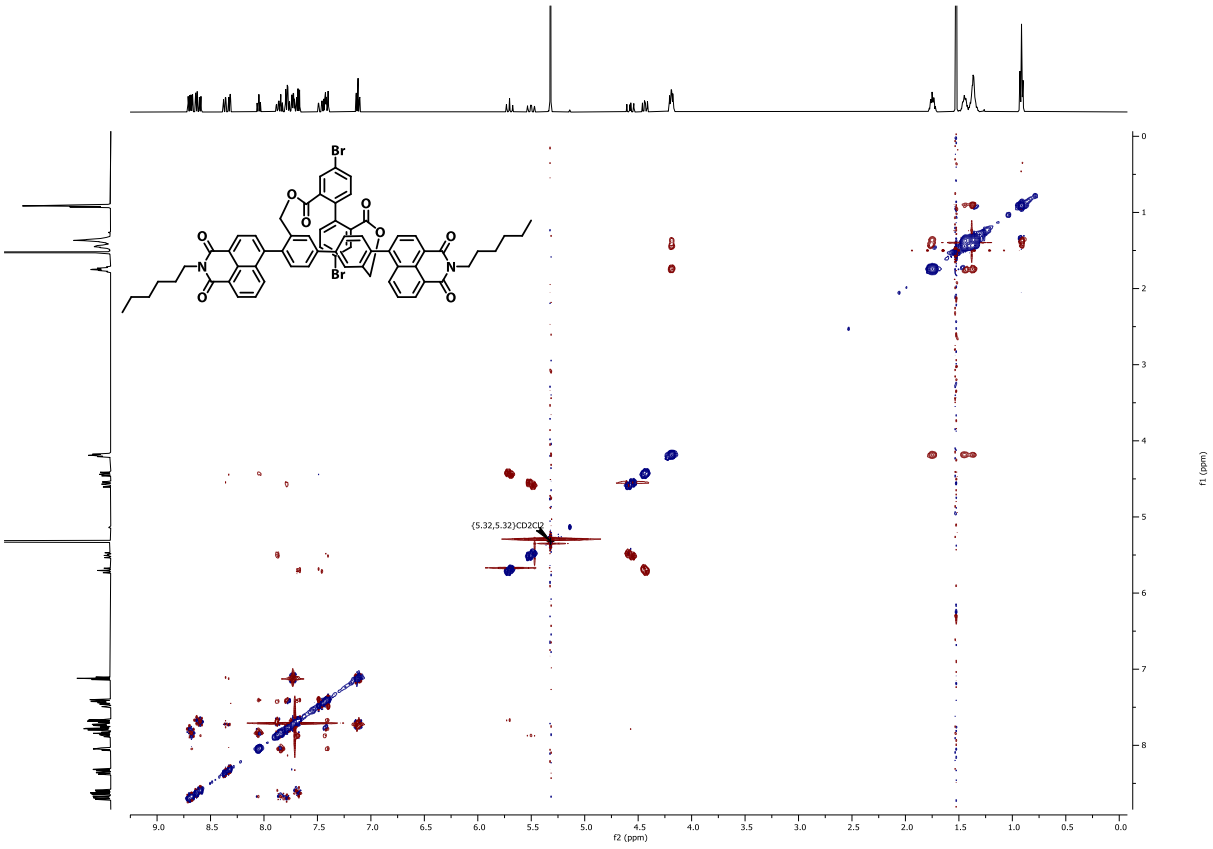
HMQC spectrum of $\mathbf{C_{Br2NI2}}$ in CD_2Cl_2



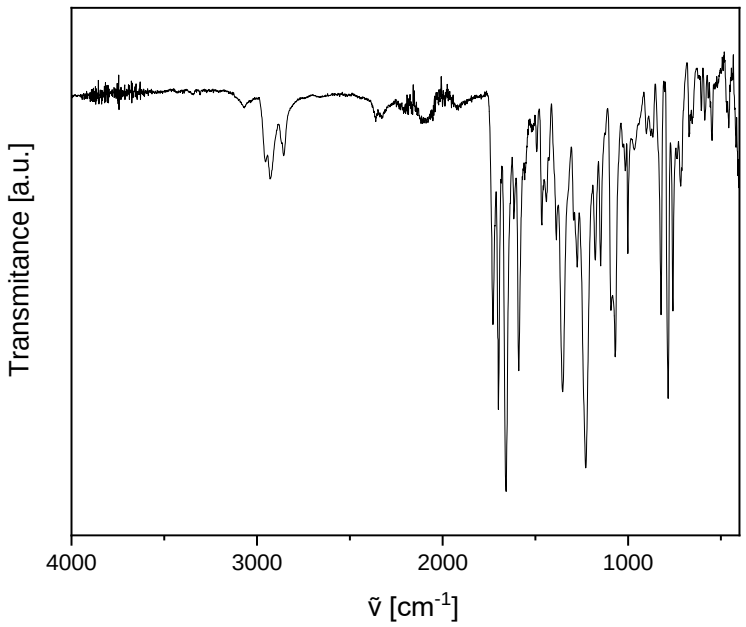
HMBC spectrum of $\mathbf{C_{Br2NI2}}$ in CD_2Cl_2



NOESY spectrum of $\mathbf{C_{Br2NI2}}$ in CD_2Cl_2



FT-IR spectrum of $\mathbf{C_{Br2NI2}}$ (neat)

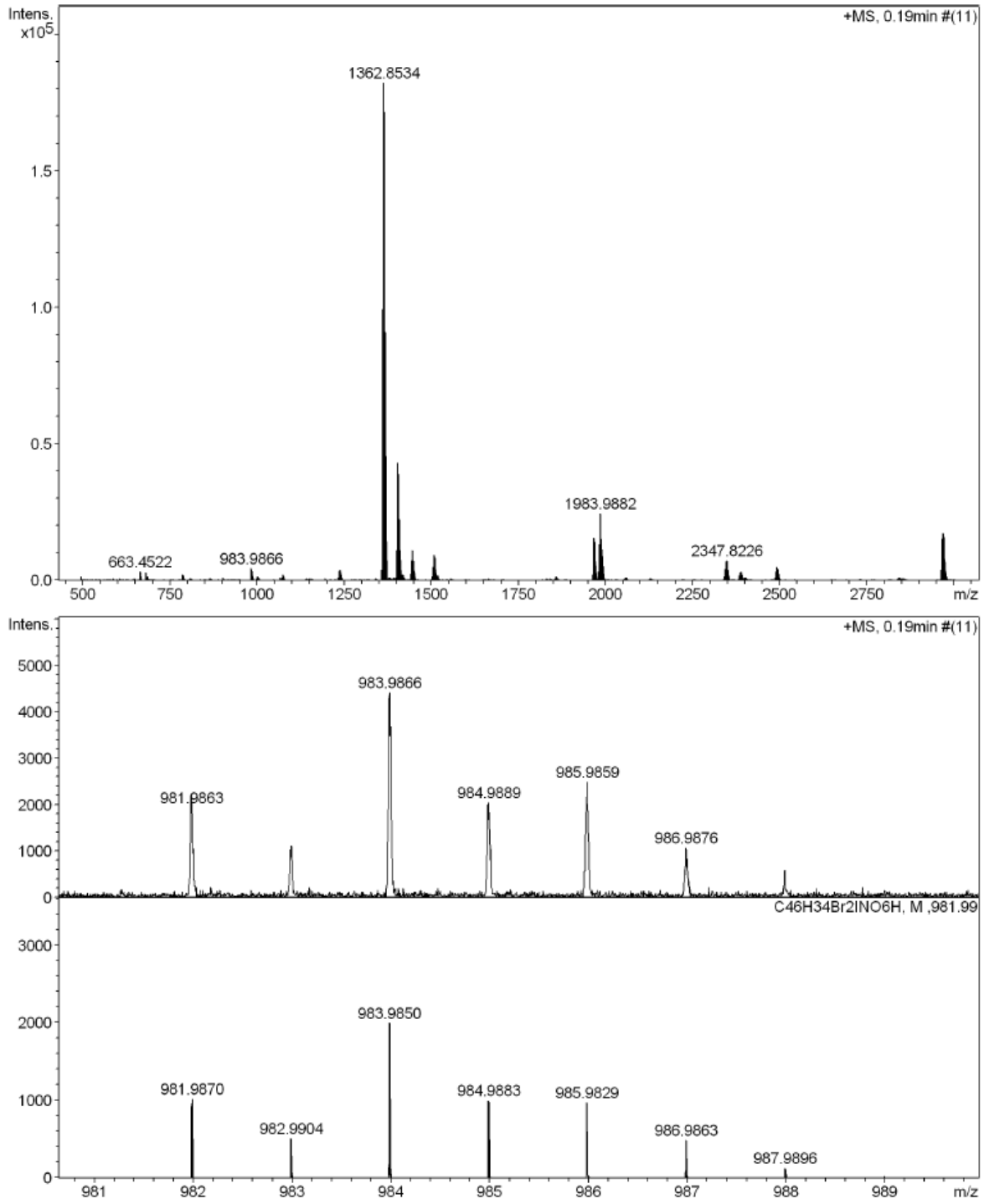


HR-ESI-MS spectrum of C_{Br2NI2}

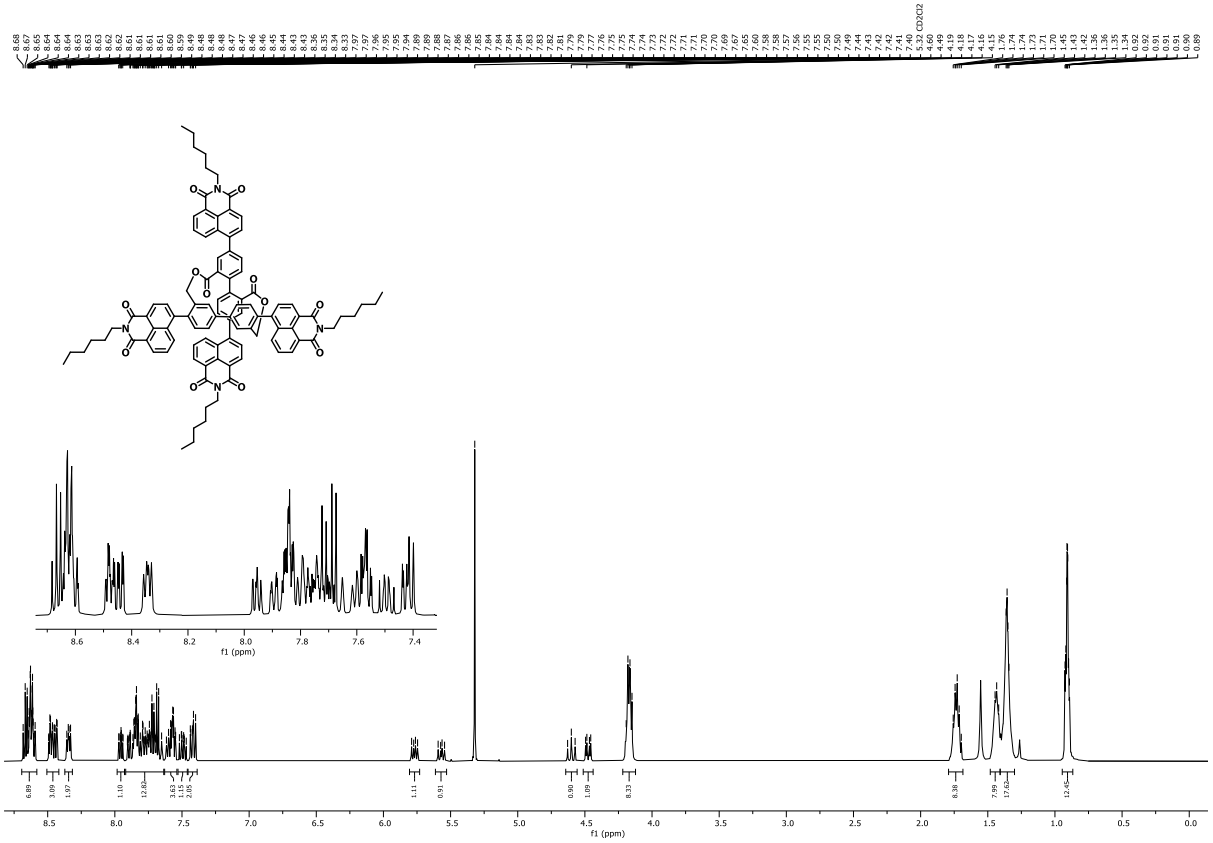
High Resolution Mass Spectrometry Report

Sample Name **KRO497-s5**
Comment

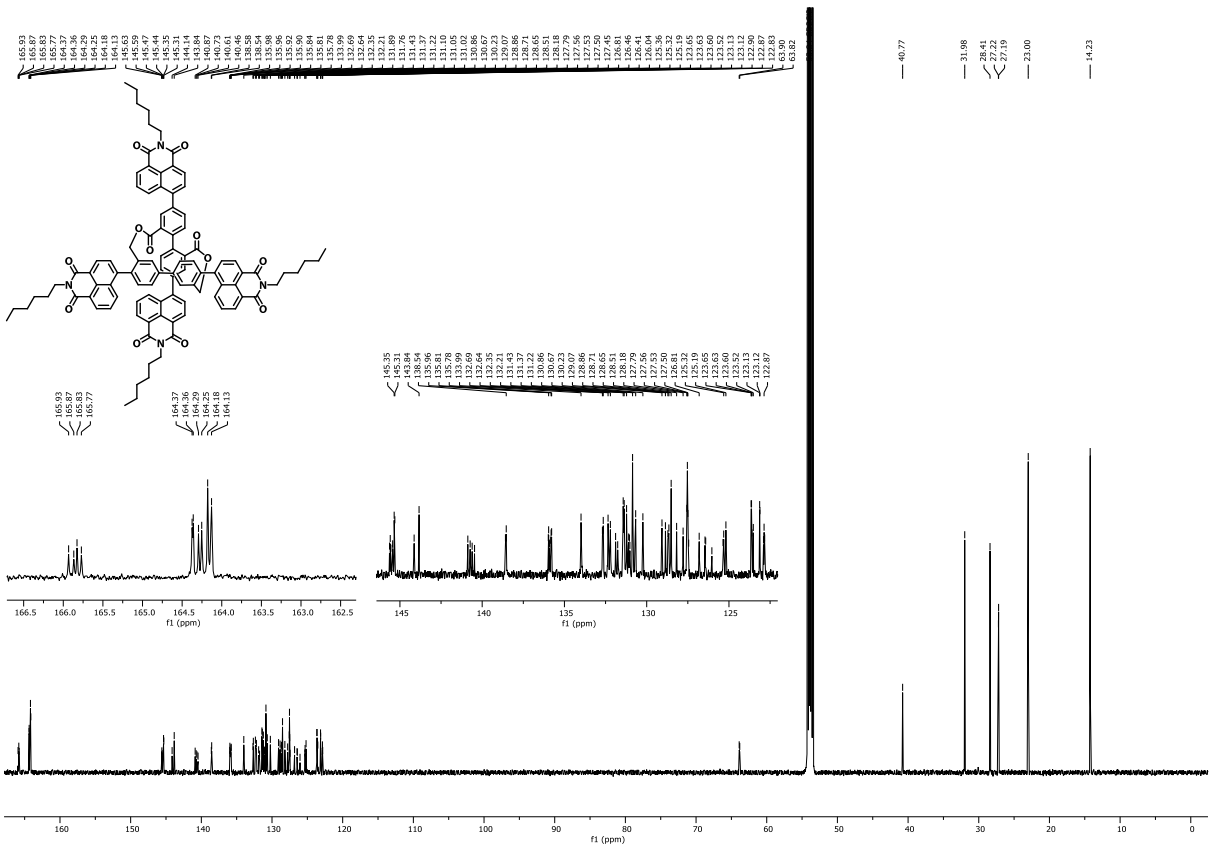
Instrument maXis 4G
Method ms_nocolumn_600-3000_pos .m



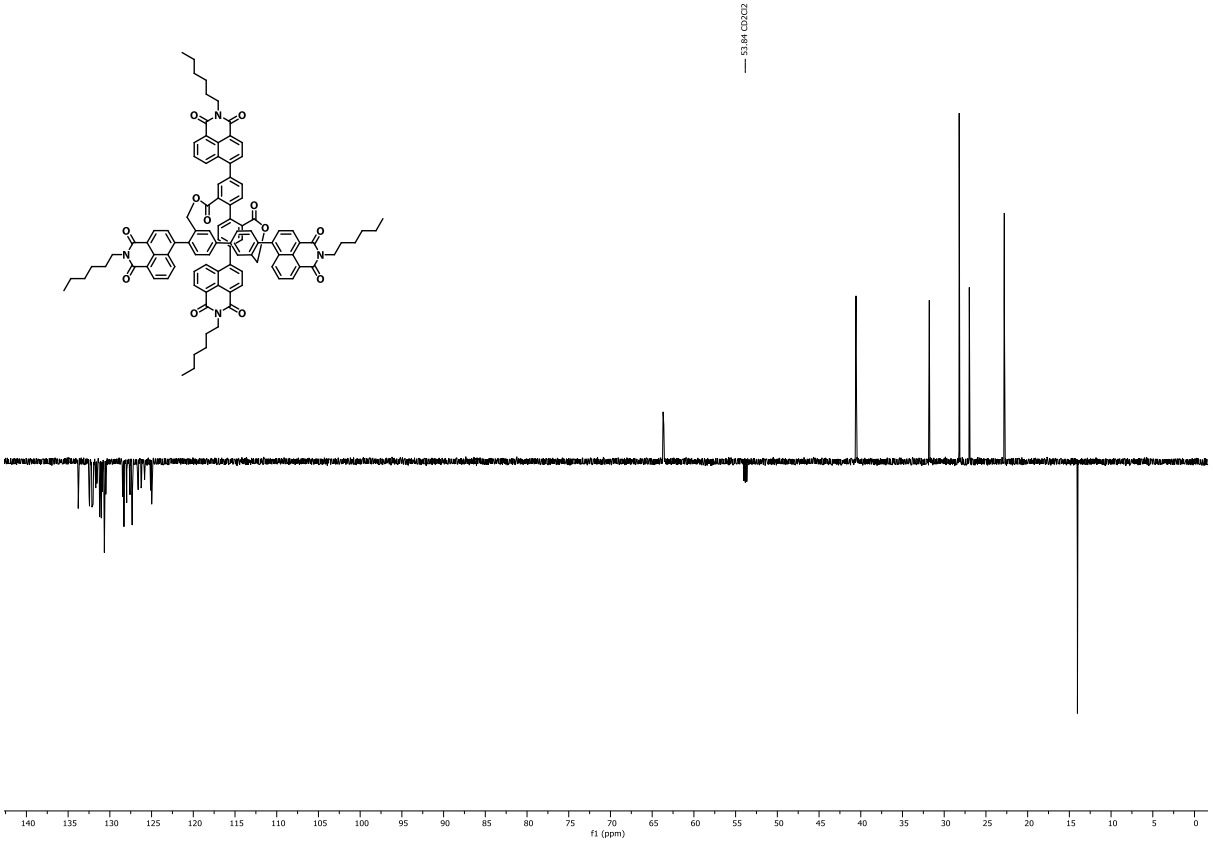
^{1}H-NMR spectrum of $\mathbf{C_{NI4}}$ in CD_2Cl_2



