Supporting Information

Series of Geländer Oligomers with orthogonal Rungs

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General Remarks

Deuterated solvents were obtained from Cambridge Isotope Laboratories, Inc. (Andover, MA, USA) or Alfa Aesar. All commercially available compounds were purchased from Sigma-Aldrich (Switzerland), Acros, Apollo Scientific, Alfa Aesar, and Fluorochem (United Kingdom). Column chromatography was performed on silica gel P60 (40-63 µm) from Silicycle^{TM}, and the solvents were HPLC grade. TLC was performed with silica gel 60 F254 aluminum plates purchased from Merck. Analytics and instruments: NMR experiments were performed on Bruker Avance III NMR spectrometers operating at 250 MHz, 400, 500, or 600 MHz proton frequencies. The instruments were equipped with a direct-observe 5 mm BBFO smart probe (250 MHz.400 MHz, 600 MHz), an indirect-detection 5 mm BBI probe (500 MHz, 600 MHz), or a four-channel cryogenic helium-cooled 5 mm QCI-F probe (600 MHz). All probes were equipped with actively shielded z-gradients (10 A). The chemical shifts are reported in ppm relative to tetramethylsilane or referenced to the residual solvent peak, and the J values are given in Hz (±0.1 Hz). Standard Bruker pulse sequences were used, and the data was processed on Topspin 3.2 (Bruker) using twofold zero-filling in the indirect dimension. The measurements are performed at room temperature. The multiplicities are written as: s=singlet, d=doublet, t=triplet, q=quartet, quint=quintet, dd=doublet of doublet, m=multiplet. UV-Vis absorption spectra were recorded at 20 °C on a Jasco V-770 Spectrophotometer. Fluorescence spectra measurements were performed on a Jasco FP-8600. CD measurements were performed on a JASCO J-1500 CD Spectrophotometer. Quantum yields were measured with Hamamatsu Quantaurus-QY, all compounds were measured three times, and the average was reported. The UV/Vis, CD, and fluorescence spectra were measured in 1 cm quartz glass cuvettes. High-pressure liquid chromatography (HPLC) and gel permeation chromatography (GPC) were performed on a Shimadzu Prominence System. For high-resolution mass spectrometry (HRMS), an HR-ESI-ToF-MS measurement was performed on a maXisTM 4G instrument from Bruker. Zn dust was activated prior to use by stirring in 0.1 M aq. HCl for several minutes, followed by washing the powder in this order with distilled water, ethanol, and diethyl ether and drying it in vacuo. The used column for analytical separation on chiral stationary phase was a Chiralpak IG, 5 µm, 4.6×250 mm. performed with a Shimadzu Prominence System equipped with SDV preparative columns from Polymer Standards Service (two Shodex columns in series, 20×600 mm each, exclusion limit: 30 000 g mol−1) with chloroform as solvent. Description of J = 5 Hz experiments.

Synthetic Procedures and Analytical Data

Dibromo phthalic anhydride,[1] 2-bromo-9-(4-nitrophenyl)-9H-carbazole (**1**), 9-(4-nitrophenyl)-2-((triisopropylsilyl)ethynyl)-carbazole (**3**), and 4-(2-((triisopropylsilyl)ethynyl)-carbazol-9-yl)aniline (**5**) and $\mathbf{EC_{Br}}$ were synthesized as previously reported,[2] all preparations of monomers and endcaps are adapted from synthetic procedures reported therein.

2,7-dibromo-9-(4-nitrophenyl)-carbazole (**2**): In an oven-dried and argon-purged 50 mL round bottom flask equipped with a septum and magnetic stirring bar, 2,7-dibromo-9H-carbazole (10 g, 30.8 mmol) and CsF (9.36 g, 61.6 mmol) were suspended in 10 mL dry DMSO. 1-Fluoro-4-nitrobenzene (13.9 g, 98.8 mmol) was added and placed under argon atmosphere. The reaction was placed in an oil bath heated to 150 °C and stirred overnight. Reaction control by LC–MS indicated complete conversion the next day, and the reaction mixture was poured into deionized water. The precipitates were collected by filtration and washed with warmed Et_2O, MeOH, and H_2O. The solids were dried at 60 °C in vacuo yielding the titular compound as a yellow powder (12.52 g, 30.8 mmol) in 91 % yield

^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.52 (d, J = 8.8 Hz, 2H), 8.34 – 8.23 (m, 2H), 7.95 (d, J = 8.3 Hz, 2H), 7.74 (*apparent* d, 2H), 7.56 (*apparent* s, 2H), 7.49 – 7.42 (m, 2H), 7.21 – 7.13 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ = 146.8, 142.6, 141.0, 127.3, 126.0, 124.9, 122.5, 121.9, 120.6, 113.0.

HR-MS (ESI-ToF, +): m/z = [M]+· Calcd. For $C_{18}H_{10}Br_2N_2O_2$: 443.9104; Found 443.9094.

9-(4-nitrophenyl)-2,7-bis((triisopropylsilyl)ethynyl)-carbazole (**4**): To a 500 mL Schlenk tube equipped with a magnetic stirring bar and septum **2** (2.00 g, 4.48 mmol) was added and dissolved in a mixture of 16 mL THF and 50 mL diisopropylamin. The mixture was sparged 30 min with argon, followed by the addition of $Pd(PPh_3)_4$ (259 mg, 224 µmol), CuI (51.2 mg, 269 µmol), and (triisopropylsilyl)acetylene (4.90 g, 6.03 mL, 26.9 mmol). The tube was sealed, placed in a pre-heated oil bath at 90 °C, and allowed to stir over night. Reaction control by LC–MS indicated complete conversion, thus, the reaction mixture was diluted with CH_2Cl_2 and filtered over a silica plug. Volatiles were removed and the crude subjected to fcc (SiO_2: 19 : 1-4 : 1=cyclohexane:toluene). The titular compound was isolated as yellow solid (2.67 g, 4.48 mmol) in 92 % yield.

^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.58 – 8.49 (m, 2H), 8.02 (d, *J* = 8.0 Hz, 2H), 7.82 – 7.70 (m, 2H), 7.49 (*apparent* s, 1H), 7.46 (dd, *J* = 8.0, 1.3 Hz, 2H), 1.13 (d, *J* = 1.9 Hz, 42H).

^{13}C NMR (101 MHz, $CDCl_3$) δ = 143.1, 140.3, 127.4, 125.9, 125.9, 123.7, 121.9, 120.7, 113.1, 107.6, 91.6, 18.8, 11.5.

HR-MS (ESI-ToF, +): m/z = $[M]^{+\cdot}$ Calcd. For $C_{40}H_{52}N_2O_2Si_2$: 648.3562; Found 648.3564.

4-(2-((triisopropylsilyl)ethynyl)-carbazol-9-yl)aniline (**7**): In a 100 mL round bottomed flask equipped with a magnetic stirring bar **6** (1.38 g, 2.13 mmol) and $SnCl_2$ dihydrate (2.94 g, 12.8 mmol) were dissolved in a mixture of 20 mL of THF and 10 mL ethanol. The reaction mixture was set under an argon atmosphere, placed in a pre-heated oil bath at 50 °C, and allowed to stir over night. LC–MS indicated complete conversion and saturated aqueous $NaHCO_3$was added. This mixture was extracted three times with CH_2Cl_2. After evaporation of volatiles an orange semisolid was quantitatively isolated (1.32 g, 2.13 mmol). NMR indicated sufficient purity and the product was used without further characterization and purification.

^{1}H NMR (400 MHz, CD_2Cl_2) δ = 8.06 – 8.00 (m, 2H), 7.41 – 7.34 (m, 4H), 7.31 – 7.21 (m, 2H), 6.95 – 6.86 (m, 2H), 3.99 (s, 2H), 1.13 (s, 42H).

General procedure for the synthesis of end capping agents (**EC$_X$**) and monomers (**M$_X$**):

In a round-bottom flask equipped with a magnetic stir bar, **1** eq. of 4-carbazol-9-yl aniline was dissolved in glacial acetic acid (0.4 M), and 1.1 of the appropriate phthalimide was added, and the reaction mixture placed in an oil bath at 120 °C. After 16 h, the reaction is allowed to cool to room temperature, and the product is collected by filtration. The product is washed with deionized H_2O and MeOH and subsequently dried *in vacuo* at 60 °C.

EC$_{Cl}$

^{1}H NMR (400 MHz, THF) δ 8.16 (dd, *J* = 7.8, 0.8 Hz, 1H), 8.13 (d, *J* = 8.1 Hz, 1H), 7.94 (t, *J* = 4.1 Hz, 1H), 7.83 (d, *J* = 4.4 Hz, 2H), 7.83 – 7.80 (m, 2H), 7.79 – 7.73 (m, 2H), 7.57 (s, 1H), 7.48 (d, *J* = 8.2 Hz, 1H), 7.45 – 7.37 (m, 2H), 7.32 – 7.24 (m, 1H), 1.16 (s, 21H).

^{13}C NMR (101 MHz, THF) δ = 166.3, 165.2, 142.8, 141.3, 137.6, 136.9, 136.5, 135.5, 132.7, 132.1, 129.2, 129.0, 128.4, 127.6, 125.5, 124.9, 124.2, 123.0, 121.7, 121.5, 121.5, 121.1, 113.9, 111.0, 109.8, 90.2, 19.3, 12.5.

HR-MS (ESI-ToF, +): m/z = $[M+H]^+$ Calcd. For $C_{37}H_{36}ClN_2O_2Si$: 603.2229; Found 603.2238.

M$_{Cl}$

^{1}H NMR (400 MHz, THF-d8) δ = 8.20 – 8.08 (*apparent* d, 2H), 7.86 – 7.77 (m, 4H), 7.56 – 7.51 (*apparent s*, 2H), 7.42 (dd, *J* = 8.1, 1.3 Hz, 2H), 1.16 (*apparent* s, 42H).

^{13}C NMR (101 MHz, THF-d8) δ = 164.0, 142.2, 137.9, 137.3, 132.7, 130.7, 130.6, 129.4, 128.6, 125.9, 124.4, 122.3, 121.5, 114.1, 109.6, 90.8, 19.3, 12.5.

HR-MS (ESI-ToF, +): m/z = $[M+H]^+$ Calcd. For $C_{48}H_{55}Cl_2N_2O_2Si_2$: 817.3174; Found 817.3185.

M$_{Br}$

^{1}H NMR (400 MHz, THF-d8) δ = 8.16 (*apparent* d, 1H), 8.13 (ad, J = 8.1 Hz, 1H), 8.01 (dd, J = 8.1, 0.9 Hz, 1H), 7.98 (dd, J = 7.4, 0.9 Hz, 1H), 7.89 – 7.80 (m, 2H), 7.79 – 7.75 (m, 2H), 7.73 (d, J = 7.7 Hz, 1H), 7.57 (*apparent* s, J = 1.1 Hz, 1H), 7.48 (*apparent* d, 1H), 7.44 – 7.38 (m, 2H), 7.27 (*apparent* t, 1H), 1.16 (*apparent* s, 22H).

^{13}C NMR (101 MHz, THF) δ = 164.2, 142.2, 140.9, 137.3, 132.9, 132.6, 129.4, 128.6, 125.9, 124.4, 122.3, 121.5, 118.4, 114.1, 109.6, 90.8, 19.3, 12.5.

HR-MS (ESI-ToF, +): m/z = $[M+Na]^+$ Calcd. For $C_{48}H_{54}Br_2N_2NaO_2Si_2$: 927.1983; Found 927.1958.

Oligomerization by reductive homocoupling:

Different size-distributions of the obtained oligomer mixture were obtained depending on the stoichiometry of EC_X to M_X; the reaction with equimolar amounts of either is described. Spectral data for A[2] matched our previous report.

Method A

A flame-dried Schlenk tube equipped with a magnetic stir bar was charged with $NiBr_2$ (10 mol%), PPh_3 (20 mol%), and Zn dust (5 eq.) and placed under an Argon atmosphere. 1 mL DMAc was added to the reaction mixture and the tube was placed in an 80 °C warm oil bath. The active species was allowed to be formed for half an hour. In a separate flame-dried Schlenk tube equipped with a magnetic stirrer, M_X and EC_X were suspended in DMAc (to 0.1 M concentration) under an Argon atmosphere. The solution of the active catalyst was added to the latter tube, and subsequently, the reaction vessel was closed. This mixture was allowed to stir for 5 days at 80 °C, cool to room temperature, and diluted with DMAc. The product was precipitated by adding deionized H_2O, collected over a pad of celite, washed with MeOH, and washed down the pad with CH_2Cl_2. After the evaporation of volatiles, the crude product was obtained. Individual oligomers were isolated using preparative GPC.

Method B

A flame-dried Schlenk tube equipped with a magnetic stir bar was charged with $NiCl_2(PPh_3)_2$ (10 mol%), PPh_3 (20 mol%), KI (3 mol%) and Zn dust (5 eq.) and placed under an Argon atmosphere. 2-Me THF (1 mL) was added to the reaction mixture, and the tube was placed in an 80 °C warm oil bath. The active species was allowed to be formed for half an hour. In a separate flame-dried Schlenk tube equipped with a magnetic stirrer, M_X and EC_x were suspended in 2-Me THF (to 0.1 M concentration) under an Argon atmosphere. The solution of the active catalyst was added to the latter tube, and subsequently, the reaction vessel was closed. This mixture was allowed to stir for 5 days at 80 °C and then cooled to room temperature. The reaction mixture is filtered through a celite pad, washed with 2-Me THF, and the volatiles evaporated. Individual oligomers were isolated using preparative GPC.

A[3]

^{1}H NMR (600 MHz, THF) δ = 8.16 – 7.99 (*several overlapping broad signals*, 14H), 7.85 – 7.80 (m, 4H), 7.78 – 7.74 (m, 2H), 7.76 – 7.72 (m, 4H), 7.72 – 7.64 (m, 2H), 7.53 (s, 2H), 7.45 – 7.41 (m, 4H), 7.40 – 7.37 (m, 4H), 7.37 – 7.34 (m, 4H), 7.24 (*apparent* t, 2H), 1.11 (s, 42H), 1.06 (s, 42H).

^{13}C NMR (151 MHz, THF) δ = 167.2, 166.9, 142.7, 142.1, 141.3, 137.5, 137.4, 136.9, 136.1, 135.9, 135.0, 133.4, 133.0, 132.8, 130.5, 129.2, 129.1, 128.4, 128.3, 127.6, 125.9, 125.5, 124.9, 124.6, 124.3, 124.1, 122.3, 121.7, 121.4, 121.4, 121.1, 113.9, 113.8, 110.9, 109.7, 109.5, 90.7, 90.1, 19.3, 19.2, 12.4, 12.4.

HR-MS (MALDI-ToF, +): m/z=[M]+ Calcd. for $C_{122}H_{124}N_6O_6Si_4$: 1880.8654; Found 1880.8646.

A[4]

^{1}H NMR (600 MHz, THF) δ = 8.20 – 8.07 (*several overlapping broad signals*, 10H), 8.07 – 8.00 (m, 8H), 7.83 (d, *J* = 8.5 Hz, 4H), 7.80 (*apparent* d, 4H), 7.74 (*apparent* d, 4H), 7.71 (*apparent* d, 8H), 7.53 (s, 2H), 7.45 – 7.40 (m, 6H), 7.39 – 7.34 (m, 8H), 7.24 (*apparent* t, 2H), 1.10 (s, 42H), 1.06 (*broad* s, 84H).

^{13}C NMR (151 MHz, THF) δ = 167.3, 167.0, 142.7, 142.2, 141.3, 137.4, 136.9, 136.2, 136.1, 135.9, 133.4, 133.0, 132.9, 130.6, 129.2, 129.2, 129.1, 129.0, 128.4, 128.3, 127.6, 125.9, 125.5, 124.9, 124.6, 124.3, 124.2, 122.3, 121.7, 121.4, 121.1, 113.9, 113.8, 110.9, 109.7, 109.5, 90.7, 90.1, 19.3, 19.2, 12.4, 12.4.

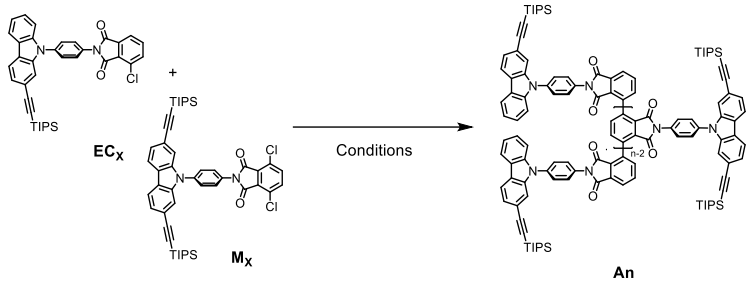
HR-MS (MALDI-ToF, +): m/z=[M]+ Calcd. for $C_{170}H_{178}N_8O_8Si_6$: 2627.2378; Found 2627.2392.

A[5]

^{1}H NMR (600 MHz, THF) δ = 8.22 (*apparent* d, 2H), 8.17 – 7.99 (*several overlapping signals*, 20H), 7.84 (*apparent* d, 6H), 7.81 (*apparent* d, 4H), 7.77 – 7.68 (*broad* m, 10H), 7.53 (s, 2H), 7.48 – 7.40 (m, 8H), 7.36 (*apparent* d, 10H), 7.24 (*apparent* t, 2H), 1.09 (s, 42H), 1.05 (*broad* s, 126H).

^{13}C NMR (151 MHz, THF) δ = 167.3, 167.0, 142.7, 142.1, 141.3, 137.9, 137.4, 136.9, 136.2, 135.9, 133.4, 133.0, 132.9, 130.6, 129.2, 129.2, 129.1, 128.4, 128.4, 128.3, 127.6, 125.9, 125.5, 124.9, 124.6, 124.3, 124.2, 122.3, 121.7, 121.4, 121.1, 113.9, 113.8, 110.9, 109.7, 109.5, 90.7, 90.1, 19.3, 19.2, 12.4, 12.4.

HR-MS (MALDI-ToF, +): m/z=[M]+ Calcd. for $C_{218}H_{232}N_{10}O_{10}Si_8$: 3373.6102; Found 3373.6201.



Scheme S1: Yamamoto-type statistical polymerization.

Table S1: Selected conditions screened for the statistical end-capped polymerization by Yamamoto type coupling.

X	eq. EC$_X$	eq. M$_X$	solvent	cat.	ligand	additive	time	temp.	yield A[2]	yield A[3]	yield A[4]	yield A[5]
Br	2	1	DMAc	$NiBr_2$	PPh_3	Zn	16 h	80 °C	27%	11%	4%	1%
Br	2	1	DMAc	$NiBr_2$	PPh_3	Zn	3 d	80 °C	4%	2%	2%	n.d
Br	2	1	THF	$Ni(PPh)_3Cl_2$	PPh_3	Zn. KI	3 d	80 °C	44%	17%	2%	n.d
Cl	1	1	2Me-THF	$Ni(PPh)_3Cl_2$	PPh_3	Zn. KI	3 d	80 °C	48%	23%	7%	4%
Cl	1	2	2Me-THF	$Ni(PPh)_3Cl_2$	PPh_3	Zn, KI	3 d	80 °C	12%	18%	16%	7%

Geländerfication

In a 250 mL round bottom flask equipped with a magnetic stir bar **A[3]** (38 mg, 20.2 µmol, 1 eq.) was dissolved in 50 ml DMSO ($4 \cdot 10^{-4}$ M) and placed in an oil bath heated to 100 °C. Subsequently, 17 mg of CuF_2 was added. The reaction was stirred for three days open to air. After the mixture cooled down to room temperature the crude product was precipitated and purified by GPC to yield **G_{BD}3** in 44% yield (11 mg, 8.78 µmol).

^{1}H NMR (600 MHz, THF-d8) δ = 8.16 (*apparent* d, 2H), 8.15 – 8.12 (m, 4H), 8.11 (d, *J* = 5.0 Hz, 2H), 8.05 (t, *J* = 7.7 Hz, 2H), 7.98 (dd, *J* = 7.9, 1.0 Hz, 2H), 7.97 (s, 2H), 7.82 – 7.75 (m, 4H), 7.71 – 7.67 (m, 4H), 7.67 – 7.65 (m, 4H), 7.64 – 7.62 (m, 2H), 7.62 – 7.58 (m, 2H), 7.46 – 7.39 (m, 4H), 7.31 – 7.25 (m, 6H).

^{13}C NMR (151 MHz, THF-d8) δ = 167.2, 167.2, 166.6, 156.8, 142.8, 142.8, 141.9, 137.1, 136.8, 136.4, 136.0, 135.5, 133.2, 133.0, 132.8, 131.0, 130.3, 129.4, 129.0, 128.6, 127.9, 125.3, 124.6, 124.6, 124.1, 122.6, 121.8, 121.7, 121.5, 121.3, 120.9, 119.9, 117.8, 117.6, 110.8, 103.8, 86.2, 85.6, 76.2, 75.5.

HR-MS (ESI-ToF, +): m/z = $[2M+2Ag]^{2+}$ Calcd. For $C_{172}H_{80}Ag_2N_{12}O_{12}$: 1359.2055; Found 1359.2047.

In a 250 mL round bottom flask equipped with a magnetic stir bar **A[4]** (20 mg, 7.61 µmol, 1 eq.) was dissolved in 75 ml DMSO (10^{-4} M) and placed in an oil bath heated to 100 °C. Subsequently, 19 mg of $CuF \cdot 2H_2O$ was added. The reaction was stirred for three days open to air. After the mixture cooled down to room temperature the crude product was precipitated and purified by GPC to yield **G_{BD}4** in 23% yield (3 mg, 1.78 µmol).

^{1}H NMR (600 MHz, THF-d8) δ 8.17 (dt, *J* = 7.8, 0.9 Hz, 2H), 8.15 – 8.14 (m, 4H), 8.13 – 8.13 (m, 4H), 8.13 – 8.11 (m, 2H), 8.06 (*apparent* t, 2H), 8.02 (*apparent* d, 2H), 8.01 (*apparent* dd, 2H), 7.82 – 7.77 (m, 4H), 7.71 – 7.67 (m, 10H), 7.66 – 7.65 (m, 2H), 7.64 – 7.63 (m, 2H), 7.62 (d, *J* = 8.3 Hz, 2H), 7.46 – 7.41 (m, 4H), 7.31 – 7.26 (m, 8H).

^{13}C NMR (151 MHz, THF-d8) δ = 137.1, 137.0, 136.8, 135.6, 129.0, 129.0, 128.7, 128.6, 127.9, 124.6, 122.8, 121.7, 121.7, 121.5, 121.2, 118.0, 117.9, 117.6, 110.9 (all signals are extracted from a HSQC experiment)

HR-MS (ESI-ToF, +): m/z = $[M+H]^+$ Calcd. For $C_{116}H_{53}N_8O_8$: 1685.3981; Found 1685.3925.

Supporting Figures

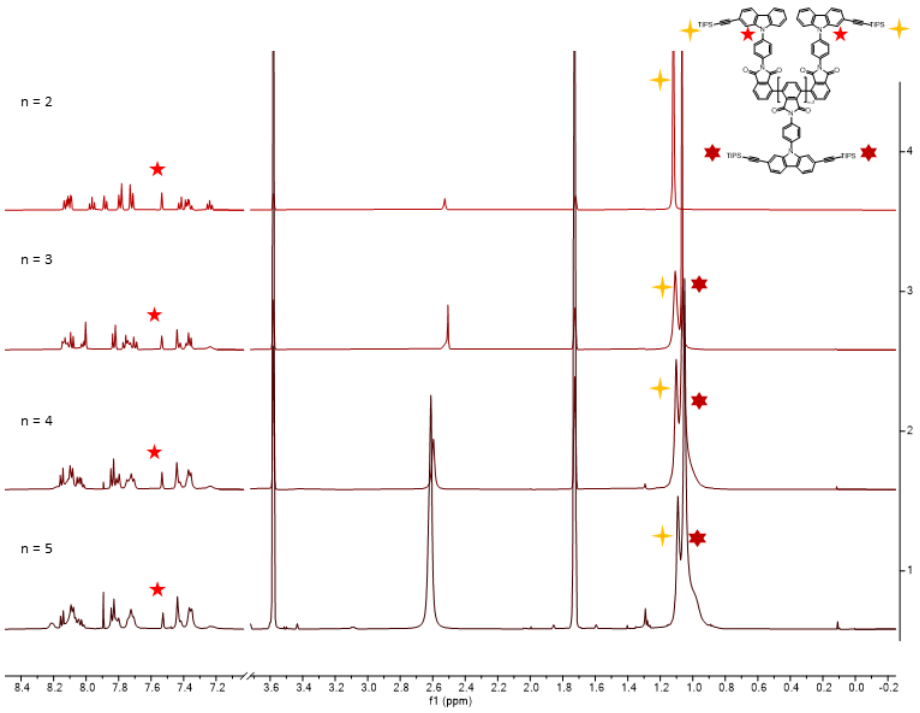


Figure S1: 1H-NMR of A[n], signals arising from the TIPS protecting group in the repeating unit are indicated in dark red six armed stars, the signals arising from the TIPS protecting group by yellow 4 armed stars, and the signal from the 1 carbazole position in the endcap by a bright red 5 armed star.

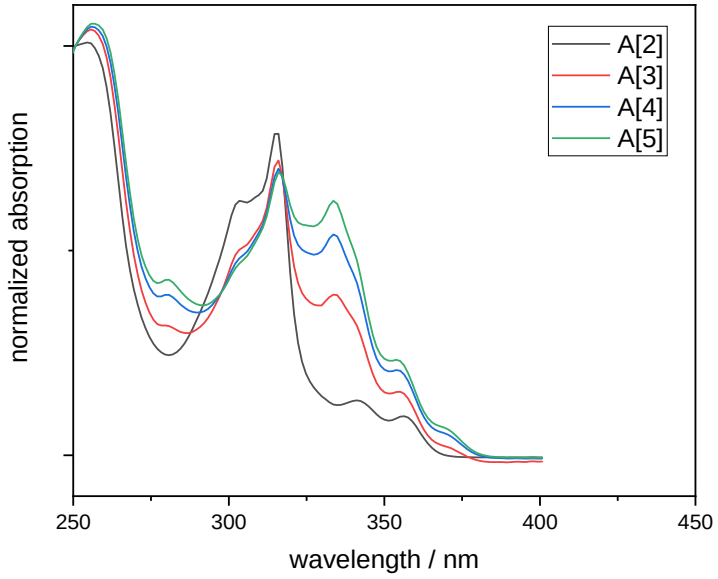


Figure S2: Normalized absorption spectra of **A[n]** extracted from the preparative GPC run in chloroform.

HPLC chromatograms

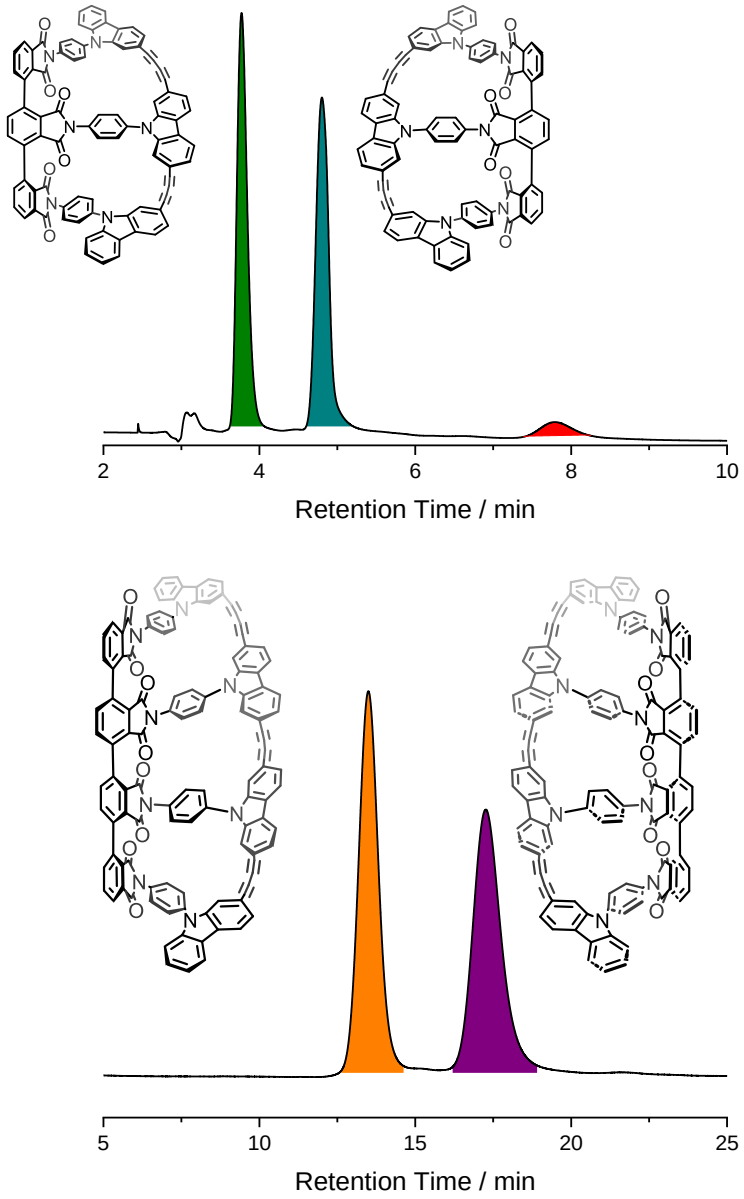


Figure S3: Chiral resolution of G_{BD}**[3]** (top) and G_{BD}**[4]** (bottom) for analytical separation. G_{BD}**[3]** was resolved on a Chiralpak™ IG column (70% CH_2Cl_2 in heptane 1 ml/min), G_{BD}**[4]** was resolved on a Chiralpak™ IBN-5 column (50% EtOAc in heptane 1 ml/min).

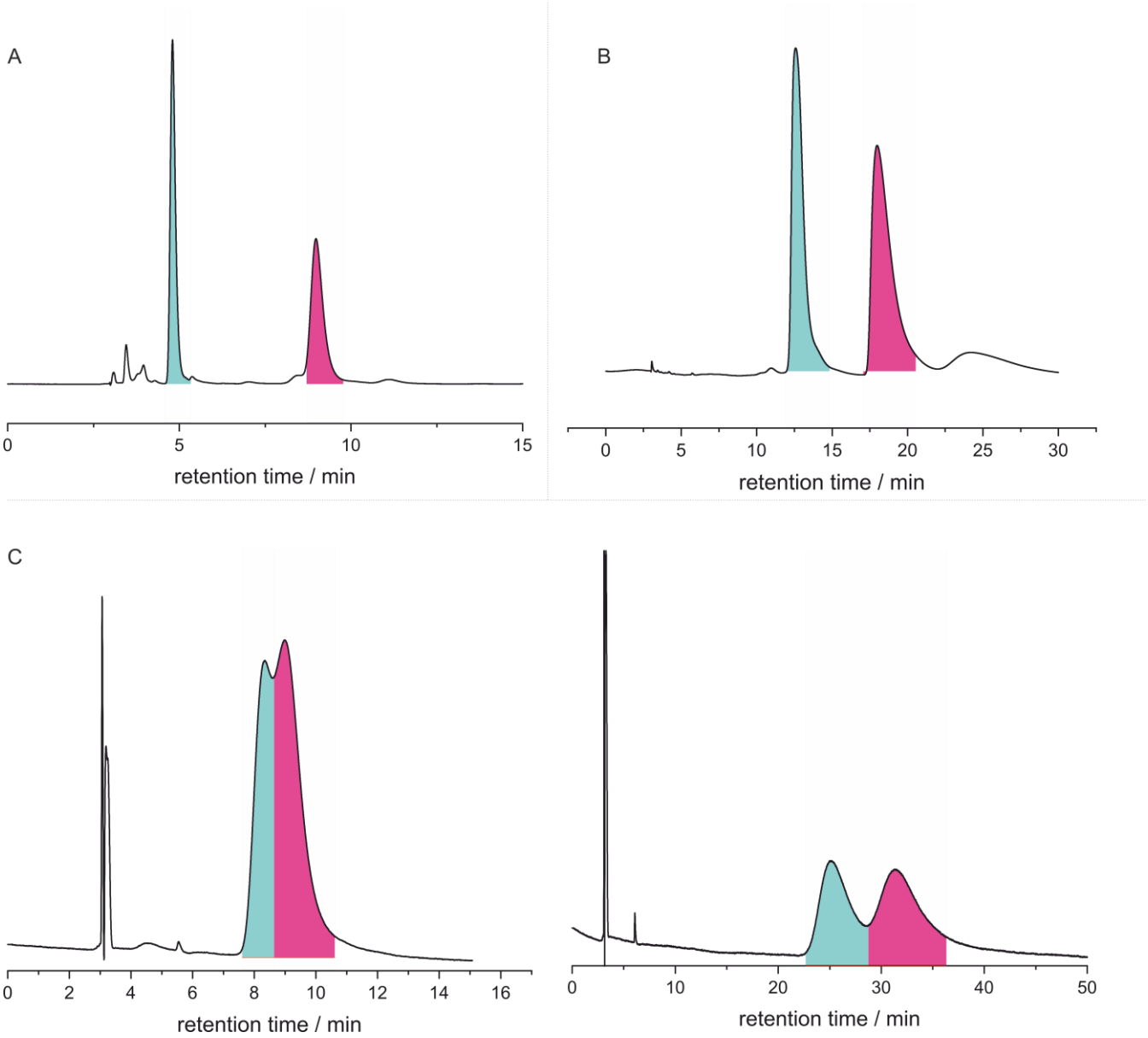


Figure S4: Analytical Chiral resolution of G_{BD}**[2-4]** on IG columns from Chiralpak™ by Daicel. Conditions: A) G_{BD}**[2]**, 1 mL/min, 50% CH_2Cl_2 in heptane. B) G_{BD}**[3]**, 1 mL/min, 50% CH_2Cl_2 in heptane. C) left: G_{BD}**[4]**, 1 mL/min, 50% CH_2Cl_2 in heptane Chiralpak™ IG. Right: G_{BD}**[4]**, 1 mL/min, 50% CH_2Cl_2 in heptane Chiralpak™ .IBN-5

Whilst the chiral resolution of G_{BD}**[2]** and G_{BD}**[3]** could be achieved with a high percentage of 70% CH_2Cl_2 in heptane on a IG (Chiralpak™) chiral stationary phase which could not be used to resolve G_{BD}**[4]**. Reducing the content to 50% CH_2Cl_2 allowed to resolve the dimeric and tetrameric species still efficiently and first (poor) separation for the tetramer was observed (Figure S4). Reducing the content to 40% CH_2Cl_2 allowed to resolve G_{BD}**[4]**. However, optimized conditions were found on a different chiral stationary phase (IBN-5 column by Chiralpak™, see Figure S3).

DFT Calculations

Optimization, frequency analysis and TD-DFT calculations were preformed using Gaussian 09 (E.01),[3] SpecDis 1.71 was used to extract the transitions and fit the calculated spectra.[4,5] The optimized geometry of **G_{BD}[2]** was reported with our previous findings,[2] but re-optimized at the B3LYP/def2-SVP level of theory for this study. **G_{BD}[3]** and **G_{BD}[4]** were optimized at B3LYP/def2-SVP level of theory. The modeled geometries are displayed below.

Determination of Torsional Angles

Mercury 2021.3.0 was used to measure the angles in the modeled structures of (*P*)-**G_{BD}[2],** (*P*)-**G_{BD}[3]** and (*P*)- **G_{BD}[4],** as well as (*P*)- **G_{BD}[3]** extracted from the solid state structure. Centroids (dummy atoms, marked in red) were calculated as pivots for measuring the angle between anchors for measuring the torsion ϕ. For ϕ, the centroids of the 7-membered scaffold of the individual phthalimides found in the axis were calculated. The torsional angle was measured from these centroids over the CC bond connecting the phthalimide units. The individual angles between the subunits were summed to determine the overall angle. The axis length was determined as the straight line connecting the carbon farthest apart in the phthalimide axis (from C6 to C6'' marked in green). The banister lengths were determined by the sum of the straight lines over a carbazole from C2 to C7 (highlighted in yellow) and the straight lines between the carbazole subunits.

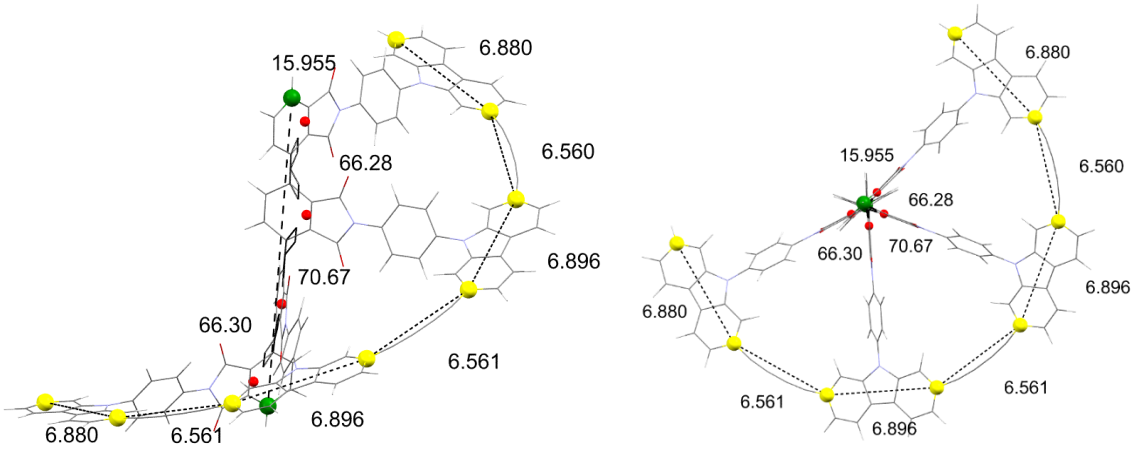


Figure S5. Measurements of key angles and distances in the model of (*P*)- **G_{BD}[4]**.

