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Supporting Information

Toward Molecular Textiles: Synthesis and Characterization of Molecular Patches

Camiel C. E. Kroonen, Antoine Hinaut, Adriano D'Addio, Alessandro Prescimone, Daniel Häussinger, Gema Navarro-Marín, Olaf Fuhr, Dieter Fenske, Ernst Meyer, and Marcel Mayor*

Supporting information

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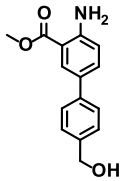
General

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. 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 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. 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, 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. All DFT calculations were performed using Gaussian 09, Revision E 0.1.[1]

Synthesis

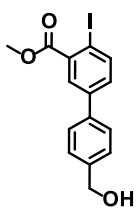


Compound 5: A 100 mL *Schlenk* flask was charged with methyl 2-amino-5-bromobenzoate **4** (3.0 g, 1 equiv.), Na_2CO_3 (3.2 g, 2.3 equiv.), 4-(Hydroxymethyl) phenylboronic acid (0.72 g, 1.1 equivl). The solids were dispersed in 65 mL Tol/$H_2$0/MeOH (4:1.5:1) and degassed with argon for 15 minutes. $Pd(PPh_3)_4$ (5 mol %) was added, tube sealed and the mixture was heated at 80°C for 5 hours. The reaction mixture was cooled down to room temperature and partioned between EtOAc and water. The organic phase was washed with water, brine, dried over sodium sulfate and concentrated in vacuo. The crude was purified by SiO_2 column chromatography (cyclohexane:EtOAc (7:3 v/v)) obtaining the product in the 2nd band as a white solid (2.2 gr, 65%).

^{1}H-NMR: (500 MHz, CD_2Cl_2) δ 8.13 (d, *J* = 2.3 Hz, 1H), 7.58 – 7.54 (m, 3H), 7.41 – 7.38 (m, 2H), 6.77 (d, *J* = 8.5 Hz, 1H), 5.82 (s, 2H), 4.69 (d, *J* = 5.4 Hz, 3H), 3.88 (s, 3H), 1.74 (t, *J* = 5.9 Hz, 1H).

^{13}C-NMR: (126 MHz, CD_2Cl_2): (126 MHz, CD2Cl2) δ 168.78, 149.03, 139.56, 132.57, 129.19, 128.64, 127.38, 126.08, 117.12, 110.90, 64.81, 51.50. Signal 168.78 is extracted from 2D-NMR.

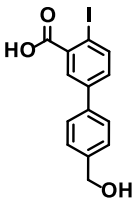
HR-ESI-MS (+): *m/z* calculated for $C_{15}H_{15}NNaO_3$ $[M+Na]^+$; 280.0944 found 280.0941.



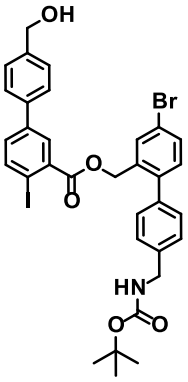
Compound 6: To a solution of p-TsOH·H_2O (890 mg, 3 equiv.) in acetonitrile (12 mL) amine **5** (404, mg 1 equiv.) was added. The resulting suspension was cooled to 0°C and a solution of $NaNO_2$ (213 mg, 2 equiv.) and KI (640 mg, 2.5 equiv.) in H_2O (4 mL) was gradually added. The reaction mixture was allowed to warm to room temperature and stirred for 16 h, before sat. $NaHCO_3$ and sat. $NaHSO_3$ solution where added. The resulting mixture was extracted with EtOAc (3 times), the organic fractions were combined, dried over sodium sulfate and concentrated under reduced pressure. The crude was purified by flash column chromatography (SiO_2, cyclohexane:EtOAc 8:2 → 7:3 v/v) obtaining the product as a white solid (520 mg, 90%).

^{1}H-NMR: (500 MHz, CD_2Cl_2): δ 8.05 (d, *J* = 8.2 Hz, 1H), 8.01 (d, *J* = 2.4 Hz, 1H), 7.63 – 7.57 (m, 2H), 7.49 – 7.43 (m, 2H), 7.41 (dd, *J* = 8.2, 2.4 Hz, 1H), 4.72 (d, *J* = 5.3 Hz, 2H), 3.93 (s, 3H), 1.85 (t, *J* = 5.7 Hz, 1H).

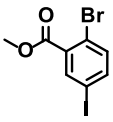
^{13}C-NMR {1H}: (126 MHz, CD_2Cl_2): δ 167.25, 142.07, 141.75, 141.21, 138.42, 136.27, 131.34, 129.66, 127.86, 127.29, 92.59, 65.01, 52.84.
HR-ESI-MS (+): *m/z* calculated for $C_{15}H_{14}IO_3$ $[M+H]^+$; 368.9982 found 368.9980.



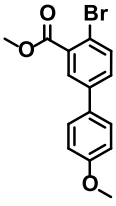
Compound 7: To a solution of ester **6** (478 mg, 1 equiv.) in MeOH (4 mL) and aqueous 1 M NaOH (2.4 mL, 3 equiv) was heated at reflux for 2 hours. After the reaction was cooled to room temperature it was diluted with 10 mL H_2O and was acidified to pH 2 with concentrated HCl. The mixture was extracted with EtOAc (3 × 10 mL), and the combined organic portions where washed with brine, dried (Na_2SO_4), filtered and concentrated in vacuo to obtain iodobenzoic acid **7** (449 mg, 98%) as a white solid.
^{1}H-NMR: (500 MHz, Acetone-d6) δ 11.67 (s, 1H), 8.16 – 8.05 (m, 2H), 7.76 – 7.62 (m, 2H), 7.56 (dd, *J* = 8.2, 2.4 Hz, 1H), 7.54 – 7.41 (m, 2H), 4.70 (s, 2H), 4.29 (s, 1H).
^{13}C-NMR {1H}: (126 MHz, Acetone-d6) δ 166.92, 142.77, 141.75, 140.96, 137.30, 136.59, 130.77, 128.80, 127.23, 126.54, 91.66, 63.32.
HR-ESI-MS (+): *m/z* calculated for $C_{14}H_{11}IO_3Na$ $[M+Na]^+$; 376.9645 found 376.9640.



Compound 2: To a 100 mL round-bottom flask acid **7** (266 mg, 1 equiv.), benzyl bromide **7'** (360 mg, 1.05 equiv.) and CsF (185 mg, 1.6 equiv.) were added and put under inert atmosphere. 5 mL dry DMF was added and the resulting mixture was stirred at r.t. for 16 hours. The mixture was diluted with EtOAc, washed 3 times with brine, dried with sodium sulfate and concentrated under reduced pressure. The corresponding crude was purified with SiO_2 column chromatography (CH_2Cl_2:EtOAc 100% → 8:2 v/v) obtaining the product as a light yellow solid (544 mg, 99 %).
^{1}H-NMR: (500 MHz, DMSO-d6) δ 8.05 (d, *J* = 8.2 Hz, 1H), 7.87 – 7.85 (m, 2H), 7.66 – 7.62 (m, 3H), 7.57 (dd, *J* = 8.2, 2.4 Hz, 1H), 7.46 – 7.40 (m, 3H), 7.39 – 7.36 (m, 2H), 7.34 – 7.31 (m, 2H), 7.28 (d, *J* = 8.2 Hz, 1H), 5.28 (s, 2H), 5.25 (t, *J* = 5.7 Hz, 1H), 4.55 (d, *J* = 5.8 Hz, 2H), 4.17 (d, *J* = 6.2 Hz, 2H), 1.40 (s, 9H).
^{13}C-NMR {1H}: (126 MHz, DMSO) δ 166.11, 155.83, 142.84, 141.08, 140.46, 140.00, 139.85, 137.00, 136.29, 136.22, 135.17, 132.07, 131.88, 131.30, 130.85, 128.74, 127.94, 127.12, 127.08, 126.29, 120.62, 92.55, 77.84, 64.51, 62.49, 43.06, 28.25.
HR-ESI-MS (+): *m/z* calculated for $C_{33}H_{31}BrINO_5Na$ $[M+Na]^+$; 750.0322 found 750.0315.

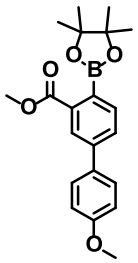


Compound 9: 2-bromo-5-iodobenzoic acid **8** (5.5 g, 1 equiv.) was dissolved in 120 mL methanol and 2.5 ml of conc. sulfuric acid (3 equiv.) was added. The reaction was heated at reflux for 4 hours before cooled down, diluted with 250 mL H_2O and extracted 3 times with TBME. The combined organics were washed with 50 mL of sat. $NaHCO_3$, 50 mL of H_2O, and 2 x with 50 mL of sat. NaCl. The organics were dried with Na_2SO_4 and filtered. The solvent was removed under vacuum yielding the compound as a yellow solid (5.0 gr, 86 %), which was used in the next step without further purification.
^{1}H-NMR: (400 MHz, CD_2Cl_2): (400 MHz, CD_2Cl_2) δ 8.10 (d, *J* = 2.3 Hz, 1H), 7.65 (dd, *J* = 8.4, 2.2 Hz, 1H), 7.40 (d, *J* = 8.4 Hz, 1H), 3.90 (s, 3H). [2]

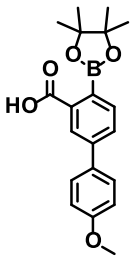


Compound 10: A 50 mL Schlenk tube was charged with methyl 2-bromo-5-iodobenzoate **9** (1.02 gr, 1 equiv.), (4-methoxyphenyl)boronic acid (505 mg, 1.2 equiv.) and K_2CO_3 (1.23 gr, 3 equiv.) and cycled between vacuum and argon for three times. The solids were dispersed in 30 mL DME/MeOH/H_2O (4:1:1) and the mixture was degassed for 15 minutes with argon. $PdCl_2$(dppf) (5 mol %) was added under inert atmosphere and the mixture was heated up to 60°C. After 16 hours the reaction mixture was cooled down to r.t., filtered over silica, diluted with EtOAc and washed with H_20. The organic phase was collected, dried over Na_2SO_4 and concentrated under reduced pressure. The obtained crude was purified via SiO_2 column chromatography (cyclohexane:EtOAc 9:1 v/v) obtaining the product in the 1st band as a white solid (670 mg, 71%).

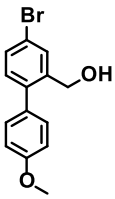
^{1}H-NMR: (500 MHz, CD_2Cl_2) δ 7.96 (d, *J* = 2.4 Hz, 1H), 7.69 (d, *J* = 8.3 Hz, 1H), 7.57 – 7.51 (m, 3H), 7.04 – 6.93 (m, 2H), 3.93 (s, 3H), 3.84 (s, 3H).
^{13}C-NMR {1H}: (126 MHz, CD_2Cl_2) δ 166.91, 160.29, 140.45, 134.96, 133.02, 131.59, 130.85, 129.57, 128.36, 119.76, 114.79, 55.75, 52.79.
HR-ESI-MS (+): *m/z* calculated for $C_{15}H_{13}BrO_3Na$ $[M+Na]^+$; 342.9940 found 342.9941.



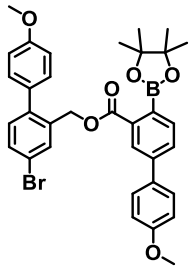
Compound 11: Bromide **10** (437 mg, 1 equiv.), bis(pinacolato)diboron (400 mg, 1.15 equiv.) and KOAc (420 mg, 3 equiv.) were added to a 25 mL flame dried *Schlenk* flask and cycled between vacuum and argon 3 times. Anhydrous dioxane (8 mL) was added and the suspension was degassed for 15 minutes with argon. $PdCl_2$(dppf) (50 mg, 5 mol%) was added and the tube was sealed and heated at 90°C for 6 hours. The reaction mixture was cooled to room temperature, filtered over silica, flushed down with EtOAc and concentrated under reduced pressure. The crude was further purified by flash column chromatography (SiO_2, Cyclohexane:EtOAc (9:1)) obtaining the product in the 2nd band as a white solid (424 mg, 85%).
^{1}H-NMR: (500 MHz, CD_2Cl_2) δ 8.13 (dd, *J* = 1.9, 0.6 Hz, 1H), 7.74 (dd, *J* = 7.7, 1.8 Hz, 1H), 7.62 – 7.57 (m, 2H), 7.55 (dd, *J* = 7.7, 0.6 Hz, 1H), 7.03 – 6.97 (m, 2H), 3.92 (s, 3H), 3.85 (s, 3H), 1.39 (s, 12H).
^{13}C-NMR {1H}: (126 MHz, CD_2Cl_2) δ 168.86, 160.14, 141.91, 134.96, 133.33, 132.65, 129.92, 128.49, 127.16, 114.69, 84.36, 55.72, 52.60, 25.06.
HR-ESI-MS (+): *m/z* calculated for $C_{21}H_{26}BO_5$ $[M+H]^+$; 369.1872, found 369.1865.



Compound 12: To a solution of methyl ester **11** (352 mg, 1 equiv.) in 9 mL THF a solution of LiOH•H_2O (120 mg, 3 equiv.) in 2 mL H_2O was added under inert atmosphere. The resulting mixture was stirred at room temperature for 1 h when TLC indicated full consumption of the starting material. The mixture was diluted with H_2O, acidified with 1M HCl followed by extraction with TBME (3 times). The organic extracts were combined and washed with brine, dried (Na_2SO_4) and concentrated to give the product as a white solid (339 mg, quant.).
^{1}H-NMR: (500 MHz, DMSO-d6) δ 8.01 (d, *J* = 1.8 Hz, 1H), 7.80 (dd, *J* = 7.7, 1.8 Hz, 1H), 7.67 – 7.62 (m, 2H), 7.47 (d, *J* = 7.6 Hz, 1H), 7.07 – 7.02 (m, 2H), 3.80 (s, 3H), 1.30 (s, 12H).
^{13}C-NMR {1H}: (126 MHz, DMSO-d6) δ 169.18, 159.23, 140.17, 135.29, 132.16, 131.50, 129.26, 127.84, 125.16, 114.50, 82.89, 55.21, 24.59.
HR-ESI-MS (+): *m/z* calculated for $C_{20}H_{24}BO_5$ $[M+H]^+$; 355.1715 found 355.1715.



Compound 14: To a 50 mL *Schlenk* tube 2-iodo-4-bromobenzyl alcohol **13** (522 mg, 1 equiv.), 4-methoxyphenylboronic acid (320 mg, 1.2 equiv.) and K_2CO_3 (720 mg, 3 equiv.) were added and cycled between vacuum and argon for three times. The solids were dispersed in 25 mL DME/H_2O (4:1) and the mixture was degassed for 15 minutes with argon. $PdCl_2$(dppf) (0.05 equiv.) was added under inert atmosphere and the mixture was heated up to 60°C. After 2.5 hours the reaction mixture was cooled down to r.t., filtered over celite, diluted in EtOAc and washed with H_20. The organic phase was collected dried with Na_2SO_4 and concentrated under vacuum. The obtained crude was purified via SiO_2 column chromatography (Cyclohexane:EtOAc 9:1 → 8:2 v/v) obtaining the product as a white solid (426 mg, 87 %).
^{1}H-NMR: (500 MHz, CD_2Cl_2): δ 7.71 (d, *J* = 2.2 Hz, 1H), 7.46 (dd, *J* = 8.2, 2.2 Hz, 1H), 7.28 – 7.22 (m, 2H), 7.14 (d, *J* = 8.1 Hz, 1H), 6.99 – 6.92 (m, 2H), 4.56 (d, *J* = 5.7 Hz, 2H), 3.84 (s, 3H), 1.73 (t, *J* = 5.8 Hz, 1H).
^{13}C-NMR {1H}: (126 MHz, CD_2Cl_2): 159.65, 141.09, 140.10, 132.14, 132.09, 131.20, 130.69, 130.48, 121.46, 114.13, 62.85, 55.69.
HR-ESI-MS (+): *m/z* calculated for $C_{14}H_{13}BrO_2Na$ $[M+Na]^+$; 314.9991 found 314.9988

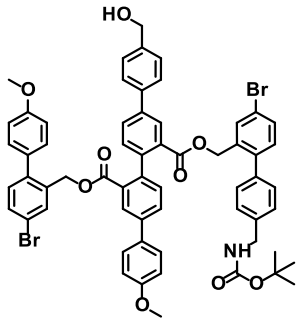


Compound 3: To a solution of acid **12** (175 mg, 1 equiv.) and alcohol **14** (145 mg, 1 equiv.) in 4 mL anhydrous CH_2Cl_2:DMF (3:1), N,N'-dicyclohexylcarbodiimide (108 mg, 1.05 equiv.) and 4-dimethylaminopyridine (6.1 mg, 0.1 equiv.) were added under inert atmosphere. The mixture was stirred at room temperature for 1.5 hours before filtered over a celite pad. The filtrate was washed with H_2O 3 times, dried with Na_2SO_4, plugged over silica and concentrated under reduced pressure. The crude was purified via SiO_2 column chromatography (pentane:CH_2Cl_2 2:8 v/v), yielding the product in the 1st band as a colorless wax (140 mg, 44%).

^{1}H-NMR: (500 MHz, CD_2Cl_2) δ 8.07 (d, *J* = 1.8 Hz, 1H), 7.76 (d, *J* = 2.2 Hz, 1H), 7.74 (dd, *J* = 7.7, 1.9 Hz, 1H), 7.60 – 7.57 (m, 2H), 7.55 (d, *J* = 7.7 Hz, 1H), 7.52 (dd, *J* = 8.2, 2.2 Hz, 1H), 7.32 – 7.28 (m, 2H), 7.20 (d, *J* = 8.2 Hz, 1H), 7.03 – 6.98 (m, 2H), 6.98 – 6.93 (m, 2H), 5.27 (s, 2H), 3.85 (s, 3H), 3.81 (s, 3H), 1.35 (s, 12H)

^{13}C-NMR {1H}: (126 MHz, CD_2Cl_2) δ 167.99, 160.16, 159.75, 141.92, 141.34, 136.13, 134.70, 133.34, 132.63, 132.29, 131.97, 131.57, 130.55, 130.18, 128.53, 127.09, 121.37, 114.70, 114.23, 84.37, 64.92, 55.73, 55.67, 24.99.

HR-ESI-MS (+): *m/z* calculated for $C_{34}H_{34}BBrO_6Na$ $[M+Na]^+$; 651.1530 found 651.1515.

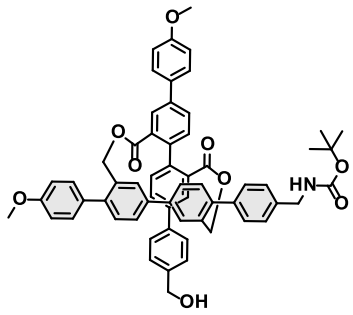


Compound 1: A 25 mL Schlenk tube was charged with boronic acid **3** (165 mg, 1 equiv.). iodo **2** (182 mg, 1 equiv.) and K_2CO_3 (104 mg, 3 equiv.). The solids were dispersed in a 10 mL THF/H_2O (4:1; v/v) mixture. The resulting suspension was degassed with argon followed by the addition of $PdCl_2$(dppf) (14 mg, 7 mol%). The mixture was heated at 60°C for 5 hours before cooled down to room temperature and filtered over a silica pad. The silica pad was flushed down with EtOAc and the filtrate was washed with H_2O. The organic layer was collected, dried with sodium sulfate and concentrated before subjected to Silica column chromatography using Cyclohexane:EtOAc (8:2 to 7:3; v/v) as eluent. The product was obtained as a white solid (222 mg, 82 %) after stripping of the volatiles.

^{1}H-NMR: (500 MHz, CD_2Cl_2): δ 8.10 – 8.09 (m, 1H), 8.07 (s, 1H), 7.72 – 7.64 (m, 2H), 7.61 – 7.57 (m, 2H), 7.57 – 7.53 (m, 2H), 7.51 – 7.46 (m, 2H), 7.37 – 7.19 (m, 8H), 7.16 – 7.11 (m, 2H), 7.10 – 7.06 (m, 2H), 7.04 – 6.98 (m, 4H), 6.87 – 6.83 (m, 2H), 4.99 – 4.95 (m, 4H), 4.92 (s, 1H), 4.75 (s, 2H), 4.24 (d, *J* = 6.0 Hz, 2H), 3.87 (s, 3H), 3.76 (s, 3H), 1.92 (s, 1H), 1.44 (s, 9H).

^{13}C-NMR {1H}: (126 MHz, CD_2Cl_2): δ 167.14, 167.00, 160.10, 159.64, 142.05, 140.92, 139.95, 139.22, 139.19, 138.94, 138.48, 135.34, 132.65, 132.58, 132.12, 131.96, 131.91, 131.74, 131.53, 131.45, 131.40, 131.30, 130.49, 130.32, 130.30, 130.12, 129.68, 129.51, 128.82, 128.47, 128.33, 127.76, 127.73, 127.51, 121.51, 121.11, 114.62, 114.13, 79.73, 65.14, 64.50, 64.44, 55.75, 55.64, 28.53.

HR-ESI-MS (+): *m/z* calculated for $C_{61}H_{53}Br_2NO_9Na$ $[M+Na]^+$; 1124.1979 found 1124.1987



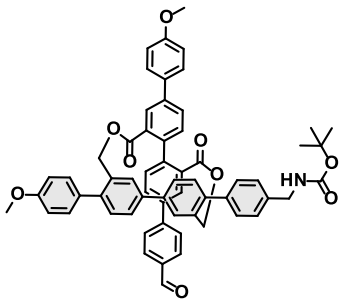
Compound C_1: Dibromo **1** (210 mg, 0.19 mmol, 1 equiv.), B_2Pin_2 (117 mg, 0.46 mmol, 2.4 equiv.) and KOAc (112 mg, 1.14 mmol, 6 equiv.) were loaded into a 25 mL flame-dried *Schlenk* tube and cycled between vacuum and argon 3 times. Dry Dioxane (6 mL) was added and the mixture was degassed with argon for 15 minutes. $PdCl_2$(dppf) (18 mg, 0.02 mmol, 0.1 equiv.) was added and the mixture was heated to 90°C. The reaction was tracked via LC-MS and after full consumption (3 hours) of the starting material the reaction was cooled down to room temperature, filtered over a silica pad, flushed down with EtOAc and concentrated under reduced pressure. The concentrate was dissolved in 100 mL THF, followed by the addition of $PdCl_2(PPh_3)_2$ (67 mg, 0.095 mmol, 0.5 equiv.) and boric acid (59 mg, 0.95 mmol, 5 equiv.). The mixture was stirred vigorously for 15 minutes before KF (114 mg, 1.9 mmol, 10 equiv.) dissolved in 10 mL H_2O was added in one portion. The mixture was stirred for 16 hours at room temperature open to the atmosphere, before it was filtered over silica and flushed down with THF. Organic volatiles

were removed under reduced pressure and the remaining aqueous phase was extracted with EtOAc 3 times. The organic phases were combined, dried with sodium sulphate and concentrated under reduced pressure. The crude was purified by SiO_2 column chromatography using Cyclohexane and EtOAc as eluent, collecting the 2nd band. The obtained yellowish solid was dispersed in MeOH and the white precipitate was collected by filtration and dried, yielding the desired compound **C_1** as an off-white solid (115 mg, 64 % over two steps).

^{1}H-NMR: (500 MHz, CD_2Cl_2): δ 8.51 (d, *J* = 2.0 Hz, 1H), 8.47 (d, *J* = 2.0 Hz, 1H), 7.87 (dd, *J* = 8.0, 2.0 Hz, 1H), 7.83 (dd, *J* = 8.0, 2.1 Hz, 1H), 7.72 – 7.67 (m, 2H), 7.66 – 7.62 (m, 2H), 7.61 – 7.56 (m, 2H), 7.46 (d, *J* = 8.3 Hz, 2H), 7.41 (d, *J* = 8.0 Hz, 1H), 7.39 – 7.28 (m, 11H), 7.02 – 6.97 (m, 4H), 5.89 – 5.84 (m, 2H), 5.03 (s, 1H), 4.94 (d, *J* = 9.1 Hz, 1H), 4.91 (d, *J* = 9.0 Hz, 1H), 4.74 – 4.70 (m, 2H), 4.36 (d, *J* = 6.1 Hz, 2H), 3.85 (s, 3H), 3.84 (s, 3H), 1.87 (s, 1H), 1.46 (s, 9H).

^{13}C-NMR {1H}: (126 MHz, CD_2Cl_2): δ 166.29, 166.17, 160.03, 159.61, 156.27 144.77, 143.92, 141.29, 140.09, 140.06, 139.67, 139.31, 139.24, 139.20, 139.08, 139.04, 134.97, 134.87, 132.55, 132.36, 132.19, 132.04, 130.73, 130.64, 130.56, 130.27, 129.63, 129.61, 129.19, 128.48, 127.82, 127.71, 127.49, 125.92, 124.87, 124.82, 114.69, 114.24, 79.65, 65.10, 64.11, 64.03, 55.71, 44.59, 28.54.

HR-ESI-MS (+): *m/z* calculated for $C_{61}H_{53}NO_9Na$ $[M+Na]^+$; 966.3603 found 966.3603

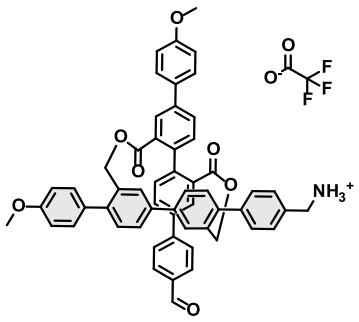


Compound C_2: Cross **C_1** (60 mg, 0.064 mmol, 1 equiv.) was dissolved in dry dichloromethane (6 mL) and cooled down to 0°C. DMP (33 mg, 1.2 equiv.) was added portion wise while cooled and after full addition the mixture was allowed to warm to room-temperature. The mixture was tracked by TLC and upon full conversion after 1 hour the mixture was quenched with sat. $NaHCO_3$ and sat. $NaHSO_3$. The aqueous phase was extracted with CH_2Cl_2 3 times and concentrated. The crude was plugged over a pad of silica (CH_2Cl_2:EtOAc 9:1) yielding the product as a white solid (52 mg, 86 %).

^{1}H-NMR: (500 MHz, CD_2Cl_2) δ 10.05 (s, 1H), 8.57 (d, *J* = 2.0 Hz, 1H), 8.48 (d, *J* = 2.1 Hz, 1H), 7.97 (d, *J* = 8.1 Hz, 2H), 7.92 (dd, *J* = 8.0, 2.0 Hz, 1H), 7.88 (d, *J* = 8.2 Hz, 2H), 7.84 (dd, *J* = 8.0, 2.0 Hz, 1H), 7.66 – 7.62 (m, 2H), 7.60 (ddd, *J* = 8.1, 6.6, 1.9 Hz, 2H), 7.46 (d, *J* = 8.0 Hz, 1H), 7.40 – 7.27 (m, 12H), 7.03 – 6.97 (m, 4H), 5.87 (dd, *J* = 14.1, 7.9 Hz, 2H), 5.03 (s, 1H), 4.94 (dd, *J* = 14.1, 3.4 Hz, 2H), 4.36 (d, *J* = 6.2 Hz, 2H), 3.85 (s, 3H), 3.84 (s, 2H), 1.46 (s, 9H).

^{13}C-NMR {1H}: (126 MHz, CD_2Cl_2) δ 192.11, 166.30, 165.94, 160.06, 159.62, 145.99, 143.60, 140.25, 139.65, 139.24, 139.21, 139.12, 138.99, 138.98, 136.05, 134.94, 134.79, 132.48, 132.43, 132.33, 131.88, 130.90, 130.75, 130.68, 130.60, 130.56, 130.33, 130.05, 129.63, 129.23, 128.48, 128.08, 128.05, 127.72, 127.64, 125.90, 124.91, 124.86, 114.71, 114.25, 79.78, 64.15, 64.12, 55.72, 44.58, 28.54.

HR-ESI-MS (+): *m/z* calculated for $C_{61}H_{51}NO_9Na$ $[M+Na]^+$; 964.3456 found 964.3455.



Compound C_M: Cross **C_2** (24 mg, 1 equiv.) was dissolved in 1 mL CH_2Cl_2 and 0.1 mL TFA was added, the mixture is stirred for 1 h. 5 mL toluene was added and the mixture was concentrated under reduced pressure yielding the product as the TFA salt (25 mg, quant.) as an off-white solid.

Reaction in NMR-Tube:

3 mg of protected amine **C_2** was dissolved in 0.75 mL CD_2Cl_2 followed by the addition of 70 µL TFA-d. The tube was shaken until homogenous and ^{1}H-NMR spectra were recorded after several time intervals. After 1 hour the spectra indicated full conversion towards the product.

^{1}H NMR (600 MHz, CD_2Cl_2:TFA-d 10:1) δ 9.98 (s, 1H), 8.60 (d, *J* = 2.0 Hz, 1H), 8.53 (d, *J* = 2.0 Hz, 1H), 8.11 – 8.06 (m, 2H), 7.97 (dd, *J* = 8.0, 2.0 Hz, 1H), 7.92 – 7.86 (m, 3H), 7.67 – 7.58 (m, 4H), 7.54 – 7.39 (m, 6H), 7.34 – 7.26 (m, 6H), 7.09 – 7.03 (m, 4H), 5.84 (d, *J* = 14.4 Hz, 2H), 5.08 (d, *J* = 14.4 Hz, 1H), 5.00 (d, *J* = 14.4 Hz, 1H), 4.40 (s, 2H), 3.94 (s, 3H), 3.93 (s, 3H).

^{1}H-NMR: (500 MHz, DMSO-d6): δ 10.07 (s, 1H), 8.54 (d, *J* = 2.1 Hz, 1H), 8.42 (d, *J* = 2.1 Hz, 1H), 8.22 (s, 3H), 8.11 (dd, *J* = 8.1, 2.1 Hz, 1H), 8.06 – 7.99 (m, 4H), 7.96 (dd, *J* = 8.1, 2.1 Hz, 1H), 7.75 – 7.67 (m, 4H), 7.60 – 7.56 (m, 2H), 7.55 – 7.48 (m, 3H), 7.40 (d, *J* = 8.0 Hz, 1H), 7.38 – 7.32 (m, 4H), 7.25 – 7.18 (m, 2H), 7.09 – 7.03 (m, 4H), 5.77 (dd, *J* = 14.6, 8.5 Hz, 2H), 5.00 (dd, *J* = 14.4, 5.4 Hz, 2H), 4.16 – 4.09 (m, 2H), 3.81 (d, *J* = 5.1 Hz, 6H).
^{13}C-NMR {1H}: (126 MHz, DMSO-d6): δ 192.76, 165.11, 164.85, 159.31, 158.84, 144.91, 144.34, 142.61, 139.15, 139.09, 137.83, 135.44, 134.20, 134.07, 131.01, 130.54, 130.28, 130.06, 129.16, 129.09, 127.87, 127.46, 127.03, 126.71, 124.74, 124.04, 114.56, 114.03, 63.92, 55.21, 55.19, 42.01.
Signals: 192.76, 165.11, 164.85, 159.31, 144.91, 144.34, 142.61, 139.15, 139.09, 137.83, 134.20, 134.07, 131.01, 130.54, 127.03, 126.71, 124.74, 124.04, 63.92 are extracted from 2D-NMR.
HR-ESI-MS (+): *m/z* calculated for $C_{56}H_{44}NO_7$ $[M+H]^+$; 842.3112, found 842.3120.

Physico-Chemical Analysis

(Chiro)-Optical analysis

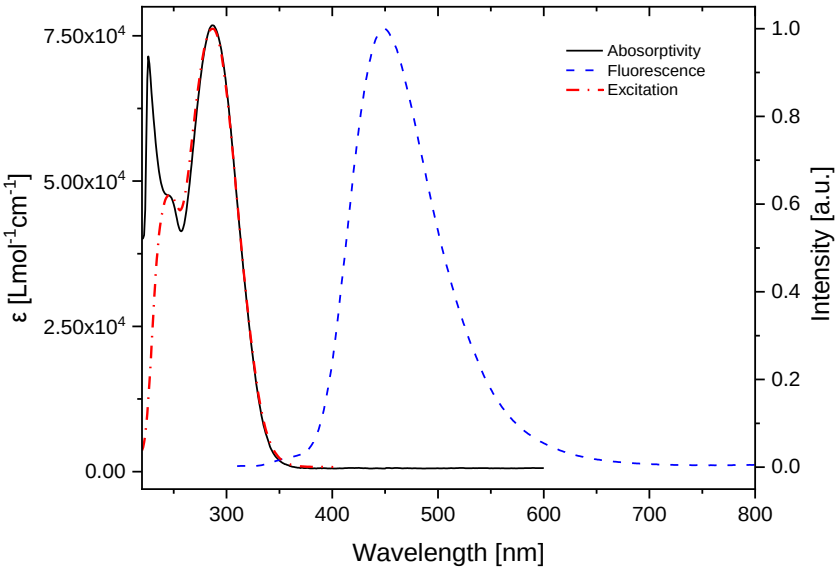


Figure S1: Absorptivity (c ~ 5*10^{-6}), normalized fluorescence (c ~ 1*10^{-6}, 287 nm) and normalized excitation (445 nm) plot in CH_2Cl_2 at 20 °C of **C_2**.

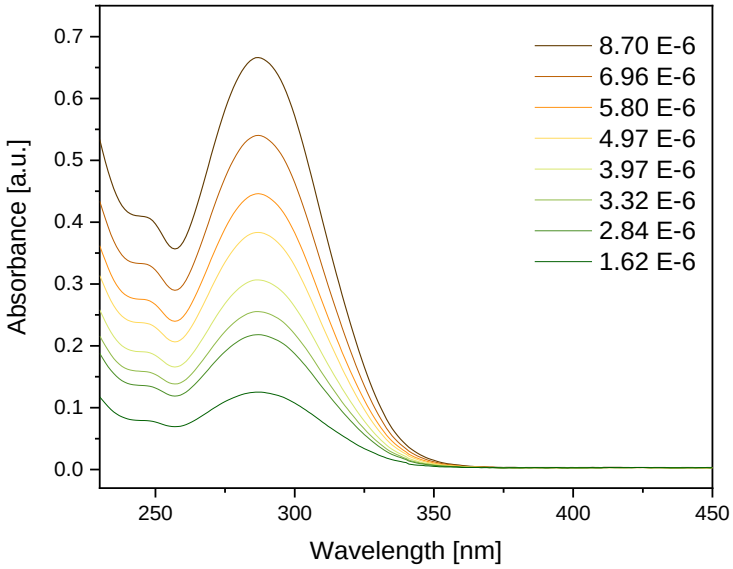


Figure S2: Dilution series of the absorption of **C_2** in CH_2Cl_2 at 20 °C.

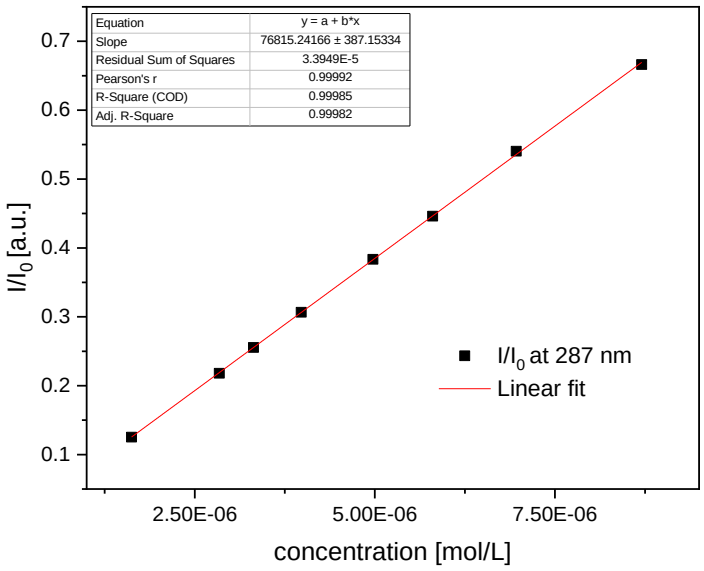


Figure S3: Linear regression of the absorption value of **C_2** at 287 nm in CH_2Cl_2 at 20 °C versus concentration.

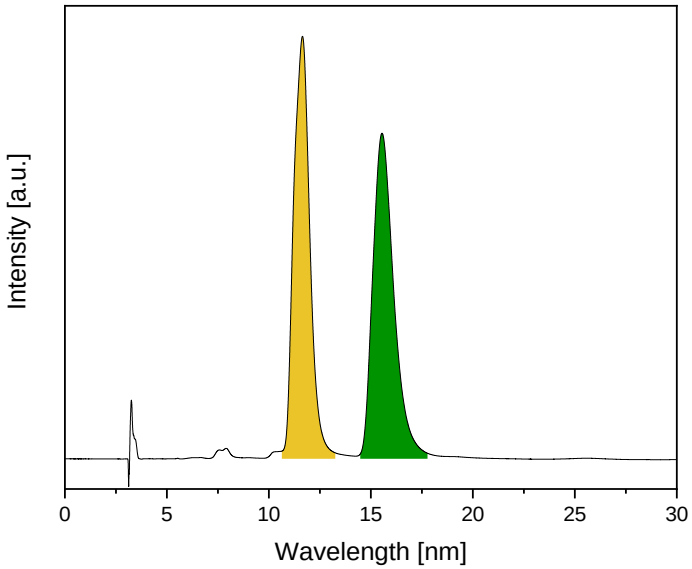


Figure S4: HPLC-chromatogram (285 nm) of *(rac)*-**C_2**, IG-Chiralpak; Heptane/CH_2Cl_2 40/60 v/v; r.t..

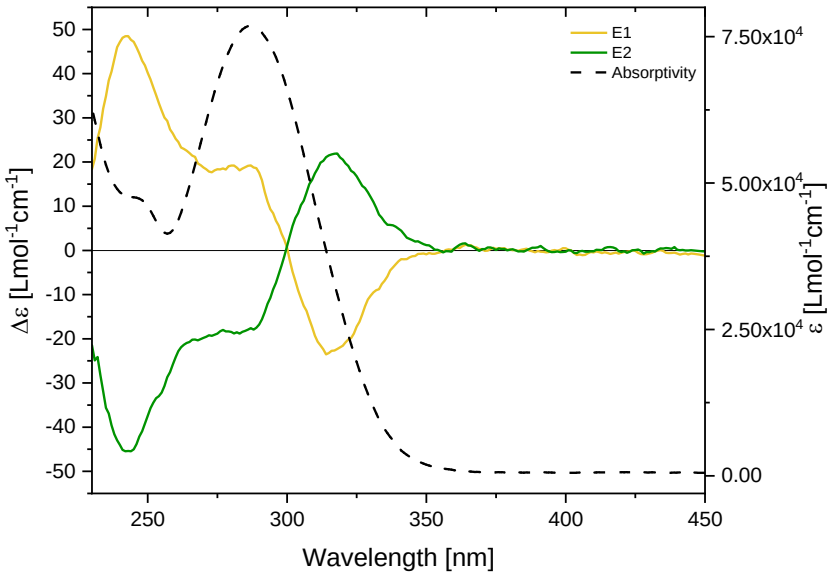


Figure S5: Molar absorptivity and CD-spectra of first eluting (E1-yellow) and second eluting enantiomer (E2-green) of **C_2** in CH_2Cl_2 at 20 °C.

TD-DFT calculation

To assign the configuration of the eluted enantiomers 60 vertical singlet and 60 vertical triplet transitions were computed at the TD-B3LYP/3-21G level of theory following the protocol described by *Pescitelli et al.*[3] and their rotary strength was fitted using the SpecDis software.[4] The geometry calculations of (*P*)-**C_2** are describe further below in this SI and the coordinates are reported further below aswell. As experimental and simulated data fitted well no additional dispersion or solvent effects were taken into account in the computation of the transitions.

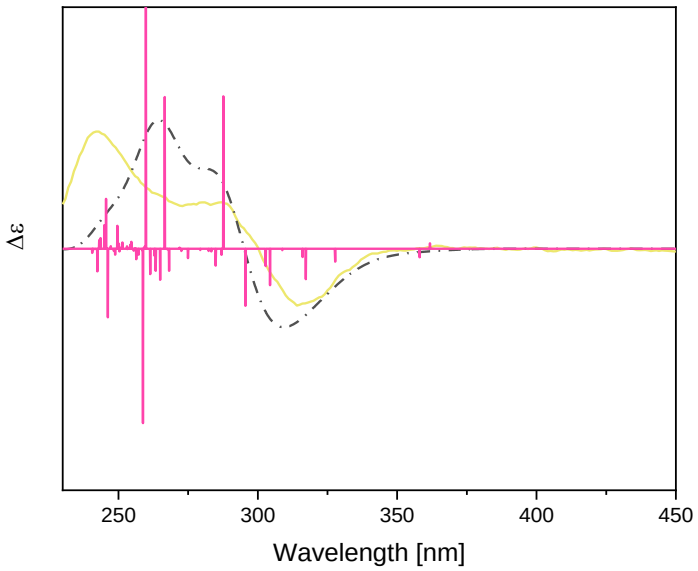


Figure S6. Experimental (yellow line) of E1 and computed (black dash dot line) spectra of (*P*)-**C_2**. The computed transitions are visualized as pink sticks. The computed spectrum was fitted with a σ = 0.2 eV and shifted by 0.1 eV to the red.

Oligomerization

In-solution synthesis

Maldi spectrum reaction control

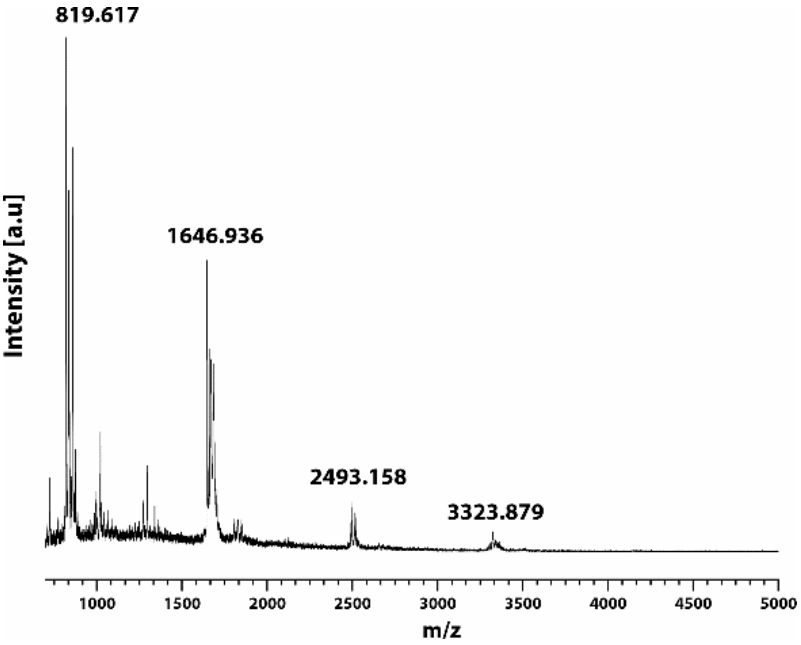


Figure S7. MALDI spectrum reaction control of $\mathbf{O_{M\text{-}I}}$ after 30 minutes indicating the presence of $\mathbf{C_M}$ (820-850 m/z), dimeric (1640-1670 m/z), trimeric (2480-2520 m/z) and tetrameric (3300-3350 m/z) species.

DOSY spectra C_2 and $O_{M\text{-}I}$

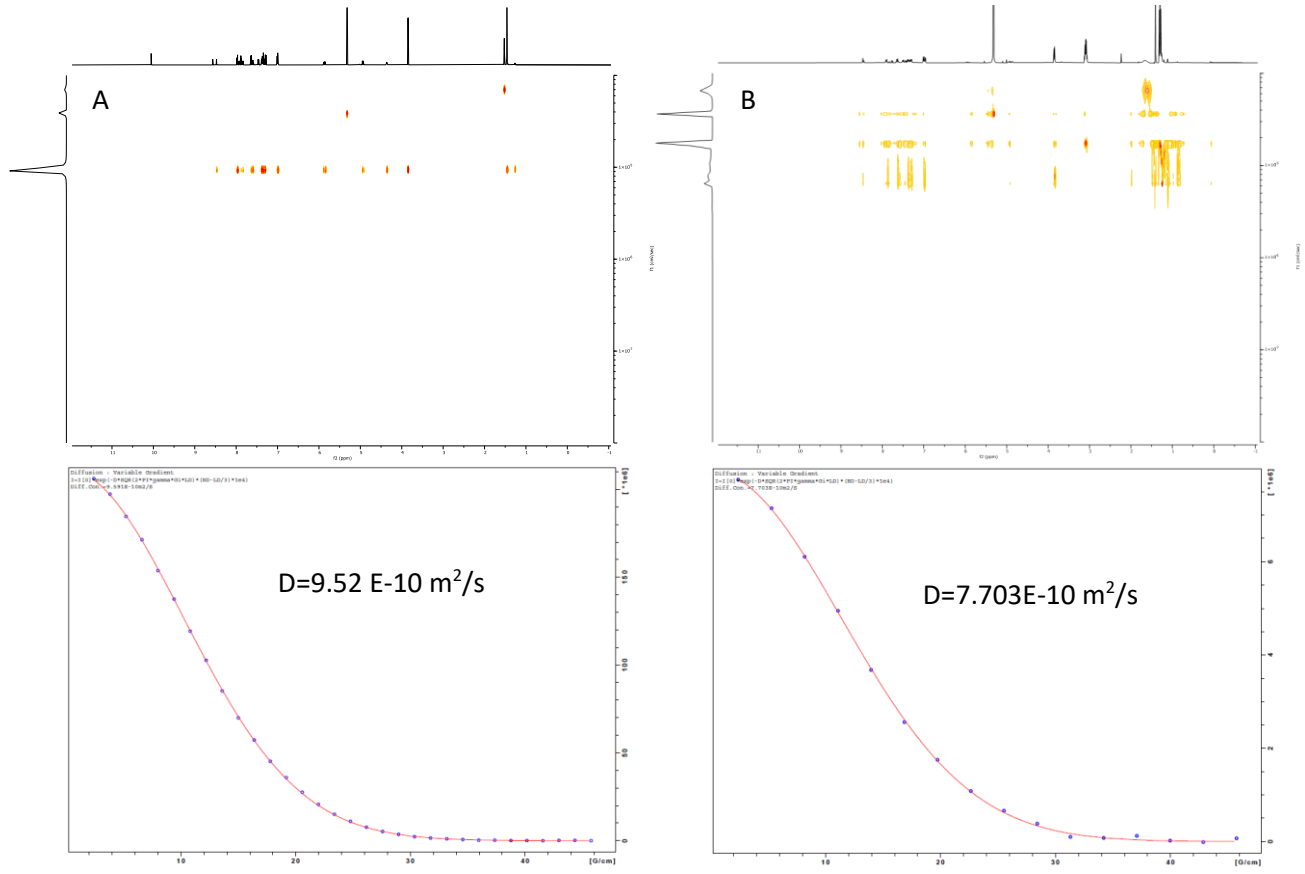


Figure S8. DOSY spectra (top) and fit (bottom) of A) $\mathbf{C_2}$ and B) $\mathbf{O_{M\text{-}I}}$ in CD_2Cl_2, 600 mHz at 25 °C.

^{1}H-NMR of $O_{M\text{-}I}$ and $O_{M\text{-}A}$

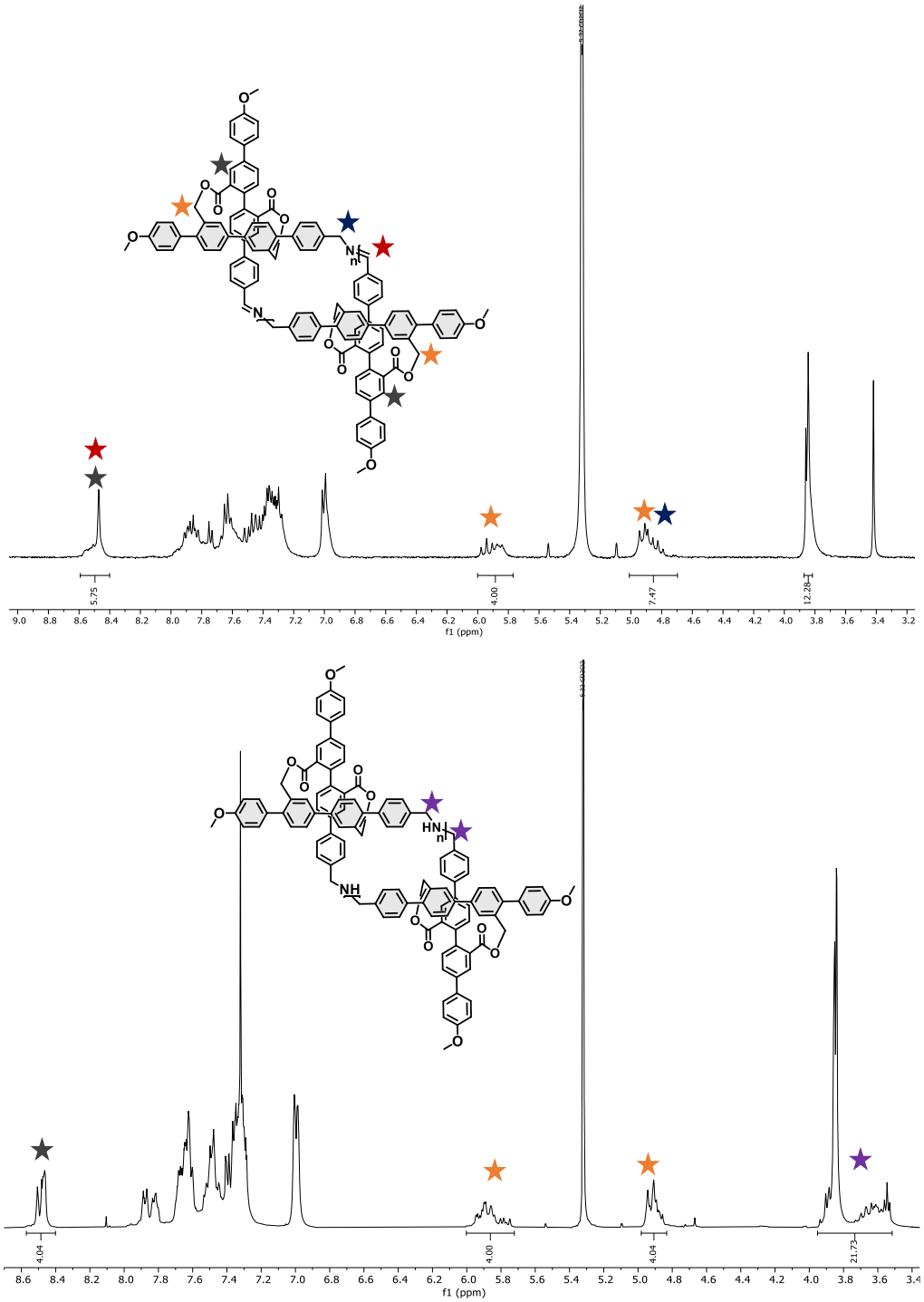


Figure S9. ^{1}H-NMR of $O_{M\text{-}I}$ and $O_{M\text{-}A}$ in CD_2Cl_2, at 20 °C. The indicated protons of imine (red), benzylic imine (blue) and benzylic amine (purple) match the expected ratio in comparison to the benzylic ester protons of the center motive (orange), considering the overlap of the methoxy signal at 3.8 ppm and phenyl proton (black) at 8.5 ppm.

Preparation and ^{1}H-NMR analysis of imine I and amine A model compound

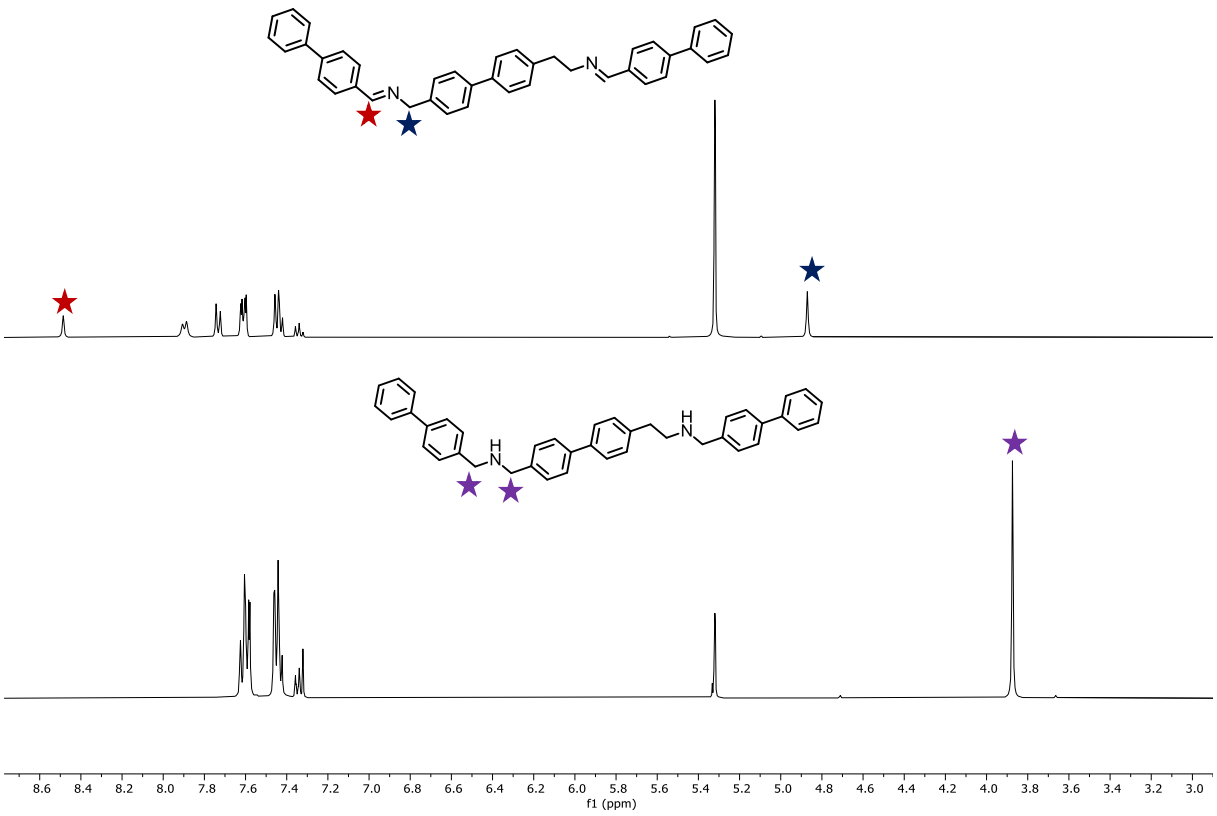
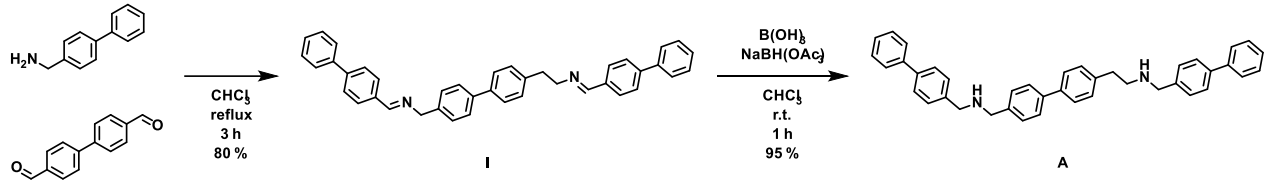


Figure S10. ^{1}H-NMR of imine **I** and amine **A** model compound in CD_2Cl_2 (400 MHz, 20 °C). Corresponding imine (red), benzylic **CH_2** imine (blue) and benzylic **CH_2** amine (purple) are indicated.