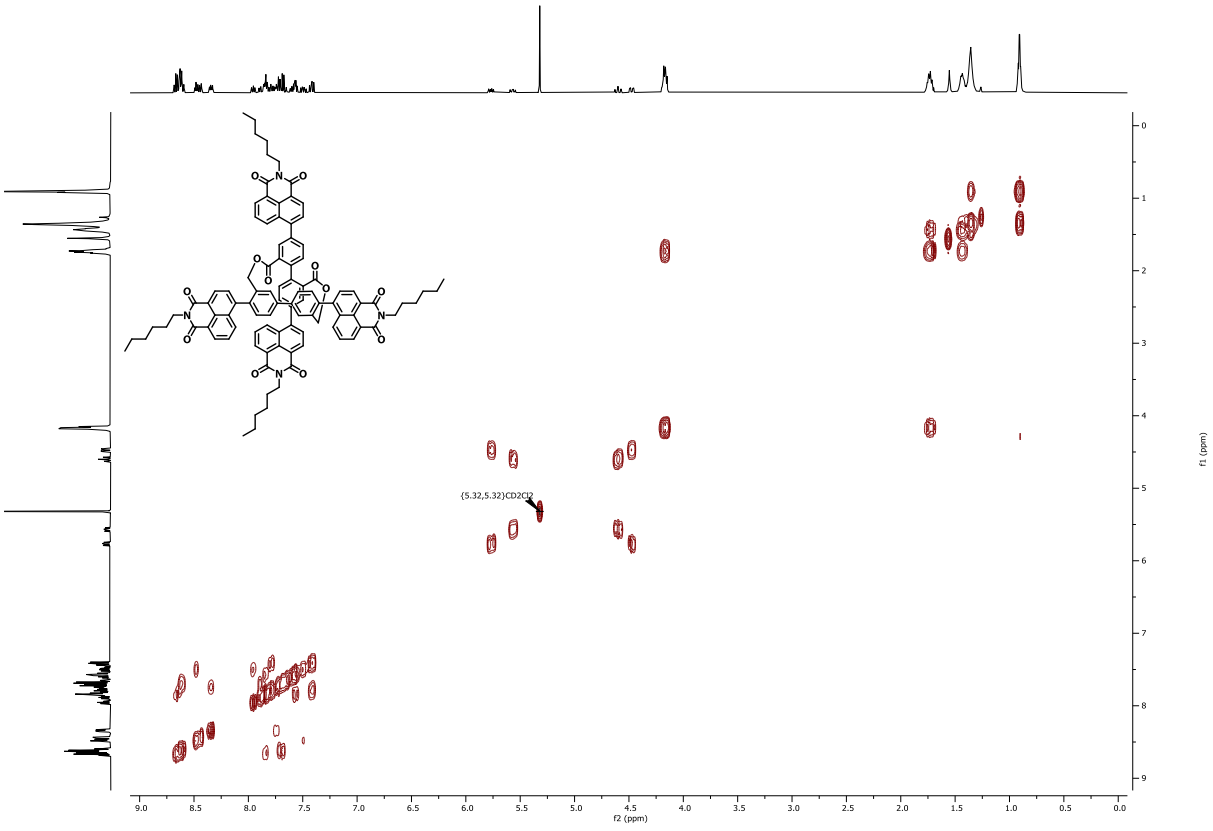
^{13}C-NMR spectrum of $\mathbf{C_{NI4}}$ in CD_2Cl_2



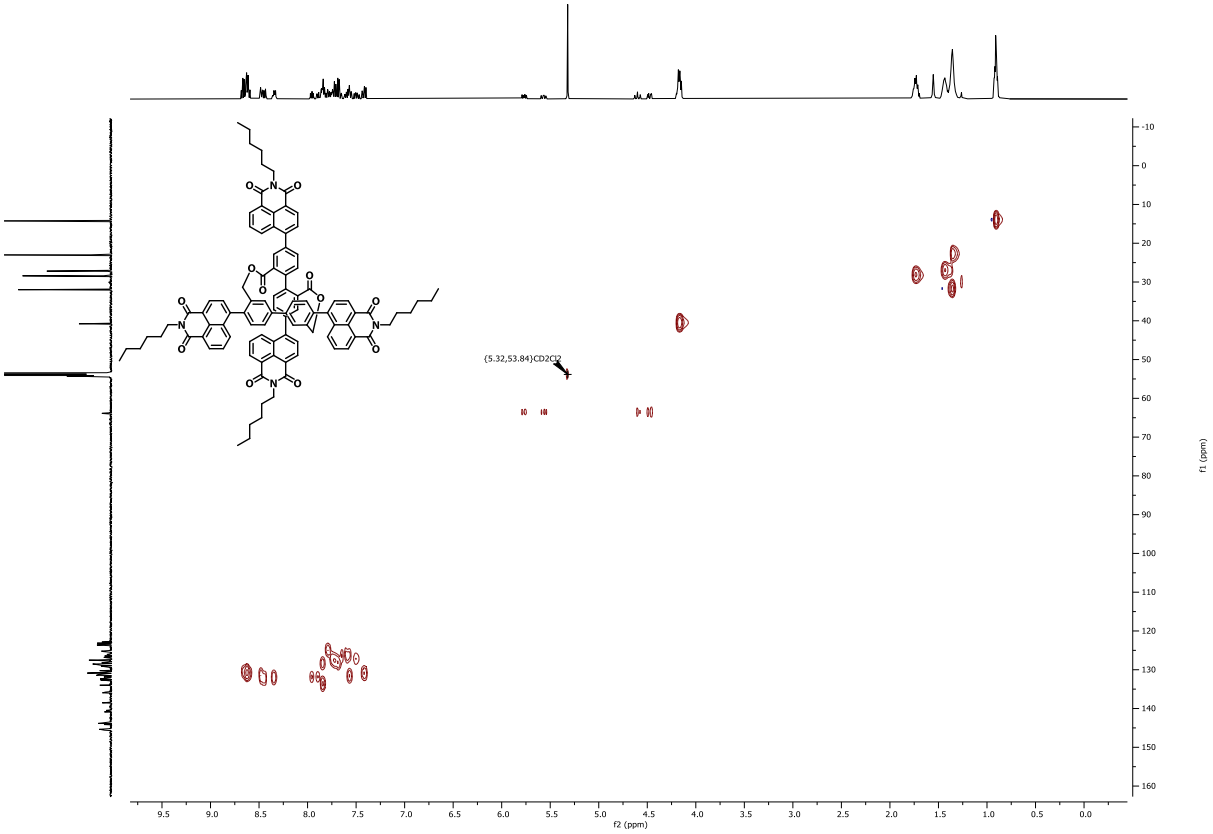
^{13}C-Dept spectrum of **C_{NI4}** in CD_2Cl_2



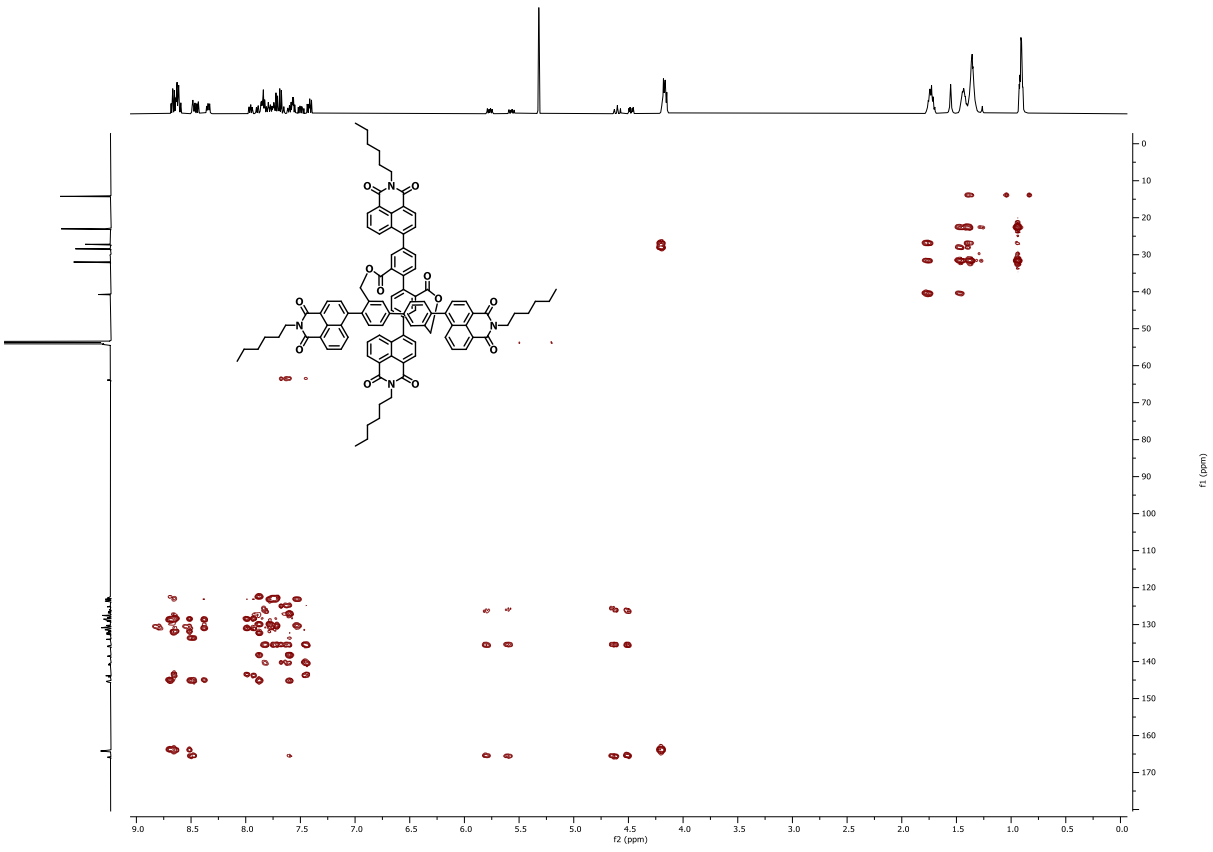
COSY spectrum of **C_{NI4}** in CD_2Cl_2



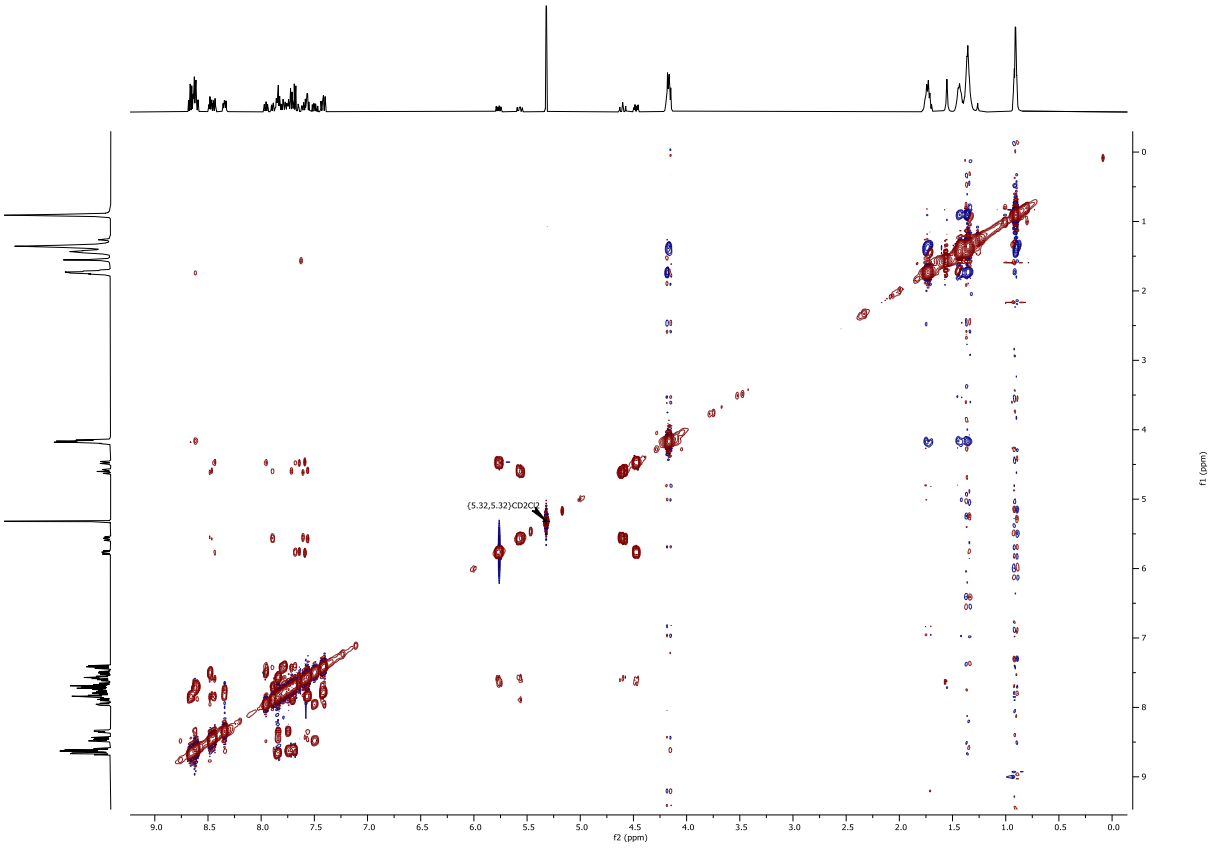
HMQC spectrum of $\mathbf{C_{NI4}}$ in CD_2Cl_2



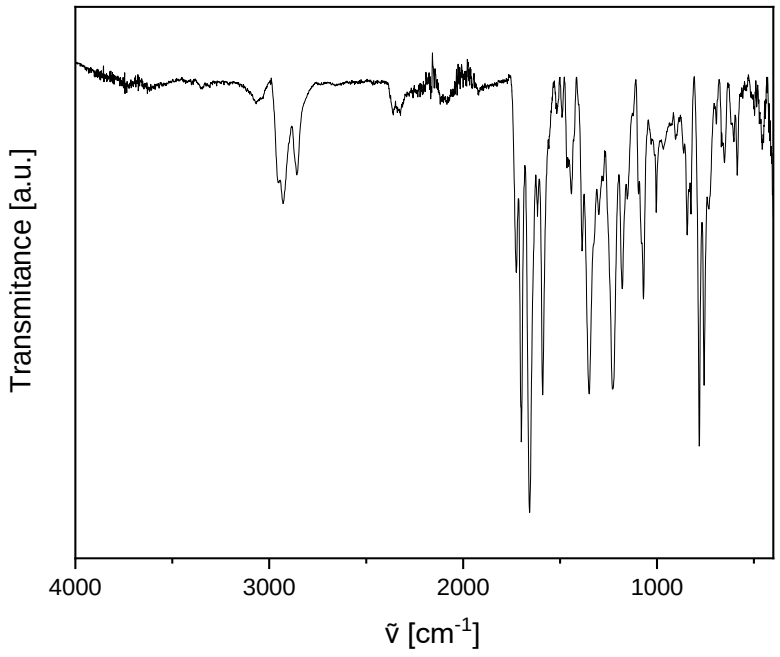
HMBC spectrum of $\mathbf{C_{NI4}}$ in CD_2Cl_2