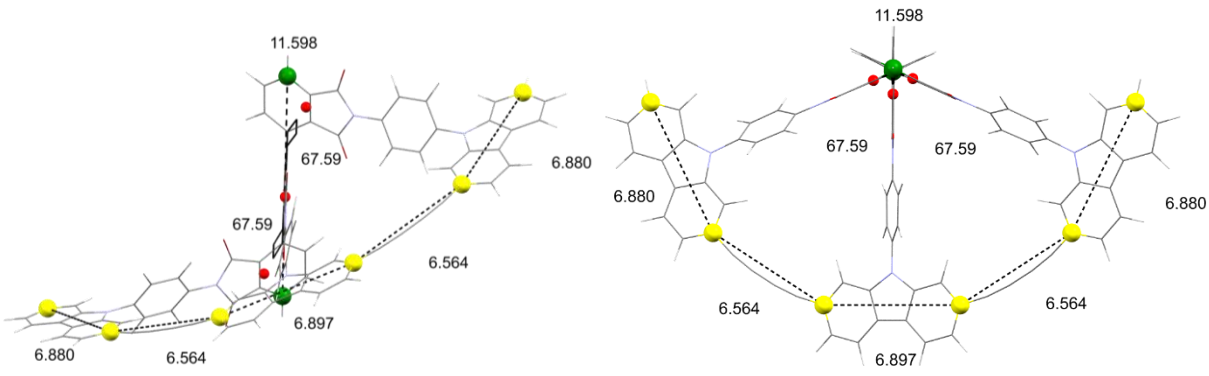


Figure S6. Measurements of key angles and distances in the model of (*P*)- **G_{BD}[3]**.

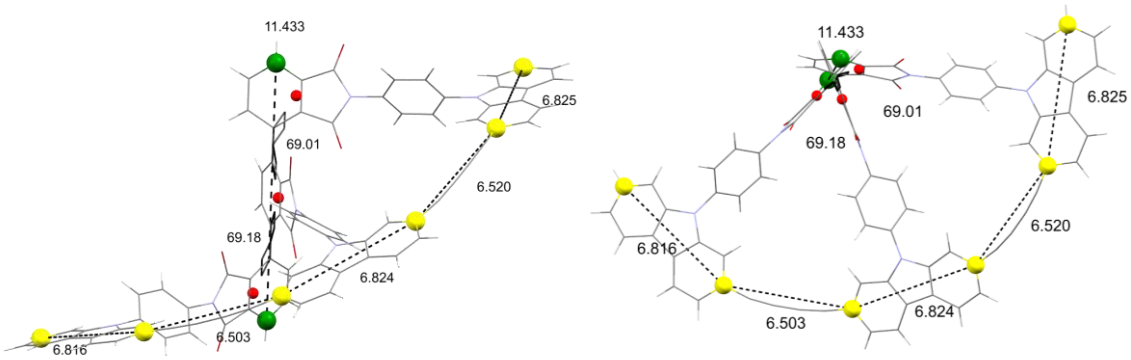


Figure S7. Measurements of key angles and distances in the X-ray structure of (*P*)- **G_{BD}[3]**.

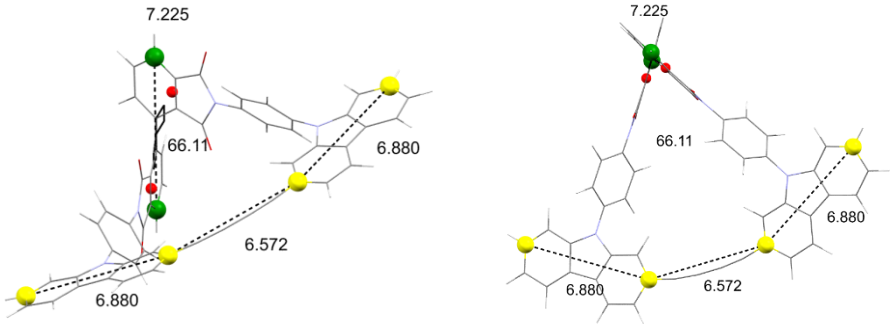


Figure S8. Measurements of key angles and distances in the model structure of (*P*)- **G_{BD}[2]**.

TD-DFT

For **G_{BD}[3]**, and **G_{BD}[4]** 50 vertical transitions were calculated at the TD-PBE0/def2-SVP level of theory polarizable continuum model (PCM) for chloroform taken in account.

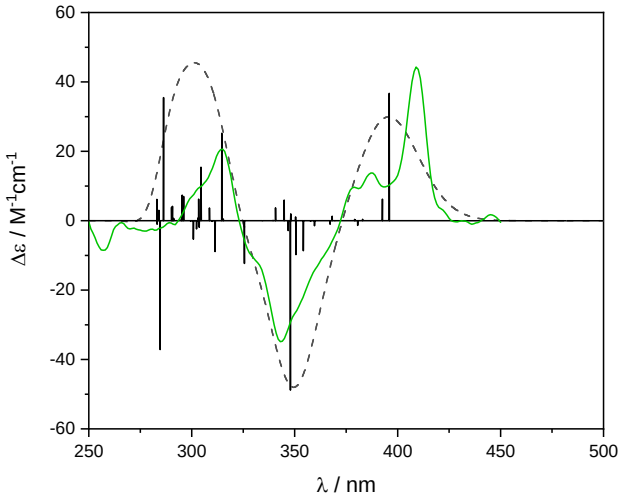


Figure S9. Experimental (green solid line) and simulated (black dashed line, fitted with σ= 0.16 eV) ECD spectrum of **G_{BD}[3].** The calculated transitions are indicated by black sticks and shifted blue by 0.3 eV. The transitions were calculated at TD-PBE0/def2-SVP level of theory.

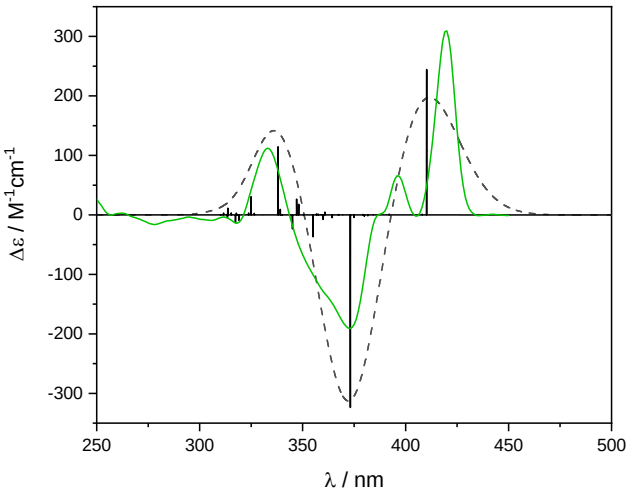


Figure S10. Experimental (green solid line) and simulated (black dashed line, fitted with σ= 0.16 eV) ECD spectrum of **G_{BD}[4].** The calculated transitions are indicated by black sticks and shifted blue by 0.3 eV. The transitions were calculated at TD-PBE0/def2-SVP level of theory.

TDM analysis

The Rotary strength R is the scalar product of the electric ($\vec{\mu}$) and magnetic ($\vec{m}$) transition dipole moments, $R = |\vec{\mu}| * |\vec{m}| \cos\theta$. We used Multiwfn[1] to analyze the transition dipole moments and visualized the data using VMD.[2] The summarized values can be found in **Table S2**. We analyzed the most intense red transition with an intense rotary strength for all three compounds TD-PBE0/def2-SVP level of theory with polarizable continuum model (PCM) for chloroform taken in account. Even though the angle θ is for all three compounds close to 90° it gets more coplanar with increasing size. Furthermore, the angles indicate moderately

large transition dipole moments. The direction of $\vec{\mu}$ is found almost parallel along the banister for **G_{BD}[2]**, **G_{BD}[3]**, and **G_{BD}[4]**, see Figure S11. Interestingly, the absolute value of $\vec{\mu}$ increases only moderately while the absolute value of $\vec{m}$ increases non linearly. These findings are in close resemblance with a series of helical PDI structures.[3]

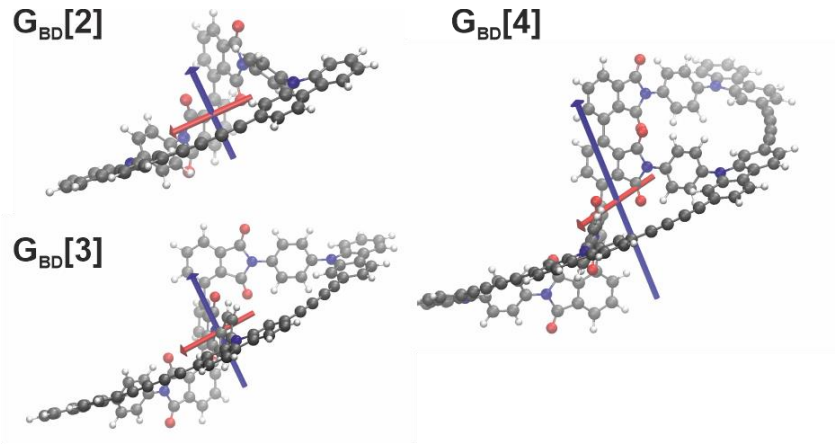


Figure S11. Visualization of the electric ($\vec{\mu}$, red) and magnetic ($\vec{m}$, blue) transition dipole moments

Table S2. Summary of values of the TDM analysis.

species	state	$\lvert\vec{\mu}\rvert$(au)	$\lvert\vec{m}\rvert$(au)	θ
G_{BD}[2]	14	5.23	6.48	90.47°
G_{BD}[3]	10	5.66	8.79	88.38°
G_{BD}[4]	7	6.11	14.78	83.86°

Crystallographic Details

Crystallographic data for compounds *(rac)*-**G_{BD}[3]** reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as supplementary information no. CCDC-2378167. Copies of the data can be obtained free of charge from https://www.ccdc.cam.ac.uk/structures/.

Experimental Details.

Single crystal X-ray diffraction data were collected on a STOE STADI VARI diffractometer with monochromated Ga Kα (1.34143 Å) radiation at low temperature. Using Olex2,[4] the structures were solved with the ShelXT[5] structure solution program using Intrinsic Phasing and refined with the ShelXL[6] refinement package using Least Squares minimization. Refinement was performed with anisotropic temperature factors for all non-hydrogen atoms; hydrogen atoms were calculated on idealized positions. Crystallographic data and refinement details are summarized in Table S3.

Table S3. Crystallographic data and refinement details for *(rac)*-**G$_{BD}$[3].**

Compound	*(rac)*-**G$_{BD}$[3]** · 8 THF
Empirical formula	$C_{118}H_{104}N_6O_{14}$
Formula weight	1830.07
Temperature/K	200
Crystal system	triclinic
Space group	$P\bar{1}$
a/Å	14.7673(5)
b/Å	16.6167(7)
c/Å	20.5716(8)
α/°	71.702(3)
β/°	89.043(3)
γ/°	88.782(3)
Volume/Å^3	4791.3(3)
Z	2
ρ_{calc}g/cm^3	1.268
μ/mm^{-1}	0.428
F(000)	1932.0
Crystal size/mm^3	0.15 × 0.04 × 0.03
Radiation	Ga Kα (λ = 1.34143)
2Θ range for data collection/°	5.208 to 110
Index ranges	–18 ≤ h ≤ 7, –20 ≤ k ≤ 20, –25 ≤ l ≤ 25
Reflections collected	63770
Independent reflections	17937 [R_{int} = 0.0560, R_{sigma} = 0.0501]
Ind. reflections with I ≥ 2σ (I)	11919
Data/restraints/parameters	17937/2/1238
Goodness-of-fit on F^2	1.071
Final R indexes [I ≥ 2σ (I)]	R_1 = 0.0811, wR_2 = 0.2404
Final R indexes [all data]	R_1 = 0.1119, wR_2 = 0.2587
Largest diff. peak/hole / e Å^{-3}	0.91/–0.63
CCDC number	2378167

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) da-si3

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: da-si3

```
Bond precision:   C-C = 0.0059 A          Wavelength=1.34143

Cell:           a=14.7673(5)       b=16.6167(7)      c=20.5716(8)
                alpha=71.702(3)    beta=89.043(3)    gamma=88.782(3)
Temperature:    200 K

                 Calculated                Reported
Volume           4791.3(3)                 4791.3(3)
Space group      P -1                      P -1
Hall group       -P 1                      -P 1
Moiety formula   C86 H40 N6 O6, 8(C4 H8 O) C86 H40 N6 O6, 8(C4 H8 O)
Sum formula      C118 H104 N6 O14          C118 H104 N6 O14
Mr               1830.07                   1830.07
Dx,g cm-3        1.268                     1.268
Z                2                         2
Mu (mm-1)        0.424                     0.428
F000             1932.0                    1932.0
F000'            1936.33
h,k,lmax                                   18,20,25
Nref                                       17937
Tmin,Tmax        0.980,0.987               0.940,0.988
Tmin'            0.938

Correction method= # Reported T Limits: Tmin=0.940 Tmax=0.988
AbsCorr = MULTI-SCAN

Data completeness=                 Theta(max)= 55.000

R(reflections)= 0.0811( 11919)                    wR2(reflections)=
                                                  0.2587( 17937)
S = 1.071                  Npar= 1238
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The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level A

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PLAT733_ALERT_1_A Torsion Calc   179.8(15), Rep     180(99) ......        9.90 s.u.-R
             C73 -C74 -C77 -C78   1_555  1_555  1_555  1_555      #  234 Check
```

Alert level B

```
PLAT097_ALERT_2_B Large Reported Max.  (Positive) Residual Density        0.91 eA-3
PLAT411_ALERT_2_B Short Inter H...H Contact  H10F     ..H88B     .        1.97 Ang.
                                                 x,1+y,z  =      1_565 Check
```

Alert level C

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DIFMN02_ALERT_2_C  The minimum difference density is < -0.1*ZMAX*0.75
            _refine_diff_density_min given =     -0.633
            Test value =     -0.600
DIFMN03_ALERT_1_C  The minimum difference density is < -0.1*ZMAX*0.75
            The relevant atom site should be identified.
DIFMX02_ALERT_1_C  The maximum difference density is > 0.1*ZMAX*0.75
            The relevant atom site should be identified.
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ...................       0.26 Report
PLAT098_ALERT_2_C Large Reported Min.  (Negative) Residual Density      -0.63 eA-3
PLAT243_ALERT_4_C High   'Solvent' Ueq as Compared to Neighbors of        C88 Check
PLAT243_ALERT_4_C High   'Solvent' Ueq as Compared to Neighbors of        C92 Check
PLAT243_ALERT_4_C High   'Solvent' Ueq as Compared to Neighbors of        C96 Check
PLAT243_ALERT_4_C High   'Solvent' Ueq as Compared to Neighbors of        O10 Check
PLAT243_ALERT_4_C High   'Solvent' Ueq as Compared to Neighbors of       C101 Check
PLAT243_ALERT_4_C High   'Solvent' Ueq as Compared to Neighbors of       C104 Check
PLAT243_ALERT_4_C High   'Solvent' Ueq as Compared to Neighbors of       C105 Check
PLAT243_ALERT_4_C High   'Solvent' Ueq as Compared to Neighbors of        O13 Check
PLAT243_ALERT_4_C High   'Solvent' Ueq as Compared to Neighbors of       C112 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of        C87 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of        C91 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of        C94 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of        C95 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of        C97 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of        C99 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of       C102 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of        O11 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of       C103 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of       C106 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of       C107 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of       C111 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of       C114 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including        O7      0.114 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including        O8      0.119 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including        O9      0.122 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       O10      0.181 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       O11      0.191 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       O13      0.181 Check
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PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C101     - C102     .       1.41 Ang.
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PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C105     - C106     .       1.42 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C109     - C110     .       1.43 Ang.
PLAT373_ALERT_2_C Long   C(sp)-C(sp)   Bond  C56      - C57      .       1.36 Ang.
PLAT373_ALERT_2_C Long   C(sp)-C(sp)   Bond  C72      - C73      .       1.36 Ang.
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PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600        310 Report
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              14 -5  2,  -2 -3  2,   5 -2  2,   6 -2  2,  -4 -1  2,  -3  0  2,
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PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .         15 Check
PLAT977_ALERT_2_C Check Negative Difference Density on H89B      .      -0.33 eA-3
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Alert level G