Scheme S1. Preparation of model compounds **I** and **A**.

Synthetic procedure I: Phenyl benzyl amine (90 mg, 0.49 mmol, 2.1 equiv.) and 4,4'-biphenylcarboxaldehyde (50 mg, 0.24 mmol, 1 equiv.) were dissolved in dry $CHCl_3$ (3 mL) under inert atmosphere and refluxed for 3 hours. The resulting mixture was concentrated under reduced pressure and the obtained solid was washed with a bit of Et_2O to obtain the product as an off-yellow solid (100 mg, 80%). **^{1}H-NMR:** (400 MHz, CD_2Cl_2) δ 8.49 (s, 2H), 7.90 (d, J = 7.9 Hz, 4H), 7.73 (d, J = 8.2 Hz, 4H), 7.65 – 7.57 (m, 8H), 7.44 (dd, J = 8.1, 6.6 Hz, 8H), 7.38 – 7.29 (m, 2H), 4.87 (s, 4H). **^{13}C-NMR {1H}:** (101 MHz, CD_2Cl_2) δ 161.66, 142.86, 141.27, 140.20, 139.20, 136.18, 129.15, 129.11, 128.86, 127.66, 127.61, 127.51, 127.36, 65.18. **HR-ESI-MS:** *m/z* calculated for $C_{40}H_{33}N_2$ $[M+H]^+$; 541.2637, found 541.2638.

Synthetic procedure A: Imine **I** (10 mg, 1 equiv.), $NaBH(OAc)_3$ (87 mg, 20 equiv.) and ground $B(OH)_3$ (23 mg, 20 equiv.) were added to a round-bottom flask. The mixture was suspended in 5 mL $CHCl_3$ and stirred at r.t. for 1 h, before it was quenched with sat. Na_2CO_3 and extracted with CH_2Cl_2 3 times. The organics were collected, dried with Na_2SO_4, filtered and concentrated to yield **A** (10 mg, 97 %). **^{1}H-NMR:** ^{1}H NMR (400 MHz, CD_2Cl_2) δ 7.64 – 7.57 (m, 12H), 7.49 – 7.41 (m, 12H), 7.38 – 7.30 (m, 2H), 3.87 (s, 8H).**^{13}C-NMR {1H}:** (101 MHz, CD_2Cl_2) δ 141.32, 140.32, 140.19, 140.04, 139.86, 129.15, 128.97, 127.56, 127.35, 127.32, 127.23, 53.22, 53.20. **HR-ESI-MS:** *m/z* calculated for $C_{40}H_{37}N_2$ $[M+H]^+$; 545.2951, found 541.2958.

SEC chromatogram of O_{M-A}

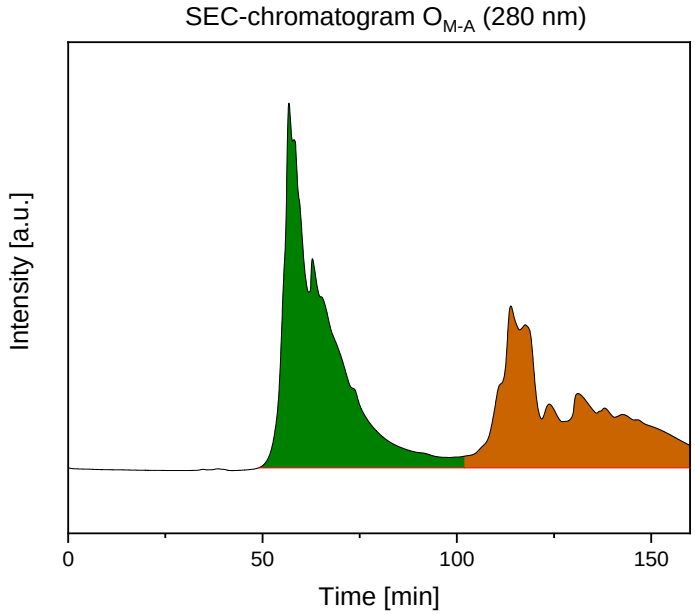


Figure S11. Size exclusion chromatography (SEC) chromatogram of **O_{M-A}**; showing cycle 1 (green) and 2 (orange) indicating the extreme smearing.

On-surface analysis with nc-AFM

Surface before annealing:

Large scale topography ncAFM image (SI Fig XXA) reveal the presence of short chains or clusters of **C_M** molecules on the Au(111) surface (see arrow). Smaller bright protrusion (see doted area) are also visible indicating the present of solvent molecules and are preferentially aligned at herringbone kinks [hin21]. The step edges are covered either with **C_M** molecules (thick protrusion) either with residual solvent molecules (thin protrusion). It is possible to zoom on the individuals **C_M** molecules or chains of **C_M** molecules, as visible in the topography and corresponding dissipation image (SI Fig XXBC). There, it is difficult to identify the different part of the molecules in the submolecular resolution images.

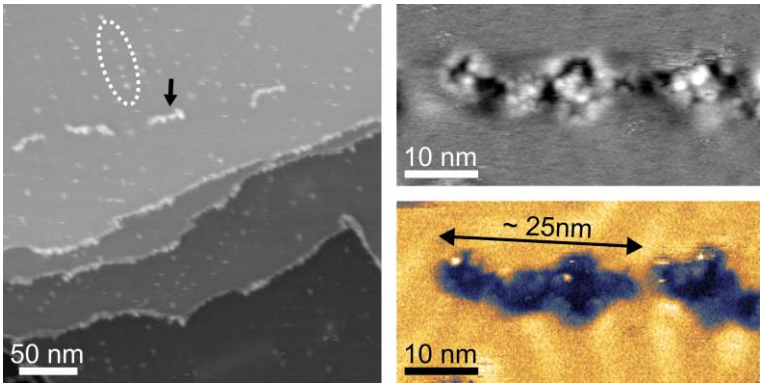


Figure S12. ncAFM topography on **C_M** on Au(111) surface as deposited. A) Large scale topography of B) topography and corresponding dissipation C) on small chains of **C_M**. Due to specific imaging conditions, contrast of the chain is lower compared to the Au(111) surface. Parameters: f_1 = 322 kHz, A_1 = 5nm. A) Δf_1 = -25 Hz. B,C) Δf_2 = -100 Hz

Surface after annealing

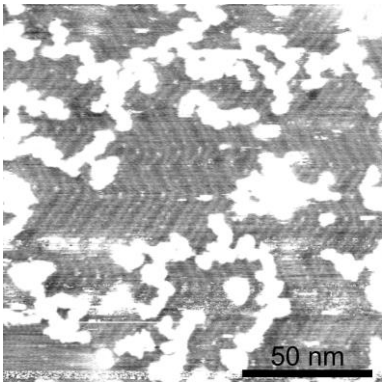


Figure S13. Same image as Figure 5a in the main manuscript with a different contrast to show the herringbone structure of the Au(111) surface. Protrusion corresponding to remaining adsorbed species are visible only at kinks of the herringbone, sign of a clean surface.

Cluster: molecular structure identification:

We created a mask from the highly dissipative region (bright color) of the second eigenmode dissipation of Figure 5 in the main manuscript. Superposing such mask on top of the pattern help us for the identification of the structures in the cluster.

The submolecular resolution image obtain in the second eigenmode frequency shift image on the island (SIFig XXA) do not present row as in the topography (Fig. 5C main manuscript). Instead, cyclic structure are visible.

It is possible to exactly superimpose the mask pattern extracted from the dissipation of the second eigenmode image on the corresponding frequency shift image. When doing the same, the mask pattern also adapt well to the row structure of the topography with all cyclic pattern on similar position of the topography.

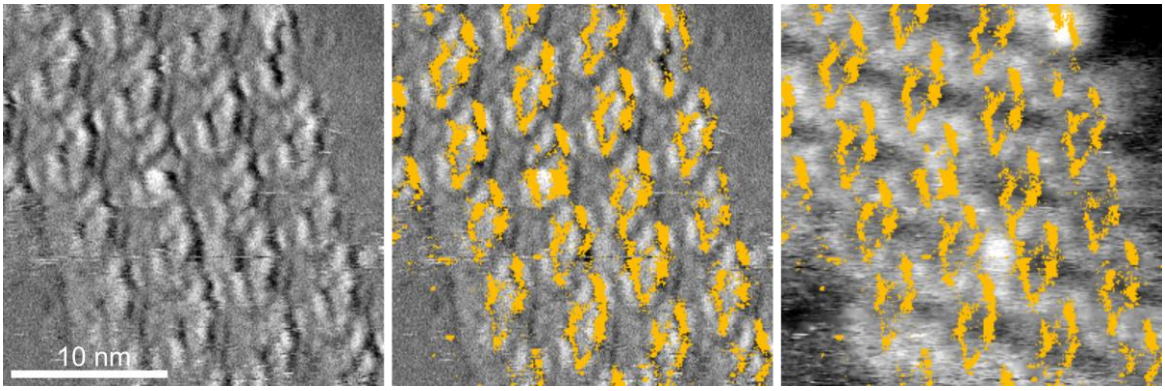


Figure S14. C_M cluster on Au(111). A) second eigenmode frequency shift image corresponding to fig 5C-D of the main manuscript. B) Mask pattern extracted from the second eigenmode dissipation superimposed on the second eigenmode frequency shift and on the C) topography images. Mask is yellow.

Parameters: A,B) f_2 = 2.3 MHz, A_2 = 200pm. C) f_1 = 322 kHz, A_1 = 8nm, Δf_1 = -60 Hz.

Geometry optimizations

The geometry of (*P*)-**C_2** was modeled from the crystal structure of (*rac*)-**C_1** and optimized by molecular mechanics to obtain an initial structure which was further refined by geometry optimization at B3LYP/3-21G level of theory and analyzed by computed frequencies.

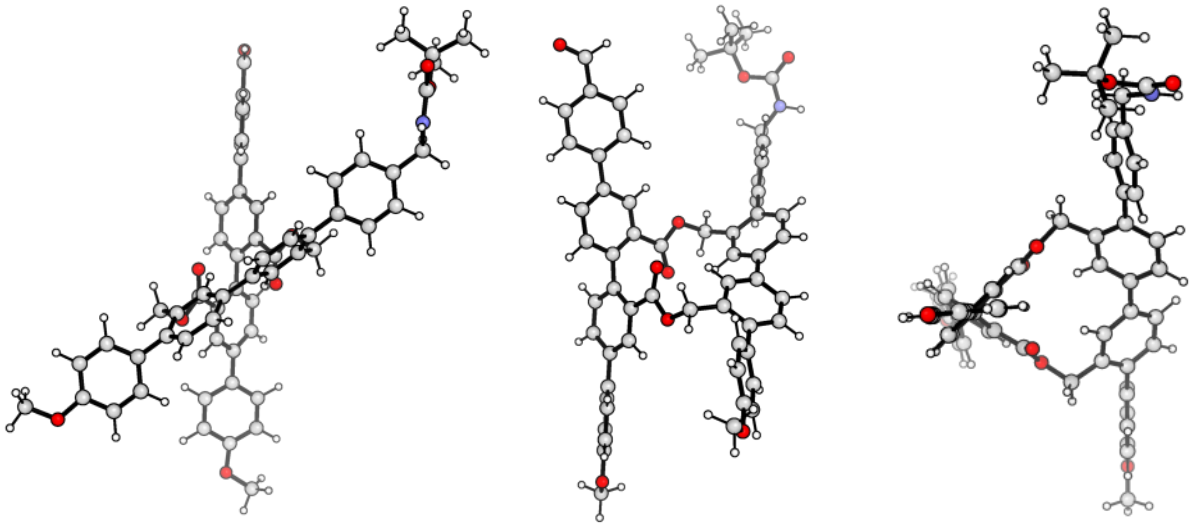


Figure S15. Geometry optimized structure of *(*P*)*-**C_2** , displayed in different orientations from left to right: front, side and top view.

The macrocyclic dimerization product of the imine condensation can either lead to a homochiral or heterochiral product. Thus, (*M, M*)-**$O_{M\text{-}I,dimer}$** and (*M, P*)-**$O_{M\text{-}I,dimer}$** were modeled from the optimized geometry from (*P*)-**C_2** and the initial guesses optimized by molecular mechanics. Both geometries were further optimized at B3LYP/6-31G* level of theory and analyzed by computed frequencies. The model of (*M, M*)- **$O_{M\text{-}I,dimer}$** has the terphenyl on the "carbonyl side" of the parent monomers on one plane and the "alcohol side" out of plane leading to a boat like structure. In contrast the model of (*M, P*)-**$O_{M\text{-}I,dimer}$** has of each parent structure the opposed side (carbonyl and alcohol side) in one plane leading to a staggered structure. Computed thermal data suggest that the homochiral product is the more stable product see Table S1.

Table S1. Thermal energies and corrections from the frequency analysis of (*M, M*)- **$O_{M\text{-}I,dimer}$** and (*M, P*)- **$O_{M\text{-}I,dimer}$** at B3LYP/6-31G* level of theory.

Species	SP E [Hartree]	ZPC [Hartree]	corr E [Hartree]	Thermal corrections [Hartree]	G [Hartree]
(*M, M*)-$O_{M\text{-}I,dimer}$	-5327.917	1.659436	-5326.257402	1.762756	-5326.154082
(*M, P*)-$O_{M\text{-}I,dimer}$	-5327.911	1.658267	-5326.25261	1.762043	-5326.148834

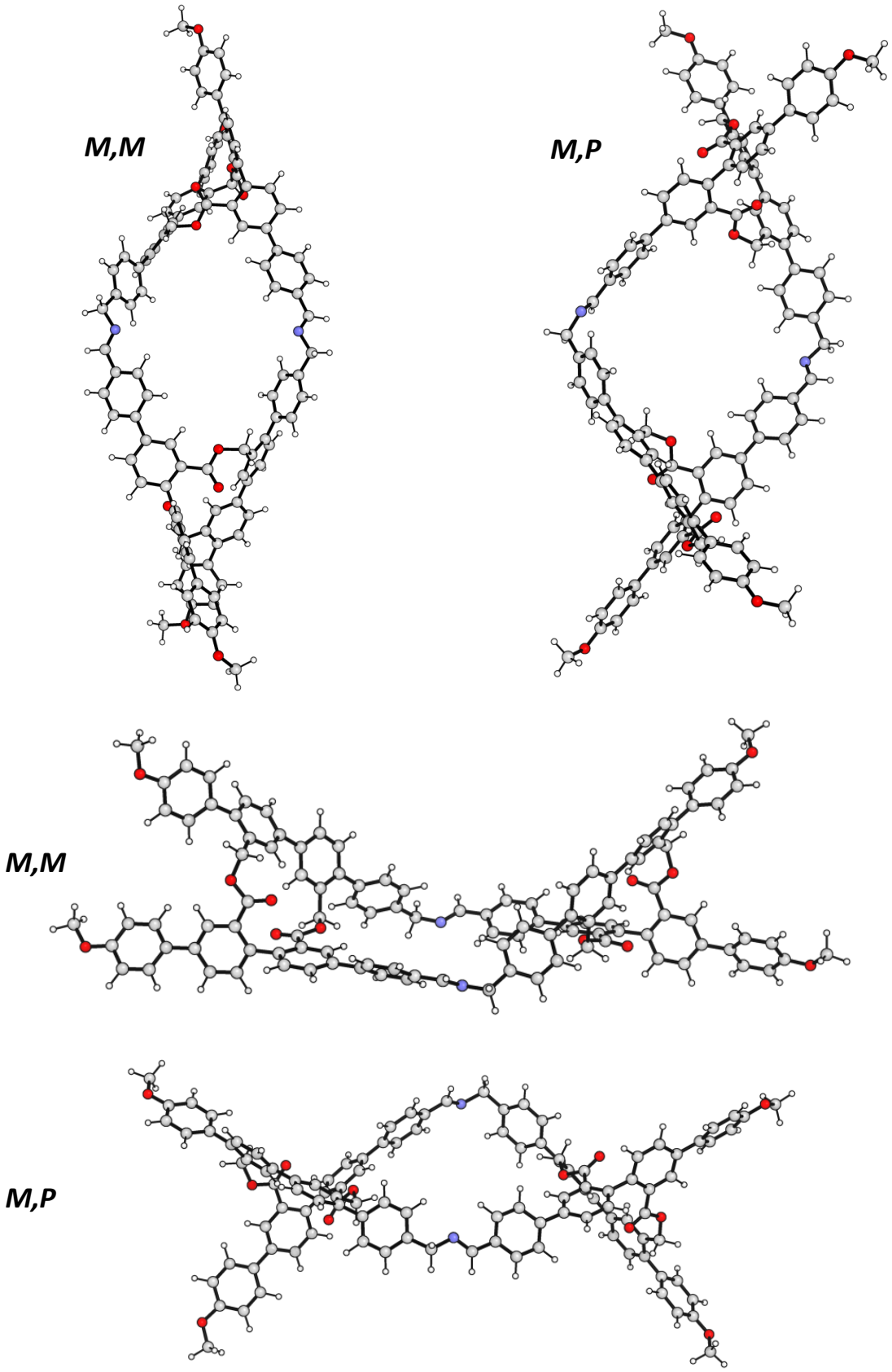


Figure S16. Geometry optimized structure of *(M,M)*-$\mathbf{O}_{\text{M-I-dimer}}$ and *(M,*P*)*-$\mathbf{O}_{\text{M-I-dimer}}$, displayed in top view orientation (top) and from the side (bottom).

Coordinates (energies in kcal)

122

(*P*)-$\mathbf{C_2}$ Energy: -1926511.1666091

O	10.05947	-1.17837	-1.69126
O	10.77937	-3.23880	-0.87296
O	-9.70383	-3.99247	3.25073
O	1.46719	0.60157	-0.78461
O	-0.71802	0.80828	-1.46291
O	-4.18791	0.05457	1.05006
O	-2.09477	0.77827	1.66005
O	6.41060	6.01826	5.23039
O	-9.55522	2.71280	-4.84145
N	8.82638	-3.03345	-2.08145
H	8.69288	-4.03699	-2.01143
C	11.22181	-0.43118	-1.09651
C	11.19620	-0.57465	0.43284
H	11.32887	-1.62360	0.70017
H	10.23737	-0.21677	0.82243
H	12.00126	0.02527	0.86961
C	12.53151	-0.95690	-1.70350
H	12.49855	-0.86214	-2.79392
H	12.65912	-2.00585	-1.43402
H	13.37289	-0.36899	-1.32233
C	10.93426	1.00995	-1.53371
H	9.96904	1.33464	-1.13391
H	10.90060	1.06725	-2.62573
H	11.72021	1.67486	-1.16211
C	9.96333	-2.54528	-1.49244
C	7.85746	-2.23904	-2.84592
H	7.90653	-2.49298	-3.91342
H	8.16712	-1.19886	-2.73013
C	6.42828	-2.42652	-2.35315
C	5.35968	-2.37896	-3.25568
H	5.55849	-2.25680	-4.31576
C	4.04377	-2.50371	-2.81000
H	3.22654	-2.49431	-3.52262
C	3.76484	-2.68027	-1.44539
C	4.84034	-2.74057	-0.54492
H	4.63663	-2.87281	0.51151
C	6.15399	-2.61502	-0.99374
H	6.97739	-2.66408	-0.29132
C	2.36354	-2.84316	-0.95821
C	1.37587	-1.85311	-1.14086
C	0.07755	-2.08943	-0.67848
H	-0.67772	-1.33733	-0.86190
C	-0.26597	-3.26209	0.00350
C	0.72049	-4.24368	0.18395
H	0.48284	-5.15648	0.71842
C	2.00959	-4.03434	-0.29884
H	2.76675	-4.79874	-0.16687
C	1.66765	-0.50526	-1.77185
H	2.70998	-0.41227	-2.06649
H	0.99600	-0.31901	-2.61350
C	-1.64615	-3.39173	0.53934
C	-2.23808	-2.27204	1.13377
H	-1.66534	-1.36201	1.25010
C	-3.55954	-2.28663	1.59099
C	-4.30999	-3.47713	1.49645
C	-3.70323	-4.61020	0.92386
H	-4.27736	-5.52731	0.85858
C	-2.39701	-4.57334	0.44330
H	-1.96572	-5.45145	-0.02406
C	-4.13988	-0.99002	2.12110
H	-5.17767	-1.10671	2.42313
H	-3.52739	-0.59588	2.93582
C	-5.71478	-3.58375	1.98751
C	-6.03392	-3.38000	3.33579
H	-5.24325	-3.14314	4.03919
C	-7.34691	-3.50415	3.79615
H	-7.55490	-3.34588	4.84565
C	-8.37093	-3.84261	2.90695
C	-8.06045	-4.05584	1.55521
H	-8.86874	-4.31286	0.88339
C	-6.75452	-3.92943	1.10422
H	-6.52809	-4.08221	0.05551
C	-10.08075	-3.78310	4.64512
H	-9.57918	-4.49595	5.31093
H	-11.15768	-3.94982	4.67347
H	-9.85646	-2.76153	4.97550
C	0.21631	1.19022	-0.75595
C	-3.09488	0.89272	0.94697
C	6.04626	4.86662	4.96944
C	4.83934	4.53097	4.19121
C	4.48932	3.20160	3.93072
H	5.10949	2.39728	4.31454
C	3.34476	2.91220	3.19365
H	3.05848	1.88295	3.01386
C	2.53032	3.94895	2.70245
C	2.89313	5.28464	2.96999
H	2.28585	6.08922	2.57233
C	4.03391	5.57022	3.70594
H	4.33804	6.58890	3.91697
C	1.30867	3.63855	1.91650

C	1.30825	2.60807	0.96962
H	2.20500	2.03620	0.77983
C	0.16476	2.30206	0.22648
C	-1.02571	3.03096	0.42265
C	-1.01693	4.06969	1.36299
H	-1.92660	4.63603	1.52122
C	0.12408	4.36877	2.10262
H	0.09099	5.15687	2.84588
C	-2.28150	2.85903	-0.38577
C	-3.28867	1.91093	-0.11476
C	-4.46587	1.89851	-0.86880
H	-5.19939	1.13541	-0.65224
C	-4.68570	2.82178	-1.89825
C	-3.68397	3.77205	-2.15444
H	-3.84087	4.51833	-2.92463
C	-2.50811	3.78857	-1.40823
H	-1.75040	4.53573	-1.61186
C	-5.94136	2.79836	-2.69114
C	-7.18332	2.54681	-2.07572
H	-7.22437	2.38850	-1.00441
C	-8.35584	2.52623	-2.81497
H	-9.31488	2.34284	-2.34890
C	-8.32954	2.75524	-4.19913
C	-7.10427	3.00362	-4.82433
H	-7.05152	3.17056	-5.89160
C	-5.92780	3.02329	-4.07416
H	-4.98207	3.18799	-4.57772
C	-9.58333	2.94416	-6.28222
H	-9.00164	2.18863	-6.82421
H	-9.20688	3.94192	-6.53880
H	-10.63479	2.86605	-6.55926
H	6.61414	3.97877	5.30938

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(*M*, *M*)-**O_{2l}** Energy: -3344359.5777743

H	-5.66697	1.82458	-1.52506
C	-3.92467	2.29392	-3.61592
C	-5.03052	1.61725	-4.16840
C	-6.37770	1.71215	-3.55428
C	-7.54027	1.69256	-4.34126
H	-7.45927	1.64677	-5.42353
C	-8.79946	1.75730	-3.75683
H	-9.68377	1.73488	-4.38697
C	-8.96582	1.84493	-2.36887
C	-7.80240	1.89893	-1.56791
C	-7.90531	2.03355	-0.08291
O	-6.69814	1.92163	0.52345
C	-6.65305	2.04492	1.97211
C	-6.59567	0.67681	2.62166
C	-7.61664	-0.22632	2.31257
C	-7.61794	-1.55123	2.76404
C	-8.71444	-2.46339	2.35713
C	-9.22105	-3.46325	3.20243
C	-10.26446	-4.27843	2.77984
C	-10.86464	-4.12945	1.51515
C	-10.37373	-3.11259	0.66673
C	-10.98800	-2.78561	-0.67990
O	-11.39692	-1.39181	-0.73785
C	-10.58349	-0.51925	-1.38341
O	-9.51775	-0.84191	-1.87533
C	-11.15010	0.86261	-1.40780
C	-12.47449	1.07244	-1.00181
C	-13.07092	2.33910	-1.02553
C	-14.47498	2.53453	-0.58871
C	-15.32027	3.45635	-1.23569
C	-16.63361	3.64325	-0.82955
C	-17.15108	2.90800	0.24711
O	-18.45253	3.16306	0.56993
C	-19.03024	2.44194	1.64629
H	-19.03005	1.36068	1.45455
H	-18.50797	2.63960	2.59182
H	-20.06056	2.79404	1.72377
C	-16.32990	1.98598	0.90596
H	-16.69773	1.41095	1.74810
H	-17.28516	4.34738	-1.33771
H	-14.94803	4.01767	-2.08832
C	-15.01053	1.81069	0.48506
H	-14.37936	1.11076	1.02545
C	-12.28947	3.41151	-1.48277
C	-10.97372	3.21654	-1.88957
H	-10.38623	4.06650	-2.22480
H	-12.70678	4.41456	-1.49691
H	-13.05514	0.21503	-0.68444
H	-11.90400	-3.34931	-0.85132
H	-10.28499	-2.96544	-1.49722
C	-11.97091	-5.05161	1.13861
C	-13.07443	-5.23339	1.99442
C	-14.09841	-6.11517	1.67878
C	-14.05096	-6.85550	0.48808
O	-15.10507	-7.69381	0.26768
C	-15.11120	-8.46576	-0.92257
H	-15.11156	-7.82890	-1.81714
H	-14.25154	-9.14762	-0.96654
H	-16.03288	-9.04987	-0.89579
C	-12.96094	-6.69841	-0.37499
H	-12.88922	-7.26652	-1.29546

H	-14.95231	-6.24535	2.33645	C	2.36003	3.16653	4.67082
H	-13.13266	-4.65744	2.91403	C	1.03656	3.27899	5.30093
C	-11.93887	-5.80588	-0.04179	C	3.45026	2.70809	5.42327
H	-11.08473	-5.71840	-0.70842	H	3.30361	2.43067	6.46505
H	-10.63125	-5.06031	3.43947	C	4.71226	2.58672	4.84993
H	-8.80838	-3.59337	4.19926	H	5.53268	2.19464	5.44368
C	-9.29955	-2.32606	1.09284	C	7.44232	3.02563	3.64278
H	-8.90086	-1.58815	0.40622	H	7.36755	3.34215	4.67924
C	-6.55379	-1.95992	3.58358	C	8.69915	2.87566	3.06747
C	-5.54921	-1.06352	3.93039	H	9.58647	3.05214	3.66852
H	-4.74347	-1.38976	4.58247	C	8.85914	2.49629	1.72869
H	-6.50399	-2.98541	3.93967	C	7.69147	2.29673	0.95725
H	-8.44563	0.12432	1.70876	C	7.78395	1.92597	-0.48752
C	-5.54375	0.26571	3.46836	O	6.57615	1.58526	-1.00214
C	-4.44974	1.17286	3.91438	C	6.50545	1.25710	-2.41622
C	-4.72670	2.38998	4.55903	C	6.48367	-0.24426	-2.62487
H	-5.75987	2.68410	4.72591	C	7.51141	-0.99136	-2.04455
C	-3.69695	3.21230	5.01077	C	7.56047	-2.38907	-2.10642
H	-3.94114	4.14856	5.50878	C	8.68468	-3.09312	-1.44401
C	-2.35630	2.84590	4.84507	C	9.32339	-4.21162	-2.00043
C	-1.25413	3.72760	5.40999	C	10.44725	-4.75609	-1.38699
N	-0.01176	3.63119	4.66482	C	10.99667	-4.20958	-0.21146
H	-1.10979	3.48767	6.48102	C	10.32604	-3.11731	0.38234
H	-1.58827	4.77326	5.36588	C	10.76419	-2.46048	1.67325
C	-2.07430	1.63655	4.20121	O	11.29056	-1.12545	1.41369
H	-1.04061	1.34522	4.04215	C	10.43622	-0.08314	1.58275
C	-3.10336	0.81347	3.74559	O	9.30351	-0.21615	2.00868
H	-2.86224	-0.11544	3.23546	C	11.03604	1.22195	1.17615
H	-5.75369	2.62548	2.17210	C	12.37001	1.27067	0.75041
H	-7.53461	2.60663	2.29055	C	12.98435	2.46465	0.35446
O	-8.94251	2.22086	0.52548	C	14.39710	2.48795	-0.09714
C	-10.36983	1.95405	-1.85307	C	15.24856	3.56325	0.22152
C	-6.53833	1.82149	-2.16795	C	16.57017	3.58953	-0.19958
C	-4.81947	0.84623	-5.32388	C	17.08992	2.53208	-0.96078
C	-3.55890	0.76205	-5.90671	O	18.39947	2.65070	-1.32624
C	-2.46320	1.43651	-5.35037	C	18.97974	1.60639	-2.09128
C	-1.14379	1.33132	-5.99022	H	18.95920	0.65048	-1.55123
H	-3.41804	0.15554	-6.79896	H	18.47357	1.48431	-3.05808
H	-5.64475	0.28654	-5.75400	H	20.01664	1.90137	-2.26252
H	-4.06488	2.91696	-2.73736	C	16.26252	1.45260	-1.29055
C	-2.66471	2.20445	-4.19113	H	16.63188	0.62648	-1.88742
H	-1.81872	2.73370	-3.76445	H	17.22640	4.41536	0.05711
C	6.27617	2.79987	2.89530	H	14.87387	4.38055	0.83167
C	4.93003	2.92980	3.50497	C	14.93487	1.44226	-0.85931
C	3.83033	3.39528	2.75658	H	14.29891	0.61025	-1.14874
H	3.97628	3.69231	1.72211	C	12.21145	3.63524	0.40507
C	2.56909	3.50891	3.32428	C	10.88750	3.60158	0.82988
H	1.72747	3.87259	2.74356	H	10.30875	4.52056	0.84906

H	12.64315	4.57965	0.08543
H	12.94326	0.35188	0.75354
H	11.57656	-2.99771	2.15914
H	9.92327	-2.36048	2.36165
C	12.25100	-4.79884	0.33279
C	13.38124	-4.00498	0.61041
C	14.56176	-4.56713	1.07625
C	14.65367	-5.95223	1.27870
O	15.85584	-6.40641	1.73911
C	16.00707	-7.79954	1.95893
H	15.30383	-8.16783	2.71771
H	15.86876	-8.37244	1.03228
H	17.02861	-7.93689	2.31819
C	13.54554	-6.76144	1.00468
H	13.58490	-7.83425	1.15577
H	15.43312	-3.95362	1.28346
H	13.33402	-2.93279	0.44082
C	12.36503	-6.17997	0.53600
H	11.50735	-6.81789	0.33928
H	10.95612	-5.59345	-1.85674
H	8.97232	-4.62537	-2.94223
C	9.18337	-2.59903	-0.23297
H	8.66350	-1.78308	0.25704
C	6.53628	-3.04838	-2.80272
C	5.51856	-2.31794	-3.40707
H	4.74027	-2.83976	-3.95739
H	6.52853	-4.13370	-2.86116
H	8.31427	-0.46179	-1.54495
C	5.46724	-0.91285	-3.34099
C	4.36389	-0.20442	-4.04819
C	4.62758	0.78454	-5.01004
H	5.65717	1.04888	-5.23772
C	3.58966	1.41300	-5.69500
H	3.82353	2.17427	-6.43652
C	2.25456	1.07107	-5.45235
C	1.14417	1.71886	-6.26343
N	-0.09091	1.87266	-5.51463
H	0.98913	1.14072	-7.19469
H	1.47511	2.72098	-6.56815
C	1.98573	0.08897	-4.49285
H	0.95565	-0.17468	-4.27262
C	3.02239	-0.53935	-3.80449
H	2.79128	-1.28993	-3.05320
H	5.58515	1.72504	-2.76348
H	7.36339	1.71804	-2.91255
O	8.81147	1.92672	-1.13904
C	10.26490	2.40700	1.21151
C	6.43103	2.44045	1.55085
H	5.55611	2.24023	0.94514
H	-1.12071	0.74978	-6.92861
H	1.00533	3.03884	6.37821

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(*M*, *P*)-**O$_{2l}$** Energy: -3344355.1036318

O	17.17340	-5.00990	0.10710
O	5.73585	-0.05230	0.71711
O	7.05080	1.64318	-0.00814
O	11.35289	-0.13348	-0.90499
O	9.53079	-1.25909	-1.64173
O	14.00495	7.68238	-2.58829
N	0.28717	2.18224	5.92196
C	1.46937	2.80312	6.49685
H	1.46777	2.56225	7.57226
H	1.44884	3.90426	6.42518
C	2.75432	2.26182	5.89131
C	3.90505	3.05420	5.83164
H	3.86683	4.08620	6.17496
C	5.10541	2.54261	5.33390
H	5.98663	3.17731	5.28964
C	5.18505	1.22191	4.87108
C	4.02554	0.43141	4.93279
H	4.06997	-0.60280	4.59958
C	2.83107	0.94060	5.43470
H	1.94353	0.31809	5.47459
C	6.46357	0.64526	4.35538
C	6.62300	0.26709	3.00469
C	7.80615	-0.34347	2.60168
H	7.89195	-0.68433	1.57790
C	8.88313	-0.55067	3.47800
C	8.73122	-0.13733	4.80866
H	9.55162	-0.25058	5.51178
C	7.53656	0.43979	5.23415
H	7.42309	0.73635	6.27369
C	5.54865	0.60294	1.98512
H	4.56054	0.28057	2.31627
H	5.52454	1.68515	1.82187
C	10.12999	-1.17090	2.96827
C	10.50127	-0.98093	1.62919
H	9.91087	-0.30745	1.02245
C	11.61906	-1.58864	1.06272
C	12.44503	-2.40439	1.86946
C	12.09697	-2.56160	3.22196
H	12.71915	-3.19645	3.84722
C	10.96075	-1.97066	3.76555
H	10.70162	-2.16276	4.80297
C	11.92630	-1.35892	-0.40717

H	13.00145	-1.26068	-0.57223	C	12.55950	4.36311	-2.81093
H	11.54684	-2.18103	-1.01982	H	12.90984	3.36095	-3.04167
C	13.66606	-3.08631	1.35718	C	13.46716	5.41206	-2.81987
C	13.63704	-3.93160	0.24038	H	14.51730	5.24553	-3.03888
H	12.69739	-4.10532	-0.27653	C	13.03701	6.72084	-2.55550
C	14.78055	-4.59400	-0.21299	C	11.68486	6.95667	-2.28256
H	14.70775	-5.24548	-1.07640	H	11.32439	7.95507	-2.06246
C	15.99503	-4.41825	0.45919	C	10.78472	5.88959	-2.27719
C	16.04451	-3.58044	1.58330	H	9.74426	6.08715	-2.03435
H	16.99466	-3.45091	2.09229	C	13.62597	9.02500	-2.33150
C	14.89874	-2.93140	2.02101	H	13.20802	9.14110	-1.32270
H	14.95566	-2.27606	2.88596	H	12.89541	9.38651	-3.06741
C	17.18220	-5.86829	-1.02234	H	14.54078	9.61499	-2.41223
H	16.51514	-6.72906	-0.88107	O	-14.42999	7.57557	-2.23402
H	18.21009	-6.22186	-1.12162	O	-5.84968	-1.20046	0.07537
H	16.89242	-5.33497	-1.93749	O	-7.77986	-2.28594	0.54896
C	6.46733	0.60203	-0.22728	O	-11.31510	0.98614	0.16446
C	10.14409	-0.21657	-1.52498	O	-9.48114	1.57321	1.35526
C	0.62614	-5.08951	-3.59056	O	-16.73431	-5.42571	1.48804
C	1.87373	-4.31465	-3.50172	N	-0.21121	-4.94083	-4.53961
C	2.65127	-4.38155	-2.33717	C	-1.47099	-5.66598	-4.46667
H	2.36402	-5.06297	-1.53917	H	-1.48041	-6.41965	-3.66031
C	3.76996	-3.56837	-2.17922	H	-1.59974	-6.20699	-5.41558
H	4.35716	-3.63106	-1.26755	C	-2.63077	-4.69915	-4.26898
C	4.15246	-2.66902	-3.18764	C	-3.71462	-5.03517	-3.45205
C	3.39698	-2.64342	-4.37595	H	-3.73992	-6.00687	-2.96320
H	3.66918	-1.94700	-5.16437	C	-4.76580	-4.13996	-3.24663
C	2.27473	-3.44543	-4.52987	H	-5.60305	-4.43918	-2.62246
H	1.67221	-3.39275	-5.43087	C	-4.76029	-2.87061	-3.84489
C	5.27733	-1.72364	-2.98417	C	-3.67743	-2.54929	-4.68243
C	5.43807	-1.08033	-1.75234	H	-3.64498	-1.56891	-5.15017
H	4.74549	-1.29272	-0.94757	C	-2.63321	-3.44469	-4.89192
C	6.43057	-0.11500	-1.53840	H	-1.79123	-3.16258	-5.51560
C	7.32739	0.21149	-2.58032	C	-5.84233	-1.86741	-3.63332
C	7.17356	-0.44933	-3.80656	C	-6.25302	-1.42721	-2.35343
H	7.86250	-0.21568	-4.61298	C	-7.20377	-0.41406	-2.25526
C	6.17121	-1.39163	-4.01321	H	-7.45029	-0.02922	-1.27438
H	6.09052	-1.88381	-4.97868	C	-7.81263	0.16763	-3.37827
C	8.36641	1.29026	-2.49978	C	-7.41714	-0.29181	-4.64226
C	9.68640	1.11231	-2.02915	H	-7.88396	0.10558	-5.53894
C	10.58321	2.19032	-2.04212	C	-6.44304	-1.27760	-4.75778
H	11.57752	2.03491	-1.64208	H	-6.14799	-1.62351	-5.74476
C	10.22557	3.45200	-2.53077	C	-5.66067	-2.02890	-1.08996
C	8.91655	3.60991	-3.01318	H	-6.10534	-3.00535	-0.88230
H	8.60761	4.56518	-3.42839	H	-4.57839	-2.14561	-1.18246
C	8.01408	2.55291	-2.99300	C	-8.82778	1.23355	-3.20010
H	7.00572	2.70330	-3.36752	C	-9.61336	1.26693	-2.03800
C	11.19414	4.57547	-2.53955	H	-9.52577	0.45246	-1.33108

C	-10.52845	2.28376	-1.77781
C	-10.71643	3.30758	-2.73381
C	-9.96167	3.25208	-3.91673
H	-10.09079	4.04139	-4.65260
C	-9.02621	2.24826	-4.14719
H	-8.42438	2.27713	-5.05095
C	-11.31597	2.27501	-0.47859
H	-10.91191	3.00460	0.22733
H	-12.36917	2.50421	-0.65797
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C	-11.63631	5.28242	-1.44396
H	-10.86582	5.14255	-0.69085
C	-12.52945	6.34657	-1.29645
H	-12.44647	6.99115	-0.42879
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C	-13.56872	5.72761	-3.39144
H	-14.33241	5.91426	-4.14016
C	-12.67239	4.67614	-3.52315
H	-12.73963	4.02399	-4.38985
C	-14.41180	8.46197	-1.12654
H	-15.22469	9.17028	-1.29667
H	-13.46199	9.00932	-1.06239
H	-14.58565	7.93107	-0.18111
C	-6.94107	-1.46055	0.84716
C	-10.34493	0.76031	1.09308
C	-0.73659	2.90700	5.69910
C	-1.99006	2.36347	5.14970
C	-2.06238	1.05212	4.65145
H	-1.16747	0.43883	4.66884
C	-3.25868	0.55080	4.15825
H	-3.30264	-0.47178	3.79373
C	-4.43091	1.33108	4.15934
C	-4.35285	2.64298	4.65295
H	-5.23792	3.27298	4.64004
C	-3.14803	3.15364	5.13042
H	-3.10526	4.17645	5.49892
C	-5.71417	0.76251	3.67681
C	-5.76943	-0.01505	2.51552
H	-4.87249	-0.15736	1.92453
C	-6.96024	-0.61464	2.07976
C	-8.15026	-0.43450	2.82027
C	-8.09252	0.36652	3.96830
H	-9.00109	0.51755	4.54358
C	-6.90729	0.95738	4.39002
H	-6.89743	1.54627	5.30317
C	-9.44857	-1.12318	2.51837
C	-10.48543	-0.58505	1.72478
C	-11.67609	-1.30547	1.54956
H	-12.46168	-0.86082	0.95119
C	-11.88823	-2.55209	2.14865
C	-10.85503	-3.06864	2.94718
H	-10.97006	-4.04385	3.41197
C	-9.66868	-2.36677	3.12423
H	-8.87696	-2.79889	3.72919
C	-13.15722	-3.29371	1.94935
C	-13.82537	-3.27493	0.71772
H	-13.39379	-2.72846	-0.11621
C	-15.01968	-3.96924	0.51760
H	-15.49563	-3.93443	-0.45574
C	-15.57542	-4.70952	1.56731
C	-14.92131	-4.74177	2.80783
H	-15.36930	-5.31190	3.61577
C	-13.73517	-4.04576	2.99011
H	-13.25880	-4.06395	3.96652
C	-17.44188	-5.42331	0.25836
H	-18.32496	-6.04420	0.41999
H	-16.84112	-5.85260	-0.55441
H	-17.75767	-4.41022	-0.02402
H	0.43612	-5.78162	-2.75222
H	-0.74451	3.98796	5.92135

Crystallographic Data

Compound 3 (CCDC-2371751)

Table S2. Crystal data and structure refinement for **3**

Formula	$C_{34}H_{34}BBrO_6$
$D_{calc.}$/ g cm^{-3}	1.390
□/mm^{-1}	1.461
Formula Weight	629.33
Colour	colourless
Shape	block-shaped
Size/mm^3	0.22×0.18×0.11
T/K	150
Crystal System	triclinic
Space Group	*P*-1
a/Å	10.0457(4)
b/Å	12.3797(4)
c/Å	13.7545(5)
□/°	94.581(3)
□/°	110.868(3)
□/°	106.192(3)
V/Å^3	1504.02(10)
Z	2
Z'	1
Wavelength/Å	1.34143
Radiation type	GaK□
□$_{min}$/°	3.301
□$_{max}$/°	55.714
Measured Refl's.	17572
Indep't Refl's	5722
Refl's I≥2 □(I)	5518
R_{int}	0.0180
Parameters	386
Restraints	0
Largest Peak	0.519
Deepest Hole	-0.623
GooF	1.042
wR_2 (all data)	0.0965
wR_2	0.0947
R_1 (all data)	0.0363
R_1	0.0347

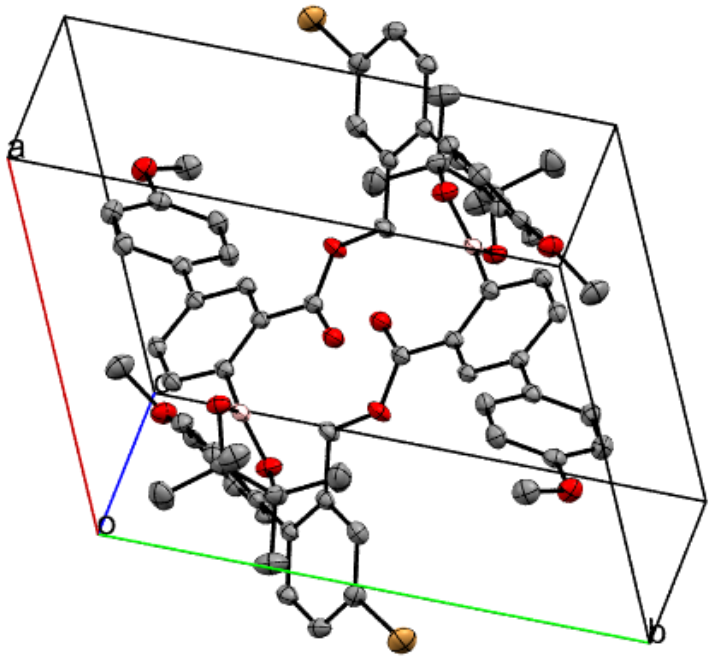


Figure S17. Unit-cell of the solid-state structure of **3**. Visualized as ORTEP representation with 50 % probability, hydrogens are omitted for clarity.

Compound C_1 (CCDC-2374177)

Table S3. Crystal data and structure refinement for **C_1**

Identification code	C_1
Empirical formula	$C_{64.5}H_{57}NO_9$
Formula weight	990.11
Temperature/K	150
Crystal system	triclinic
Space group	P-1
a/Å	8.4822(8)
b/Å	19.6804(15)
c/Å	34.006(4)
α/°	94.828(7)
β/°	95.563(8)
γ/°	97.248(7)
Volume/Å^3	5578.0(9)
Z	4
ρ_{calc}g/cm^3	1.179
μ/mm^{-1}	0.399
F(000)	2092.0
Crystal size/mm^3	0.24 × 0.2 × 0.03
Radiation	GaKα (λ = 1.34143)
2Θ range for data collection/°	3.956 to 118.2
Index ranges	-10 ≤ h ≤ 5, -24 ≤ k ≤ 24, -42 ≤ l ≤ 43
Reflections collected	59228
Independent reflections	23242 [R_{int} = 0.0158, R_{sigma} = 0.0190]
Data/restraints/parameters	23242/2/1342
Goodness-of-fit on F^2	1.047
Final R indexes [I>=2σ (I)]	R_1 = 0.0935, wR_2 = 0.2657
Final R indexes [all data]	R_1 = 0.1151, wR_2 = 0.2859
Largest diff. peak/hole / e Å^{-3}	1.27/-0.73

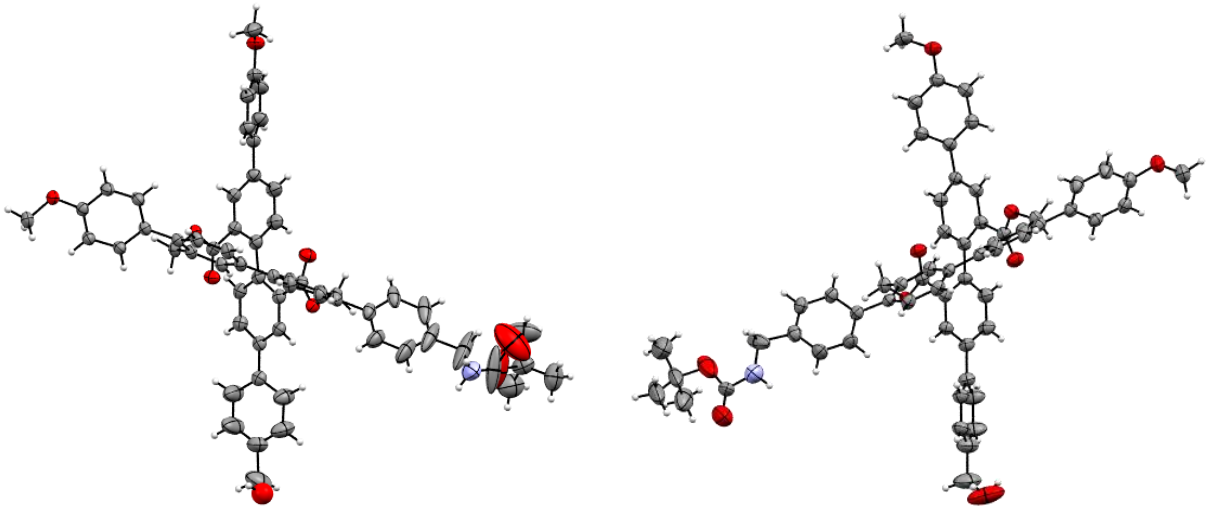


Figure S18. Solid state structure of (***M***)-$\mathbf{C_1}$ (left) and (***P***)-$\mathbf{C_1}$ (right). Visualized as ORTEP representation with 50 % probability, solvent molecules are omitted for clarity.

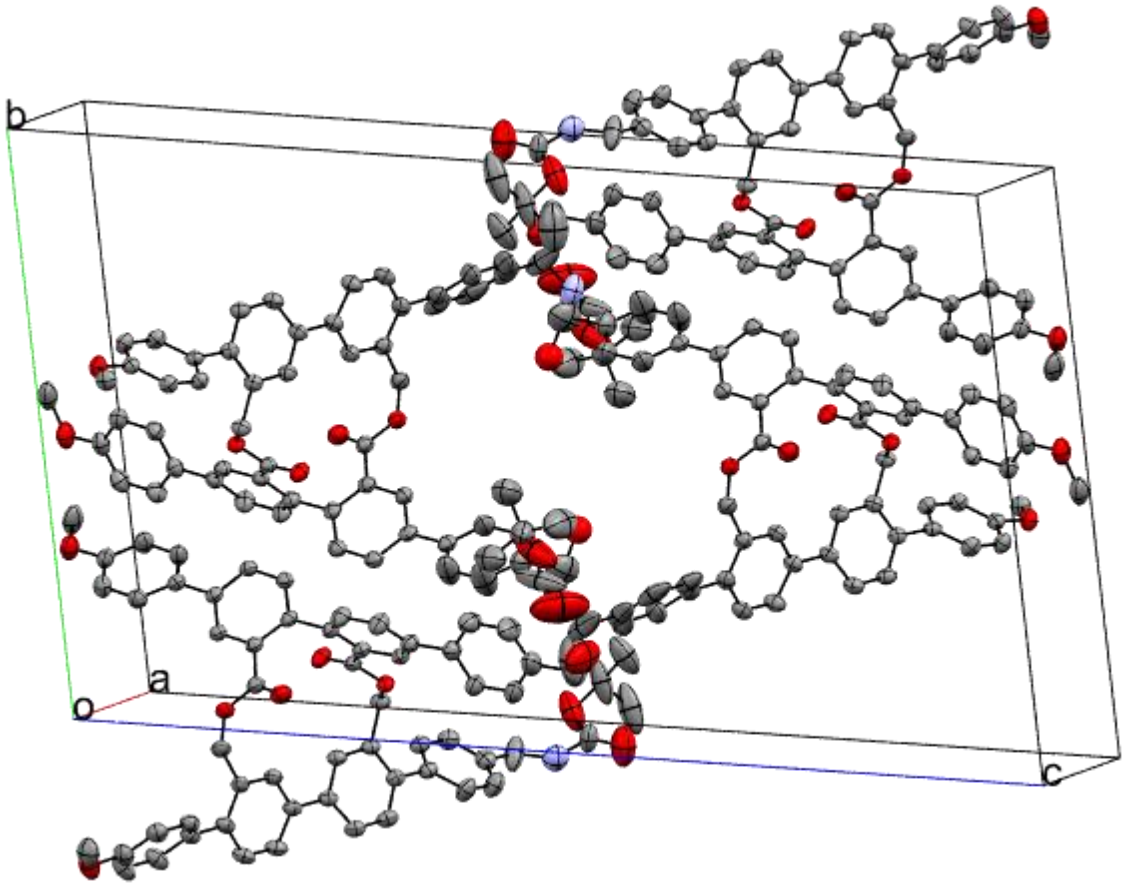


Figure S19. Unit-cell of the solid-state structure of $\mathbf{C_1}$. Visualized as ORTEP representation with 50 % probability, hydrogens are omitted for clarity.

References

[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, Gaussian 09, Revision E.01.

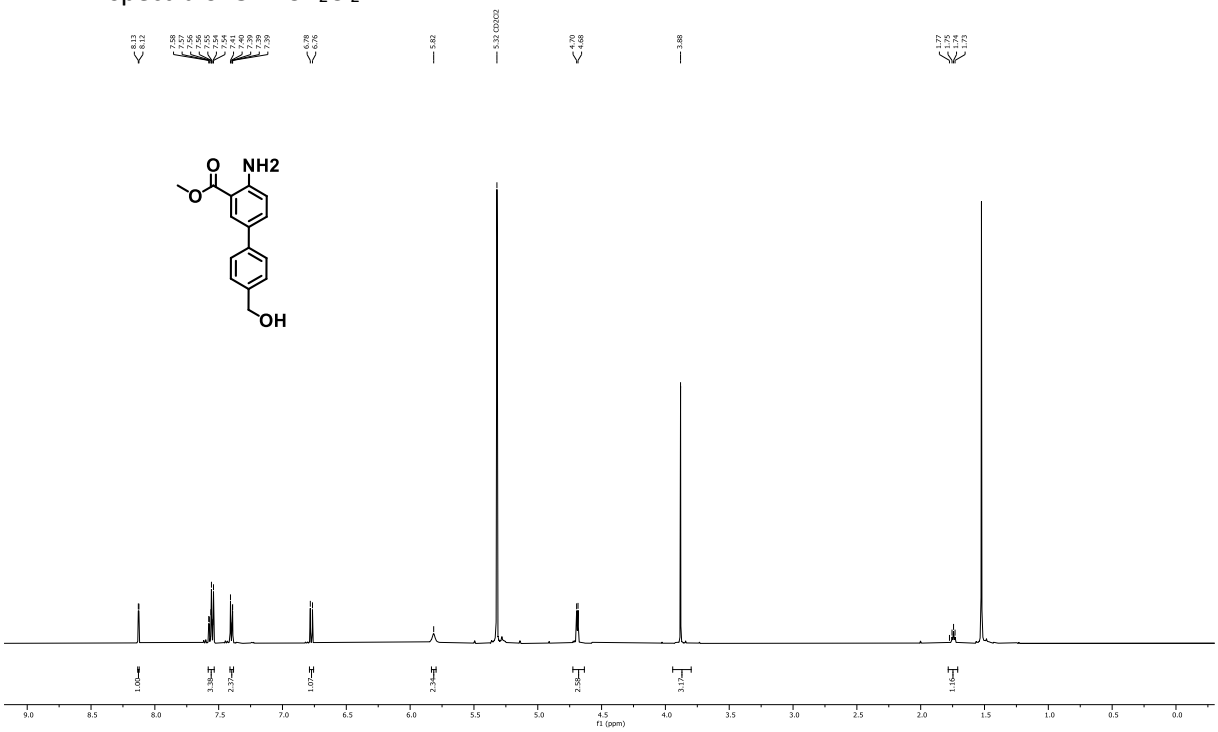
[2] J. J. Dressler, S. A. Miller, B. T. Meeuwsen, A. M. S. Riel, B. J. Dahl, *Tetrahedron* **2015**, *71*, 283–292.