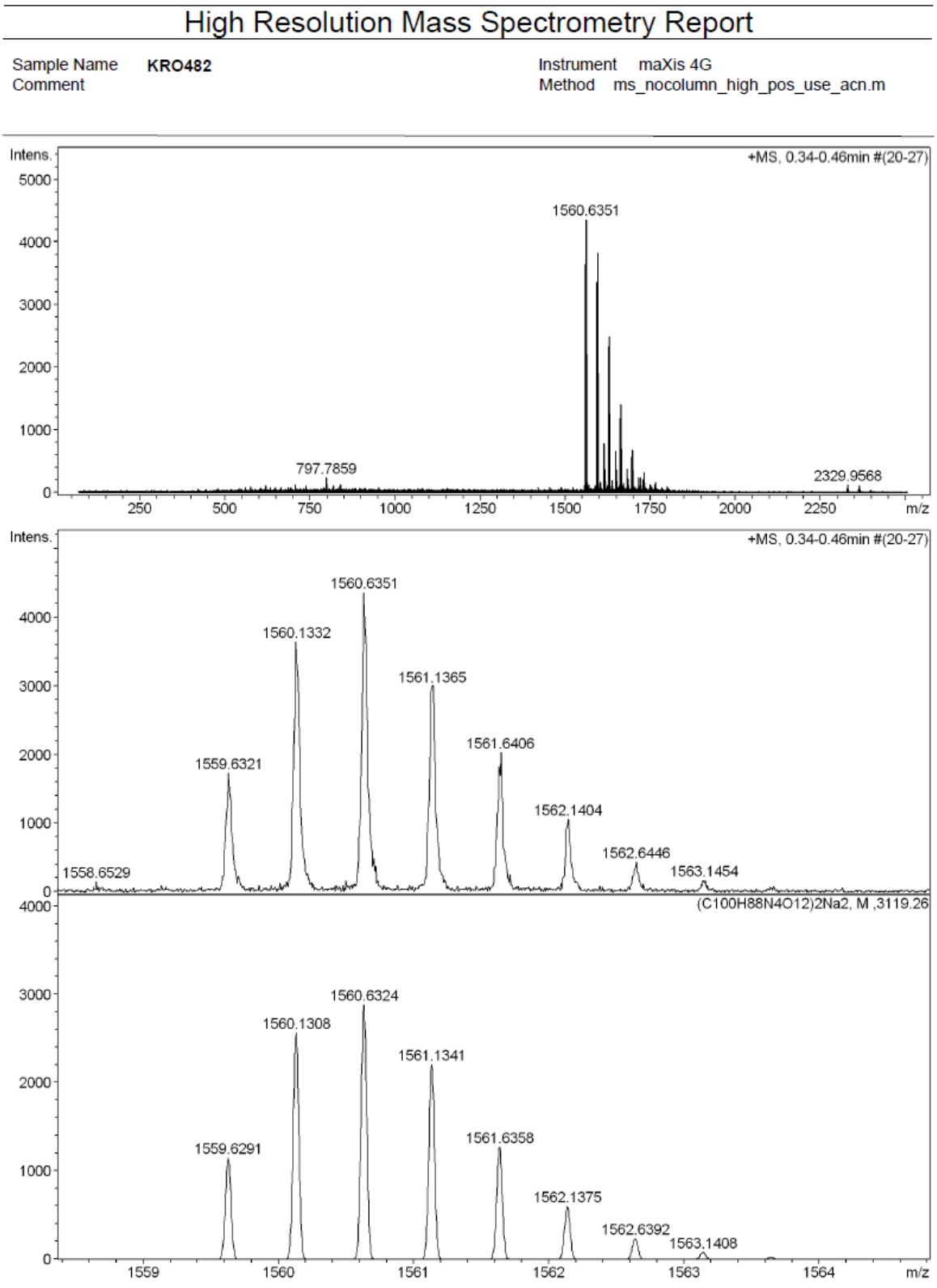
NOESY spectrum of $\mathbf{C_{NI4}}$ in CD_2Cl_2



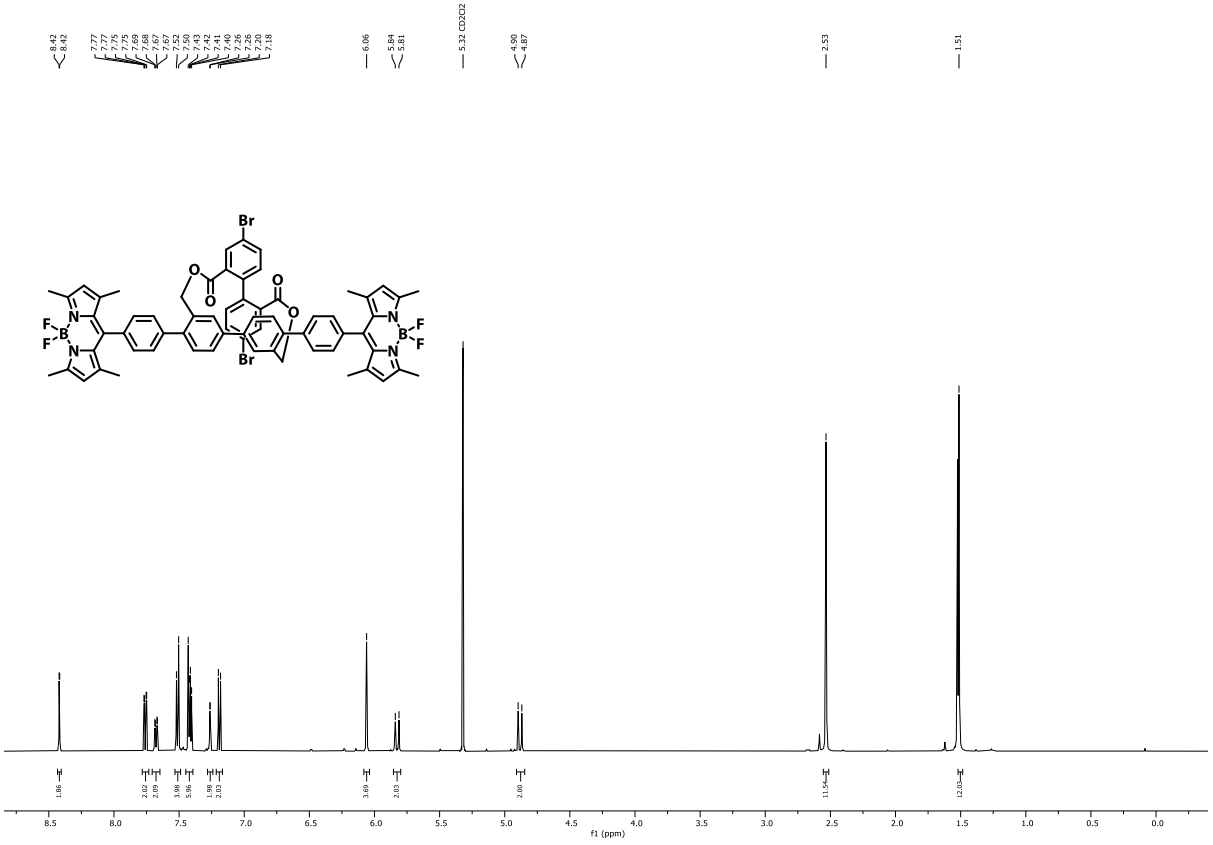
FT-IR spectrum of $\mathbf{C_{NI4}}$ (neat)



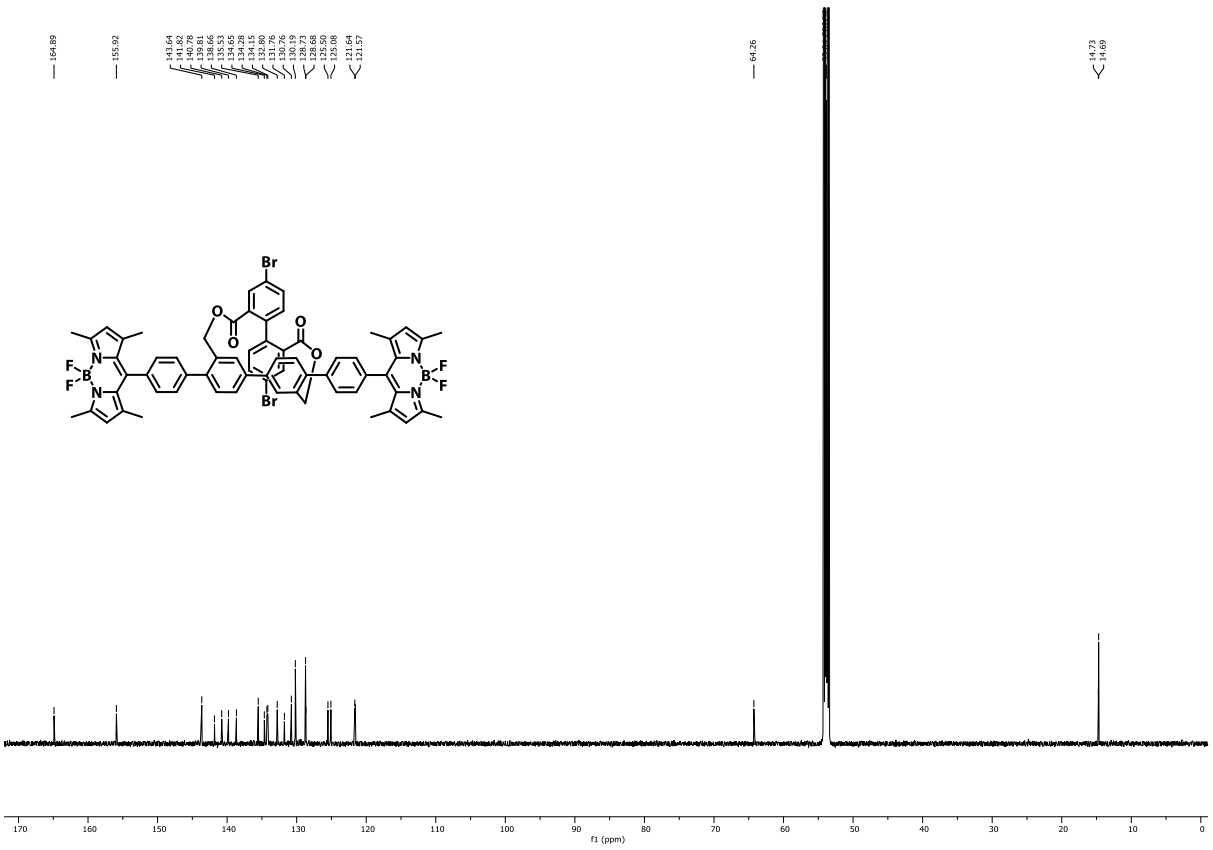
HR-ESI-MS spectrum of C_{NI4}



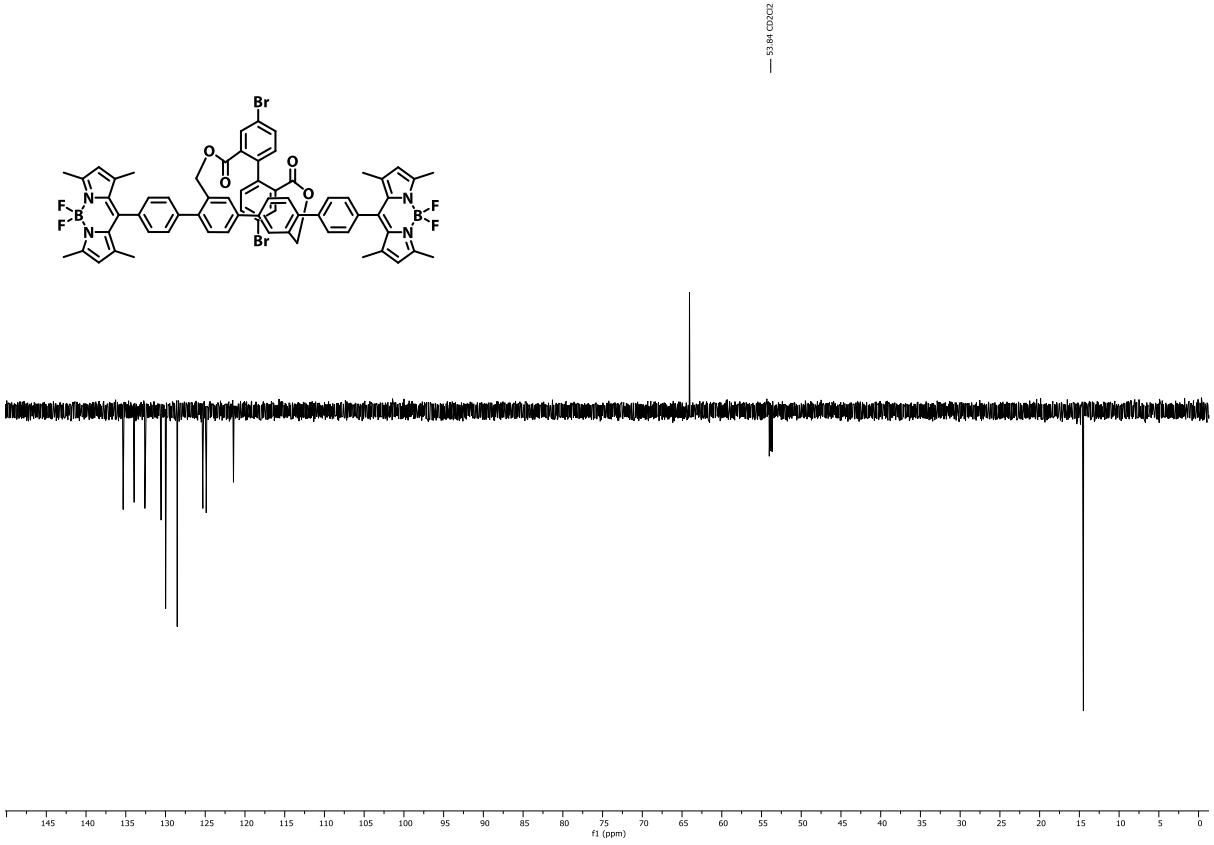
^{1}H-NMR spectrum of $\mathbf{C_{Br2BY2}}$ in CD_2Cl_2



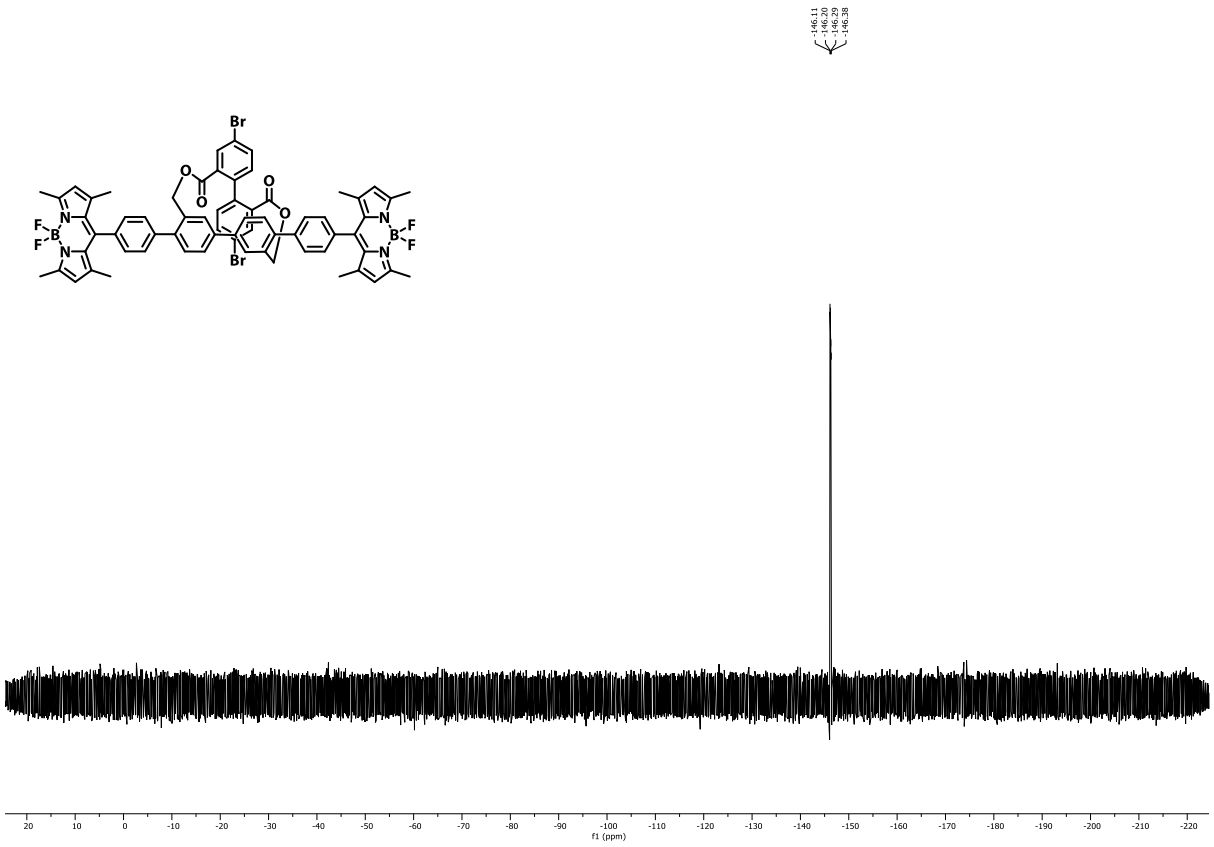
^{13}C-NMR spectrum of $\mathbf{C_{Br2BY2}}$ in CD_2Cl_2



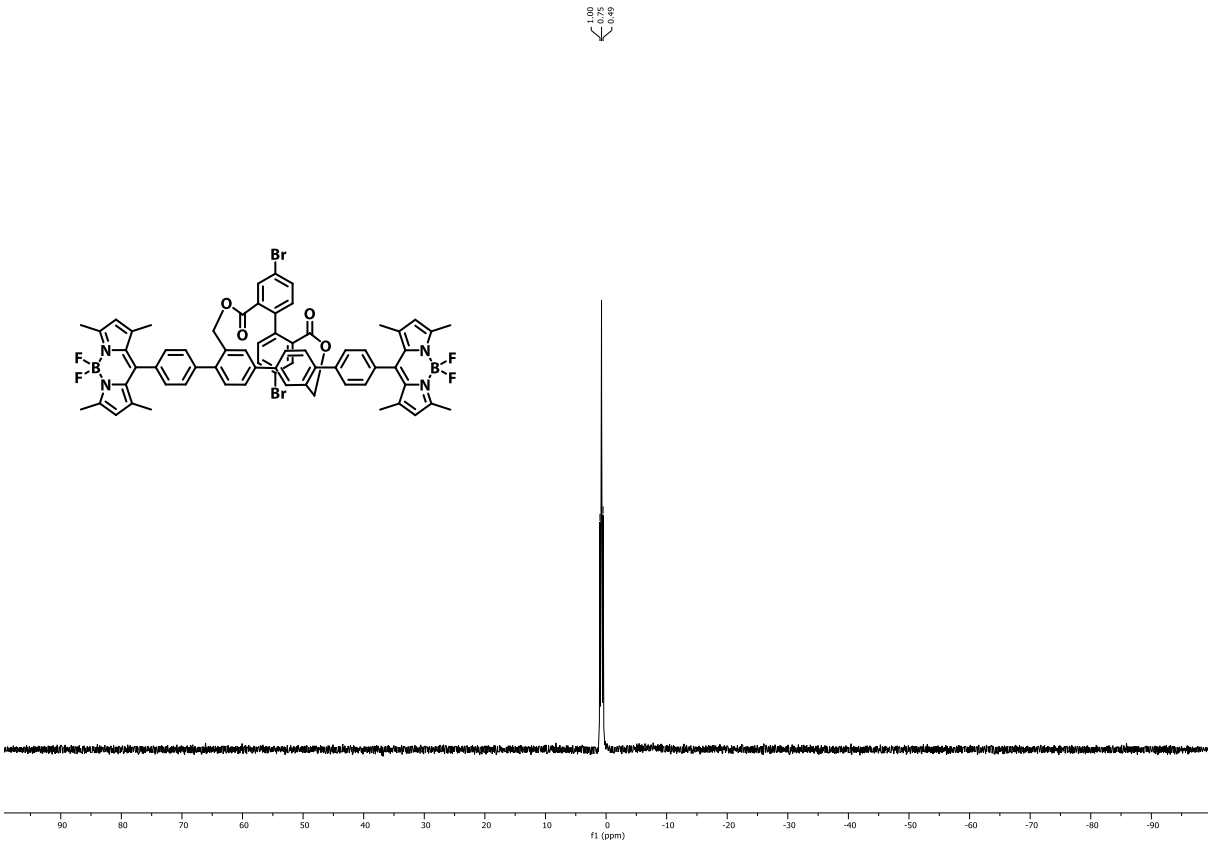
^{13}C-Dept spectrum of $\mathbf{C_{Br2BY2}}$ in CD_2Cl_2