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ABSMU01_ALERT_1_G  Calculation of _exptl_absorpt_correction_mu
                   not performed for this radiation type.
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          3 Note
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical          ? Check
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.18 Report
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)      0.003 Degree
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          2 Report
PLAT300_ALERT_4_G Atom Site Occupancy of O14A       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C115       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C116       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C117       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C118       Constrained at        0.5 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of H11L       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H11M       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H11N       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H11O       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H11P       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H11Q       Constrained at        0.5 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of C18B       Constrained at        0.5 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of H15A       Constrained at        0.5 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of H16B       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H17A       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H17B       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H18A       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H18B       Constrained at        0.5 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  9  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 10  )       100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  9  )       6.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 10  )       6.50 Check
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C52      - C55       .       1.43 Ang.
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C58      - C61       .       1.43 Ang.
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C68      - C71       .       1.43 Ang.
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C74      - C77       .       1.42 Ang.
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PLAT398_ALERT_2_G Deviating  C-O-C   Angle From 120 for O11       .      107.0 Degree
PLAT398_ALERT_2_G Deviating  C-O-C   Angle From 120 for O12       .      108.4 Degree
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PLAT411_ALERT_2_G Short Inter H...H Contact  H11N     ..H32       .       1.95 Ang.
                                                     x,y,z  =      1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  O8       ..C8        .       2.94 Ang.
                                                     x,y,z  =      1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  O11      ..C1        .       2.93 Ang.
                                                     x,y,z  =      1_555 Check
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C15B     --C16B             1.93 Ang.
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #         13 Check
PLAT822_ALERT_4_G CIF-embedded .res Contains Negative PART Numbers          1 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         2 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .    Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          2 Note
               0  1  0,   0  0  1,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         16 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          1 Note
               1 -2  1,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        3.6 Low
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities .......    Please Check
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res ..      110.0 Degree
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          1 Info
PLAT984_ALERT_1_G The  C-f'=    0.0148 Deviates from the B&C-Value     0.0137 Check
PLAT984_ALERT_1_G The  N-f'=    0.0253 Deviates from the B&C-Value     0.0241 Check
PLAT984_ALERT_1_G The  O-f'=    0.0412 Deviates from the B&C-Value     0.0389 Check
```

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  1 ALERT level A = Most likely a serious problem - resolve or explain
  2 ALERT level B = A potentially serious problem, consider carefully
 47 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 64 ALERT level G = General information/check it is not something unexpected

 10 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 38 ALERT type 2 Indicator that the structure model may be wrong or deficient
  8 ALERT type 3 Indicator that the structure quality may be low
 56 ALERT type 4 Improvement, methodology, query or suggestion
  2 ALERT type 5 Informative message, check
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

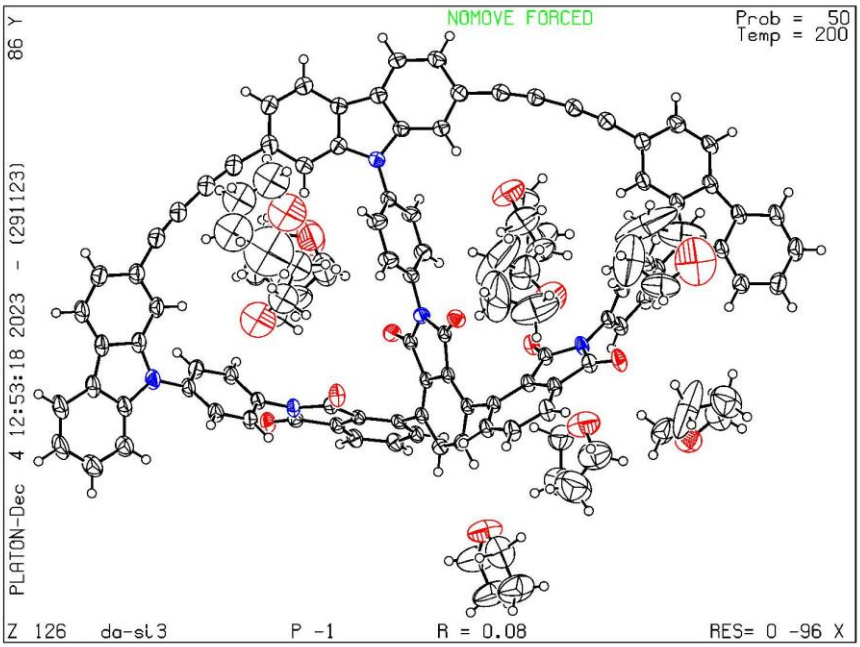
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 29/11/2023; check.def file version of 14/09/2023

Datablock da-si3 - ellipsoid plot



NMR Spectra

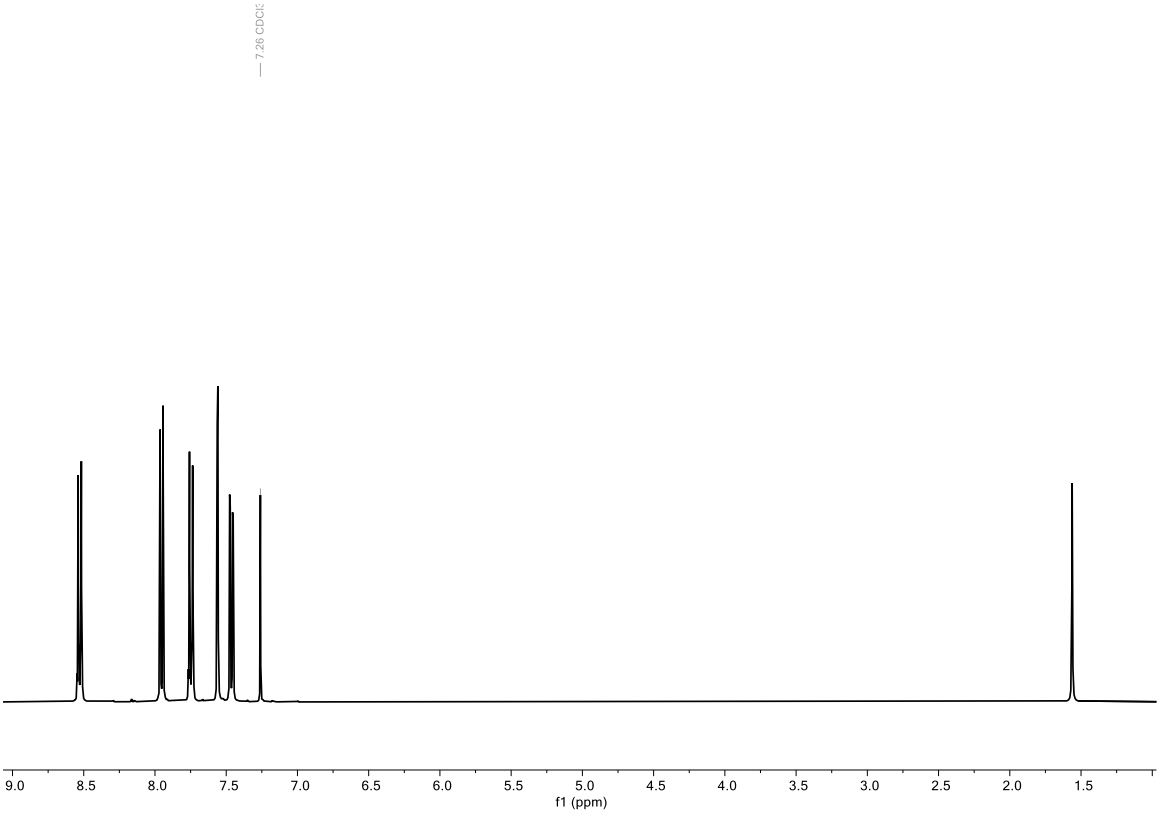


Figure S12. ^{1}H-NMR(400MHz, THF-d8, 298K) of **2**.

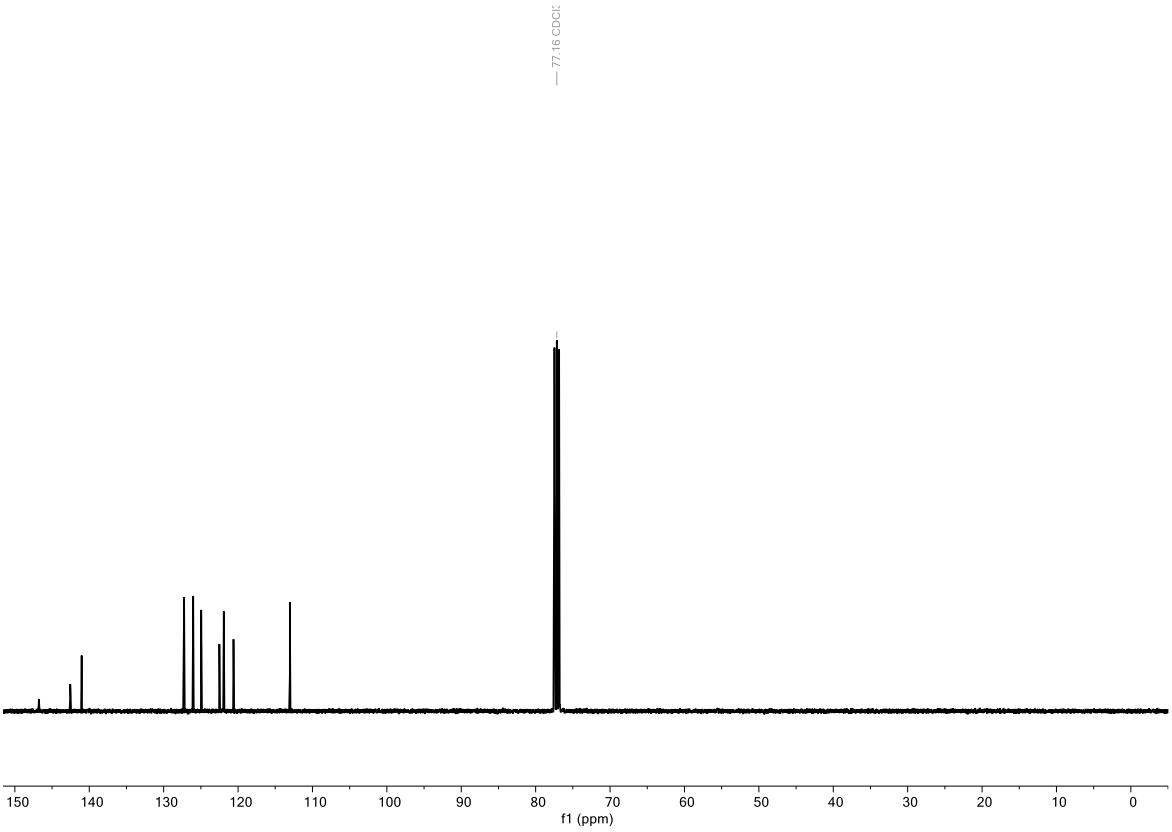


Figure S13. ^{13}C-NMR(101 MHz, THF-d8, 298K) of **2**.

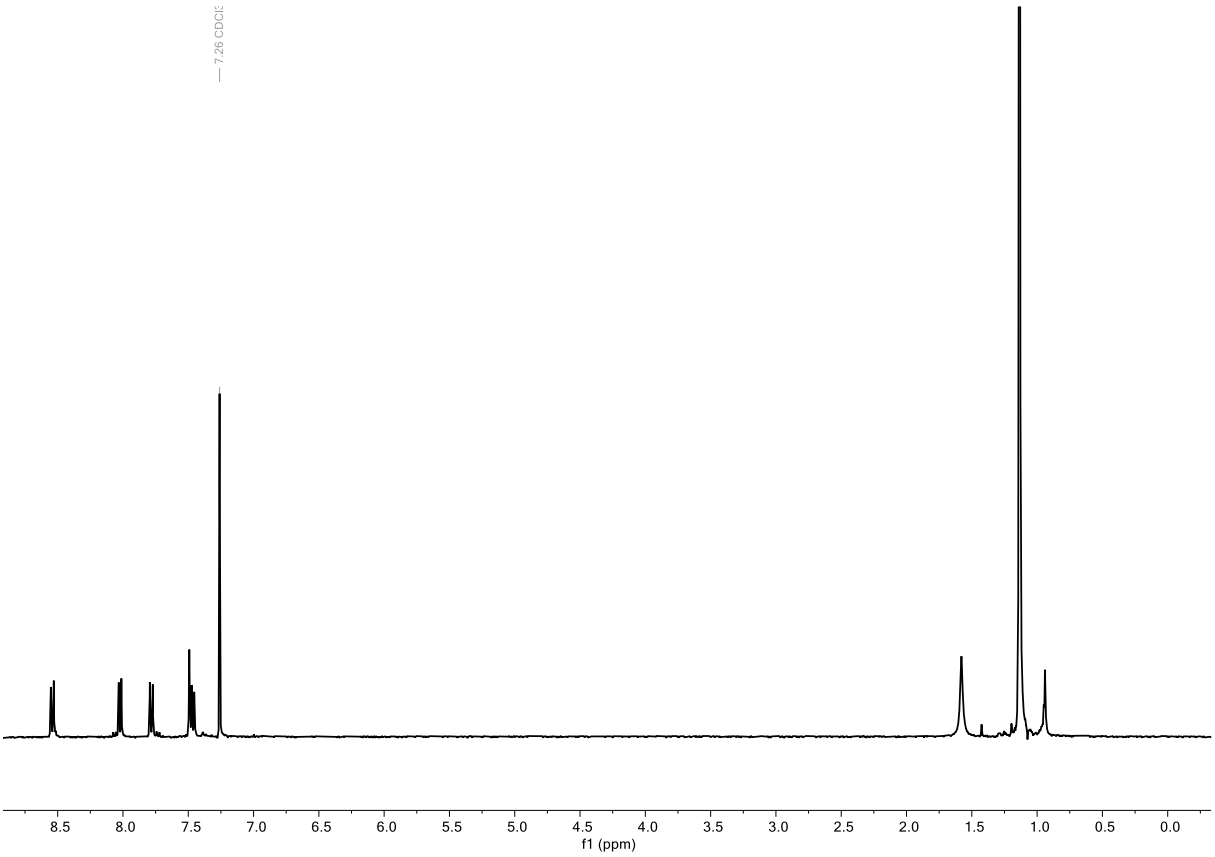


Figure S14. ^{1}H-NMR(400MHz, THF-d8, 298K) of **4**.

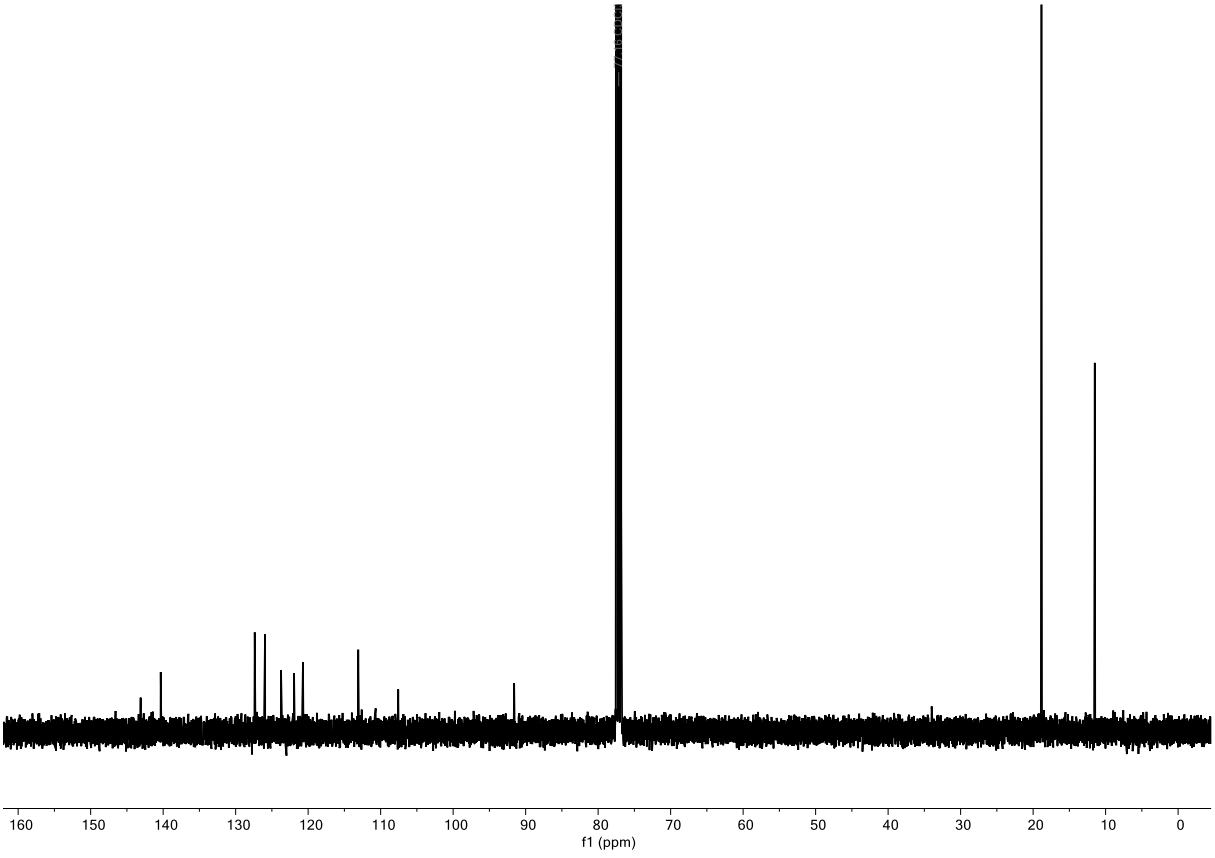


Figure S15. ^{13}C-NMR(101 MHz, THF-d8, 298K) of **4**.

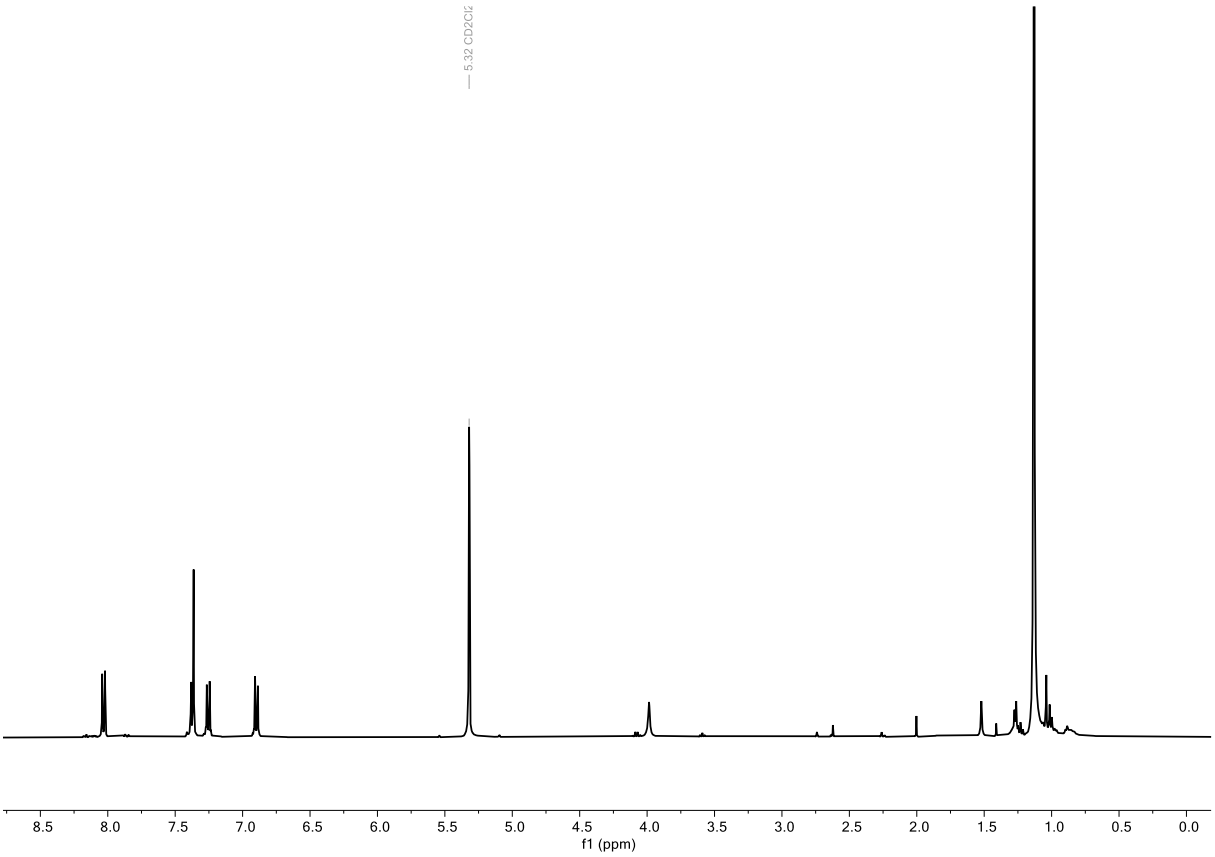


Figure S16. ^{1}H-NMR(400MHz, THF-d8, 298K) of **6**.

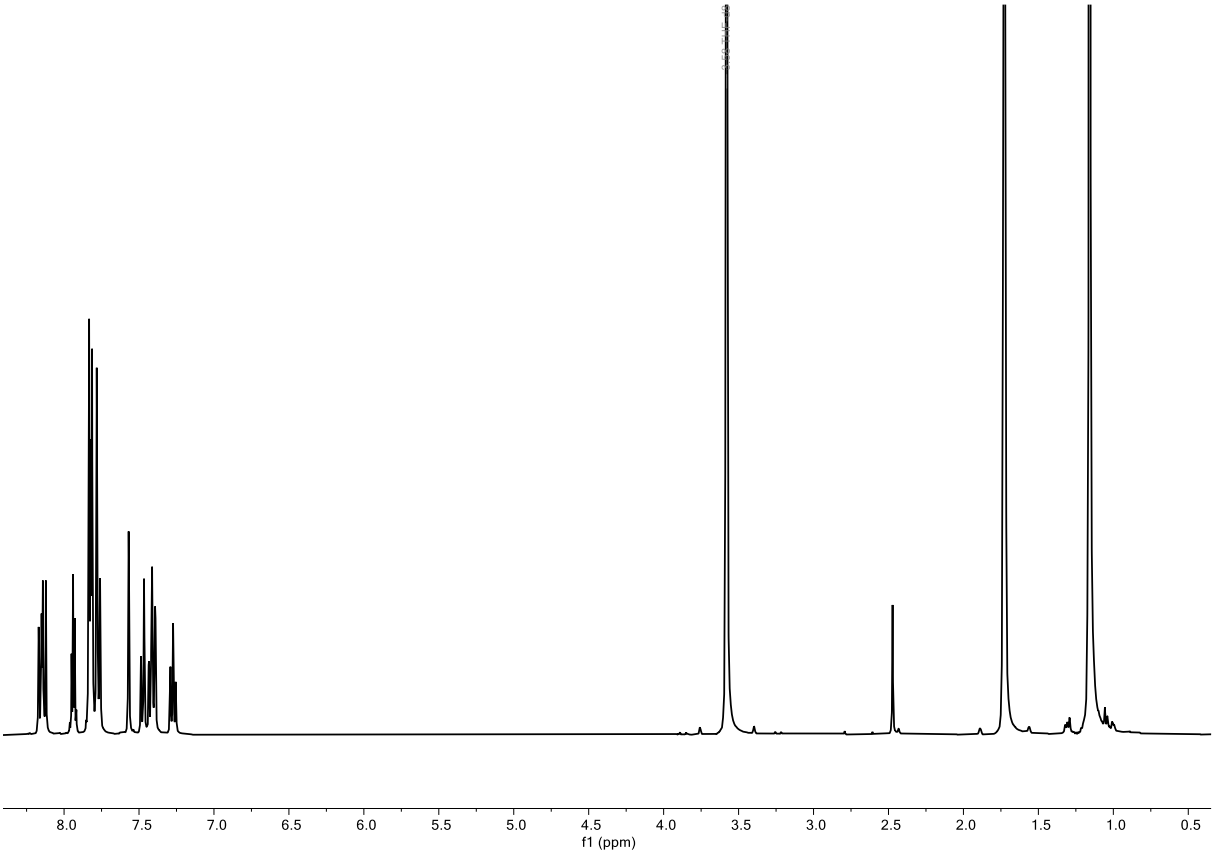


Figure S17. ^{1}H-NMR(400MHz, THF-d8, 298K) of $\mathbf{EC_{Cl}}$.

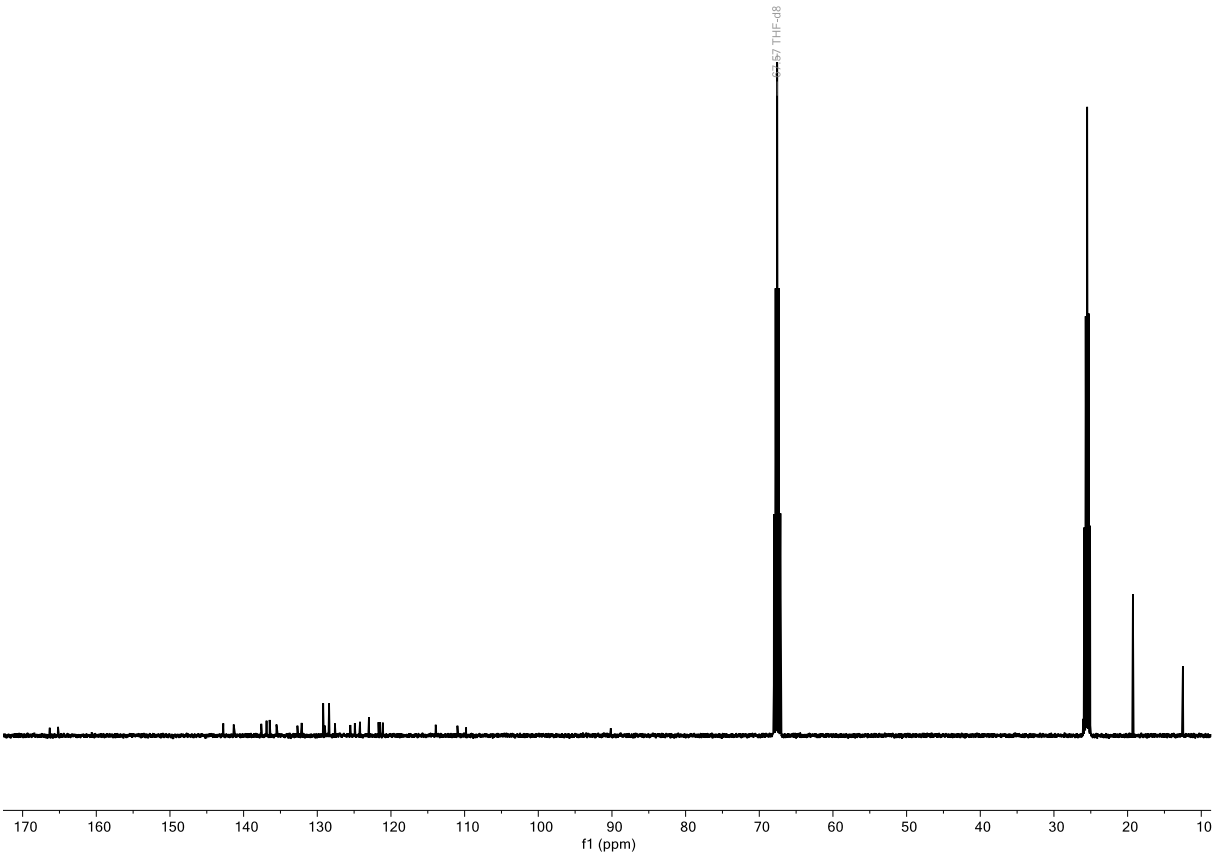


Figure S18. ^{13}C-NMR(101 MHz, THF-d8, 298K) of $\mathbf{EC_{Cl}}$.

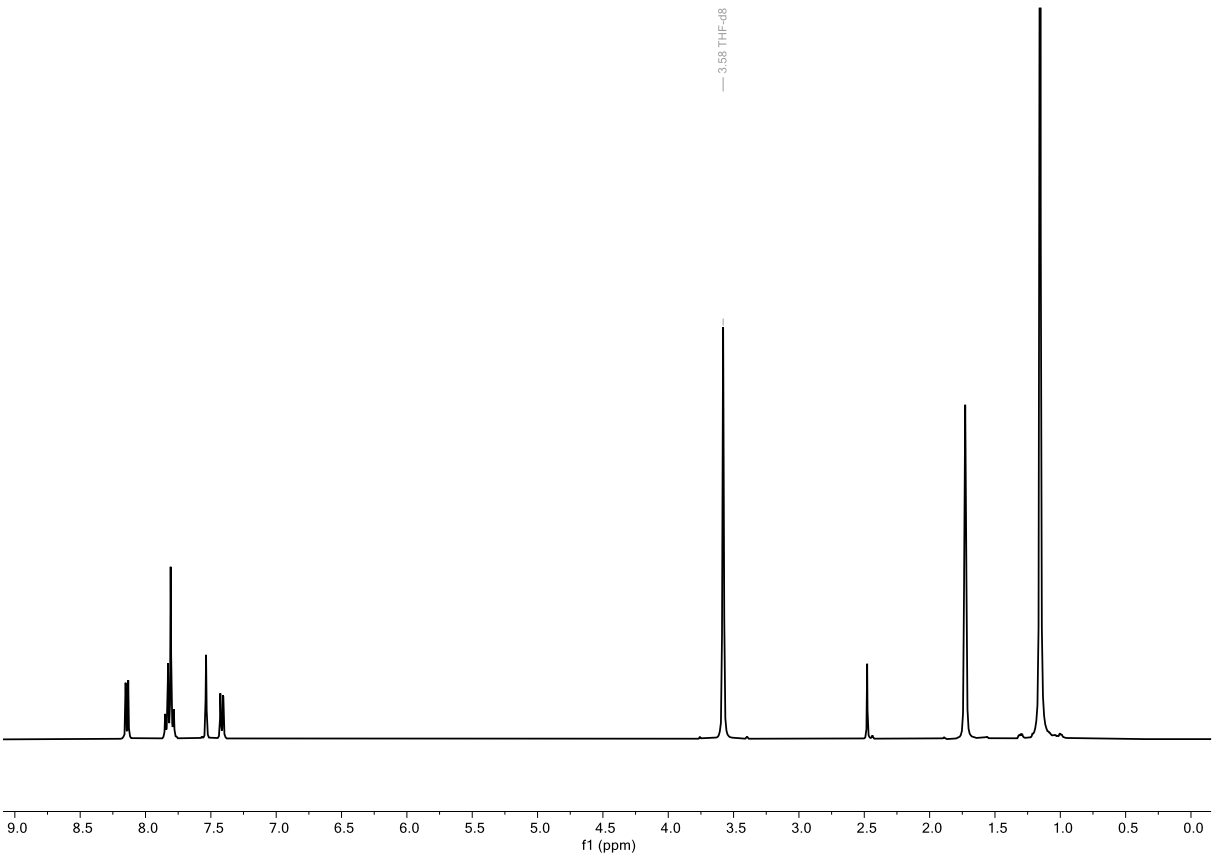


Figure S19. ^{1}H-NMR(400MHz, THF-d8, 298K) of $\mathbf{M_{Cl}}$.

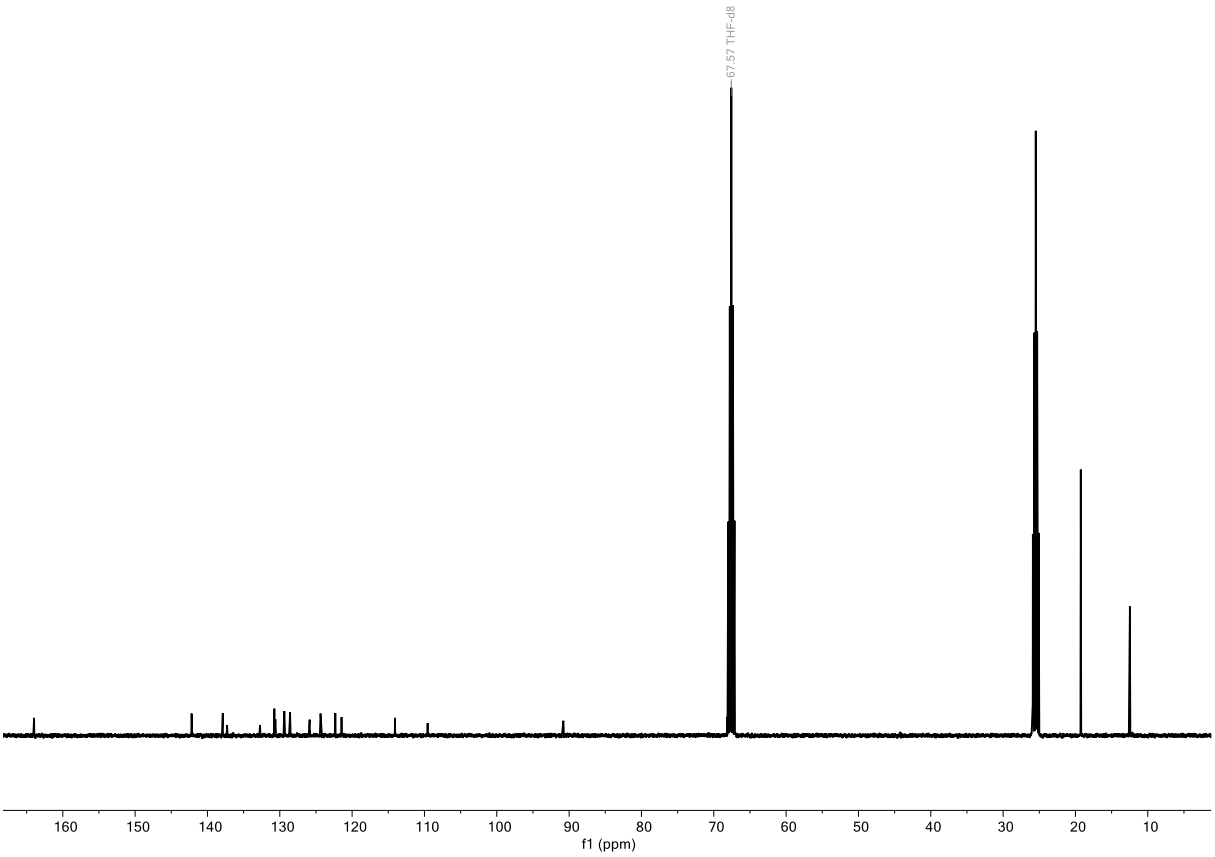


Figure S20. ^{13}C-NMR(101 MHz, THF-d8, 298K) of $\mathbf{M_{Cl}}$.

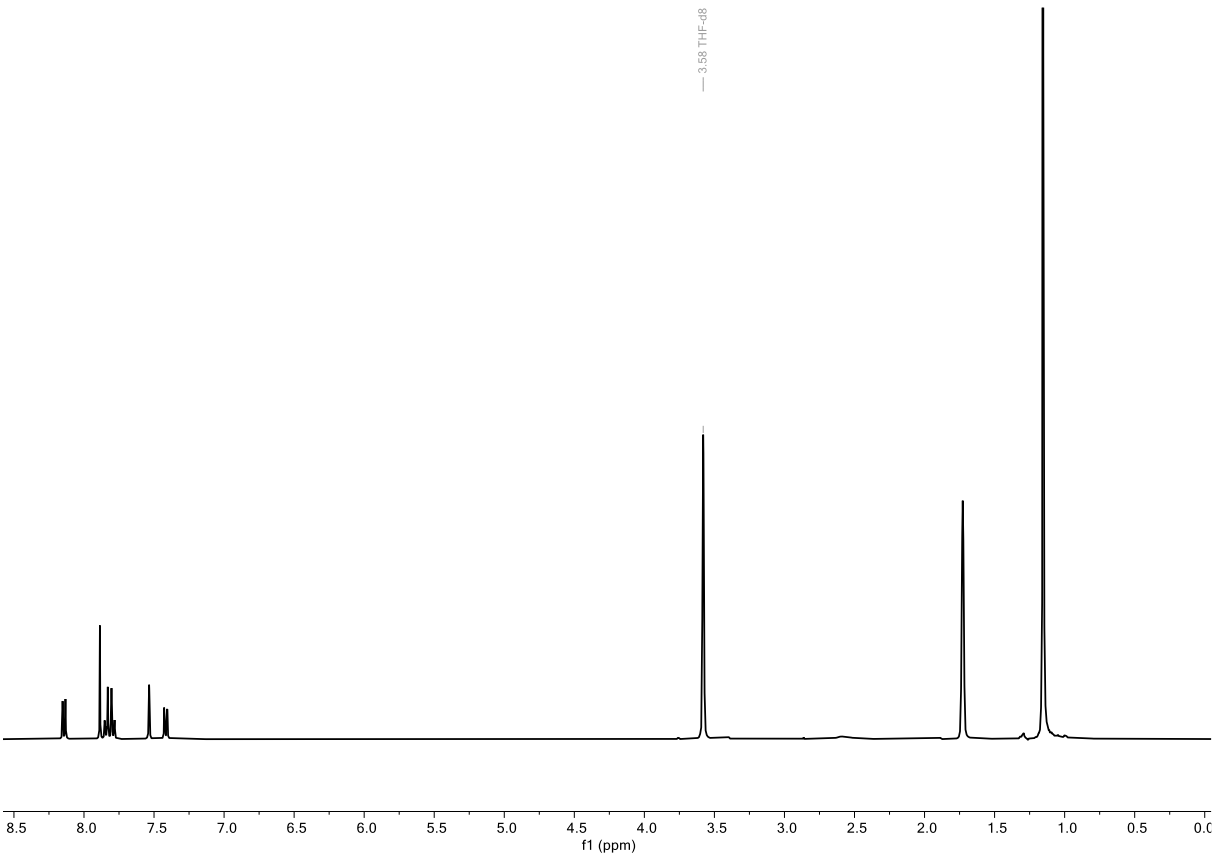


Figure S21. ^{1}H-NMR(400MHz, THF-d8, 298K) of $\mathbf{M_{Br}}$.

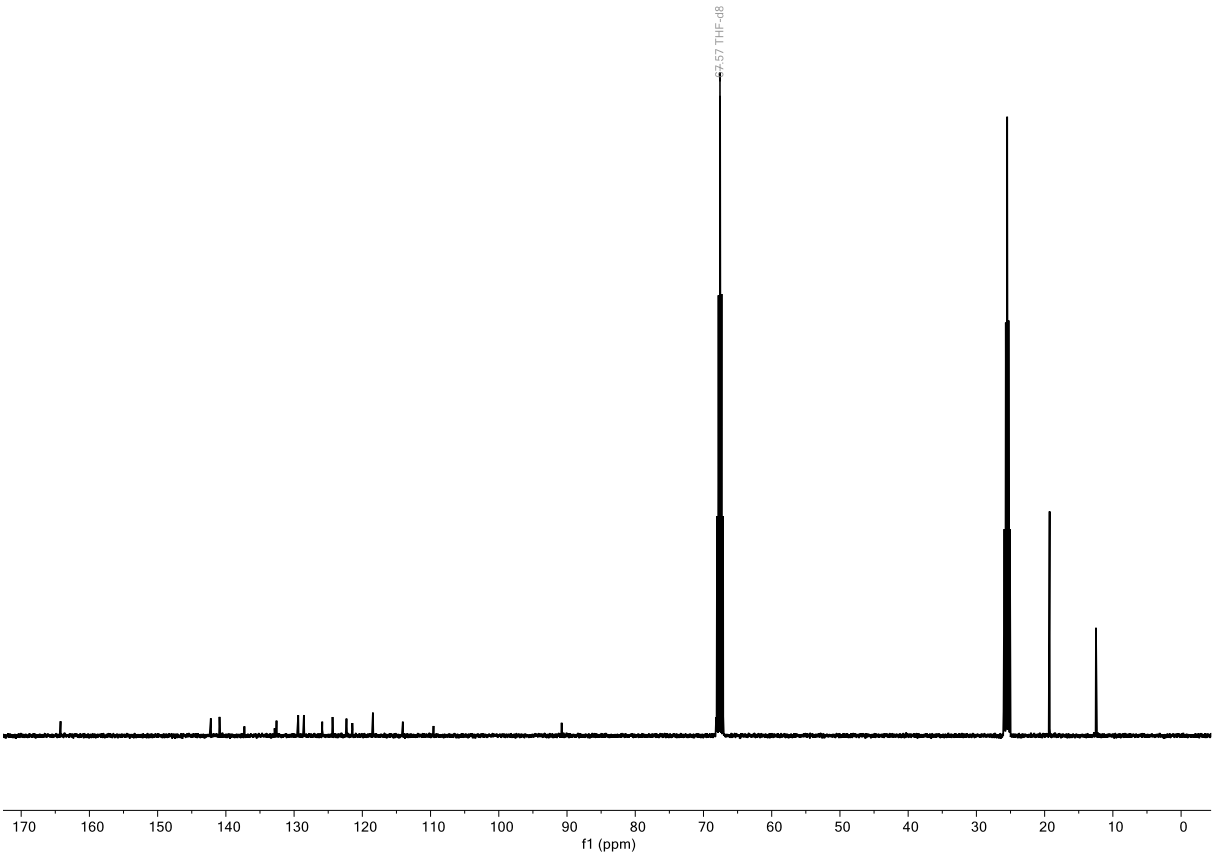


Figure S22. ^{13}C-NMR(101 MHz, THF-d8, 298K) of $\mathbf{M_{Br}}$.

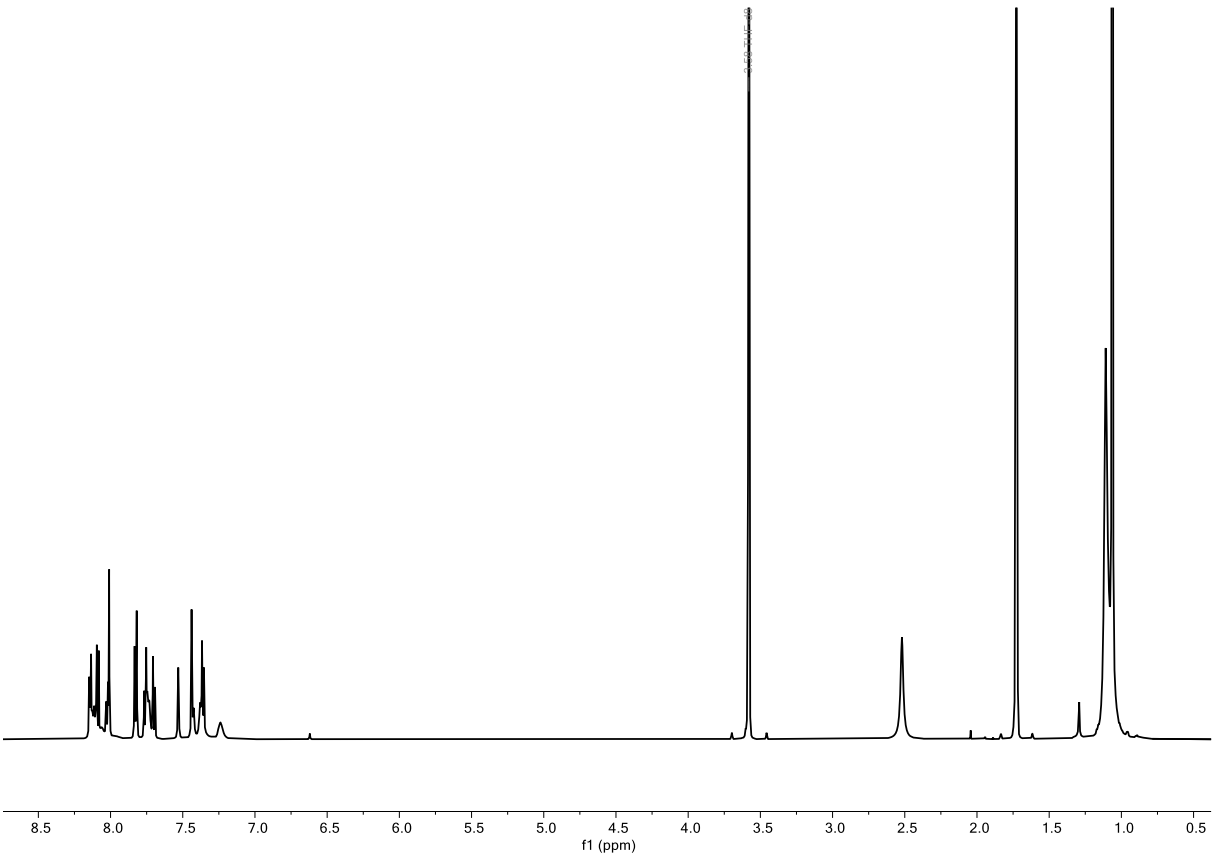


Figure S23. ^{1}H-NMR(600MHz, THF-d8, 298K) of **A[3]**.

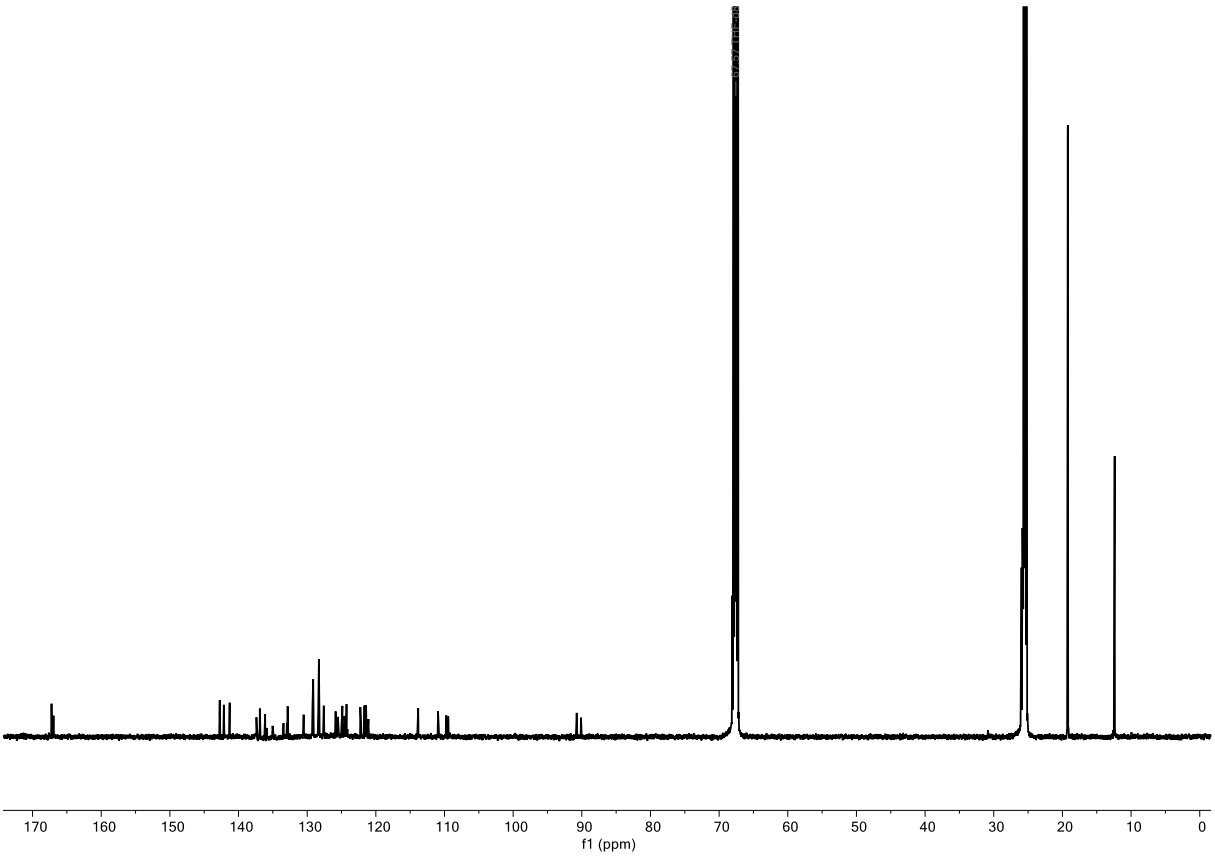


Figure S24. ^{13}C-NMR(151 MHz, THF-d8, 298K) of **A[3]**.

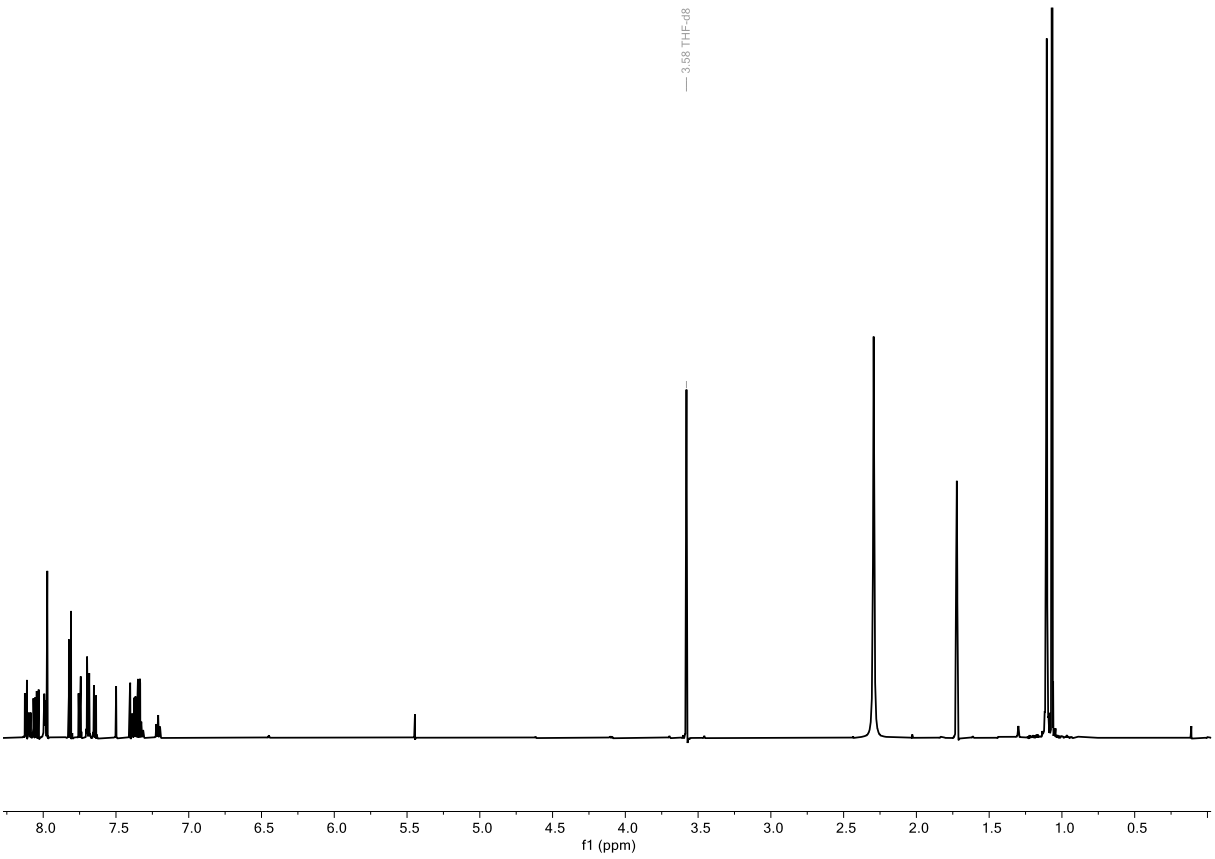


Figure S25. ^{1}H-NMR(600MHz, THF-d8, 333K) of **A[3]**.

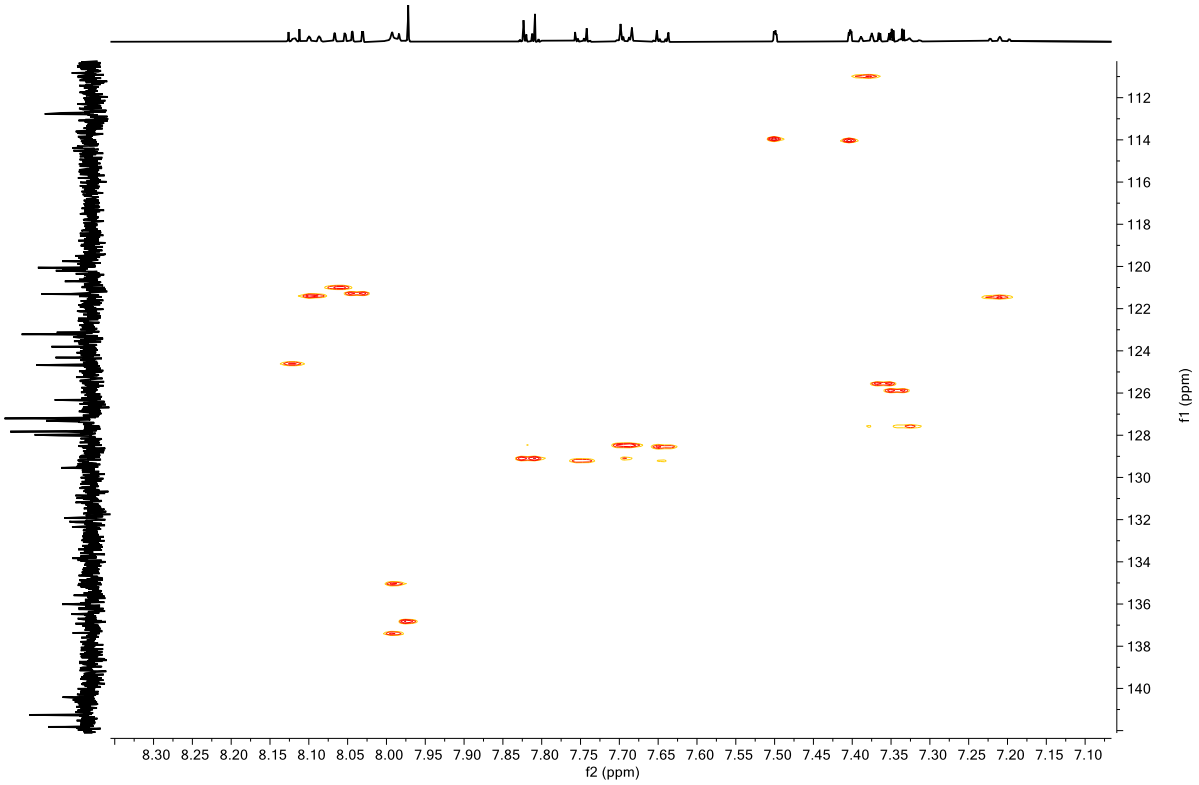


Figure S26. High resolution HSQC-NMR(600MHz, THF-d8, 333K) of **A[3]**.

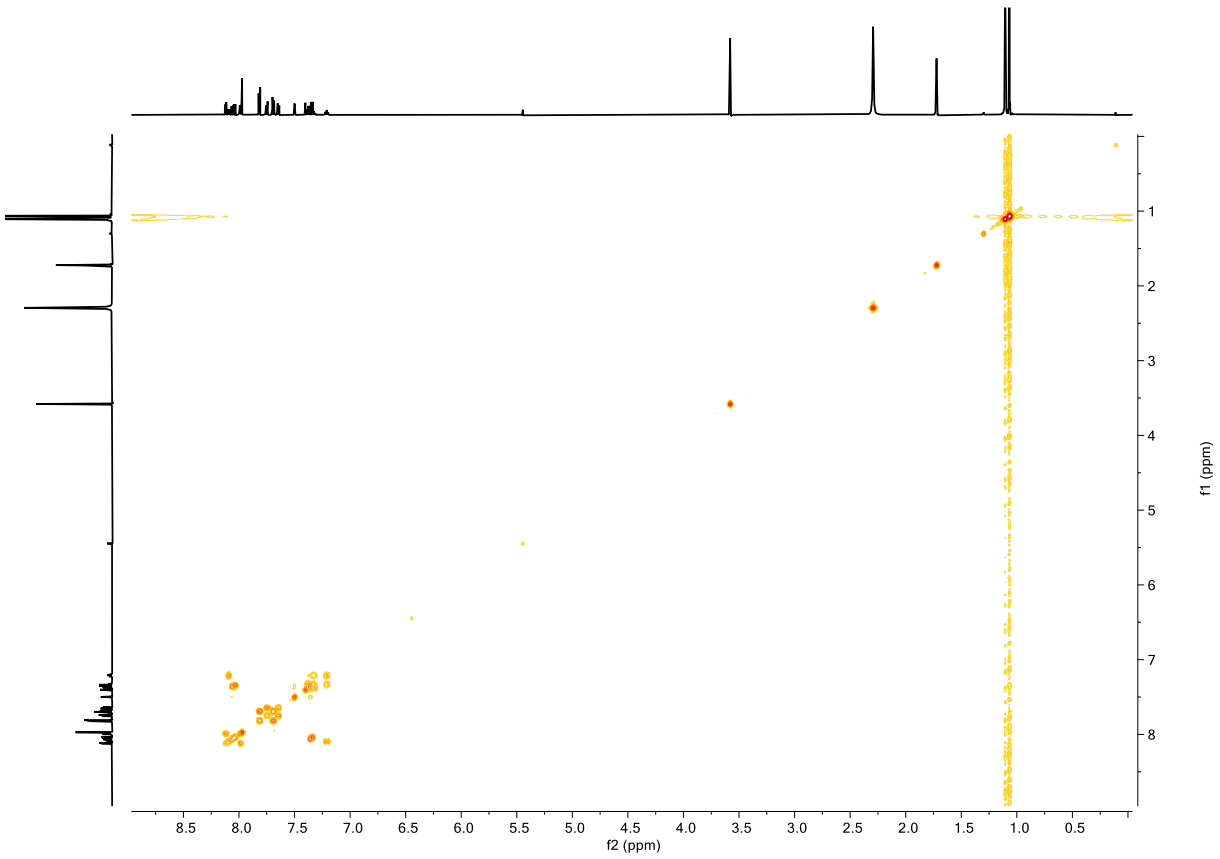


Figure S27. COSY-NMR(600MHz, THF-d8, 333K) of **A[3]**.

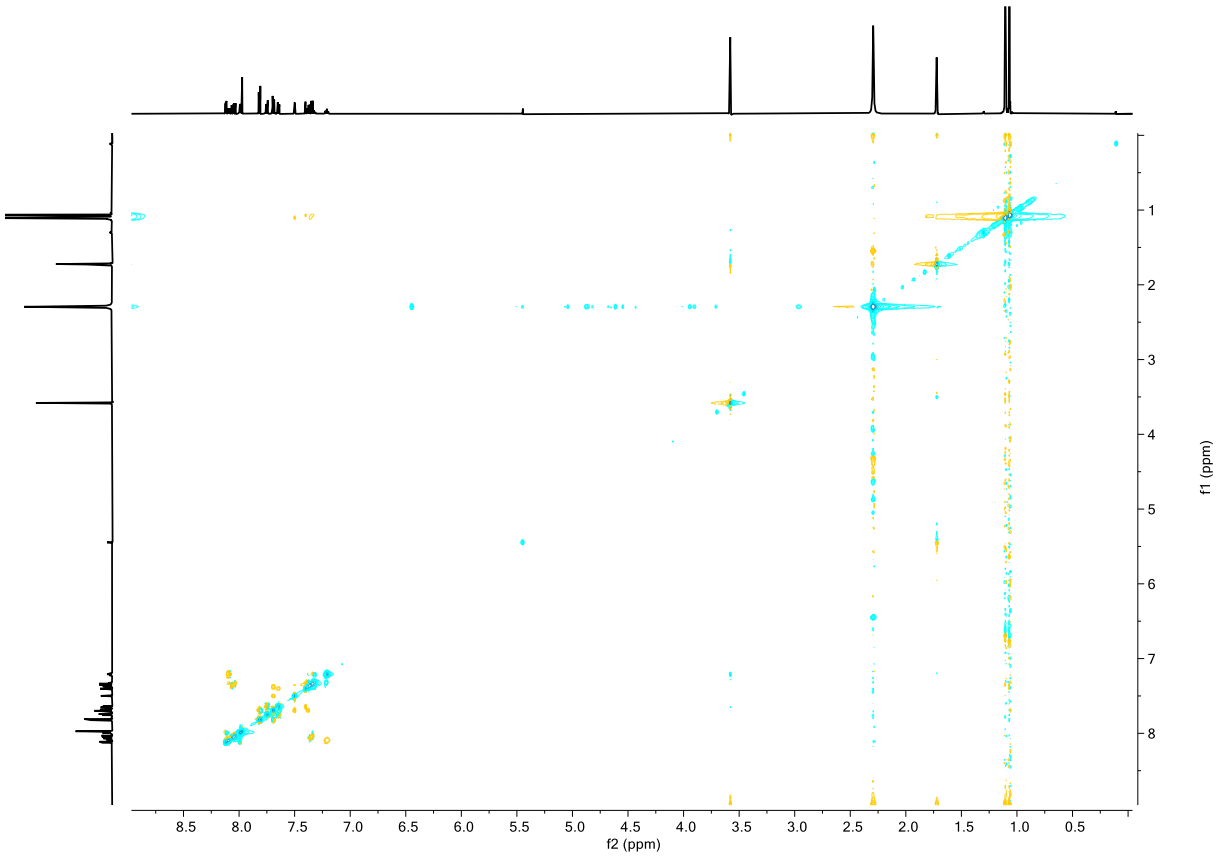


Figure S28. NOESY-NMR(600 MHz, THF-d8, 333 K) of **A[3]**

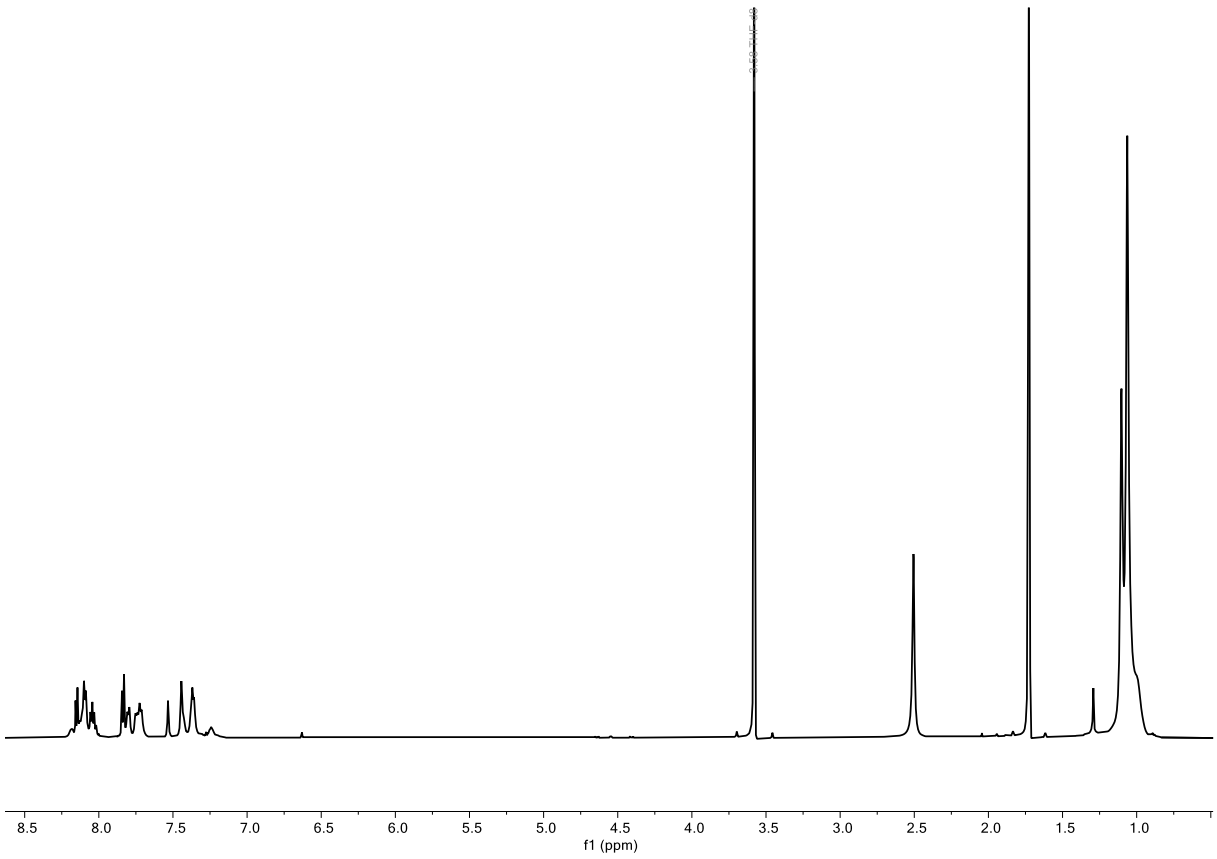


Figure S29. ^{1}H-NMR(600 MHz, THF-d8, 298 K) of **A[4]**

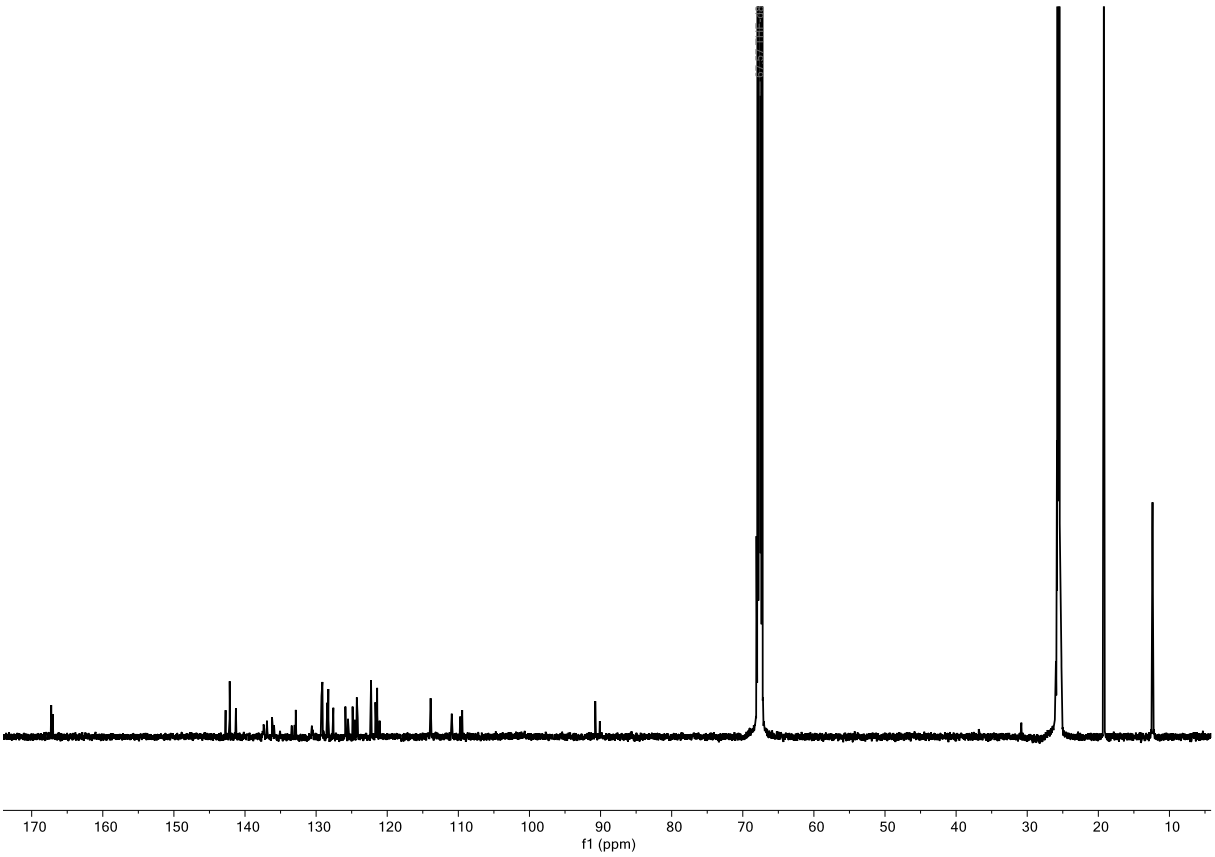


Figure S30. ^{13}C-NMR(151 MHz, THF-d8, 298 K) of **A[4]**

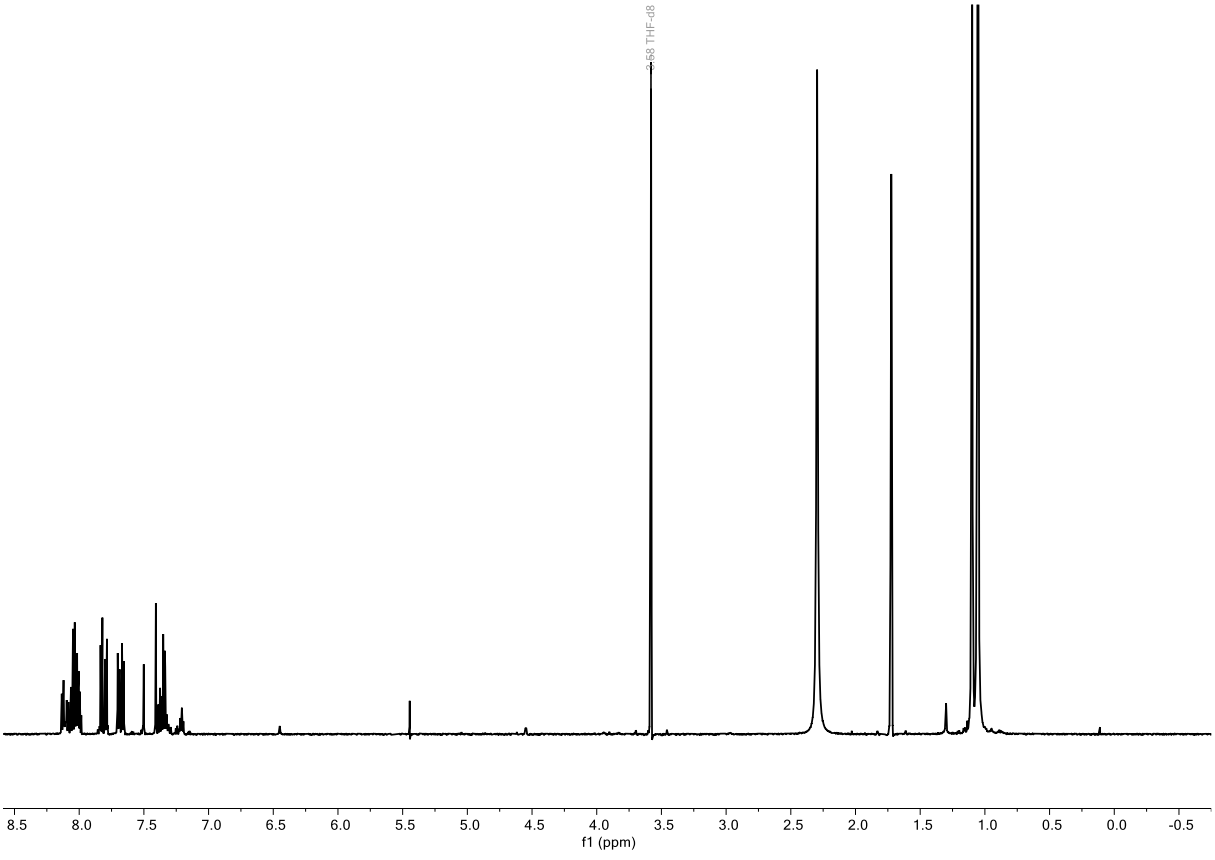


Figure S31. ^{1}H-NMR(600 MHz, THF-d8, 333 K) of **A[4]**

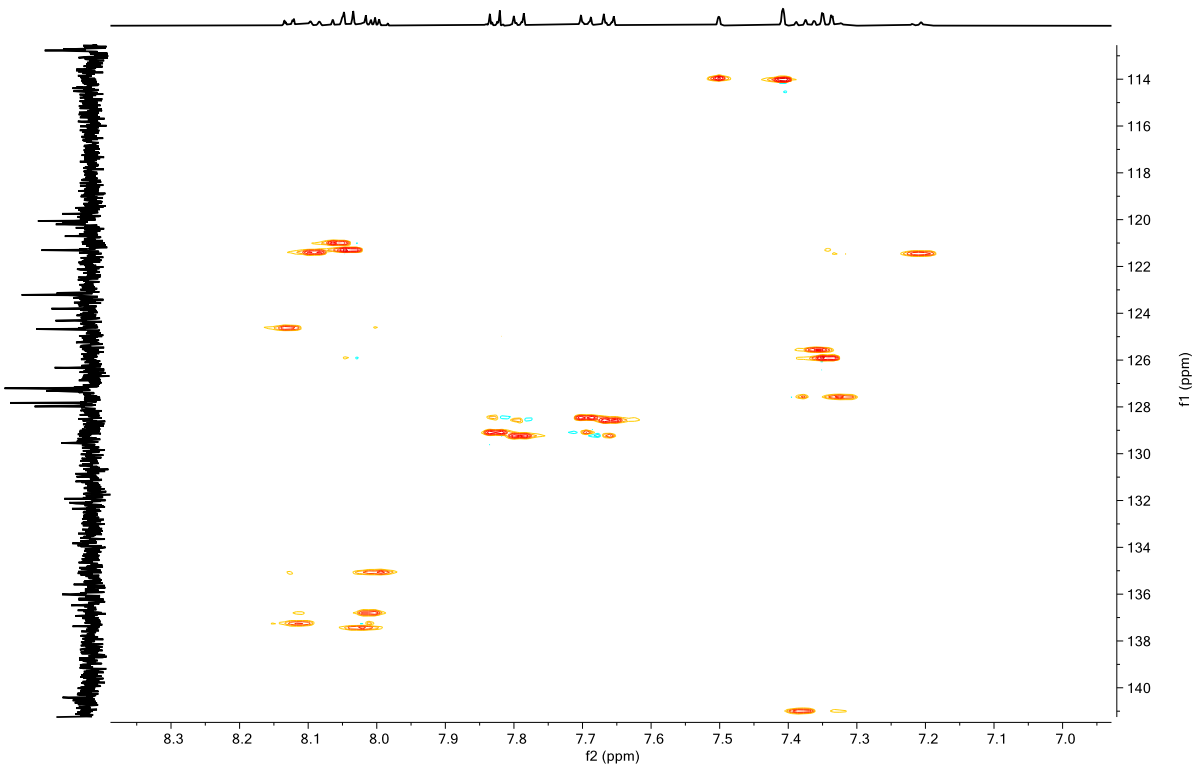


Figure S32. High resolution HSQC-NMR(600 MHz, THF-d8, 333 K) of **A[4]**

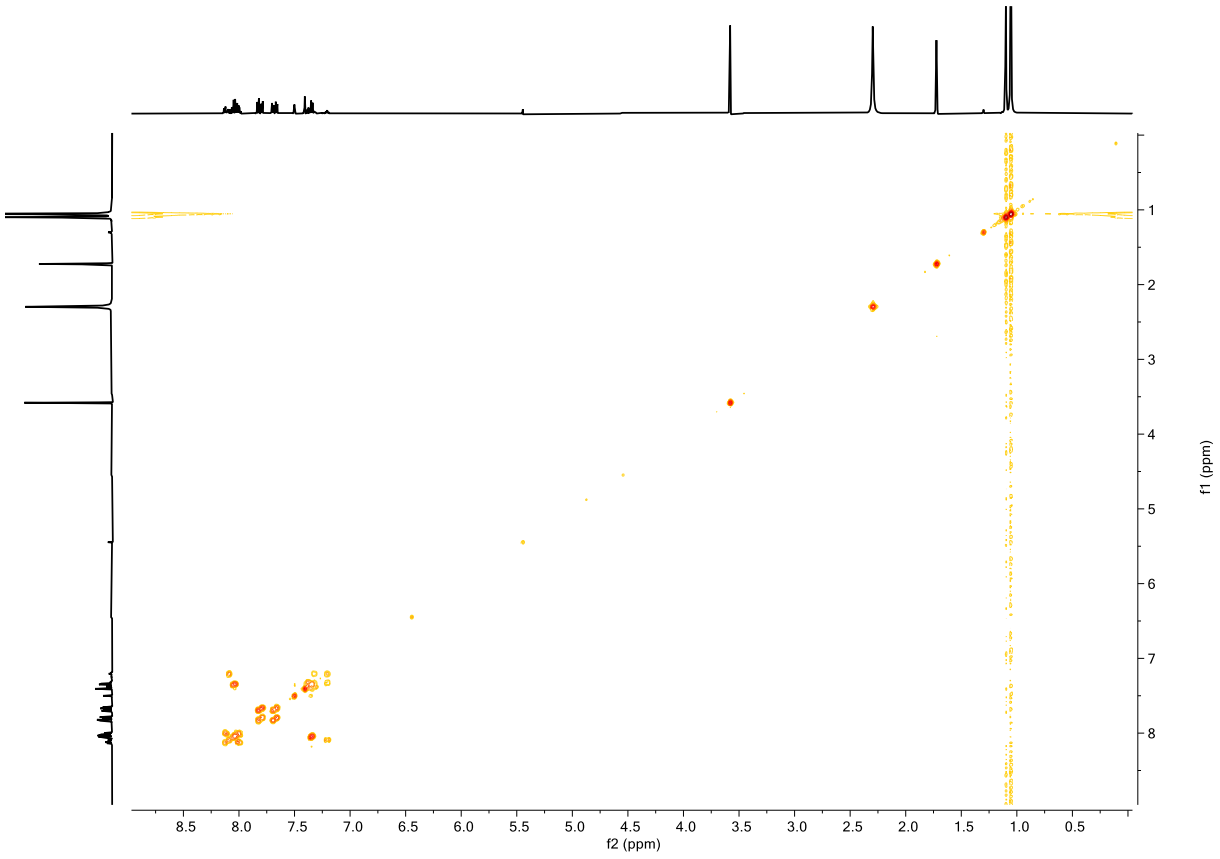


Figure S33. COSY-NMR(600 MHz, THF-d8, 333 K) of **A[4]**

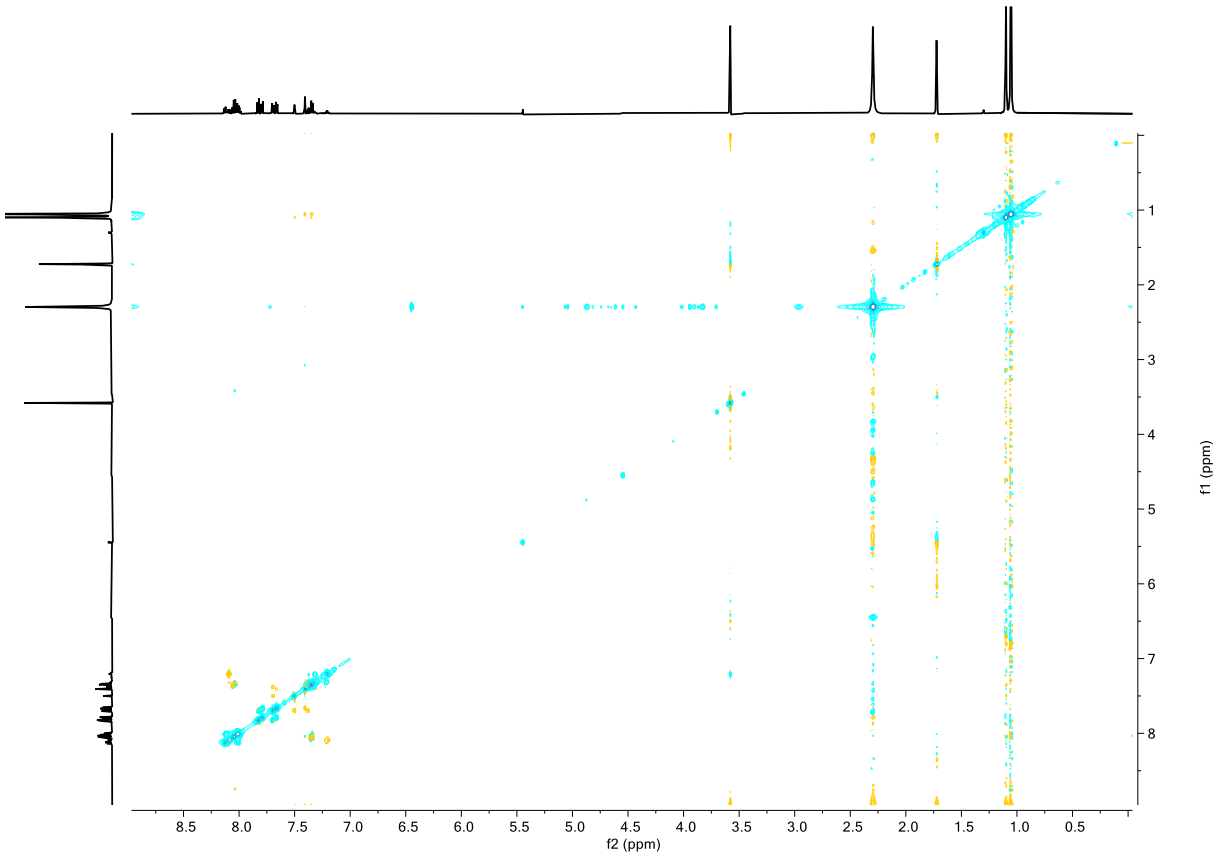


Figure S34. NOESY-NMR(600 MHz, THF-d8, 333 K) of **A[4]**

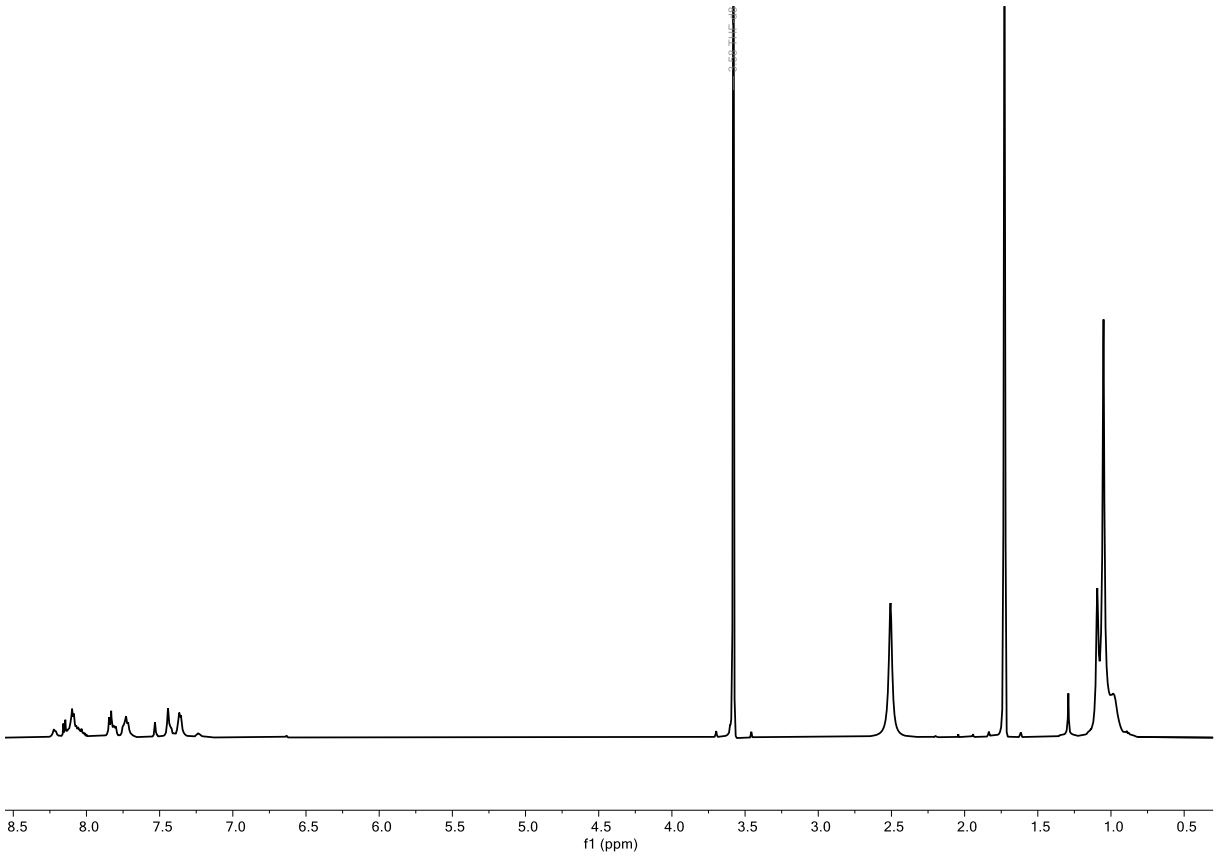


Figure S35. ^{1}H-NMR(600 MHz, THF-d8, 298 K) of **A[5]**

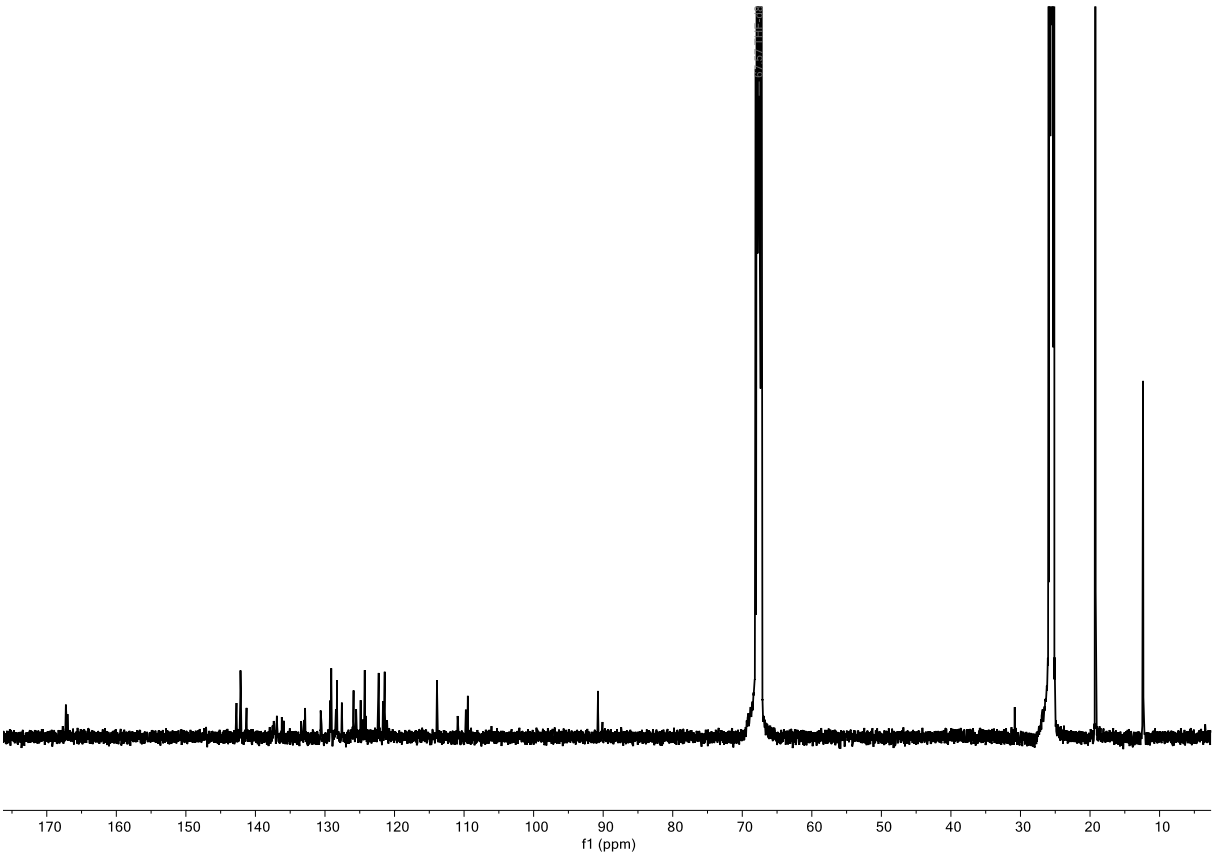


Figure S36. ^{13}C-NMR(126 MHz, THF-d8, 298 K) of **A[5]**

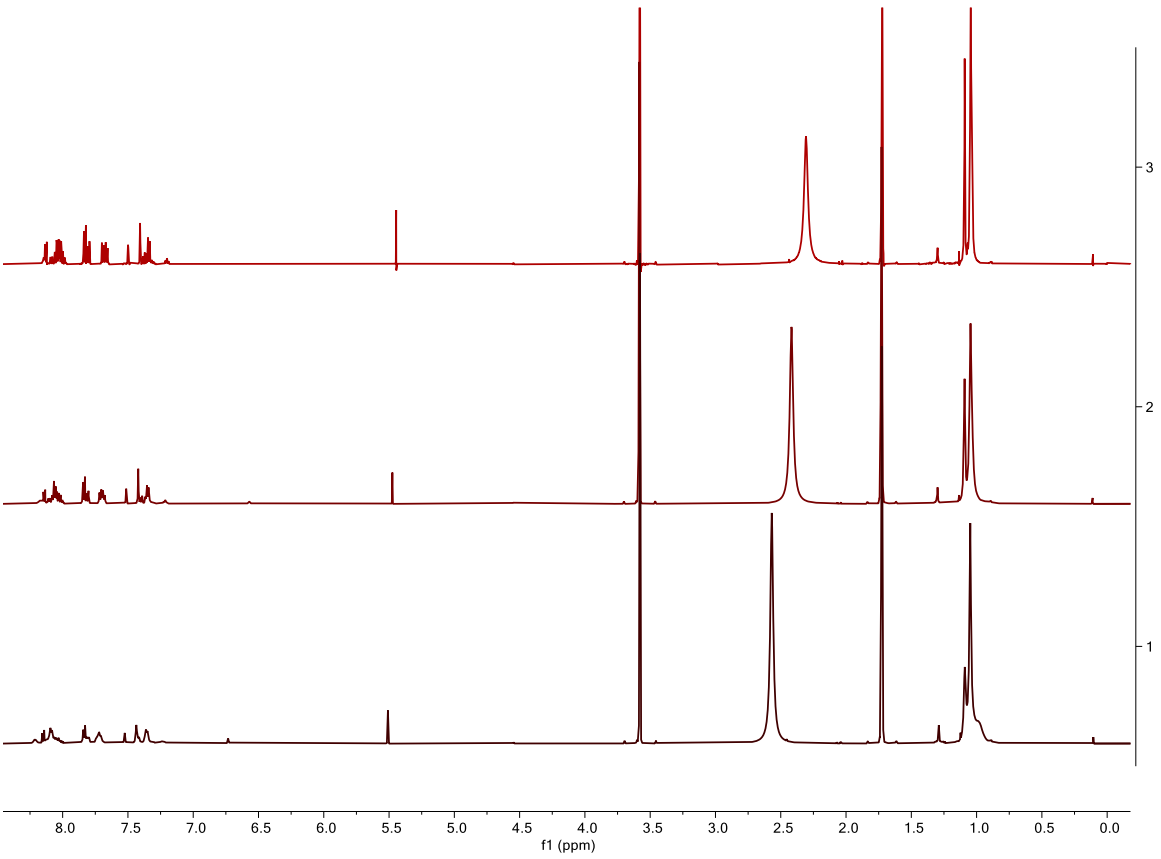


Figure S37. ^{1}C-NMR(600 MHz, THF-d8) of **A[5]**, top to bottom 333 K, 318 K, and 293 K..

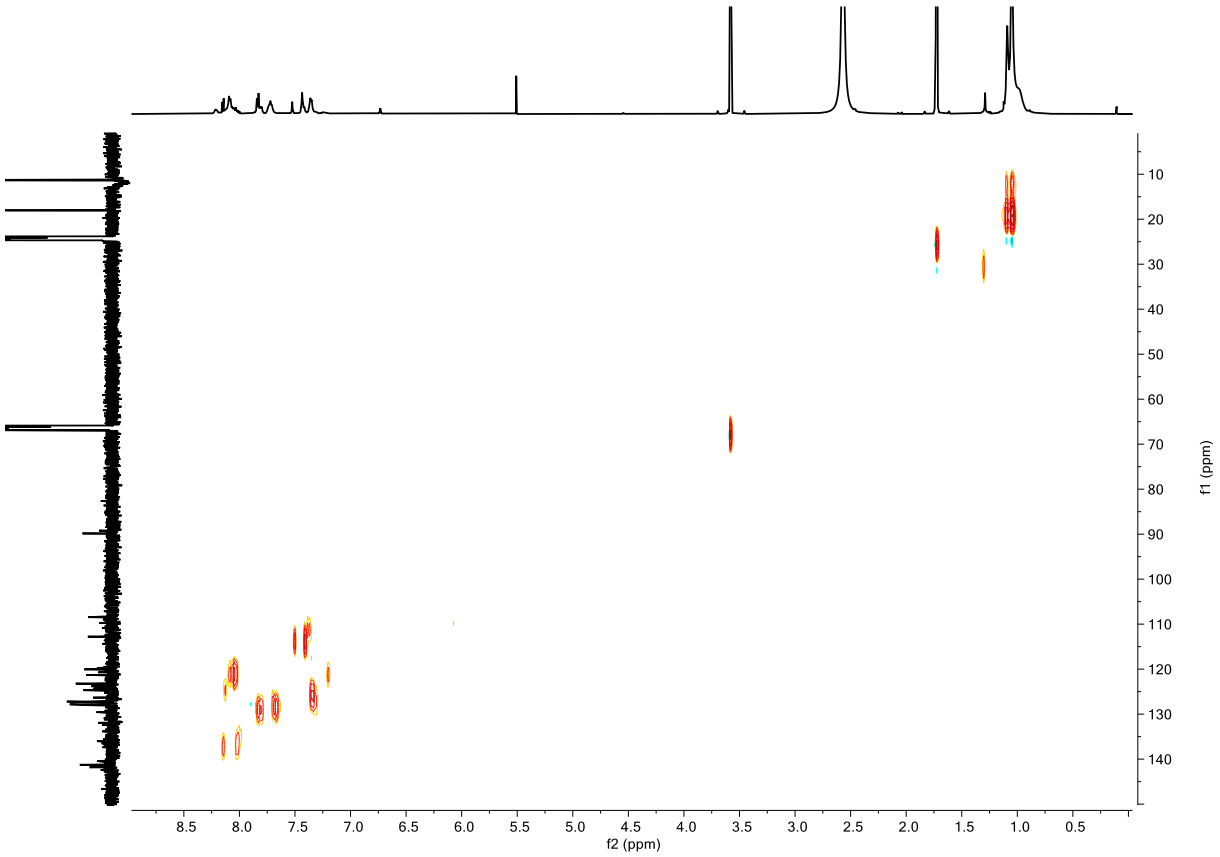


Figure S38. HSQC-NMR(600 MHz, THF-d8, 333 K) of **A[5].**

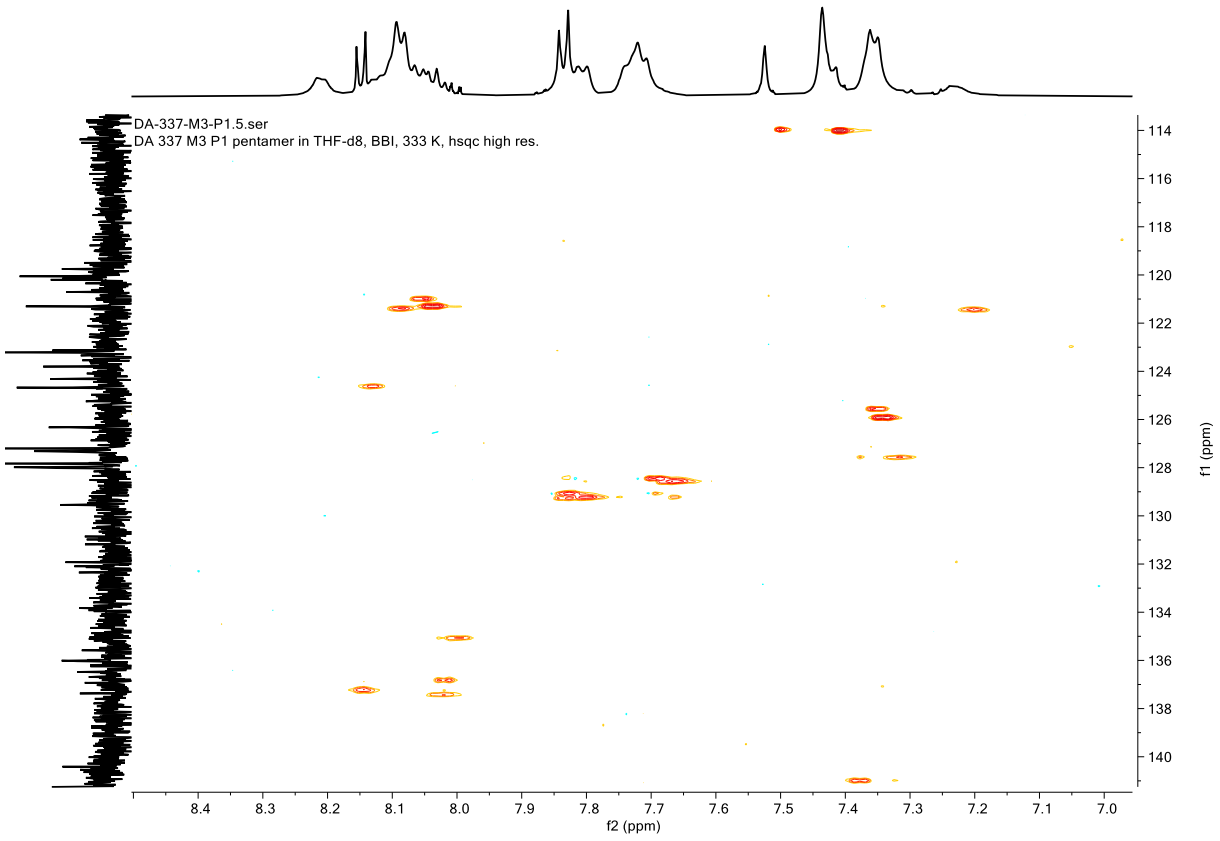


Figure S39. High resolution HSQC-NMR(600 MHz, THF-d8, 333 K) of **A[5].**

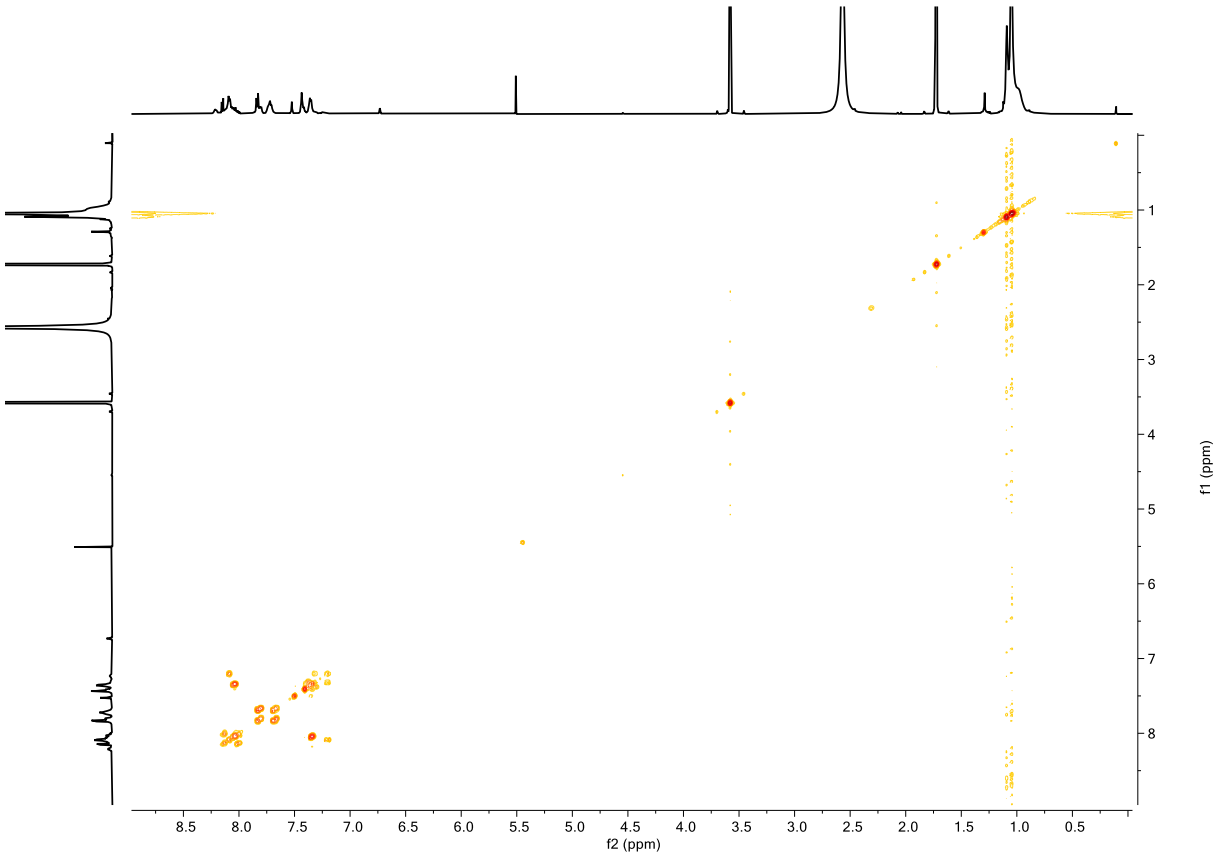


Figure S40. COSY-NMR(600 MHz, THF-d8, 333 K) of **A[5].**

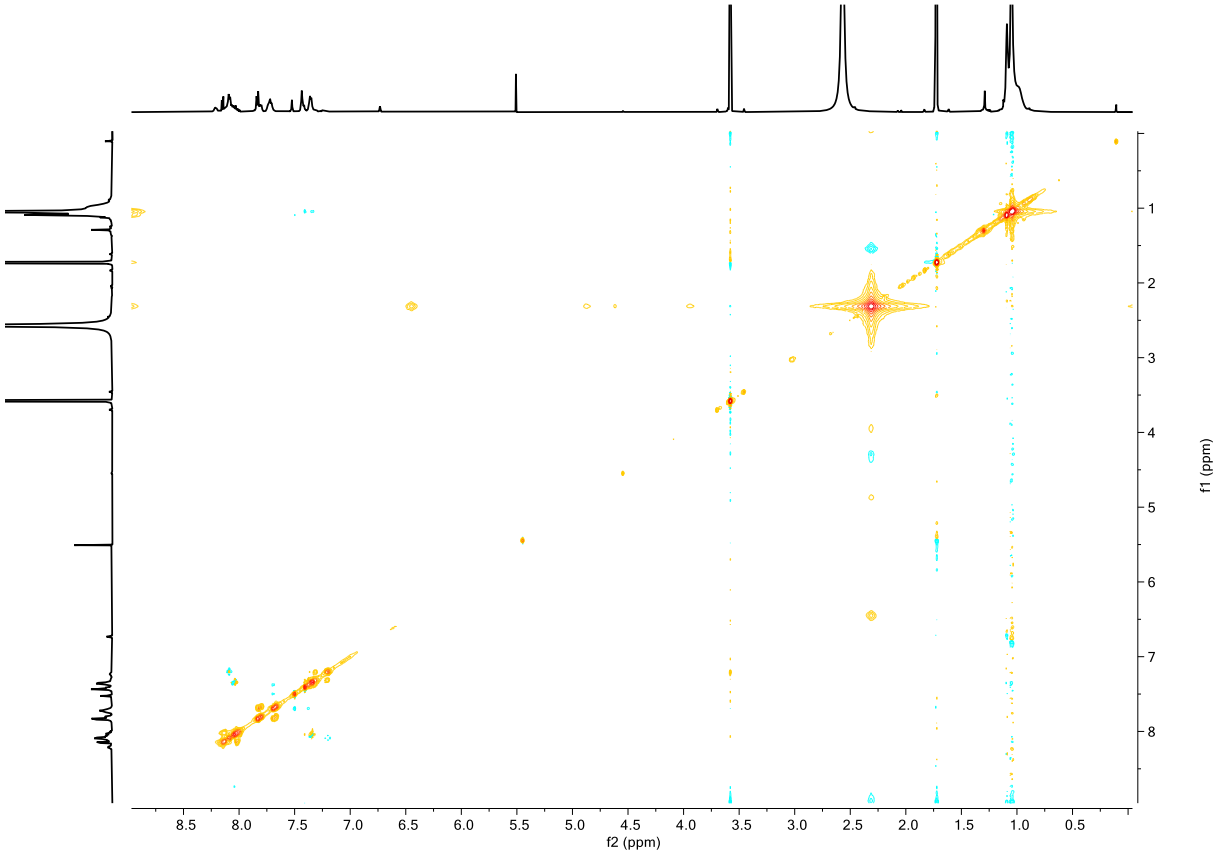


Figure S41. NOSY-NMR(600 MHz, THF-d8, 333 K) of **A[5].**

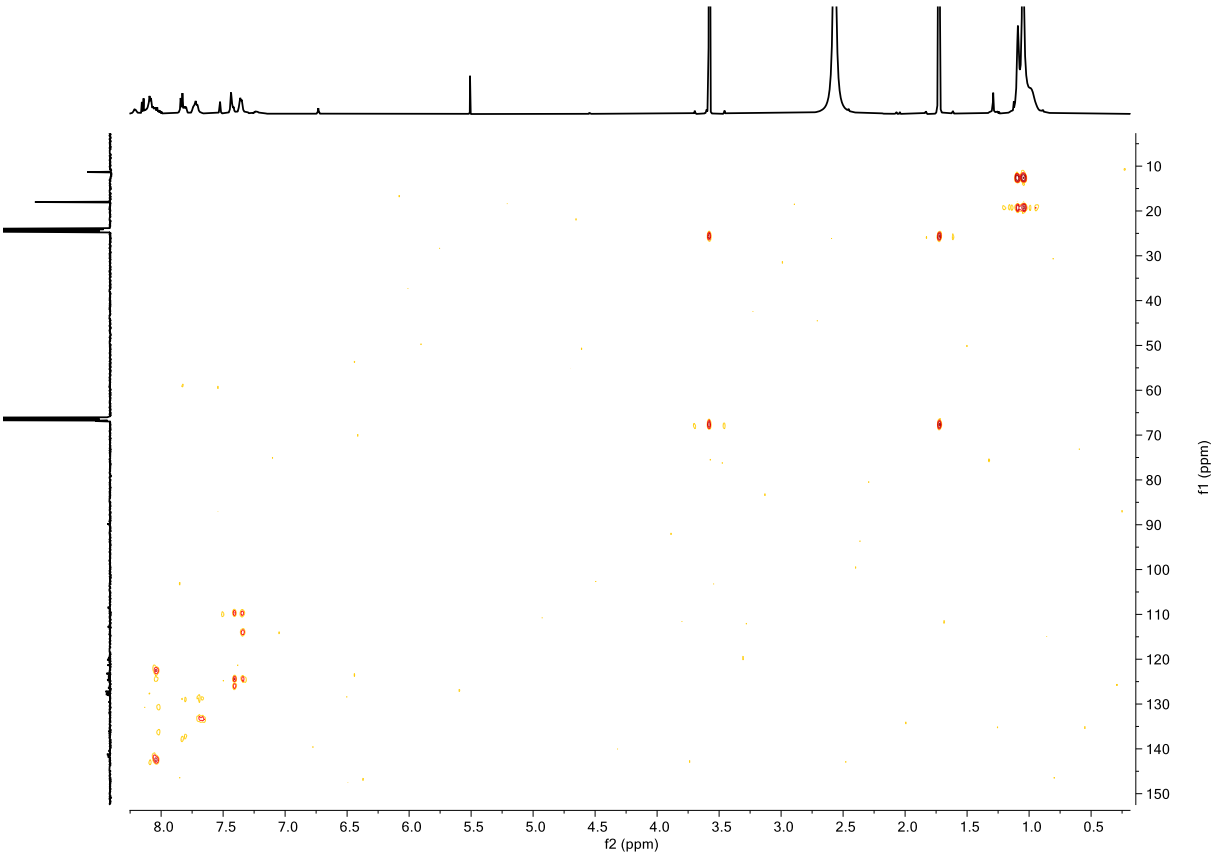


Figure S42. HMBC-NMR(600 MHz, THF-d8, 333 K) of **A[5].**

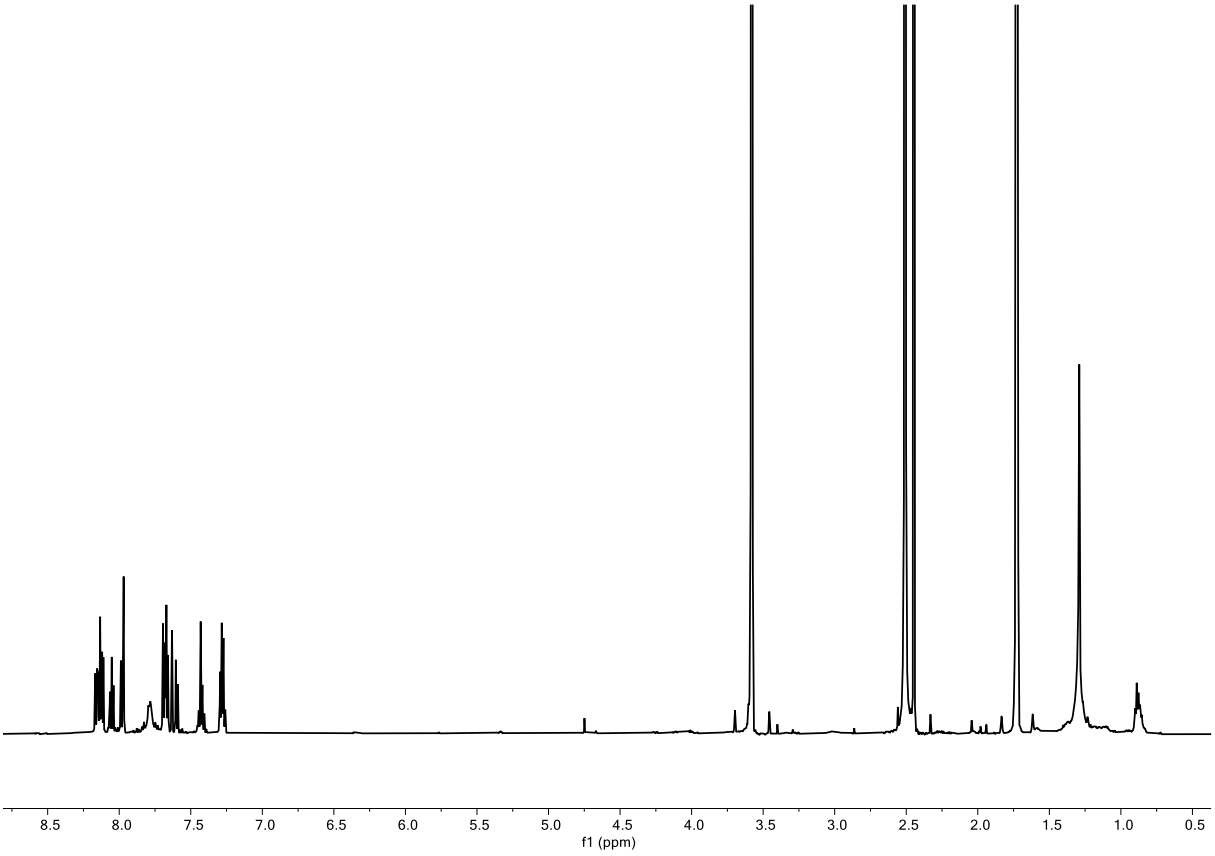


Figure S43. ^{1}H-NMR(600 MHz, THF-d8, 298 K) of $\mathbf{G_{BD}3}$

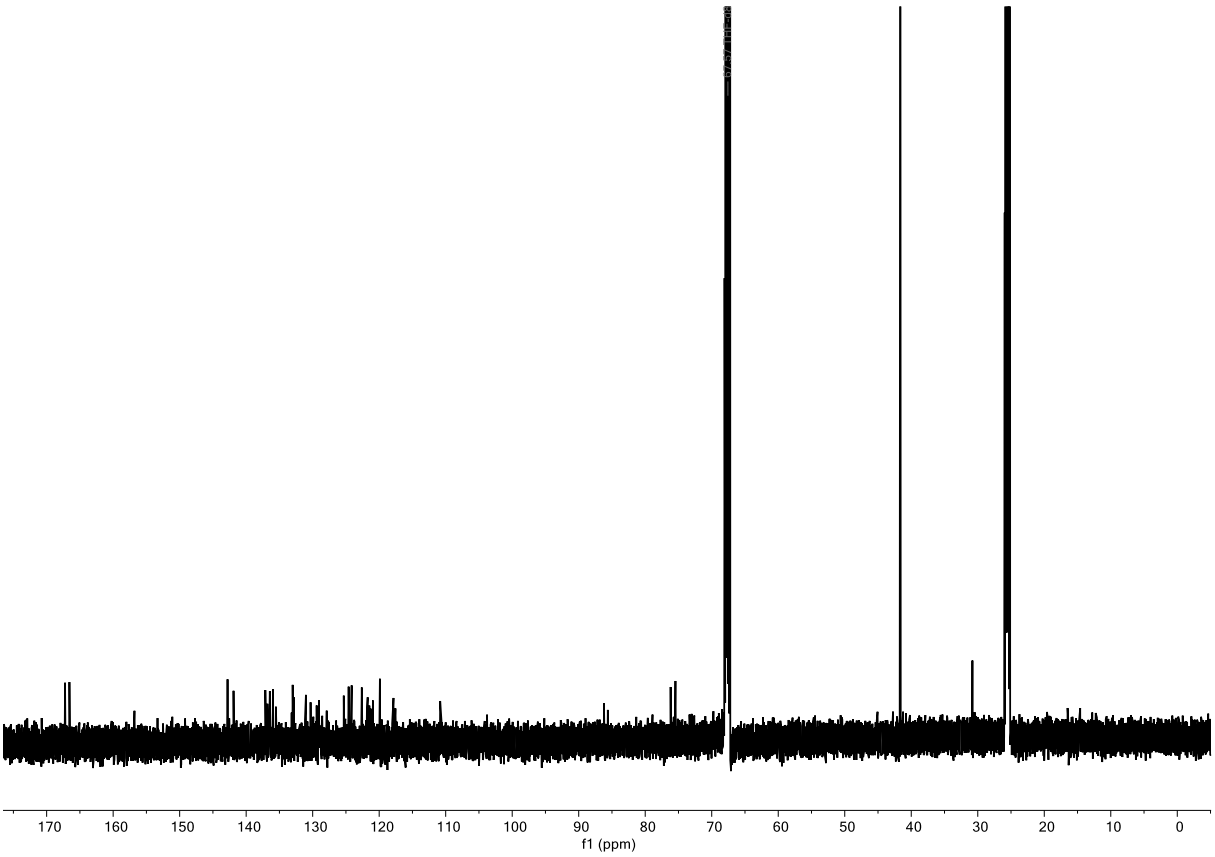