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

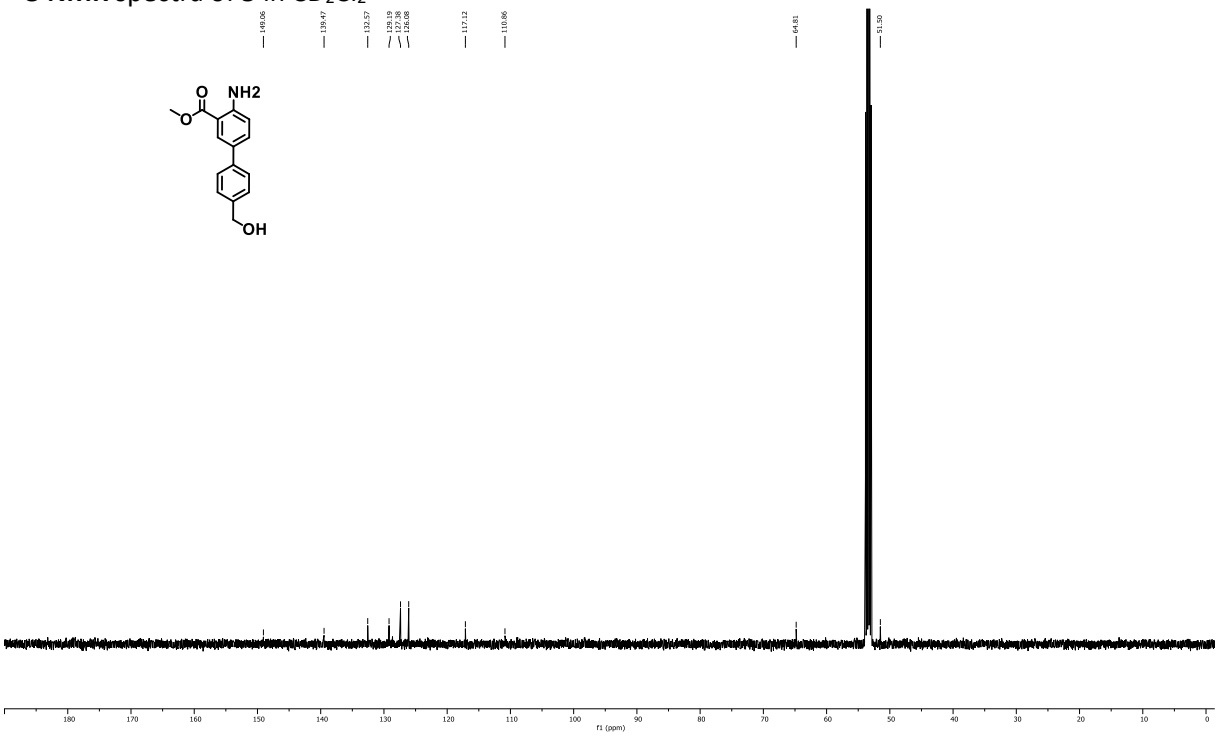
[4] T. Bruhn, A. Schaumlöffel, Y. Hemberger, G. Bringmann, *Chirality* **2013**, *25*, 243–249.

NMR and HR-ESI-MS spectra

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



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

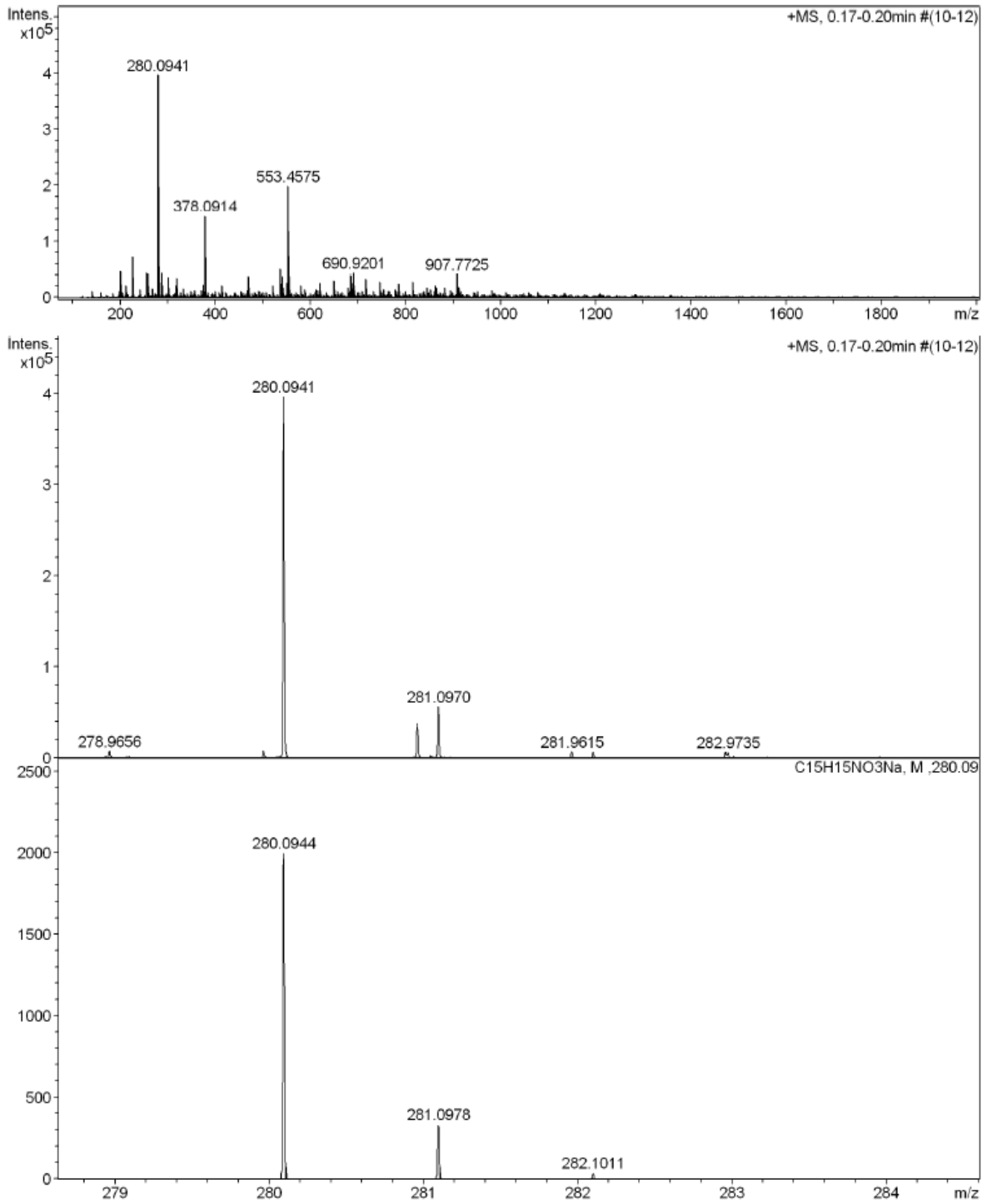


HR-ESI-MS spectra of **5** in CD_2Cl_2

High Resolution Mass Spectrometry Report

Sample Name **KRO-310**
Comment

Instrument maXis 4G
Method ms_nocolumn_mid_pos.m



High Resolution Mass Spectrometry Report

Measured m/z vs. theoretical m/z

Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e^- Conf	z
280.0941	1	C 15 H 15 N Na O 3	100.00	280.0944	0.3	1.0	13.4	8.5	even	1+

Mass list

#	m/z	I %	I
1	141.0028	2.8	11191
2	198.9929	2.9	11676
3	201.1097	12.1	47970
4	212.9720	5.4	21406
5	226.0861	18.7	74087
6	227.0891	3.0	11999
7	242.9823	3.8	14994
8	256.9617	11.2	44424
9	258.1119	10.8	42698
10	266.9812	4.3	17215
11	280.0941	100.0	397163
12	280.9609	9.6	37998
13	281.0970	14.3	56764
14	286.9719	11.5	45586
15	301.0742	3.7	14783
16	302.0756	9.3	37105
17	316.9822	5.3	20918
18	319.2597	3.0	12009
19	320.0860	8.9	35202
20	327.0006	2.5	9982
21	334.1012	4.4	17285
22	348.0803	2.7	10890
23	356.9742	3.2	12830
24	370.9900	3.4	13488
25	374.0902	5.7	22570
26	378.0914	36.7	145878
27	379.0943	6.7	26600
28	400.0728	2.8	11020
29	414.9794	5.3	21182
30	441.2957	2.5	10001
31	452.9564	3.0	11912
32	467.0997	3.5	14010
33	469.3269	9.7	38531
34	470.3301	3.1	12300
35	482.9664	2.6	10342
36	490.9331	3.1	12191
37	492.9482	2.9	11496
38	502.0080	2.7	10617
39	506.9638	2.6	10267
40	520.9437	5.4	21507
41	536.1632	3.4	13509
42	537.1976	13.2	52572
43	538.2008	4.5	17861
44	541.1185	9.5	37913
45	542.1194	4.5	17961
46	543.1168	3.4	13341
47	550.9543	6.7	26799
48	553.4575	50.2	199383
49	554.4606	19.0	75421
50	555.4636	3.8	14986
51	580.9647	5.6	22257
52	588.9309	3.9	15565
53	590.9458	2.5	9917
54	610.9754	3.6	14405
55	615.1377	3.4	13650
56	618.9417	6.7	26560
57	648.9526	7.5	29801
58	656.9190	3.0	11734
59	678.9631	4.5	18004
60	682.9462	3.0	11875
61	685.4337	10.0	39604
62	686.4369	4.5	18035

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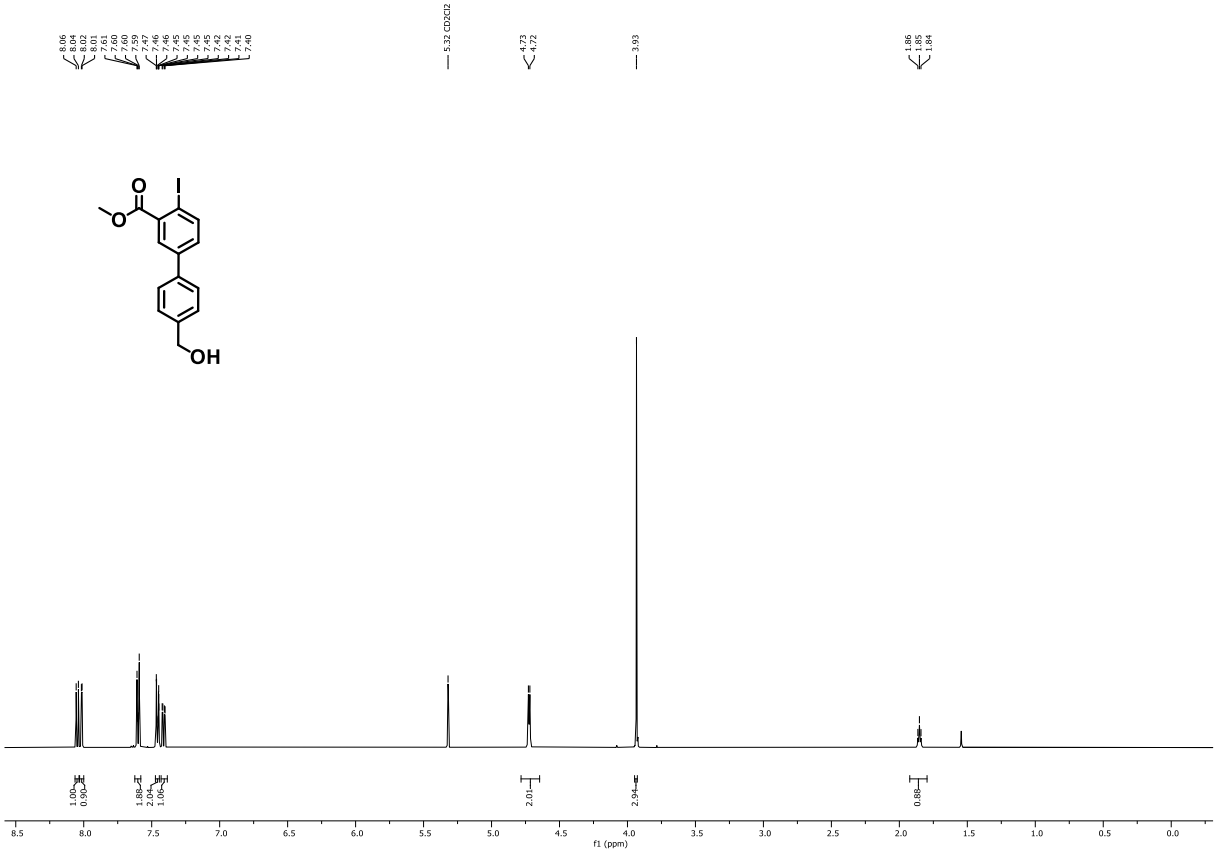
#	m/z	I %	I
63	686.9292	6.8	27055
64	688.9265	4.4	17277
65	689.1563	3.4	13318
66	690.9201	11.3	44777
67	691.9215	3.4	13364
68	697.9516	2.6	10394
69	708.9736	2.8	10954
70	716.9402	8.4	33554
71	731.9463	3.0	11816
72	746.9512	7.2	28418
73	750.9342	2.6	10474
74	754.9175	3.9	15596
75	763.1757	2.9	11543
76	765.9403	3.0	11754
77	776.9616	3.7	14574
78	780.9447	3.0	12095
79	784.9287	6.4	25607
80	799.9340	2.8	10966
81	814.9387	7.0	27813
82	839.9329	2.9	11563
83	844.9495	4.6	18223
84	848.9333	2.5	9882
85	852.9163	3.8	14936
86	860.9488	3.0	11738
87	862.9435	5.5	21993
88	863.9415	4.4	17607
89	882.9272	4.7	18836
90	893.9447	3.5	14025
91	907.7725	10.6	41919
92	908.7762	6.6	26309
93	909.7824	3.2	12899
94	912.9383	4.6	18190
95	916.9500	3.0	11732
96	942.9496	2.7	10662
97	950.9151	2.8	10982
98	980.9266	3.3	13114
99	1010.9385	2.7	10671
100	1078.9263	2.6	10282

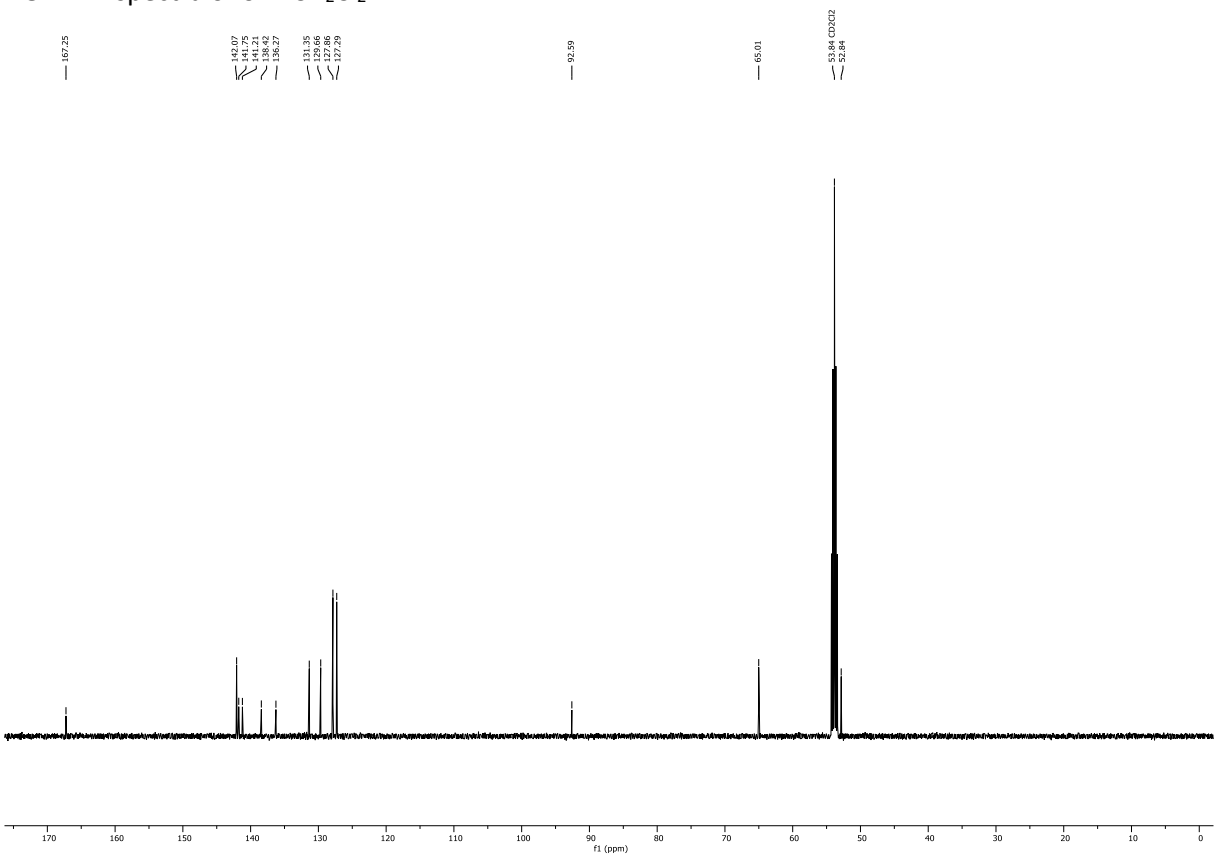
Acquisition Parameter

General	Fore Vacuum	3.40e+000 mBar	High Vacuum	1.24e-007 mBar	Source Type	ESI
	Scan Begin	75 m/z	Scan End	2000 m/z	Ion Polarity	Positive
Source	Set Nebulizer	2.0 Bar	Set Capillary	4500 V	Set Dry Gas	8.0 l/min
	Set Dry Heater	200 °C	Set End Plate Offset	-500 V		
Quadrupole	Set Ion Energy (MS only)	4.0 eV				
Coll. Cell	Collision Energy	8.0 eV	Set Collision Cell RF	600.0 Vpp	100.0 Vpp	
Ion Cooler	Set Ion Cooler Transfer Time	75.0 µs	Set Ion Cooler Pre Pulse Storage Time	10.0 µs		

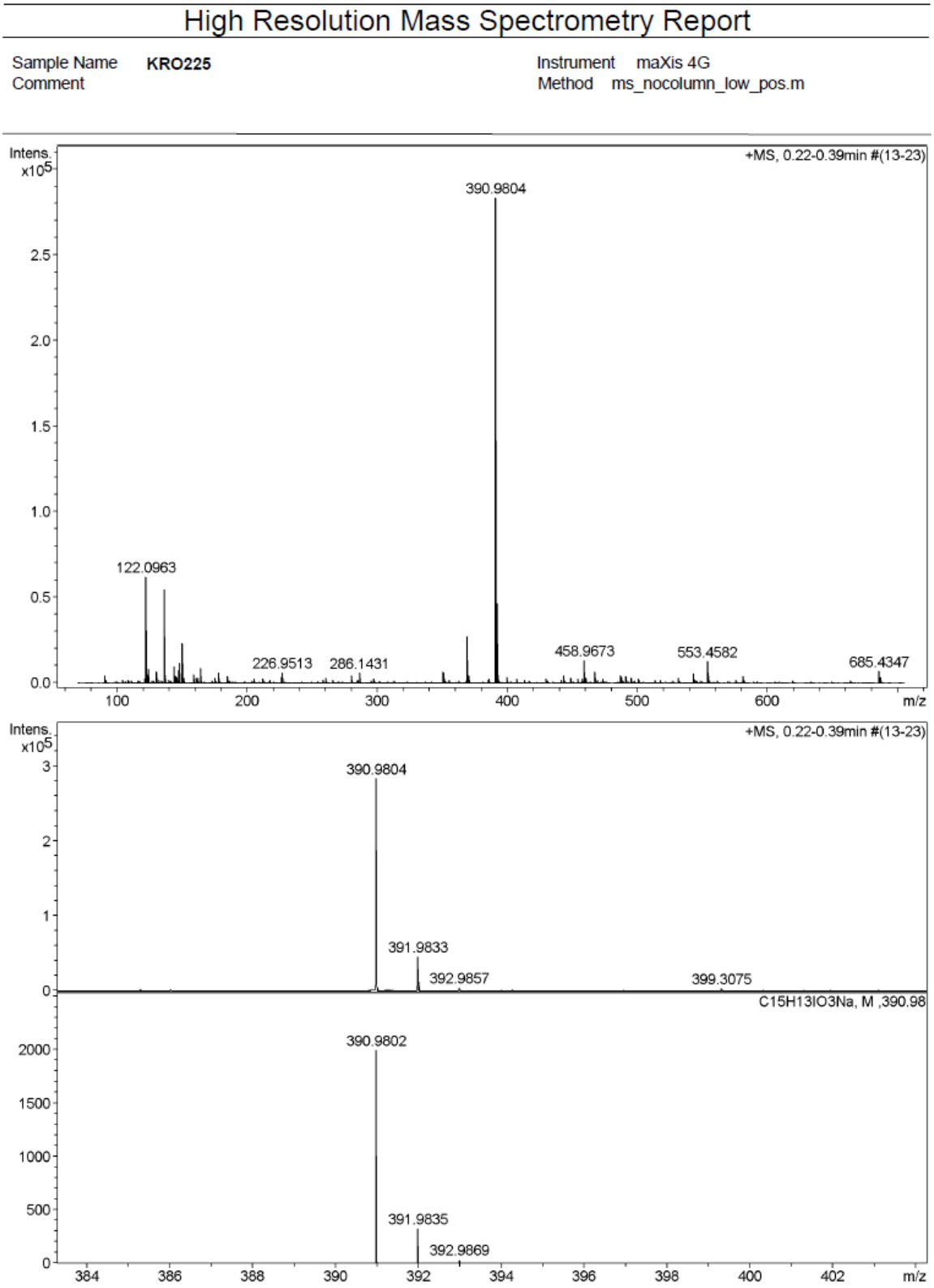
^{1}H-NMR spectra of **6** in CD_2Cl_2



^{13}C-NMR spectra of **6** in CD_2Cl_2



HR-ESI-MS spectra of **6**



High Resolution Mass Spectrometry Report

Measured m/z vs. theoretical m/z

Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e^- Conf	z
368.9980	1	C 15 H 14 I O 3	100.00	368.9982	0.2	0.6	10.7	8.5	even	1+
386.0245	1	C 15 H 17 I N O 3	100.00	386.0248	0.3	0.7	96.4	7.5	even	
390.9804	1	C 15 H 13 I Na O 3	100.00	390.9802	-0.3	-0.7	0.9	8.5	even	
406.9543	1	C 15 H 13 I K O 3	100.00	406.9541	-0.2	-0.5	93.1	8.5	even	

Mass list

#	m/z	I %	I
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2	91.5046	0.6	1838
3	103.9552	0.8	2157
4	108.0807	0.8	2187
5	111.0201	0.5	1496
6	121.0885	0.8	2293
7	122.0963	21.9	62075
8	123.0806	1.2	3497
9	123.0990	1.8	5148
10	124.0867	2.8	7982
11	128.1069	0.6	1586
12	129.9874	0.6	1697
13	130.1589	2.3	6649
14	131.9618	0.7	2124
15	134.0962	0.5	1498
16	136.1120	19.3	54822
17	137.1152	1.8	5176
18	139.9877	0.6	1757
19	143.9589	3.4	9766
20	144.9822	1.4	3886
21	145.9544	1.3	3747
22	146.9802	0.7	2117
23	147.0915	2.7	7793
24	147.9310	4.1	11702
25	148.0873	0.7	2101
26	148.1120	0.8	2160
27	149.9306	3.9	11050
28	150.1276	8.2	23199
29	151.1307	1.0	2862
30	158.9640	1.8	5089
31	161.1073	1.0	2948
32	162.1275	1.0	2845
33	164.1432	3.0	8613
34	175.1229	1.1	3130
35	178.1588	2.1	5951
36	184.9856	1.4	3992
37	186.9809	0.5	1538
38	205.0600	0.8	2290
39	212.1431	0.8	2378
40	217.1041	0.6	1698
41	226.0862	1.2	3448
42	226.1590	0.5	1483
43	226.9513	2.2	6194
44	258.1124	0.7	1997
45	260.2008	1.1	3050
46	265.9625	0.7	2120
47	280.0703	1.7	4732
48	285.1355	0.7	2076
49	286.1431	2.1	6015
50	297.0725	0.8	2225
51	313.0681	0.5	1475
52	350.2662	2.3	6607
53	350.9876	2.1	5903
54	355.2821	0.7	1887
55	368.9980	9.7	27388
56	370.0015	1.6	4439
57	385.2912	0.6	1829
58	386.0245	0.8	2235
59	390.9804	100.0	283495

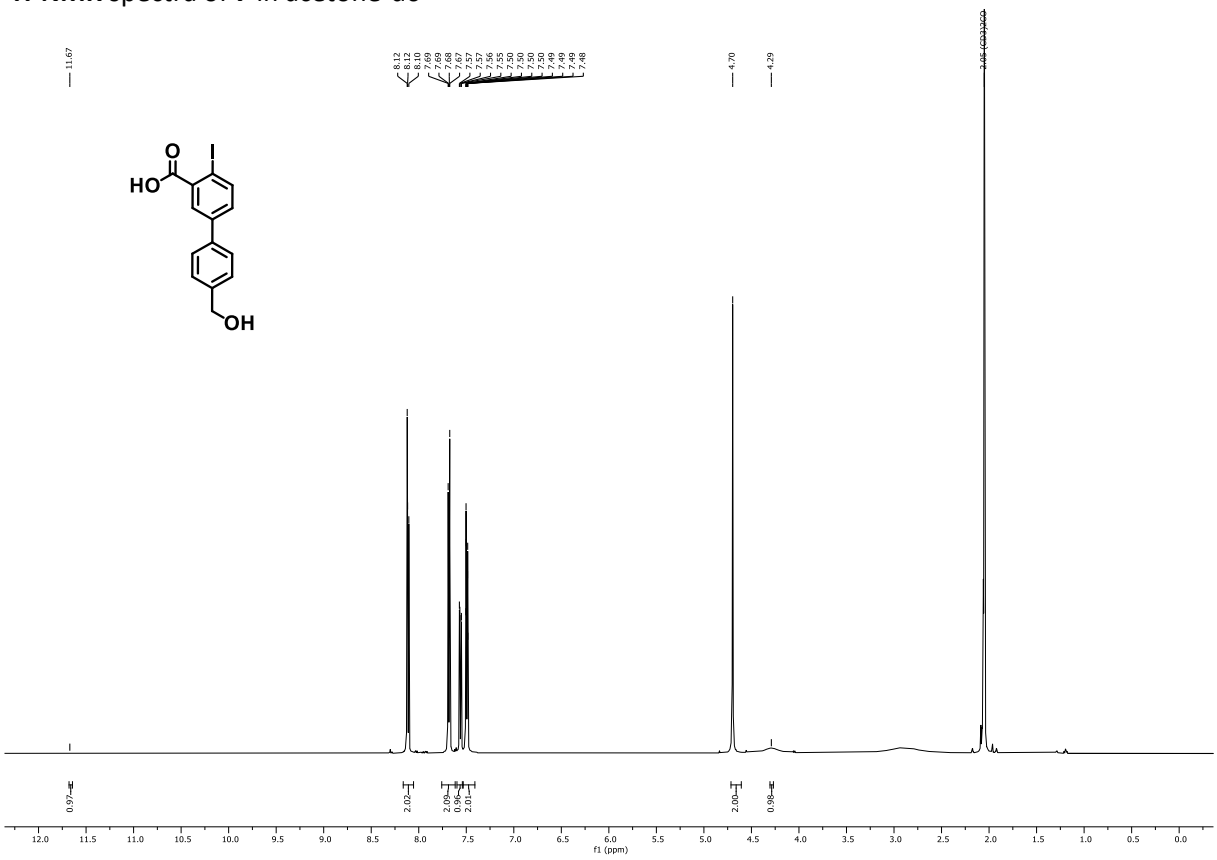
High Resolution Mass Spectrometry Report

#	m/z	I %	I
60	391.9833	16.3	46299
61	392.9857	1.7	4945
62	399.3075	1.3	3695
63	406.9543	0.9	2680
64	413.3233	0.7	1993
65	429.3183	0.9	2589
66	441.2971	0.6	1838
67	443.3336	1.6	4538
68	448.9384	1.0	2872
69	453.7855	0.8	2384
70	457.3489	0.9	2530
71	458.9673	4.7	13455
72	459.9701	1.0	2752
73	467.0109	2.3	6419
74	468.0144	0.5	1532
75	469.3279	0.8	2195
76	473.3439	0.8	2384
77	486.8226	1.5	4351
78	487.3601	1.3	3739
79	487.8233	0.5	1553
80	490.8177	1.4	3949
81	494.8118	1.0	2773
82	500.3005	0.8	2323
83	500.8026	0.5	1508
84	501.3754	0.7	1950
85	513.7834	0.6	1760
86	517.3715	0.7	1891
87	531.3861	1.0	2894
88	543.0419	1.9	5458
89	544.0454	0.6	1841
90	545.4015	0.5	1468
91	553.4582	4.5	12786
92	554.4618	1.7	4723
93	561.3962	0.5	1483
94	575.4121	0.7	2030
95	580.9529	1.4	3900
96	581.4549	0.7	1867
97	581.9521	0.7	2000
98	619.4382	0.6	1608
99	685.4347	2.5	6993
100	686.4382	1.2	3267

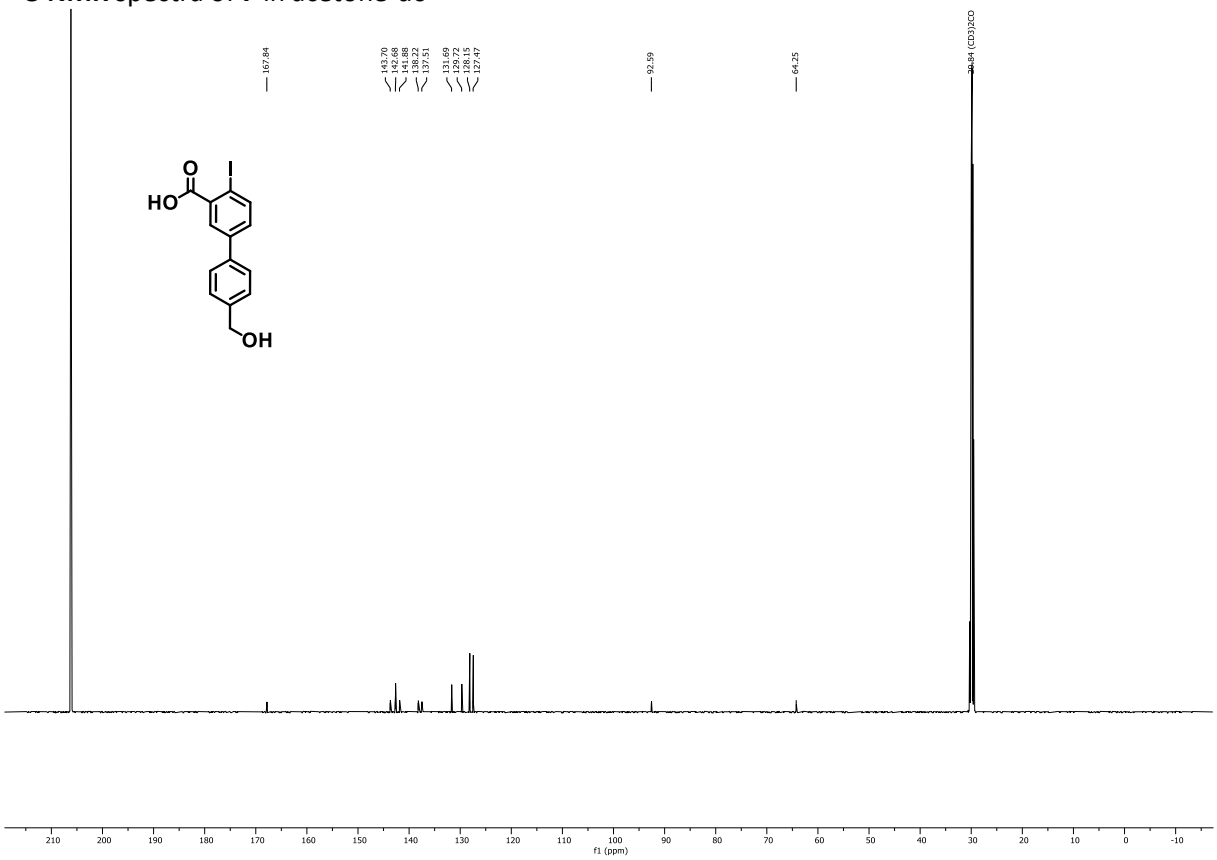
Acquisition Parameter

General	Fore Vacuum	3.38e+000 mBar	High Vacuum	9.12e-008 mBar	Source Type	ESI
	Scan Begin	75 m/z	Scan End	700 m/z	Ion Polarity	Positive
Source	Set Nebulizer	2.0 Bar	Set Capillary	4500 V	Set Dry Gas	8.0 l/min
	Set Dry Heater	200 °C	Set End Plate Offset	-500 V		
Quadrupole	Set Ion Energy (MS only)	4.0 eV				
Coll. Cell	Collision Energy	8.0 eV	Set Collision Cell RF	350.0 Vpp	55.0 Vpp	
Ion Cooler	Set Ion Cooler Transfer Time	55.0 µs	Set Ion Cooler Pre Pulse Storage Time		7.0 µs	

^{1}H-NMR spectra of **7** in acetone-d6



^{13}C-NMR spectra of **7** in acetone-d6

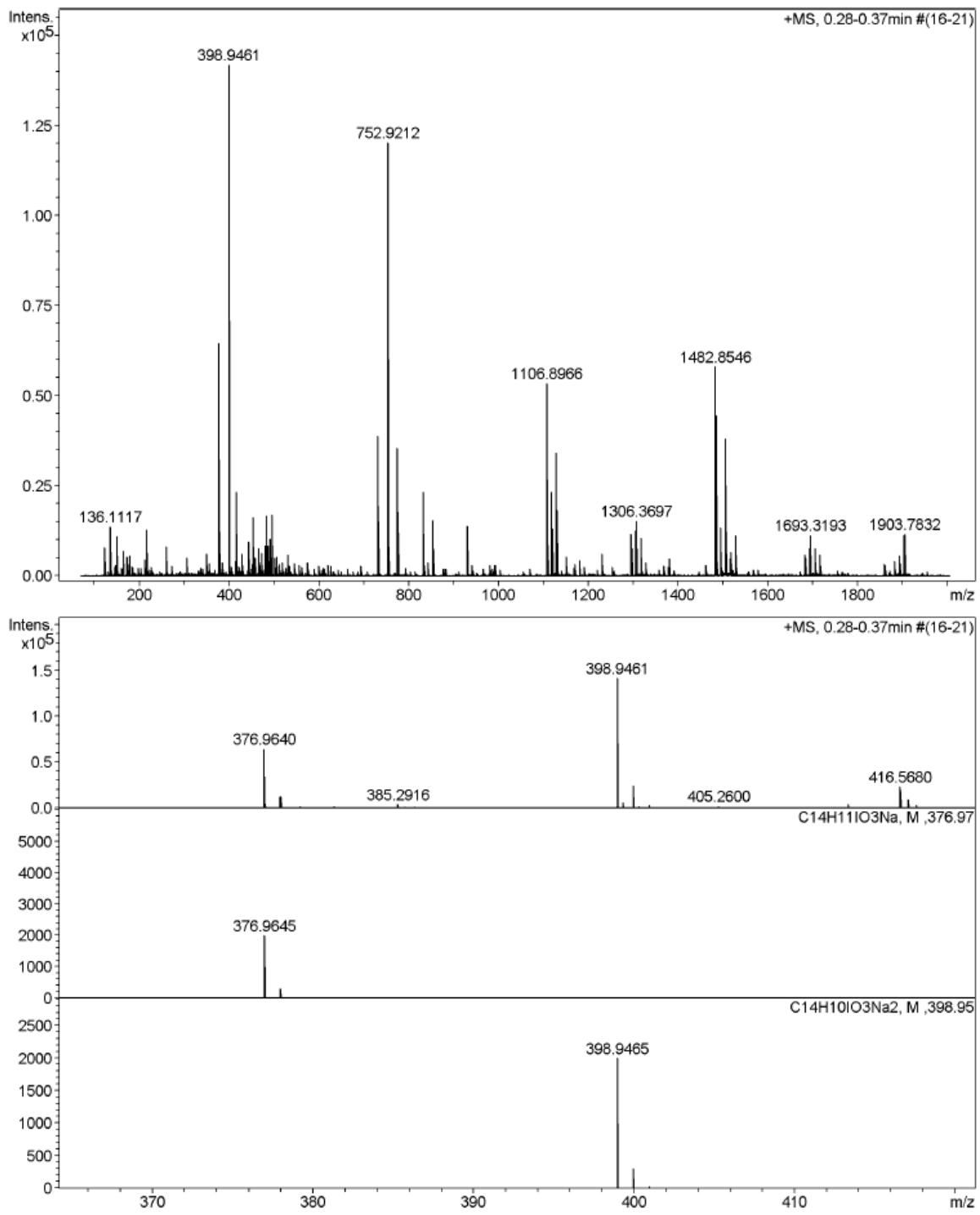


HR-ESI-MS spectra of **7**

High Resolution Mass Spectrometry Report

Sample Name **KRO-227**
Comment

Instrument maXis 4G
Method ms_nocolumn_mid_pos.m



High Resolution Mass Spectrometry Report

Measured m/z vs. theoretical m/z

Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e¯ Conf	z
354.9818	1	C 14 H 12 I O 3	100.00	354.9826	0.8	2.2	88.0	8.5	even	1+
376.9640	1	C 14 H 11 I Na O 3	100.00	376.9645	0.5	1.3	24.4	8.5	even	
398.9461	1	C 14 H 10 I Na 2 O 3	100.00	398.9465	0.3	0.9	14.4	8.5	even	
730.9391	1	C 28 H 22 I 2 Na O 6	100.00	730.9398	0.6	0.9	46.0	16.5	even	

Mass list

#	m/z	I %	I
1	122.0961	5.7	8041
2	136.1117	9.7	13728
3	150.1276	7.9	11193
4	164.1432	4.9	6897
5	173.0782	3.9	5490
6	178.1586	4.0	5648
7	217.1043	9.1	12874
8	260.2002	4.9	6884
9	261.1303	5.8	8217
10	305.1562	3.7	5270
11	350.2657	4.3	6153
12	376.9640	45.6	64679
13	377.9675	8.8	12512
14	398.9461	100.0	141897
15	399.3068	4.6	6576
16	399.9494	17.6	25011
17	416.5680	16.4	23231
18	417.0696	6.7	9545
19	429.3178	4.3	6080
20	443.3334	6.7	9563
21	453.7845	11.5	16377
22	457.3487	3.6	5106
23	466.9330	5.5	7850
24	471.7949	4.6	6537
25	481.8163	6.0	8479
26	483.2581	11.8	16761
27	483.7592	7.3	10421
28	485.8106	3.6	5127
29	487.3596	6.0	8518
30	490.8165	7.2	10255
31	494.8110	12.1	17112
32	501.3753	3.7	5186
33	505.2399	3.8	5369
34	531.3851	4.1	5850
35	730.9391	27.5	38973
36	731.9429	10.8	15261
37	752.9212	84.8	120374
38	753.9246	30.4	43104
39	754.9274	5.9	8332
40	774.9027	25.0	35469
41	775.9063	8.5	12047
42	832.1286	16.4	23301
43	833.1318	6.5	9209
44	854.1109	10.9	15426
45	855.1132	5.0	7128
46	929.9089	9.8	13857
47	930.4104	8.3	11739
48	930.9127	4.1	5810
49	1106.8966	37.7	53534
50	1107.3990	6.5	9161
51	1107.9005	21.4	30418
52	1108.9030	6.2	8815
53	1117.8880	14.8	21018
54	1118.3903	16.5	23401
55	1118.8922	9.4	13311
56	1119.3945	3.7	5251
57	1128.8781	24.2	34295
58	1129.8818	12.9	18341
59	1130.8853	3.7	5295

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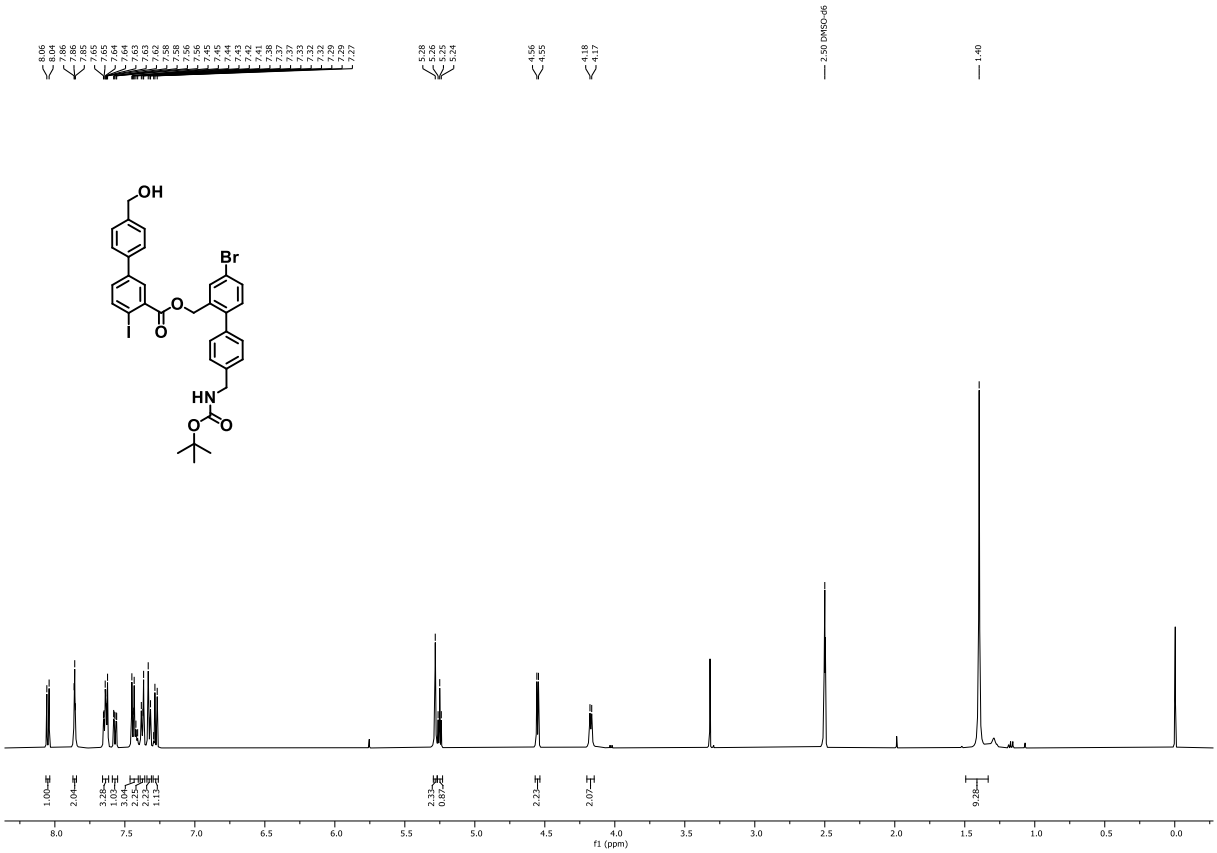
#	m/z	I %	I
60	1150.8592	3.9	5489
61	1230.0665	4.4	6239
62	1294.8762	6.3	8953
63	1295.3784	7.7	10956
64	1295.8809	5.5	7842
65	1305.8664	9.0	12745
66	1306.3697	10.8	15386
67	1306.8708	7.3	10418
68	1316.8574	6.5	9290
69	1317.3606	7.4	10507
70	1317.8604	4.5	6359
71	1482.8546	41.0	58128
72	1483.3569	8.8	12486
73	1483.8578	31.5	44641
74	1484.8609	11.0	15586
75	1493.8464	6.3	8907
76	1494.3479	9.6	13552
77	1494.8498	7.3	10352
78	1495.3504	3.6	5115
79	1504.8370	26.8	38088
80	1505.3390	9.5	13463
81	1505.8400	20.5	29068
82	1506.8433	6.7	9501
83	1516.3293	4.8	6769
84	1526.8184	8.0	11344
85	1527.3218	4.4	6304
86	1527.8226	6.5	9271
87	1682.3297	4.3	6035
88	1682.8295	3.6	5171
89	1692.8174	5.4	7667
90	1693.3193	8.0	11398
91	1693.8201	6.5	9174
92	1704.3090	5.4	7638
93	1704.8118	4.9	6979
94	1715.3014	4.1	5874
95	1892.2917	4.0	5742
96	1892.7936	3.9	5472
97	1902.7785	5.8	8168
98	1903.2817	8.1	11436
99	1903.7832	8.3	11714
100	1904.2858	4.8	6843

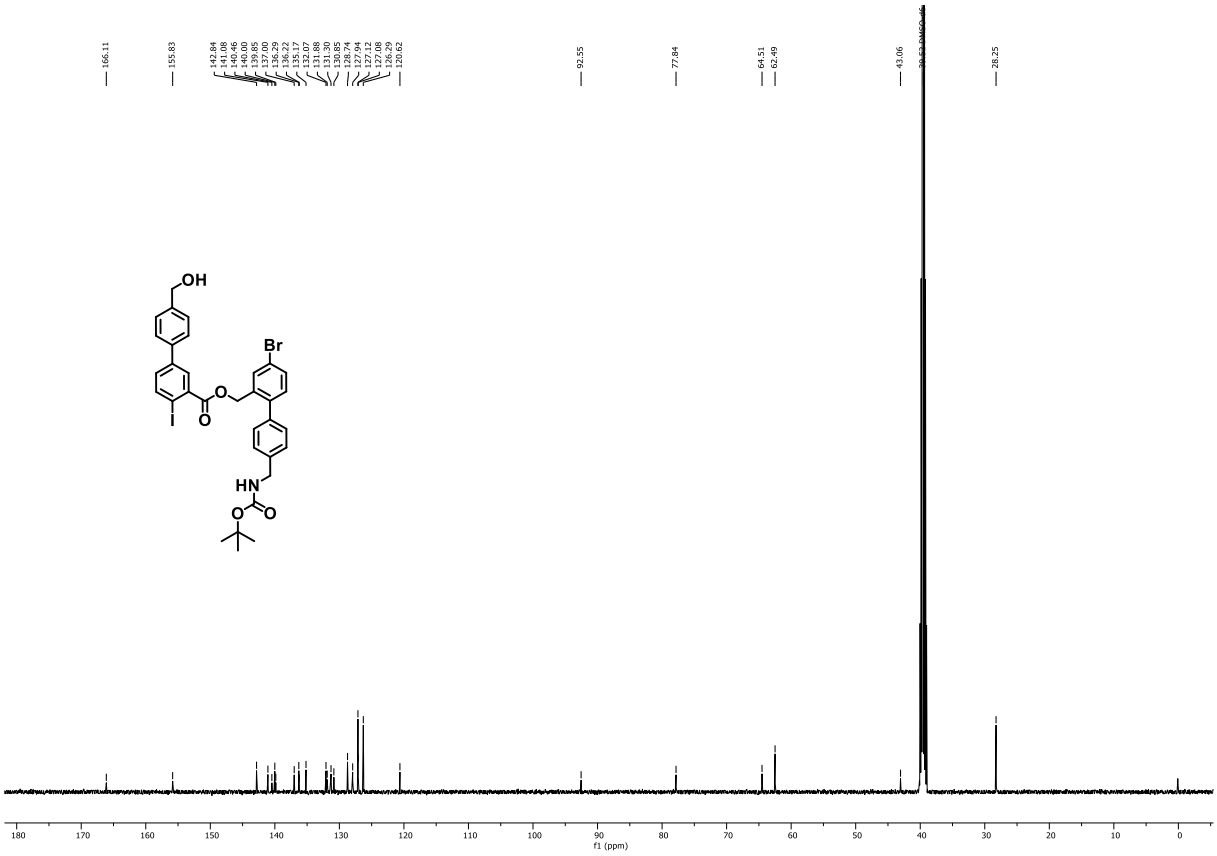
Acquisition Parameter

General	Fore Vacuum	3.38e+000 mBar	High Vacuum	9.09e-008 mBar	Source Type	ESI
	Scan Begin	75 m/z	Scan End	2000 m/z	Ion Polarity	Positive
Source	Set Nebulizer	2.0 Bar	Set Capillary	4500 V	Set Dry Gas	8.0 l/min
	Set Dry Heater	200 °C	Set End Plate Offset	-500 V		
Quadrupole	Set Ion Energy (MS only)	4.0 eV				
Coll. Cell	Collision Energy	8.0 eV	Set Collision Cell RF	600.0 Vpp	100.0 Vpp	
Ion Cooler	Set Ion Cooler Transfer Time	75.0 µs	Set Ion Cooler Pre Pulse Storage Time		10.0 µs	

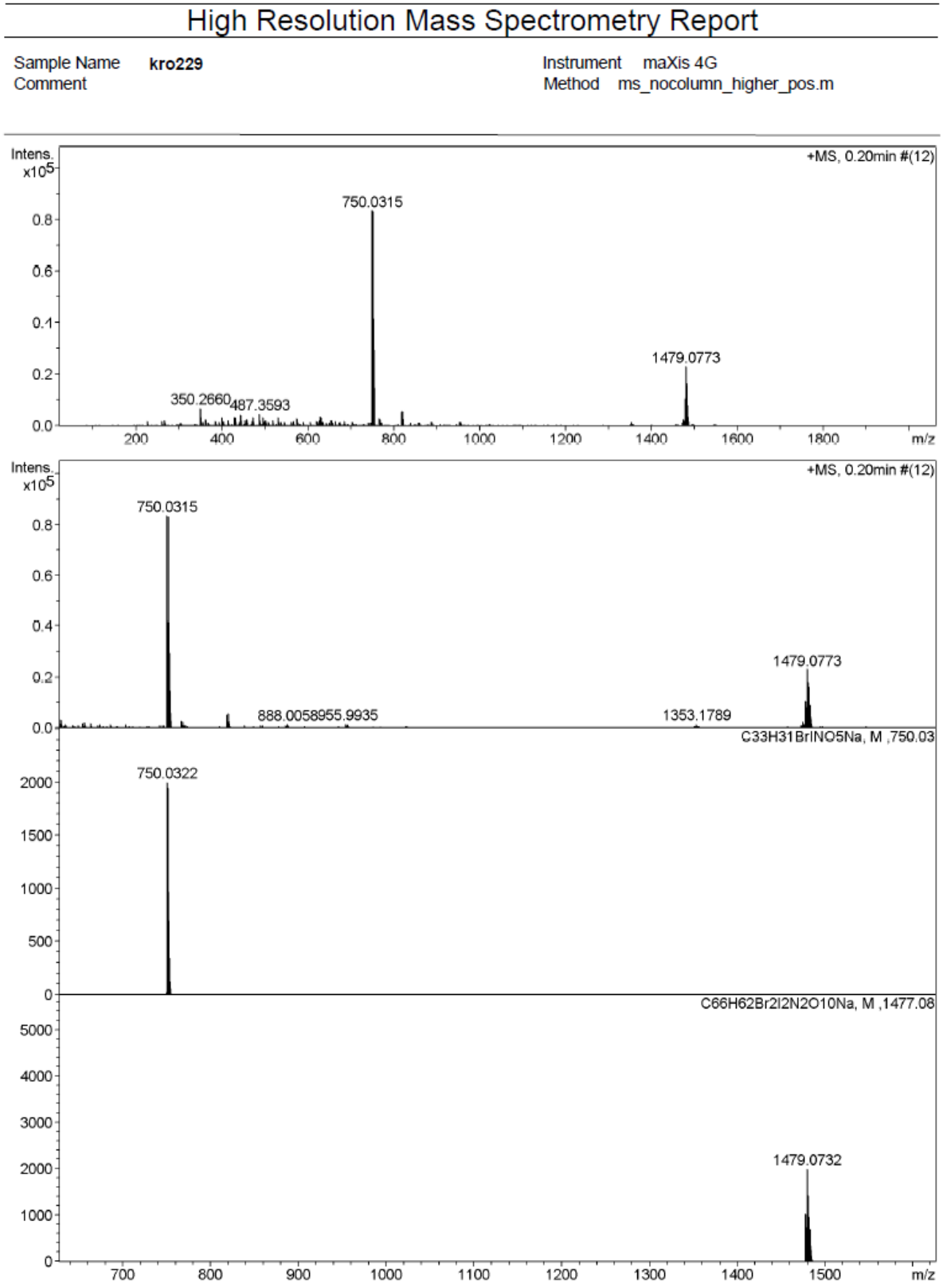
[1]H-NMR spectra of **2** in DMSO-d6



[13]C-NMR spectra of **2** in DMSO-d6


166.11
155.83
142.84
141.08
140.66
140.00
139.85
137.00
136.29
136.22
135.17
132.07
131.88
131.30
130.85
128.74
127.94
127.12
127.08
126.39
120.62
92.55
77.84
64.51
62.49
43.06
28.25
OH
Br
I
O
O
HN
O
O
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

HR-ESI-MS spectra of **2**



High Resolution Mass Spectrometry Report

Measured m/z vs. theoretical m/z

Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e¯ Conf	z
750.0315	1	C 33 H 31 Br I N Na O 5	100.00	750.0322	0.8	1.0	19.1	17.5	even	1+
1477.0767	1	C 66 H 62 Br 2 I 2 N 2 Na O 10	100.00	1477.0753	-1.4	-1.0	43.5	34.5	even	

Mass list

#	m/z	I %	I
1	226.9530	2.3	1916
2	260.2010	2.1	1738
3	265.9628	2.6	2185
4	302.9827	1.4	1152
5	350.2660	8.1	6768
6	351.2691	1.8	1534
7	355.2814	1.7	1434
8	362.9263	3.0	2541
9	369.2976	1.5	1288
10	385.2916	2.1	1775
11	394.2549	1.6	1316
12	399.3078	4.0	3373
13	400.3100	1.3	1066
14	401.9362	1.8	1480
15	403.0970	2.1	1722
16	413.3232	2.4	2042
17	429.3181	3.8	3133
18	430.9133	4.0	3344
19	440.4069	1.5	1266
20	441.2963	1.8	1476
21	443.3334	5.1	4255
22	444.3364	1.7	1453
23	453.7854	2.8	2337
24	457.3487	2.9	2459
25	469.9243	2.3	1913
26	471.7945	1.4	1180
27	473.3437	3.9	3250
28	487.3593	5.3	4440
29	488.3627	1.6	1350
30	494.8114	4.1	3389
31	498.9003	2.3	1944
32	501.3753	2.5	2079
33	506.9440	1.9	1560
34	517.3693	2.4	1984
35	531.3863	4.1	3389
36	532.3874	1.5	1217
37	537.9118	1.6	1317
38	545.4023	1.9	1589
39	561.3968	1.9	1578
40	566.8877	2.4	1976
41	575.4114	3.3	2788
42	589.4266	1.8	1504
43	605.4232	1.8	1474
44	605.8986	1.6	1302
45	619.4368	2.4	1968
46	624.1345	1.8	1490
47	626.1321	2.4	2020
48	627.9959	4.3	3582
49	628.9994	1.5	1218
50	629.9944	4.0	3332
51	630.9969	1.5	1225
52	634.8750	2.0	1649
53	649.4481	1.3	1081
54	653.9763	2.4	2025
55	655.9732	2.6	2162
56	663.4641	2.4	1998
57	673.8861	1.6	1365
58	685.4342	2.0	1656
59	702.8634	1.9	1586
60	750.0315	100.0	83508
61	751.0346	34.8	29082