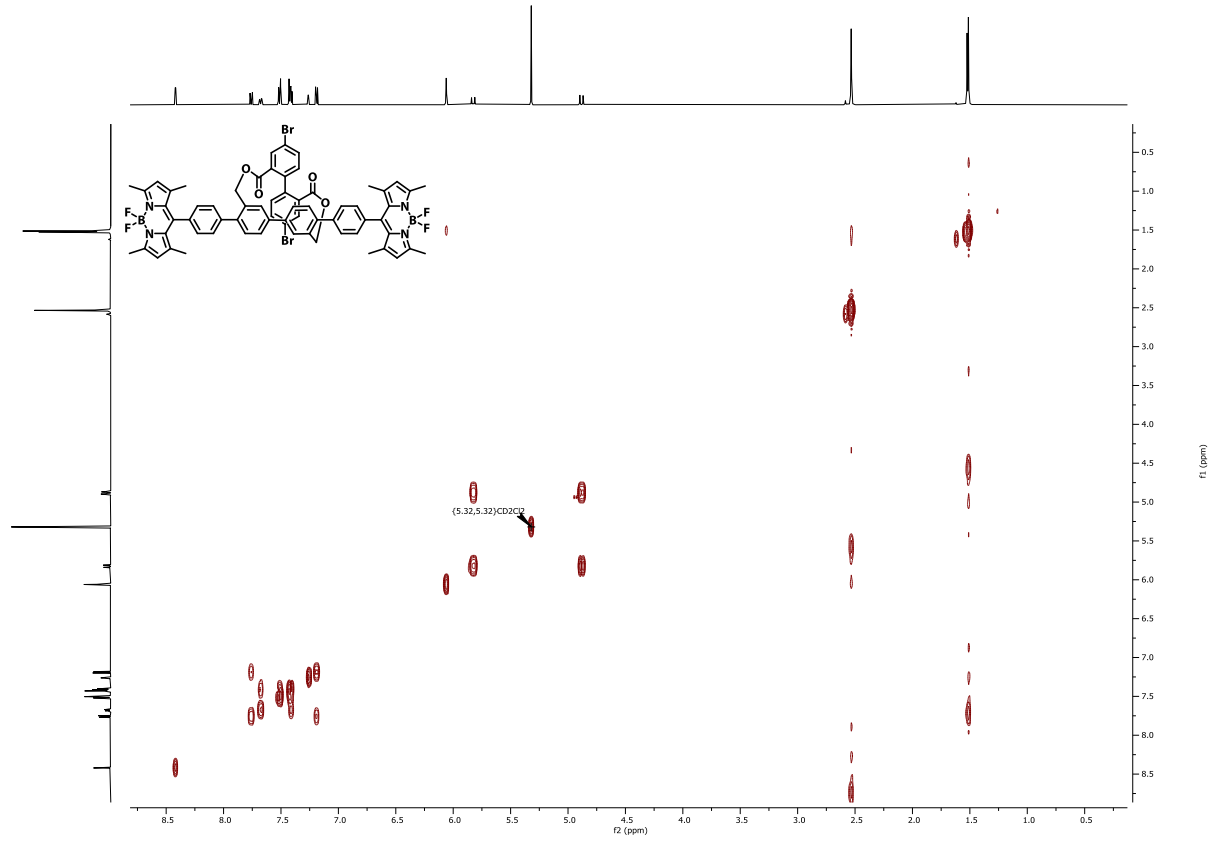
^{19}F-NMR spectrum of $\mathbf{C_{Br2BY2}}$ in CD_2Cl_2



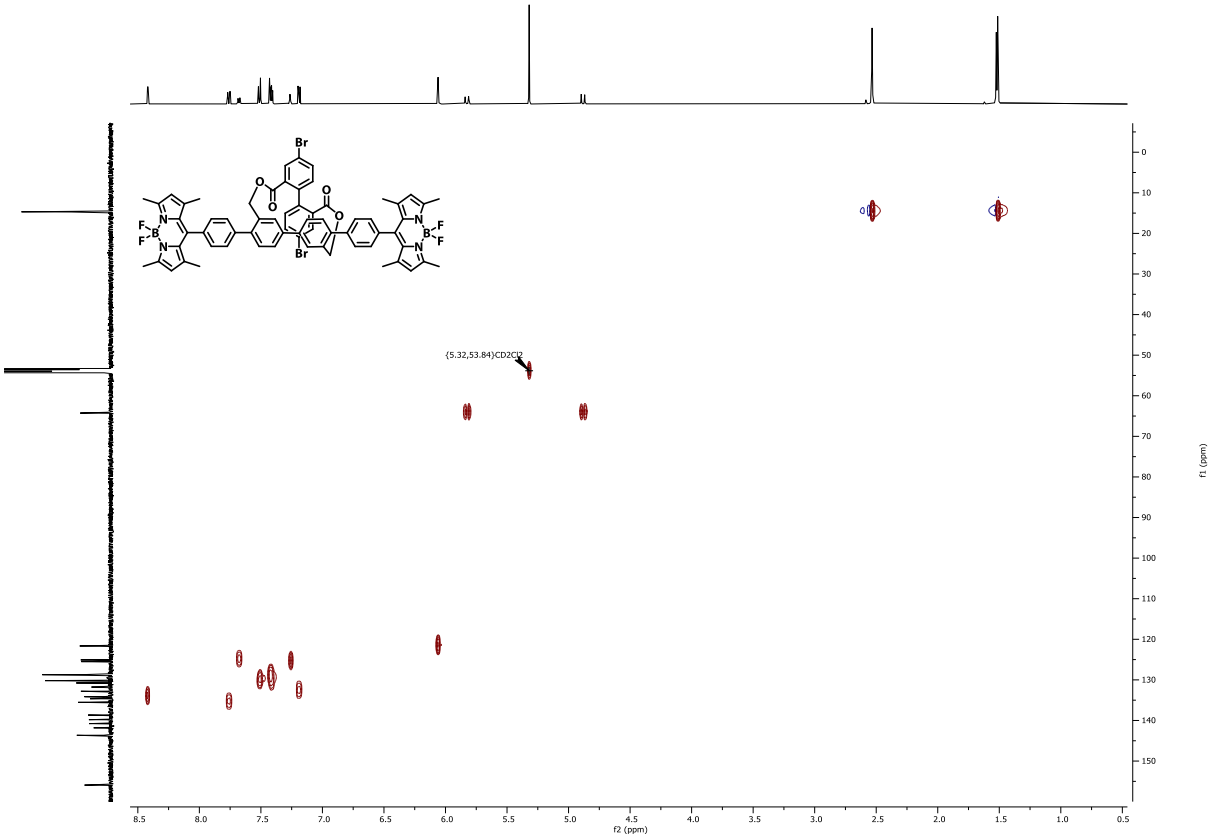
^{11}B-NMR spectrum of **C_{Br2BY2}** in CD_2Cl_2



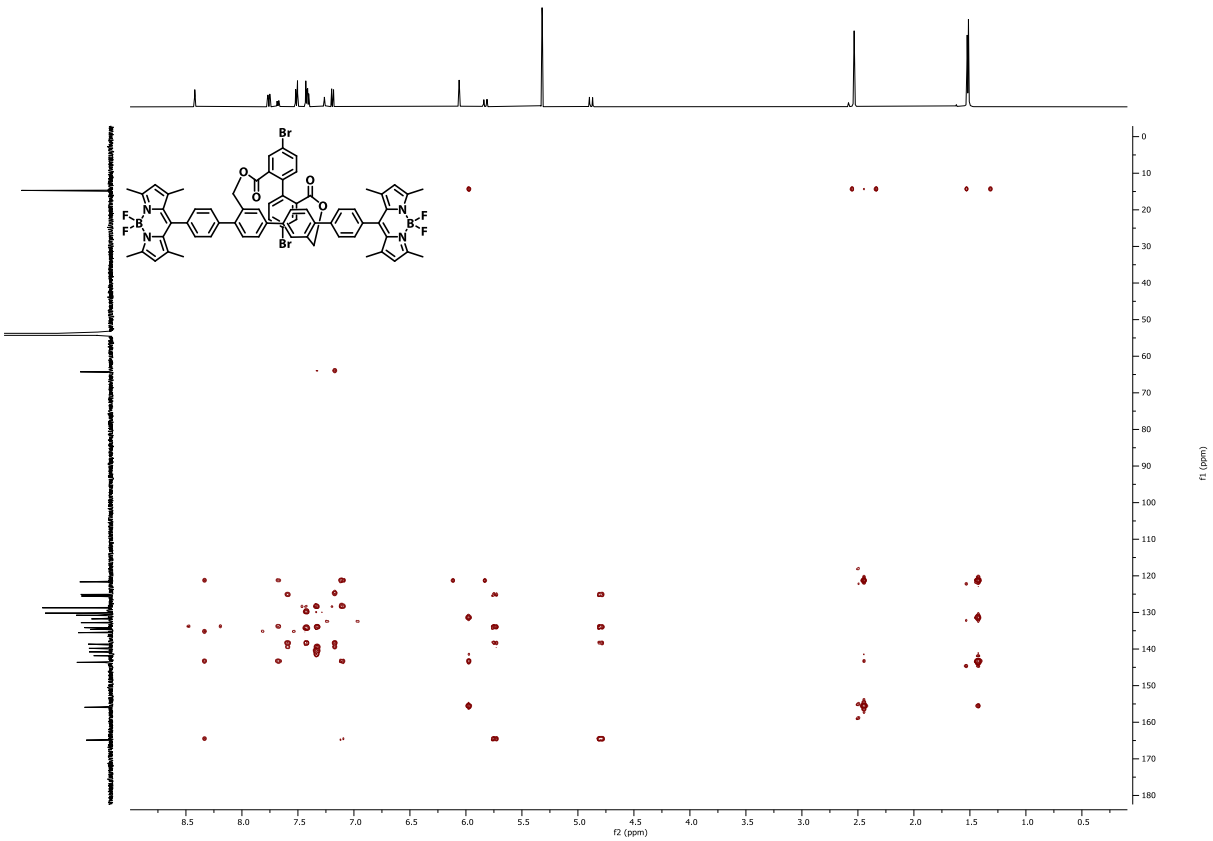
COSY spectrum of **C_{Br2BY2}** in CD_2Cl_2



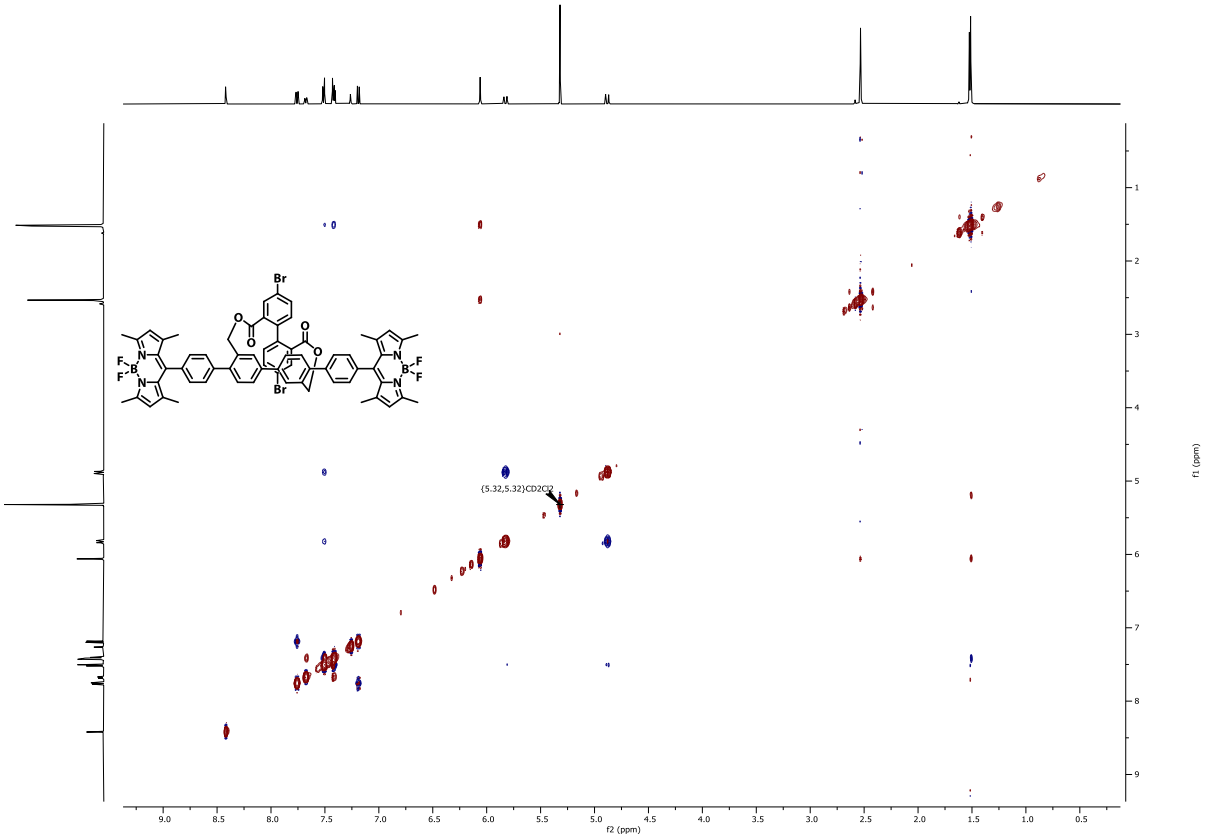
HMQC spectrum of $\mathbf{C_{Br2BY2}}$ in CD_2Cl_2



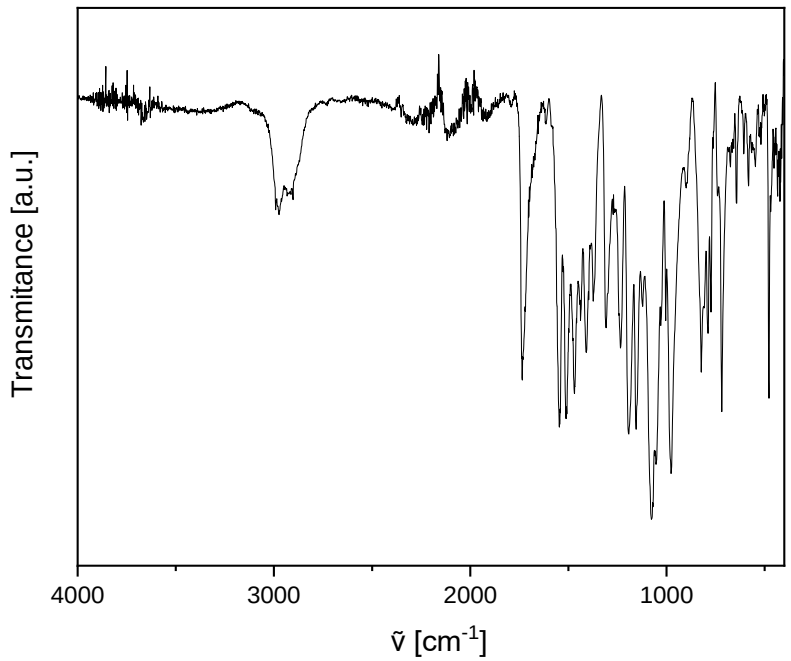
HMBC spectrum of $\mathbf{C_{Br2BY2}}$ in CD_2Cl_2