Figure S44. ^{13}C-NMR(151 MHz, THF-d8, 298 K) of $\mathbf{G_{BD}3}$

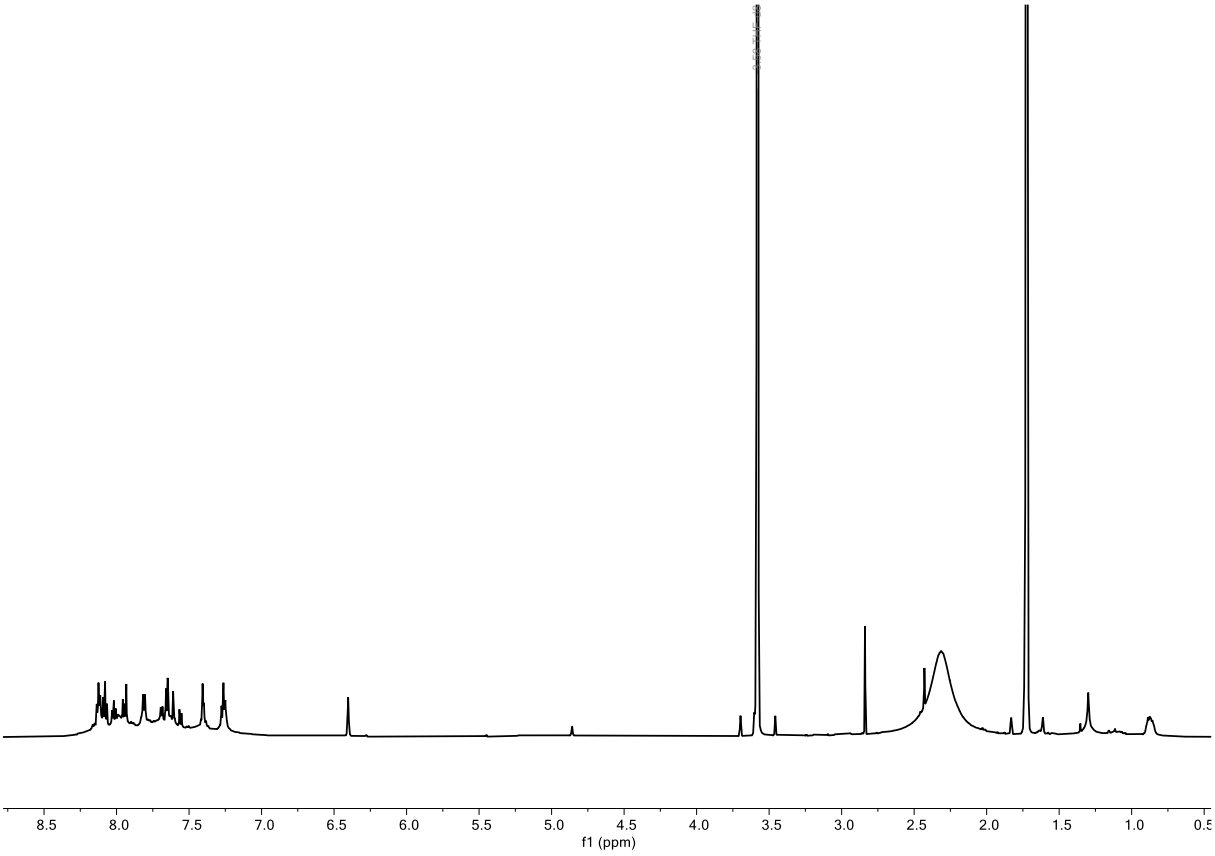


Figure S45. ^{1}H-NMR(600 MHz, THF-d8, 333 K) of $\mathbf{G_{BD}3}$

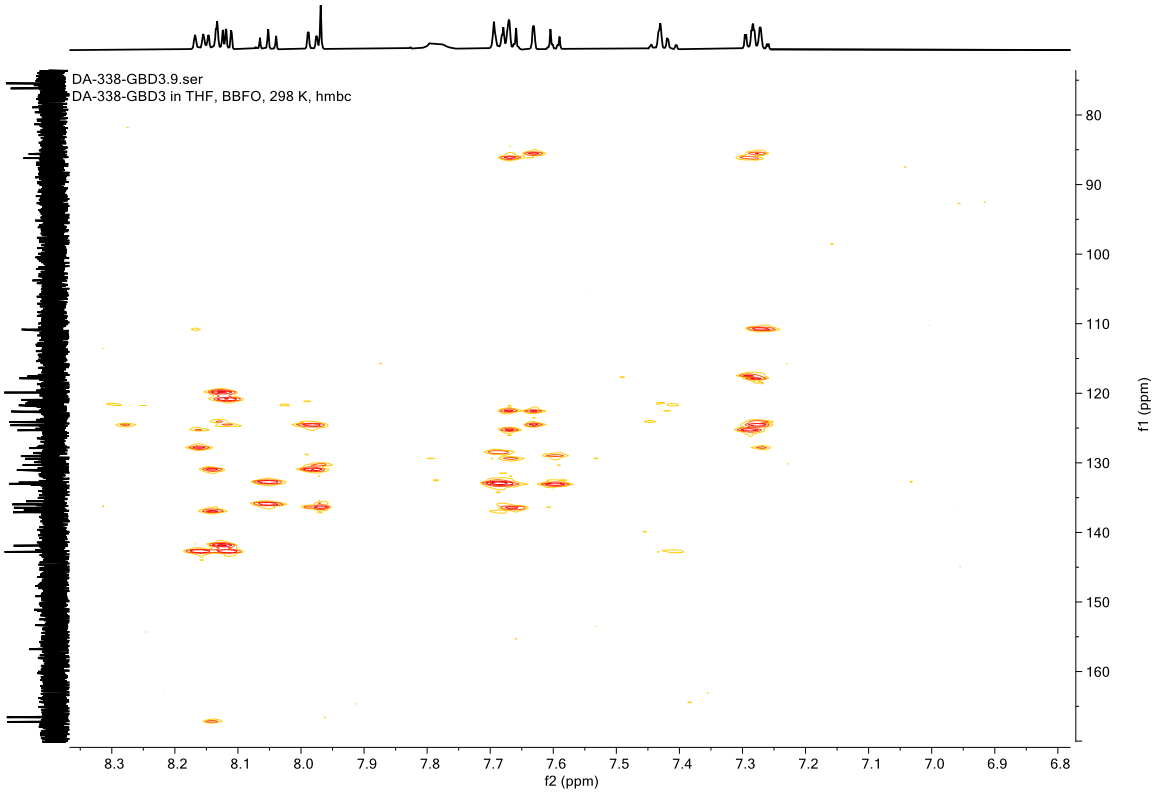


Figure S46. HMBC-NMR(600 MHz, THF-d8, 298 K) of $\mathbf{G_{BD}3}$

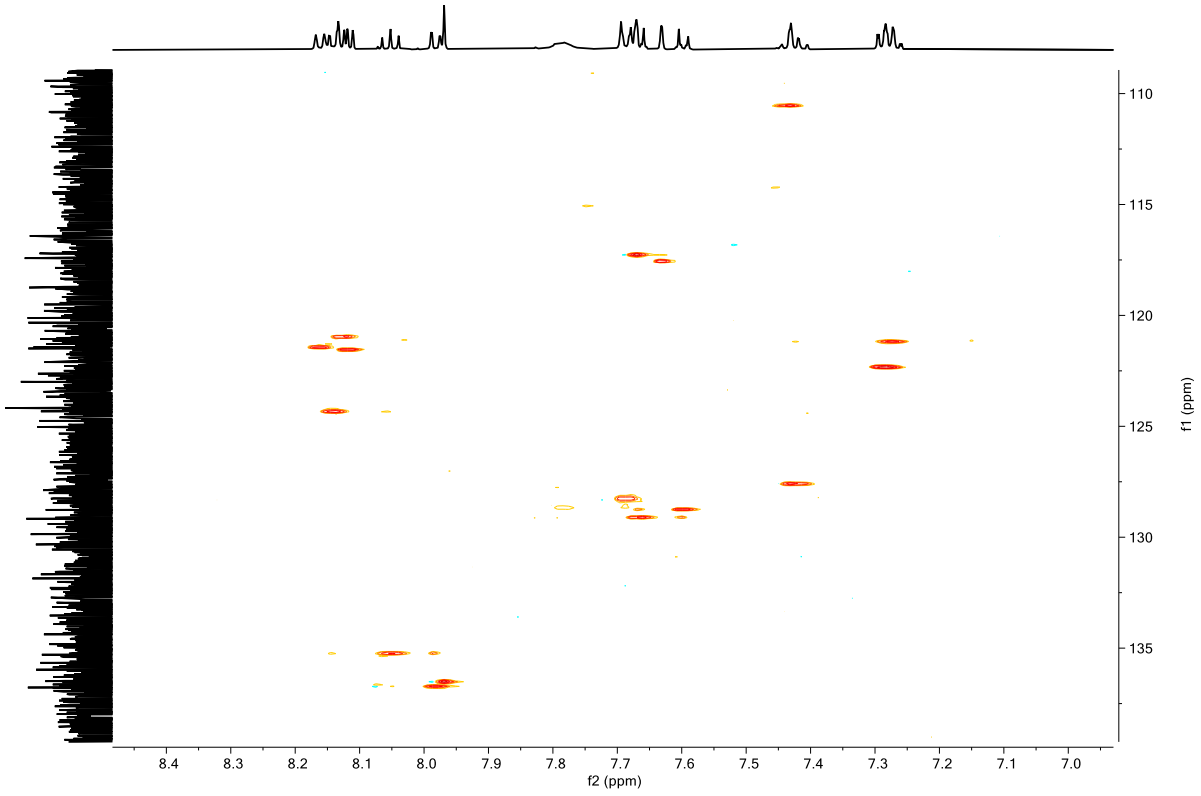


Figure S47. High resolution HSQC-NMR(600 MHz, THF-d8, 298 K) of $\mathbf{G_{BD}3}$

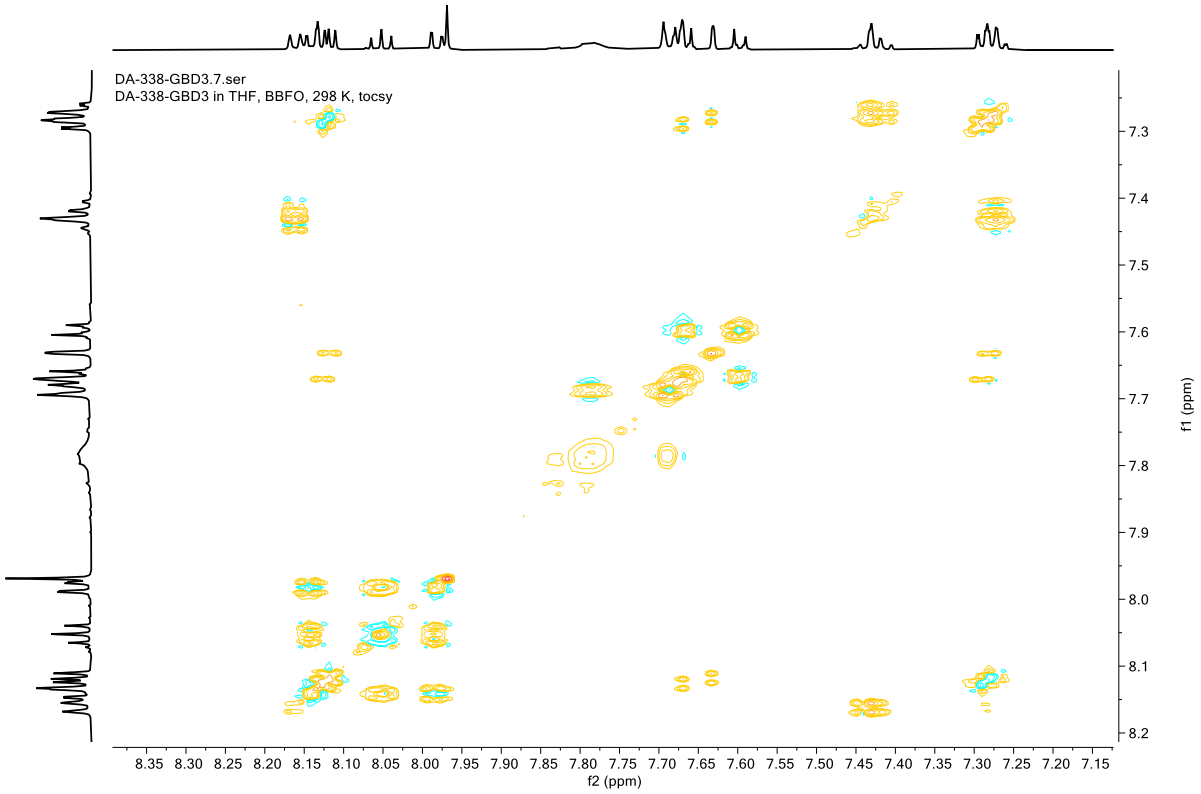


Figure S48. TOCSY-NMR(600 MHz, THF-d8, 298 K) of $\mathbf{G_{BD}3}$

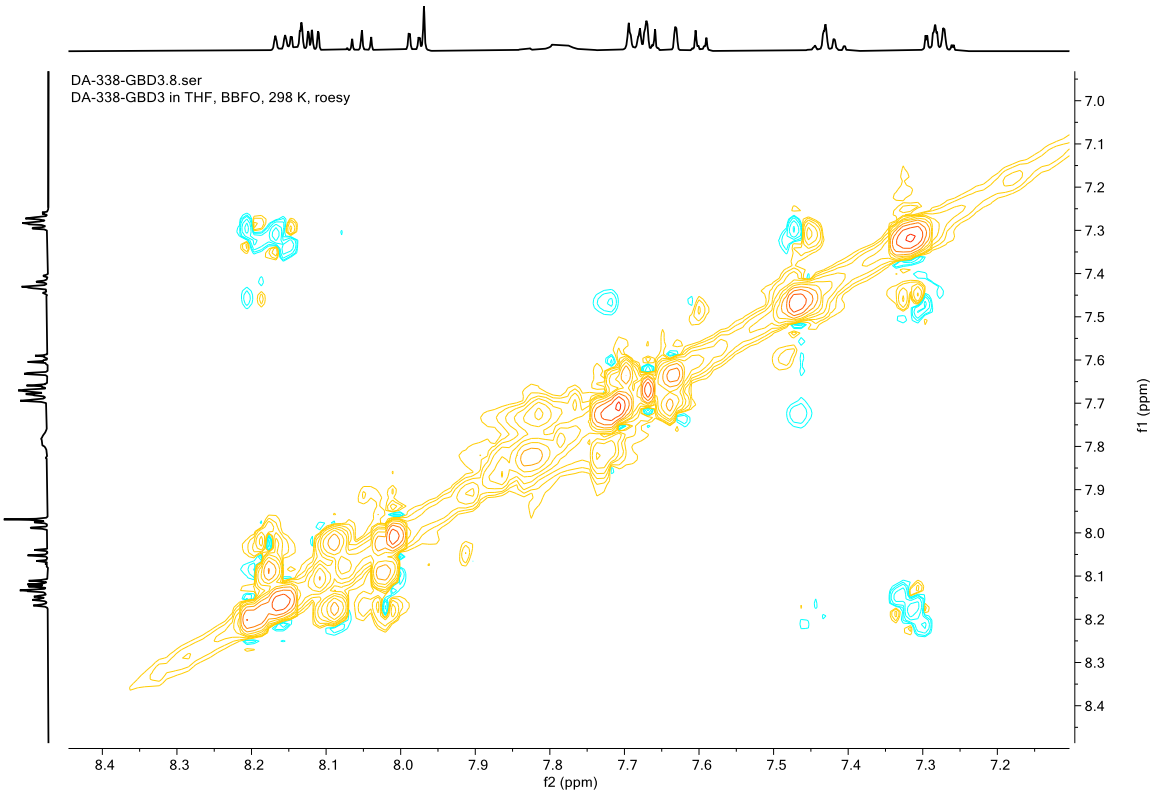


Figure S49. ROESY-NMR(600 MHz, THF-d8, 298 K) of $\mathbf{G_{BD}3}$

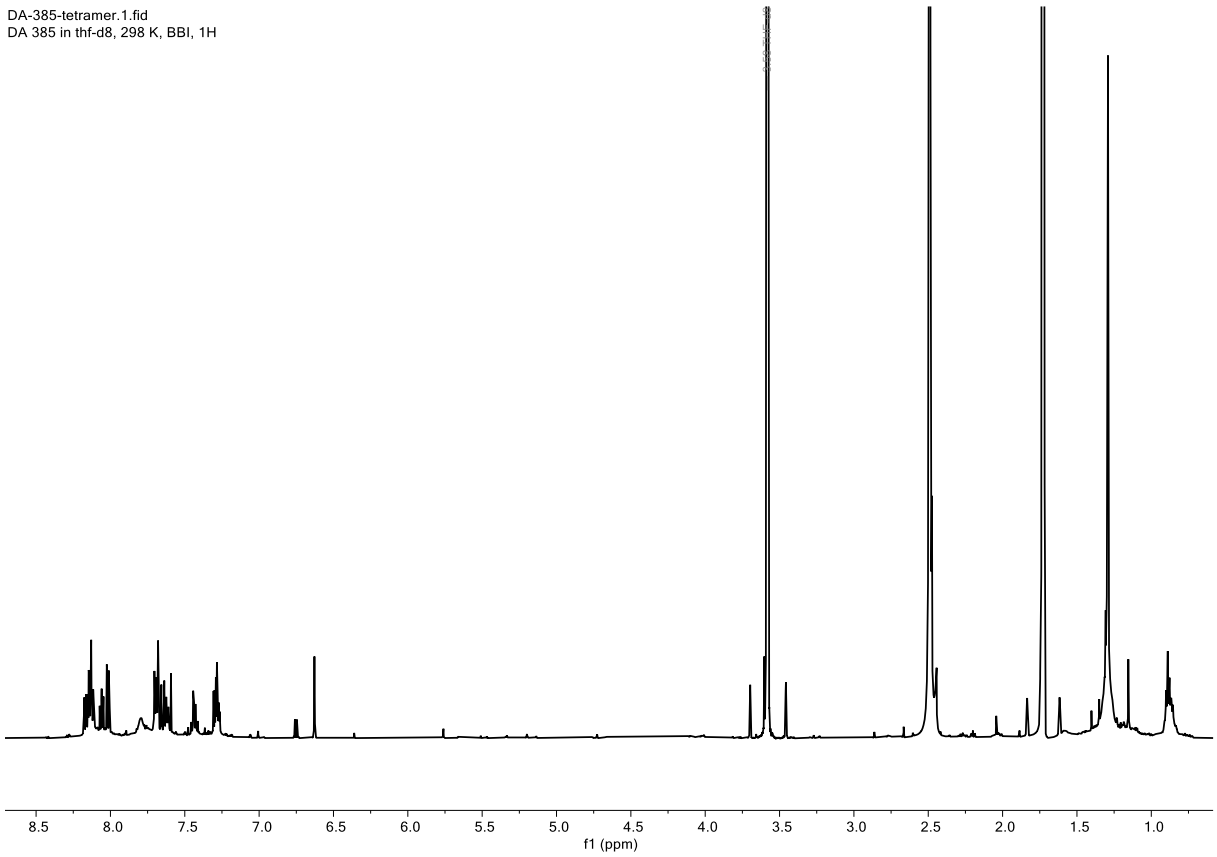


Figure S50. ^{1}H-NMR(600 MHz, THF-d8, 298 K) of **G_{BD}4**

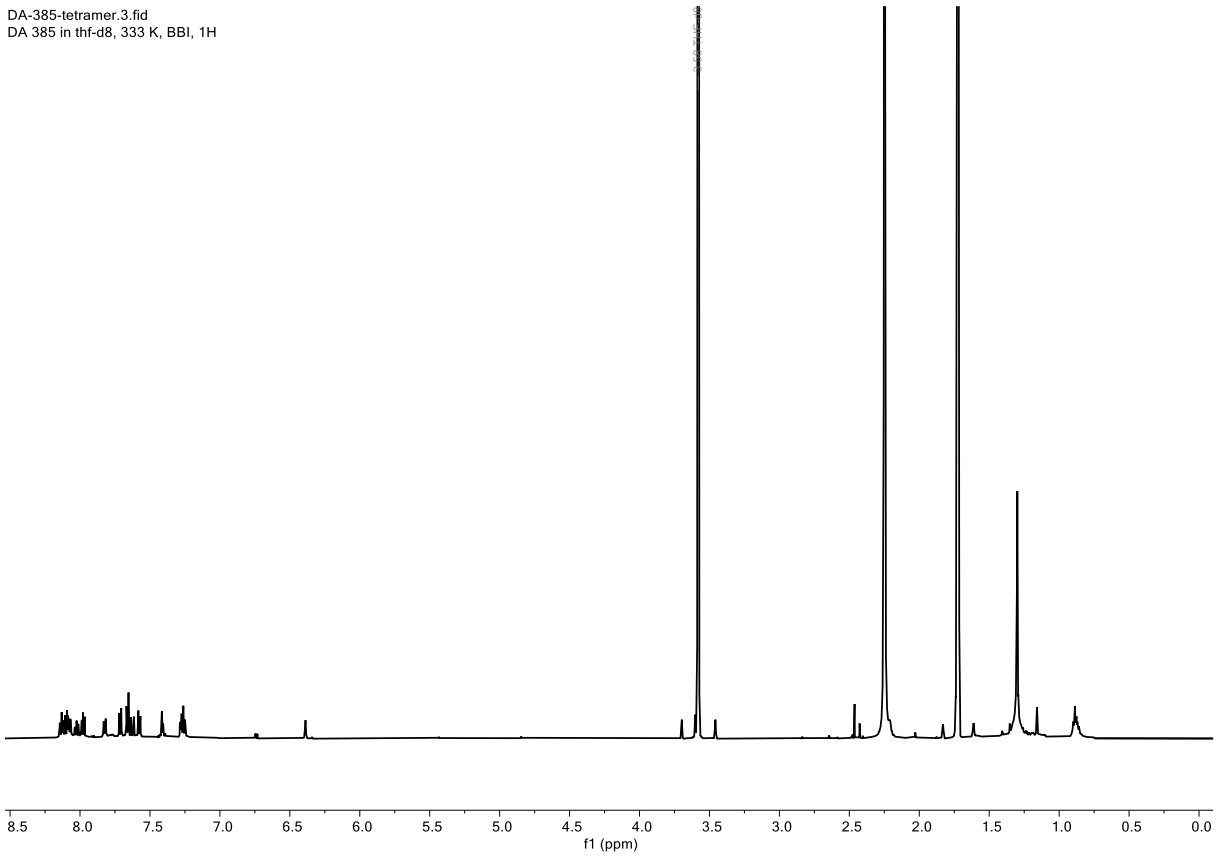


Figure S51. ^{1}H-NMR(600 MHz, THF-d8, 333 K) of **G_{BD}4**

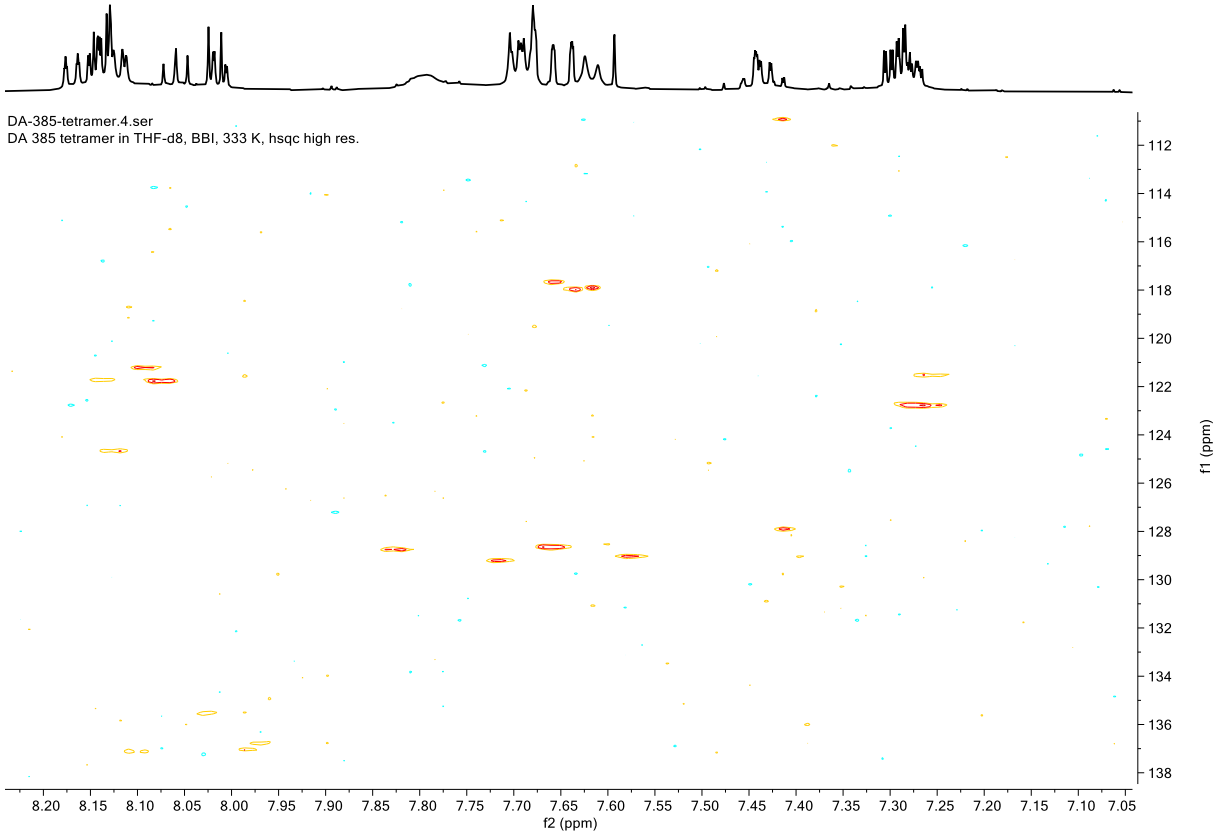


Figure S52. High resolution HSQC-NMR(600 MHz, THF-d8, 333 K) of **G_{BD}4**

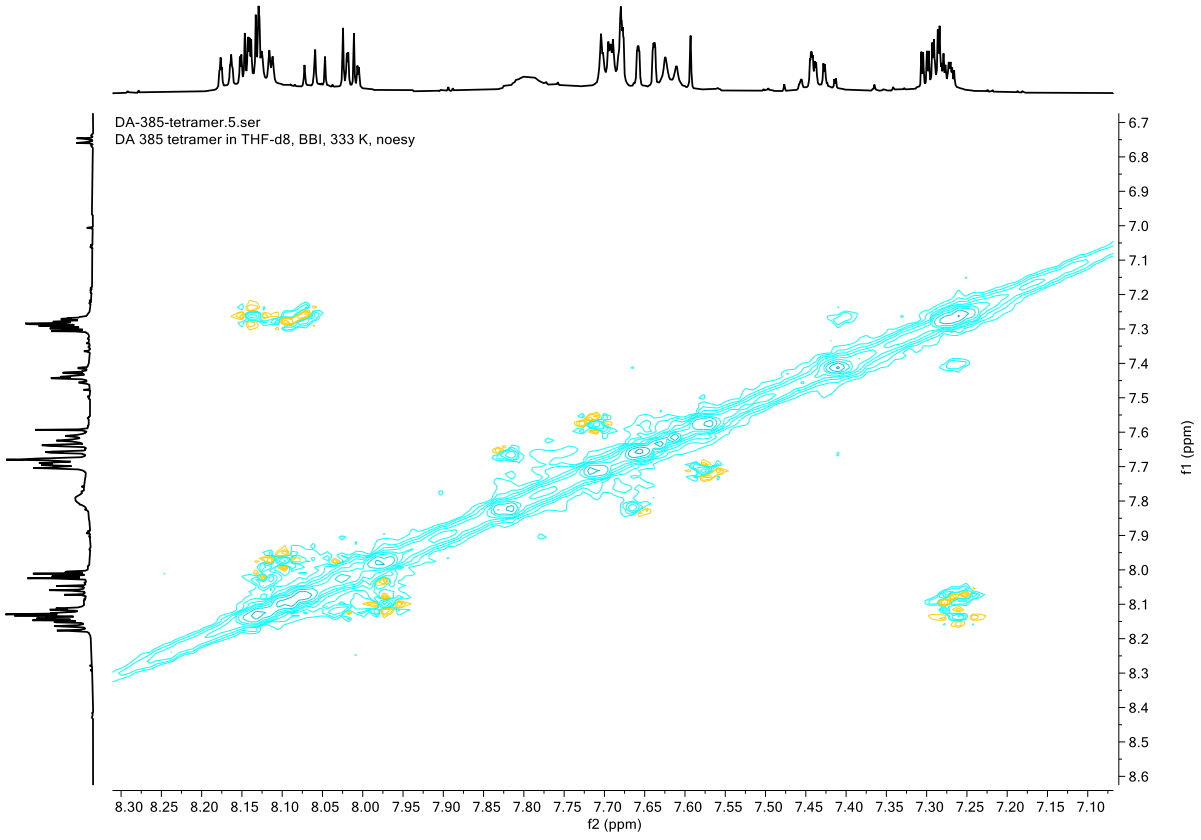


Figure S53. NOESY-NMR(600 MHz, THF-d8, 333 K) of **G_{BD}4**

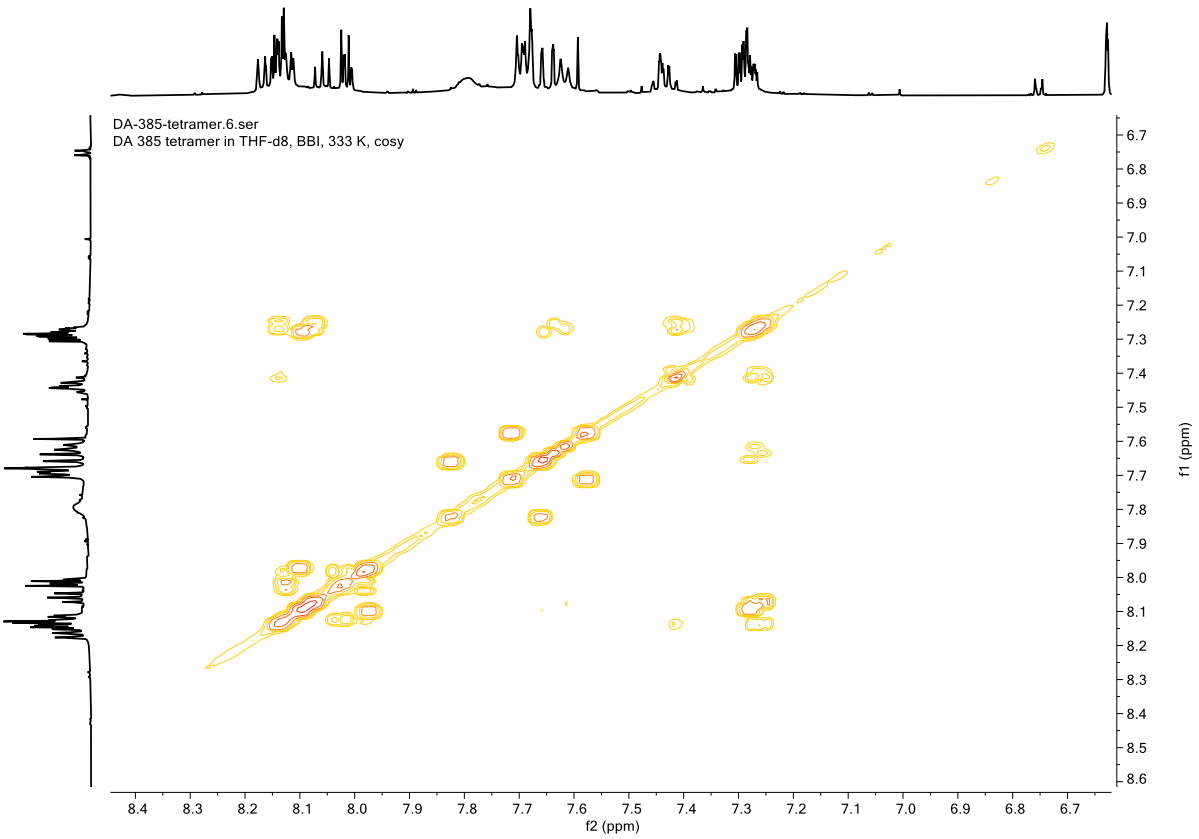
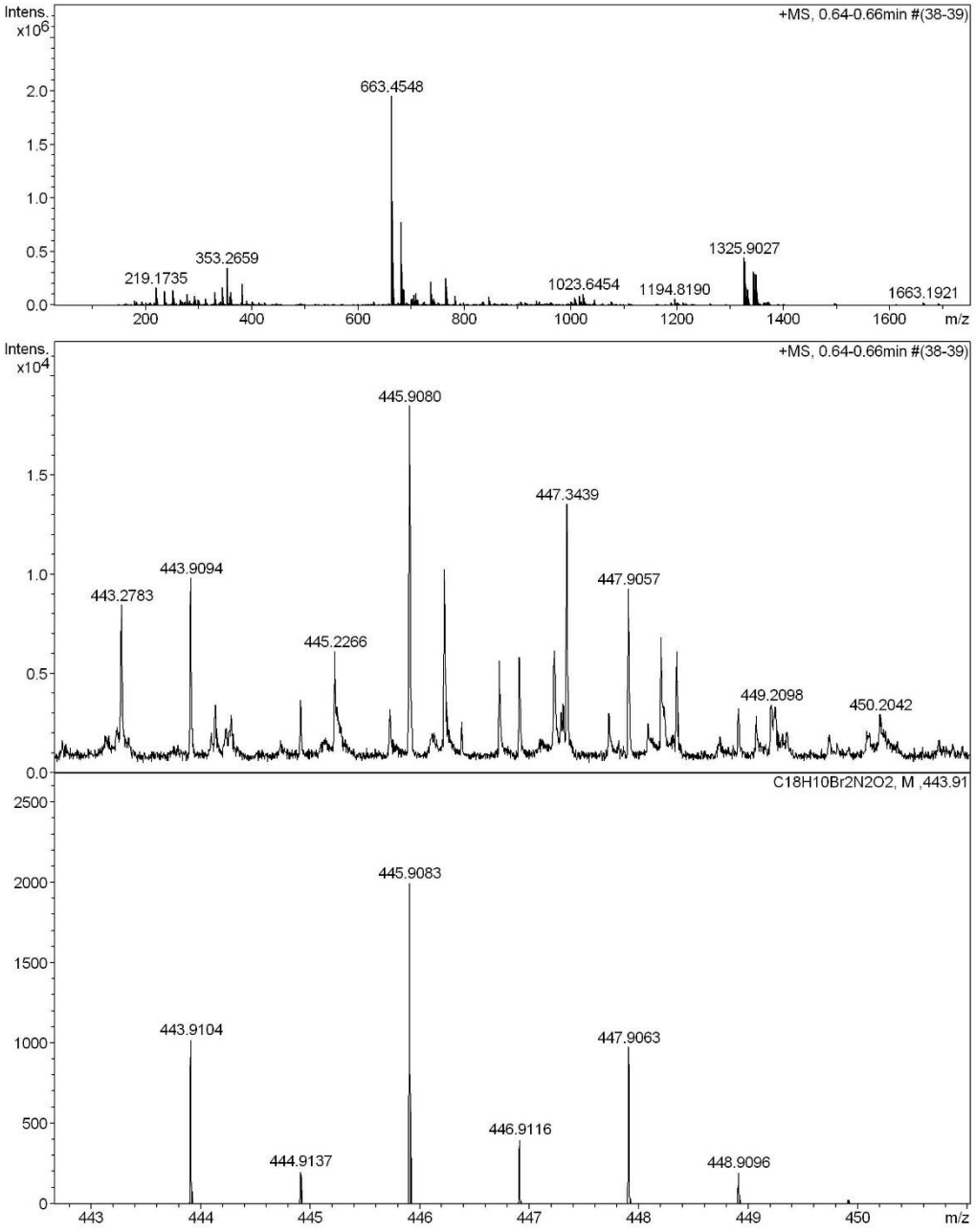


Figure S54. COSY-NMR(600 MHz, THF-d8, 333 K) of $\mathbf{G_{BD}4}$

High Resolution Mass Spectrometry Report

Sample Name **DA-418 DI**
Comment manually injected

Instrument maXis 4G
Method 22 Direct_pos_mid.m



Bruker Compass DataAnalysis 4.0 Acquisition Date 14.05.2024 13:59:51 Page 1 of 3

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
443.9094	1	C 18 H 10 Br 2 N 2 O 2	100.00	443.9104	1.0	2.1	64.7	14.0	odd	1+

Mass list

#	m/z	I %	I
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2	183.0770	1.7	33564
3	193.9781	1.7	33916
4	219.1735	8.4	164566
5	220.1786	1.7	32951
6	221.1162	3.6	70026
7	235.1683	6.9	133985
8	251.1633	7.0	137645
9	253.1788	3.8	73570
10	265.9994	1.9	37967
11	266.0357	2.9	56528
12	269.1737	1.8	34748
13	269.9863	1.8	34737
14	275.1608	1.9	36222
15	277.1779	5.5	107097
16	279.1579	1.6	32177
17	284.0030	2.4	47318
18	291.1558	4.5	87753
19	294.2055	2.7	53428
20	299.1610	3.0	58313
21	301.1401	2.5	48807
22	313.2728	3.4	66937
23	331.2836	6.5	126621
24	341.3041	1.8	36051
25	345.2031	8.5	166569
26	346.2061	1.8	35292
27	353.2659	18.0	352116
28	354.2689	3.8	73468
29	359.3148	4.2	82517
30	361.1979	6.3	123571
31	381.2971	10.4	202830
32	382.3001	2.3	44840
33	391.2832	2.2	43602
34	401.2163	2.0	38827
35	413.2653	1.6	32175
36	629.4384	2.0	38224
37	663.4548	100.0	1955228
38	664.4578	40.8	796819
39	665.4605	8.3	161721
40	680.4810	40.0	781765
41	681.4841	16.2	316878
42	682.4867	3.7	73008
43	683.5430	2.1	40797
44	685.4358	7.7	150693
45	686.4389	3.5	67728
46	699.5954	2.9	56849
47	700.6267	3.1	59939
48	705.5826	4.9	95291
49	706.5857	2.3	44858
50	708.5116	5.9	114449
51	709.5147	2.8	54999
52	711.5742	2.7	52804
53	723.4875	1.8	36066
54	736.5068	11.5	224540
55	736.5406	3.3	64683
56	737.5099	5.5	107523
57	737.5443	1.9	37150
58	742.4970	3.2	63295
59	743.5003	1.7	32857
60	764.5748	13.1	256184
61	765.5782	6.8	132798
62	766.5807	1.9	37352

High Resolution Mass Spectrometry Report

#	m/z	I %	I
63	781.5065	4.6	89619
64	782.5090	2.4	47206
65	835.5248	1.7	32798
66	845.5251	4.2	82316
67	846.5280	2.3	44579
68	905.4241	1.9	37484
69	934.6406	2.4	46983
70	939.6215	2.1	41103
71	999.7392	1.7	33732
72	1007.6517	3.5	67601
73	1008.6546	2.6	50619
74	1015.7135	4.7	91789
75	1016.7167	3.3	65035
76	1018.6903	2.1	40264
77	1023.6454	5.6	110310
78	1024.6486	3.7	72178
79	1043.6532	1.7	33938
80	1043.7444	2.9	55761
81	1044.7477	2.0	39745
82	1075.7130	1.8	34747
83	1194.8190	3.2	61873
84	1195.8223	2.5	48936
85	1325.9027	22.8	446075
86	1326.9061	21.1	413010
87	1327.9089	9.2	180495
88	1328.9113	2.9	57296
89	1331.9104	7.5	146981
90	1332.9135	6.7	131549
91	1333.9164	3.2	61851
92	1342.9290	16.3	319191
93	1343.9323	15.2	296350
94	1344.9350	6.7	131328
95	1345.9375	2.1	42027
96	1347.8844	14.9	291633
97	1348.8878	14.2	277908
98	1349.8905	6.4	126063
99	1350.8931	2.0	40042
100	1370.9589	1.7	33746

Acquisition Parameter

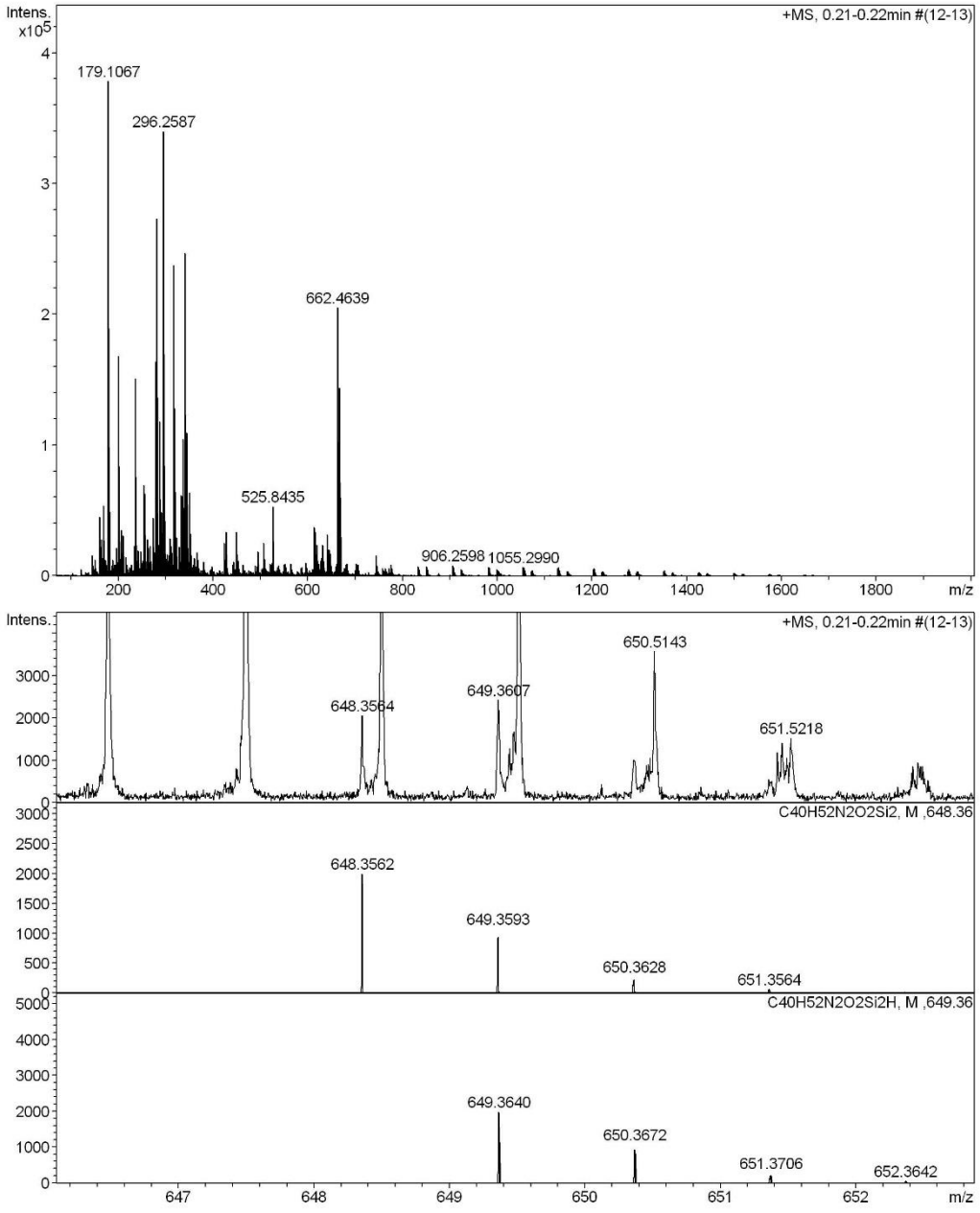
General	Fore Vacuum	2.31e+000 mBar	High Vacuum	1.09e-007 mBar	Source Type	ESI
	Scan Begin	75 m/z	Scan End	1700 m/z	Ion Polarity	Positive
Source	Set Nebulizer	0.4 Bar	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
	Set Dry Heater	180 °C	Set End Plate Offset	-500 V		
Quadrupole	Set Ion Energy (MS only)	4.0 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		

Figure S55. HR-MS report of **2**.

High Resolution Mass Spectrometry Report

Sample Name **DA-327**
Comment

Instrument maXis 4G
Method ms_nocolumn_75-1000_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
648.3564	1	C 40 H 52 N 2 O 2 Si 2	100.00	648.3562	-0.2	-0.3	235.2	18.0	odd	1+

Mass list

#	m/z	I %	I
1	144.9821	4.1	15663
2	161.0960	11.9	45083
3	165.0908	7.4	27967
4	169.0859	14.2	53806
5	170.1175	4.5	17012
6	179.1067	100.0	378366
7	180.1130	26.2	99148
8	196.1329	4.8	18159
9	197.1169	5.7	21626
10	201.0886	44.5	168543
11	202.0918	5.5	20741
12	203.1429	7.0	26659
13	207.1741	9.3	35045
14	210.1100	8.2	31184
15	211.0962	3.7	14037
16	217.1046	3.8	14327
17	235.1689	6.1	22994
18	236.1766	8.3	31357
19	237.1234	40.0	151414
20	238.1265	5.3	20069
21	239.1487	6.3	23975
22	242.2475	5.2	19729
23	249.1482	5.0	18962
24	253.1796	18.4	69695
25	254.1830	3.5	13058
26	254.2477	4.1	15342
27	256.2634	16.8	63417
28	261.1307	7.4	27884
29	263.2369	5.8	21864
30	267.1588	3.9	14909
31	268.2270	6.1	23158
32	274.2740	11.8	44479
33	278.2474	4.7	17856
34	279.0932	19.8	75046
35	279.2316	7.0	26671
36	280.0964	3.9	14812
37	280.2636	43.3	163684
38	281.2667	8.6	32690
39	282.2793	72.3	273459
40	283.2823	12.6	47826
41	284.2939	7.3	27446
42	288.1332	31.2	117869
43	289.1384	7.2	27226
44	290.2092	6.0	22845
45	292.2263	12.8	48471
46	294.2424	8.7	33074
47	296.2587	89.9	340189
48	297.2617	17.5	66253
49	298.2738	22.4	84643
50	299.2771	4.6	17408
51	301.0752	3.4	12815
52	304.2610	4.4	16698
53	308.2206	4.2	16020
54	310.2374	7.7	29004
55	312.2530	6.0	22780
56	314.2686	4.7	17736
57	318.2406	62.9	237837
58	319.2435	12.1	45816
59	320.2560	33.9	128313
60	321.2591	6.0	22526
61	323.2216	7.8	29615
62	328.2482	5.9	22195

High Resolution Mass Spectrometry Report

#	m/z	I %	I
63	332.2196	16.3	61550
64	334.2352	16.1	61104
65	336.2509	27.6	104344
66	337.2540	5.6	21001
67	340.2487	65.3	247076
68	341.2517	12.6	47618
69	345.2039	29.0	109666
70	346.2066	5.8	21995
71	350.2302	16.9	64000
72	351.2333	3.6	13496
73	352.2456	8.6	32406
74	361.1776	3.6	13667
75	366.2251	4.8	18273
76	424.3422	6.7	25308
77	427.3782	9.0	34089
78	449.3603	8.9	33666
79	494.8122	5.0	18911
80	507.3771	6.6	25109
81	508.3819	3.5	13147
82	525.8435	14.1	53202
83	613.4917	9.9	37431
84	614.4948	3.8	14407
85	615.5065	8.9	33790
86	619.3900	6.3	23700
87	620.3926	3.8	14373
88	629.4864	3.7	13952
89	631.5018	6.2	23470
90	640.4553	8.4	31720
91	642.4699	5.3	19893
92	645.4811	5.4	20334
93	647.4963	4.6	17451
94	662.4639	54.3	205397
95	663.4666	22.1	83569
96	664.4687	5.4	20384
97	667.4189	38.1	144223
98	668.4220	15.9	60055
99	669.4247	3.8	14406
100	744.6114	4.2	15862

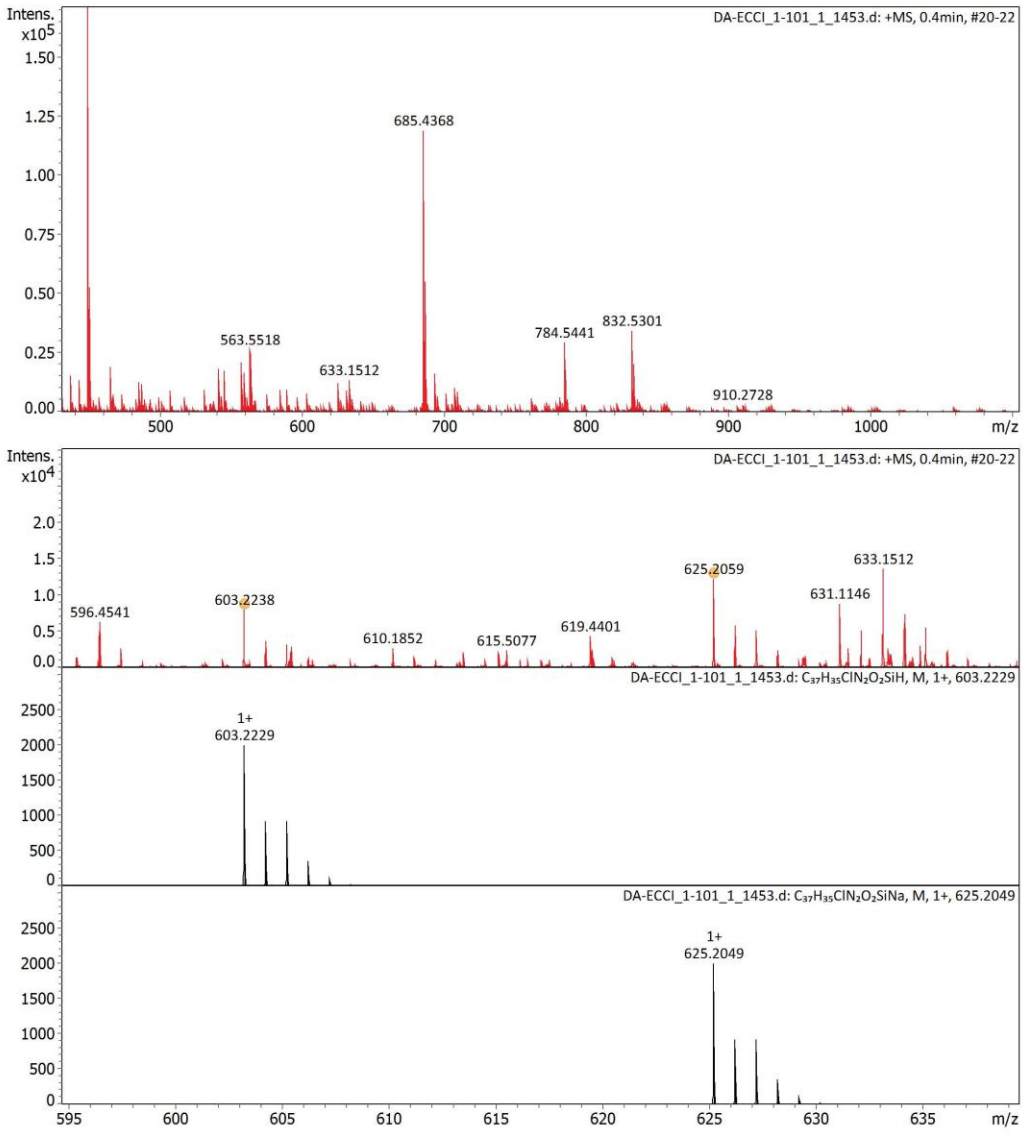
Acquisition Parameter

General	Fore Vacuum	2.48e+000 mBar	High Vacuum	9.70e-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 Vpp	
Ion Cooler	Set Ion Cooler Transfer Time	75.0 µs	Set Ion Cooler Pre Pulse Storage Time	10.0 µs		

Figure S56. HR-MS report of **4**.

High Resolution Mass Spectrometry Report

Sample Name	**DA-ECCI**	Instrument	maXis II
Comment		Method	ms_nocolumn_pos_mid.m



High Resolution Mass Spectrometry Report

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¯ Conf	N-Rule
603.2238	1	C37H36ClN2O2Si	603.2229	-1.4	80.3	1	100.00	25.0	even	ok
625.2059	1	C37H35ClN2NaO2Si	625.2049	-1.7	27.2	1	100.00	25.0	even	ok

#	m/z	Res.	S/N	I	I %	FWHM
1	90.9767	22079	1186.4	31446	1.4	0.0041
2	103.9557	23733	2769.1	73188	3.2	0.0044
3	105.9538	24995	1304.4	34409	1.5	0.0042
4	122.0965	23732	42689.8	1140765	50.2	0.0051
5	123.0922	22867	4128.9	110443	4.9	0.0054
6	123.0998	24635	4274.0	114323	5.0	0.0050
7	124.0872	23943	790.3	21148	0.9	0.0052
8	130.1591	24277	1812.6	48522	2.1	0.0054
9	131.9619	25964	3136.3	83953	3.7	0.0051
10	133.9600	26091	1413.6	37903	1.7	0.0051
11	136.1122	24805	7002.6	187843	8.3	0.0055
12	137.1079	24687	1065.8	28595	1.3	0.0056
13	137.1148	21238	680.0	18243	0.8	0.0065
14	144.9822	26382	3549.2	97152	4.3	0.0055
15	146.9804	26183	1615.5	44485	2.0	0.0056
16	147.0918	25555	3654.6	100713	4.4	0.0058
17	148.0875	23192	763.0	21076	0.9	0.0064
18	150.1278	25343	4664.0	129219	5.7	0.0059
19	157.0765	24255	687.8	19216	0.8	0.0065
20	158.9641	25424	2099.6	58867	2.6	0.0063
21	159.0917	25122	11488.5	322189	14.2	0.0063
22	160.0951	25986	1347.8	37836	1.7	0.0062
23	161.1074	25889	582.4	16369	0.7	0.0062
24	164.1435	26181	1866.0	52564	2.3	0.0063
25	164.5873	26273	1649.1	46483	2.0	0.0063