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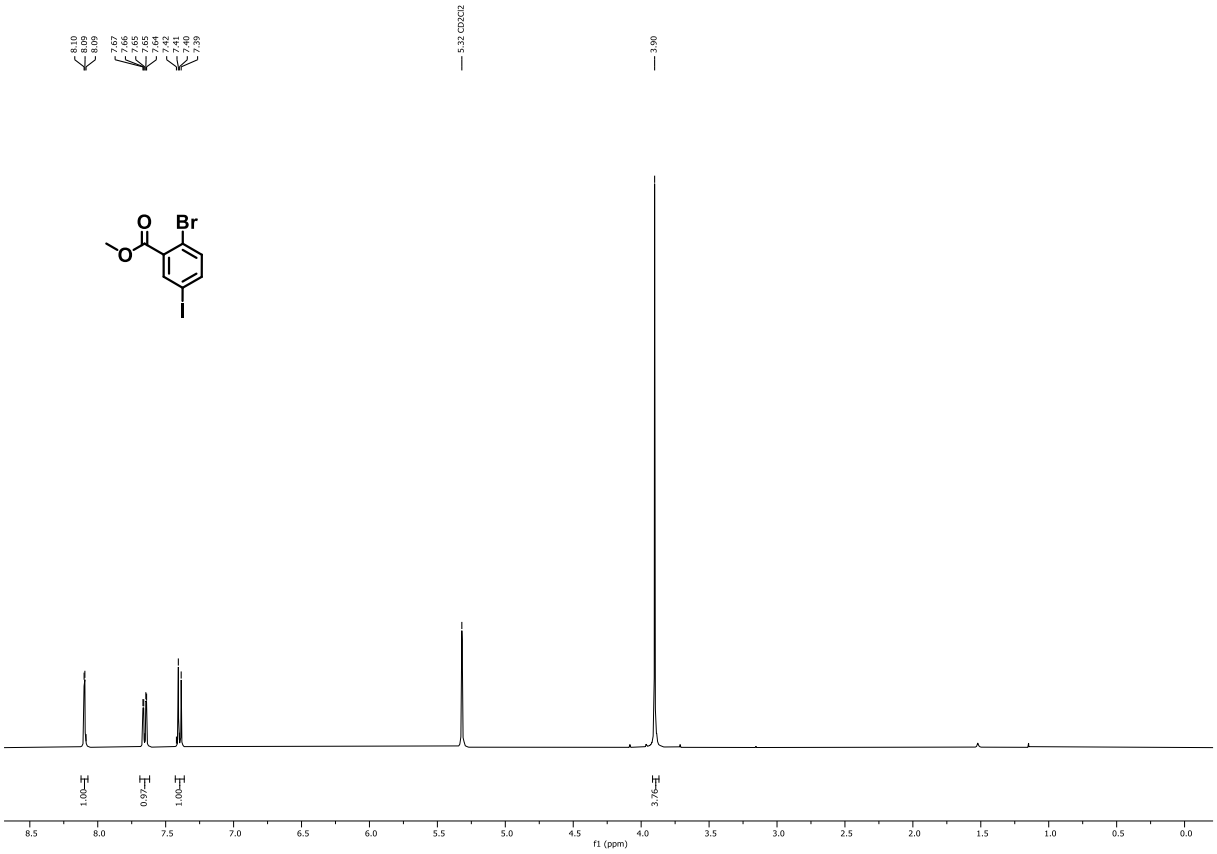
#	m/z	I %	I
62	752.0299	99.8	83344
63	753.0321	35.5	29622
64	754.0347	6.9	5742
65	766.0040	3.3	2783
66	768.0018	2.9	2397
67	770.8502	1.5	1254
68	771.0920	1.3	1097
69	818.0196	6.4	5314
70	819.0225	2.8	2363
71	820.0167	6.8	5640
72	821.0199	2.3	1902
73	838.8378	1.3	1091
74	857.0284	1.3	1121
75	859.0293	1.4	1203
76	886.0041	1.6	1310
77	888.0058	1.8	1478
78	953.9937	1.6	1355
79	955.9935	1.9	1576
80	1353.1789	1.9	1608
81	1472.1222	1.3	1089
82	1473.1263	1.5	1285
83	1474.1198	2.9	2449
84	1475.1282	1.7	1429
85	1476.1216	2.0	1669
86	1477.0767	12.7	10623
87	1478.0812	10.0	8354
88	1479.0773	27.5	22983
89	1480.0808	21.8	18189
90	1481.0761	19.3	16140
91	1482.0788	11.1	9296
92	1483.0817	4.1	3436
93	1484.0827	1.4	1154

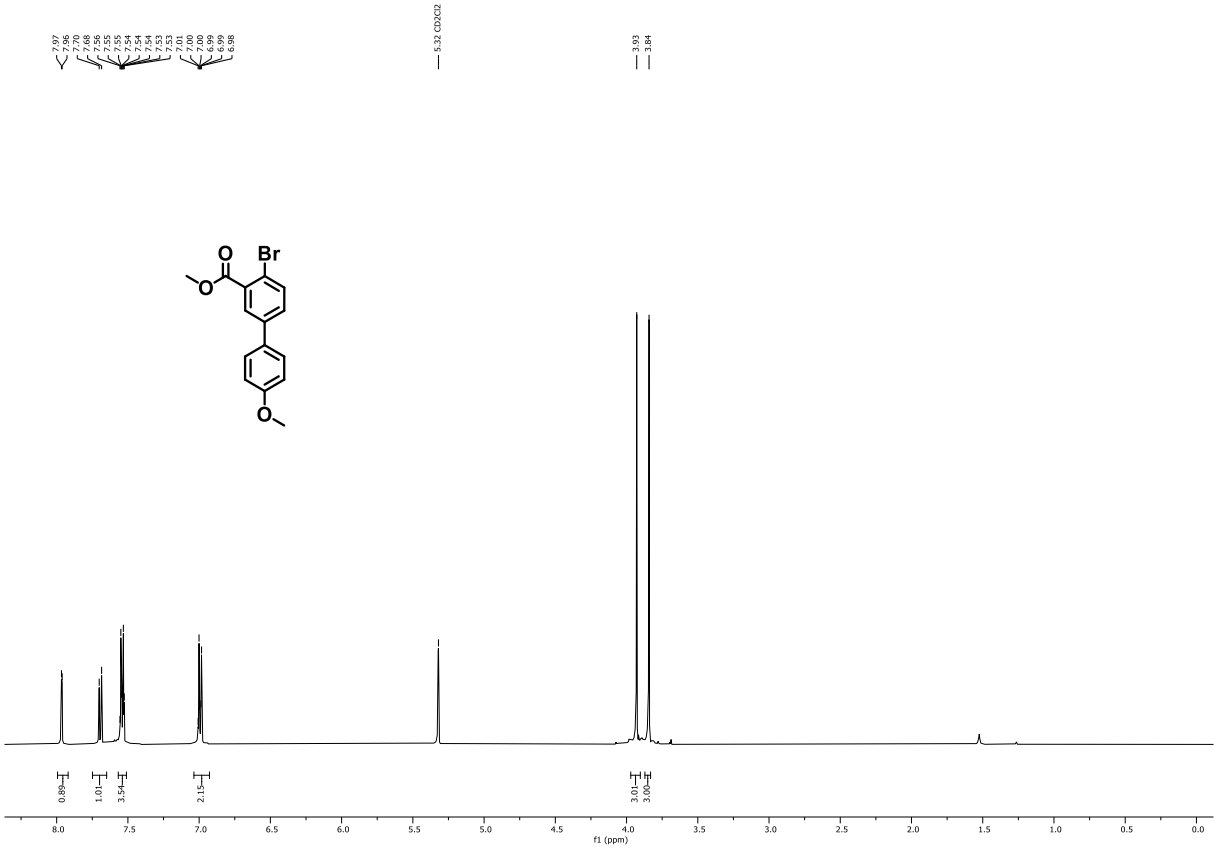
Acquisition Parameter

General	Fore Vacuum	3.36e+000 mBar	High Vacuum	9.15e-008 mBar	Source Type	ESI
	Scan Begin	75 m/z	Scan End	2000 m/z	Ion Polarity	Positive
Source	Set Nebulizer	2.0 Bar	Set Capillary	4500 V	Set Dry Gas	8.0 l/min
	Set Dry Heater	200 °C	Set End Plate Offset	-500 V		
Quadrupole	Set Ion Energy (MS only)	4.0 eV				
Coll. Cell	Collision Energy	8.0 eV	Set Collision Cell RF	600.0 Vpp	100.0 Vpp	
Ion Cooler	Set Ion Cooler Transfer Time	100.0 µs	Set Ion Cooler Pre Pulse Storage Time	18.0 µs		

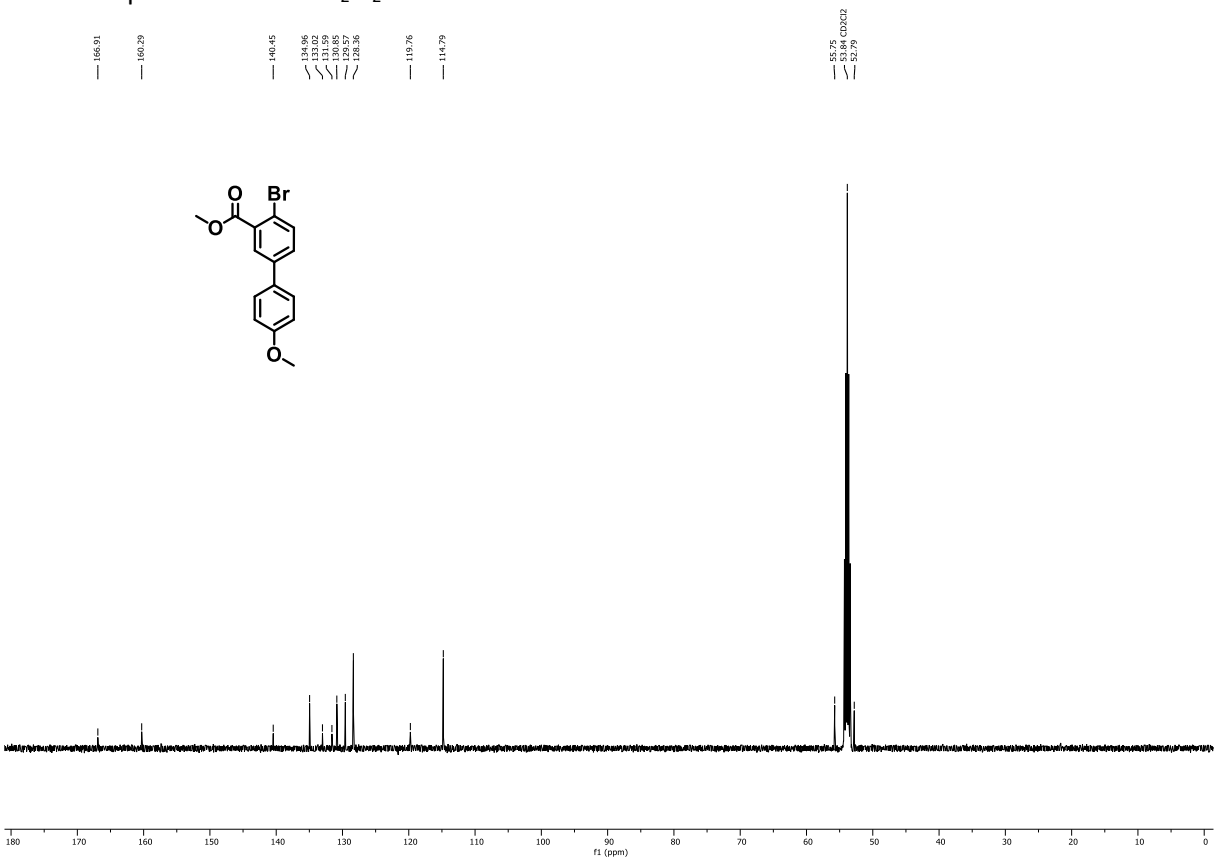
^{1}H-NMR spectra of **9** in CD_2Cl_2



^{1}H-NMR spectra of **10** in CD_2Cl_2



^{13}C-NMR spectra of **10** in CD_2Cl_2

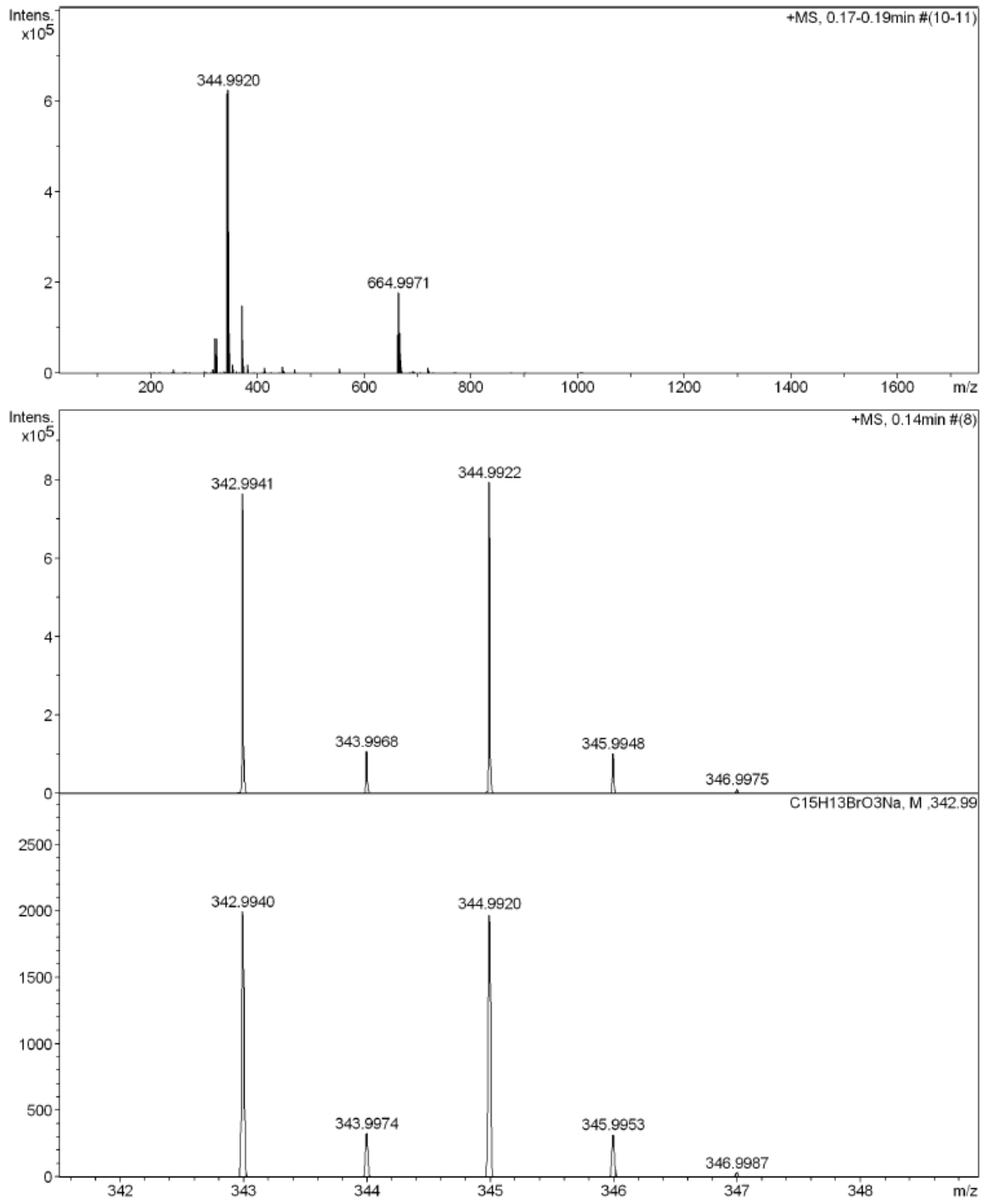


HR-ESI-MS spectra of **10**

High Resolution Mass Spectrometry Report

Sample Name **kro262**
Comment

Instrument maXis 4G
Method 22 Direct_pos_mid.m



High Resolution Mass Spectrometry Report

Measured m/z vs. theoretical m/z

Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e¯ Conf	z
342.9941	1	C 15 H 13 Br Na O 3	100.00	342.9940	-0.1	-0.2	23.8	8.5	even	1+

Mass list

#	m/z	I %	I
1	173.0779	0.2	1826
2	198.1038	0.4	3253
3	205.0592	0.5	3622
4	217.1045	0.5	3789
5	239.0876	0.2	1938
6	241.0286	0.4	3382
7	242.0932	1.3	9956
8	243.0997	0.4	3178
9	257.0972	0.2	1833
10	261.1306	0.2	1989
11	261.9982	0.3	2220
12	263.9962	0.3	2069
13	265.0826	0.2	1790
14	273.1669	0.3	2756
15	301.1406	0.6	4461
16	304.2606	0.6	4714
17	313.2341	0.3	2168
18	317.1165	1.3	10185
19	318.1205	0.3	2544
20	321.0115	11.5	91809
21	322.0146	1.8	14242
22	323.0097	10.9	86932
23	324.0127	1.8	14214
24	325.0158	0.2	1848
25	331.2090	0.3	2224
26	337.1041	0.3	2069
27	338.0378	0.6	4501
28	340.0359	0.6	4629
29	341.1133	0.4	3068
30	342.9330	0.2	1874
31	342.9941	96.3	766136
32	343.9968	13.7	109365
33	344.9303	0.3	2185
34	344.9922	100.0	795616
35	345.9948	13.1	104504
36	346.9975	1.6	12684
37	349.1415	0.4	3201
38	353.2654	3.2	25465
39	354.2683	0.5	4317
40	360.3230	0.8	6316
41	361.3273	0.2	1901
42	365.1058	0.2	1882
43	371.1250	23.3	185302
44	372.1281	5.1	40657
45	373.1312	0.7	5596
46	381.2969	2.5	19501
47	382.2998	0.6	5142
48	393.2969	0.4	3465
49	394.2254	0.3	2120
50	409.0404	0.3	2278
51	410.9796	0.3	2077
52	412.9784	0.2	1937
53	413.2651	2.0	15980
54	414.2686	0.5	4282
55	421.3272	0.3	2046
56	425.2138	0.3	2460
57	441.2970	0.5	3973
58	447.3441	2.4	18792
59	448.3466	0.8	6228
60	449.0348	0.7	5254
61	449.3568	0.3	2720
62	451.0337	0.6	5097

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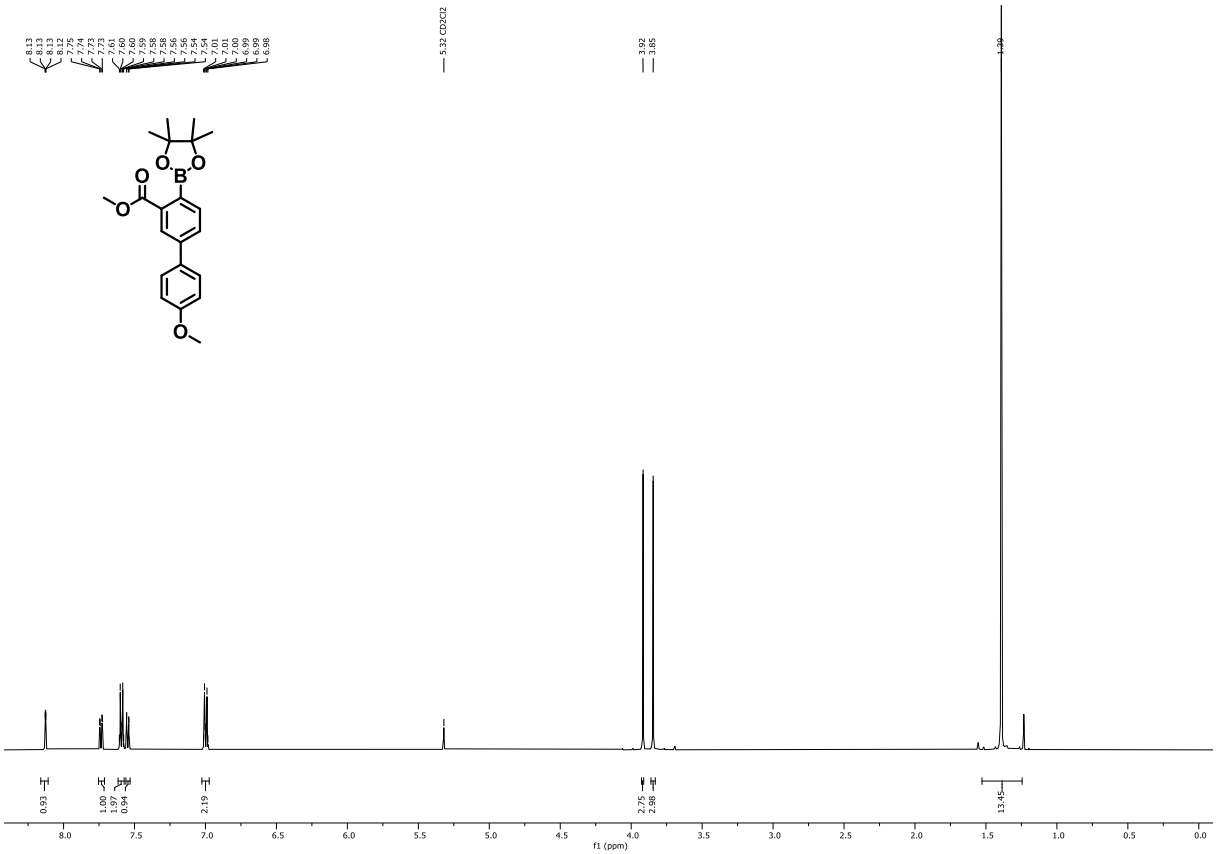
#	m/z	I %	I
63	469.3283	1.4	11185
64	470.3318	0.4	2978
65	553.4582	1.8	14562
66	554.4622	0.7	5600
67	662.9991	12.9	103001
68	664.0022	4.1	32822
69	664.9972	28.1	223478
70	666.0003	9.0	71780
71	666.9957	13.8	109860
72	667.9981	4.5	36185
73	669.0013	1.0	7957
74	685.4347	0.4	2970
75	691.1299	0.8	6418
76	692.1320	0.3	2544
77	693.1284	0.8	6290
78	694.1304	0.4	3117
79	701.4003	0.3	2061
80	705.5819	0.4	3018
81	719.2607	2.0	15652
82	720.2633	1.0	7668
83	721.2647	0.3	2349
84	721.5770	1.2	9328
85	722.5803	0.6	4424
86	729.4326	0.3	2149
87	733.2712	0.2	1824
88	767.3494	0.4	3356
89	769.0399	0.2	1786
90	769.3469	0.4	2908
91	771.0389	0.3	2544
92	789.3318	0.3	2054
93	797.1714	0.2	1866
94	875.4643	0.3	2289
95	901.5956	0.3	2634
96	902.5994	0.2	1808
97	1005.4396	0.5	3601
98	1006.4427	0.3	2442
99	1007.4384	0.6	4450
100	1008.4399	0.3	2285

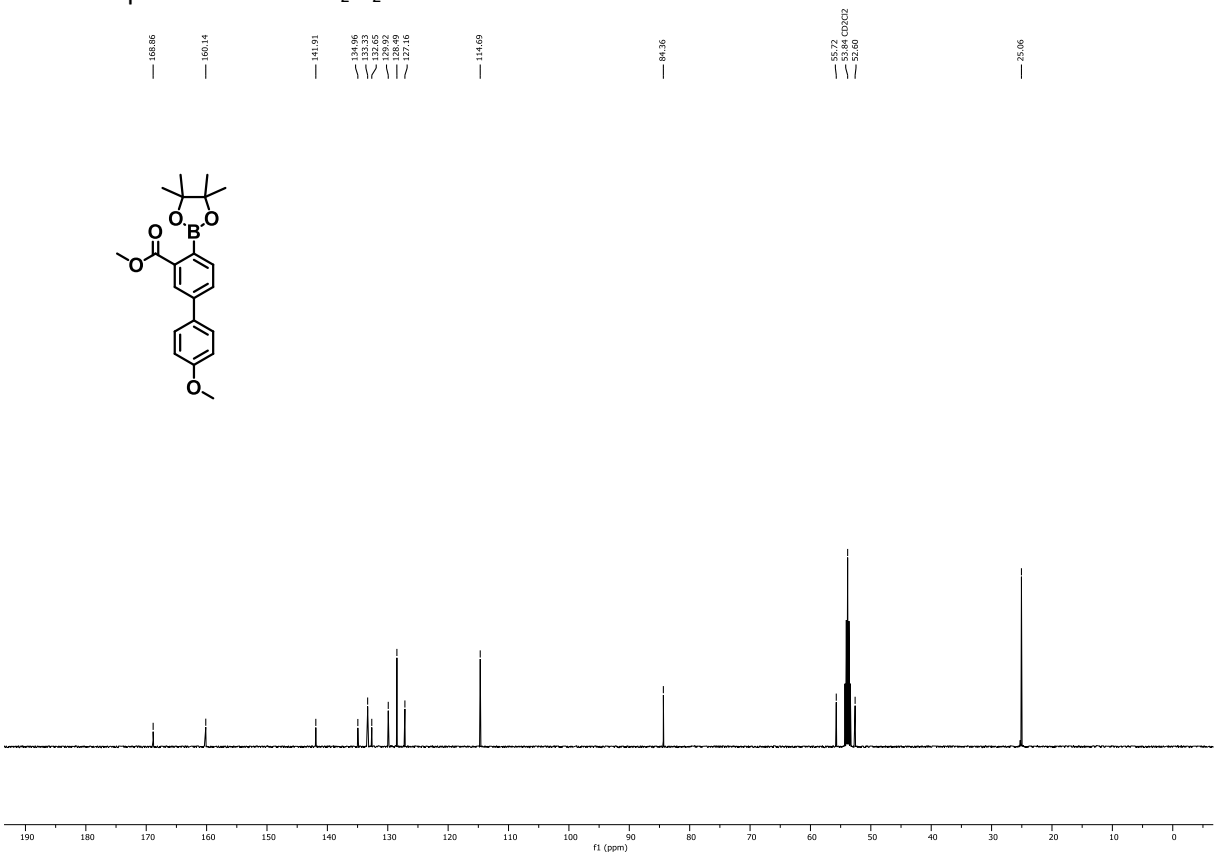
Acquisition Parameter

General	Fore Vacuum	3.39e+000 mBar	High Vacuum	8.71e-008 mBar	Source Type	ESI
	Scan Begin	75 m/z	Scan End	1700 m/z	Ion Polarity	Positive
Source	Set Nebulizer	0.4 Bar	Set Capillary	3600 V	Set Dry Gas	4.0 l/min
	Set Dry Heater	180 °C	Set End Plate Offset	-500 V		
Quadrupole	Set Ion Energy (MS only)	4.0 eV				
Coll. Cell	Collision Energy	8.0 eV	Set Collision Cell RF	350.0 Vpp	100.0 Vpp	
Ion Cooler	Set Ion Cooler Transfer Time	75.0 µs	Set Ion Cooler Pre Pulse Storage Time		10.0 µs	

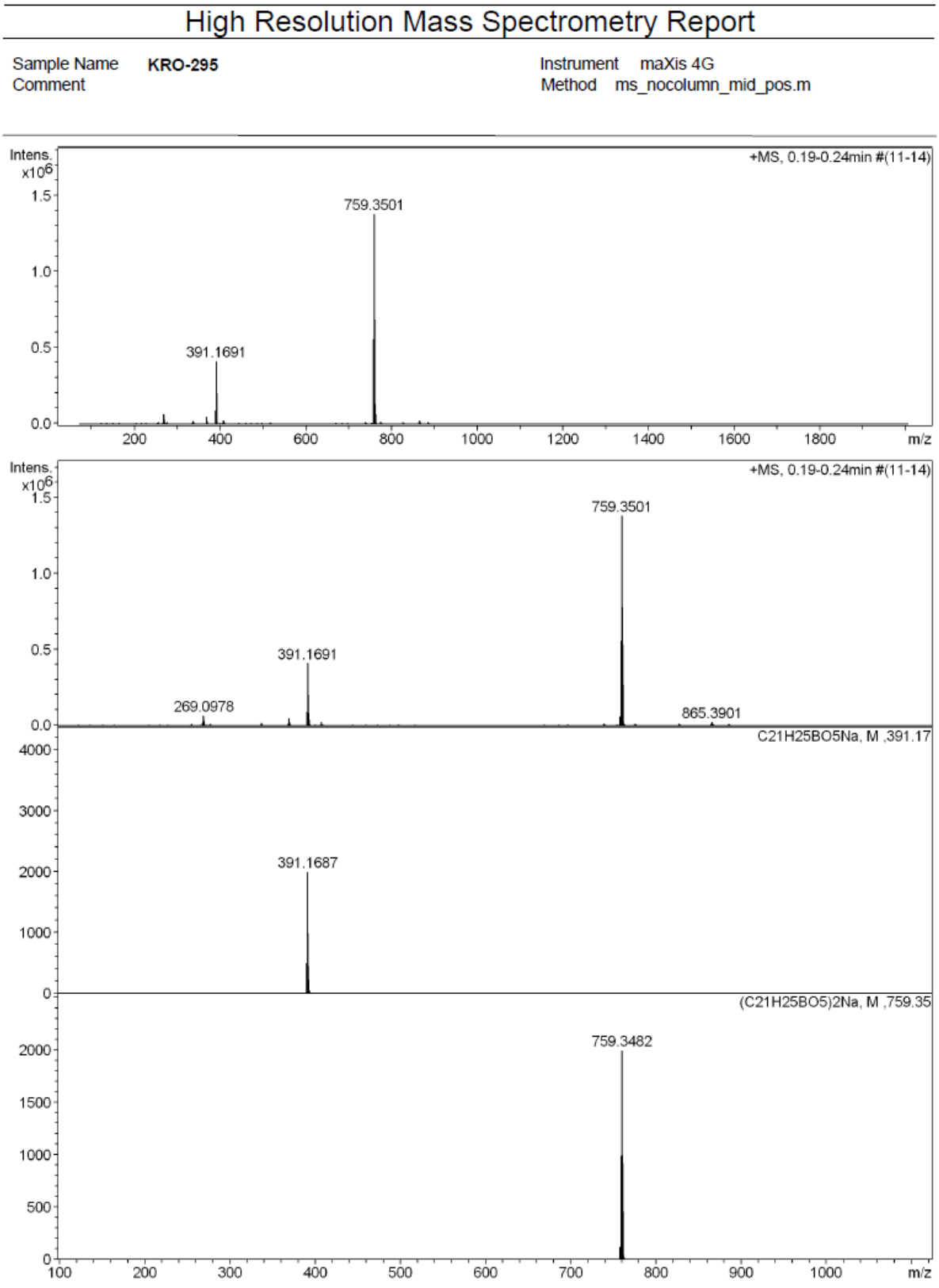
^{1}H-NMR spectra of **11** in CD_2Cl_2



^{13}C-NMR spectra of **11** in CD_2Cl_2



HR-ESI-MS spectra of **11**



High Resolution Mass Spectrometry Report

Measured m/z vs. theoretical m/z

Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e¯ Conf	z
369.1865	1	C 21 H 26 B O 5	100.00	369.1872	0.3	0.7	6.9	9.5	even	1+
391.1691	1	C 21 H 25 B Na O 5	100.00	391.1691	0.0	0.1	15.7	9.5	even	
407.1423	1	C 21 H 25 B K O 5	100.00	407.1430	0.3	0.8	15.8	9.5	even	
754.3927	1	C 42 H 54 B 2 N O 10	100.00	754.3942	0.2	0.2	52.2	17.5	even	
759.3501	1	C 42 H 50 B 2 Na O 10	100.00	759.3496	-0.5	-0.7	19.8	18.5	even	
775.3222	1	C 42 H 50 B 2 K O 10	100.00	775.3235	-0.0	-0.1	29.0	18.5	even	

Mass list

#	m/z	I %	I
1	122.0964	0.2	2434
2	136.1121	0.3	3836
3	150.1277	0.2	3127
4	164.1435	0.2	2436
5	178.1589	0.2	2242
6	205.0597	0.3	3848
7	212.1431	0.1	1947
8	217.1044	0.2	3192
9	226.9511	0.4	4949
10	254.0852	0.2	3130
11	255.0821	0.8	10898
12	265.9619	0.3	3464
13	268.1012	1.0	14444
14	269.0978	4.7	65202
15	270.1011	0.8	10504
16	273.1670	0.2	2558
17	276.1782	0.2	3347
18	277.1751	0.7	9079
19	336.1636	0.3	4255
20	337.1603	1.2	15942
21	338.1635	0.3	3562
22	368.1895	0.8	10535
23	369.1865	3.2	44268
24	370.1895	0.7	10204
25	371.1249	0.2	2118
26	371.1922	0.1	1986
27	390.1719	6.3	86897
28	391.1691	29.7	410862
29	392.1719	6.0	83451
30	393.1743	0.9	11861
31	399.3074	0.2	2315
32	406.1454	0.4	5322
33	407.1423	1.5	20616
34	408.1450	0.4	5300
35	409.1426	0.2	2386
36	429.3180	0.2	2096
37	443.3335	0.2	2749
38	459.1558	0.4	4892
39	473.3437	0.2	2399
40	487.3593	0.2	2531
41	497.2098	0.4	5353
42	498.1667	0.2	2782
43	516.2573	0.2	2085
44	517.2533	0.4	4839
45	531.3855	0.2	2179
46	669.2545	0.2	2454
47	685.4338	0.2	3352
48	696.3134	0.2	2350
49	697.3109	0.4	5643
50	698.3146	0.2	2252
51	738.3073	0.2	2388
52	739.3037	0.7	10205
53	740.3077	0.3	4301
54	753.3949	0.2	2875
55	754.3927	0.5	6984
56	755.3965	0.2	3151
57	757.3544	4.3	59575

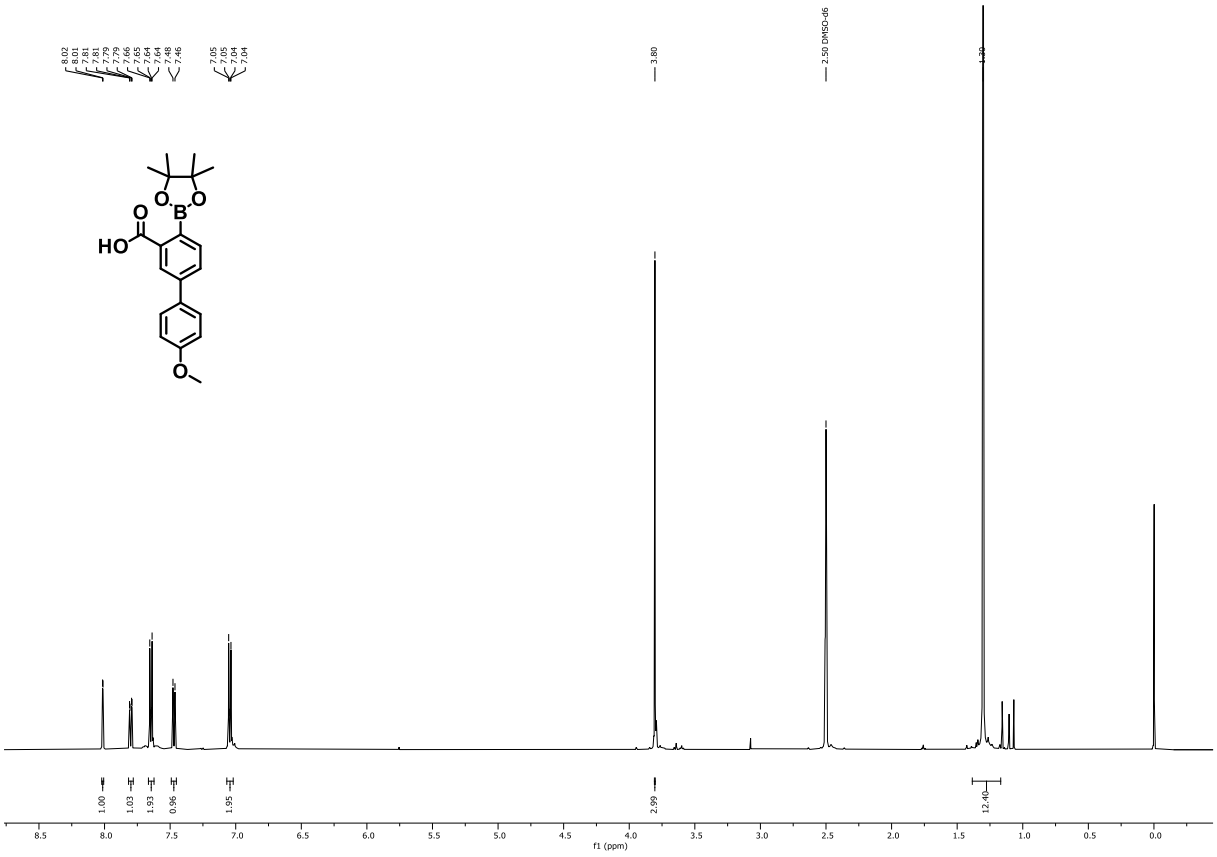
High Resolution Mass Spectrometry Report

#	m/z	I %	I
58	758.3522	40.5	558910
59	758.8044	0.2	2106
60	759.0540	0.2	2311
61	759.0847	0.1	2069
62	759.1274	0.2	2431
63	759.1510	0.2	2315
64	759.2100	0.2	2978
65	759.3501	100.0	1381693
66	759.6651	0.2	2874
67	759.6836	0.2	2326
68	759.6985	0.2	2405
69	759.7034	0.2	2354
70	759.7442	0.2	2589
71	759.7951	0.2	2996
72	759.8715	0.1	2057
73	759.8933	0.2	2299
74	759.9172	0.2	2575
75	760.0383	0.2	2841
76	760.0625	0.2	2286
77	760.0841	0.1	2069
78	760.1218	0.1	2016
79	760.1591	0.2	2285
80	760.1936	0.1	2062
81	760.2451	0.1	1978
82	760.3524	38.6	533021
83	761.3546	9.5	131568
84	762.3567	1.7	23940
85	763.3591	0.3	4493
86	774.3256	0.4	5586
87	775.3222	0.9	13065
88	776.3253	0.4	5698
89	777.3240	0.2	2182
90	826.3374	0.3	4108
91	827.3352	0.7	9124
92	828.3383	0.3	4175
93	864.3923	0.7	9048
94	865.3901	1.6	22477
95	866.3921	0.8	10413
96	867.3953	0.2	3292
97	884.4358	0.4	5176
98	885.4336	0.6	8438
99	886.4372	0.3	3722
100	1053.6164	0.1	1950

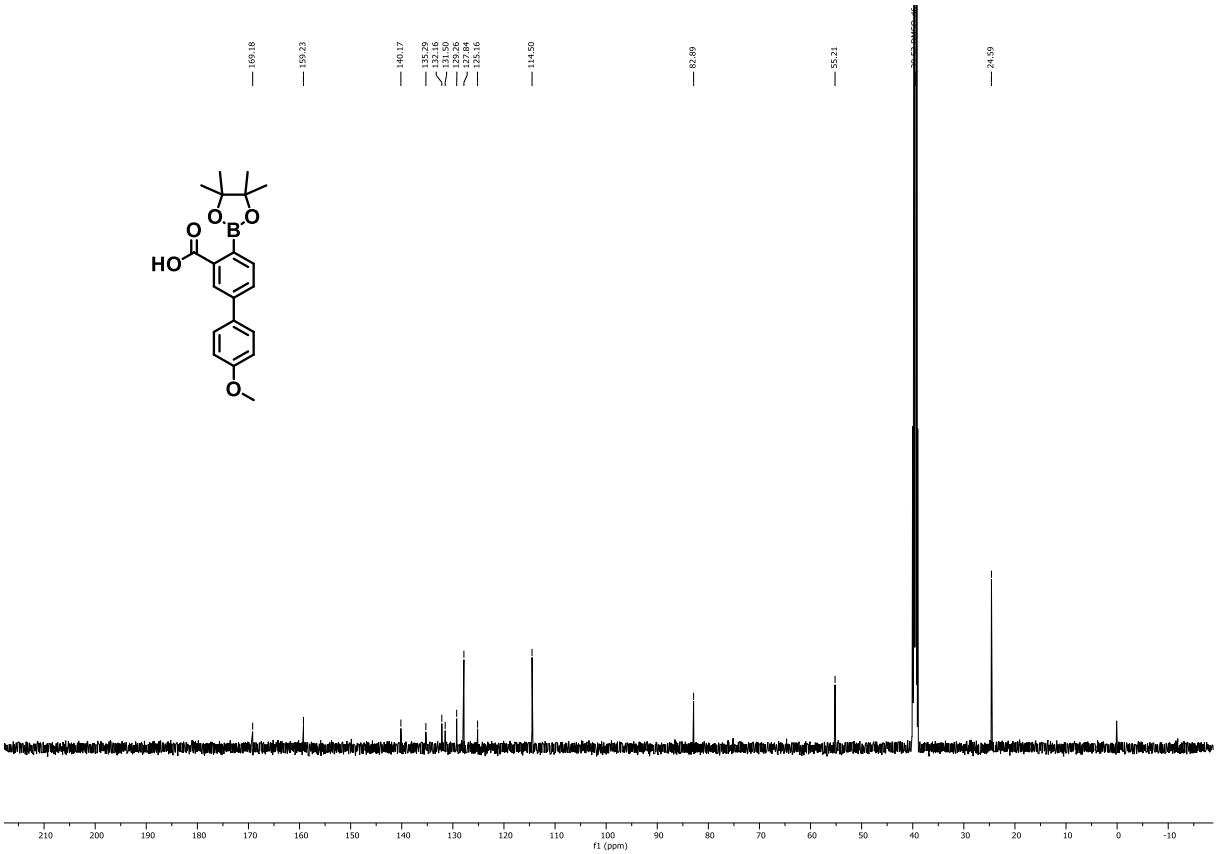
Acquisition Parameter

General	Fore Vacuum	3.08e+000 mBar	High Vacuum	9.09e-008 mBar	Source Type	ESI
	Scan Begin	75 m/z	Scan End	2000 m/z	Ion Polarity	Positive
Source	Set Nebulizer	2.0 Bar	Set Capillary	4500 V	Set Dry Gas	8.0 l/min
	Set Dry Heater	200 °C	Set End Plate Offset	-500 V		
Quadrupole	Set Ion Energy (MS only)	4.0 eV				
Coll. Cell	Collision Energy	8.0 eV	Set Collision Cell RF	600.0 Vpp	100.0 Vpp	
Ion Cooler	Set Ion Cooler Transfer Time	75.0 µs	Set Ion Cooler Pre Pulse Storage Time	10.0 µs		

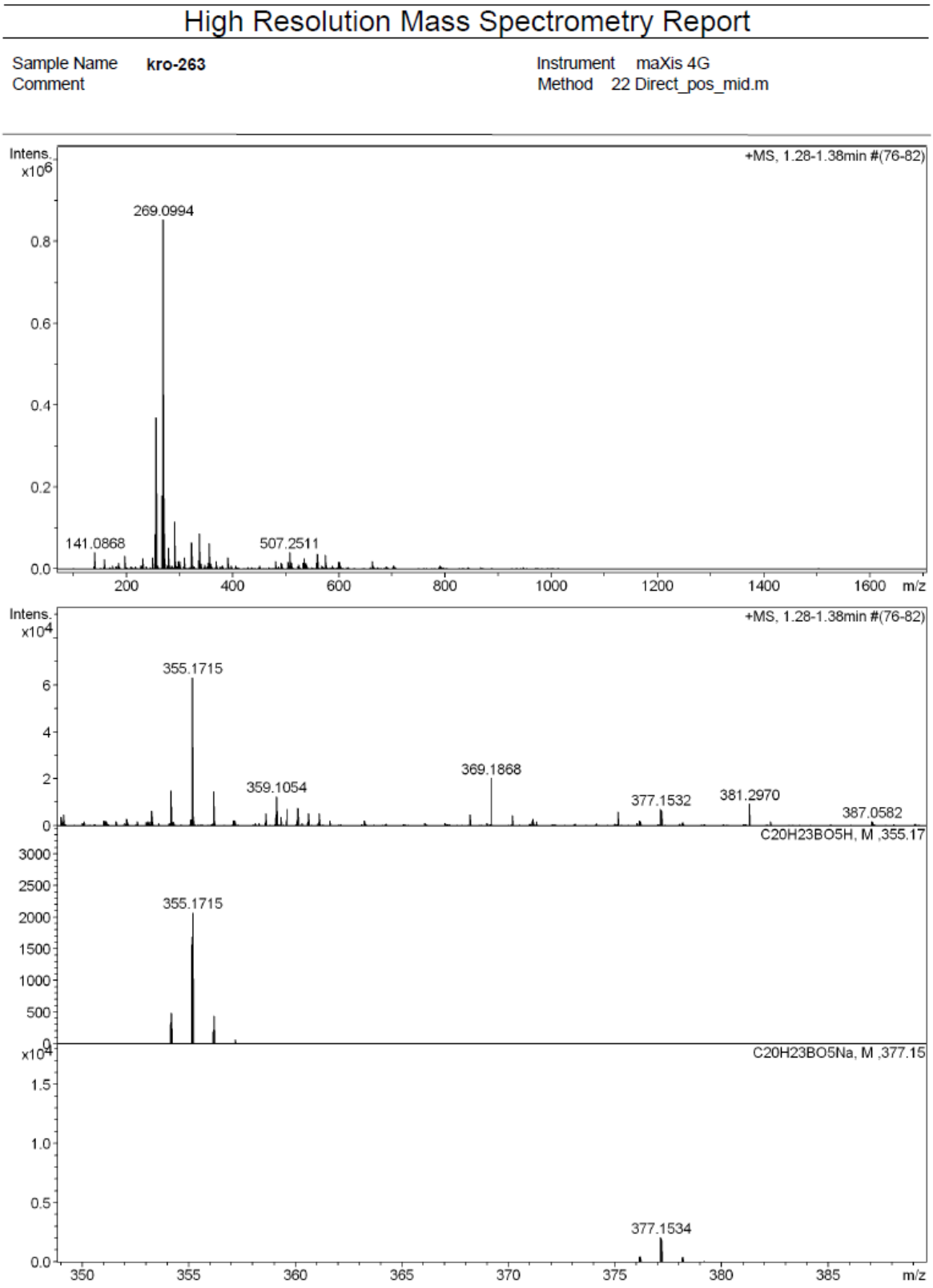
^{1}H-NMR spectra of **12** in DMSO-d6



^{13}C-NMR spectra of **12** in DMSO-d6



HR-ESI-MS spectra of **12**



High Resolution Mass Spectrometry Report

Measured m/z vs. theoretical m/z

Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e¯ Conf	z
355.1715	1	C 20 H 24 B O 5	100.00	355.1715	-0.0	-0.1	10.8	9.5	even	1+
377.1532	1	C 20 H 23 B Na O 5	100.00	377.1534	-0.1	-0.3	47.1	9.5	even	

Mass list

#	m/z	I %	I
1	141.0868	4.8	40780
2	159.1178	2.9	24578
3	173.1533	1.0	8337
4	183.0802	1.0	8311
5	185.0960	1.8	15122
6	197.0963	1.9	15900
7	197.1301	3.9	33196
8	209.1139	0.9	7386
9	227.1260	1.0	8340
10	229.1037	1.0	8432
11	231.0998	3.0	25914
12	237.2065	0.9	7901
13	249.2067	3.4	28958
14	254.0867	10.1	85948
15	255.0836	43.5	371304
16	256.0865	6.2	52673
17	259.1886	1.1	9738
18	267.0942	0.9	7783
19	268.1025	21.2	181346
20	269.0994	100.0	853438
21	270.1024	14.0	119856
22	271.1044	1.7	14105
23	271.1888	20.3	173051
24	272.1263	2.0	17297
25	272.1921	3.1	26051
26	277.0649	1.1	9644
27	279.0939	6.3	53385
28	280.0972	1.3	10826
29	281.1729	0.9	7255
30	286.1251	1.2	10058
31	290.0842	3.2	27721
32	291.0808	13.8	117947
33	292.0839	2.2	19197
34	295.0755	1.0	8188
35	297.1299	2.3	19352
36	299.1201	1.6	13483
37	301.1172	0.9	8065
38	301.1416	2.3	19254
39	308.0942	0.9	7400
40	309.0911	3.4	29293
41	309.1299	2.1	18017
42	322.1101	1.7	14904
43	323.1067	7.7	65687
44	324.1099	1.4	11900
45	327.1403	0.9	7818
46	336.1646	2.6	22106
47	337.1612	10.2	87024
48	338.1643	2.2	18969
49	341.2300	1.5	12951
50	347.1221	1.3	11484
51	354.1748	1.8	15106
52	355.1715	7.4	63248
53	356.1748	1.7	14702
54	359.1054	1.5	12722
55	359.6057	0.8	7226
56	360.1042	0.9	7547
57	369.1868	2.4	20371
58	377.1532	0.8	7192
59	381.2970	1.1	9404
60	391.1686	3.4	28725
61	392.1713	0.9	7323

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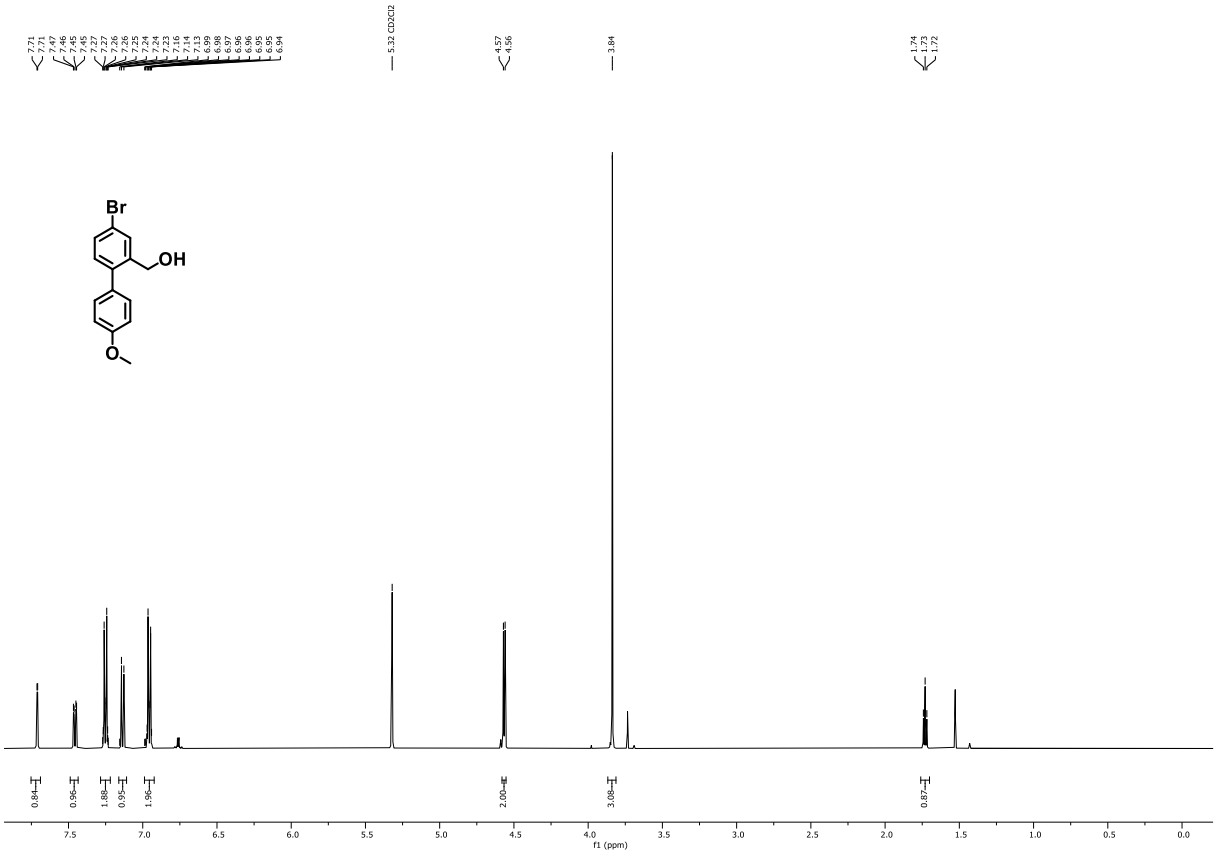
#	m/z	I %	I
62	397.1214	1.0	8291
63	406.1709	1.1	9371
64	451.1530	1.1	9324
65	480.6670	1.4	11780
66	481.1662	2.3	19411
67	481.6672	1.2	10192
68	491.3786	1.9	16092
69	493.3577	1.6	13446
70	505.1605	2.1	18161
71	506.2543	1.1	9581
72	507.2511	4.8	40803
73	508.2542	1.4	11975
74	511.2158	1.8	15217
75	525.0811	1.4	12050
76	533.1776	1.9	16595
77	534.1832	1.4	12170
78	535.1827	3.1	26237
79	536.1855	1.4	11619
80	537.1807	2.0	16778
81	538.1824	1.1	9617
82	539.1787	1.3	10730
83	558.1721	1.9	16554
84	559.1691	4.4	37632
85	560.1720	1.5	12561
86	567.2082	1.2	10364
87	574.2713	1.0	8561
88	575.2681	4.1	35415
89	576.2717	1.3	11280
90	587.0965	1.2	10310
91	599.2343	2.1	17803
92	600.2368	0.9	7526
93	601.1122	2.1	18336
94	601.2319	1.1	9373
95	602.1152	0.9	7914
96	602.9577	1.0	8859
97	663.4512	2.3	19669
98	664.4545	1.1	9088
99	703.1844	1.0	8436
100	789.2583	1.1	9461