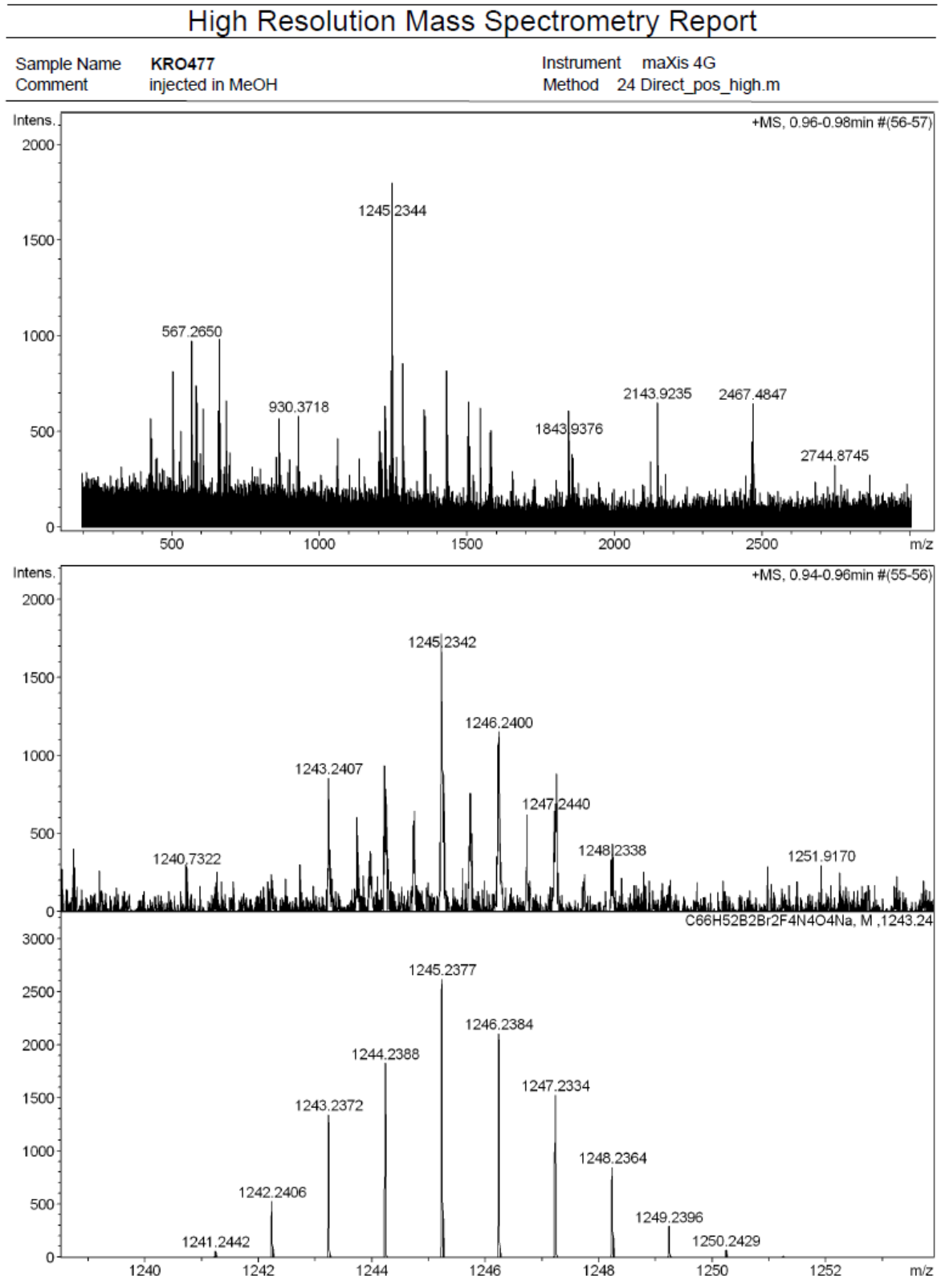
NOESY spectrum of $\mathbf{C_{Br2BY2}}$ in CD_2Cl_2



FT-IR spectrum of $\mathbf{C_{Br2BY2}}$ (neat)



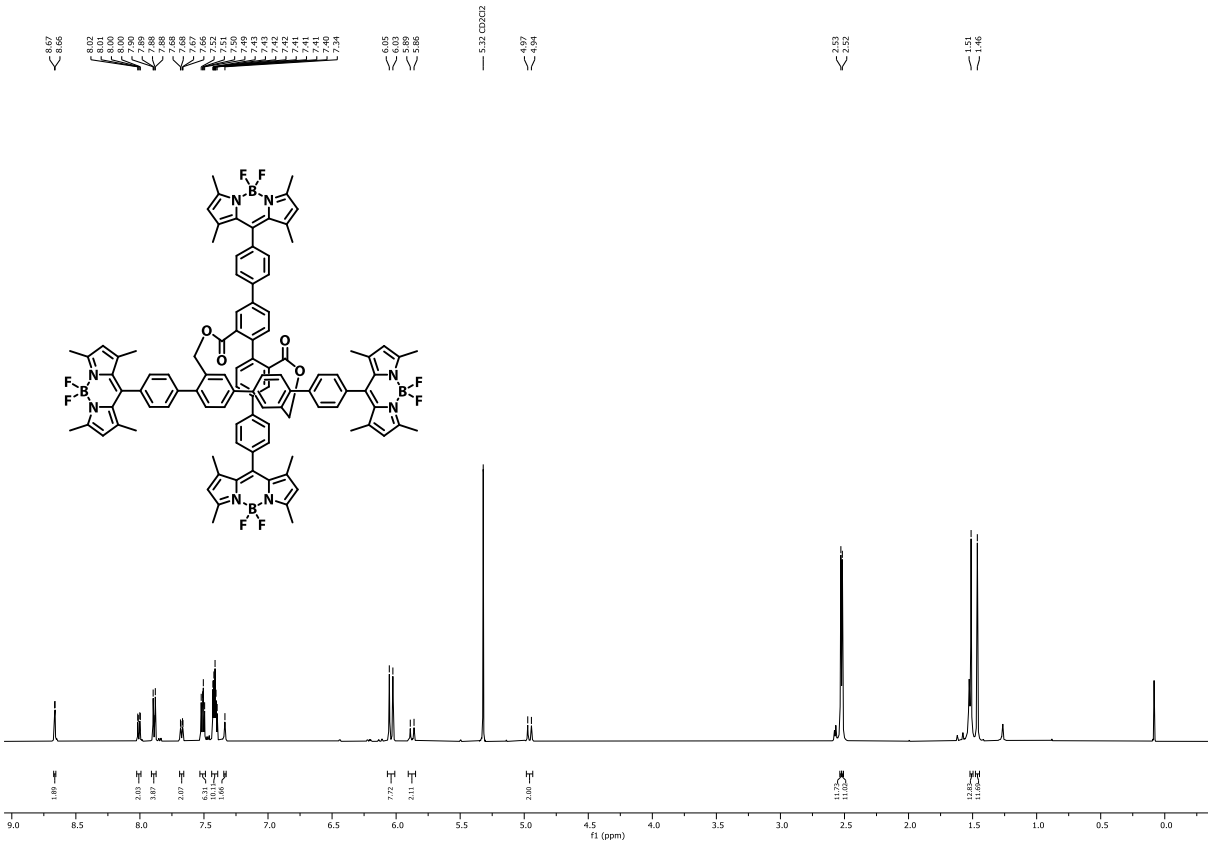
HR-ESI-MS spectrum of C_{Br2BY2}



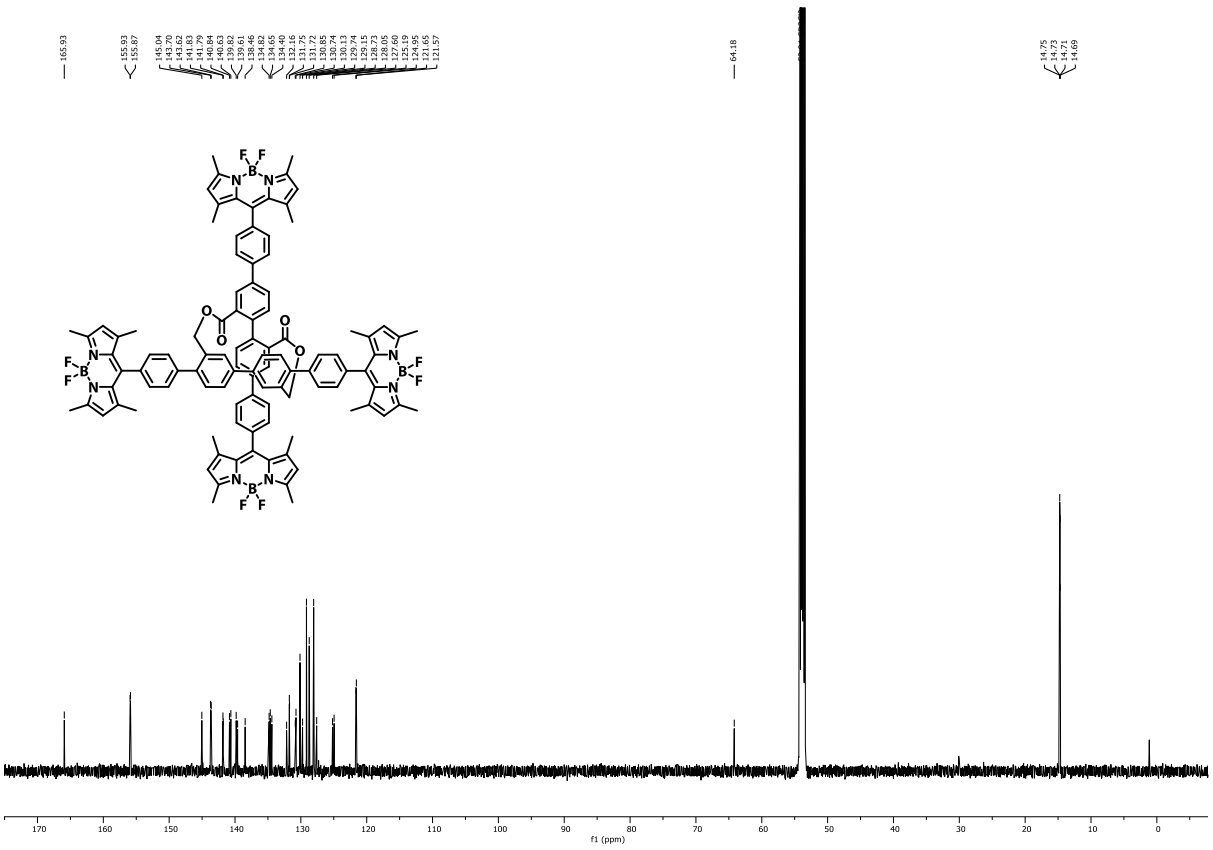
Measured m/z vs. theoretical m/z

Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e¯ Conf	z
1243.2407	1	C 66 H 52 B 2 Br 2 F 4 N 4 Na O 4	100.00	1243.2372	-3.4	-2.8	109.2	40.5	even	1+
2441.5071	1	C 132 H 105 B 4 Br 4 F 8 N 8 O 8	100.00	2441.5087	1.6	0.7	540.2	80.5	even	

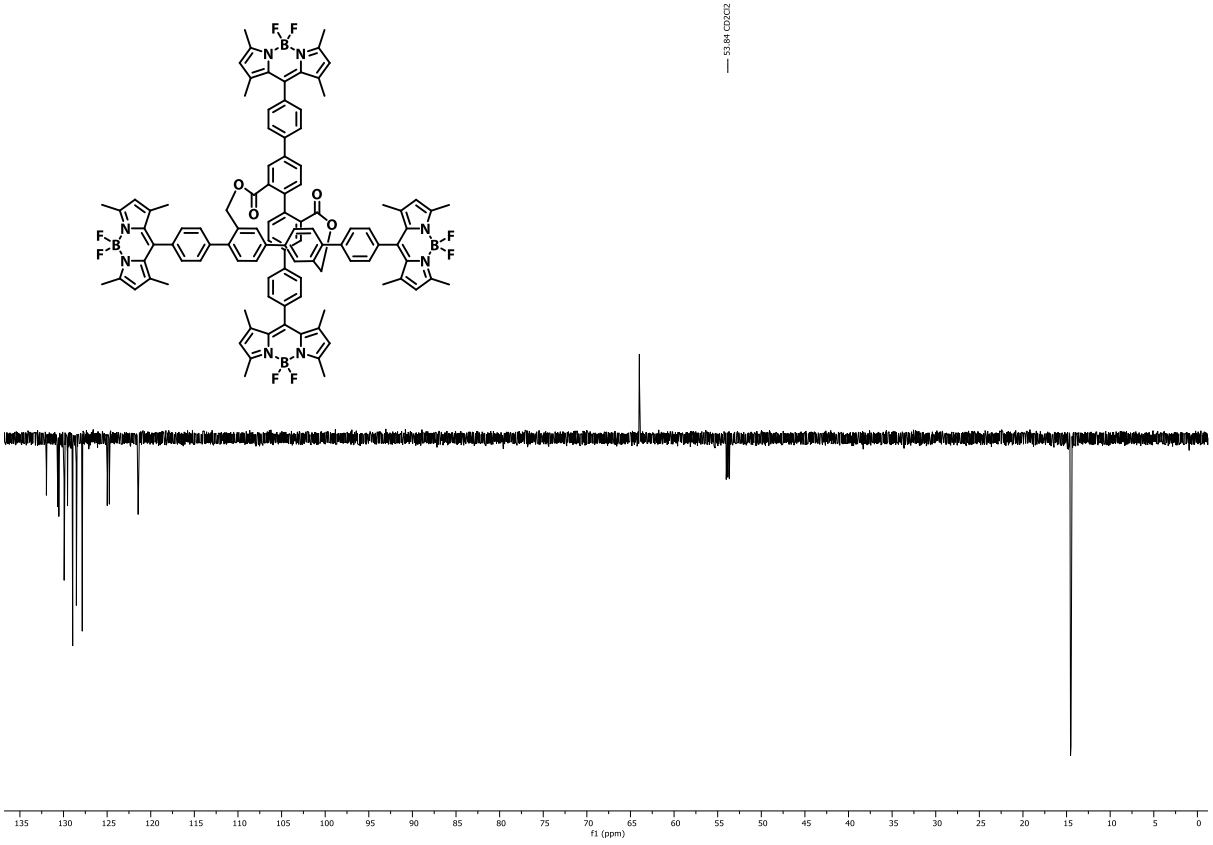
^{1}H-NMR spectrum of $\mathbf{C_{BY4}}$ in CD_2Cl_2



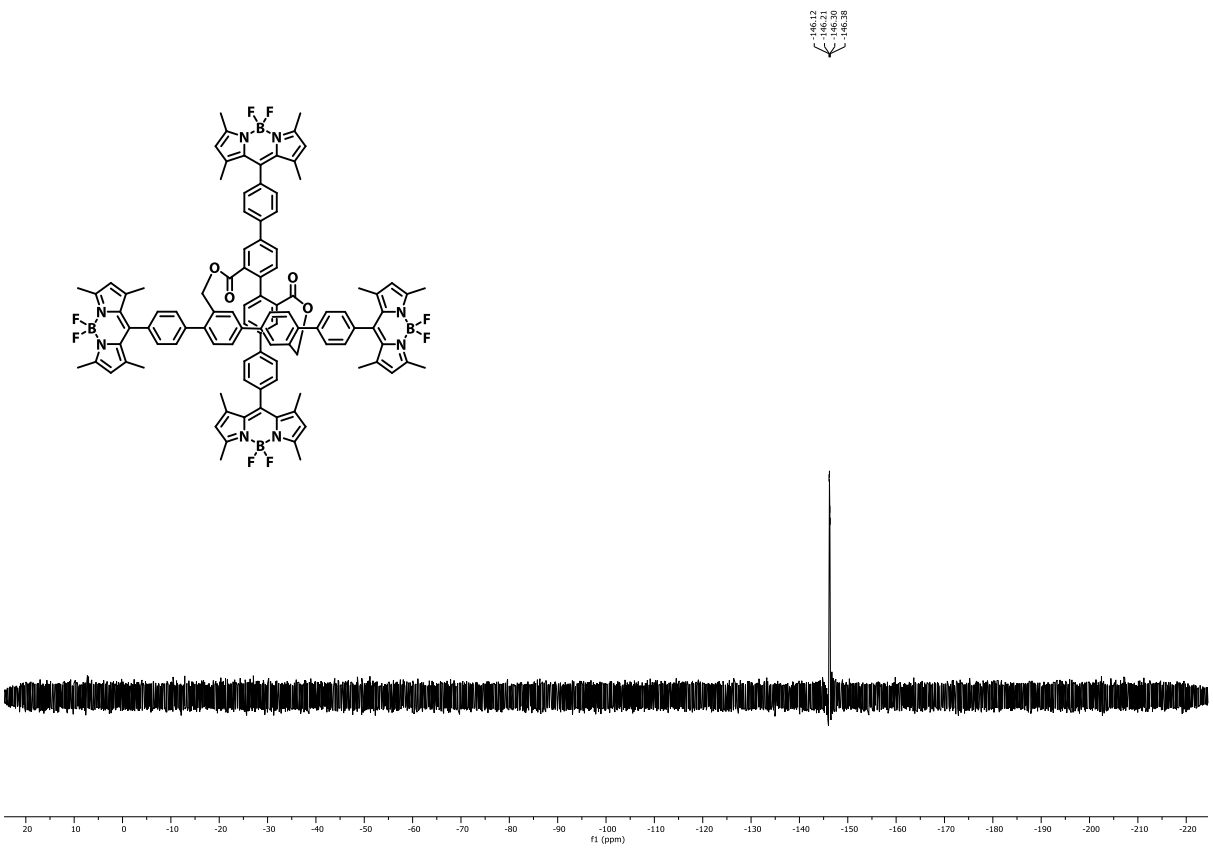
^{13}C-NMR spectrum of $\mathbf{C_{BY4}}$ in CD_2Cl_2