26	169.0757	25594	3266.2	92861	4.1	0.0066
27	170.0822	25617	79896.3	2271697	100.0	0.0066
28	170.1563	41964	804.5	22873	1.0	0.0041
29	171.0856	25028	10068.4	286143	12.6	0.0068
30	172.0890	21971	636.8	18088	0.8	0.0078
31	173.0783	25460	926.2	26281	1.2	0.0068
32	175.1231	27613	829.5	23503	1.0	0.0063
33	178.1590	27100	2672.1	75910	3.3	0.0066
34	183.0917	27312	3212.3	92362	4.1	0.0067
35	185.1138	24952	576.7	16632	0.7	0.0074
36	186.0089	27855	573.8	16580	0.7	0.0067
37	186.2216	26597	820.3	23710	1.0	0.0070
38	194.1153	26432	675.7	20041	0.9	0.0073
39	205.0600	28026	1596.2	47716	2.1	0.0073
40	211.1229	27929	802.9	24423	1.1	0.0076
41	213.1392	24489	634.9	19364	0.9	0.0087
42	215.1254	28291	909.5	27827	1.2	0.0076
43	216.0995	28528	521.7	15973	0.7	0.0076
44	217.1045	27399	1041.8	31962	1.4	0.0079
45	226.1591	28852	1618.7	50300	2.2	0.0078
46	226.9515	29330	1431.3	44532	2.0	0.0077
47	229.1411	29825	1909.3	59607	2.6	0.0077
48	230.2479	29444	1747.5	54680	2.4	0.0078
49	254.2479	30513	901.1	29196	1.3	0.0083
50	256.2635	29622	1738.1	56252	2.5	0.0087
51	261.1309	29943	593.8	19193	0.8	0.0087
52	262.1802	30243	2862.9	92471	4.1	0.0087
53	263.1837	29146	505.1	16304	0.7	0.0090
54	273.1674	30326	900.4	29151	1.3	0.0090
55	274.2742	30943	1293.6	42124	1.9	0.0089
56	280.2637	30564	1310.2	43274	1.9	0.0092
57	282.2792	29359	14544.2	480970	21.2	0.0096
58	283.2826	30586	3079.7	101756	4.5	0.0093

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#	m/z	Res.	S/N	I	I %	FWHM
59	284.2934	21155	632.5	20922	0.9	0.0134
60	288.2535	30882	1520.8	50783	2.2	0.0093
61	292.2249	30147	467.4	15773	0.7	0.0097
62	294.9391	32751	701.8	23815	1.0	0.0090
63	296.2586	31217	921.0	31338	1.4	0.0095
64	299.1619	31440	547.7	18850	0.8	0.0095
65	302.2456	30893	552.5	19380	0.9	0.0098
66	304.2612	30718	4667.6	164623	7.2	0.0099
67	304.3001	32117	500.0	17633	0.8	0.0095
68	305.2646	31142	962.6	33983	1.5	0.0098
69	308.2200	31992	463.0	16375	0.7	0.0096
70	318.2405	31230	4943.8	178357	7.9	0.0102
71	319.2440	30945	996.6	35976	1.6	0.0103
72	320.2561	30732	4566.0	165059	7.3	0.0104
73	321.2596	30305	883.6	31946	1.4	0.0106
74	328.1669	31771	2050.2	75274	3.3	0.0103
75	329.1703	29700	511.3	18836	0.8	0.0111
76	334.2356	32163	674.5	25204	1.1	0.0104
77	336.2511	31342	5577.1	209813	9.2	0.0107
78	337.2545	32202	1178.7	44469	2.0	0.0105
79	350.2305	32465	763.6	29462	1.3	0.0108
80	352.2255	30016	568.8	22020	1.0	0.0117
81	353.2665	32754	1399.3	54334	2.4	0.0108
82	381.2979	33755	1511.2	60695	2.7	0.0113
83	393.3480	32789	456.0	18785	0.8	0.0120
84	437.1940	33806	350.3	15623	0.7	0.0129
85	449.2861	34225	574.2	26169	1.2	0.0131
86	449.3605	33891	3921.4	178733	7.9	0.0133
87	450.3640	34221	1150.9	52527	2.3	0.0132
88	465.3343	33878	416.4	19128	0.8	0.0137
89	541.1217	36198	355.3	18145	0.8	0.0149
90	545.3305	36286	337.2	17379	0.8	0.0150
91	557.0955	35996	401.2	21151	0.9	0.0155
92	559.1322	36141	314.9	16654	0.7	0.0155
93	563.5518	35191	496.5	26365	1.2	0.0160
94	685.4368	36723	2082.8	119043	5.2	0.0187
95	686.4401	37935	964.8	55133	2.4	0.0181
96	693.1936	38554	281.6	16085	0.7	0.0180
97	784.5441	38298	563.5	29435	1.3	0.0205
98	785.5472	37458	341.8	17826	0.8	0.0210
99	832.5301	38870	713.2	34473	1.5	0.0214
100	833.5338	37966	420.3	20298	0.9	0.0220

Acquisition Parameter

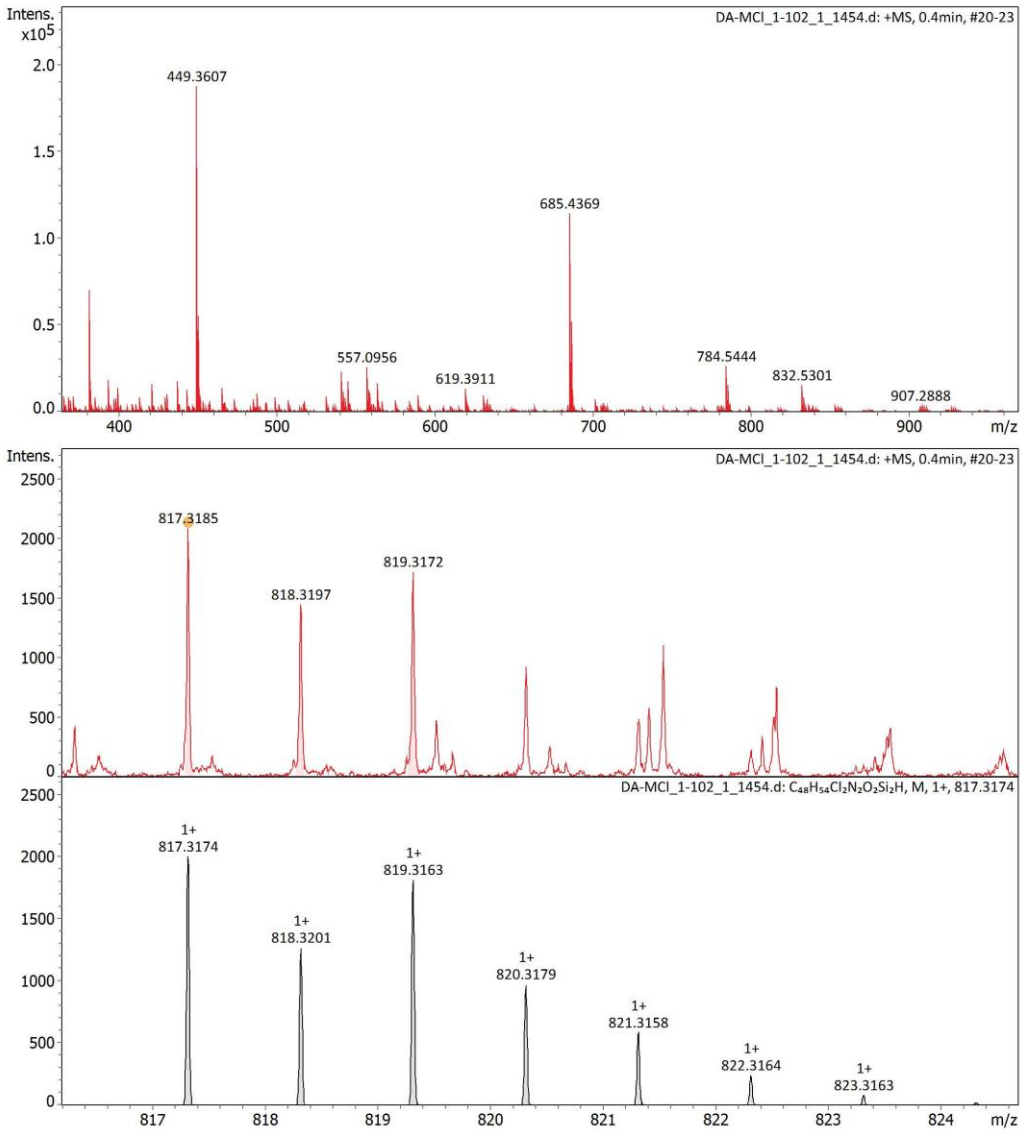
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	220 °C
Scan Begin	75 m/z	Set End Plate Offset	-500 V	Set Dry Gas	9.0 l/min
Scan End	1700 m/z	Set Collision Cell RF	350.0 Vpp	Set Ion Energy (MS only)	4.0 eV

Bruker Compass DataAnalysis 5.3 Acquisition Date 3/7/2024 3:10:48 PM Page 3 of 3

Figure S57. HR-MS report of **EC$_{Cl}$**.

High Resolution Mass Spectrometry Report

Sample Name	**DA-MCI**	Instrument	maXis II
Comment		Method	ms_nocolumn_pos_mid.m



High Resolution Mass Spectrometry Report

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¯ Conf	N-Rule
817.3185	1	C48H55Cl2N2O2Si2	817.3174	-1.4	223.6	1	100.00	30.0	even	ok
839.3012	1	C48H54Cl2N2NaO2Si2	839.2993	-2.2	121.8	1	100.00	30.0	even	ok

#	m/z	Res.	S/N	I	I %	FWHM
1	90.9767	21985	1699.1	37560	3.4	0.0041
2	103.9557	23907	3202.5	71002	6.3	0.0043
3	105.9539	24843	1493.4	33059	3.0	0.0043
4	122.0965	23608	50050.5	1119754	100.0	0.0052
5	123.0922	23409	5211.4	116648	10.4	0.0053
6	123.0998	24803	5118.1	114560	10.2	0.0050
7	124.0873	23895	969.7	21716	1.9	0.0052
8	130.1592	24565	2049.0	45888	4.1	0.0053
9	131.9618	26094	3692.4	82906	7.4	0.0051
10	133.9601	26188	1712.0	38532	3.4	0.0051
11	136.1122	25035	8355.7	188311	16.8	0.0054
12	137.1079	24887	1286.0	28986	2.6	0.0055
13	137.1149	21263	825.7	18609	1.7	0.0064
14	144.9822	26441	4196.8	96275	8.6	0.0055
15	146.9805	26059	1936.4	44644	4.0	0.0056
16	147.0918	25823	4762.1	109859	9.8	0.0057
17	148.0875	23774	955.6	22103	2.0	0.0062
18	148.0947	25183	614.8	14218	1.3	0.0059
19	150.1279	25595	5597.5	129895	11.6	0.0059
20	151.1244	21806	563.5	13057	1.2	0.0069
21	151.1305	21047	615.2	14256	1.3	0.0072
22	157.0765	23583	840.4	19661	1.8	0.0067
23	158.9642	25609	2990.2	70142	6.3	0.0062
24	159.0918	25467	3905.4	91640	8.2	0.0062
25	161.1074	25946	756.6	17783	1.6	0.0062
26	164.1435	26690	2206.9	52077	4.7	0.0062
27	169.0757	25833	1921.5	45775	4.1	0.0065
28	170.0823	25519	45209.4	1076927	96.2	0.0067
29	171.0857	25111	5683.6	135376	12.1	0.0068
30	173.0785	26516	1060.1	25249	2.3	0.0065
31	175.1230	27121	1098.0	26072	2.3	0.0065
32	178.1591	26836	3067.6	73117	6.5	0.0066
33	183.0918	27824	904.1	21915	2.0	0.0066
34	185.1145	21752	681.5	16600	1.5	0.0085
35	186.0088	28155	648.7	15830	1.4	0.0066
36	186.2217	26793	1014.5	24760	2.2	0.0070
37	194.1154	26704	716.4	18041	1.6	0.0073
38	205.0601	28177	2297.3	58275	5.2	0.0073
39	215.1255	28351	1206.2	31195	2.8	0.0076
40	217.1046	28219	894.8	23221	2.1	0.0077
41	226.1592	29249	917.3	24195	2.2	0.0077
42	226.9516	29247	2059.4	54401	4.9	0.0078
43	229.1411	29770	2121.9	56249	5.0	0.0077
44	230.2479	29824	2181.0	57893	5.2	0.0077
45	254.2480	30095	909.8	25035	2.2	0.0084
46	256.2636	29519	1714.2	47167	4.2	0.0087
47	262.1802	30204	3305.7	91969	8.2	0.0087
48	263.1836	30280	618.6	17226	1.5	0.0087
49	273.1675	30222	917.2	25721	2.3	0.0090
50	274.2743	30646	1727.6	48795	4.4	0.0089
51	278.2462	28756	447.1	12818	1.1	0.0097
52	280.2637	30324	1268.3	36423	3.3	0.0092
53	282.2793	29454	14577.7	418626	37.4	0.0096
54	283.2827	30652	3047.6	87447	7.8	0.0092
55	284.2935	21582	657.8	18889	1.7	0.0132
56	288.2536	30799	1234.7	35692	3.2	0.0094
57	294.9393	32354	1003.5	29513	2.6	0.0091
58	296.2587	30776	827.9	24397	2.2	0.0096

High Resolution Mass Spectrometry Report

#	m/z	Res.	S/N	I	I %	FWHM
59	299.1621	31148	706.5	21045	1.9	0.0096
60	301.1413	31484	462.8	13991	1.2	0.0096
61	302.2456	31208	577.5	17562	1.6	0.0097
62	304.2613	30961	5017.1	153659	13.7	0.0098
63	304.3003	32107	552.1	16908	1.5	0.0095
64	305.2647	30852	1015.0	31108	2.8	0.0099
65	308.2200	31641	436.3	13381	1.2	0.0097
66	318.2407	31680	4562.1	141941	12.7	0.0100
67	319.2440	30881	900.7	28056	2.5	0.0103
68	320.2562	31012	4148.5	129245	11.5	0.0103
69	321.2597	30652	838.9	26113	2.3	0.0105
70	326.3784	32431	461.5	14468	1.3	0.0101
71	328.1671	31718	620.3	19573	1.7	0.0103
72	334.2356	32759	633.7	20345	1.8	0.0102
73	336.2512	31548	5235.9	169328	15.1	0.0107
74	337.2546	31911	1055.2	34258	3.1	0.0106
75	338.3420	32445	412.0	13419	1.2	0.0104
76	350.2305	31634	692.2	23101	2.1	0.0111
77	352.2257	30661	547.0	18351	1.6	0.0115
78	353.2666	32573	1858.6	62601	5.6	0.0108
79	354.2691	25703	422.7	14272	1.3	0.0138
80	362.9269	32434	401.4	13681	1.2	0.0112
81	381.2980	33730	2001.6	70225	6.3	0.0113
82	382.3015	32911	469.1	16494	1.5	0.0116
83	393.3481	33458	504.4	18248	1.6	0.0118
84	399.3087	33609	377.7	13822	1.2	0.0119
85	421.2542	35161	421.4	16173	1.4	0.0120
86	437.1939	33857	449.6	17813	1.6	0.0129
87	449.2862	34543	716.2	29089	2.6	0.0130
88	449.3607	33705	4618.5	187569	16.8	0.0133
89	450.3641	34202	1364.6	55522	5.0	0.0132
90	465.3347	33972	344.2	14136	1.3	0.0137
91	541.1216	36925	504.3	22989	2.1	0.0147
92	545.3307	36844	391.3	17985	1.6	0.0148
93	557.0956	35790	551.9	25807	2.3	0.0156
94	563.5521	36581	358.9	16880	1.5	0.0154
95	619.3911	35972	281.4	13454	1.2	0.0172
96	685.4369	37608	2412.9	114238	10.2	0.0182
97	686.4405	38317	1100.8	52115	4.7	0.0179
98	784.5444	38297	639.7	26404	2.4	0.0205
99	785.5471	34388	375.4	15462	1.4	0.0228
100	832.5301	38558	409.9	15381	1.4	0.0216

Acquisition Parameter

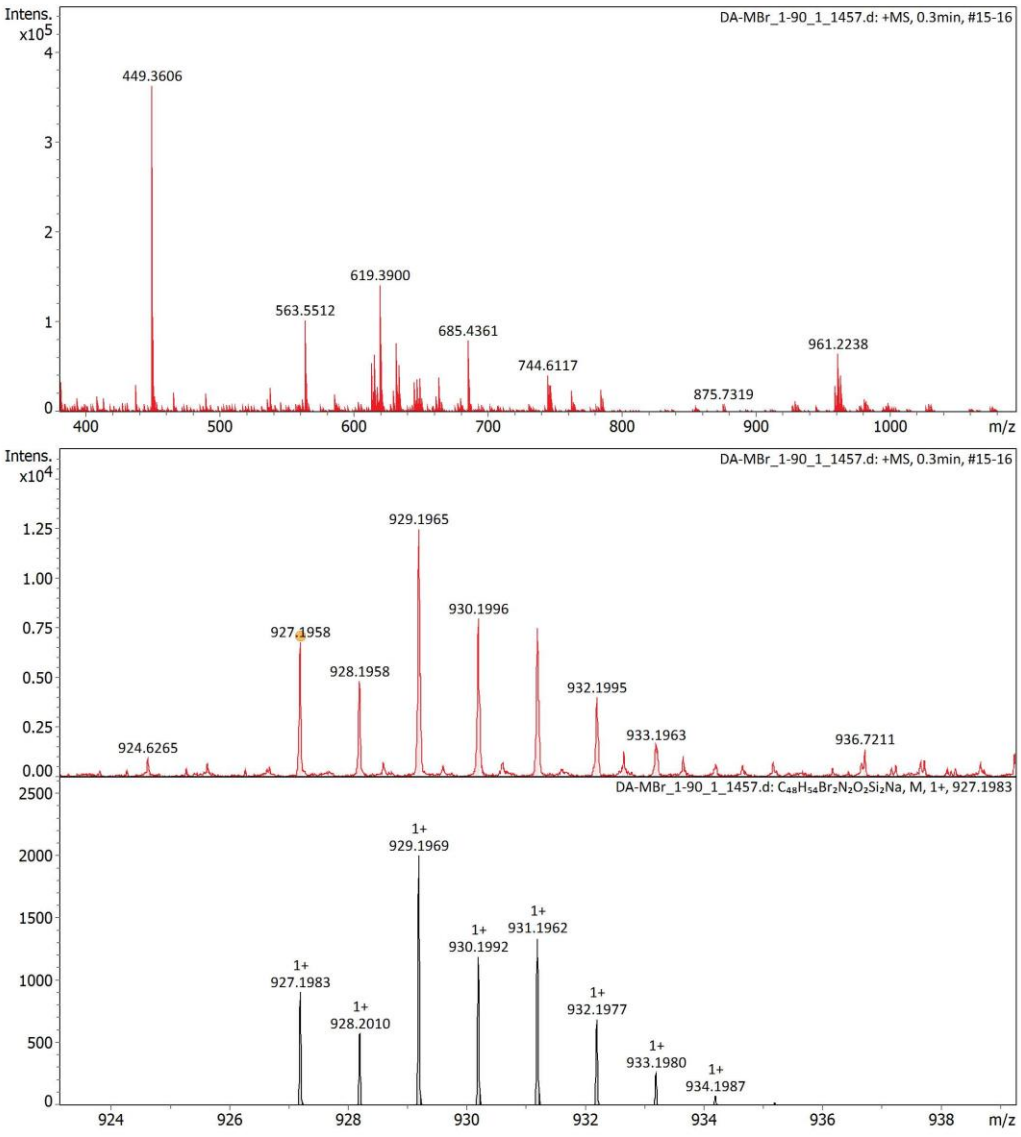
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	220 °C
Scan Begin	75 m/z	Set End Plate Offset	-500 V	Set Dry Gas	9.0 l/min
Scan End	1700 m/z	Set Collision Cell RF	350.0 Vpp	Set Ion Energy (MS only)	4.0 eV

Bruker Compass DataAnalysis 5.3 Acquisition Date 3/7/2024 3:12:56 PM Page 3 of 3

Figure S58. HR-MS report of **M**$_{Cl}$.

High Resolution Mass Spectrometry Report

Sample Name	**DA-MBr**	Instrument	maXis II