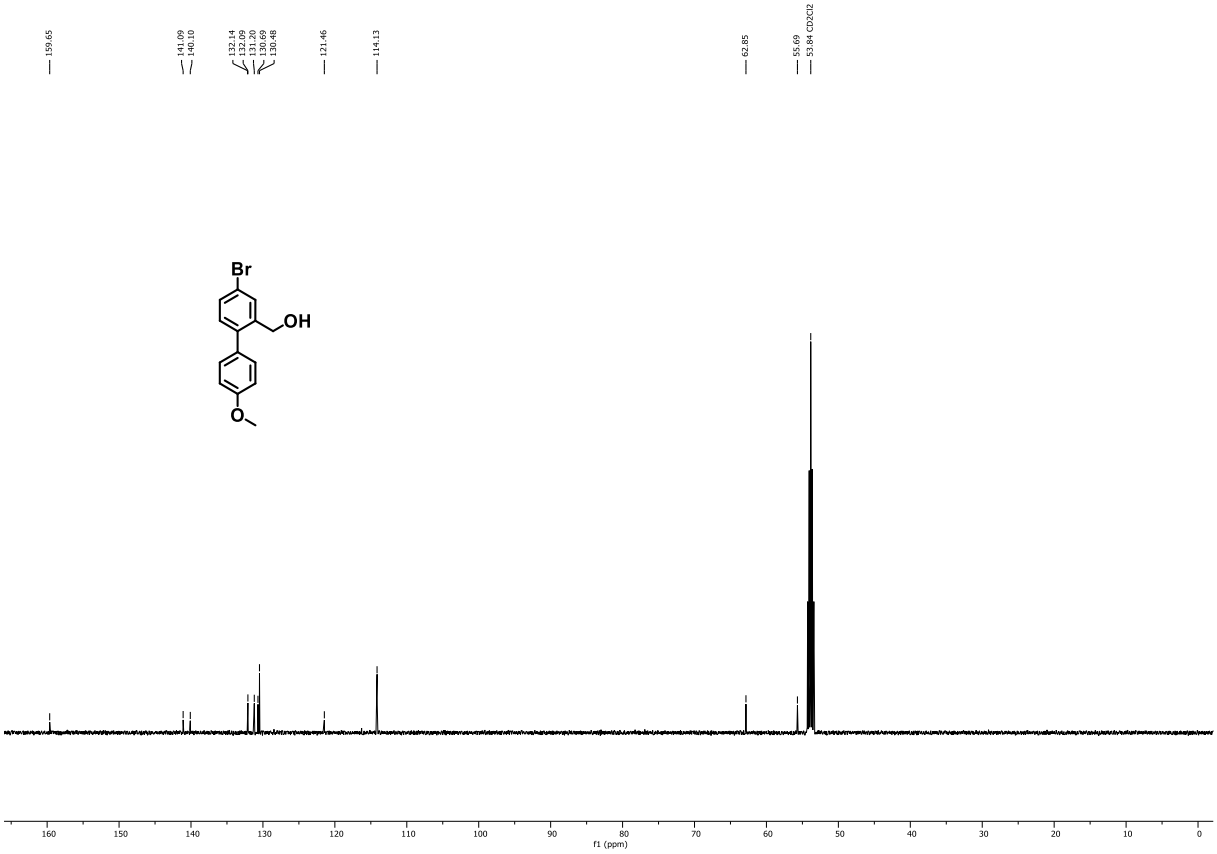
Acquisition Parameter

General	Fore Vacuum	3.46e+000 mBar	High Vacuum	8.93e-008 mBar	Source Type	ESI
	Scan Begin	75 m/z	Scan End	1700 m/z	Ion Polarity	Positive
Source	Set Nebulizer	0.4 Bar	Set Capillary	3600 V	Set Dry Gas	4.0 l/min
	Set Dry Heater	180 °C	Set End Plate Offset	-500 V		
Quadrupole	Set Ion Energy (MS only)	4.0 eV				
Coll. Cell	Collision Energy	8.0 eV	Set Collision Cell RF	350.0 Vpp	100.0 Vpp	
Ion Cooler	Set Ion Cooler Transfer Time	75.0 µs	Set Ion Cooler Pre Pulse Storage Time		10.0 µs	

^{1}H-NMR spectra of **14** in CD_2Cl_2



^{13}C-NMR spectra of **14** in CD_2Cl_2

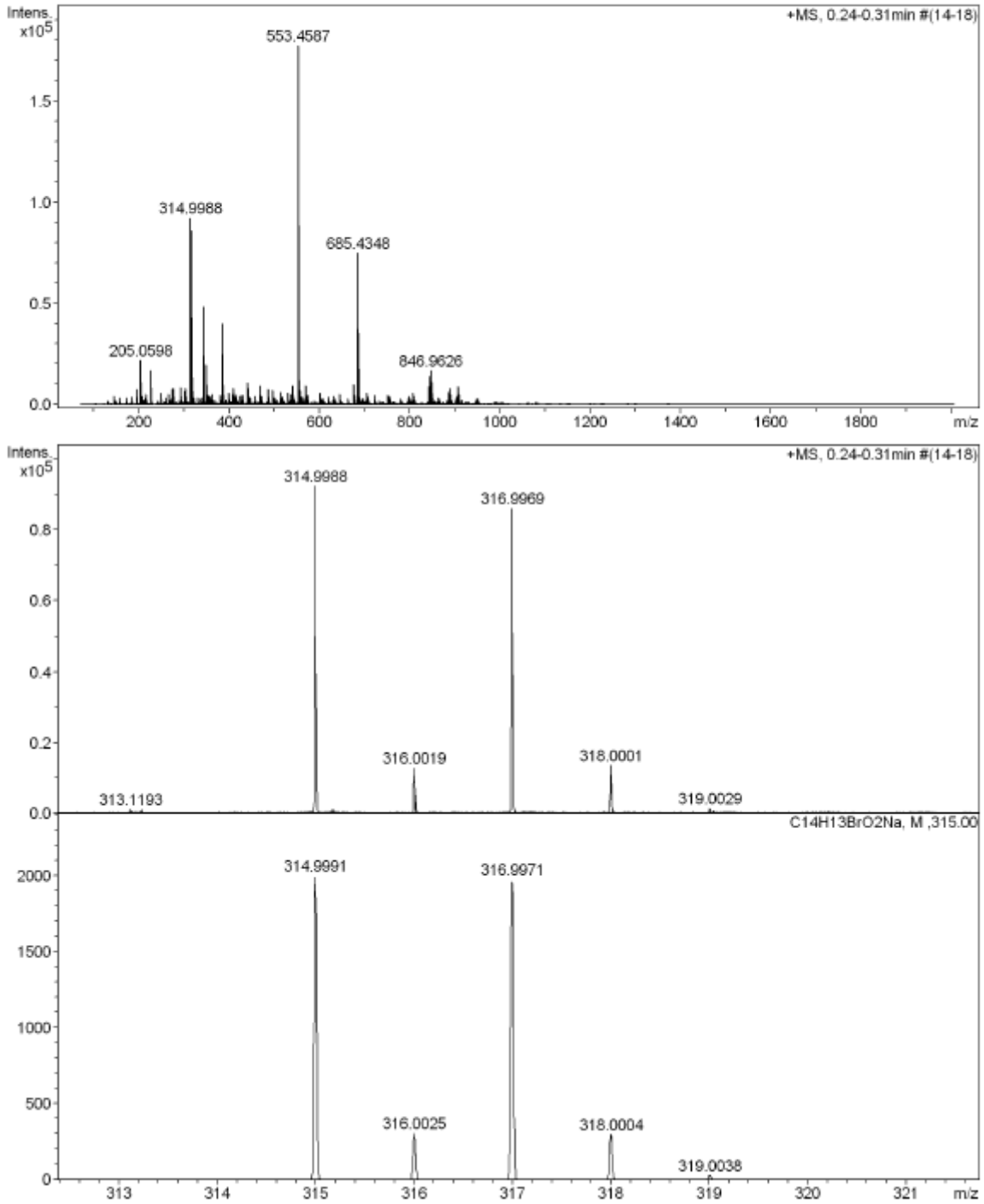


HR-MS spectra of **14**

High Resolution Mass Spectrometry Report

Sample Name **KRO217**
Comment

Instrument maXis 4G
Method ms_nocolumn_mid_pos.m



High Resolution Mass Spectrometry Report

Measured m/z vs. theoretical m/z

Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	z
314.9988	1	C 14 H 13 Br Na O 2	100.00	314.9991	0.3	0.9	24.7	7.5	even	1+

Mass list

#	m/z	I %	I
1	144.9820	2.5	4397
2	185.1145	2.3	4105
3	196.0879	4.3	7638
4	205.0598	12.3	21823
5	209.0213	2.5	4487
6	216.9226	2.7	4710
7	217.1045	3.0	5325
8	226.9513	9.4	16744
9	249.1092	3.1	5568
10	249.1568	2.4	4199
11	267.0624	2.9	5152
12	275.0063	4.2	7536
13	277.0050	4.5	7986
14	293.1354	2.2	3926
15	294.1095	4.8	8510
16	301.0749	3.7	6500
17	303.1377	4.5	8033
18	314.9988	52.1	92453
19	316.0019	7.3	13009
20	316.9969	48.6	86288
21	318.0001	7.7	13686
22	343.1300	27.3	48378
23	344.1334	6.6	11696
24	350.2660	11.2	19871
25	351.2690	2.7	4703
26	353.2657	2.8	5049
27	355.2810	2.4	4214
28	358.9793	2.5	4361
29	362.9258	3.1	5523
30	381.2965	2.8	4944
31	385.1407	22.7	40293
32	385.2916	2.7	4736
33	386.1441	5.7	10165
34	399.3071	3.4	6007
35	409.0409	4.6	8175
36	413.3227	2.2	3939
37	415.0424	3.1	5425
38	417.0393	2.2	3870
39	425.2862	2.6	4547
40	429.3176	2.9	5065
41	430.9133	2.7	4740
42	441.2970	6.1	10907
43	443.3338	4.5	7912
44	457.3485	2.4	4340
45	469.3250	5.4	9515
46	473.3439	2.4	4295
47	487.3596	4.3	7716
48	497.3955	4.0	7042
49	513.3390	3.6	6348
50	517.3699	2.2	3984
51	531.3858	3.3	5800
52	537.3935	3.1	5458
53	541.1199	5.2	9272
54	542.1207	2.5	4428
55	553.4587	100.0	177467
56	554.4617	36.1	64137
57	555.4649	6.8	12108
58	557.0937	2.9	5111
59	557.3647	4.1	7317
60	559.1297	2.2	3865
61	561.3964	2.1	3714
62	569.4322	5.3	9341

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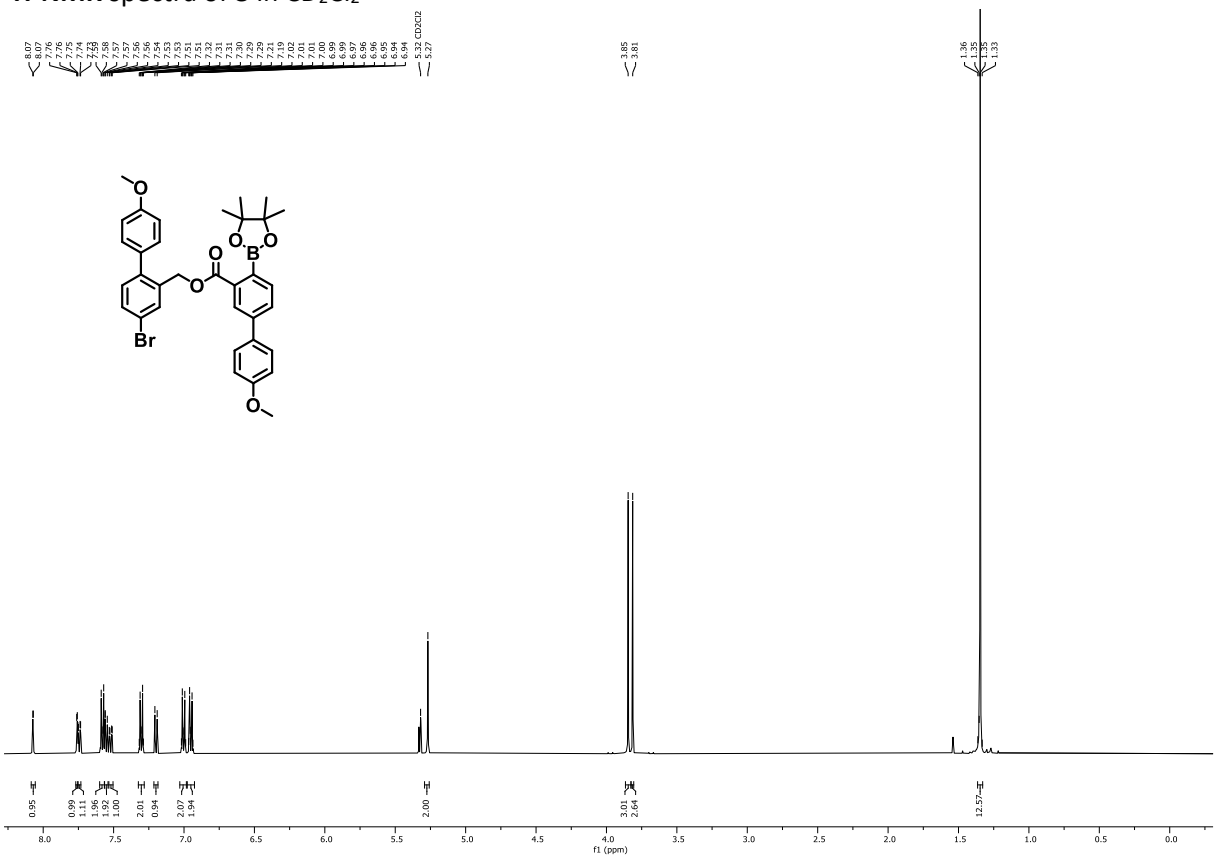
#	m/z	I %	I
63	575.4118	2.7	4860
64	601.3910	3.3	5916
65	619.4385	2.1	3739
66	633.1486	2.4	4196
67	645.4171	3.0	5304
68	677.1446	5.6	9871
69	678.1479	2.7	4795
70	685.4348	42.2	74888
71	686.4378	19.9	35388
72	687.4401	4.8	8455
73	689.4437	2.3	4045
74	705.5811	3.4	5975
75	707.1681	2.1	3701
76	721.5761	2.6	4622
77	750.4059	2.8	4909
78	752.9320	2.2	3816
79	754.9311	2.6	4547
80	798.8798	2.5	4459
81	808.0302	3.4	5996
82	810.0295	2.5	4395
83	842.9580	3.1	5421
84	843.9631	5.0	8818
85	844.9619	7.9	14066
86	845.9638	5.9	10498
87	846.9626	9.5	16931
88	847.9651	4.3	7656
89	848.9632	6.3	11156
90	849.9656	2.7	4715
91	885.9768	2.1	3733
92	886.9749	3.5	6250
93	887.9758	3.0	5343
94	888.9748	4.4	7875
95	889.9766	2.2	3819
96	890.9750	3.1	5425
97	904.9219	2.6	4605
98	906.9226	2.1	3662
99	907.7708	5.2	9204
100	908.7748	3.1	5447

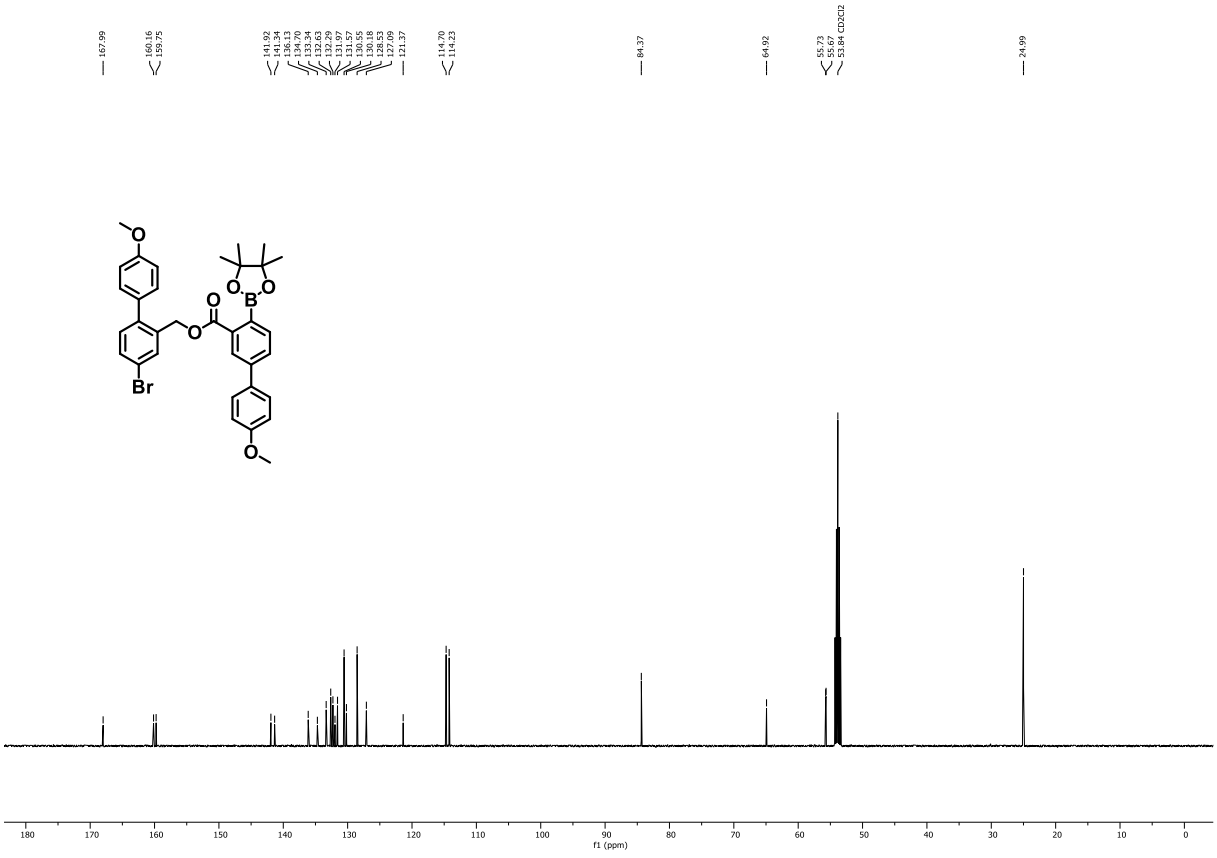
Acquisition Parameter

General	Fore Vacuum	3.36e+000 mBar	High Vacuum	9.05e-008 mBar	Source Type	ESI
	Scan Begin	75 m/z	Scan End	2000 m/z	Ion Polarity	Positive
Source	Set Nebulizer	2.0 Bar	Set Capillary	4500 V	Set Dry Gas	8.0 l/min
	Set Dry Heater	200 °C	Set End Plate Offset	-500 V		
Quadrupole	Set Ion Energy (MS only)	4.0 eV				
Coll. Cell	Collision Energy	8.0 eV	Set Collision Cell RF	600.0 Vpp	100.0 Vpp	
Ion Cooler	Set Ion Cooler Transfer Time	75.0 µs	Set Ion Cooler Pre Pulse Storage Time		10.0 µs	

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



^{13}C-NMR spectra of **3** in CD_2Cl_2

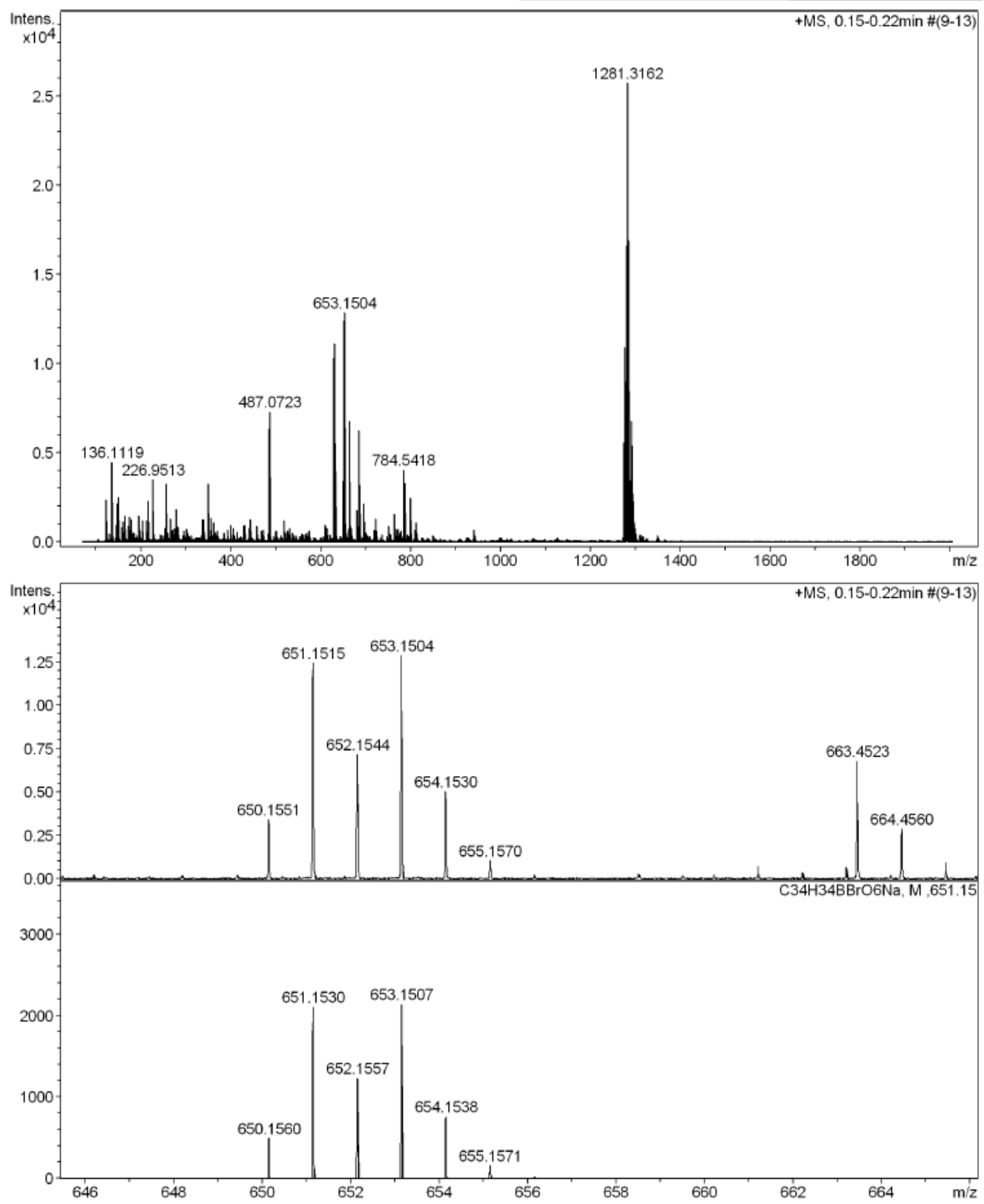


HR-ESI-MS spectra of **3**

High Resolution Mass Spectrometry Report

Sample Name **kro277**
Comment

Instrument maXis 4G
Method ms_nocolumn_mid_pos.m



High Resolution Mass Spectrometry Report

Measured m/z vs. theoretical m/z

Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e¯ Conf	z
651.1515	1	C 34 H 34 B Br Na O 6	100.00	651.1530	0.9	1.4	27.1	17.5	even	1+
1279.3179	1	C 68 H 68 B 2 Br 2 Na O 12	100.00	1279.3158	-2.1	-1.6	55.1	34.5	even	

Mass list

#	m/z	I %	I
1	122.0962	9.2	2377
2	136.1119	17.4	4485
3	147.0915	7.0	1811
4	147.9309	8.4	2165
5	149.9307	8.6	2213
6	150.1278	9.9	2553
7	161.1072	4.6	1189
8	164.1430	5.7	1477
9	175.1229	5.5	1416
10	178.1587	4.9	1259
11	196.0880	5.8	1492
12	205.0599	4.7	1218
13	212.1431	4.8	1231
14	217.1044	9.0	2309
15	226.9513	13.7	3523
16	255.0820	12.7	3261
17	265.9622	5.2	1329
18	279.0933	7.2	1862
19	337.1603	5.1	1303
20	338.3406	5.0	1278
21	350.2659	12.7	3279
22	355.1699	5.3	1376
23	362.9259	4.4	1123
24	443.3331	5.0	1274
25	485.0739	24.7	6367
26	486.0771	8.8	2272
27	487.0723	28.5	7336
28	487.3595	4.3	1116
29	488.0757	10.3	2649
30	517.2941	4.8	1230
31	519.2955	4.4	1121
32	628.1738	9.9	2554
33	629.1698	40.1	10313
34	630.1729	23.5	6038
35	631.1688	43.3	11146
36	632.1715	15.7	4031
37	650.1551	13.3	3429
38	651.1515	48.3	12435
39	652.1544	27.9	7185
40	653.1504	50.0	12876
41	654.1530	19.6	5040
42	655.1570	4.1	1057
43	663.4523	26.4	6793
44	664.4560	11.3	2898
45	680.4789	6.9	1787
46	685.4346	24.3	6256
47	686.4385	12.5	3210
48	695.4893	8.5	2176
49	696.4939	4.5	1148
50	722.4907	5.2	1350
51	764.5734	6.2	1592
52	784.5418	15.9	4082
53	785.5429	11.5	2966
54	786.5359	13.0	3334
55	787.5364	5.3	1353
56	798.5561	9.6	2471
57	799.5597	5.8	1501
58	812.5735	4.4	1140
59	1273.3640	8.2	2111
60	1274.3612	21.8	5600
61	1275.3629	29.1	7478

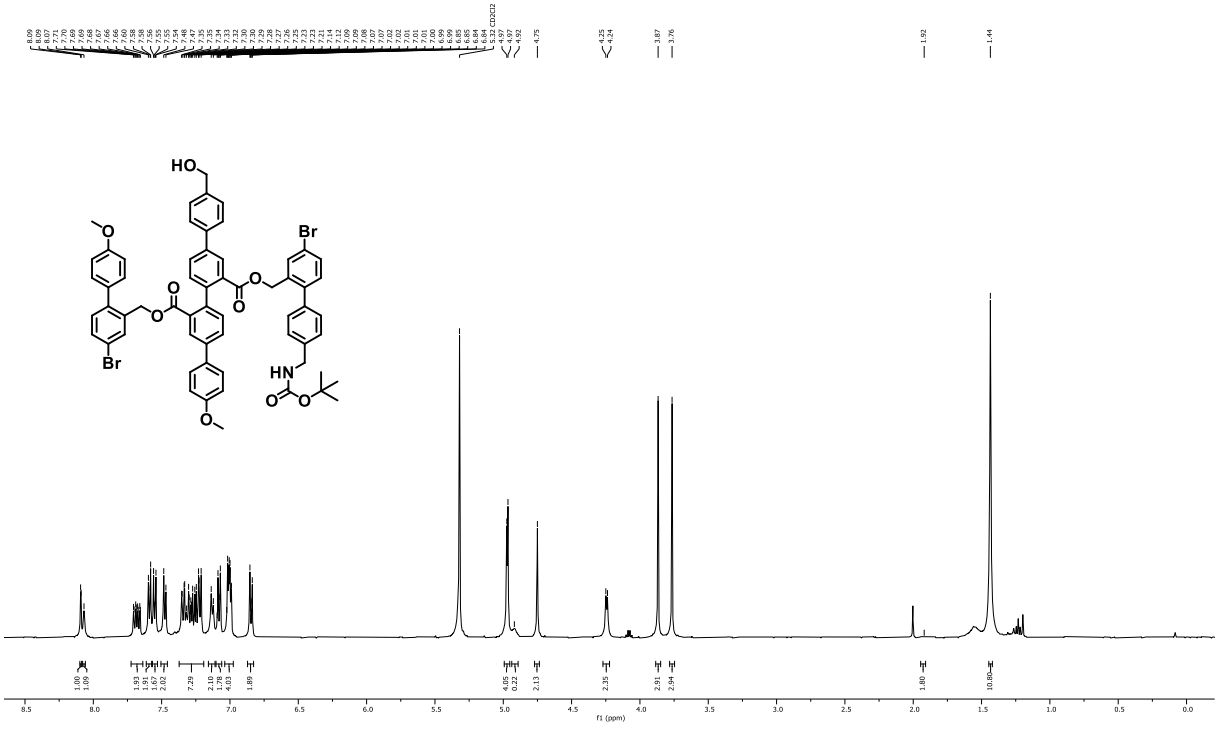
High Resolution Mass Spectrometry Report

#	m/z	I %	I
62	1276.3611	42.6	10964
63	1277.3615	35.0	9006
64	1278.3564	33.4	8603
65	1279.3179	51.8	13317
66	1280.3186	64.6	16631
67	1281.3162	100.0	25728
68	1282.3177	76.1	19574
69	1283.3154	65.7	16903
70	1284.3165	34.5	8876
71	1285.3185	11.5	2969
72	1288.3746	5.4	1387
73	1289.3716	13.6	3501
74	1290.3740	17.2	4437
75	1291.3711	26.4	6797
76	1292.3724	21.1	5427
77	1293.3698	17.3	4453
78	1294.3726	9.1	2343

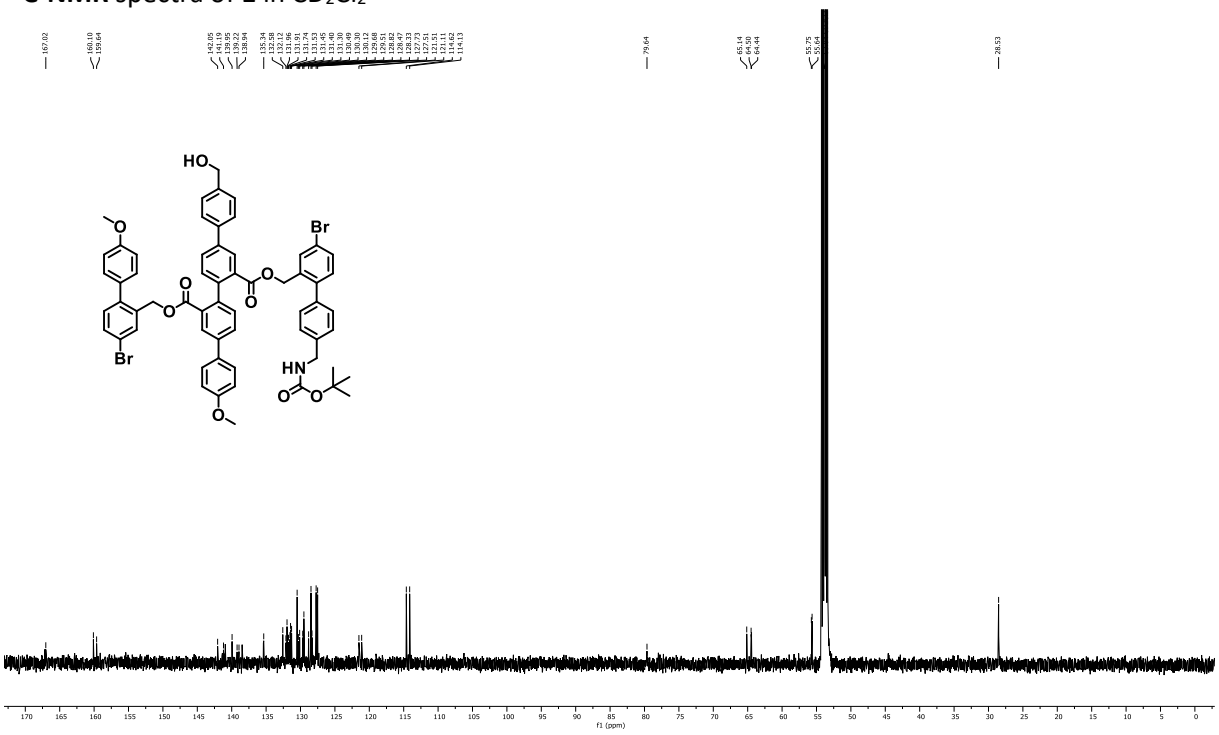
Acquisition Parameter

General	Fore Vacuum	3.36e+000 mBar	High Vacuum	1.02e-007 mBar	Source Type	ESI
	Scan Begin	75 m/z	Scan End	2000 m/z	Ion Polarity	Positive
Source	Set Nebulizer	2.0 Bar	Set Capillary	4500 V	Set Dry Gas	8.0 l/min
	Set Dry Heater	200 °C	Set End Plate Offset	-500 V		
Quadrupole	Set Ion Energy (MS only)	4.0 eV				
Coll. Cell	Collision Energy	8.0 eV	Set Collision Cell RF	600.0 Vpp	100.0 Vpp	
Ion Cooler	Set Ion Cooler Transfer Time	75.0 µs	Set Ion Cooler Pre Pulse Storage Time	10.0 µs		

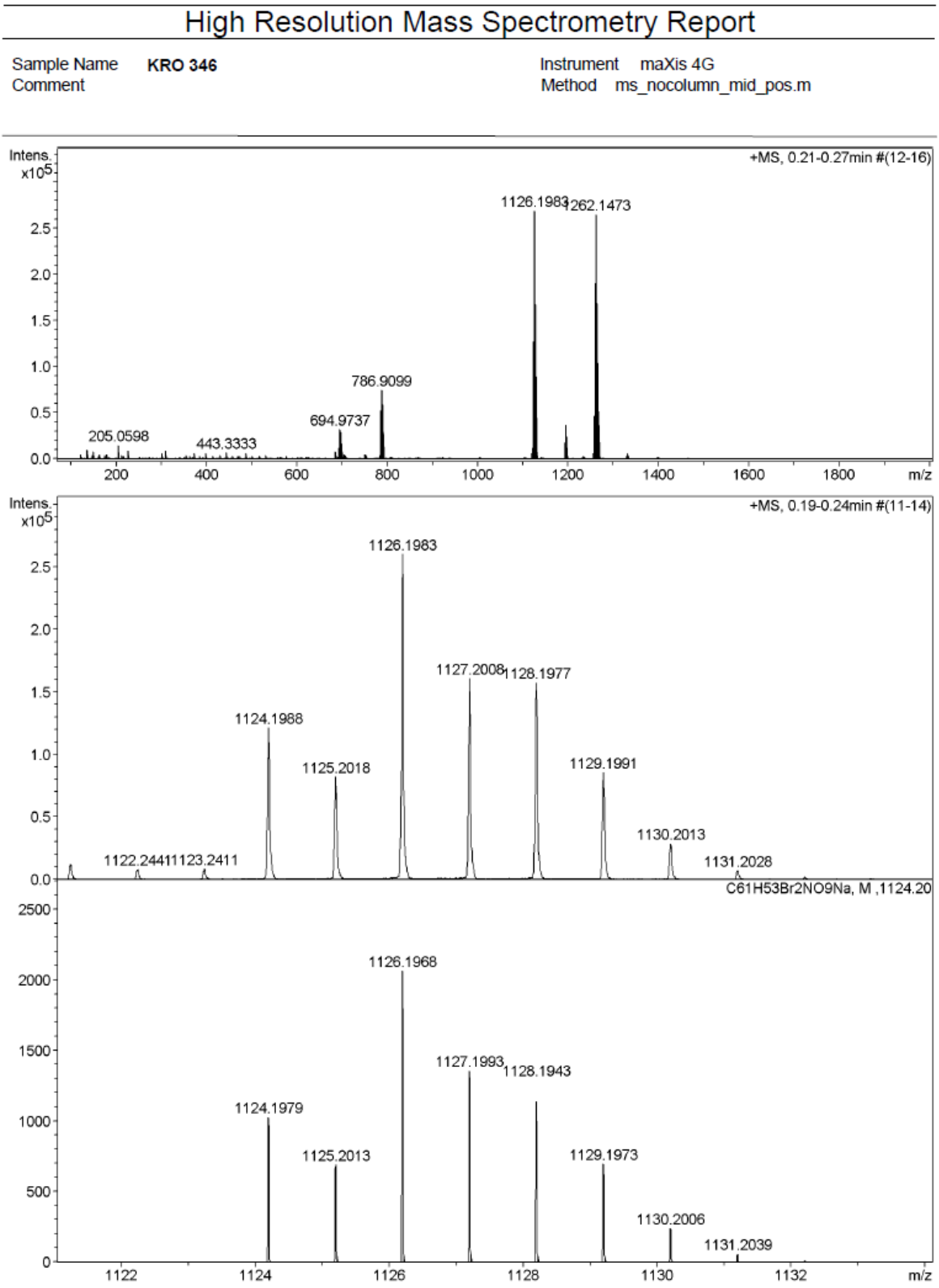
^{1}H-NMR spectra of **1** in CD_2Cl_2



^{13}C-NMR spectra of **1** in CD_2Cl_2



HR-MS spectra of **1**



High Resolution Mass Spectrometry Report

Measured m/z vs. theoretical m/z

Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	z
1124.1988	1	C 61 H 53 Br 2 N Na O 9	100.00	1124.1979	-0.9	-0.8	17.5	34.5	even	1+

Mass list

#	m/z	I %	I
1	122.0961	1.4	4302
2	136.1119	3.2	9485
3	147.0914	1.2	3522
4	150.1276	2.5	7535
5	161.1074	0.9	2697
6	164.1430	1.6	4679
7	175.1225	1.4	4185
8	178.1588	1.6	4760
9	205.0598	4.9	14697
10	212.1431	1.3	3888
11	213.1459	1.0	2992
12	217.1044	1.2	3510
13	226.1587	0.9	2560
14	226.9512	3.4	10120
15	301.0749	2.0	6064
16	309.1303	3.0	9024
17	355.2813	1.5	4607
18	362.9257	1.4	4252
19	372.1947	2.1	6254
20	385.2917	1.0	3066
21	399.3071	2.0	6055
22	413.3229	1.0	3025
23	429.3182	1.3	3987
24	430.9132	1.4	4117
25	443.3333	2.4	7027
26	457.3487	1.2	3497
27	469.3266	1.2	3633
28	473.3433	1.2	3685
29	487.3592	1.9	5750
30	498.9005	0.9	2568
31	501.3756	1.0	2878
32	517.3703	1.1	3157
33	531.3859	1.3	3862
34	566.8878	1.0	3047
35	575.4115	1.2	3559
36	685.4340	2.6	7888
37	686.4374	1.2	3637
38	691.9823	1.1	3126
39	692.9757	3.8	11188
40	693.9748	6.7	19924
41	694.9738	10.3	30542
42	695.9747	4.9	14622
43	696.9728	9.4	28009
44	697.9754	3.8	11407
45	698.9729	5.3	15769
46	699.9758	2.0	5949
47	700.9724	1.2	3699
48	702.8626	0.9	2580
49	704.0036	1.3	3901
50	705.0018	1.8	5278
51	707.0013	1.3	3948
52	750.0307	1.8	5397
53	752.0293	1.9	5611
54	782.9109	1.3	4007
55	783.9138	1.5	4381
56	784.9093	9.3	27752
57	785.9105	19.3	57310
58	786.9100	26.8	79880
59	787.9120	9.5	28357
60	788.9092	21.7	64494
61	789.9119	7.7	22980
62	790.9102	10.0	29894

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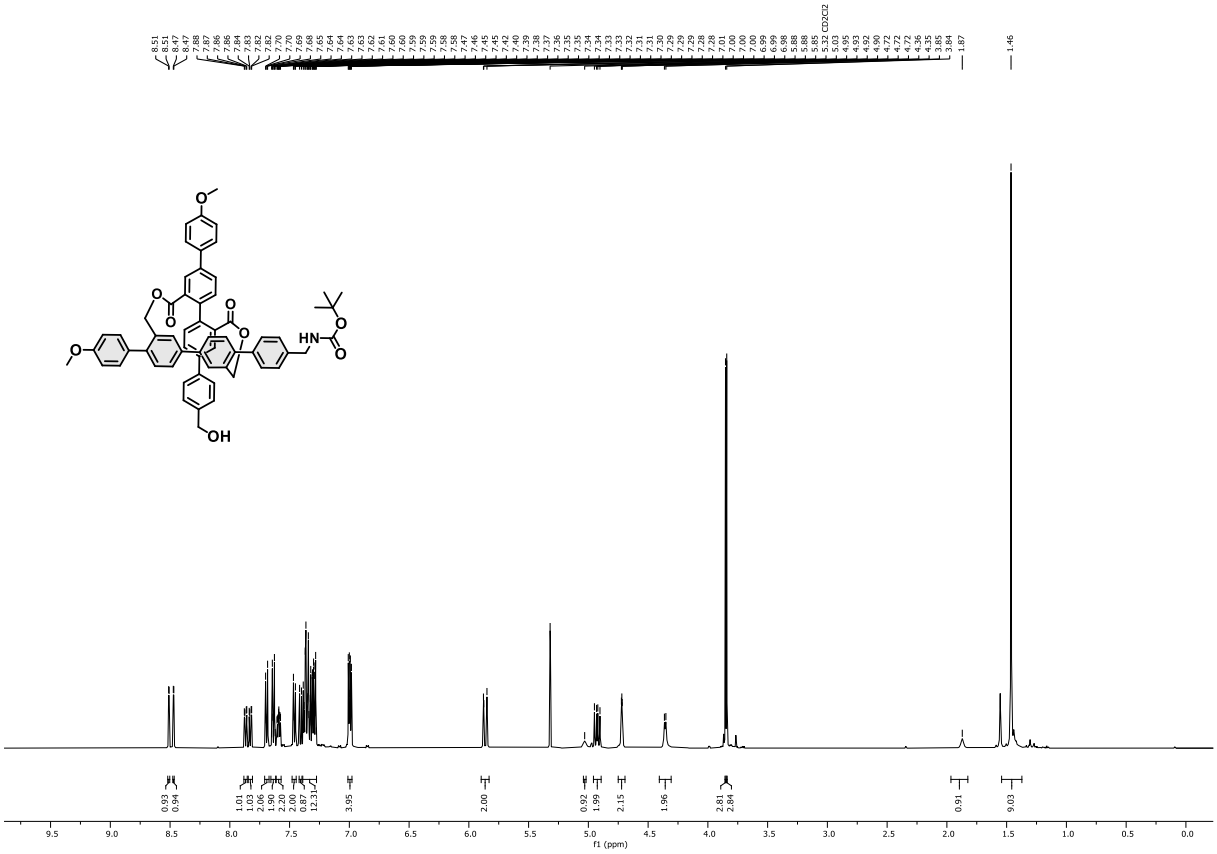
#	m/z	I %	I
63	791.9127	3.6	10816
64	921.7499	1.1	3167
65	1004.1604	0.9	2779
66	1119.2424	2.0	6073
67	1120.2456	1.4	4161
68	1121.2414	4.2	12630
69	1122.2441	2.7	8130
70	1123.2411	2.9	8505
71	1124.1988	40.8	121389
72	1125.2018	27.7	82394
73	1126.1983	87.4	260260
74	1127.2008	54.1	161042
75	1128.1977	53.0	157795
76	1129.1991	28.9	85930
77	1130.2013	9.7	28868
78	1131.2028	2.5	7327
79	1192.1862	5.2	15364
80	1193.1894	3.4	10110
81	1194.1849	10.3	30710
82	1195.1882	6.8	20236
83	1196.1851	6.9	20686
84	1197.1866	3.8	11183
85	1198.1897	1.3	3888
86	1256.1469	2.1	6361
87	1257.1500	3.3	9884
88	1258.1468	17.5	52155
89	1259.1479	39.4	117240
90	1260.1476	72.8	216781
91	1261.1481	69.7	207364
92	1262.1473	100.0	297652
93	1263.1491	58.3	173520
94	1264.1473	63.3	188493
95	1265.1492	38.8	115480
96	1266.1482	26.5	78953
97	1267.1485	14.0	41535
98	1268.1511	4.9	14628
99	1269.1543	1.3	4011
100	1330.1579	1.2	3457

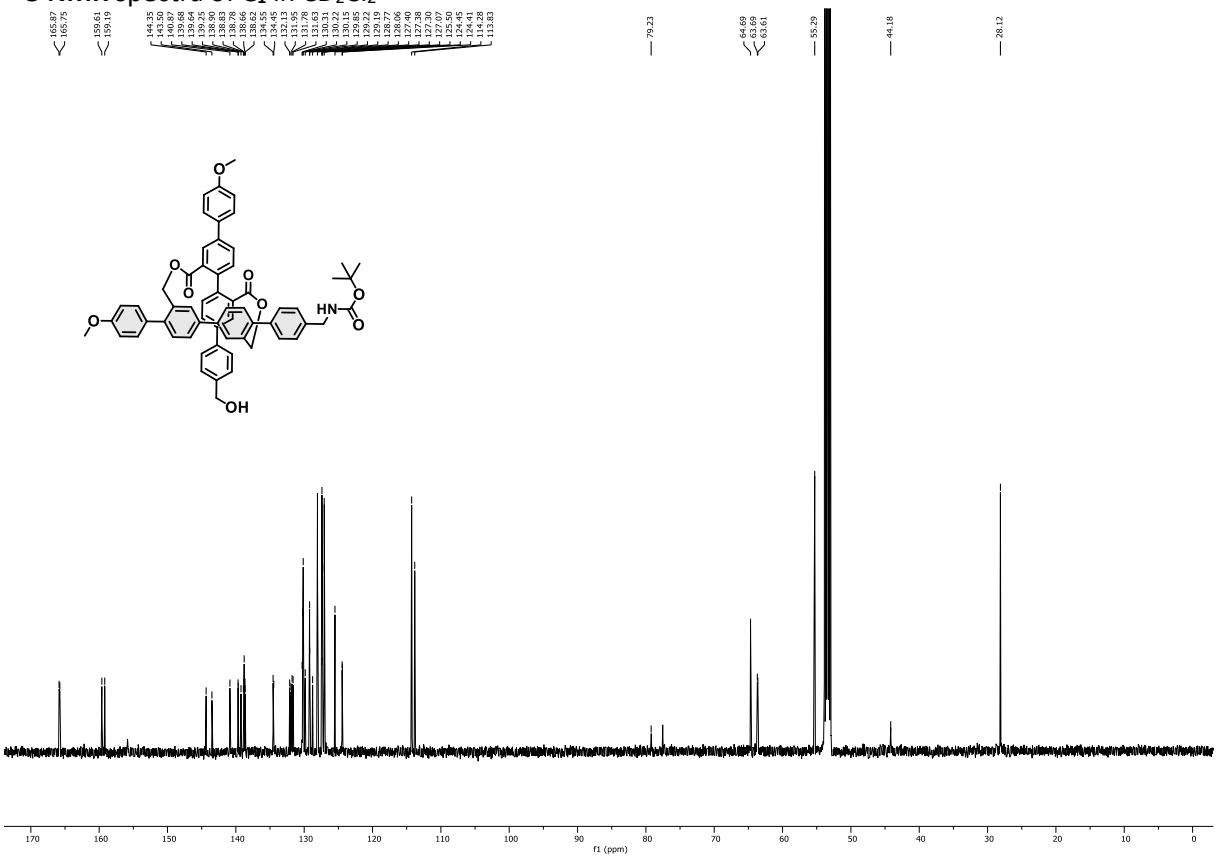
Acquisition Parameter

General	Fore Vacuum	3.07e+000 mBar	High Vacuum	1.34e-007 mBar	Source Type	ESI
	Scan Begin	75 m/z	Scan End	2000 m/z	Ion Polarity	Positive
Source	Set Nebulizer	2.0 Bar	Set Capillary	4500 V	Set Dry Gas	8.0 l/min
	Set Dry Heater	200 °C	Set End Plate Offset	-500 V		
Quadrupole	Set Ion Energy (MS only)	4.0 eV				
Coll. Cell	Collision Energy	8.0 eV	Set Collision Cell RF	600.0 Vpp	100.0 Vpp	
Ion Cooler	Set Ion Cooler Transfer Time	75.0 µs	Set Ion Cooler Pre Pulse Storage Time	10.0 µs		

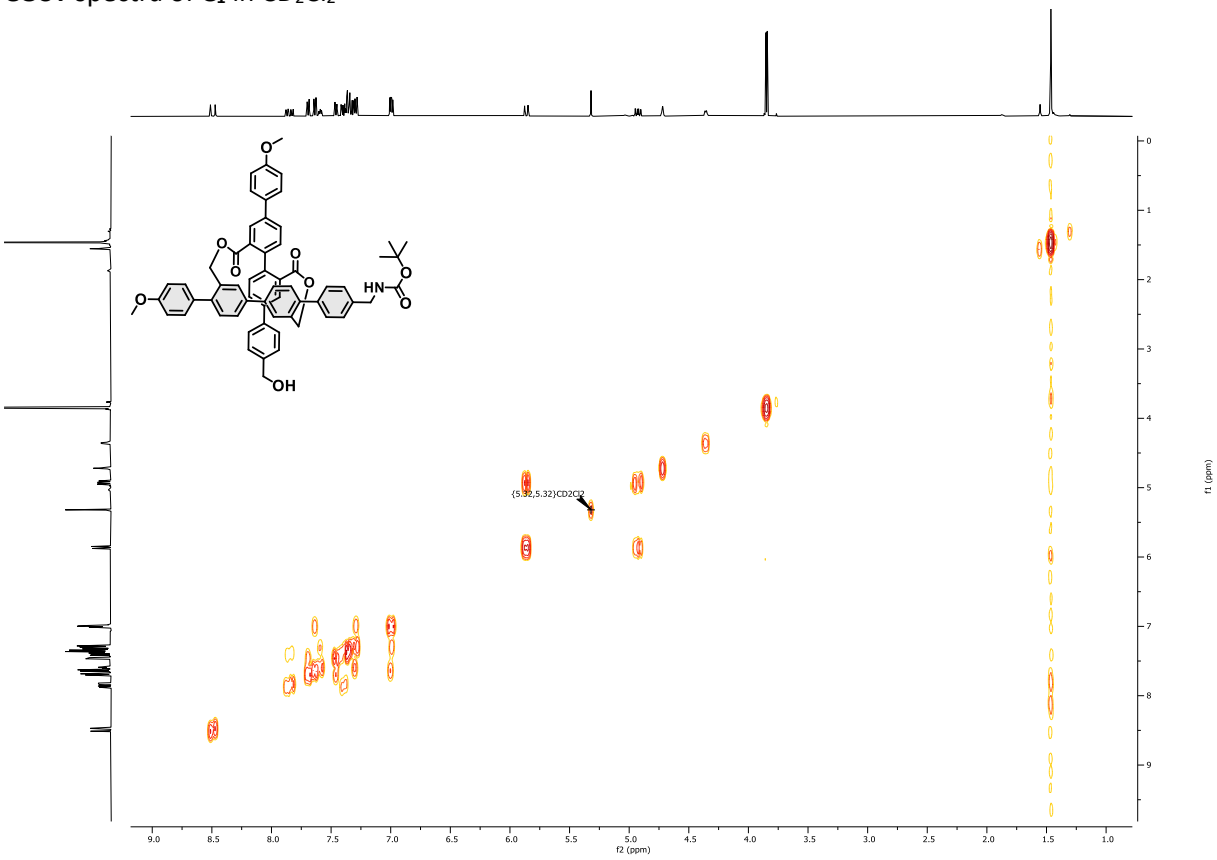
^{1}H-NMR spectra of **C_1** in CD_2Cl_2



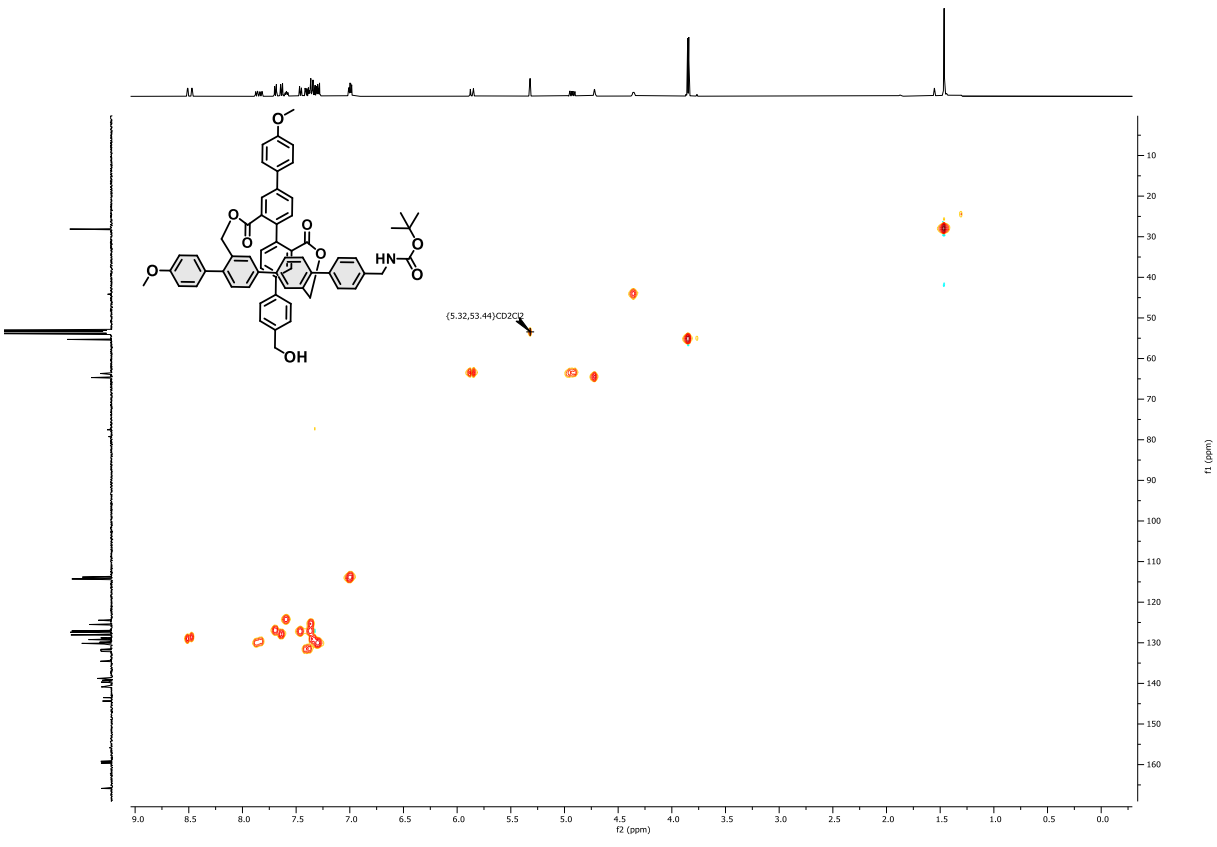
^{13}C-NMR spectra of **C_1** in CD_2Cl_2