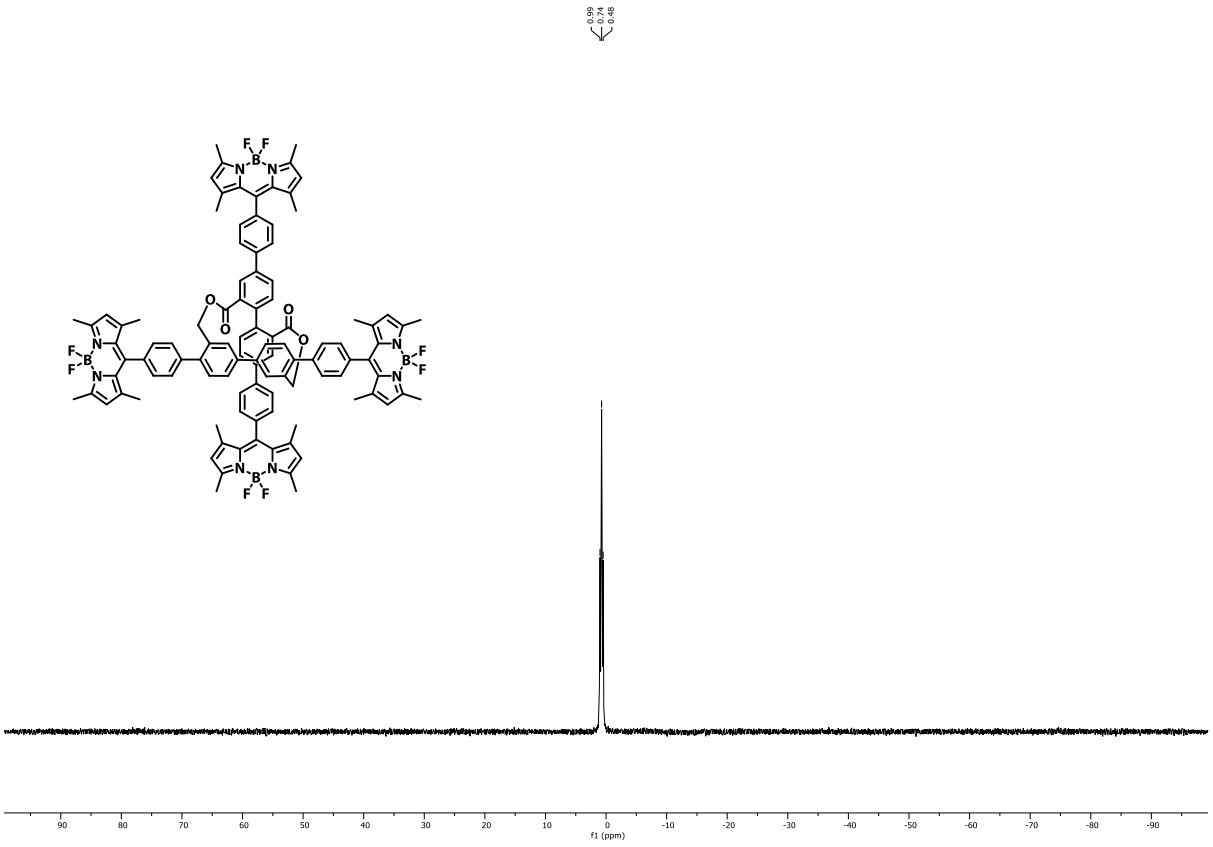
^{13}C-Dept spectrum of **C_{BY4}** in CD_2Cl_2



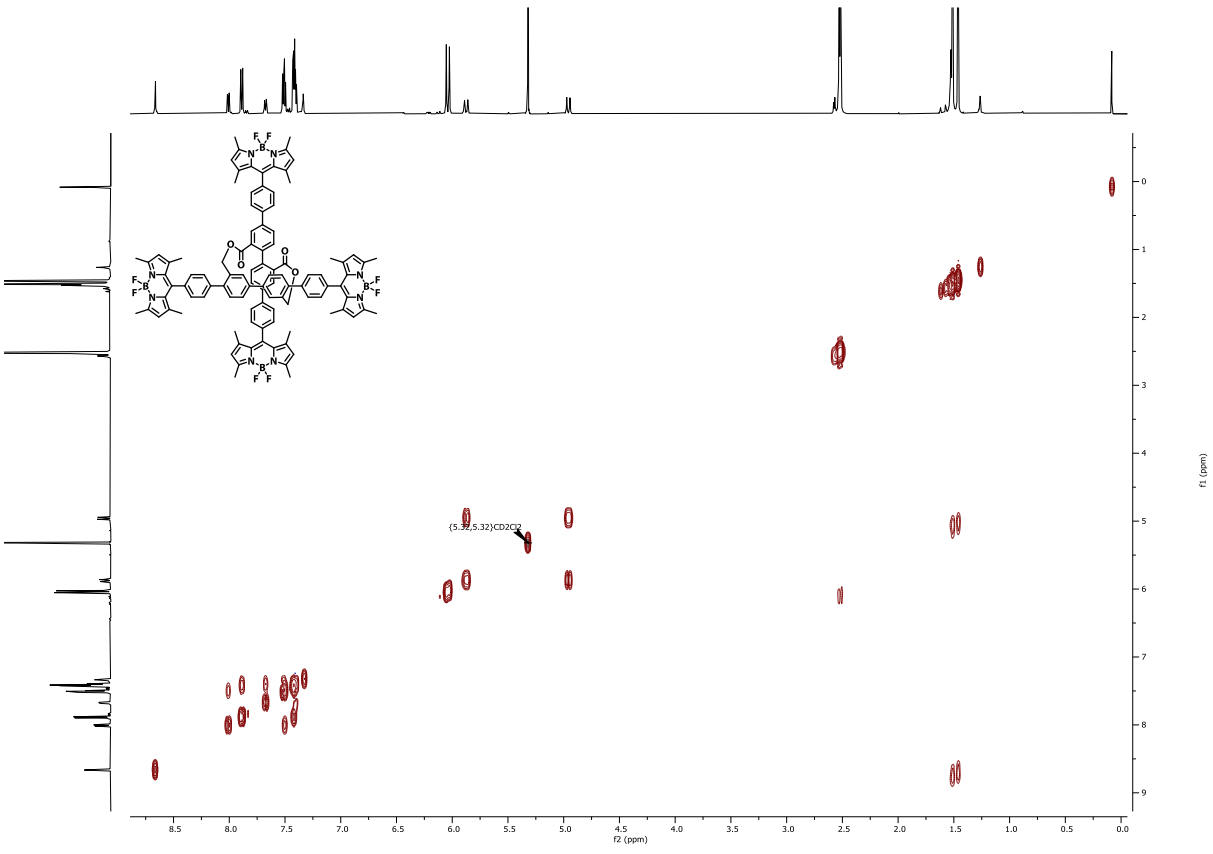
^{19}F-NMR spectrum of **C_{BY4}** in CD_2Cl_2



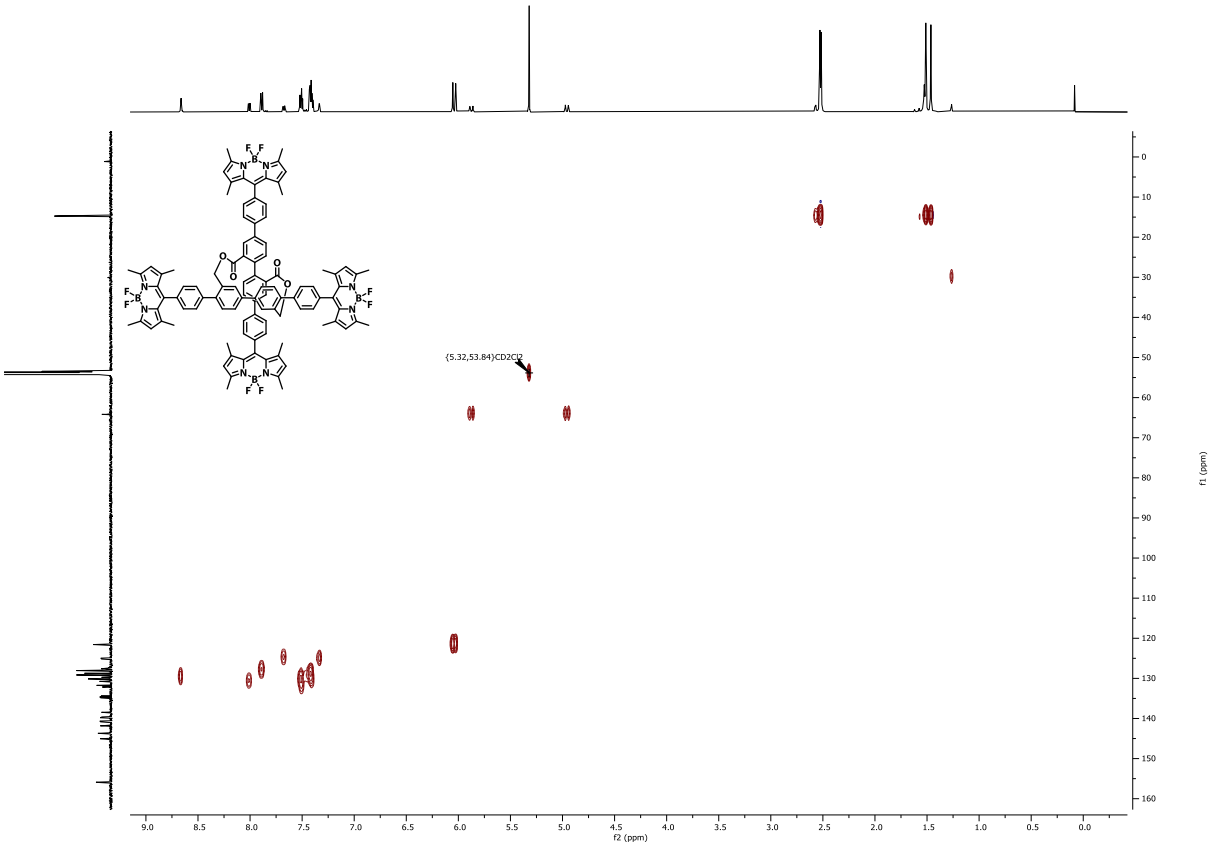
^{11}B-NMR spectrum of **C_{BY4}** in CD_2Cl_2



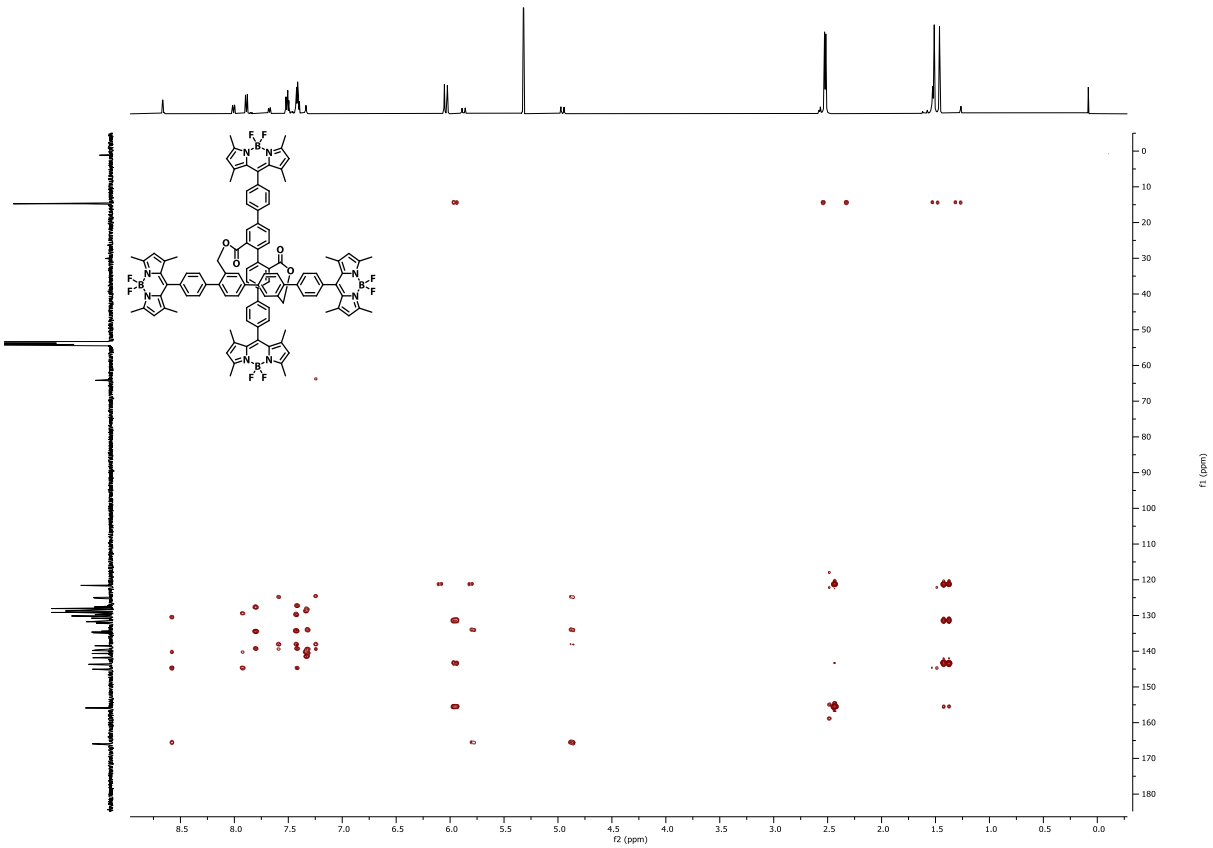
COSY spectrum of **C_{BY4}** in CD_2Cl_2



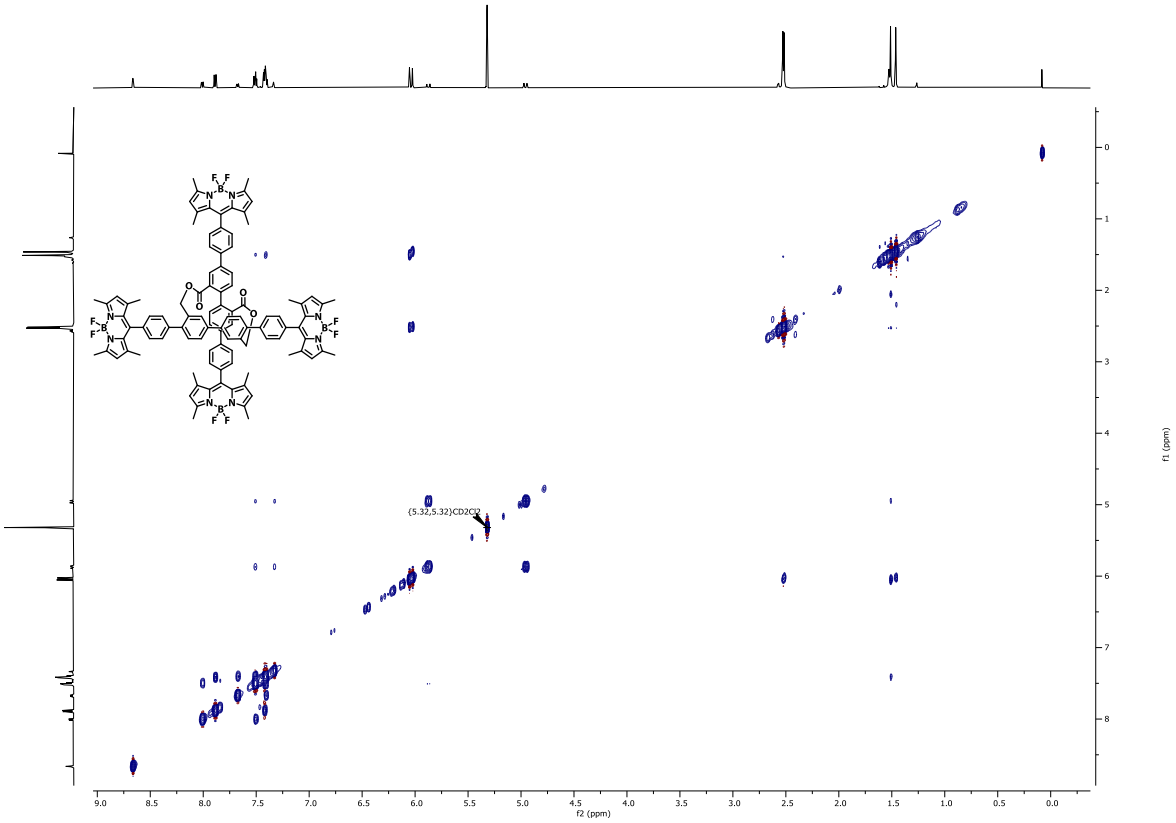
HMQC spectrum of $\mathbf{C_{BY4}}$ in CD_2Cl_2



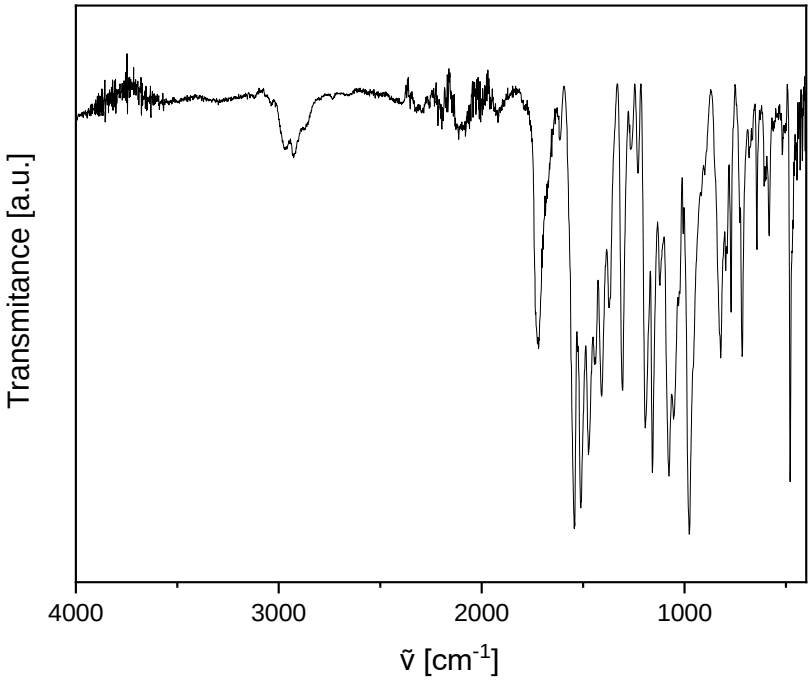
HMBC spectrum of $\mathbf{C_{BY4}}$ in CD_2Cl_2



NOESY spectrum of $\mathbf{C_{BY4}}$ in CD_2Cl_2



FT-IR spectrum of $\mathbf{C_{BY4}}$ (neat)