Comment		Method	ms_nocolumn_pos_mid.m



High Resolution Mass Spectrometry Report

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¯ Conf	N-Rule
927.1958	1	C48H54Br2N2NaO2Si2	927.1983	2.7	58.6	1	100.00	28.0	even	ok

#	m/z	Res.	S/N	I	I %	FWHM
1	90.9785	21757	1324.8	50477	5.2	0.0042
2	102.1296	23851	1052.8	40021	4.2	0.0043
3	103.9574	23842	904.4	34363	3.6	0.0044
4	122.0982	23530	25049.1	950742	98.7	0.0052
5	123.0944	23915	1543.8	58558	6.1	0.0051
6	123.1015	24823	2606.6	98864	10.3	0.0050
7	130.1608	24345	1220.8	46421	4.8	0.0053
8	131.9635	26232	994.9	37899	3.9	0.0050
9	136.1138	25011	3850.0	146888	15.3	0.0054
10	144.9838	26823	1165.6	44675	4.6	0.0054
11	147.0934	25560	1242.9	47753	5.0	0.0058
12	150.1294	25440	2389.5	91925	9.5	0.0059
13	158.9657	25268	2139.1	82731	8.6	0.0063
14	164.1450	26389	910.1	35381	3.7	0.0062
15	170.0838	25941	1906.1	74521	7.7	0.0066
16	178.1605	27158	1241.3	48677	5.1	0.0066
17	194.1166	27136	856.2	35550	3.7	0.0072
18	201.0900	28029	1171.0	49478	5.1	0.0072
19	210.1115	27561	1037.6	45449	4.7	0.0076
20	217.1060	28416	1396.4	61905	6.4	0.0076
21	226.1426	27851	1335.3	60539	6.3	0.0081
22	226.9527	28988	1424.1	64628	6.7	0.0078
23	229.1422	28925	662.1	30101	3.1	0.0079
24	230.2490	28603	2936.2	133646	13.9	0.0080
25	254.1375	29710	555.9	26750	2.8	0.0086
26	254.2490	29937	536.0	25791	2.7	0.0085
27	256.2645	29311	1370.2	66168	6.9	0.0087
28	261.1320	30019	1120.3	55923	5.8	0.0087
29	262.1811	29883	1385.8	69334	7.2	0.0088
30	274.2751	30096	2995.0	154973	16.1	0.0091
31	275.2786	29494	538.5	28085	2.9	0.0093
32	276.2310	30011	481.6	25228	2.6	0.0092
33	278.2469	28911	825.2	43390	4.5	0.0096
34	280.2645	30088	1537.2	81280	8.4	0.0093
35	282.2801	29120	7269.6	385458	40.0	0.0097
36	283.2836	30086	1527.8	80984	8.4	0.0094
37	290.2101	30915	1450.7	78824	8.2	0.0094
38	290.2701	30435	842.4	45801	4.8	0.0095
39	292.2259	29838	1406.3	76863	8.0	0.0098
40	294.9400	32072	523.7	28799	3.0	0.0092
41	296.2593	29929	2977.8	164129	17.0	0.0099
42	297.2628	30512	629.8	34791	3.6	0.0097
43	298.2749	29461	790.5	43895	4.6	0.0101
44	302.2464	31123	690.9	39626	4.1	0.0097
45	304.2620	30268	6761.7	391041	40.6	0.0101
46	305.1581	30541	512.1	29699	3.1	0.0100
47	305.2654	30167	1388.4	80528	8.4	0.0101
48	308.2206	30848	1159.3	67982	7.1	0.0100
49	318.2412	30522	15750.8	962990	100.0	0.0104
50	318.3017	34505	424.4	25946	2.7	0.0092
51	319.2446	30559	3168.7	194034	20.1	0.0104
52	320.2567	30153	12383.3	758426	78.8	0.0106
53	321.2602	30507	2507.1	153509	15.9	0.0105
54	332.2205	31895	1550.6	97539	10.1	0.0104
55	334.2164	22845	772.7	48880	5.1	0.0146
56	334.2360	31312	2179.8	137906	14.3	0.0107
57	335.2394	29246	422.8	26845	2.8	0.0115
58	336.2517	30884	14185.8	902481	93.7	0.0109
59	337.2550	30902	2884.9	184068	19.1	0.0109

High Resolution Mass Spectrometry Report

#	m/z	Res.	S/N	I	I %	FWHM
60	338.2610	17191	411.3	26291	2.7	0.0197
61	345.2044	32460	507.2	32835	3.4	0.0106
62	350.2309	31623	3386.3	220894	22.9	0.0111
63	351.2343	31516	687.8	45038	4.7	0.0111
64	352.2265	24774	1242.3	81611	8.5	0.0142
65	352.2464	31087	1875.3	123209	12.8	0.0113
66	353.2510	23635	397.4	26214	2.7	0.0149
67	353.2667	29117	453.1	29889	3.1	0.0121
68	354.2625	26758	467.2	30898	3.2	0.0132
69	359.2046	31479	435.5	28979	3.0	0.0114
70	366.2258	31928	549.4	36963	3.8	0.0115
71	368.2414	31708	1261.7	85113	8.8	0.0116
72	381.2984	33300	482.9	33439	3.5	0.0115
73	437.1939	34019	399.8	30001	3.1	0.0129
74	449.3606	33221	4706.0	362049	37.6	0.0135
75	450.3641	33421	1373.5	105869	11.0	0.0135
76	537.5357	35550	304.9	26775	2.8	0.0151
77	563.5512	35153	1120.8	101955	10.6	0.0160
78	564.5548	36328	463.2	42150	4.4	0.0155
79	613.4918	36061	554.7	53930	5.6	0.0170
80	615.5070	34734	651.8	63610	6.6	0.0177
81	617.5218	32052	289.5	28335	2.9	0.0193
82	619.3900	36367	1439.2	140967	14.6	0.0170
83	620.3928	34632	764.8	74947	7.8	0.0179
84	621.3931	27590	257.5	25234	2.6	0.0225
85	631.5022	36286	767.0	75940	7.9	0.0174
86	632.5058	35010	305.7	30285	3.1	0.0181
87	633.5173	32957	524.9	52068	5.4	0.0192
88	645.4815	35706	335.6	33339	3.5	0.0181
89	647.4968	34216	366.4	36480	3.8	0.0189
90	649.5123	33030	378.6	37753	3.9	0.0197
91	663.4920	34964	387.1	38724	4.0	0.0190
92	685.4361	37241	782.0	79289	8.2	0.0184
93	686.4394	36991	359.7	36503	3.8	0.0186
94	744.6117	37139	388.4	40790	4.2	0.0200
95	746.6263	32989	273.5	28745	3.0	0.0226
96	784.5437	36847	234.3	25296	2.6	0.0213
97	959.2257	39547	308.3	28936	3.0	0.0243
98	961.2238	38807	683.7	63996	6.6	0.0248
99	962.2263	38658	400.0	37360	3.9	0.0249
100	963.2230	36964	430.5	40144	4.2	0.0261

Acquisition Parameter

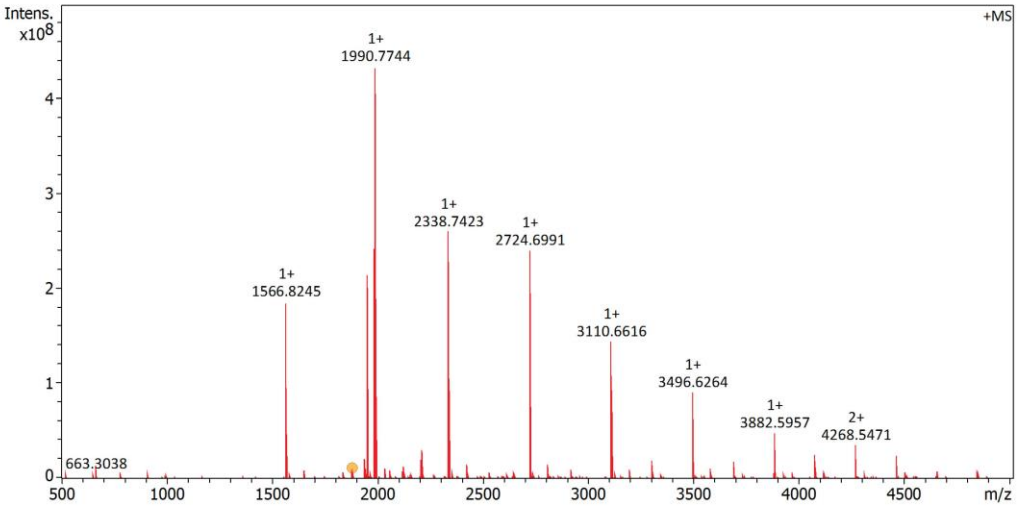
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	220 °C
Scan Begin	75 m/z	Set End Plate Offset	-500 V	Set Dry Gas	9.0 l/min
Scan End	1700 m/z	Set Collision Cell RF	350.0 Vpp	Set Ion Energy (MS only)	4.0 eV

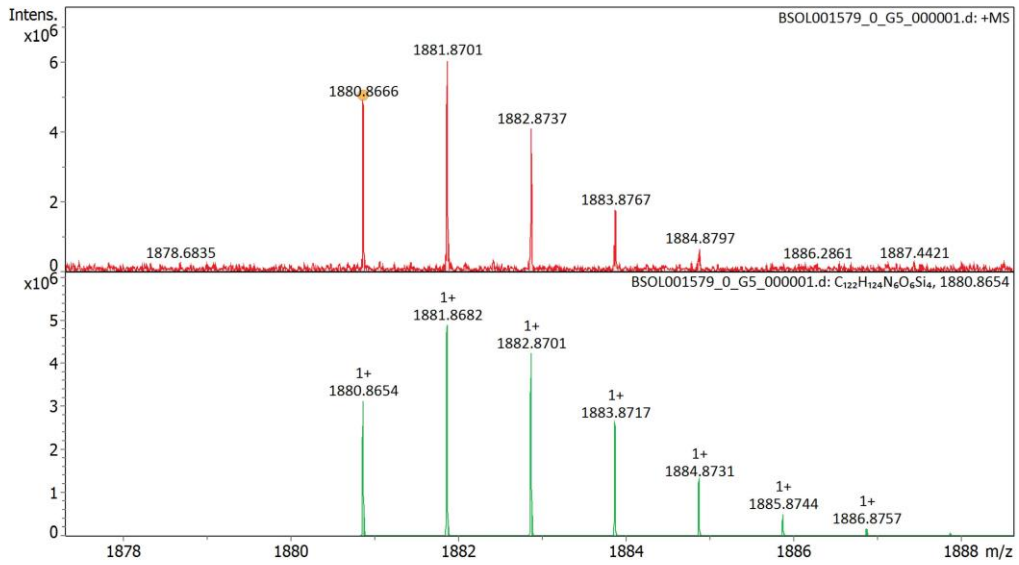
Bruker Compass DataAnalysis 5.3 Acquisition Date 3/7/2024 3:19:21 PM Page 3 of 3

Figure S59. HR-MS report of $\mathbf{M_{Br}}$.

Acquisition Parameter

Method:	MALDI_MS_POS_500-5000_2M_16AvScans			Acquisition Date:	17.12.2021 14:50:05
File Name:	D:\Data\ETH Data\BSOL0015xx\BSOL001579_0_G5_000001.d			Operator:	Daniel Wirz
Source	Dual (MALDI/ESI)	Polarity	Positive	Nebulizer Gas	1.3 bar
Broadband Low Mass	500.4 m/z			Drying Gas Flow Rate	3.7 L/min
Broadband High Mass	5000.0 m/z	Laser Power	32.0 lp	Capillary	4500.0 V
No. of Cell Fills	1			Drying Gas	200.0 °C
Apodization	Full-Sine	Time of Flight to Detector	0.004 sec	Temperature	





Evaluation Spectra / Validation Formula:

#	Ion Formula	Adduct	m/z	z	Meas. m/z	mSigma	N-Rule	err [mDa]	err [ppm]
1	C122H124N6O6Si4	M	1880.8654	1+	1880.8666	146.2	ok	-1.2	-0.6

Calibration Info:

Internal calibration

Date:	17.12.2021 14:51:49
Polarity:	Positive
Calibration spectrum:	+MS: Scan
Reference mass list:	MALDI: DCTB Matrix + Na-PFHA Cluster (pos)
Calibration mode:	Quadratic
Standard deviation:	0.721 ppm

Reference m/z	Resulting m/z	Intensity	Error [ppm]
250.1464			
251.1543			
273.1362			
332.2009			
408.9481			
500.2934			
501.3013			
523.2832			
750.4404			
751.4483			
773.4302			
794.9069			
1000.5874			
1001.5953			
1023.5772			
1180.8657			
1566.8246	1566.8245	186279136	-0.066
1952.7834	1952.7839	215077968	0.248
2338.7423	2338.7423	259881392	0.035
2724.7011	2724.6991	240395008	-0.747
3110.6599	3110.6616	144229904	0.542
3496.6188			
3882.5776			
4268.5365			
4654.4953			
5040.4541			
5426.4130			
5812.3718			
6198.3307			
6584.2895			
6970.2483			
7356.2072			
7742.1660			
8128.1249			
8514.0837			
8900.0425			
9286.0014			
9671.9602			

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	1566.8245	192333	4875.9	43.0	0.0081
2	1567.8279	182081	1232.2	10.9	0.0086
3	1940.5373	152790	453.7	4.8	0.0127
4	1952.7839	148878	4672.3	49.6	0.0131
5	1953.7869	155528	1698.2	18.0	0.0126
6	1987.7714	151862	5178.3	56.3	0.0131
7	1988.7747	149276	7646.6	83.1	0.0133
8	1989.7725	146356	7467.9	81.2	0.0136
9	1990.7744	158025	9196.7	100.0	0.0126
10	1990.7883	324414	1929.0	21.0	0.0061
11	1991.7627	174907	559.0	6.1	0.0114
12	1991.7765	142446	5011.4	54.5	0.0140
13	1992.7679	175872	718.6	7.8	0.0113
14	1992.7808	139809	1939.6	21.1	0.0143
15	1993.7721	170595	506.4	5.5	0.0117
16	1993.7855	160079	650.4	7.1	0.0125
17	2209.6608	106343	411.1	4.7	0.0208
18	2210.6634	127353	608.6	7.0	0.0174
19	2211.6667	110630	433.0	5.0	0.0200
20	2338.7423	131062	4951.8	60.0	0.0178
21	2339.7451	129943	2025.9	24.5	0.0180
22	2340.7483	129694	505.6	6.1	0.0180
23	2724.6991	112353	4111.9	55.5	0.0243
24	2725.7018	113630	2088.7	28.2	0.0240
25	2726.7050	113394	575.7	7.8	0.0240
26	3110.6616	87079	2275.0	33.3	0.0357
27	3111.6659	93963	1468.5	21.5	0.0331
28	3112.6690	98113	495.0	7.3	0.0317
29	3496.6264	82843	1285.9	21.1	0.0422
30	3497.6309	85989	900.7	14.8	0.0407
31	3498.6338	85489	293.9	4.8	0.0409
32	3882.5957	74700	639.9	11.2	0.0520
33	3883.5992	74978	516.8	9.0	0.0518
34	4076.0496	68752	324.7	5.9	0.0593
35	4076.5499	65424	275.0	5.0	0.0623
36	4268.5471	75071	481.8	8.2	0.0569
37	4269.0476	73017	278.7	4.8	0.0585
38	4269.5489	74766	474.4	8.1	0.0571
39	4461.9859	69550	324.0	5.5	0.0642
40	4462.4883	68885	305.6	5.2	0.0648

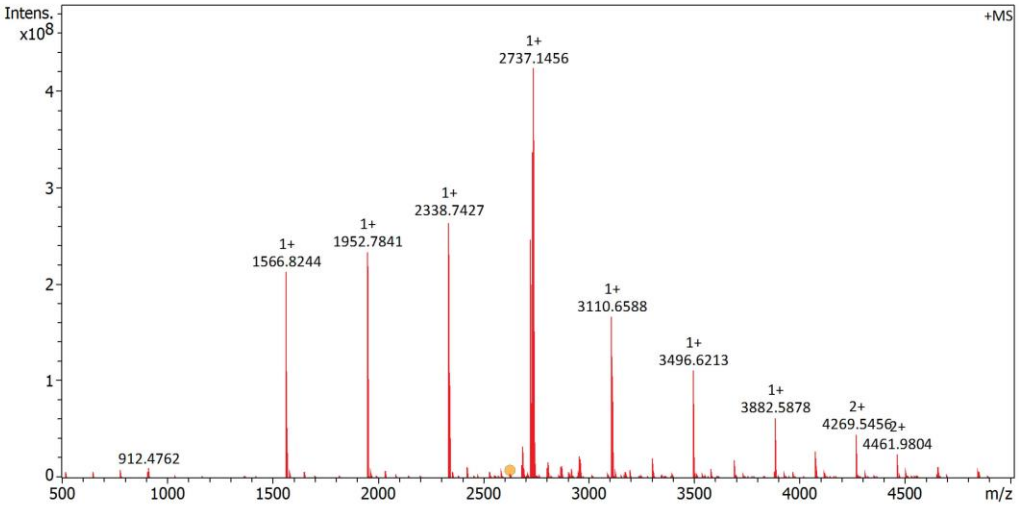
#	m/z	Res.	S/N	I %	FWHM
1	1880.8654	162516		64.1	0.0116
2	1881.8682	162603		100.0	0.0116
3	1882.8701	162689		86.6	0.0116
4	1883.8717	162776		53.6	0.0116
5	1884.8731	162862		26.1	0.0116
6	1885.8744	162949		10.5	0.0116
7	1886.8757	163035		3.6	0.0116
8	1887.8770	163122		1.1	0.0116
9	1888.8783	163208		0.3	0.0116

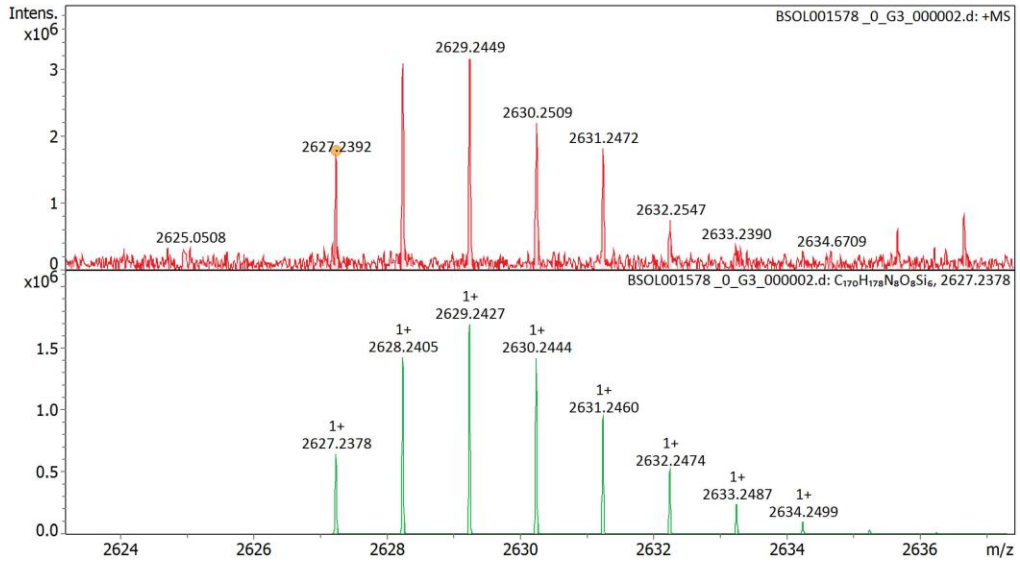
BSOL001578 Adriano D'Addio/ - DA-337-M3-P2 - DCM - DCTB+Ag 1:10:1

ETH Eidgenössische Technische Hochschule Zürich Swiss Federal Institute of Technology Zurich

Acquisition Parameter

Method:	MALDI_MS_POS_500-5000_2M_16AvScans			Acquisition Date:	17.12.2021 14:39:02