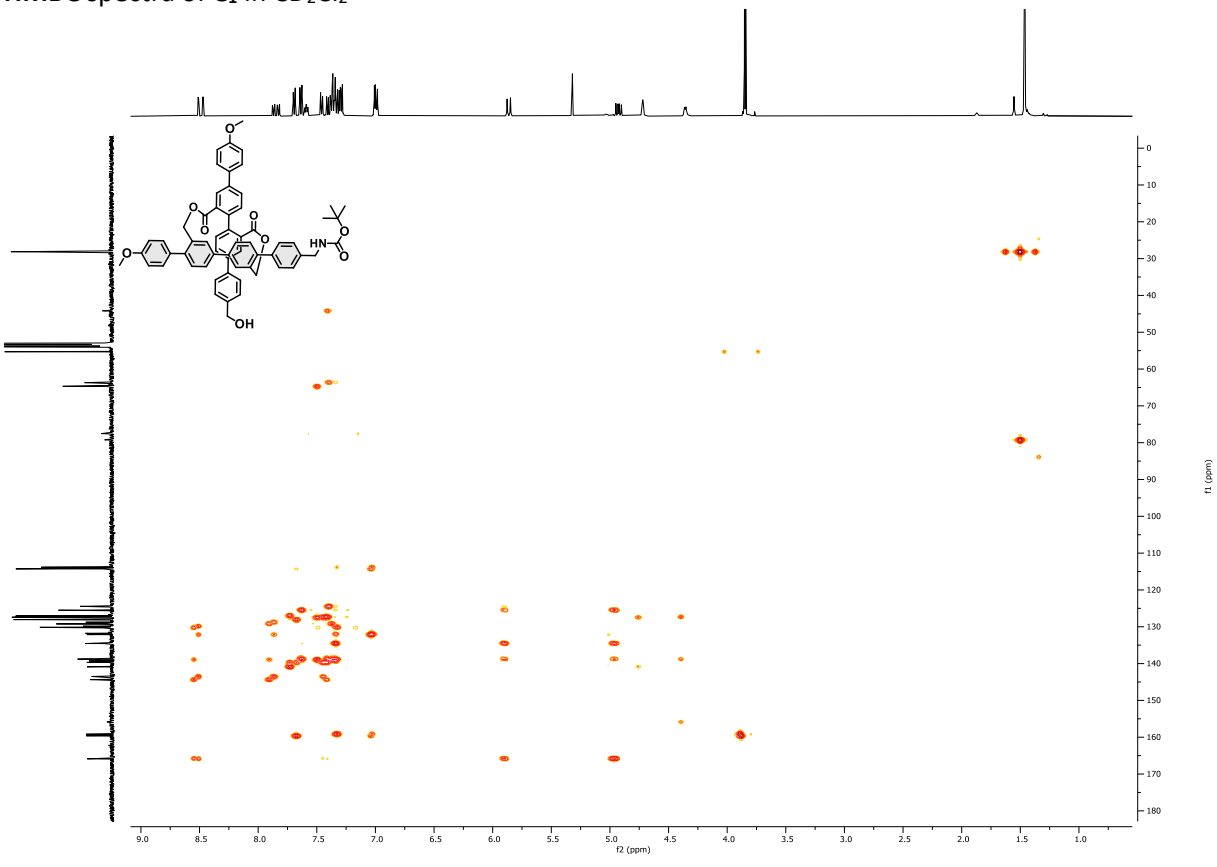
COSY spectra of **C_1** in CD_2Cl_2



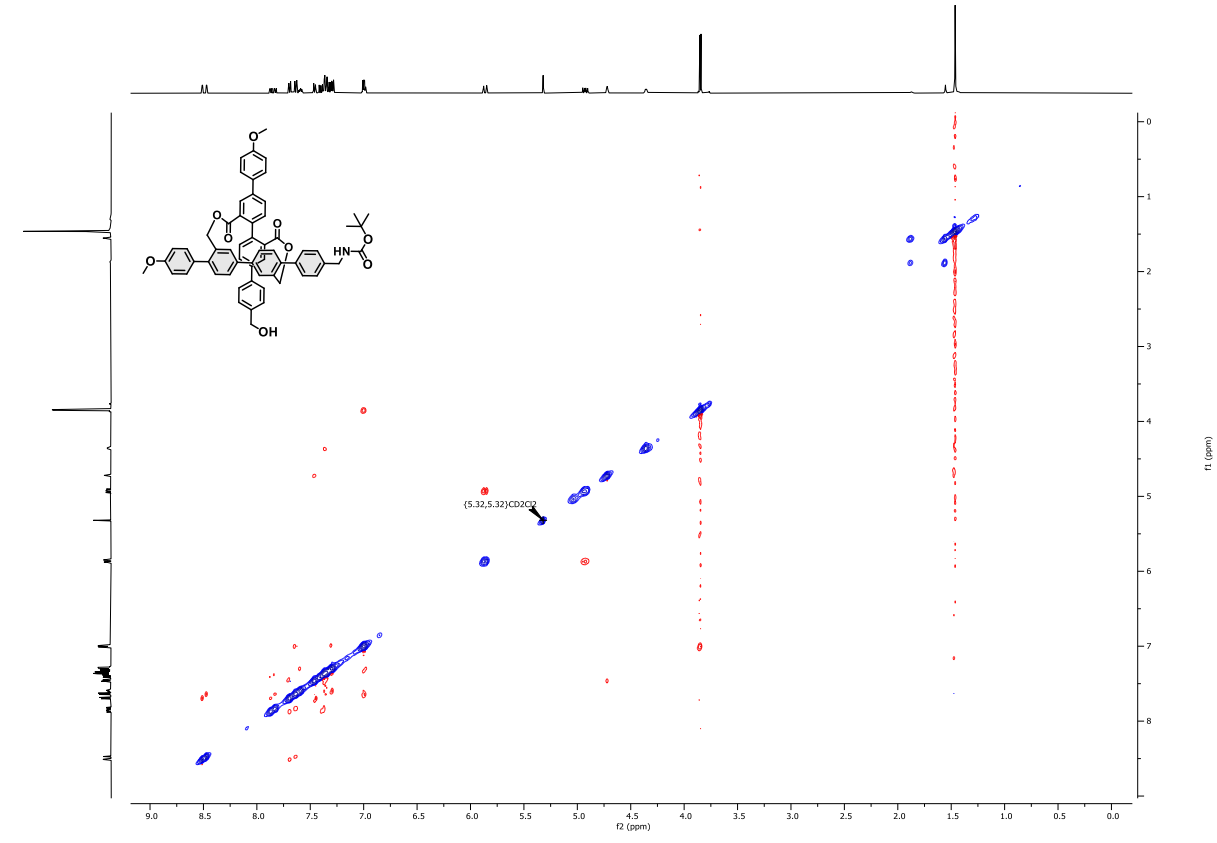
HMQC spectra of **C_1** in CD_2Cl_2



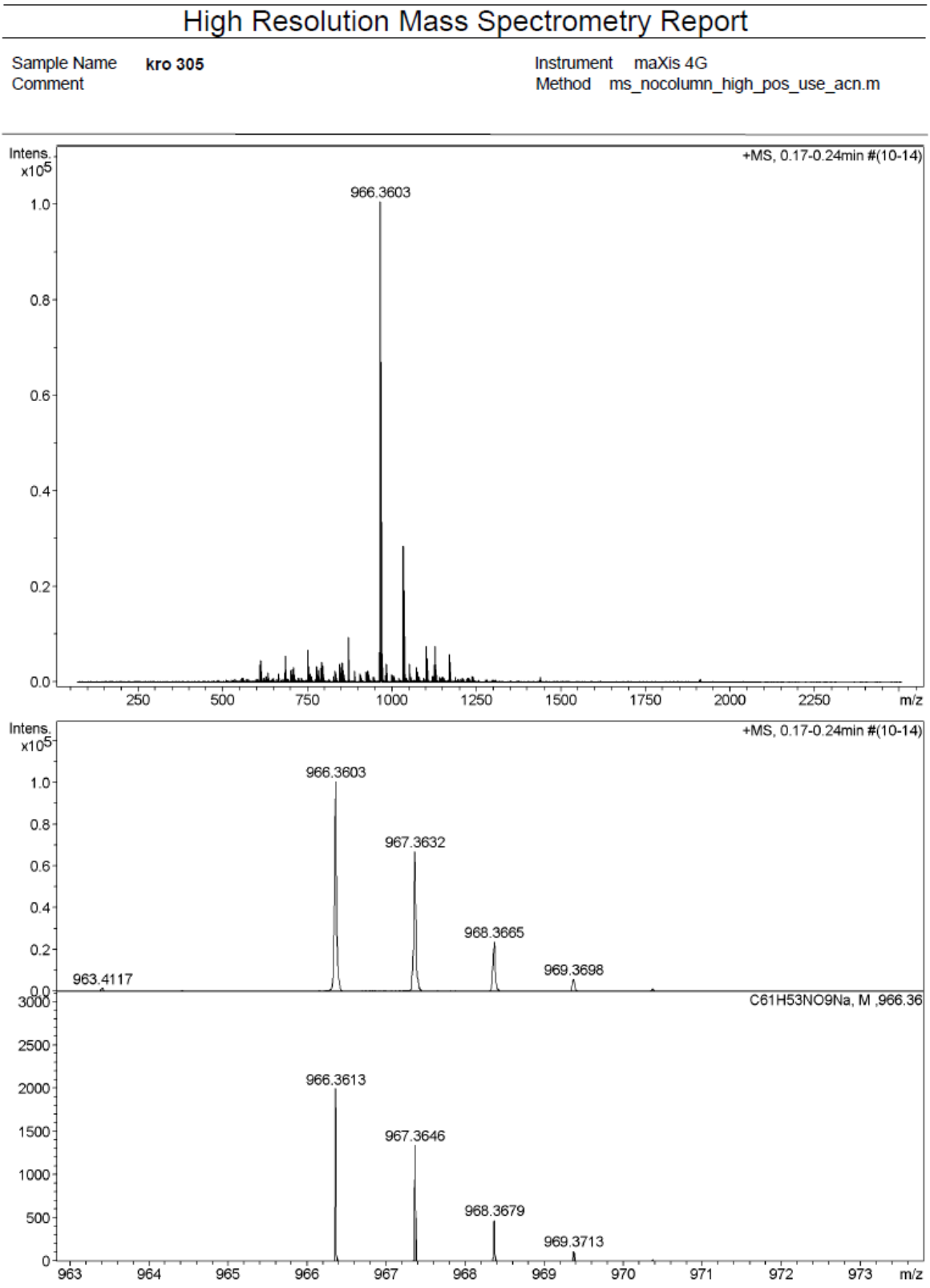
HMBC spectra of **C_1** in CD_2Cl_2



NOESY spectra of **C_1** in CD_2Cl_2



HR-MS spectra of **C_1**



High Resolution Mass Spectrometry Report

Measured m/z vs. theoretical m/z

Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	z
966.3603	1	C 61 H 53 N Na O 9	100.00	966.3613	0.9	0.9	1.3	35.5	even	1+

Mass list

#	m/z	I %	I
1	610.1833	3.6	3631
2	611.1869	4.6	4596
3	612.1850	2.2	2216
4	633.1490	1.9	1934
5	663.4558	1.5	1535
6	684.2004	2.0	2054
7	685.4339	5.5	5583
8	686.1999	1.5	1462
9	686.4371	2.7	2707
10	702.2121	2.5	2528
11	703.2133	1.6	1653
12	707.1675	2.7	2749
13	708.1669	1.7	1705
14	709.1658	1.5	1512
15	709.3787	3.1	3127
16	710.3817	1.5	1476
17	711.3782	1.5	1559
18	750.4056	6.8	6880
19	751.4086	3.1	3083
20	752.4047	3.4	3380
21	753.3544	1.6	1623
22	753.4073	1.8	1829
23	755.3553	1.7	1691
24	758.2201	1.9	1881
25	759.2205	1.7	1679
26	776.2314	3.3	3277
27	777.2313	2.2	2209
28	778.2303	1.9	1879
29	781.1851	2.5	2503
30	782.1863	2.1	2096
31	783.1844	1.7	1735
32	791.3739	2.9	2951
33	792.3729	4.2	4232
34	793.3766	1.8	1814
35	794.3737	3.4	3458
36	795.3763	1.5	1471
37	796.3747	1.9	1906
38	832.2383	2.4	2372
39	833.2392	1.8	1801
40	834.2377	1.6	1627
41	844.3255	3.8	3803
42	845.3284	2.3	2282
43	850.2489	3.0	3063
44	851.2499	2.4	2431
45	852.2473	1.8	1834
46	852.2930	3.9	3962
47	853.2978	2.5	2562
48	855.2051	2.5	2552
49	856.2054	1.9	1941
50	857.2050	1.7	1692
51	870.3044	9.4	9506
52	871.3084	5.8	5877
53	872.3108	2.4	2434
54	888.3163	2.4	2443
55	889.3175	1.7	1753
56	906.2580	1.8	1830
57	907.2588	1.5	1481
58	908.2566	1.4	1439
59	924.2694	2.3	2268
60	925.2691	1.9	1934
61	926.2686	1.9	1874
62	929.2243	2.3	2293

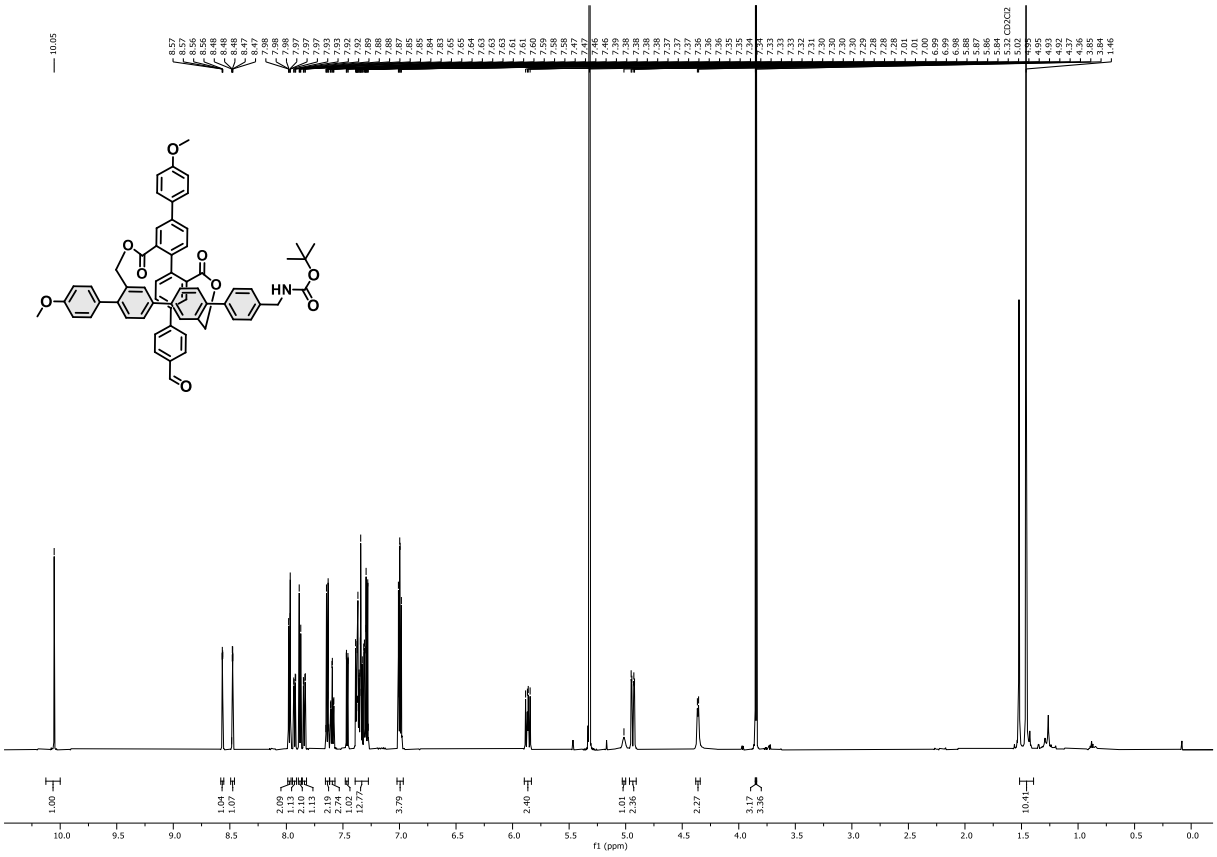
High Resolution Mass Spectrometry Report

#	m/z	I %	I
63	930.2239	1.6	1591
64	961.4037	6.2	6256
65	962.4070	4.1	4149
66	963.4117	1.6	1658
67	966.3603	100.0	100647
68	967.3632	66.7	67130
69	968.3665	23.8	23976
70	969.3698	6.1	6139
71	980.2766	1.4	1454
72	982.3338	3.8	3868
73	983.3364	2.9	2923
74	999.2903	1.6	1599
75	1000.2864	1.4	1409
76	1003.2413	1.5	1492
77	1034.3472	28.4	28604
78	1035.3504	19.1	19246
79	1036.3533	7.3	7317
80	1037.3560	1.8	1799
81	1050.3215	1.6	1602
82	1051.3341	3.9	3938
83	1052.3386	2.5	2507
84	1073.3580	3.1	3072
85	1074.2991	1.6	1597
86	1074.3613	2.2	2215
87	1102.3347	7.6	7644
88	1103.3375	4.9	4942
89	1104.3406	2.1	2104
90	1124.1959	3.6	3595
91	1125.2008	2.3	2321
92	1126.1951	7.6	7643
93	1127.1981	4.6	4607
94	1128.1952	4.4	4399
95	1129.1978	2.7	2767
96	1170.3212	5.8	5849
97	1170.4930	2.1	2088
98	1171.3250	4.3	4306
99	1171.4967	1.6	1594
100	1172.3293	1.6	1621

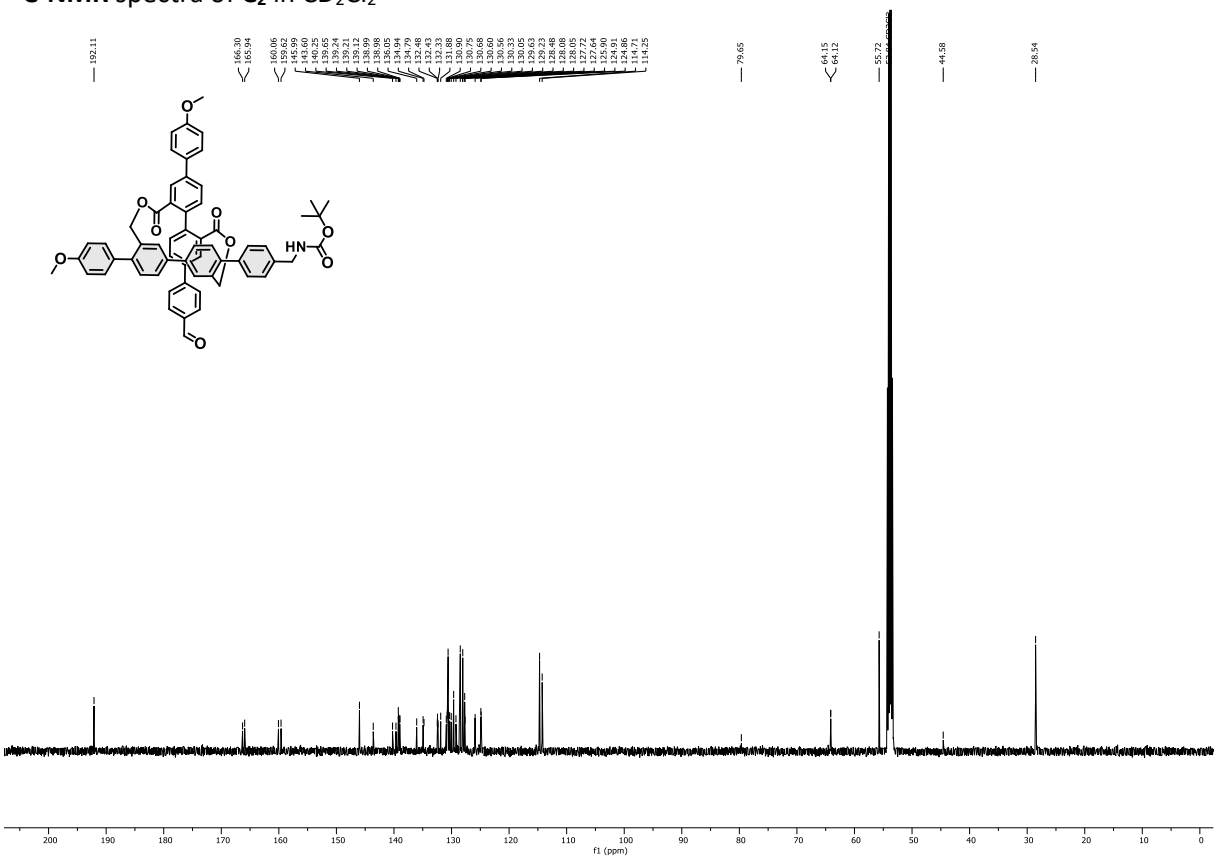
Acquisition Parameter

General	Fore Vacuum	3.36e+000 mBar	High Vacuum	1.20e-007 mBar	Source Type	ESI
	Scan Begin	75 m/z	Scan End	2500 m/z	Ion Polarity	Positive
Source	Set Nebulizer	2.0 Bar	Set Capillary	4500 V	Set Dry Gas	8.0 l/min
	Set Dry Heater	200 °C	Set End Plate Offset	-500 V		
Quadrupole	Set Ion Energy (MS only)	4.0 eV				
Coll. Cell	Collision Energy	12.0 eV	Set Collision Cell RF	2000.0 Vpp	800.0 Vpp	
Ion Cooler	Set Ion Cooler Transfer Time	120.0 µs	Set Ion Cooler Pre Pulse Storage Time	18.0 µs		

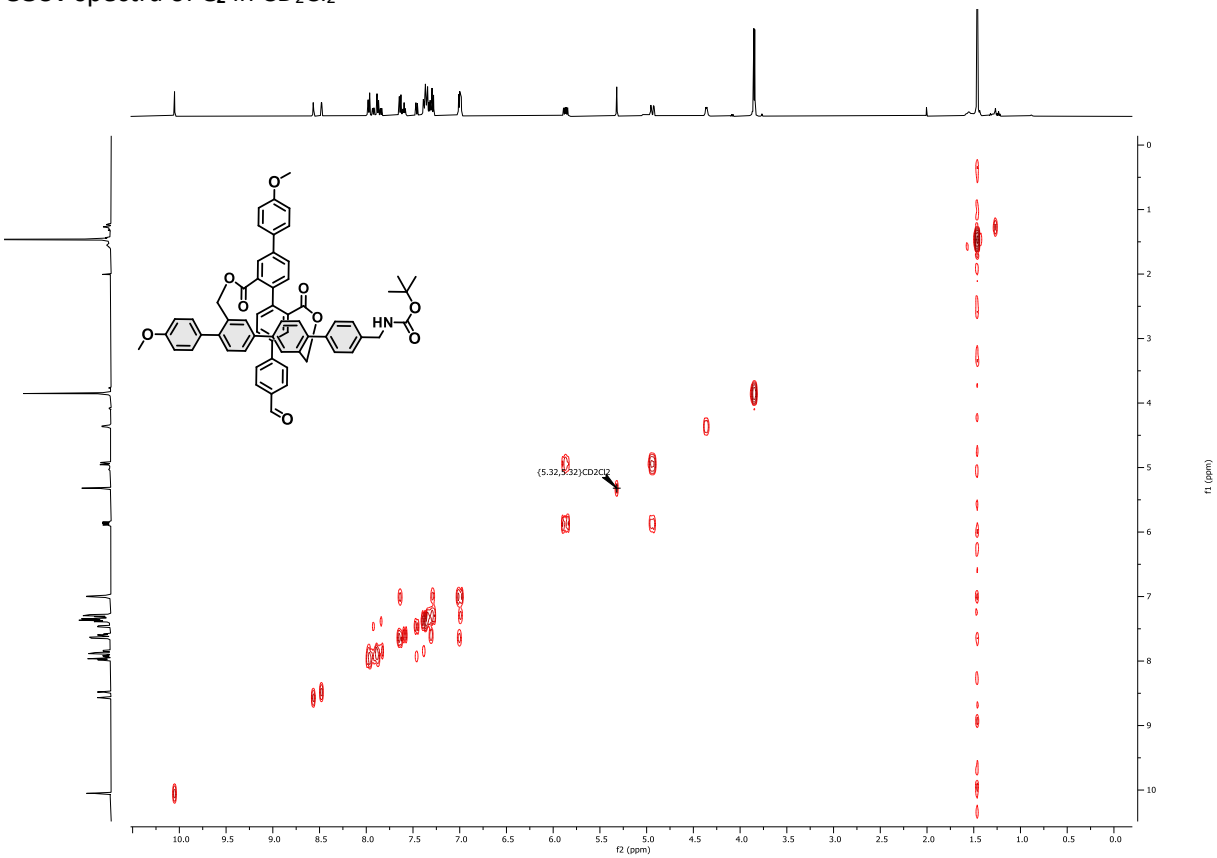
^{1}H-NMR spectra of **C_2** in CD_2Cl_2



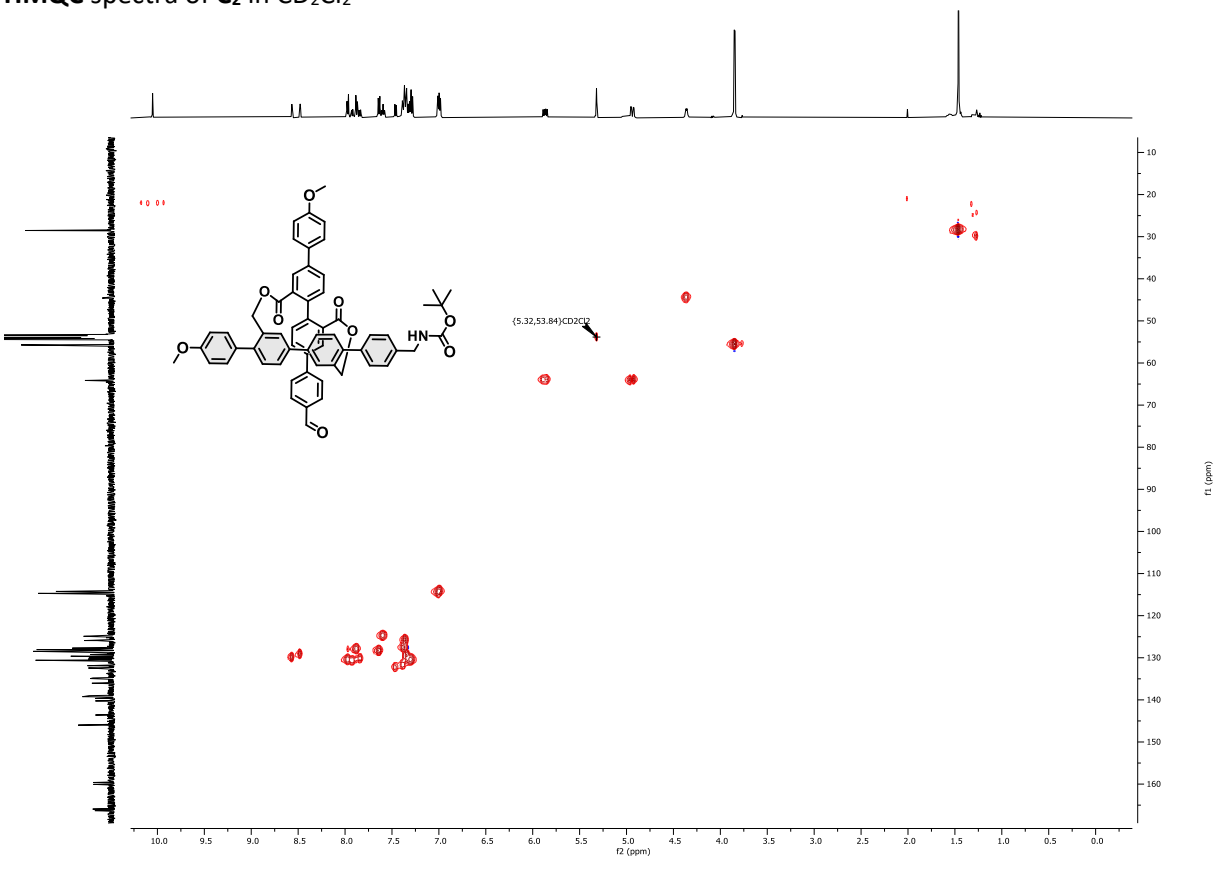
^{13}C-NMR spectra of **C_2** in CD_2Cl_2



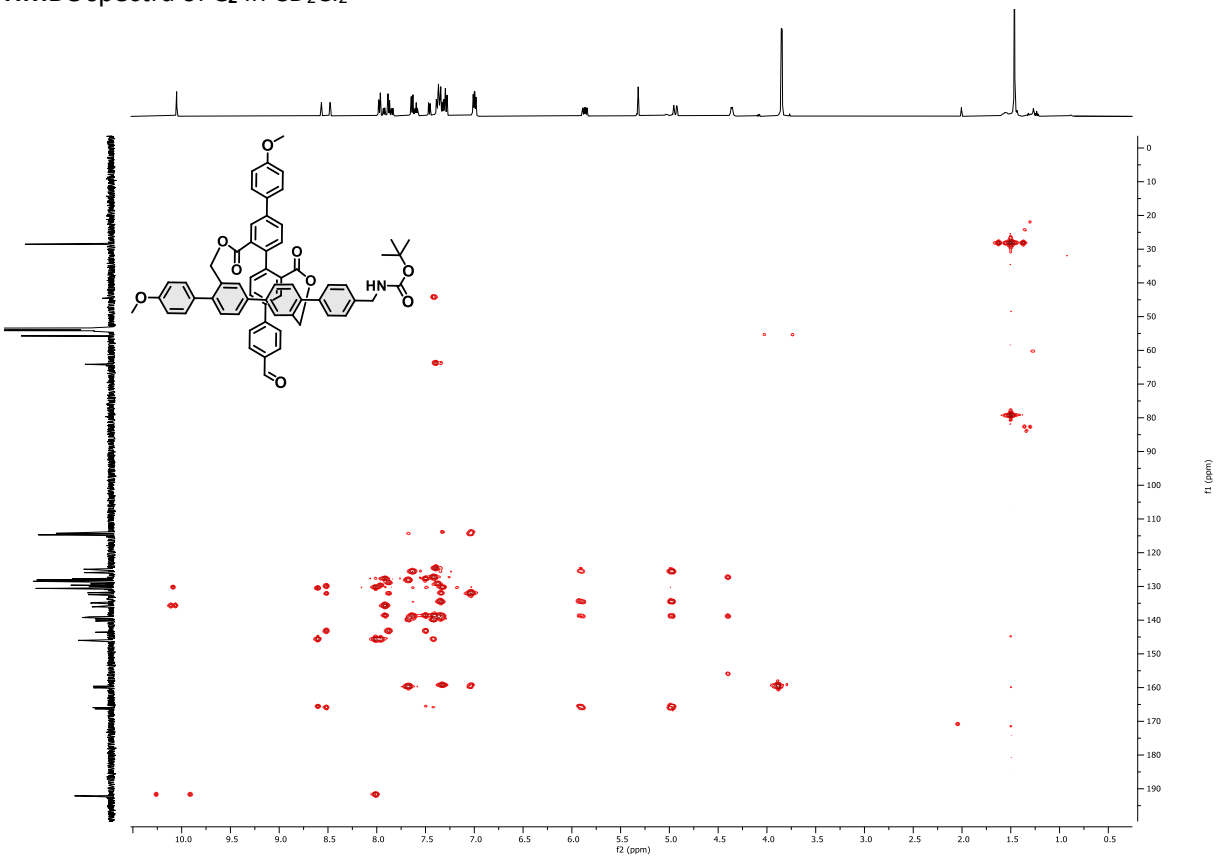
COSY spectra of **C_2** in CD_2Cl_2



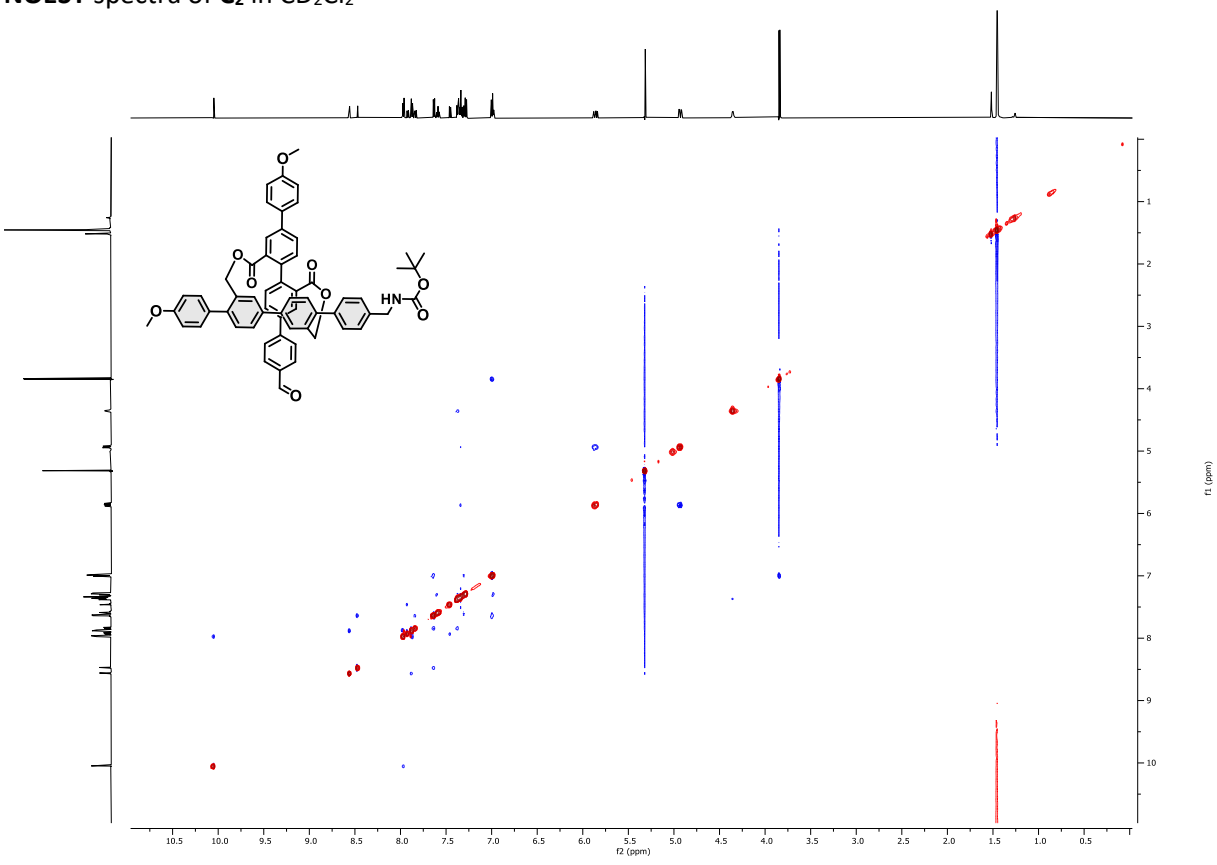
HMQC spectra of **C_2** in CD_2Cl_2



HMBC spectra of **C_2** in CD_2Cl_2



NOESY spectra of **C_2** in CD_2Cl_2

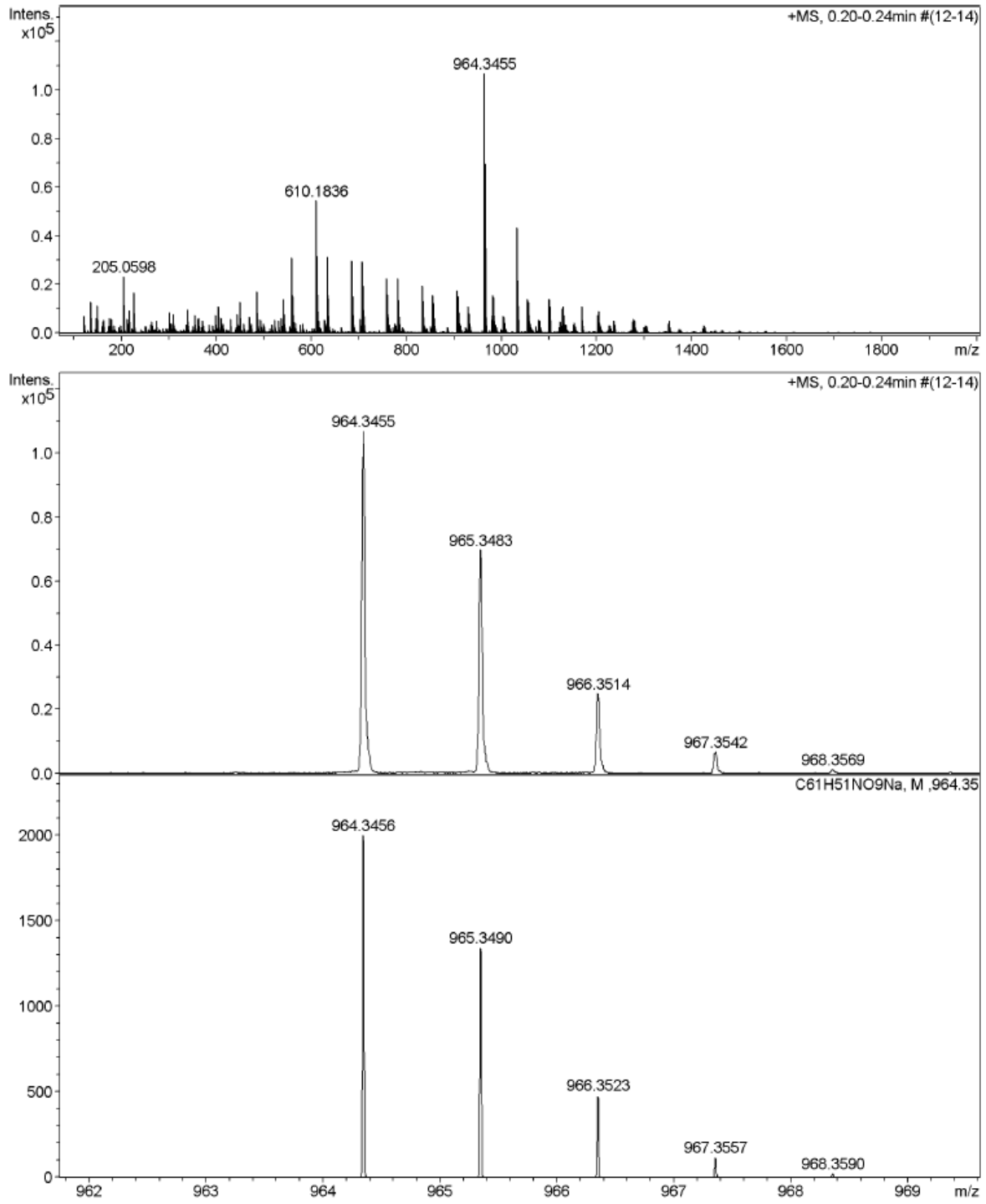


HR-ESI-MS spectra of **C_2**

High Resolution Mass Spectrometry Report

Sample Name **KRO 395**
Comment

Instrument maXis 4G
Method ms_nocolumn_mid_pos.m



High Resolution Mass Spectrometry Report

Measured m/z vs. theoretical m/z

Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e¯ Conf	z
964.3455	1	C 61 H 51 N Na O 9	100.00	964.3456	0.1	0.1	8.1	36.5	even	1+

Mass list

#	m/z	I %	I
1	122.0963	6.6	7068
2	136.1120	12.0	12858
3	147.0917	6.1	6519
4	150.1275	10.6	11326
5	175.1227	5.9	6317
6	205.0598	21.8	23382
7	212.1431	5.7	6063
8	217.1045	8.7	9343
9	226.9514	15.7	16778
10	301.0749	8.2	8787
11	309.1307	7.5	8051
12	339.1292	9.1	9747
13	355.2814	7.2	7662
14	361.2344	5.8	6161
15	362.9257	6.0	6419
16	399.3072	7.1	7649
17	405.2603	10.2	10877
18	411.0931	6.0	6402
19	443.3336	7.5	7994
20	449.2868	12.0	12843
21	469.3274	6.3	6781
22	485.1122	15.9	17052
23	486.1127	7.0	7508
24	487.3594	5.8	6165
25	536.1643	6.1	6528
26	541.1199	13.0	13956
27	542.1204	7.3	7815
28	559.1308	29.0	31079
29	560.1313	14.4	15383
30	561.1287	11.2	12026
31	610.1836	51.0	54617
32	611.1840	29.7	31823
33	612.1822	20.3	21737
34	613.1817	8.6	9177
35	633.1495	29.6	31662
36	634.1502	18.1	19384
37	635.1474	13.6	14526
38	684.2019	28.1	30032
39	685.2032	18.2	19468
40	685.4347	24.9	26612
41	686.2007	14.2	15248
42	686.4378	11.4	12230
43	687.2004	6.1	6534
44	707.1681	27.6	29586
45	708.1691	18.3	19601
46	709.1666	14.1	15123
47	710.1661	6.8	7229
48	758.2208	21.1	22612
49	759.2218	14.9	15914
50	760.2199	12.3	13132
51	761.2189	6.2	6672
52	781.1871	21.0	22519
53	782.1878	14.9	15988
54	783.1845	12.9	13818
55	784.1842	6.6	7030
56	832.2392	18.2	19437
57	833.2407	15.4	16534
58	834.2385	12.4	13307
59	835.2386	6.9	7377
60	855.2061	14.6	15655
61	856.2064	11.7	12533
62	857.2044	9.7	10339

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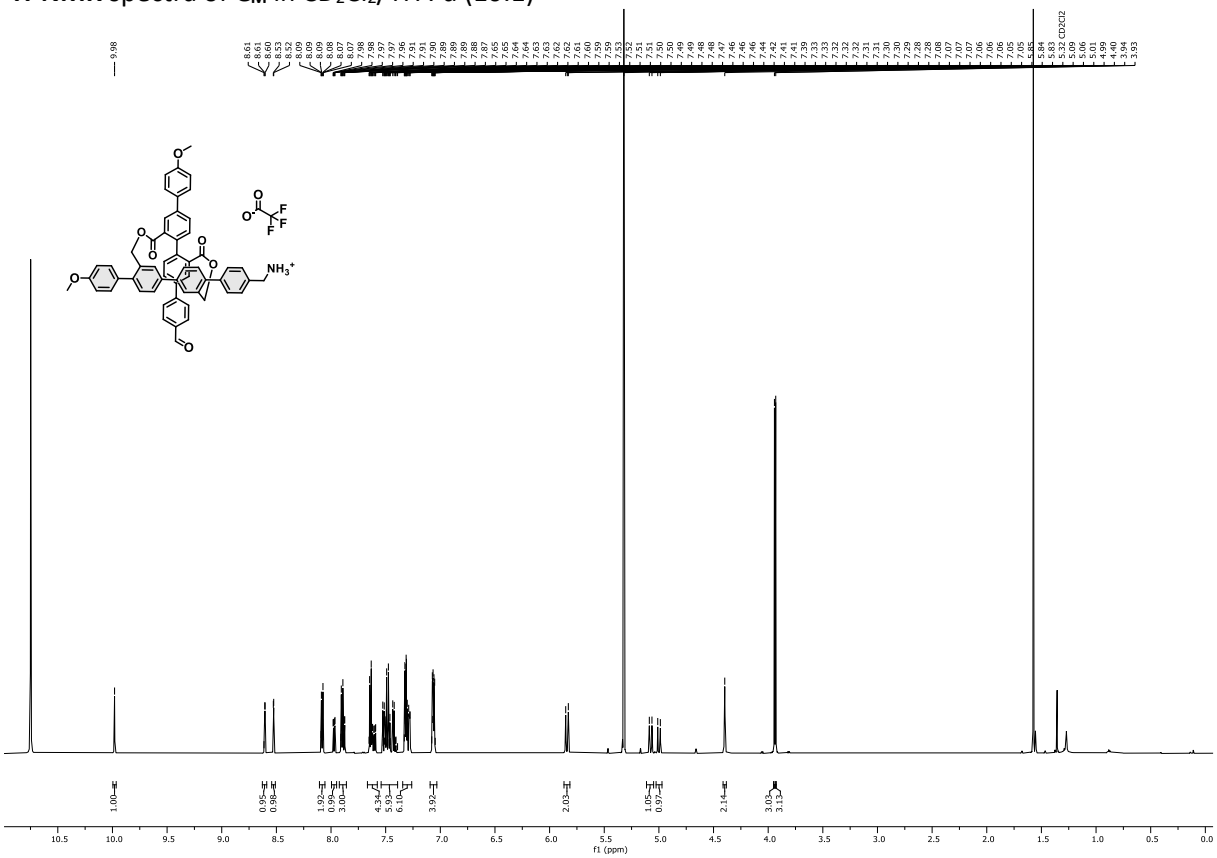
#	m/z	I %	I
63	858.2025	5.9	6362
64	906.2586	16.4	17526
65	907.2592	14.1	15099
66	908.2577	13.2	14109
67	909.2571	8.2	8768
68	929.2245	10.2	10880
69	930.2257	8.3	8908
70	931.2234	7.8	8330
71	964.3455	100.0	107022
72	965.3483	65.2	69813
73	966.3514	23.4	25046
74	967.3542	6.4	6817
75	980.2771	14.7	15785
76	981.2782	14.0	14980
77	982.2766	13.9	14872
78	983.2766	7.9	8434
79	1003.2435	6.7	7176
80	1004.2446	6.4	6884
81	1005.2418	6.1	6491
82	1032.3324	40.6	43455
83	1033.3356	28.3	30248
84	1034.3394	10.5	11248
85	1054.2968	11.6	12432
86	1055.2967	13.0	13938
87	1056.2955	12.2	13061
88	1057.2958	7.9	8402
89	1100.3200	13.3	14243
90	1101.3235	10.2	10921
91	1128.3147	9.5	10155
92	1129.3164	10.1	10860
93	1130.3149	10.1	10770
94	1131.3151	6.9	7433
95	1168.3077	10.3	11003
96	1169.3111	6.8	7329
97	1202.3350	6.8	7241
98	1203.3357	7.2	7682
99	1204.3336	8.5	9087
100	1205.3330	5.8	6198

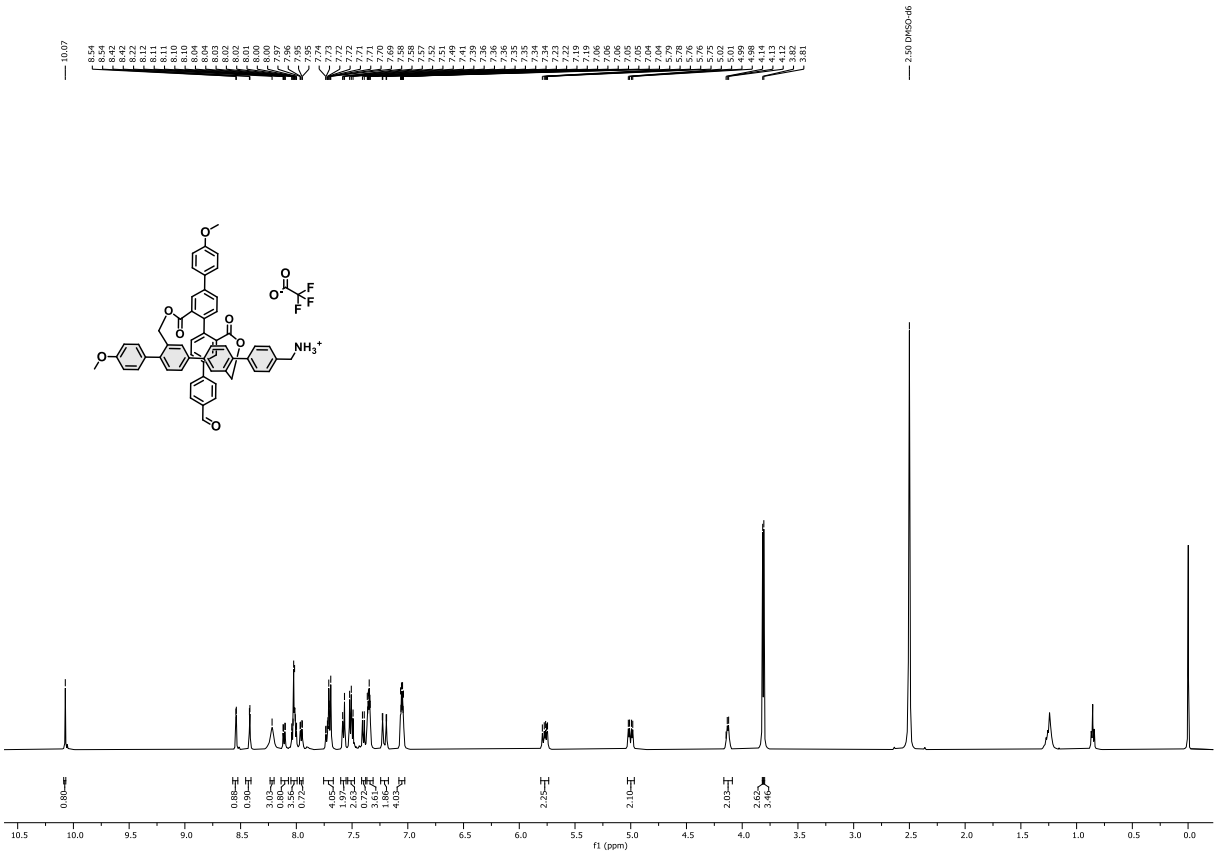
Acquisition Parameter

General	Fore Vacuum	3.09e+000 mBar	High Vacuum	1.34e-007 mBar	Source Type	ESI
	Scan Begin	75 m/z	Scan End	2000 m/z	Ion Polarity	Positive
Source	Set Nebulizer	2.0 Bar	Set Capillary	4500 V	Set Dry Gas	8.0 l/min
	Set Dry Heater	200 °C	Set End Plate Offset	-500 V		
Quadrupole	Set Ion Energy (MS only)	4.0 eV				
Coll. Cell	Collision Energy	8.0 eV	Set Collision Cell RF	600.0 Vpp	100.0 Vpp	
Ion Cooler	Set Ion Cooler Transfer Time	75.0 µs	Set Ion Cooler Pre Pulse Storage Time	10.0 µs		

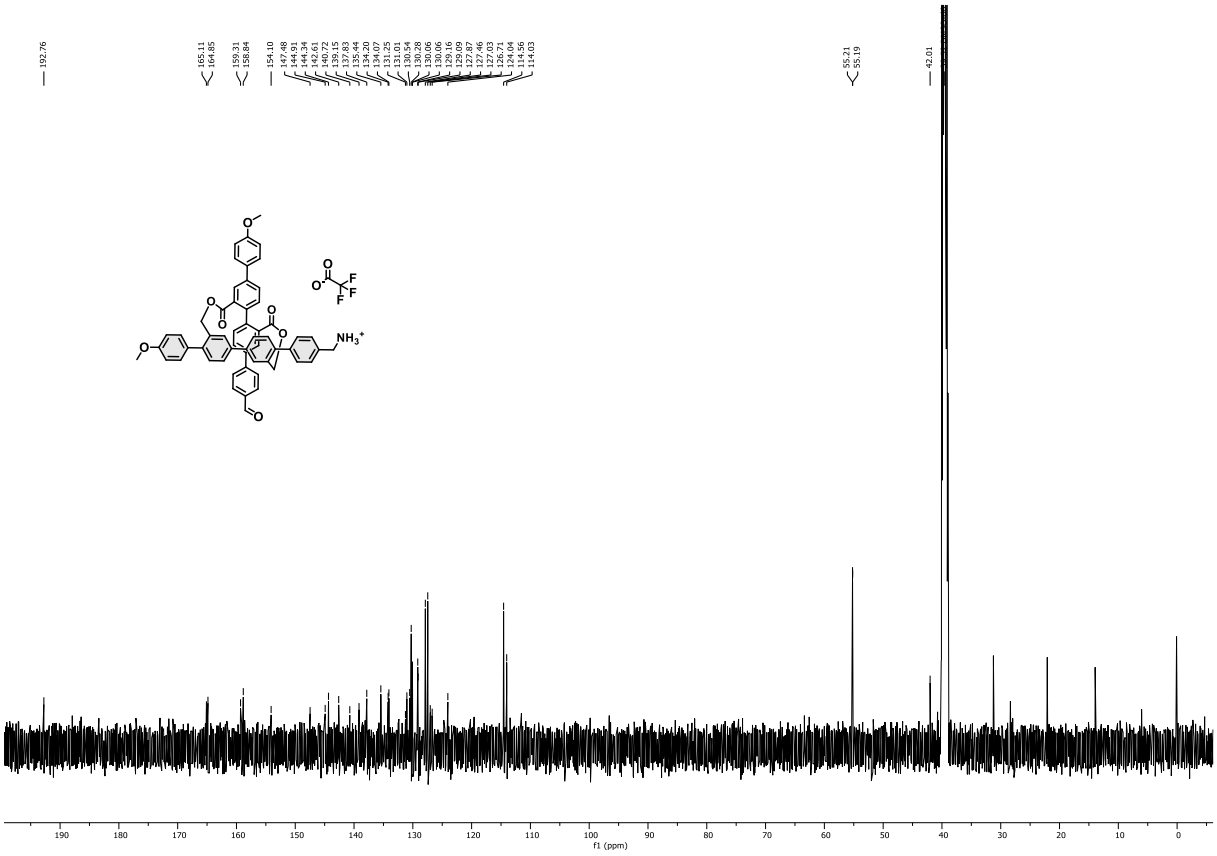
^{1}H-NMR spectra of **C_M** in CD_2Cl_2/TFA-d (10:1)