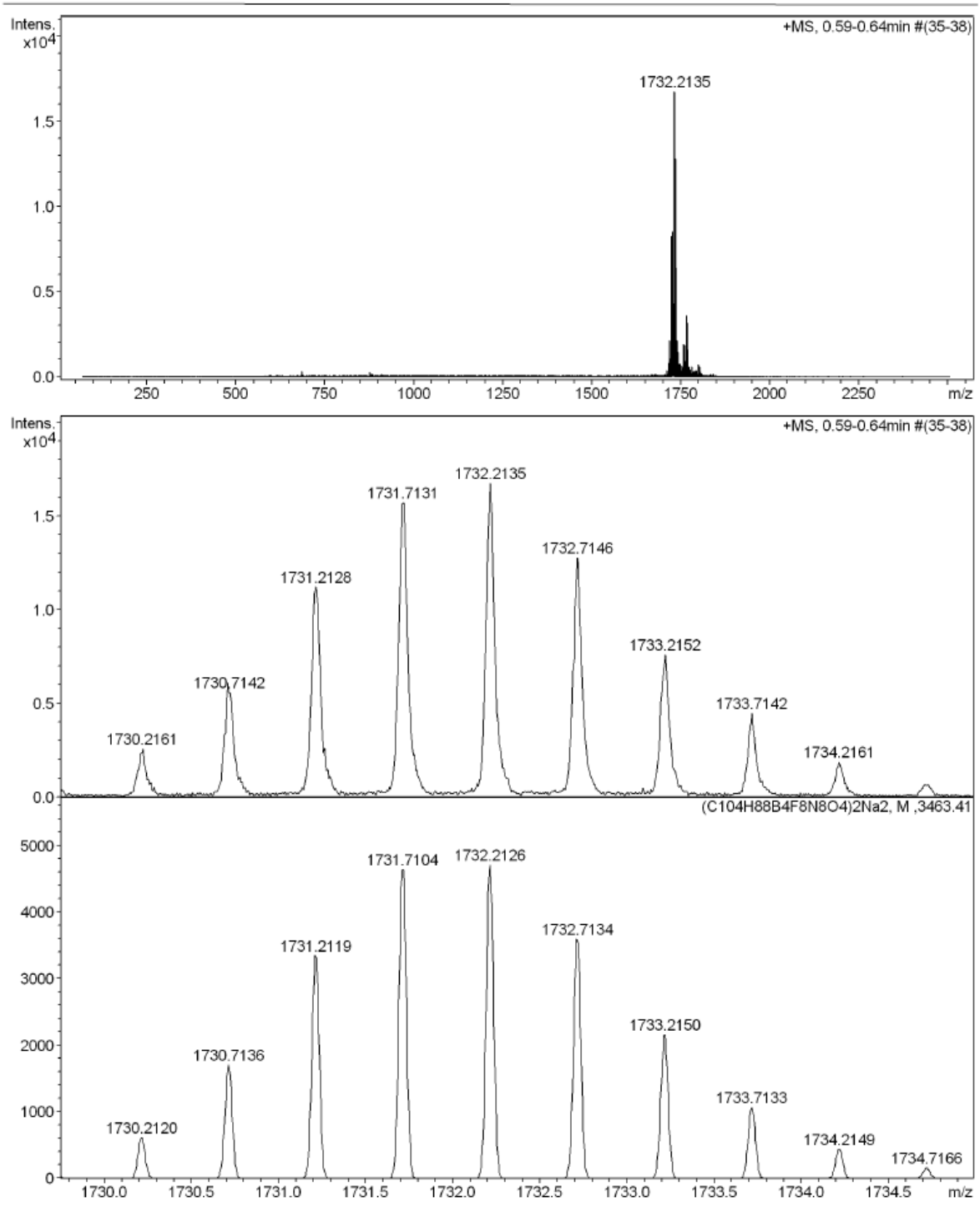


HR-ESI-MS spectrum of C_{BY4}

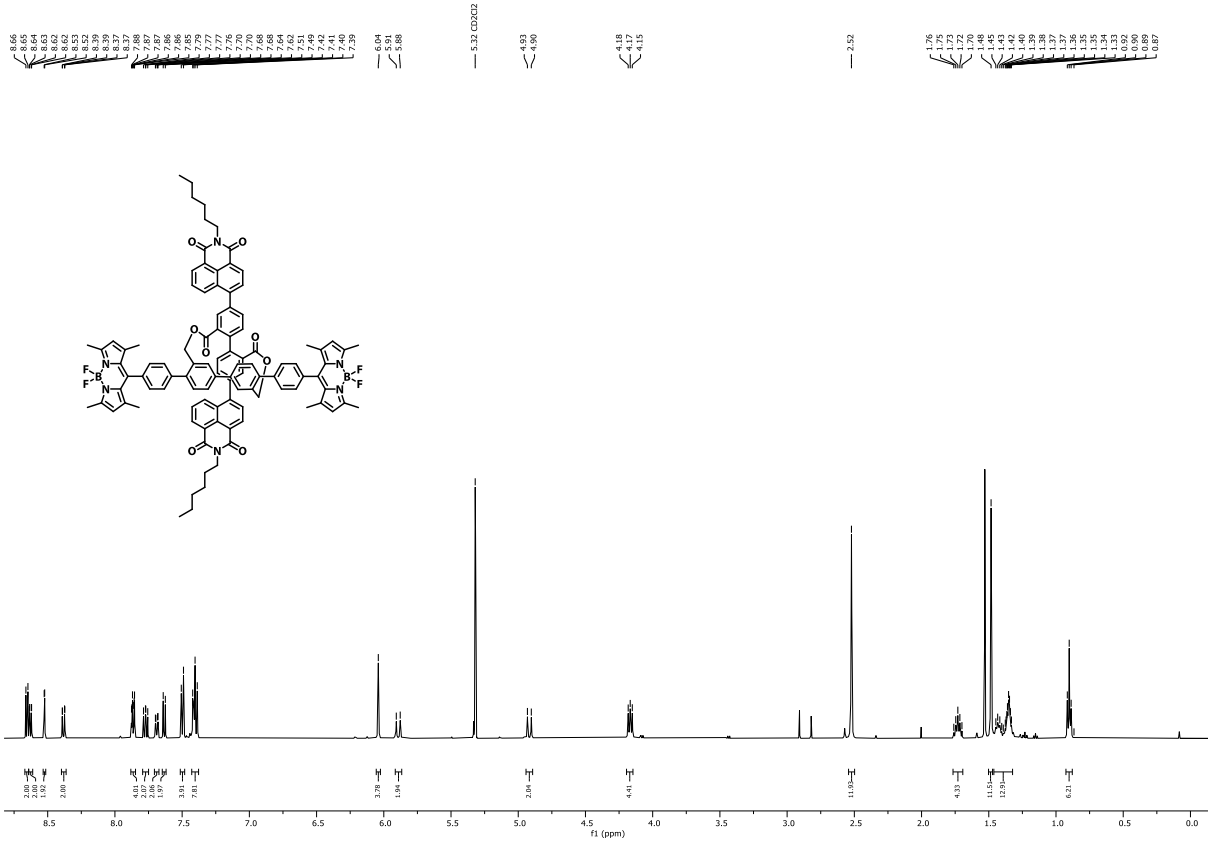
High Resolution Mass Spectrometry Report

Sample Name **KRO480**
Comment

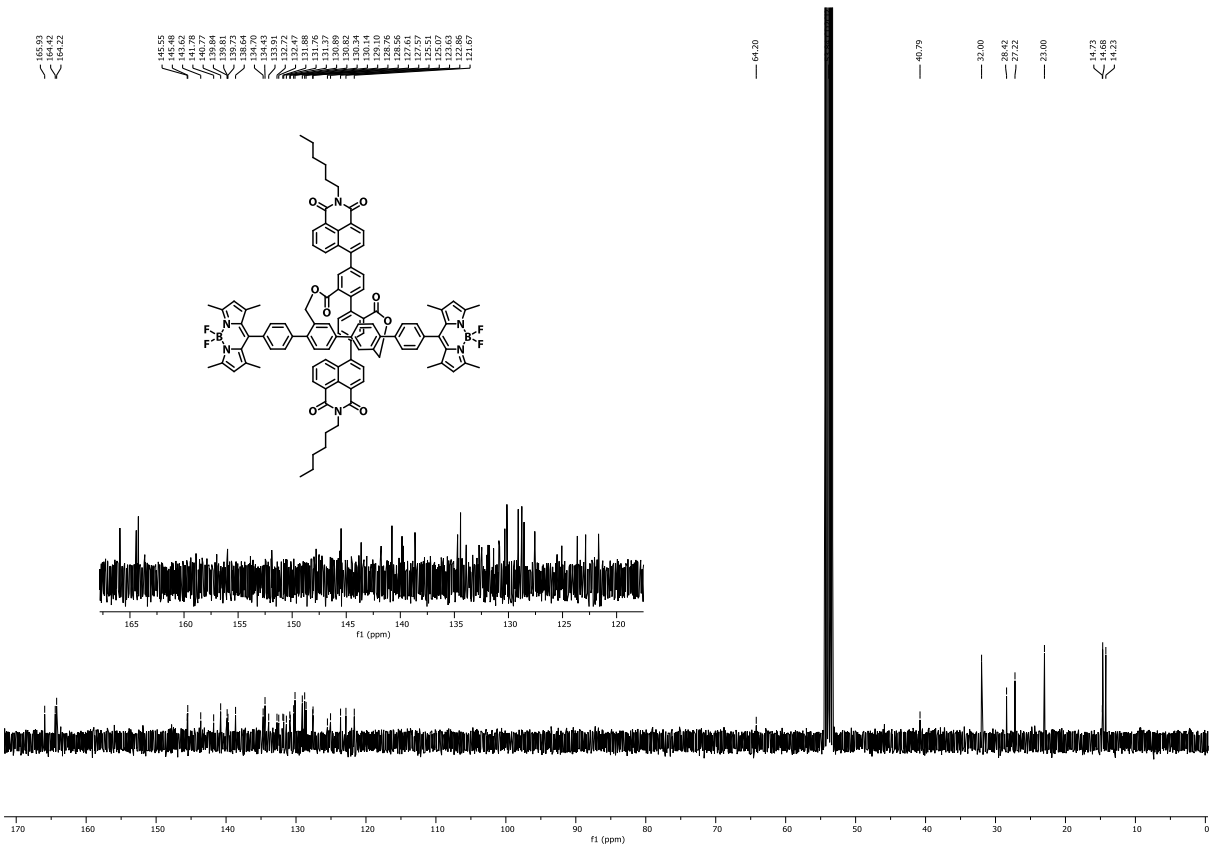
Instrument maXis 4G
Method ms_nocolumn_high_pos_use_acn.m



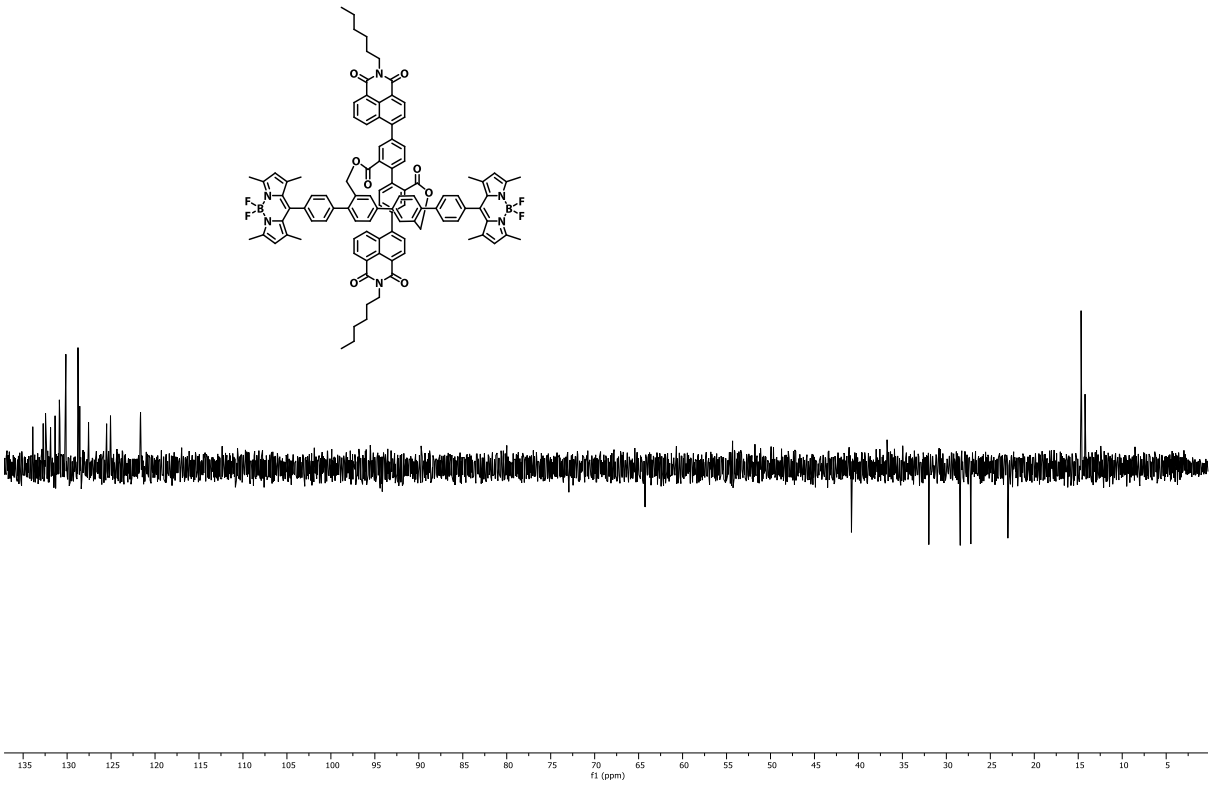
^{1}H-NMR spectrum of $\mathbf{C_{NI2BY2}}$ in CD_2Cl_2



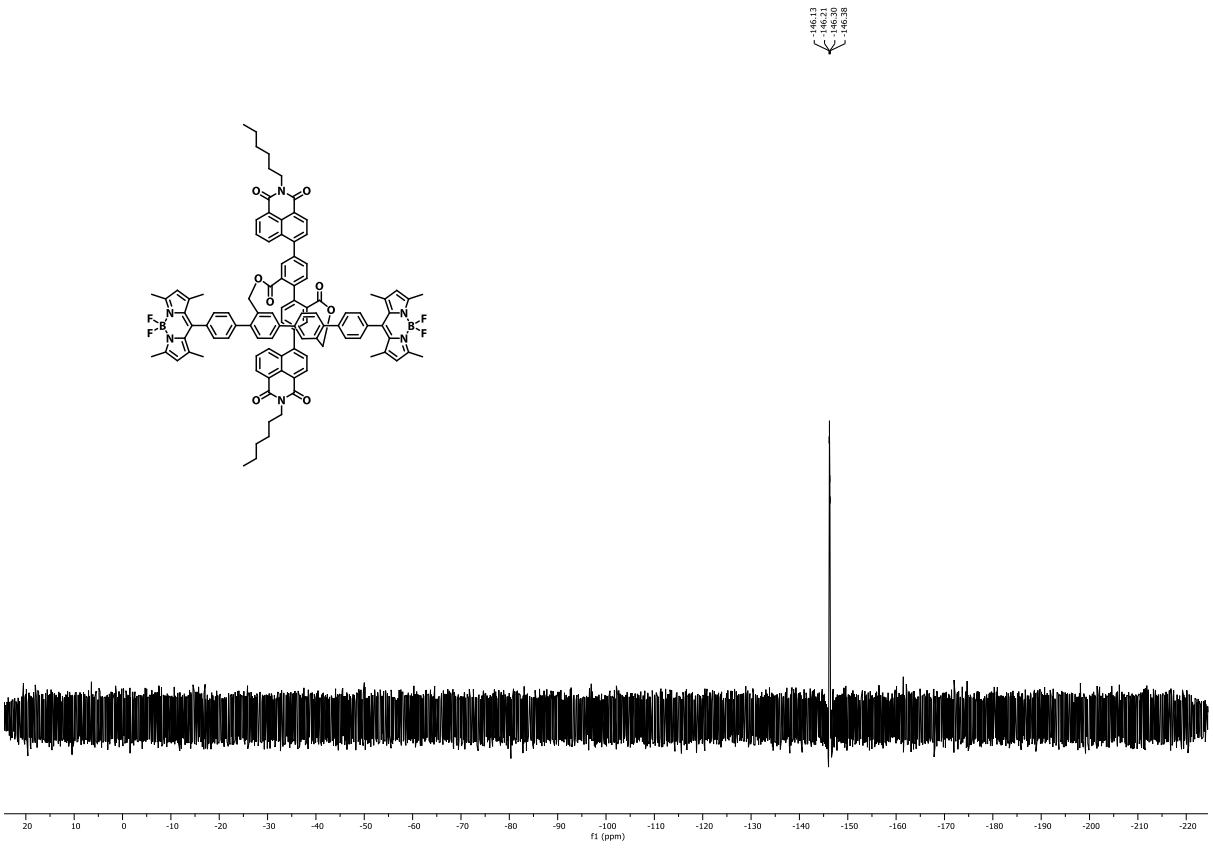
^{13}C-NMR spectrum of $\mathbf{C_{NI2BY2}}$ in CD_2Cl_2