File Name:	D:\Data\ETH Data\BSOL0015xx\BSOL001578 _0_G3_000002.d			Operator:	Daniel Wirz
Source	Dual (MALDI/ESI)	Polarity	Positive	Nebulizer Gas	1.3 bar
Broadband Low Mass	500.4 m/z			Drying Gas Flow Rate	3.7 L/min
Broadband High Mass	5000.0 m/z	Laser Power	32.0 lp	Capillary	4500.0 V
No. of Cell Fills	1			Drying Gas	200.0 °C
Apodization	Full-Sine	Time of Flight to Detector	0.004 sec	Temperature	





BSOL001578 Adriano D'Addio/ - DA-337-M3-P2 - DCM - DCTB+Ag 1:10:1

ETH Eidgenössische Technische Hochschule Zürich Swiss Federal Institute of Technology Zurich

Evaluation Spectra / Validation Formula:

#	Ion Formula	Adduct	m/z	z	Meas. m/z	mSigma	N-Rule	err [mDa]	err [ppm]
1	C170H178N8O8Si6	M	2627.2378	1+	2627.2392	89.7	ok	-1.4	-0.5

Calibration Info:

Internal calibration

Date:	17.12.2021 14:40:59
Polarity:	Positive
Calibration spectrum:	+MS: Scan
Reference mass list:	MALDI: DCTB Matrix + Na-PFHA Cluster (pos)
Calibration mode:	Quadratic
Standard deviation:	0.721 ppm

Reference m/z	Resulting m/z	Intensity	Error [ppm]
250.1464			
251.1543			
273.1362			
332.2009			
408.9481			
500.2934			
501.3013			
523.2832			
750.4404			
751.4483			
773.4302			
794.9069			
1000.5874			
1001.5953			
1023.5772			
1180.8657			
1566.8246	1566.8244	213067040	-0.113
1952.7834	1952.7841	234032112	0.362
2338.7423	2338.7427	266039216	0.167
2724.7011	2724.6990	246330880	-0.759
3110.6599	3110.6588	166825936	-0.360
3496.6188	3496.6213	111774848	0.732
3882.5776			
4268.5365			
4654.4953			
5040.4541			
5426.4130			
5812.3718			
6198.3307			
6584.2895			
6970.2483			
7356.2072			
7742.1660			
8128.1249			
8514.0837			
8900.0425			
9286.0014			
9671.9602			

Mass List:

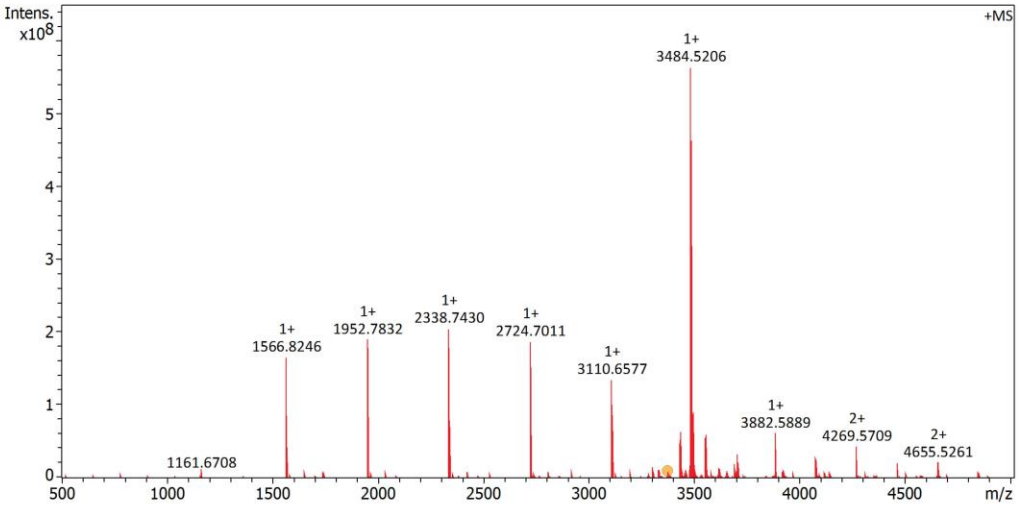
#	m/z	Res.	S/N	I %	FWHM
1	1566.8244	196111	5628.6	50.4	0.0080
2	1567.8282	185410	1384.4	12.4	0.0085
3	1952.7841	154331	5434.8	55.3	0.0127
4	1953.7873	155132	1961.7	20.0	0.0126
5	2338.7427	133027	5220.4	62.9	0.0176
6	2339.7454	130382	2138.9	25.8	0.0179
7	2340.7484	129328	524.3	6.3	0.0181
8	2685.9079	99483	328.6	5.3	0.0270
9	2686.9088	104556	481.4	7.8	0.0257
10	2687.9103	105152	488.6	7.9	0.0256
11	2688.9111	95677	384.1	6.2	0.0281
12	2724.6990	113319	3622.5	58.2	0.0240
13	2724.7252	168186	439.1	7.1	0.0162
14	2725.7018	113845	1810.3	29.1	0.0239
15	2726.7049	112855	481.8	7.8	0.0242
16	2734.1412	112024	1781.9	28.6	0.0244
17	2735.1446	107331	3626.9	58.3	0.0255
18	2736.1447	100758	4977.7	80.0	0.0272
19	2737.1456	107685	6224.0	100.0	0.0254
20	2738.1472	104228	5178.3	83.2	0.0263
21	2739.1475	91016	3097.0	49.8	0.0301
22	2740.1503	72532	1443.9	23.2	0.0378
23	2741.1548	72440	656.4	10.6	0.0378
24	2957.0379	99191	324.7	5.1	0.0298
25	2958.0398	94353	348.6	5.5	0.0314
26	3110.6588	89624	2533.9	39.4	0.0347
27	3111.6627	97756	1609.1	25.0	0.0318
28	3112.6657	101985	542.8	8.5	0.0305
29	3304.1345	96226	303.2	5.0	0.0343
30	3496.6213	85336	1512.2	26.4	0.0410
31	3497.6254	88698	1041.6	18.2	0.0394
32	3498.6284	89096	368.6	6.5	0.0393
33	3882.5878	81373	797.2	14.8	0.0477
34	3883.5905	81290	665.8	12.4	0.0478
35	4076.0448	70424	347.5	6.6	0.0579
36	4076.5480	66533	276.7	5.3	0.0613
37	4268.5419	76605	595.3	10.7	0.0557
38	4269.0437	75122	347.4	6.2	0.0568
39	4269.5456	75793	605.0	10.8	0.0563
40	4461.9804	69051	327.2	5.9	0.0646

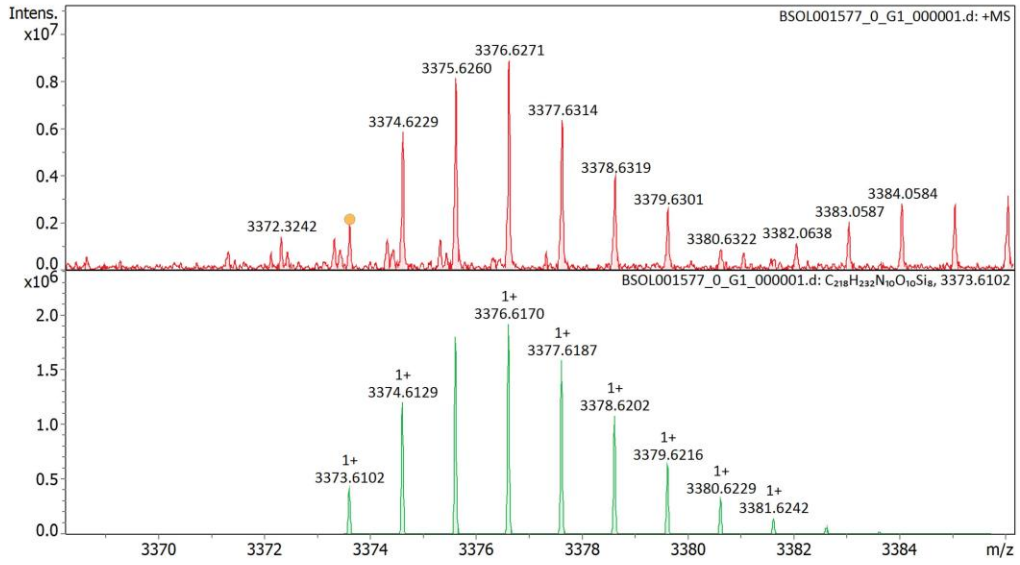
#	m/z	Res.	S/N	I %	FWHM
1	2627.2378	113557		38.3	0.0231
2	2628.2405	113600		84.1	0.0231
3	2629.2427	113643		100.0	0.0231
4	2630.2444	113687		84.0	0.0231
5	2631.2460	113730		55.4	0.0231
6	2632.2474	113773		30.3	0.0231
7	2633.2487	113817		14.2	0.0231
8	2634.2499	113860		5.8	0.0231
9	2635.2512	113903		2.1	0.0231
10	2636.2524	113946		0.7	0.0231
11	2637.2536	113990		0.2	0.0231

Figure S60. HR-MS report of **A[4]**.

Acquisition Parameter

Method:	MALDI_MS_POS_500-5000_2M_16AvScans			Acquisition Date:	17.12.2021 14:27:03
File Name:	D:\Data\ETH Data\BSOL0015xx\BSOL001577_0_G1_000001.d			Operator:	
Source	Dual (MALDI/ESI)	Polarity	Positive	Nebulizer Gas	1.3 bar
Broadband Low Mass	500.4 m/z			Drying Gas Flow Rate	3.7 L/min
Broadband High Mass	5000.0 m/z	Laser Power	34.6 lp	Capillary	4500.0 V
No. of Cell Fills	1			Drying Gas	200.0 °C
Apodization	Full-Sine	Time of Flight to Detector	0.004 sec	Temperature	





BSOL001577 Adriano D'Addio/ - DA-337-M3-P1 - DCM - DCTB+Ag 1:10:1

ETH Eidgenössische Technische Hochschule Zürich Swiss Federal Institute of Technology Zurich

Evaluation Spectra / Validation Formula:

#	Ion Formula	Adduct	m/z	z	Meas. m/z	mSigma	N-Rule	err [mDa]	err [ppm]
1	C218H232N10O10Si8	M	3373.6102	1+	3373.6201	60.8	ok	-9.9	-2.9

Calibration Info:

Internal calibration

Date:	17.12.2021 14:31:40
Polarity:	Positive
Calibration spectrum:	+MS: Scan
Reference mass list:	MALDI: DCTB Matrix + Na-PFHA Cluster (pos)
Calibration mode:	Quadratic
Standard deviation:	0.575 ppm

Reference m/z	Resulting m/z	Intensity	Error [ppm]
250.1464			
251.1543			
273.1362			
332.2009			
408.9481			
500.2934			
501.3013			
523.2832			
750.4404			
751.4483			
773.4302			
794.9069			
1000.5874			
1001.5953			
1023.5772			
1180.8657			
1566.8246	1566.8246	166675280	0.005
1952.7834	1952.7832	190861200	-0.113
2338.7423	2338.7430	206008576	0.335
2724.7011	2724.7011	188013168	-0.003
3110.6599	3110.6577	136381216	-0.721
3496.6188	3496.6205	89869624	0.504
3882.5776			
4268.5365			
4654.4953			
5040.4541			
5426.4130			
5812.3718			
6198.3307			
6584.2895			
6970.2483			
7356.2072			
7742.1660			
8128.1249			
8514.0837			
8900.0425			
9286.0014			
9671.9602			

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	1566.8246	198264	4412.2	29.5	0.0079
2	1567.8287	192654	1106.5	7.4	0.0081
3	1952.7832	152885	4395.5	33.8	0.0128
4	1953.7869	143834	1379.8	10.6	0.0136
5	2338.7430	132220	4194.4	36.5	0.0177
6	2339.7459	124999	1616.6	14.1	0.0187
7	2724.7011	110834	3501.2	33.3	0.0246
8	2725.7044	106372	1645.1	15.6	0.0256
9	3110.6577	92184	1266.5	24.1	0.0337
10	3111.6614	93807	800.7	15.3	0.0332
11	3432.2873	71399	293.9	5.4	0.0481
12	3433.2880	73452	454.3	8.3	0.0467
13	3434.2875	78299	612.1	11.2	0.0439
14	3435.2874	76239	597.2	10.9	0.0451
15	3436.2886	74606	515.7	9.4	0.0461
16	3437.2892	69993	350.1	6.4	0.0491
17	3480.5128	81136	915.6	15.1	0.0429
18	3481.5148	76100	2425.0	39.9	0.0457
19	3482.5157	68671	4137.9	68.1	0.0507
20	3483.0971	85703	316.2	5.2	0.0406
21	3483.5185	66776	5830.7	95.9	0.0522
22	3484.5206	64551	6079.4	100.0	0.0540
23	3485.5192	71827	4992.9	82.1	0.0485
24	3486.5187	71008	3359.1	55.3	0.0491
25	3487.5204	67892	1944.6	32.0	0.0514
26	3488.5258	63349	1048.5	17.3	0.0551
27	3489.5296	68540	536.8	8.9	0.0509
28	3496.6205	79238	965.8	15.9	0.0441
29	3497.6243	80731	705.3	11.6	0.0433
30	3552.4475	78177	449.9	7.4	0.0454
31	3553.4484	77104	602.4	9.9	0.0461
32	3554.4498	76805	637.6	10.5	0.0463
33	3555.4514	75858	537.1	8.9	0.0469
34	3556.4522	75743	392.3	6.5	0.0470
35	3704.4236	78797	340.7	5.3	0.0470
36	3705.4237	79072	376.3	5.8	0.0469
37	3882.5889	73801	718.1	11.1	0.0526
38	3883.5931	73961	613.2	9.5	0.0525
39	4268.5682	73503	532.4	7.5	0.0581
40	4269.5709	73610	562.1	7.9	0.0580

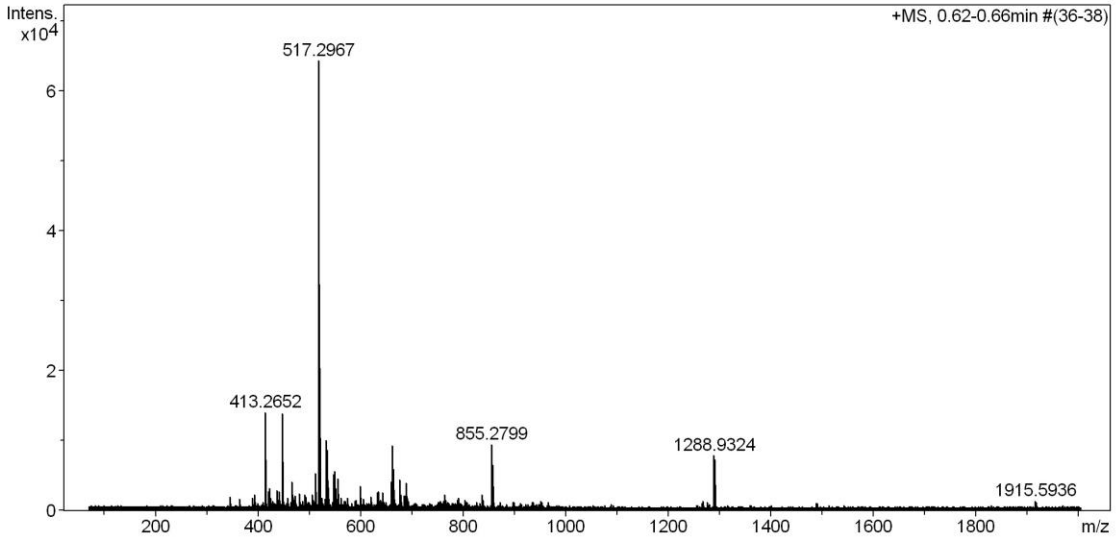
#	m/z	Res.	S/N	I %	FWHM
1	3373.6102	86133		22.1	0.0392
2	3374.6129	86158		62.6	0.0392
3	3375.6151	86184		94.5	0.0392
4	3376.6170	86209		100.0	0.0392
5	3377.6187	86235		82.6	0.0392
6	3378.6202	86260		56.5	0.0392
7	3379.6216	86286		33.1	0.0392
8	3380.6229	86312		17.0	0.0392
9	3381.6242	86337		7.8	0.0392
10	3382.6254	86363		3.2	0.0392
11	3383.6266	86388		1.2	0.0392
12	3384.6278	86414		0.4	0.0392
13	3385.6290	86439		0.1	0.0392

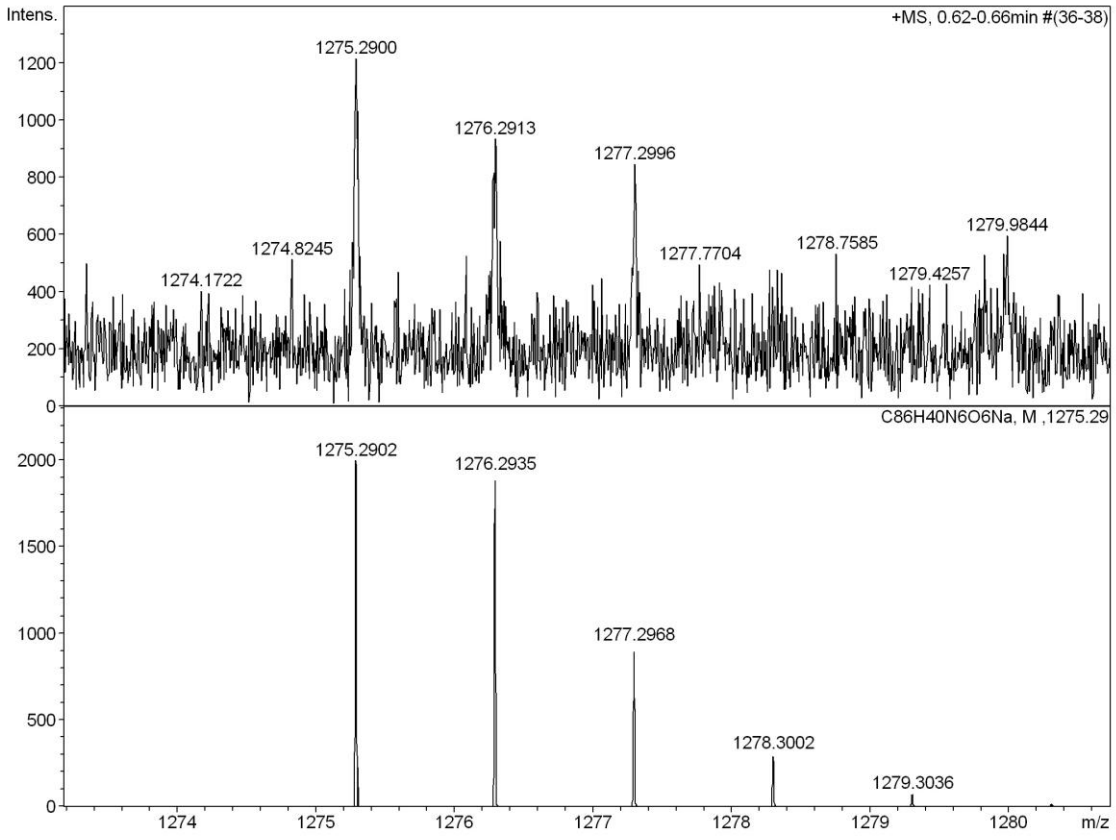
Bruker Daltonics solariX ETH - MS-Service LOC - D-CHAB Page 2 of 2

Figure S60. HR-MS report of **A[5]**.

High Resolution Mass Spectrometry Report

Sample Name	**DA 338**	Instrument	maXis 4G
Comment	direct injection manually. dissolved in THF,. ANalyzed in Meoh+fa 0.1%	Method	24 Direct_pos_high.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
1275.2900	1	C 86 H 40 N 6 Na O 6	100.00	1275.2902	0.1	0.1	138.1	69.5	even	1+

Mass list

#	m/z	I %	I
1	345.2023	3.0	1958
2	365.1053	2.7	1734
3	389.2510	2.9	1856
4	393.2092	3.7	2398
5	393.2970	3.2	2041
6	413.2652	21.9	14072
7	413.3238	4.2	2717
8	414.2694	6.9	4440
9	421.2322	4.4	2803
10	423.1817	2.3	1502
11	423.2205	4.9	3182
12	425.1815	3.0	1904
13	425.2154	3.0	1941
14	437.2358	4.6	2948
15	441.2971	4.3	2740
16	441.3561	2.5	1603
17	447.2922	2.3	1478
18	447.3443	21.7	13971
19	448.3483	6.4	4089
20	457.3490	2.8	1821
21	467.2463	6.4	4131
22	469.3254	3.1	1999
23	471.2059	2.4	1517
24	473.3449	3.5	2239
25	481.2615	3.8	2436
26	491.2429	3.7	2395
27	493.2439	3.2	2026
28	505.2781	3.7	2399
29	507.2420	2.4	1527
30	511.2733	8.4	5384
31	512.2761	2.3	1469
32	517.2967	100.0	64316
33	517.3709	3.5	2229
34	518.2997	33.0	21199
35	519.2965	91.4	58777
36	520.2995	31.8	20477
37	521.3030	5.7	3680
38	525.2795	2.5	1630
39	531.3862	2.4	1536