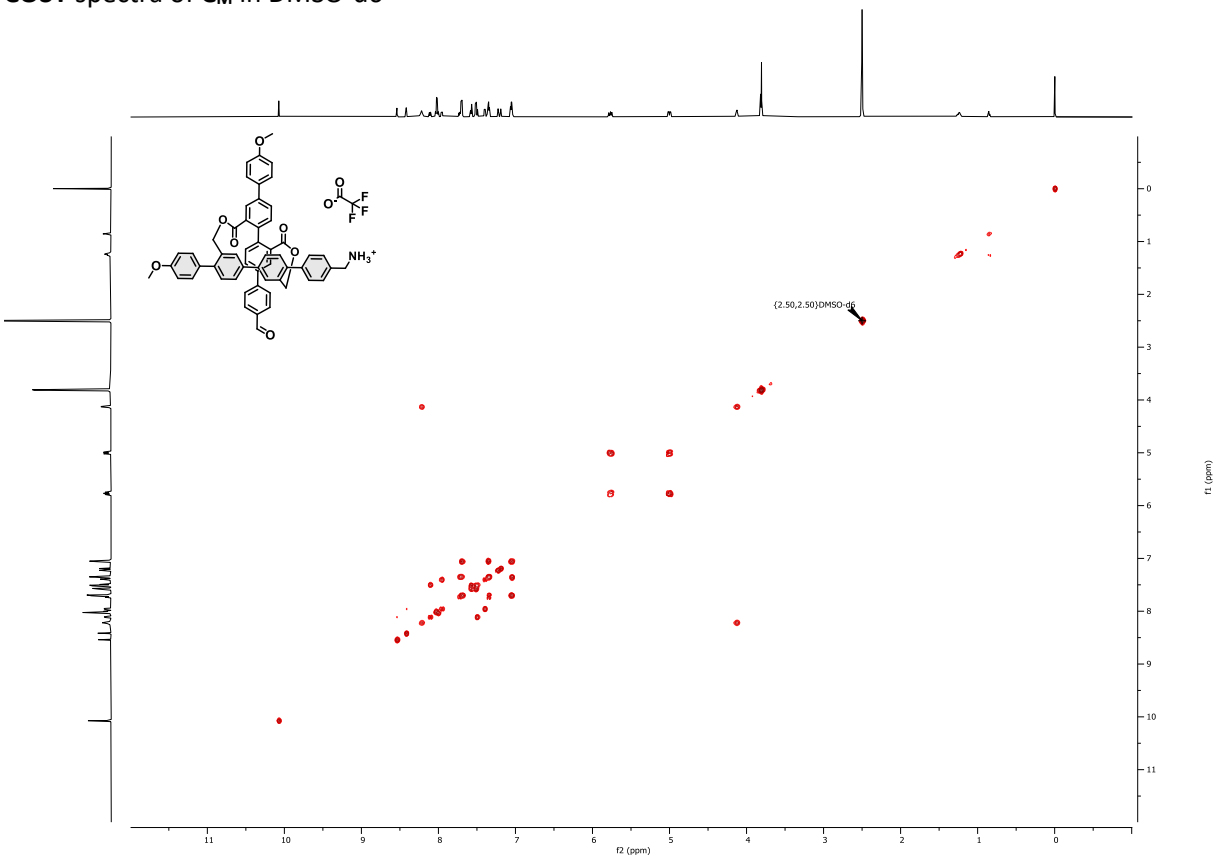
^{1}H-NMR spectra of **C_M** in DMSO-d6



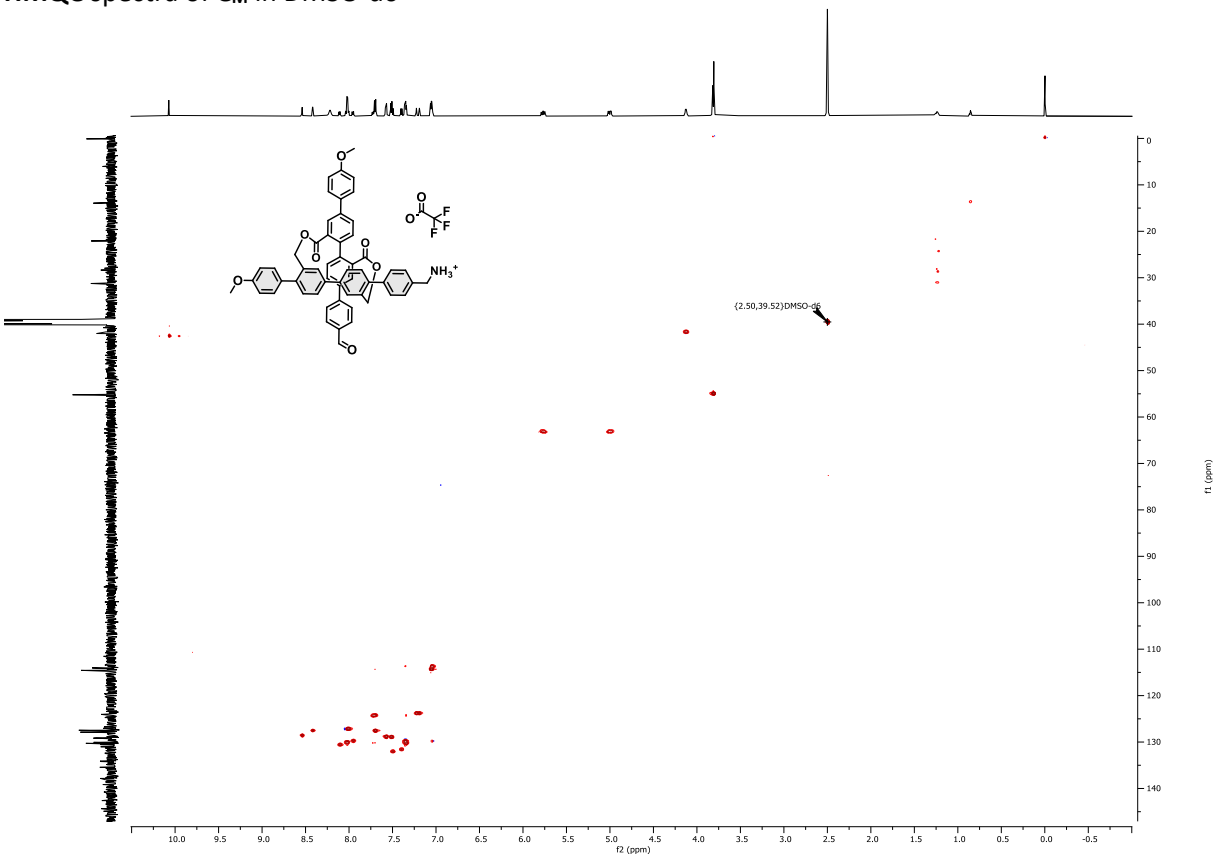
^{13}C-NMR spectra of **C_M** in DMSO-d6



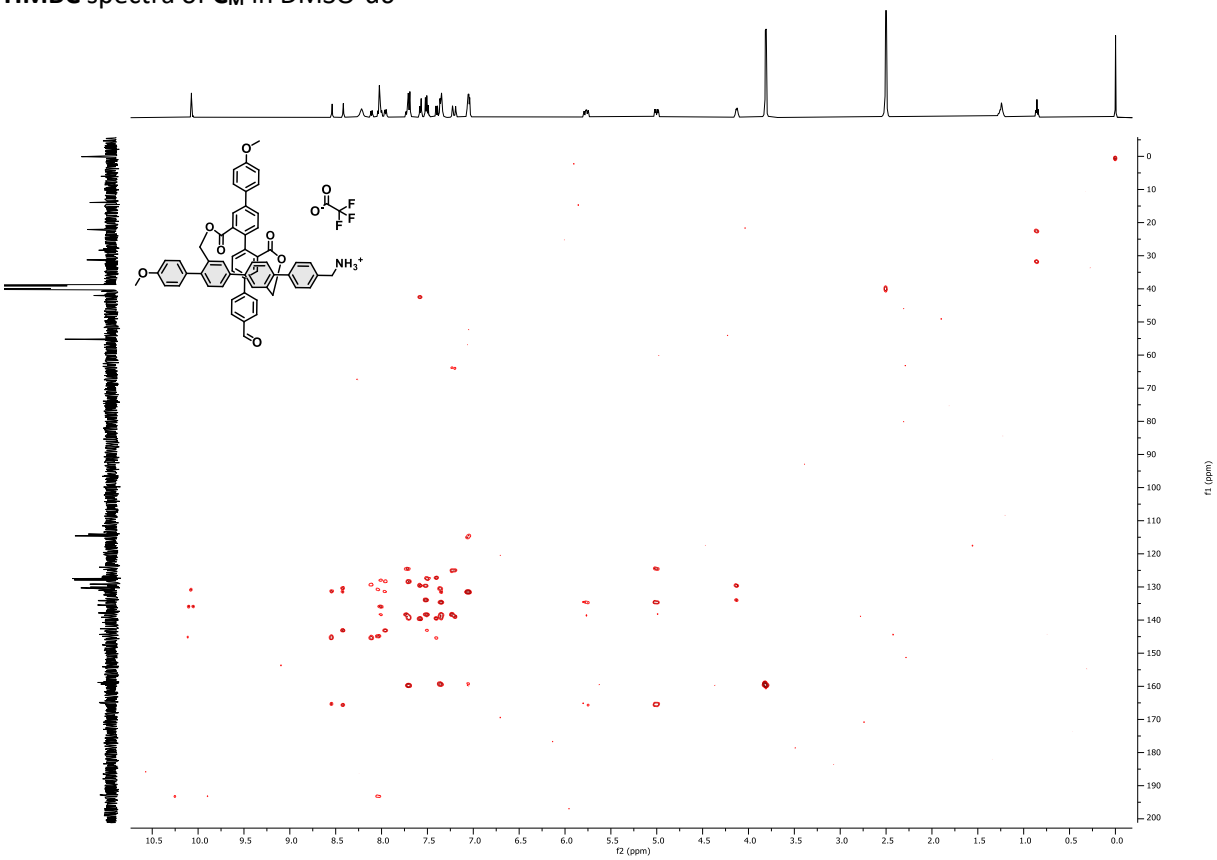
COSY spectra of **C_M** in DMSO-d6



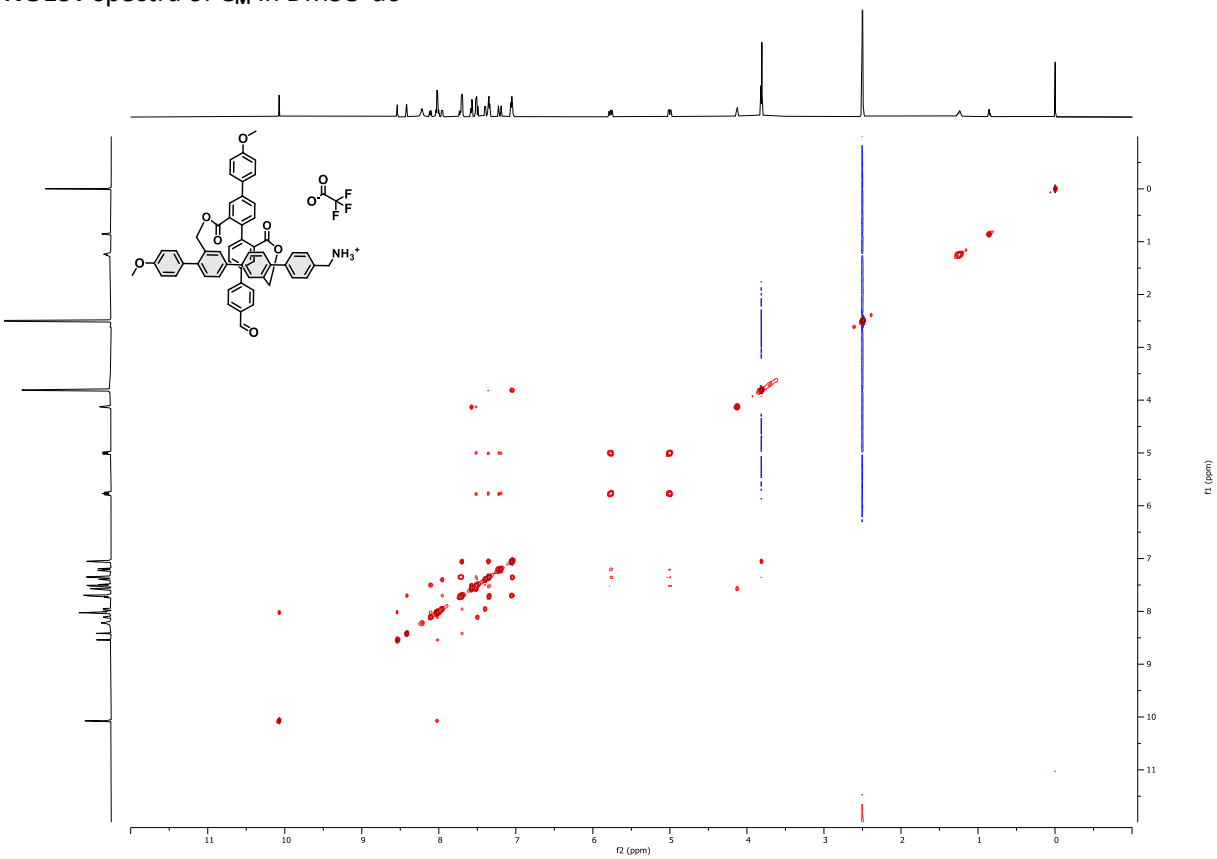
HMQC spectra of **C_M** in DMSO-d6



HMBC spectra of **C_M** in DMSO-d6



NOESY spectra of $\mathbf{C_M}$ in DMSO-d6



HR-ESI-MS spectra of **C_M**

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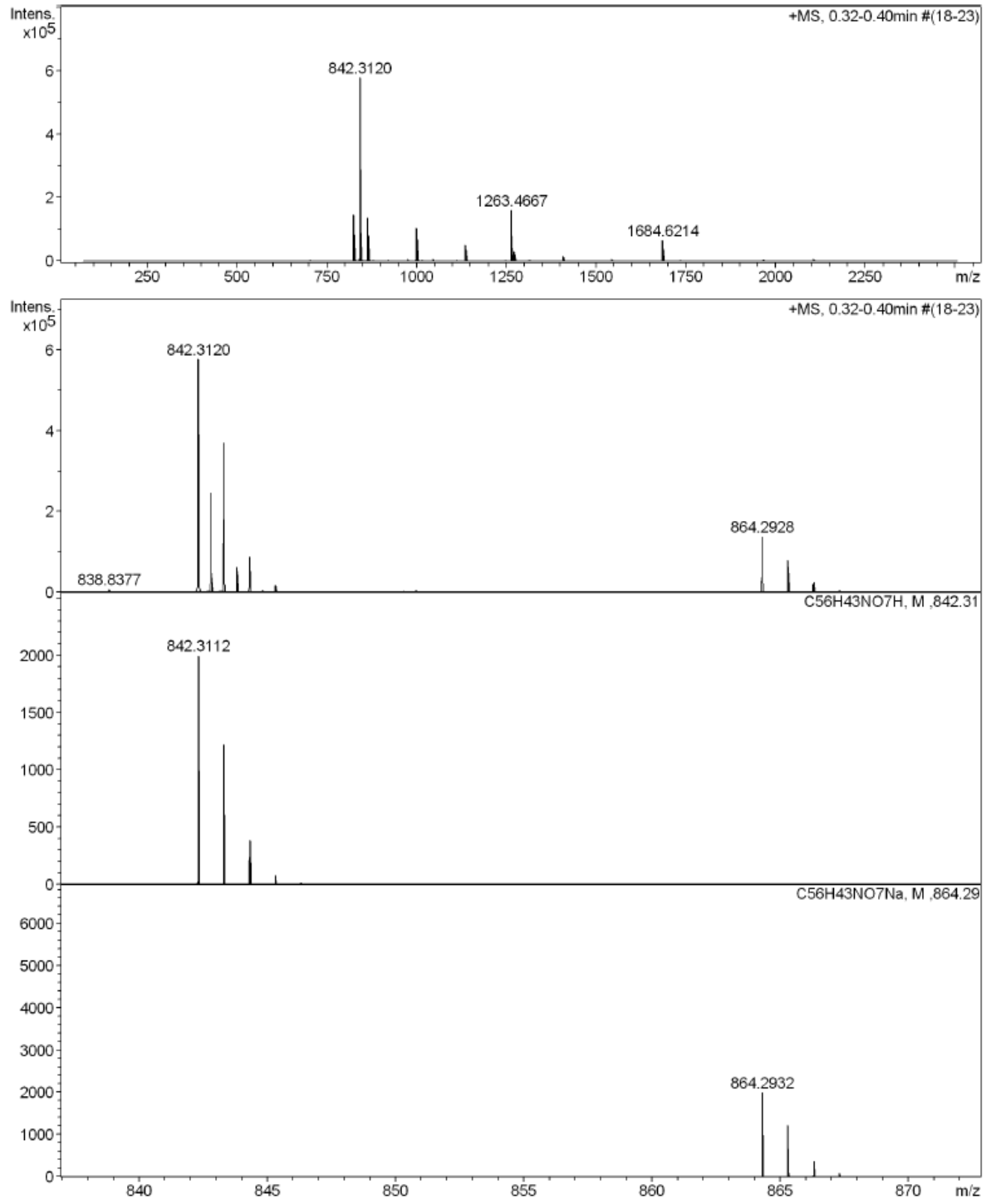
Sample Name **KRO382**
Comment

Instrument maXis 4G
Method ms_nocolumn_high_pos_use_acn.m



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Measured m/z vs. theoretical m/z

Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e¯ Conf	z
842.3120	1	C 56 H 44 N O 7	100.00	842.3112	-0.7	-0.9	25.4	35.5	even	1+
864.2928	1	C 56 H 43 N Na O 7	100.00	864.2932	0.3	0.4	15.3	35.5	even	

Mass list

#	m/z	I %	I
1	702.8630	0.5	2754
2	707.1672	0.3	1965
3	825.2845	25.1	144763
4	826.2875	14.3	82742
5	827.2906	4.6	26355
6	828.2935	1.1	6533
7	838.8377	1.3	7601
8	842.3120	100.0	577364
9	842.6740	0.3	1993
10	842.8135	43.0	248013
11	843.1496	0.4	2125
12	843.1635	0.4	2155
13	843.2073	0.4	2255
14	843.3151	64.3	371024
15	843.8162	11.0	63766
16	844.3174	15.4	88831
17	844.8181	1.1	6256
18	845.3199	2.8	16223
19	846.3234	0.5	3167
20	850.3088	0.7	3863
21	850.8102	0.7	4323
22	851.3122	0.5	3149
23	858.3055	0.5	2892
24	864.2928	24.0	138314
25	865.2959	13.9	80481
26	866.2987	4.5	26127
27	867.3018	1.1	6380
28	880.2686	0.6	3418
29	881.2748	0.3	2009
30	920.3567	0.4	2462
31	974.8130	1.0	5770
32	996.3891	0.5	2605
33	997.3914	0.4	2167
34	1000.2680	18.3	105900
35	1001.2710	11.9	68476
36	1002.2736	4.0	22979
37	1003.2757	0.9	5368
38	1016.2437	0.4	2491
39	1046.4432	1.1	6185
40	1047.4454	0.7	4178
41	1096.4976	0.4	2029
42	1110.7875	0.7	4074
43	1136.2425	9.1	52707
44	1137.2456	6.2	36077
45	1138.2490	2.2	12904
46	1139.2525	0.6	3254
47	1204.2304	0.4	2126
48	1246.7626	0.4	2516
49	1262.9644	14.1	81614
50	1263.4667	27.6	159571
51	1263.9684	25.2	145521
52	1264.4696	16.1	92686
53	1264.9709	7.3	42390
54	1265.4719	2.9	16733
55	1265.9739	1.1	6416
56	1270.9598	0.5	3031
57	1271.4631	0.8	4397
58	1271.9642	0.7	3840
59	1272.2176	5.5	31745
60	1272.4653	0.4	2562
61	1273.2211	3.6	21068

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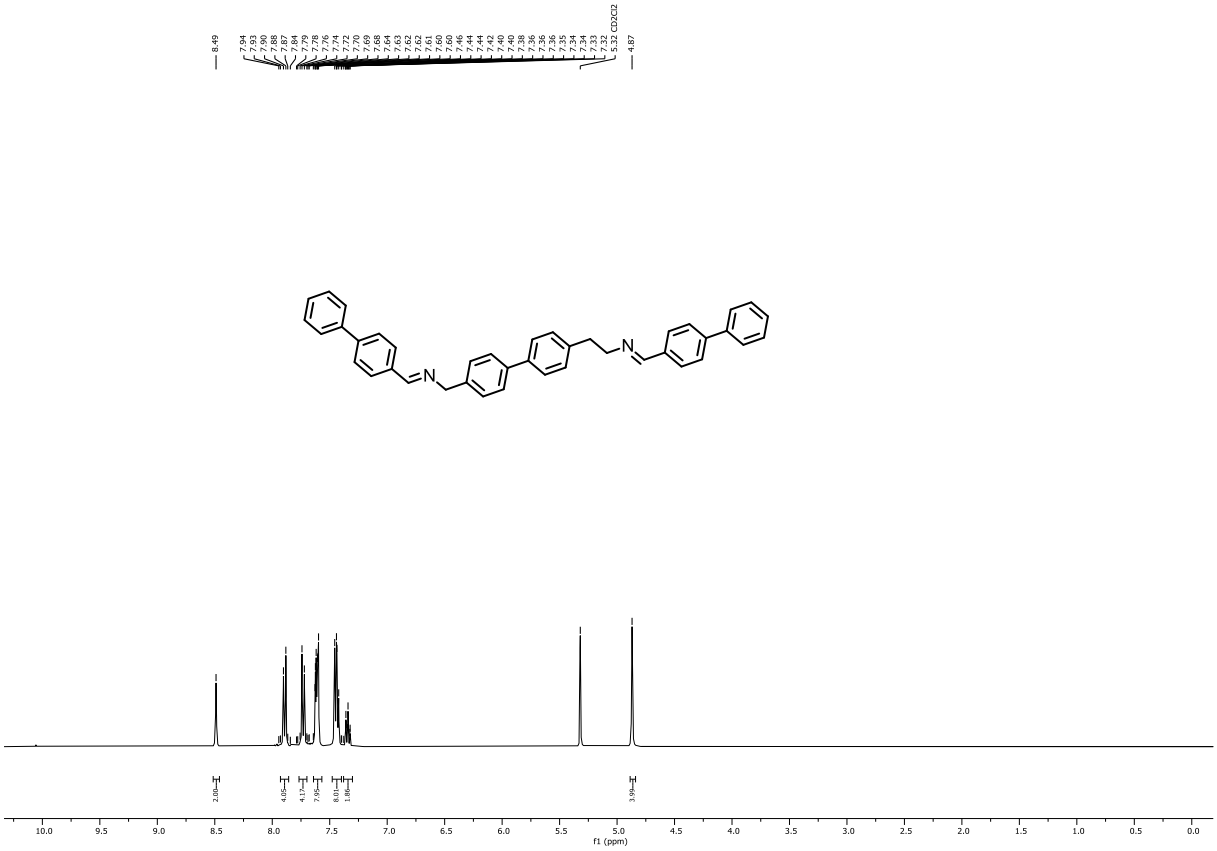
#	m/z	I %	I
62	1274.2243	1.5	8577
63	1275.2265	0.4	2422
64	1312.9933	0.4	2260
65	1313.4945	0.7	4158
66	1313.9960	0.7	4261
67	1314.4975	0.5	2858
68	1408.1921	2.8	16377
69	1409.1953	2.1	12180
70	1410.1980	0.8	4869
71	1544.1669	1.0	5949
72	1545.1698	0.7	4273
73	1683.6161	4.4	25125
74	1683.9522	0.4	2566
75	1684.1192	7.1	41034
76	1684.2865	0.6	3634
77	1684.6214	11.3	65126
78	1684.9560	0.8	4346
79	1685.1230	7.3	42182
80	1685.2902	0.6	3623
81	1685.6246	6.1	35312
82	1686.1252	2.4	13869
83	1686.6261	1.5	8925
84	1687.1264	0.4	2424
85	1687.6283	0.3	1931
86	1692.6163	0.4	2049
87	1706.6011	0.4	2256
88	1734.1459	0.3	1934
89	1734.6479	0.4	2436
90	1735.1497	0.4	2188
91	1964.7217	0.5	2719
92	1965.0566	0.6	3717
93	1965.3906	0.7	3848
94	1965.7240	0.6	3344
95	1966.0601	0.4	2391
96	2104.7698	0.5	2779
97	2105.2736	0.8	4568
98	2105.7754	0.9	5380
99	2106.2752	0.7	3813
100	2106.7790	0.4	2467

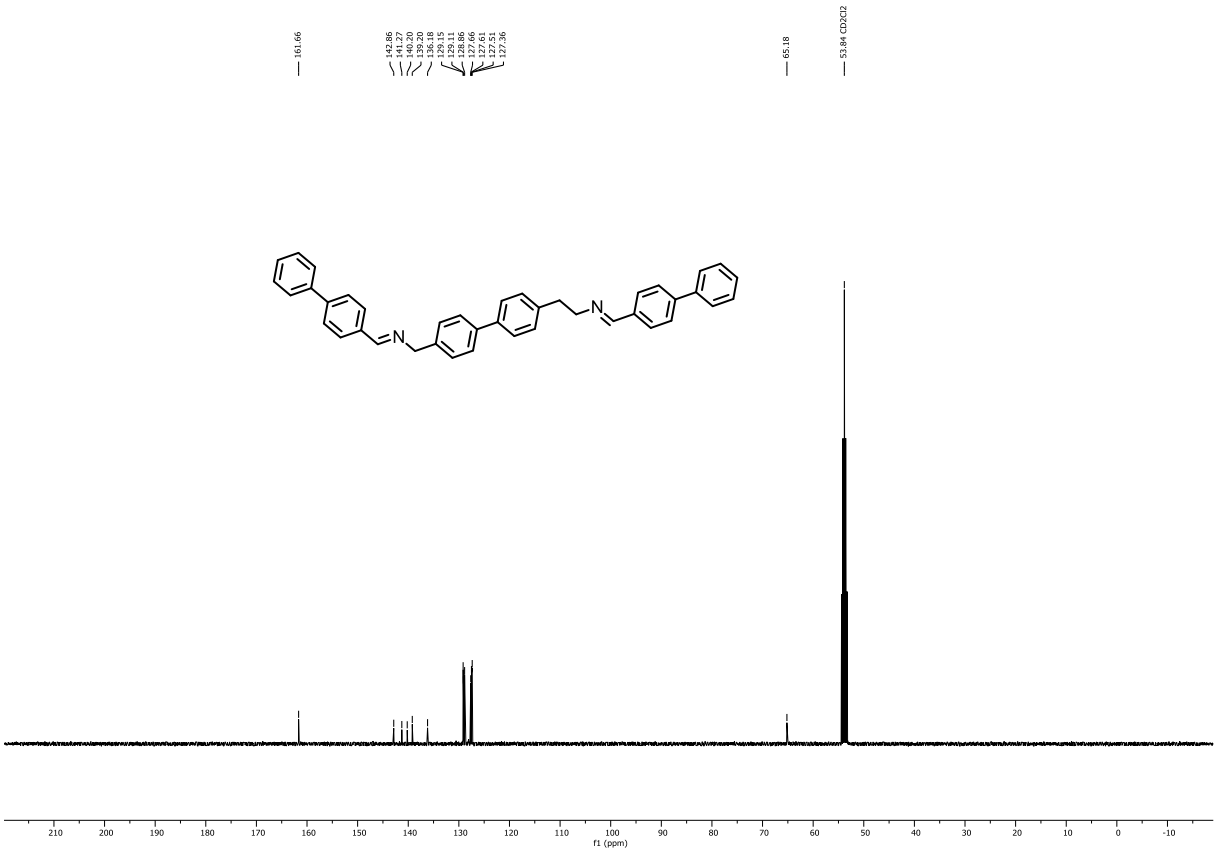
Acquisition Parameter

General	Fore Vacuum	3.08e+000 mBar	High Vacuum	1.05e-007 mBar	Source Type	ESI
	Scan Begin	75 m/z	Scan End	2500 m/z	Ion Polarity	Positive
Source	Set Nebulizer	2.0 Bar	Set Capillary	4500 V	Set Dry Gas	8.0 l/min
	Set Dry Heater	200 °C	Set End Plate Offset	-500 V		
Quadrupole	Set Ion Energy (MS only)	4.0 eV				
Coll. Cell	Collision Energy	12.0 eV	Set Collision Cell RF	2000.0 Vpp	800.0 Vpp	
Ion Cooler	Set Ion Cooler Transfer Time	120.0 µs	Set Ion Cooler Pre Pulse Storage Time	18.0 µs		

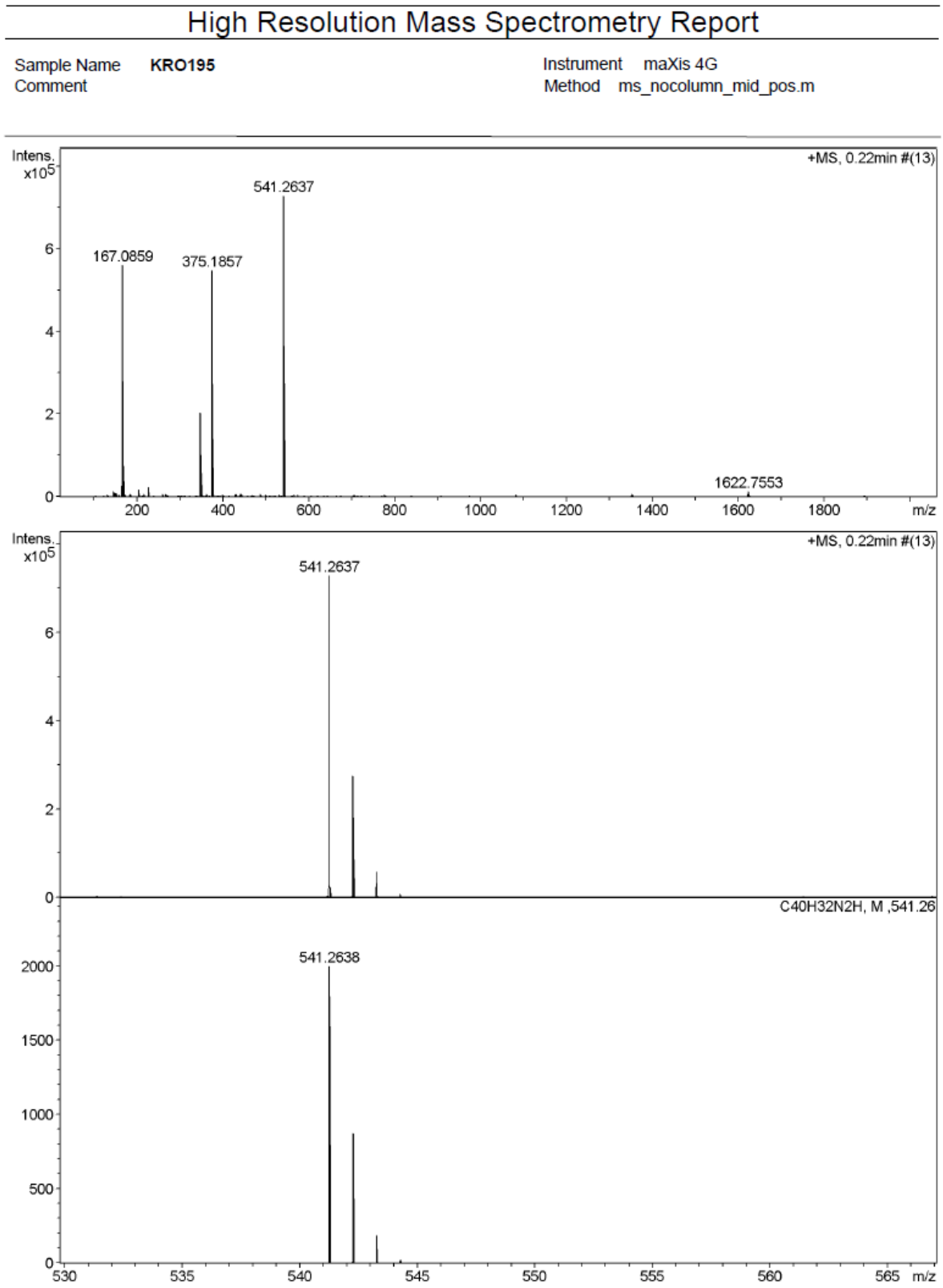
^{1}H-NMR spectra of **I** in **CD_2Cl_2**



^{13}C-NMR spectra of **I** in **CD_2Cl_2**



HR-ESI-MS spectra of **I**



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Measured m/z vs. theoretical m/z

Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e¯ Conf	z
541.2637	1	C 40 H 33 N 2	100.00	541.2638	0.2	0.3	33.5	25.5	even	1+

Mass list

#	m/z	I %	I
1	103.9553	0.3	2432
2	121.9662	0.3	2298
3	131.9621	0.8	5808
4	133.9603	0.4	3076
5	144.9821	1.8	13201
6	146.9804	0.9	6497
7	147.9312	1.3	9824
8	149.9306	1.2	8955
9	152.0620	1.1	8217
10	158.9640	0.6	4059
11	165.0698	3.6	26336
12	166.0758	0.9	6273
13	167.0859	76.9	560662
14	168.0889	10.4	75474
15	169.0924	0.8	5538
16	173.0784	0.7	5294
17	183.0781	0.4	2598
18	184.1114	0.6	4071
19	185.1146	0.9	6314
20	205.0597	2.5	17887
21	215.1248	0.5	3405
22	217.1047	0.9	6615
23	226.9510	3.3	24296
24	260.2001	1.1	7773
25	261.1303	0.4	2580
26	265.9620	0.9	6556
27	271.1147	0.3	2382
28	271.1355	0.8	5888
29	273.1663	0.3	2236
30	294.9383	0.4	2880
31	302.9818	0.5	3385
32	337.2348	0.4	2926
33	341.2650	0.3	2306
34	348.1744	28.1	204766
35	349.1774	8.2	59684
36	350.1802	1.0	7466
37	350.2659	2.6	19290
38	351.2693	0.6	4326
39	355.2810	0.5	3404
40	362.9256	1.0	7563
41	369.2975	0.3	2508
42	375.1857	75.1	547173
43	376.1703	11.8	86337
44	376.1877	19.4	141024
45	377.1732	3.7	26702
46	377.1895	2.8	20487
47	378.1760	0.6	4264
48	385.2922	0.5	3608
49	394.2554	0.4	2582
50	399.3069	0.7	5405
51	413.3230	0.5	3428
52	429.3178	0.6	4100
53	430.9130	1.0	7557
54	441.2962	0.8	5992
55	443.3331	1.0	7116
56	457.3488	0.5	3600
57	467.3158	0.5	3595
58	469.9236	0.4	2652
59	473.3434	0.5	3776
60	487.3592	0.9	6292
61	498.9003	0.6	4541
62	501.3745	0.5	3632

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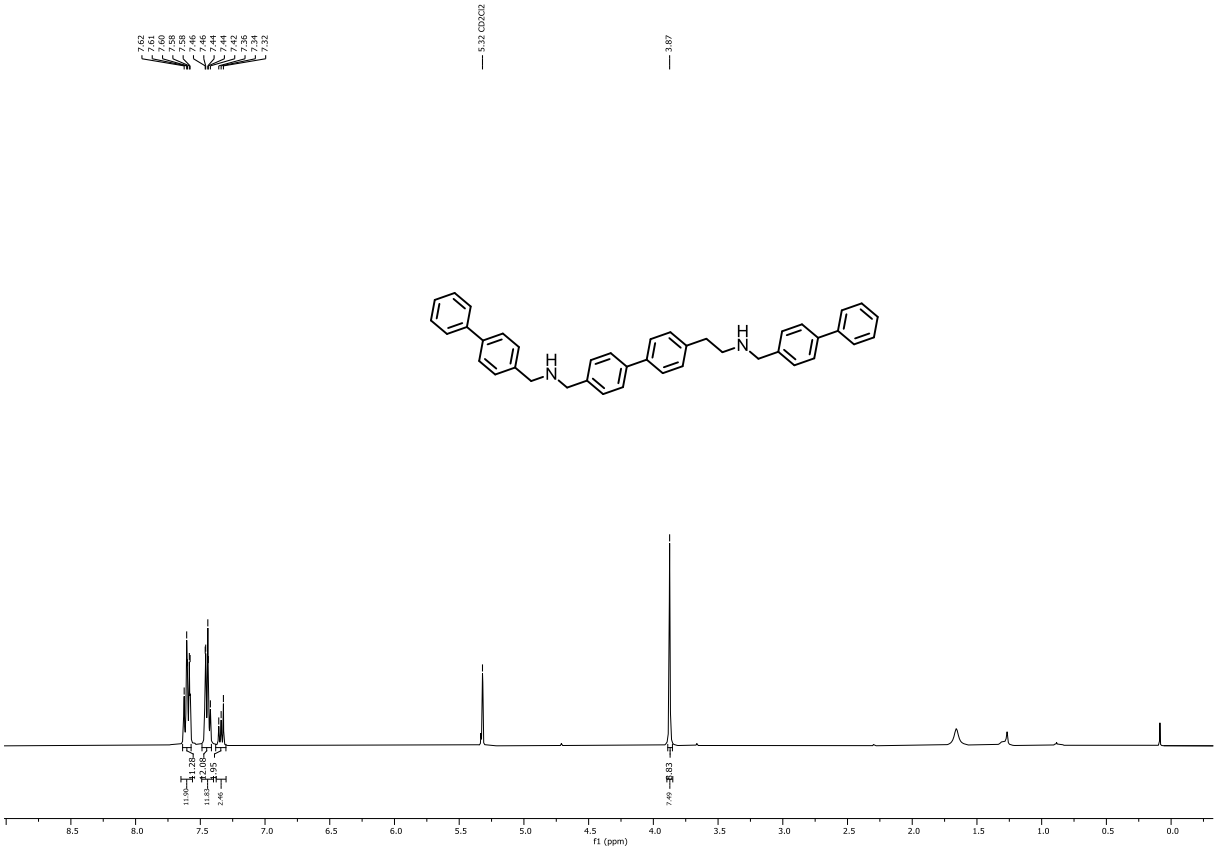
#	m/z	I %	I
63	506.9442	0.4	2984
64	517.3712	0.4	3250
65	523.3227	0.3	2302
66	531.3861	0.7	4796
67	541.2637	100.0	728684
68	542.2666	37.9	275902
69	543.2693	8.1	58802
70	544.2725	1.1	7832
71	545.4017	0.4	2697
72	566.8876	0.6	4244
73	575.4111	0.6	4014
74	619.4368	0.3	2441
75	634.8753	0.5	3634
76	702.8617	0.5	3658
77	705.5793	0.6	4070
78	721.5755	0.4	2634
79	770.8493	0.3	2463
80	776.2606	0.6	4724
81	777.2617	0.5	3362
82	778.2578	0.3	2391
83	838.8346	0.3	2456
84	1081.5133	0.5	3911
85	1082.5146	0.4	3206
86	1351.6315	0.5	3321
87	1352.1370	0.9	6817
88	1352.6357	0.9	6830
89	1353.1362	0.8	5836
90	1353.6404	0.4	3233
91	1621.7534	0.6	4624
92	1622.2550	1.0	7513
93	1622.7553	1.8	13108
94	1623.2581	1.2	8452
95	1623.7594	1.1	8017
96	1624.2633	0.5	3549
97	1624.7618	0.3	2232
98	1892.8765	0.4	2908
99	1893.3703	0.3	2311
100	1893.8781	0.3	2190

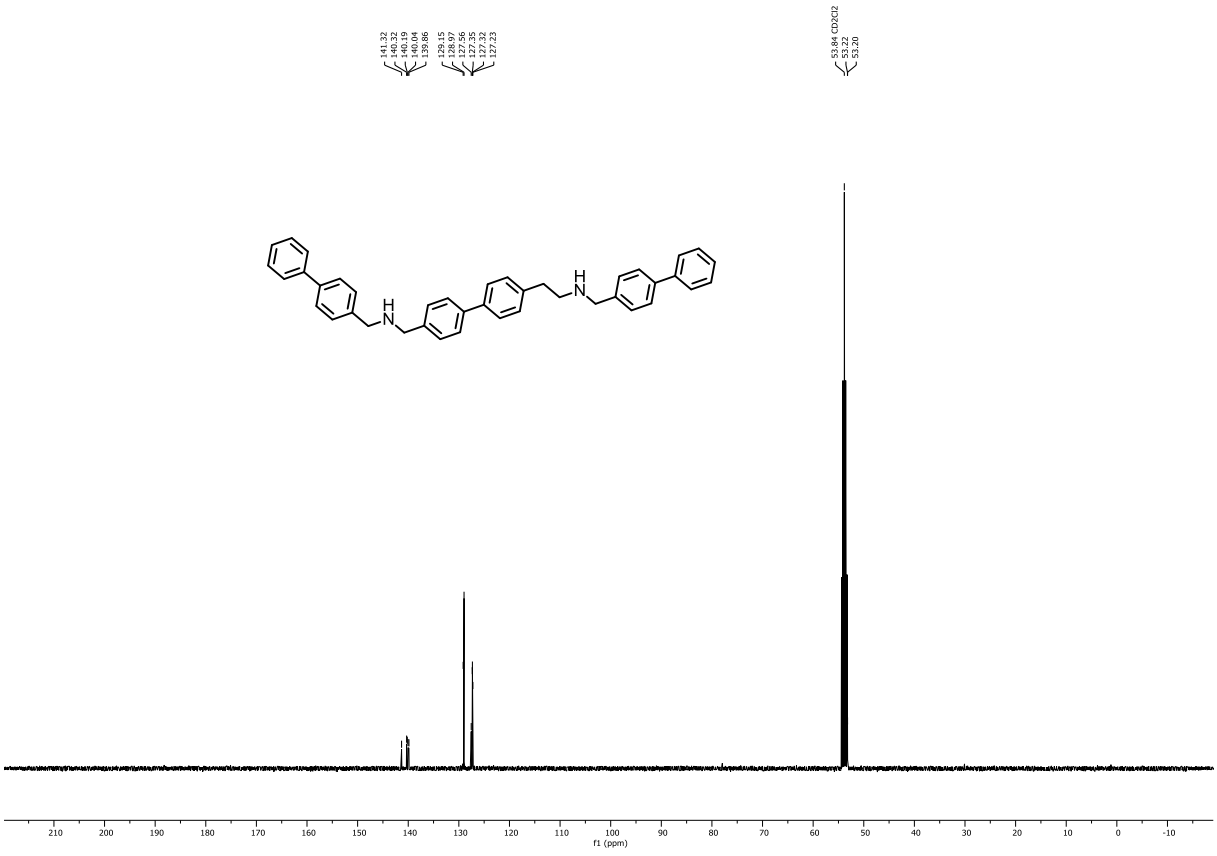
Acquisition Parameter

General	Fore Vacuum	3.46e+000 mBar	High Vacuum	1.14e-007 mBar	Source Type	ESI
	Scan Begin	75 m/z	Scan End	2000 m/z	Ion Polarity	Positive
Source	Set Nebulizer	2.0 Bar	Set Capillary	4500 V	Set Dry Gas	8.0 l/min
	Set Dry Heater	200 °C	Set End Plate Offset	-500 V		
Quadrupole	Set Ion Energy (MS only)	4.0 eV				
Coll. Cell	Collision Energy	8.0 eV	Set Collision Cell RF	600.0 Vpp	100.0 Vpp	
Ion Cooler	Set Ion Cooler Transfer Time	75.0 µs	Set Ion Cooler Pre Pulse Storage Time		10.0 µs	

^{1}H-NMR spectra of **A** in **CD_2Cl_2**



^{13}C-NMR spectra of **A** in **CD_2Cl_2**

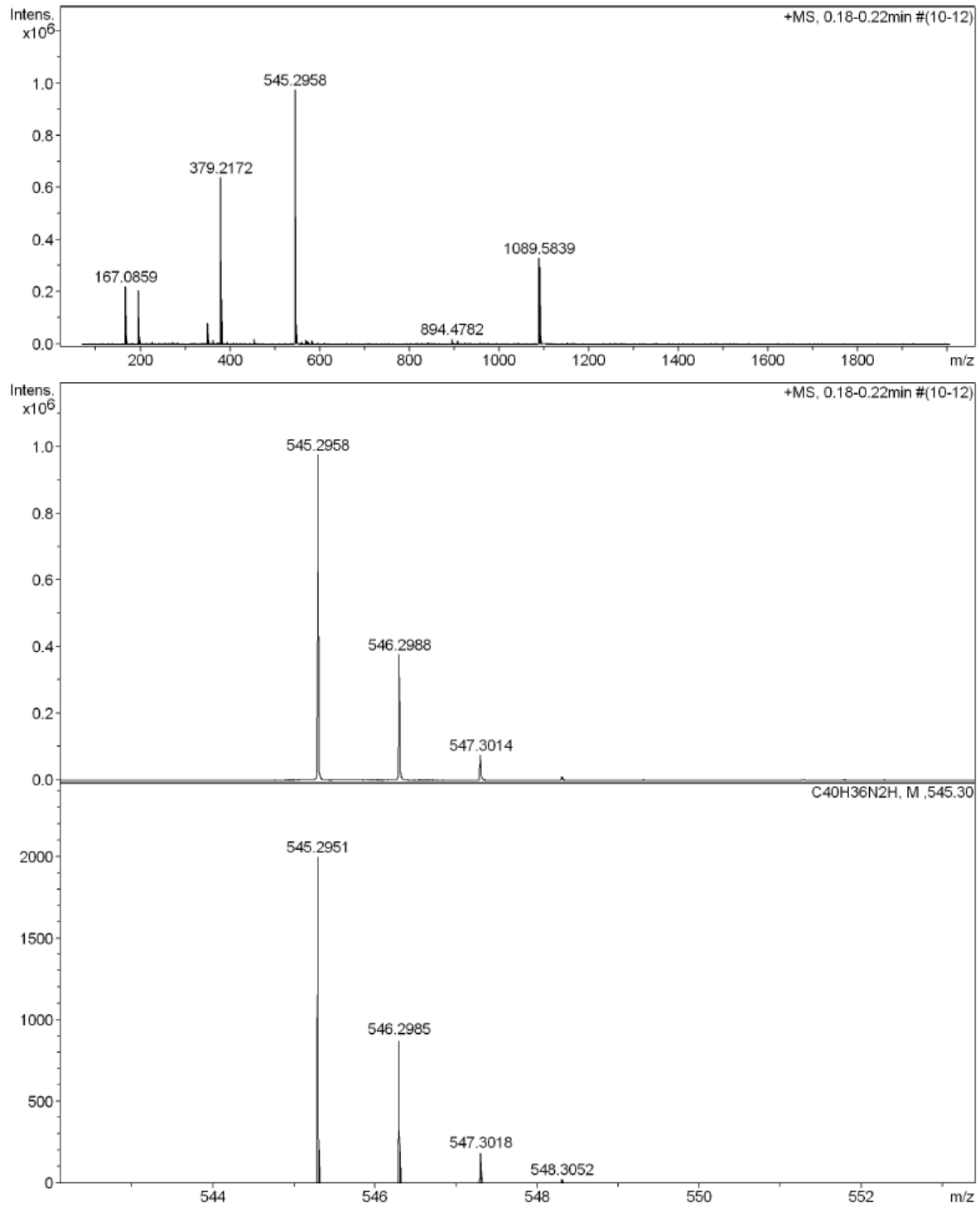


HR-ESI-MS spectra of **A**

High Resolution Mass Spectrometry Report

Sample Name **KRO505**
Comment

Instrument maXis 4G
Method ms_nocolumn_75-1000_pos.m



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Measured m/z vs. theoretical m/z

Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e¯ Conf	z
545.2958	1	C 40 H 37 N 2	100.00	545.2951	-0.6	-1.1	30.9	23.5	even	1+
567.2764	1	C 40 H 36 N 2 Na	100.00	567.2771	0.6	1.1	27.3	23.5	even	
583.2501	1	C 40 H 36 K N 2	100.00	583.2510	0.9	1.6	22.8	23.5	even	
1089.5839	1	C 80 H 73 N 4	100.00	1089.5830	-0.9	-0.8	11.3	46.5	even	

Mass list

#	m/z	I %	I
1	167.0859	22.6	221116
2	168.0890	3.4	32889
3	169.0928	0.3	2674
4	196.1123	21.0	205563
5	197.0963	0.3	3233
6	197.1154	3.2	31118
7	198.1184	0.3	2762
8	226.9513	0.9	8596
9	273.1512	0.9	8567
10	273.6530	0.5	4468
11	280.2633	0.2	2399
12	282.2790	0.7	6425
13	296.2578	0.3	2467
14	304.2610	0.2	2341
15	333.1637	0.3	2563
16	350.1902	8.3	80647
17	351.1931	2.1	20468
18	352.1965	0.3	3131
19	362.1901	1.7	16522
20	362.9261	0.3	2495
21	363.1929	0.5	5151
22	370.7035	0.4	4235
23	371.2046	0.3	2969
24	375.1850	0.6	6191
25	378.1848	1.9	18119
26	379.1886	0.7	7279
27	379.2172	65.5	639690
28	380.2013	4.1	39883
29	380.2199	17.7	172528
30	381.2047	1.3	12402
31	381.2226	2.4	23412
32	382.2259	0.3	2557
33	393.1955	0.8	7962
34	393.2320	0.4	3991
35	394.1797	0.7	6612
36	395.1827	0.3	2518
37	395.2097	0.2	2259
38	407.2475	0.5	4436
39	430.9130	0.3	2656
40	453.7426	2.1	20256
41	454.2441	1.7	16752
42	454.7457	0.6	5669
43	536.1649	0.3	2971
44	545.2958	100.0	976961
45	546.2988	38.6	376663
46	547.3014	7.7	75589
47	548.3046	1.1	10562
48	559.3103	0.9	8584
49	560.3139	0.3	3385
50	561.2894	0.3	2566
51	567.2764	1.5	15120
52	568.2798	0.6	5943
53	573.2531	1.1	11152
54	573.2876	0.3	2864
55	573.3258	0.7	7033
56	574.2562	0.5	5230
57	574.3230	0.9	8422
58	575.2659	0.3	3129
59	575.3245	0.4	4064

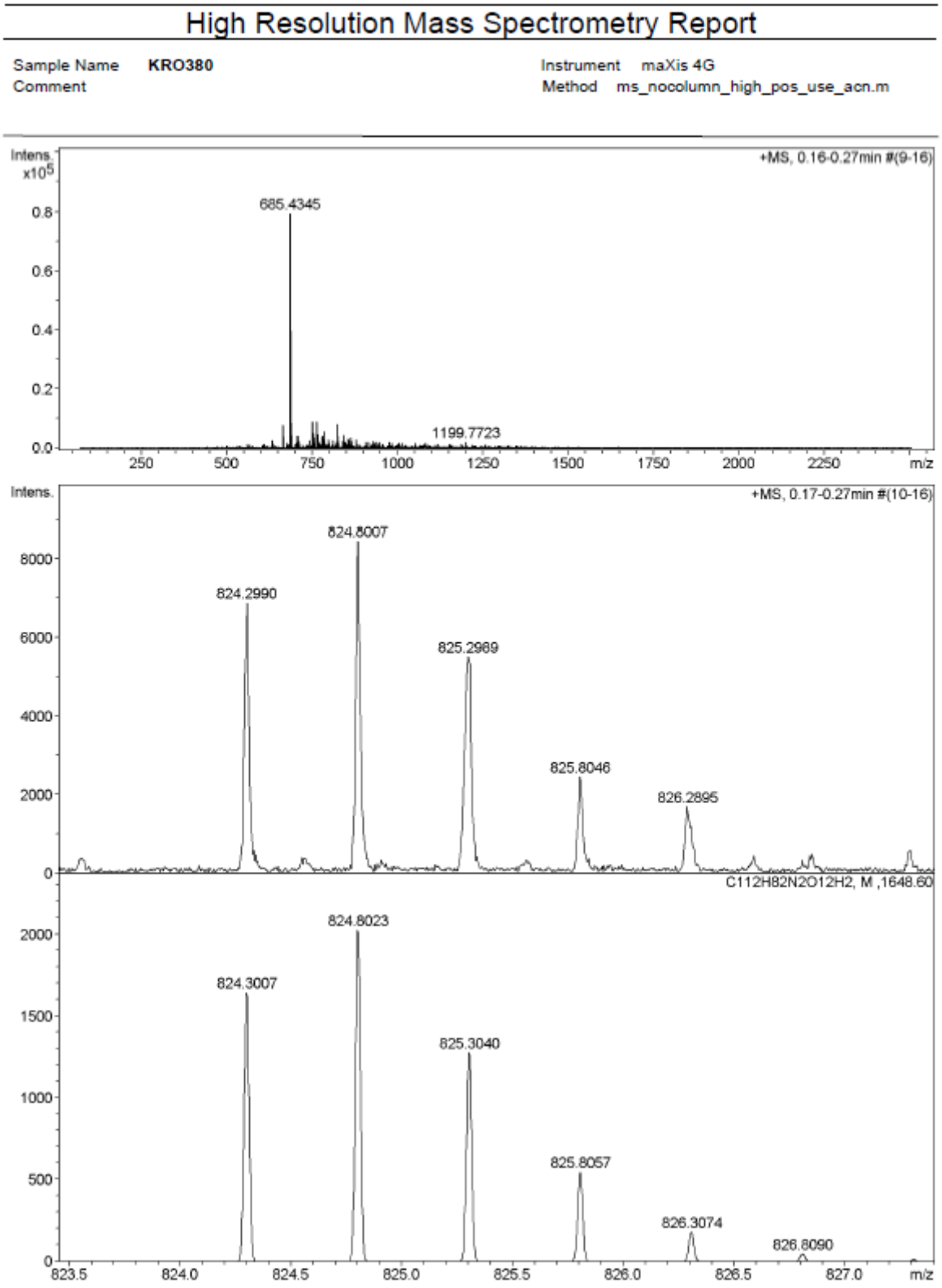
High Resolution Mass Spectrometry Report

#	m/z	I %	I
60	583.2501	1.2	12030
61	584.2535	0.6	5405
62	595.2349	0.4	3679
63	610.1830	0.4	3789
64	611.1835	0.2	2416
65	635.2640	0.3	2906
66	684.2021	0.2	2312
67	711.3719	0.4	4038
68	712.3746	0.3	2567
69	740.3987	0.3	2484
70	823.3806	0.2	2132
71	823.4453	0.2	2096
72	826.5665	0.3	3259
73	840.5446	0.5	4403
74	841.5484	0.3	2883
75	842.5591	0.4	3868
76	843.5641	0.2	2393
77	894.4782	2.2	21249
78	895.4807	1.6	15603
79	896.4845	0.6	5984
80	906.4775	1.3	12859
81	907.4810	0.9	8811
82	908.4829	0.3	3344
83	924.4869	0.4	3788
84	925.4907	0.3	2661
85	937.4832	0.2	2315
86	963.6022	0.2	2249
87	991.6332	0.2	2191
88	1089.5839	34.0	331709
89	1090.5872	30.1	294445
90	1091.5902	12.4	120801
91	1092.5926	3.5	33982
92	1093.5956	0.8	7708
93	1117.5393	0.2	2286
94	1118.5442	0.2	2356
95	1139.5229	0.2	2345
96	1140.5269	0.2	2146
97	1151.5046	0.7	6875
98	1152.5073	0.6	5672
99	1153.5063	0.5	5231
100	1154.5076	0.3	3306

Acquisition Parameter

General	Fore Vacuum	2.39e+000 mBar	High Vacuum	1.28e-007 mBar	Source Type	ESI
	Scan Begin	75 m/z	Scan End	2000 m/z	Ion Polarity	Positive
Source	Set Nebulizer	2.0 Bar	Set Capillary	4500 V	Set Dry Gas	8.0 l/min
	Set Dry Heater	200 °C	Set End Plate Offset	-500 V		
Quadrupole	Set Ion Energy (MS only)	4.0 eV				
Coll. Cell	Collision Energy	8.0 eV	Set Collision Cell RF	500.0 Vpp	100.0 Vpp	
Ion Cooler	Set Ion Cooler Transfer Time	75.0 µs	Set Ion Cooler Pre Pulse Storage Time	10.0 µs		

HR-ESI-MS spectra of $\mathbf{O}_{\mathbf{M\text{-}I\text{-}dimer}}$



High Resolution Mass Spectrometry Report

Measured m/z vs. theoretical m/z

Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	z
824.2990	1	C 112 H 84 N 2 O 12	100.00	824.3007	1.7	2.0	39.4	72.0	even	2+