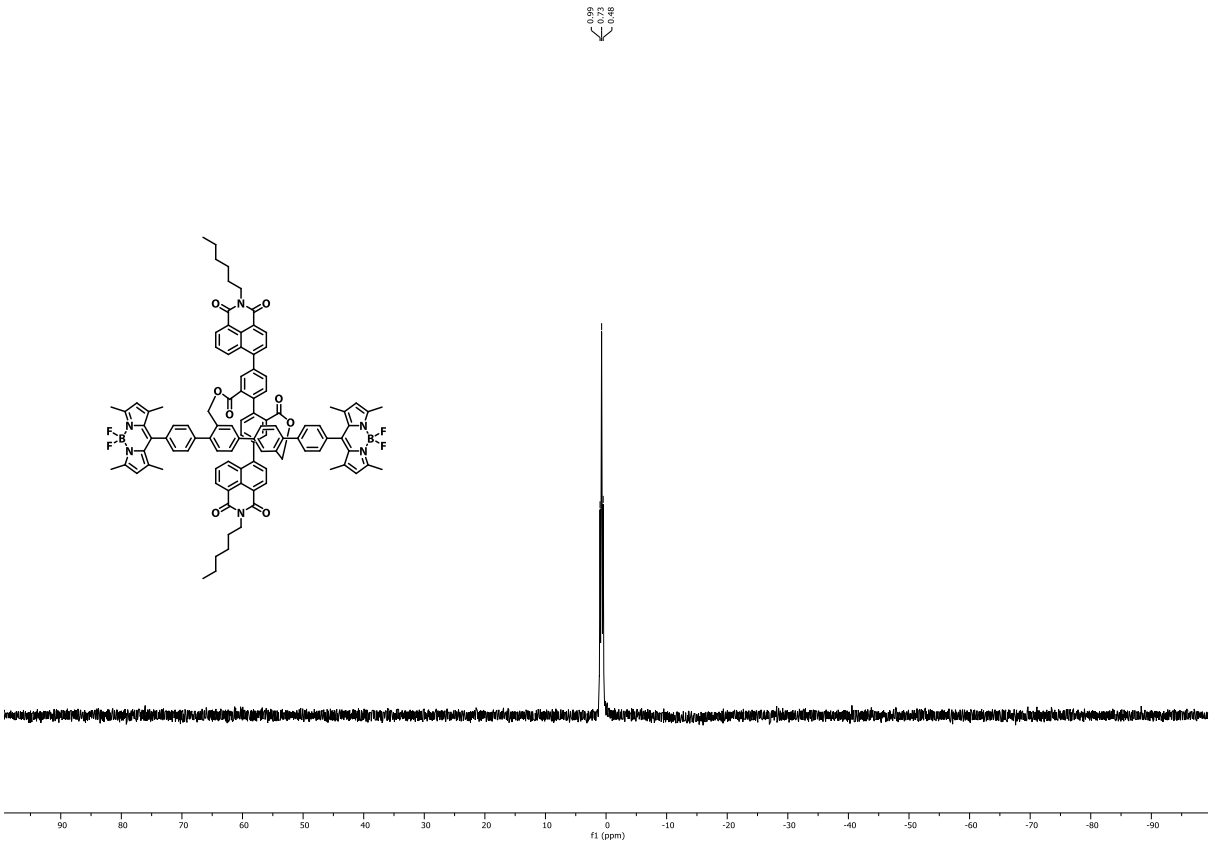
^{13}C-Dept spectrum of **C_{NI2BY2}** in CD_2Cl_2



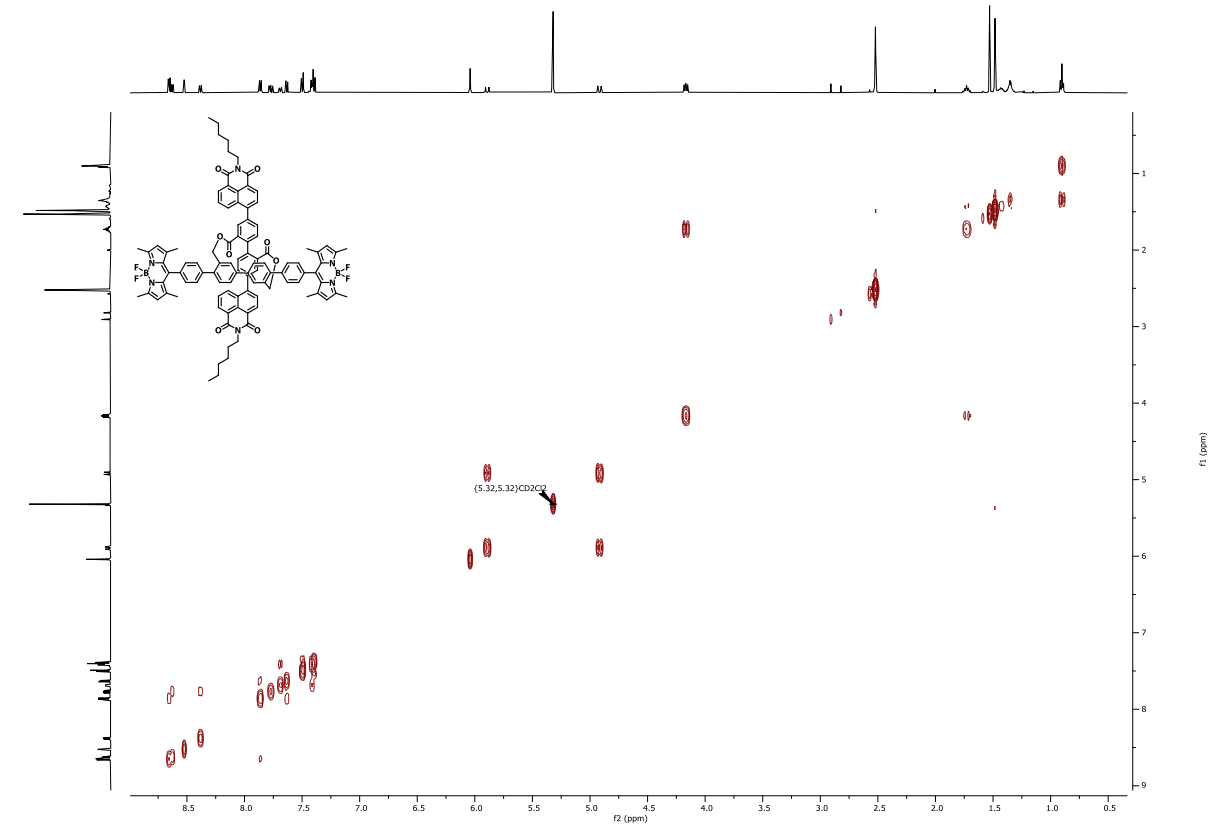
^{19}F-NMR spectrum of **C_{NI2BY2}** in CD_2Cl_{2kk}



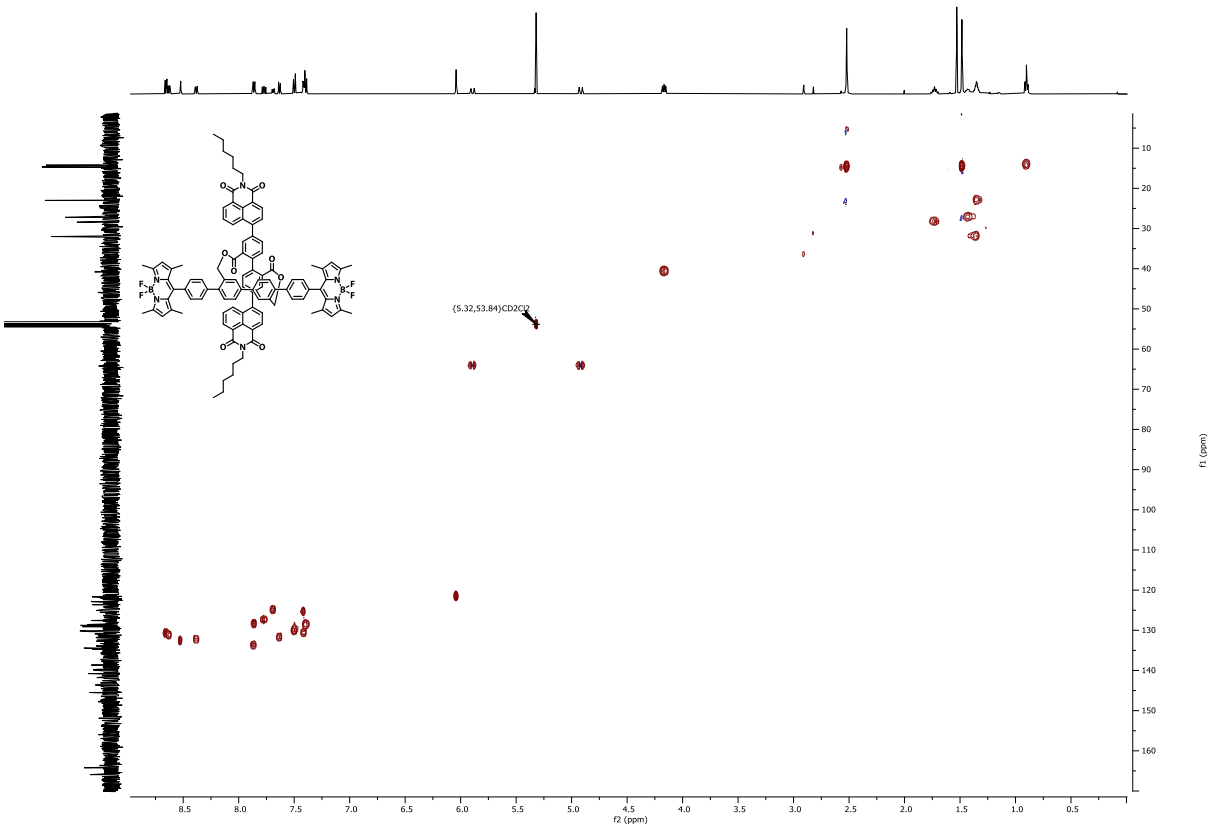
^{11}B-NMR spectrum of **C_{NI2BY2}** in CD_2Cl_2



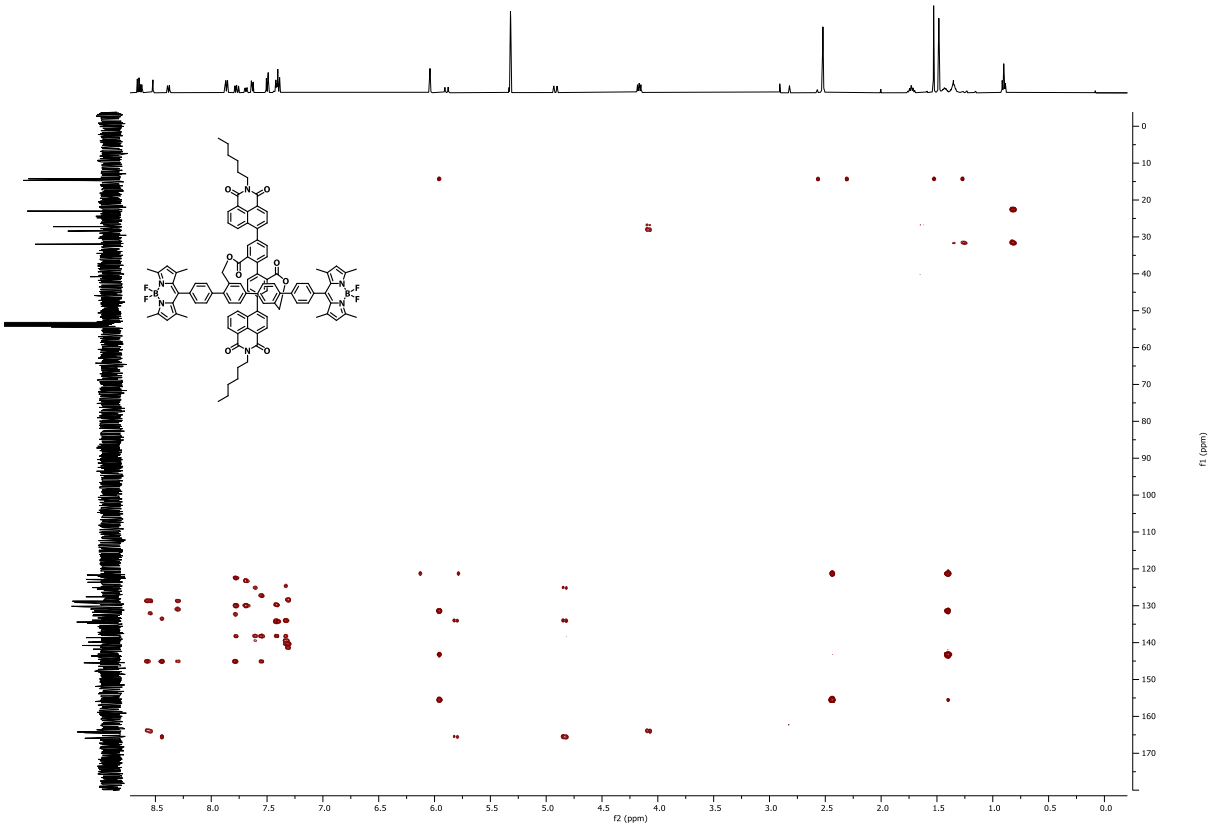
COSY spectrum of **C_{NI2BY2}** in CD_2Cl_2



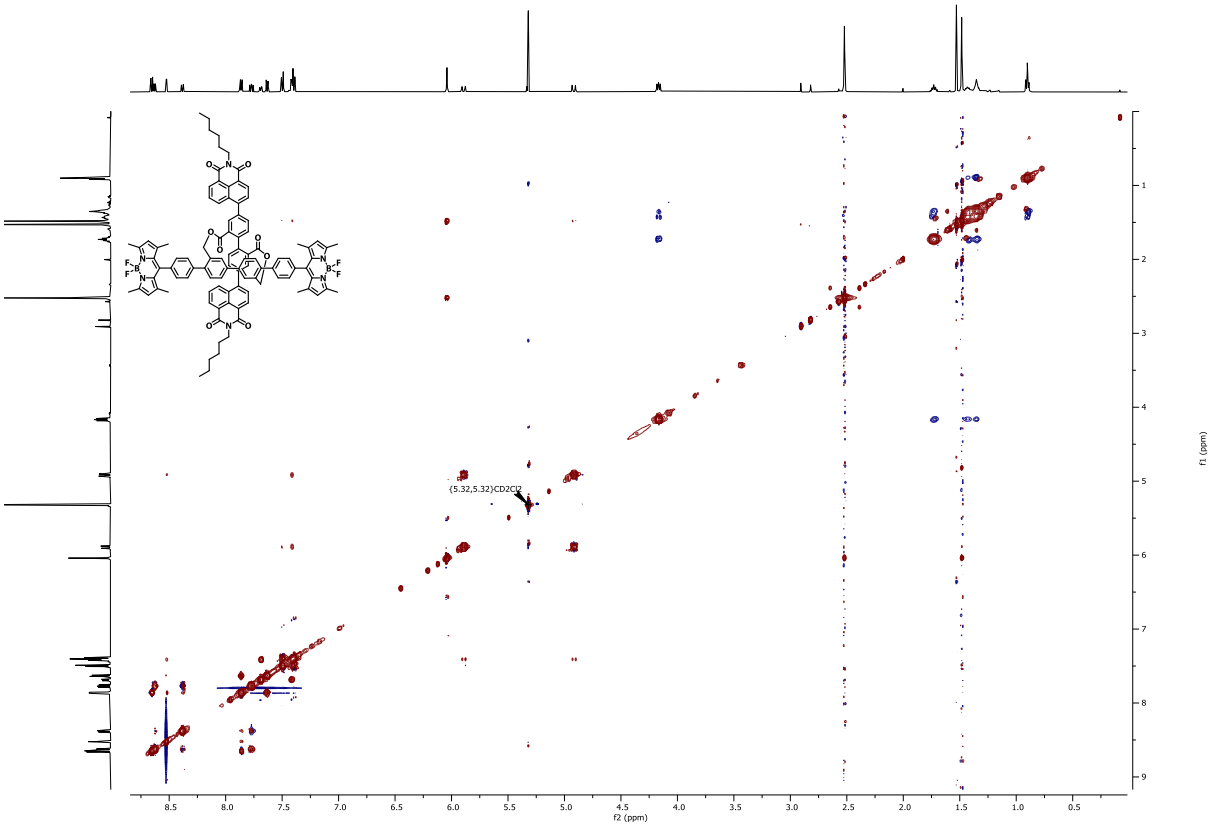
HMQC spectrum of $\mathbf{C_{NI2BY2}}$ in CD_2Cl_2



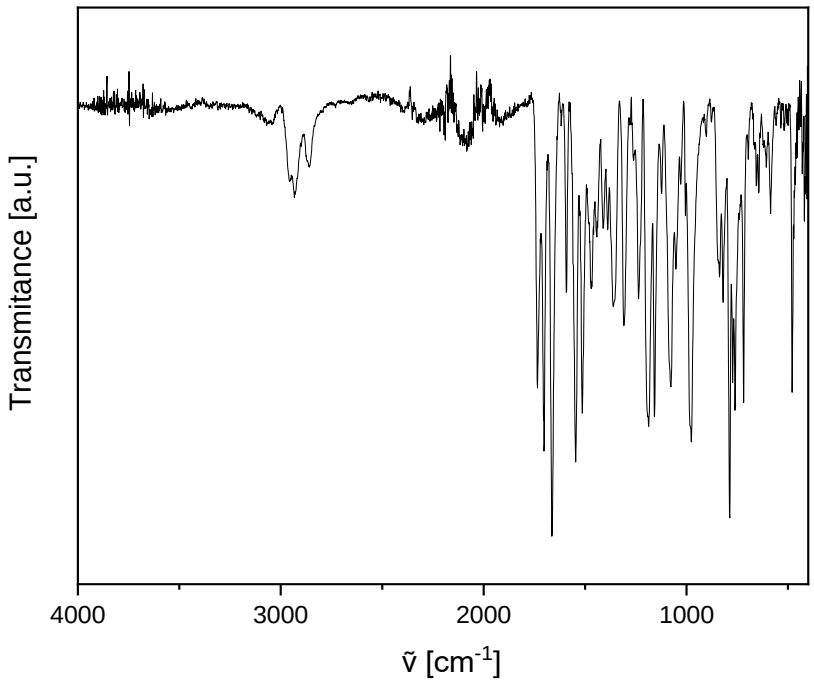
HMBC spectrum of $\mathbf{C_{NI2BY2}}$ in CD_2Cl_2



NOESY spectrum of $\mathbf{C_{NI2BY2}}$ in CD_2Cl_2



FT-IR spectrum of $\mathbf{C_{NI2BY2}}$ (neat)



HR-ESI-MS spectrum of C_{NI2BY2}