Mass list

#	m/z	I %	I
1	559.1310	1.9	1551
2	610.1839	1.6	1300
3	633.1490	3.1	2516
4	634.1500	2.1	1661
5	635.1478	1.6	1289
6	663.4525	9.9	8006
7	664.4555	5.2	4218
8	665.4576	1.7	1332
9	673.8863	1.9	1560
10	680.4781	1.7	1402
11	685.4345	100.0	80641
12	686.4377	47.5	38318
13	687.4407	11.0	8859
14	688.4429	2.0	1587
15	701.4085	1.8	1435
16	702.8631	1.9	1546
17	707.1672	5.5	4470
18	708.1681	3.5	2842
19	708.5102	2.2	1736
20	709.1657	3.2	2603
21	709.3798	5.3	4266
22	710.1656	1.6	1310
23	710.3817	2.6	2077
24	711.3787	2.8	2246
25	712.8967	1.9	1494
26	741.8743	3.1	2487
27	750.4052	11.4	9178
28	751.4089	6.0	4821
29	752.4051	6.2	4982
30	753.3546	4.3	3431
31	753.4117	3.5	2839
32	754.3582	2.1	1716
33	755.3546	4.4	3563
34	756.3580	1.9	1544
35	764.5723	12.0	9655
36	765.5757	6.2	4967
37	766.5800	1.7	1407
38	770.8509	1.9	1533
39	776.2304	1.7	1386
40	778.5520	5.0	3993
41	779.5545	2.6	2120
42	780.8849	2.0	1598
43	781.1864	5.1	4138
44	782.1874	3.5	2810
45	783.1861	3.2	2559
46	784.1848	2.0	1576
47	784.5406	6.7	5383
48	785.5430	4.7	3763
49	786.5392	2.0	1626
50	792.6039	2.0	1591
51	798.5569	3.5	2799
52	799.5597	2.1	1677
53	809.8612	3.0	2457
54	821.4082	2.7	2187
55	824.2990	8.5	6884
56	824.8007	10.5	8457
57	825.2989	6.8	5520
58	825.8046	3.0	2457
59	826.2895	2.1	1700
60	838.8373	2.9	2338
61	842.3096	6.0	4858
62	843.3139	4.2	3360

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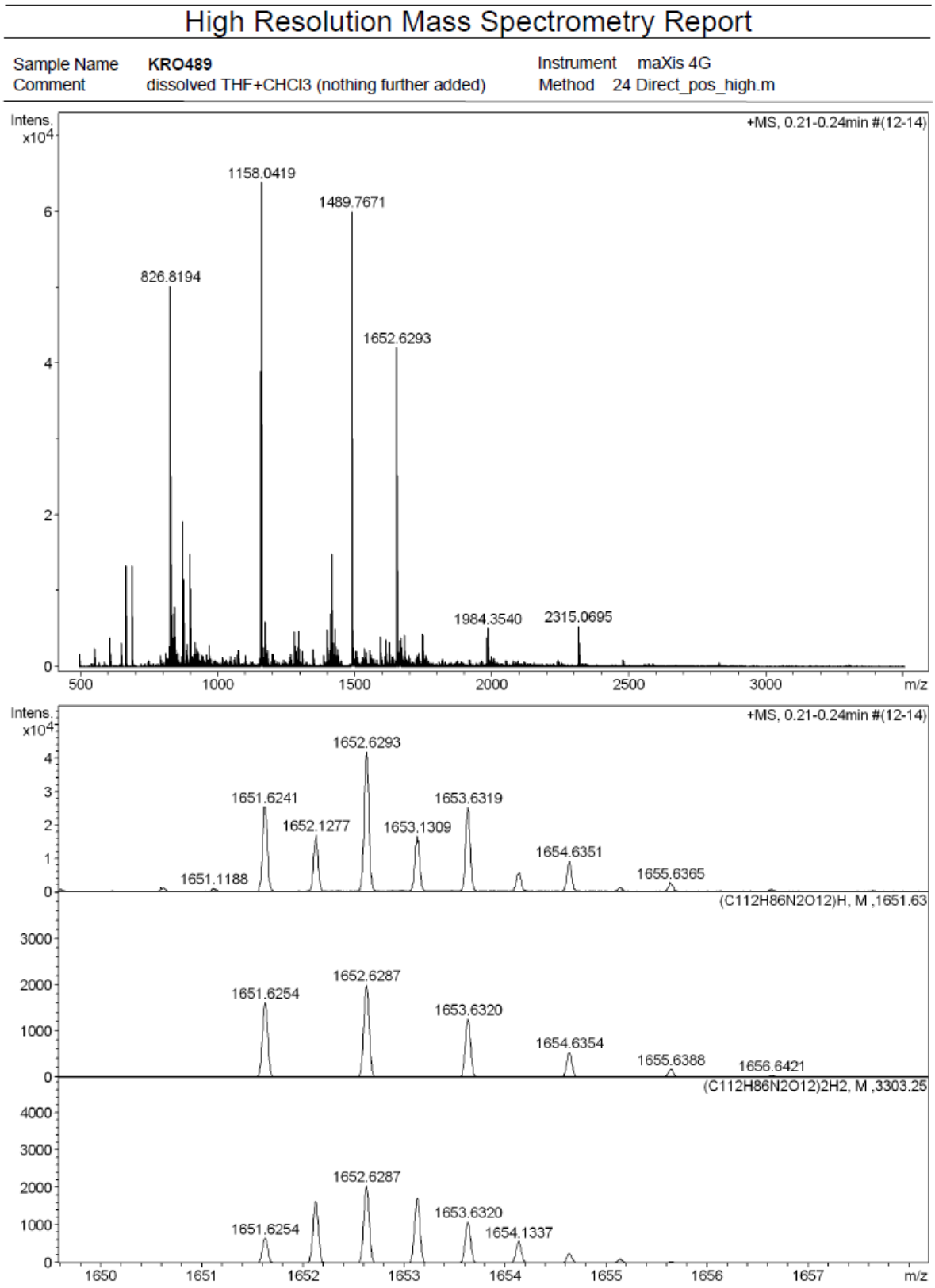
#	m/z	I %	I
63	848.8722	2.2	1814
64	850.2495	1.6	1294
65	855.2059	4.0	3237
66	856.2067	3.1	2525
67	857.2053	3.1	2532
68	858.2026	1.6	1305
69	864.2919	4.8	3860
70	865.2963	3.2	2584
71	877.8488	3.6	2935
72	906.8249	1.8	1464
73	907.7711	2.7	2153
74	908.7745	1.7	1337
75	916.8610	2.3	1849
76	929.2239	2.7	2205
77	930.2252	2.6	2079
78	931.2244	2.6	2130
79	932.2234	1.6	1319
80	932.2779	2.9	2374
81	933.2823	1.7	1399
82	939.5949	2.3	1858
83	940.5986	1.8	1440
84	945.8362	2.4	1920
85	957.3831	1.8	1429
86	974.8134	1.6	1293
87	975.7587	2.4	1963
88	976.7620	1.6	1260
89	984.8466	2.0	1593
90	1000.2700	1.7	1408
91	1003.2440	2.0	1633
92	1004.2454	2.3	1831
93	1005.2417	2.0	1632
94	1013.8228	1.9	1522
95	1052.8351	1.8	1484
96	1077.2612	1.6	1252
97	1078.2648	1.6	1253
98	1081.8121	1.9	1493
99	1199.7723	2.7	2155
100	1200.7780	2.0	1620

Acquisition Parameter

General	Fore Vacuum	3.07e+000 mBar	High Vacuum	9.18e-008 mBar	Source Type	ESI
	Scan Begin	75 m/z	Scan End	2500 m/z	Ion Polarity	Positive
Source	Set Nebulizer	2.0 Bar	Set Capillary	4500 V	Set Dry Gas	8.0 l/min
	Set Dry Heater	200 °C	Set End Plate Offset	-500 V		
Quadrupole	Set Ion Energy (MS only)	4.0 eV				
Coll. Cell	Collision Energy	12.0 eV	Set Collision Cell RF	2000.0 Vpp	800.0 Vpp	
Ion Cooler	Set Ion Cooler Transfer Time	120.0 µs	Set Ion Cooler Pre Pulse Storage Time	18.0 µs		

HR-ESI-MS spectra of $\mathbf{O}_{\text{M-A-dimer}}$



High Resolution Mass Spectrometry Report

Measured m/z vs. theoretical m/z

Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e¯ Conf	z
1651.6241	1	C 112 H 87 N 2 O 12	100.00	1651.6254	1.3	0.8	88.2	70.5	even	1+

Mass list

#	m/z	I %	I
1	607.3971	6.0	3814
2	647.4630	4.9	3098
3	663.4573	20.9	13369
4	664.4605	9.4	6017
5	685.4387	20.9	13328
6	686.4417	9.3	5963
7	825.2862	28.8	18419
8	826.3160	67.7	43242
9	826.8194	78.7	50229
10	827.3185	57.9	36976
11	827.8223	21.3	13606
12	828.3156	10.3	6586
13	835.3230	5.2	3350
14	835.8253	5.9	3797
15	840.3322	11.0	7056
16	840.8348	12.5	7960
17	841.3356	8.4	5333
18	842.3111	4.6	2933
19	870.3425	20.6	13176
20	871.3462	12.6	8019
21	872.3572	30.0	19159
22	873.3606	18.1	11555
23	874.3633	5.7	3661
24	896.3579	6.0	3806
25	898.3727	23.2	14811
26	899.3757	16.1	10281
27	900.3836	12.6	8035
28	901.3898	5.8	3700
29	916.3809	5.1	3274
30	967.3555	4.5	2878
31	1157.5397	61.1	39000
32	1158.0419	100.0	63862
33	1158.5437	89.6	57217
34	1159.0451	51.4	32843
35	1159.5456	22.5	14400
36	1160.0467	9.8	6243
37	1171.5535	7.0	4465
38	1172.0563	9.4	6000
39	1172.5586	7.9	5033
40	1173.0597	4.6	2944
41	1280.2116	6.5	4169
42	1280.7137	7.3	4645
43	1281.2143	4.4	2830
44	1294.2270	7.1	4518
45	1294.7285	7.4	4720
46	1295.2299	4.5	2850
47	1399.3271	7.5	4804
48	1399.8298	7.5	4760
49	1400.3307	5.4	3424
50	1412.8400	5.2	3305
51	1413.3432	10.9	6975
52	1413.8452	10.2	6521
53	1414.3456	8.6	5498
54	1414.7079	13.0	8318
55	1415.2095	22.7	14480
56	1415.7114	23.2	14819
57	1416.2129	16.6	10574
58	1416.7157	9.0	5777
59	1422.3484	4.9	3146
60	1427.3584	7.5	4781
61	1427.8596	7.8	4955
62	1428.3635	5.0	3223

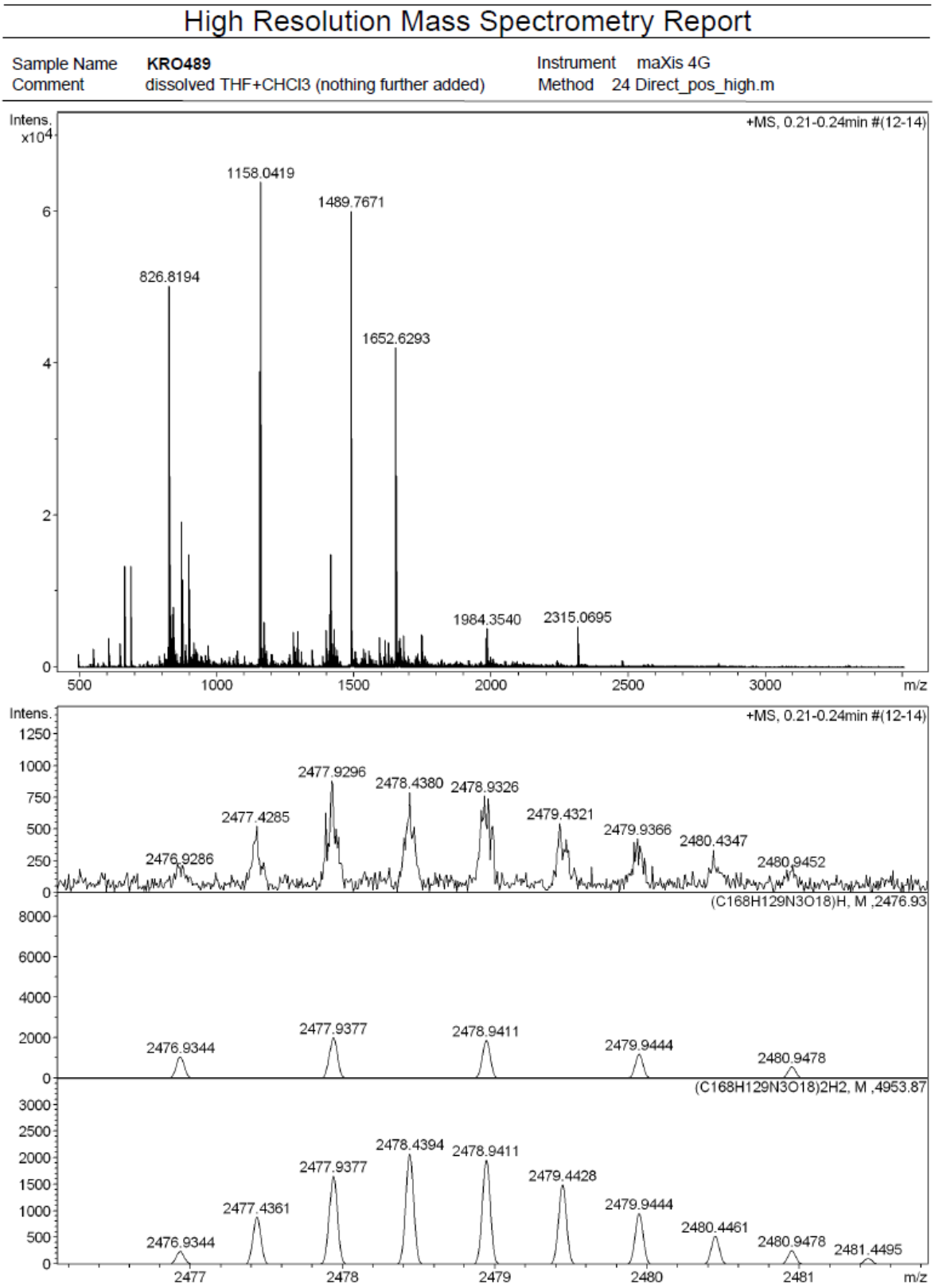
High Resolution Mass Spectrometry Report

#	m/z	I %	I
63	1488.7635	40.9	26126
64	1489.2652	86.5	55251
65	1489.7671	94.0	60049
66	1490.2684	72.5	46277
67	1490.7696	39.7	25380
68	1491.2715	18.6	11905
69	1491.7731	6.8	4319
70	1592.7523	5.2	3300
71	1593.2536	6.2	3991
72	1611.9358	5.6	3585
73	1612.4393	4.4	2832
74	1625.9515	5.1	3265
75	1651.6241	39.9	25502
76	1652.1277	26.9	17173
77	1652.6293	66.0	42118
78	1653.1309	26.1	16683
79	1653.6319	39.6	25299
80	1654.1344	9.1	5832
81	1654.6351	14.6	9355
82	1666.1408	4.9	3155
83	1666.6407	6.0	3823
84	1667.1436	5.5	3505
85	1679.6540	5.3	3409
86	1680.6565	6.5	4120
87	1681.6598	4.5	2848
88	1746.4335	5.7	3614
89	1746.9362	6.8	4352
90	1747.4355	6.6	4216
91	1747.9371	4.7	2993
92	1983.3501	6.0	3861
93	1983.8516	7.3	4663
94	1984.3540	8.0	5119
95	1984.8558	5.9	3783
96	1985.3557	4.4	2825
97	2314.0632	4.8	3080
98	2315.0695	8.4	5382
99	2316.0720	7.4	4714
100	2317.0783	4.4	2798

Acquisition Parameter

General	Fore Vacuum	2.61e+000 mBar	High Vacuum	9.50e-008 mBar	Source Type	ESI
	Scan Begin	500 m/z	Scan End	3500 m/z	Ion Polarity	Positive
Source	Set Nebulizer	0.4 Bar	Set Capillary	3600 V	Set Dry Gas	4.0 l/min
	Set Dry Heater	180 °C	Set End Plate Offset	-500 V		
Quadrupole	Set Ion Energy (MS only)	4.0 eV				
Coll. Cell	Collision Energy	70.0 eV	Set Collision Cell RF	2000.0 Vpp	300.0 Vpp	
Ion Cooler	Set Ion Cooler Transfer Time	142.0 µs	Set Ion Cooler Pre Pulse Storage Time		22.0 µs	

HR-ESI-MS spectra of $\mathbf{O}_{\text{M-A-trimer}}$



High Resolution Mass Spectrometry Report

Measured m/z vs. theoretical m/z

Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	z
1651.6241	1	C 112 H 87 N 2 O 12	100.00	1651.6254	1.3	0.8	88.2	70.5	even	1+

Mass list

#	m/z	I %	I
1	607.3971	6.0	3814
2	647.4630	4.9	3098
3	663.4573	20.9	13369
4	664.4605	9.4	6017
5	685.4387	20.9	13328
6	686.4417	9.3	5963
7	825.2862	28.8	18419
8	826.3160	67.7	43242
9	826.8194	78.7	50229
10	827.3185	57.9	36976
11	827.8223	21.3	13606
12	828.3156	10.3	6586
13	835.3230	5.2	3350
14	835.8253	5.9	3797
15	840.3322	11.0	7056
16	840.8348	12.5	7960
17	841.3356	8.4	5333
18	842.3111	4.6	2933
19	870.3425	20.6	13176
20	871.3462	12.6	8019
21	872.3572	30.0	19159
22	873.3606	18.1	11555
23	874.3633	5.7	3661
24	896.3579	6.0	3806
25	898.3727	23.2	14811
26	899.3757	16.1	10281
27	900.3836	12.6	8035
28	901.3898	5.8	3700
29	916.3809	5.1	3274
30	967.3555	4.5	2878
31	1157.5397	61.1	39000
32	1158.0419	100.0	63862
33	1158.5437	89.6	57217
34	1159.0451	51.4	32843
35	1159.5456	22.5	14400
36	1160.0467	9.8	6243
37	1171.5535	7.0	4465
38	1172.0563	9.4	6000
39	1172.5586	7.9	5033
40	1173.0597	4.6	2944
41	1280.2116	6.5	4169
42	1280.7137	7.3	4645
43	1281.2143	4.4	2830
44	1294.2270	7.1	4518
45	1294.7285	7.4	4720
46	1295.2299	4.5	2850
47	1399.3271	7.5	4804
48	1399.8298	7.5	4760
49	1400.3307	5.4	3424
50	1412.8400	5.2	3305
51	1413.3432	10.9	6975
52	1413.8452	10.2	6521
53	1414.3456	8.6	5498
54	1414.7079	13.0	8318
55	1415.2095	22.7	14480
56	1415.7114	23.2	14819
57	1416.2129	16.6	10574
58	1416.7157	9.0	5777
59	1422.3484	4.9	3146
60	1427.3584	7.5	4781
61	1427.8596	7.8	4955
62	1428.3635	5.0	3223

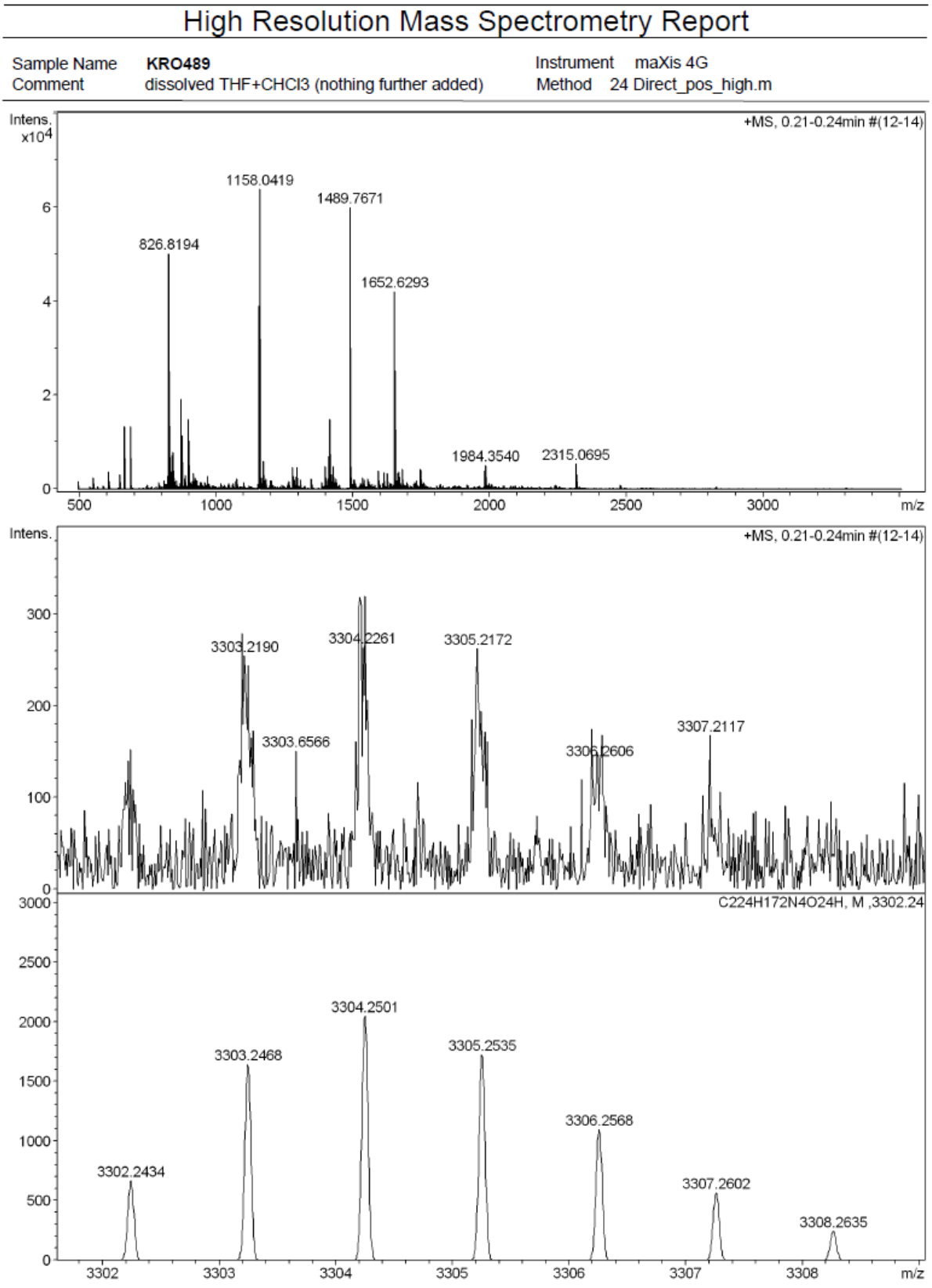
High Resolution Mass Spectrometry Report

#	m/z	I %	I
63	1488.7635	40.9	26126
64	1489.2652	86.5	55251
65	1489.7671	94.0	60049
66	1490.2684	72.5	46277
67	1490.7696	39.7	25380
68	1491.2715	18.6	11905
69	1491.7731	6.8	4319
70	1592.7523	5.2	3300
71	1593.2536	6.2	3991
72	1611.9358	5.6	3585
73	1612.4393	4.4	2832
74	1625.9515	5.1	3265
75	1651.6241	39.9	25502
76	1652.1277	26.9	17173
77	1652.6293	66.0	42118
78	1653.1309	26.1	16683
79	1653.6319	39.6	25299
80	1654.1344	9.1	5832
81	1654.6351	14.6	9355
82	1666.1408	4.9	3155
83	1666.6407	6.0	3823
84	1667.1436	5.5	3505
85	1679.6540	5.3	3409
86	1680.6565	6.5	4120
87	1681.6598	4.5	2848
88	1746.4335	5.7	3614
89	1746.9362	6.8	4352
90	1747.4355	6.6	4216
91	1747.9371	4.7	2993
92	1983.3501	6.0	3861
93	1983.8516	7.3	4663
94	1984.3540	8.0	5119
95	1984.8558	5.9	3783
96	1985.3557	4.4	2825
97	2314.0632	4.8	3080
98	2315.0695	8.4	5382
99	2316.0720	7.4	4714
100	2317.0783	4.4	2798

Acquisition Parameter

General	Fore Vacuum	2.61e+000 mBar	High Vacuum	9.50e-008 mBar	Source Type	ESI
	Scan Begin	500 m/z	Scan End	3500 m/z	Ion Polarity	Positive
Source	Set Nebulizer	0.4 Bar	Set Capillary	3600 V	Set Dry Gas	4.0 l/min
	Set Dry Heater	180 °C	Set End Plate Offset	-500 V		
Quadrupole	Set Ion Energy (MS only)	4.0 eV				
Coll. Cell	Collision Energy	70.0 eV	Set Collision Cell RF	2000.0 Vpp	300.0 Vpp	
Ion Cooler	Set Ion Cooler Transfer Time	142.0 µs	Set Ion Cooler Pre Pulse Storage Time		22.0 µs	

HR-ESI-MS spectra of $\mathbf{O}_{\text{M-A-tetramer}}$



High Resolution Mass Spectrometry Report

Measured m/z vs. theoretical m/z

Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e¯ Conf	z
1651.6241	1	C 112 H 87 N 2 O 12	100.00	1651.6254	1.3	0.8	88.2	70.5	even	1+

Mass list

#	m/z	I %	I
1	607.3971	6.0	3814
2	647.4630	4.9	3098
3	663.4573	20.9	13369
4	664.4605	9.4	6017
5	685.4387	20.9	13328
6	686.4417	9.3	5963
7	825.2862	28.8	18419
8	826.3160	67.7	43242
9	826.8194	78.7	50229
10	827.3185	57.9	36976
11	827.8223	21.3	13606
12	828.3156	10.3	6586
13	835.3230	5.2	3350
14	835.8253	5.9	3797
15	840.3322	11.0	7056
16	840.8348	12.5	7960
17	841.3356	8.4	5333
18	842.3111	4.6	2933
19	870.3425	20.6	13176
20	871.3462	12.6	8019
21	872.3572	30.0	19159
22	873.3606	18.1	11555
23	874.3633	5.7	3661
24	896.3579	6.0	3806
25	898.3727	23.2	14811
26	899.3757	16.1	10281
27	900.3836	12.6	8035
28	901.3898	5.8	3700
29	916.3809	5.1	3274
30	967.3555	4.5	2878
31	1157.5397	61.1	39000
32	1158.0419	100.0	63862
33	1158.5437	89.6	57217
34	1159.0451	51.4	32843
35	1159.5456	22.5	14400
36	1160.0467	9.8	6243
37	1171.5535	7.0	4465
38	1172.0563	9.4	6000
39	1172.5586	7.9	5033
40	1173.0597	4.6	2944
41	1280.2116	6.5	4169
42	1280.7137	7.3	4645
43	1281.2143	4.4	2830
44	1294.2270	7.1	4518
45	1294.7285	7.4	4720
46	1295.2299	4.5	2850
47	1399.3271	7.5	4804
48	1399.8298	7.5	4760
49	1400.3307	5.4	3424
50	1412.8400	5.2	3305
51	1413.3432	10.9	6975
52	1413.8452	10.2	6521
53	1414.3456	8.6	5498
54	1414.7079	13.0	8318
55	1415.2095	22.7	14480
56	1415.7114	23.2	14819
57	1416.2129	16.6	10574
58	1416.7157	9.0	5777
59	1422.3484	4.9	3146
60	1427.3584	7.5	4781
61	1427.8596	7.8	4955
62	1428.3635	5.0	3223

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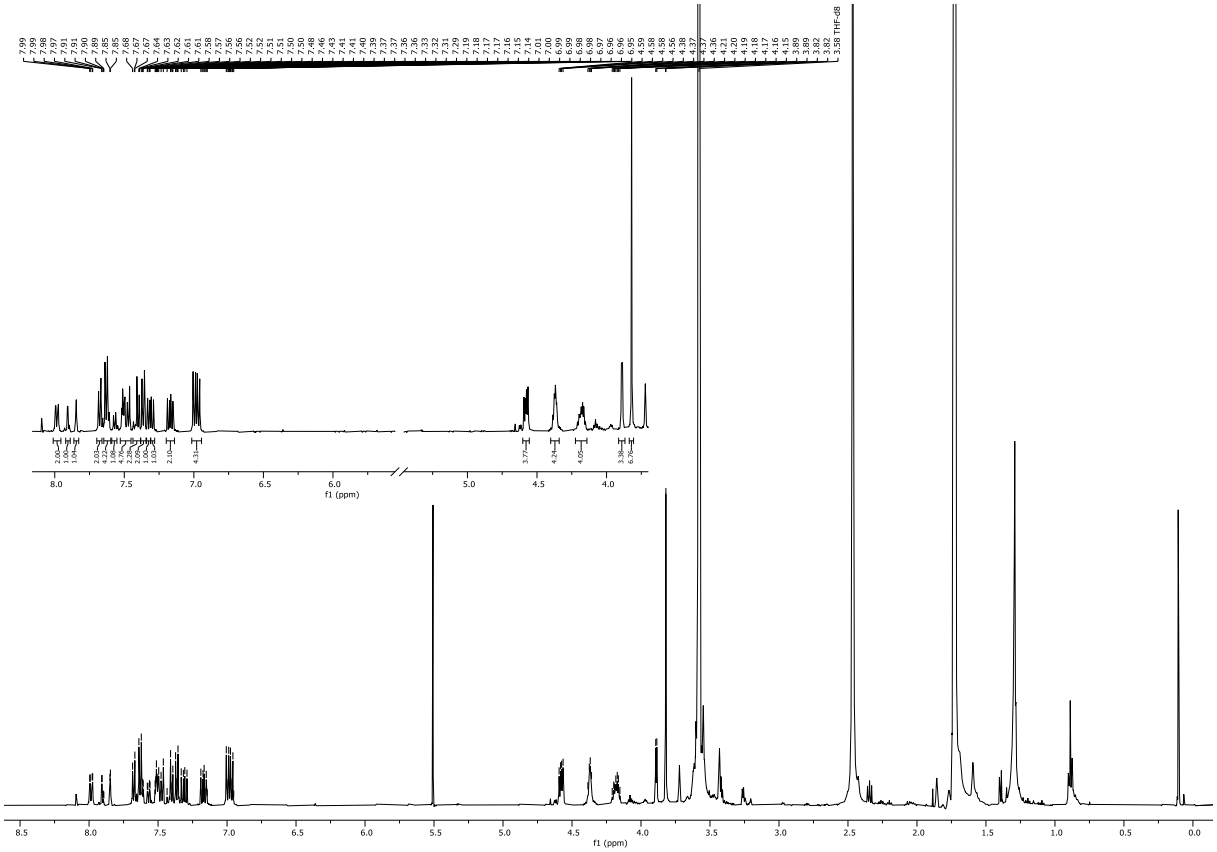
#	m/z	I %	I
63	1488.7635	40.9	26126
64	1489.2652	86.5	55251
65	1489.7671	94.0	60049
66	1490.2684	72.5	46277
67	1490.7696	39.7	25380
68	1491.2715	18.6	11905
69	1491.7731	6.8	4319
70	1592.7523	5.2	3300
71	1593.2536	6.2	3991
72	1611.9358	5.6	3585
73	1612.4393	4.4	2832
74	1625.9515	5.1	3265
75	1651.6241	39.9	25502
76	1652.1277	26.9	17173
77	1652.6293	66.0	42118
78	1653.1309	26.1	16683
79	1653.6319	39.6	25299
80	1654.1344	9.1	5832
81	1654.6351	14.6	9355
82	1666.1408	4.9	3155
83	1666.6407	6.0	3823
84	1667.1436	5.5	3505
85	1679.6540	5.3	3409
86	1680.6565	6.5	4120
87	1681.6598	4.5	2848
88	1746.4335	5.7	3614
89	1746.9362	6.8	4352
90	1747.4355	6.6	4216
91	1747.9371	4.7	2993
92	1983.3501	6.0	3861
93	1983.8516	7.3	4663
94	1984.3540	8.0	5119
95	1984.8558	5.9	3783
96	1985.3557	4.4	2825
97	2314.0632	4.8	3080
98	2315.0695	8.4	5382
99	2316.0720	7.4	4714
100	2317.0783	4.4	2798

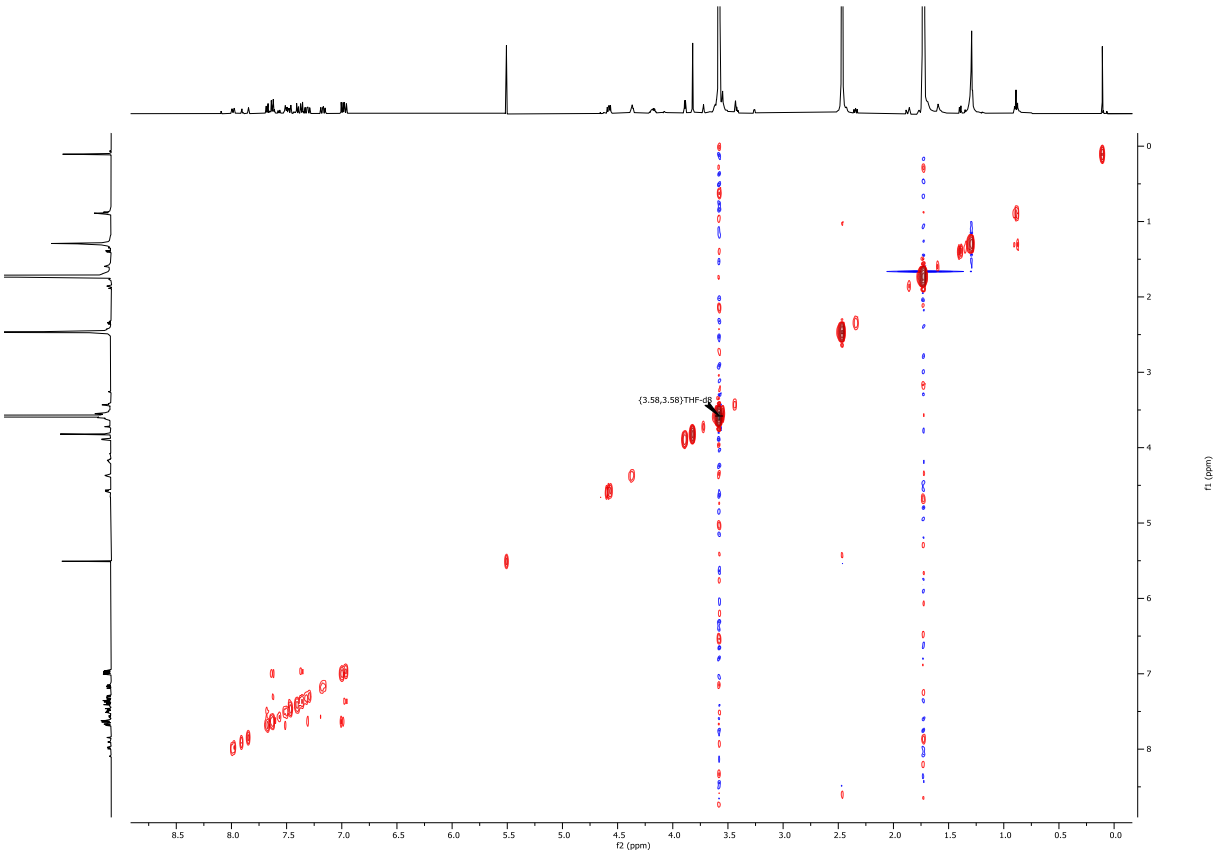
Acquisition Parameter

General	Fore Vacuum	2.61e+000 mBar	High Vacuum	9.50e-008 mBar	Source Type	ESI
	Scan Begin	500 m/z	Scan End	3500 m/z	Ion Polarity	Positive
Source	Set Nebulizer	0.4 Bar	Set Capillary	3600 V	Set Dry Gas	4.0 l/min
	Set Dry Heater	180 °C	Set End Plate Offset	-500 V		
Quadrupole	Set Ion Energy (MS only)	4.0 eV				
Coll. Cell	Collision Energy	70.0 eV	Set Collision Cell RF	2000.0 Vpp	300.0 Vpp	
Ion Cooler	Set Ion Cooler Transfer Time	142.0 µs	Set Ion Cooler Pre Pulse Storage Time	22.0 µs		

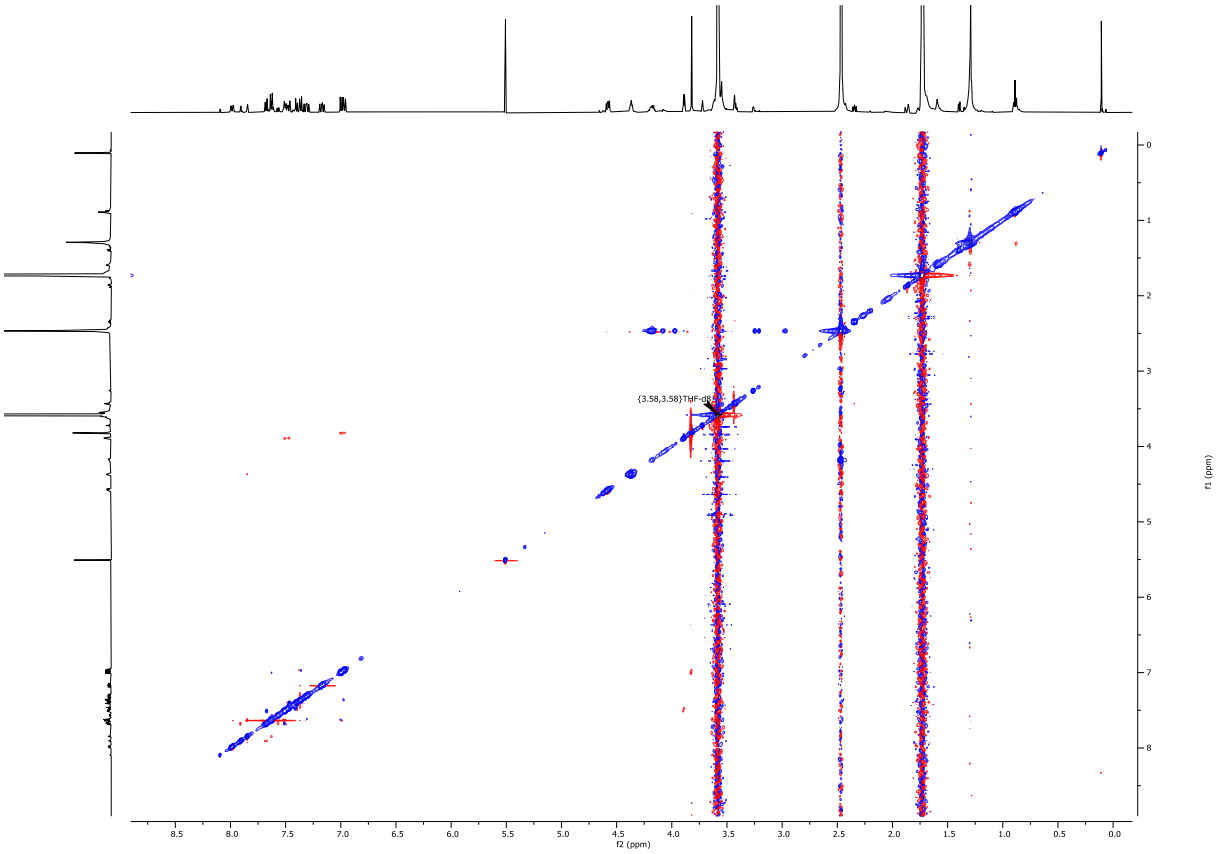
^{1}H-NMR spectra of **$O_{M\text{-}C}$** in **THF-d8**



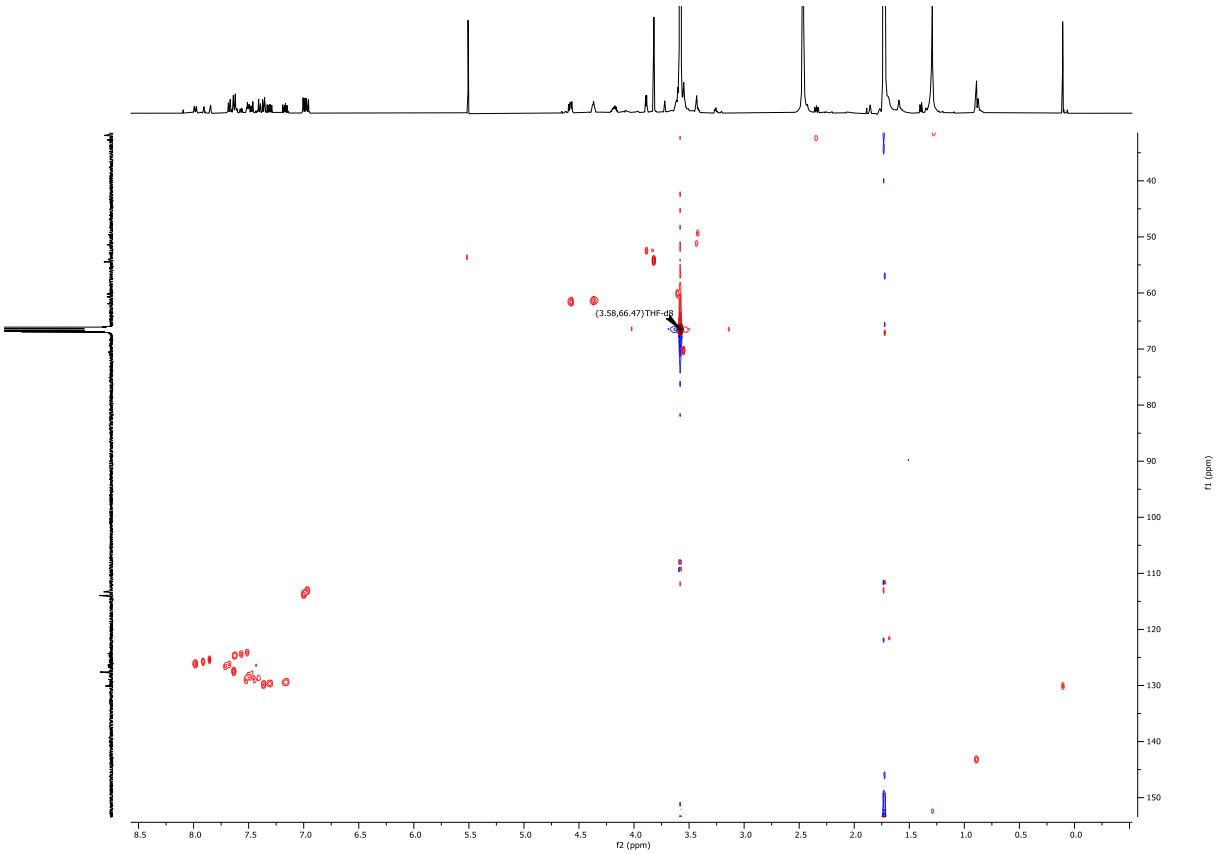
COSY spectra of **$O_{M\text{-}C}$** in **THF-d8**



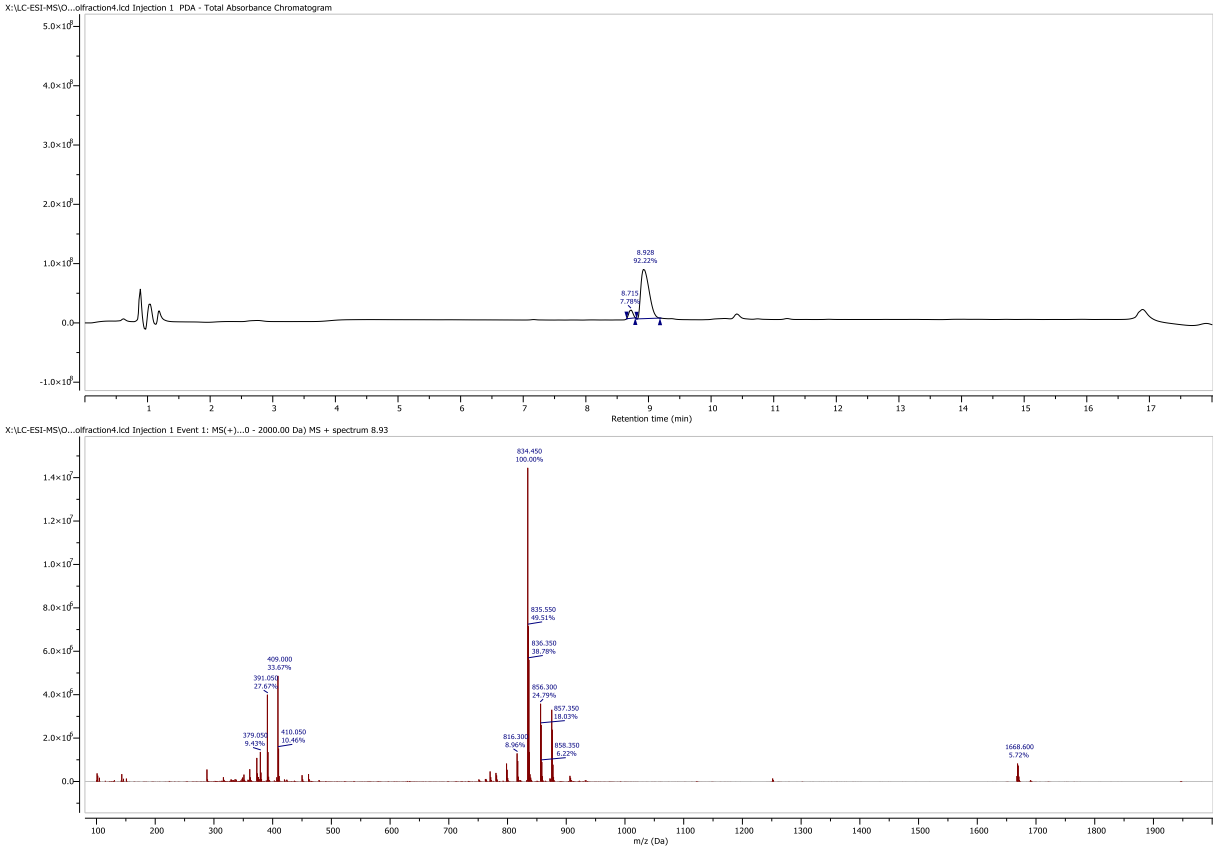
NOESY spectra of $\mathbf{O_{M\text{-}C}}$ in **THF-d8**



HMQC spectra of $\mathbf{O_{M\text{-}C}}$ in **THF-d8**



LC-MS of $O_{M\text{-}C}$



HR-ESI-MS of $\mathbf{O}_{M\text{-}C}$

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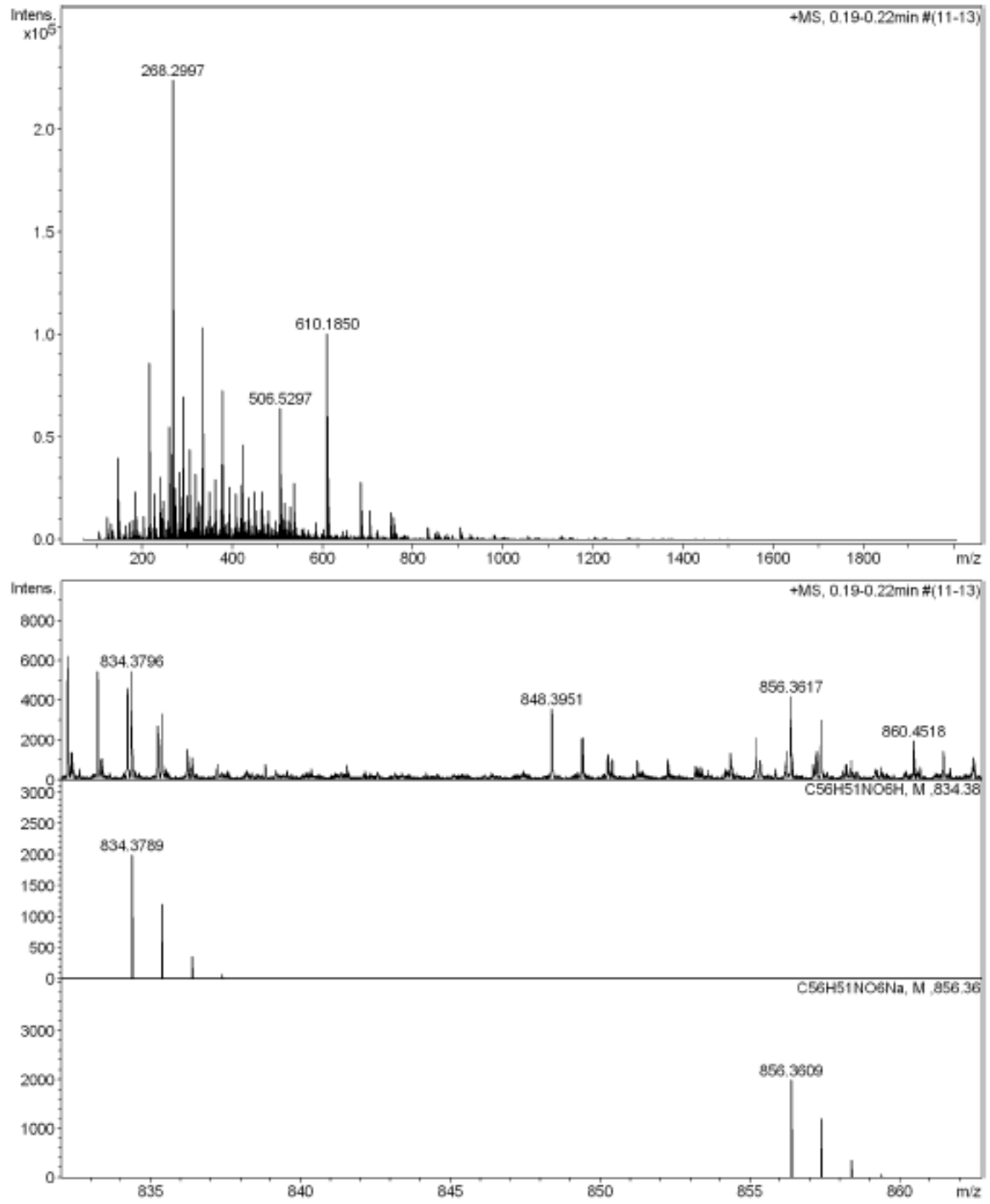
Sample Name **KRO511**
Comment

Instrument maXis 4G
Method ms_nocolumn_75-1000_pos.m



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Measured m/z vs. theoretical m/z

Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e^- Conf	z
834.3796	1	C 56 H 52 N O 6	100.00	834.3789	-0.7	-0.8	20.8	31.5	even	1+
856.3617	1	C 56 H 51 N Na O 6	100.00	856.3609	-0.8	-0.9	102.3	31.5	even	

Mass list

#	m/z	I %	I
1	122.0959	4.9	10939
2	131.9617	3.4	7715
3	144.9818	17.9	40132
4	146.9799	8.5	18946
5	150.1271	4.1	9261
6	173.0780	3.7	8379
7	178.1585	4.3	9564
8	186.0082	10.6	23682
9	188.0064	4.5	10147
10	205.0596	5.2	11699
11	217.1043	38.5	86283
12	218.1076	3.5	7898
13	226.9511	10.1	22557
14	227.0353	5.3	11926
15	240.2681	6.0	13392
16	242.2838	13.8	30922
17	245.0990	4.8	10747
18	247.1148	8.4	18711
19	259.1147	4.2	9400
20	261.1307	24.6	55151
21	266.0710	3.4	7651
22	266.2839	18.6	41680
23	267.2871	4.0	9008
24	268.2997	100.0	223998
25	269.3029	19.8	44335
26	270.3145	7.2	16082
27	273.1666	11.3	25360
28	274.2736	7.0	15737
29	275.1097	7.4	16666
30	282.2788	14.8	33123
31	284.2941	3.7	8337
32	289.1256	9.3	20832
33	291.1412	31.2	69791
34	292.1445	3.9	8798
35	299.1098	9.6	21556
36	301.1253	3.4	7698
37	303.1413	5.8	13026
38	305.1207	4.8	10797
39	305.1569	19.7	44113
40	319.1362	14.4	32257
41	320.2557	5.2	11615
42	324.3620	8.3	18555
43	331.1363	7.5	16861
44	333.1518	15.5	34747
45	335.1676	46.4	103828
46	336.1709	6.8	15172
47	347.1674	4.1	9166
48	349.1468	10.5	23564
49	349.1833	9.5	21172
50	361.1466	3.6	8026
51	363.1626	13.2	29661
52	365.1777	4.2	9400
53	375.1626	6.6	14789
54	377.1783	16.4	36756
55	379.1939	32.7	73164
56	380.1976	5.7	12670
57	385.2922	3.4	7630
58	391.1579	3.7	8323
59	393.1731	11.6	25877
60	407.1888	10.2	22793
61	409.2039	3.8	8462

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#	m/z	I %	I
62	419.1889	4.9	10889
63	421.2044	11.9	26600
64	423.2202	20.6	46201
65	424.2235	3.8	8427
66	429.3186	4.0	8999
67	435.1836	4.2	9418
68	437.1994	9.3	20781
69	449.1722	10.4	23406
70	450.1758	3.5	7776
71	451.2150	6.4	14411
72	463.2148	3.3	7497
73	465.2309	6.7	15032
74	467.2467	10.4	23307
75	479.2096	3.5	7880
76	480.2530	3.5	7886
77	481.2258	6.5	14493
78	495.2413	4.1	9279
79	506.5297	28.6	64102
80	507.5330	11.3	25316
81	509.2570	4.1	9244
82	511.2725	4.6	10259
83	517.1600	8.1	18177
84	525.2518	4.1	9166
85	528.5116	7.3	16384
86	536.1658	12.4	27711
87	537.1664	6.0	13378
88	538.1639	4.0	8931
89	585.1478	3.7	8388
90	610.1850	44.9	100609
91	611.1855	26.9	60149
92	612.1835	18.0	40362
93	613.1833	7.3	16346
94	684.2041	12.6	28301
95	685.2045	7.8	17541
96	685.4362	4.7	10589
97	686.2028	6.3	14122
98	705.5829	6.4	14430
99	750.4075	6.0	13407
100	758.2224	5.0	11135

Acquisition Parameter

General	Fore Vacuum	2.39e+000 mBar	High Vacuum	9.94e-008 mBar	Source Type	ESI
	Scan Begin	75 m/z	Scan End	2000 m/z	Ion Polarity	Positive
Source	Set Nebulizer	2.0 Bar	Set Capillary	4500 V	Set Dry Gas	8.0 l/min
	Set Dry Heater	200 °C	Set End Plate Offset	-500 V		
Quadrupole	Set Ion Energy (MS only)	4.0 eV				
Coll. Cell	Collision Energy	8.0 eV	Set Collision Cell RF	500.0 Vpp	100.0 V_{pp}	
Ion Cooler	Set Ion Cooler Transfer Time	75.0 µs	Set Ion Cooler Pre Pulse Storage Time		10.0 µs	