40	533.2914	15.6	10049
41	534.2951	5.3	3386
42	535.2909	12.6	8123
43	536.2942	5.2	3334
44	547.2701	8.0	5169
45	548.2759	2.7	1718
46	549.2756	8.7	5604
47	550.2812	3.1	2011
48	551.2865	4.9	3168
49	555.2996	7.2	4624
50	561.3992	3.0	1937
51	575.4143	2.8	1813
52	591.1924	2.4	1557
53	599.3257	5.6	3595
54	600.3271	2.7	1745
55	605.4241	2.8	1775
56	619.4384	3.1	2016
57	633.3786	4.2	2698
58	635.3822	4.2	2732
59	639.4217	2.4	1538
60	643.3507	4.0	2560
61	659.1705	6.4	4109
62	660.1749	3.6	2324

High Resolution Mass Spectrometry Report

#	m/z	I %	I
63	661.1699	14.4	9275
64	661.4097	2.5	1637
65	662.1738	5.2	3363
66	662.2845	4.5	2863
67	663.1698	9.3	5998
68	663.2854	2.3	1472
69	663.4605	3.6	2295
70	664.1726	3.9	2482
71	665.1667	2.5	1611
72	677.1666	2.6	1681
73	677.3782	7.0	4494
74	678.3813	3.7	2374
75	685.4362	3.4	2163
76	686.1936	3.3	2137
77	687.3785	2.5	1606
78	688.1895	6.2	3980
79	689.1617	3.2	2080
80	690.1850	3.0	1922
81	763.1777	3.5	2267
82	764.1780	2.6	1646
83	765.1757	2.5	1626
84	789.4980	2.3	1481
85	791.4991	2.9	1896
86	837.1971	2.3	1500
87	837.6215	3.4	2209
88	838.6219	2.4	1519
89	855.2799	14.8	9523
90	856.2817	10.2	6547
91	857.2801	10.3	6651
92	858.2809	6.2	4007
93	1287.4293	4.6	2991
94	1287.9299	7.8	5034
95	1288.4314	10.8	6947
96	1288.9324	12.3	7937
97	1289.4348	11.4	7358
98	1289.9339	8.2	5296
99	1290.4336	5.3	3381
100	1290.9380	2.3	1508

Acquisition Parameter

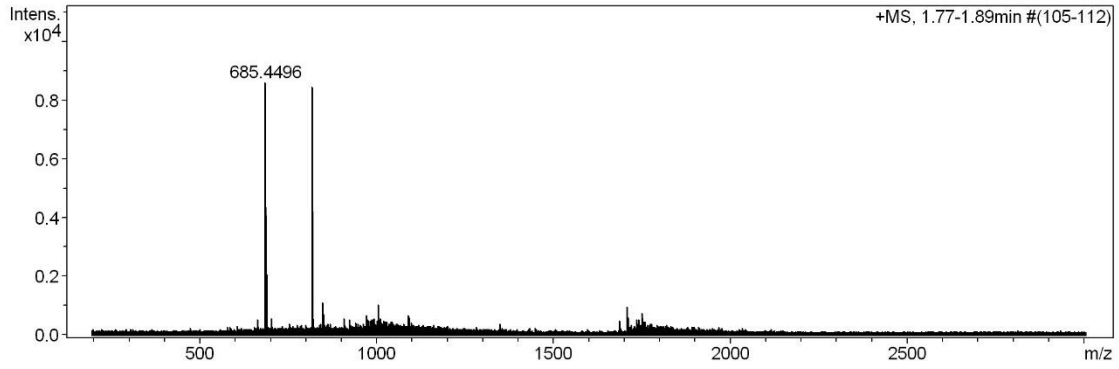
General	Fore Vacuum	3.46e+000 mBar	High Vacuum	1.07e-007 mBar	Source Type	ESI
	Scan Begin	75 m/z	Scan End	2000 m/z	Ion Polarity	Positive
Source	Set Nebulizer	0.4 Bar	Set Capillary	3600 V	Set Dry Gas	4.0 l/min
	Set Dry Heater	180 °C	Set End Plate Offset	-500 V		
Quadrupole	Set Ion Energy (MS only)	4.0 eV				
Coll. Cell	Collision Energy	10.0 eV	Set Collision Cell RF	1000.0 Vpp	300.0 Vpp	
Ion Cooler	Set Ion Cooler Transfer Time	160.0 µs	Set Ion Cooler Pre Pulse Storage Time		18.0 µs	

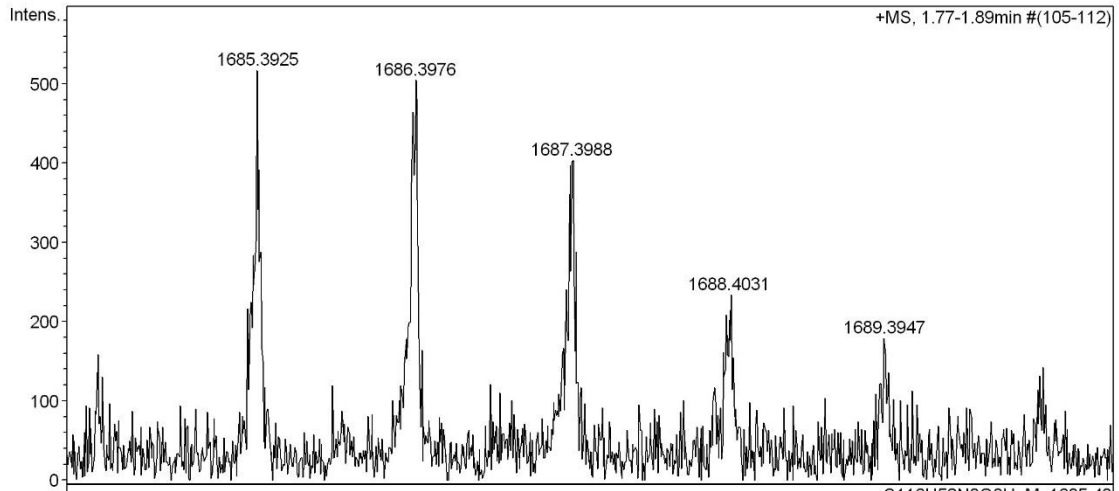
Figure S62. HR-MS report of G_{BD}**[3]**.

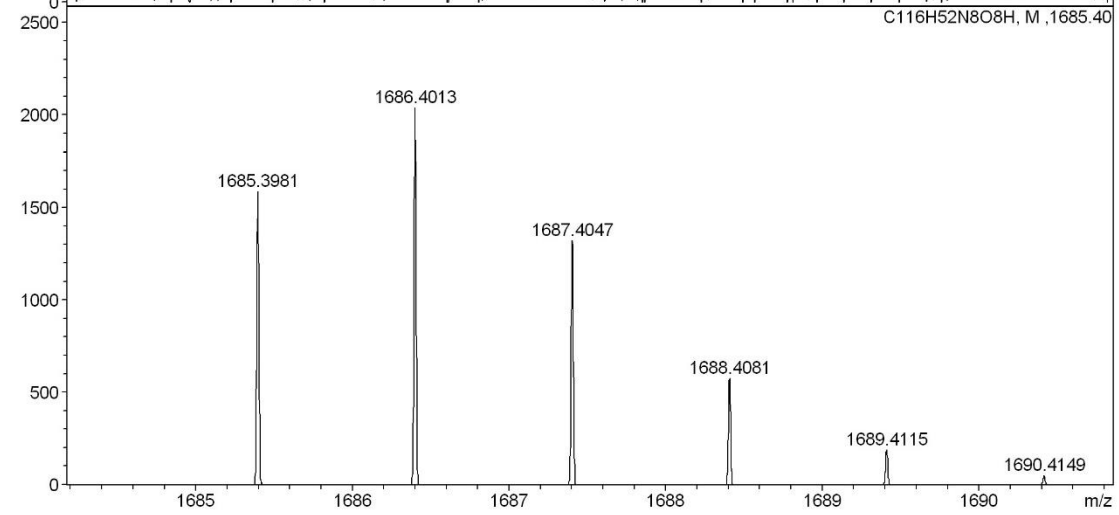
High Resolution Mass Spectrometry Report

Sample Name **DA-385**
Comment

Instrument maXis 4G
Method 24 Direct_pos_high.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
1684.3795	1	C 116 H 52 N 8 O 8	100.00	1684.3903	10.7	6.4	310.1	95.0	odd	1+
1685.3925	1	C 116 H 53 N 8 O 8	100.00	1685.3981	5.6	3.3	160.0	94.5	even	
1707.3782	1	C 116 H 52 N 8 Na O 8	100.00	1707.3800	1.8	1.1	178.1	94.5	even	
1723.3608	1	C 116 H 52 K N 8 O 8	100.00	1723.3540	-6.9	-4.0	653.7	94.5	even	
1748.3973	1	C 118 H 55 N 9 Na O 8	100.00	1748.4066	9.3	5.3	430.1	95.5	even	

Mass list

#	m/z	I %	I
1	663.4695	6.3	544
2	685.4496	100.0	8602
3	686.4532	47.7	4106
4	687.4545	12.8	1098
5	701.4217	6.8	583
6	753.3633	4.6	394
7	755.3647	4.8	413
8	816.3205	98.6	8480
9	817.3235	63.9	5495
10	818.3276	22.5	1939
11	819.3295	4.9	425
12	848.3096	13.1	1124
13	849.3109	8.5	727
14	850.3182	6.9	593
15	851.3276	4.9	418
16	861.5254	4.4	380
17	867.3222	4.5	391
18	907.7774	6.6	565
19	908.7815	4.8	416
20	924.2188	6.2	530
21	939.7644	4.3	369
22	942.2137	5.0	433
23	945.7399	4.5	391
24	953.7401	4.2	361
25	961.6337	4.5	383
26	963.7035	4.5	383
27	971.7530	7.7	665
28	972.7594	5.9	509
29	975.6119	6.4	550
30	976.6199	5.4	468
31	977.6213	5.9	508
32	983.2056	5.8	500
33	985.7323	6.4	555
34	987.7401	5.5	469
35	989.5900	6.2	530
36	990.5972	4.7	407
37	991.6063	4.6	394
38	992.6092	4.4	377
39	993.6201	6.6	571
40	995.6331	4.7	404
41	997.6521	4.2	364
42	1001.7222	5.7	490
43	1003.5712	8.6	743
44	1003.7431	12.1	1039
45	1004.5765	4.9	425
46	1004.7468	6.6	567
47	1005.5845	4.3	374
48	1005.6616	4.9	420
49	1005.7481	4.3	369
50	1006.5872	4.4	380
51	1007.5953	4.8	412
52	1008.6102	4.4	381
53	1009.6157	5.9	511
54	1011.6323	4.8	410
55	1015.6271	4.6	395
56	1017.6278	4.8	411
57	1019.5626	4.5	391
58	1019.7215	5.8	495

High Resolution Mass Spectrometry Report

#	m/z	I %	I
59	1021.5870	5.0	433
60	1022.5761	5.5	473
61	1023.5905	5.1	435
62	1025.6067	5.1	441
63	1026.6120	4.5	386
64	1027.6203	5.2	452
65	1029.6347	4.2	365
66	1037.5771	4.5	391
67	1047.5997	4.7	403
68	1055.6514	4.6	396
69	1057.5972	4.5	388
70	1067.6200	4.3	374
71	1089.6274	7.4	637
72	1090.6306	7.2	623
73	1098.6590	5.0	427
74	1099.6662	4.3	367
75	1119.6722	4.3	371
76	1348.8834	4.7	403
77	1685.3925	6.0	518
78	1686.3976	4.8	417
79	1687.3988	4.7	402
80	1707.3782	7.7	667
81	1708.3819	11.2	964
82	1709.3847	7.0	603
83	1710.3913	5.7	491
84	1733.3859	4.4	381
85	1734.3780	5.0	431
86	1735.3843	4.8	410
87	1739.3854	6.1	528
88	1740.3873	4.8	417
89	1741.3842	5.2	444
90	1747.3981	4.2	365
91	1749.3744	7.6	655
92	1750.3769	8.6	743
93	1751.3815	7.8	673
94	1756.3761	4.4	374
95	1757.3736	5.6	479
96	1758.3837	4.7	404
97	1759.3832	5.1	441
98	1760.3855	4.5	384
99	1775.3663	4.6	399
100	1777.3696	4.4	382

Acquisition Parameter

General	Fore Vacuum	3.21e+000 mBar	High Vacuum	9.22e-008 mBar	Source Type	ESI
	Scan Begin	200 m/z	Scan End	3000 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		

Figure S63. HR-MS report of G_{BD}**[4]**.

Cartesians of optimized geometries

92
GBD2-b3lyp-def2svp-freq.out Energy: -1674726.8044058
O -1.46279 3.00841 0.79491
O -3.53335 3.17126 -3.31769
O 1.46280 3.00842 -0.79491
O 3.53336 3.17125 3.31769
N -2.68965 2.77046 -1.17424
N -5.56559 -1.92474 0.10282
N 5.56559 -1.92474 -0.10283
N 2.68966 2.77046 1.17424
C -1.75506 3.39421 -0.31072
C -1.25827 4.60025 -1.04604
C -0.35707 5.59810 -0.65424
C -0.16408 6.65684 -1.56533
H 0.53231 7.45615 -1.30031
C -0.81782 6.70196 -2.80336
H -0.62458 7.53950 -3.47792
C -1.70759 5.68957 -3.18325
H -2.22896 5.70443 -4.14243
C -1.91179 4.65536 -2.27799
C -2.81975 3.47718 -2.39499
C -3.42171 1.59281 -0.85204
C -4.01479 1.45307 0.41133
H -3.90112 2.23969 1.15664
C -4.72394 0.29398 0.72550
H -5.16425 0.17317 1.71724
C -4.86756 -0.72820 -0.22272
C -4.28846 -0.57601 -1.49030
H -4.40529 -1.36791 -2.23267
C -3.56029 0.57107 -1.80225
H -3.11222 0.68010 -2.78926
C -6.92942 -2.04955 0.37190
C -7.92798 -1.06816 0.36926
H -7.69546 -0.02641 0.14121
C -9.23164 -1.46778 0.66566
H -10.02923 -0.72042 0.67085
C -9.54082 -2.81113 0.95477
H -10.57242 -3.08903 1.18316
C -8.54511 -3.78649 0.94837
H -8.78923 -4.82894 1.16792
C -7.22444 -3.41376 0.65433
C -4.97720 -3.18493 0.21588
C -5.97504 -4.14005 0.55522
C -5.60148 -5.48244 0.73333
H -6.35105 -6.23465 0.99113
C -4.26834 -5.85158 0.58932
H -3.96648 -6.89065 0.73112
C -3.27475 -4.88653 0.26957
C -3.63731 -3.53702 0.07698
H -2.87423 -2.79692 -0.16390
C -1.89543 -5.22118 0.15720
C -0.67967 -5.34546 0.05436
C 0.67967 -5.34546 -0.05432
C 1.89542 -5.22118 -0.15716
C 4.97719 -3.18493 -0.21588
C 3.63731 -3.53702 -0.07696
H 2.87423 -2.79692 0.16392
C 3.27475 -4.88653 -0.26954
C 4.26834 -5.85158 -0.58929
H 3.96647 -6.89066 -0.73109
C 5.60147 -5.48245 -0.73331
H 6.35103 -6.23465 -0.99111
C 5.97504 -4.14006 -0.55522
C 6.92941 -2.04956 -0.37192
C 7.22444 -3.41377 -0.65434
C 8.54510 -3.78650 -0.94839
H 8.78922 -4.82895 -1.16795
C 9.54081 -2.81114 -0.95481
H 10.57240 -3.08904 -1.18321
C 9.23163 -1.46778 -0.66571
H 10.02922 -0.72043 -0.67091
C 7.92798 -1.06816 -0.36930
H 7.69546 -0.02641 -0.14125
C 4.86757 -0.72820 0.22271
C 4.72393 0.29398 -0.72551
H 5.16424 0.17316 -1.71725
C 4.01478 1.45307 -0.41134
H 3.90111 2.23969 -1.15664
C 3.42172 1.59281 0.85204
C 3.56030 0.57107 1.80225
H 3.11224 0.68011 2.78926
C 4.28848 -0.57601 1.49029
H 4.40530 -1.36791 2.23267
C 1.75507 3.39422 0.31073
C 1.25828 4.60025 1.04605
C 0.35708 5.59810 0.65425
C 0.16408 6.65684 1.56534
H -0.53231 7.45615 1.30033
C 0.81782 6.70195 2.80338
H 0.62458 7.53949 3.47794
C 1.70760 5.68957 3.18326
H 2.22896 5.70442 4.14244
C 1.91180 4.65536 2.27799
C 2.81976 3.47718 2.39499

138
GBD3-B3LYP-def2svp-freq.out Energy: -2559092.8137672
C -0.38999 -3.03763 0.57609
C 0.38997 -3.03761 -0.57612
C 0.80152 -4.22123 -1.20044
C 0.38253 -5.41526 -0.58534
C -0.38258 -5.41528 0.58522
C -0.80155 -4.22126 1.20036
C -0.63539 -1.62004 0.97491
N 0.00001 -0.80158 0.00002
C 0.63538 -1.62001 -0.97490
O -1.24889 -1.23633 1.94202
O 1.24889 -1.23628 -1.94200
C 0.00001 0.63197 0.00004
C -0.84910 1.35450 0.86088
C -0.83219 2.74844 0.86850
C 0.00001 3.46695 0.00005
C 0.83222 2.74845 -0.86841
C 0.84913 1.35450 -0.86079
N 0.00001 4.88739 0.00004
C -1.12488 5.70833 -0.11924
C -0.71879 7.07255 -0.07620
C 0.71881 7.07255 0.07617
C 1.12490 5.70833 0.11928
C -2.45975 5.34984 -0.28918
C -3.42568 6.37278 -0.39493
C -3.02791 7.73641 -0.34251
C -1.69016 8.08163 -0.19011
C 1.69019 8.08163 0.19002
C 3.02794 7.73641 0.34244
C 3.42571 6.37278 0.39494
C 2.45977 5.34984 0.28924
C -4.78542 5.97824 -0.54287
C -5.89919 5.47635 -0.65276
C 4.78544 5.97824 0.54290
C 5.89920 5.47633 0.65281
C 2.91961 -3.79345 -2.55515
C 3.62363 -3.84988 -3.75509
C 3.07194 -4.37279 -4.91850
C 1.76308 -4.86346 -4.83528
C 1.04975 -4.81144 -3.63026
C 1.60427 -4.26235 -2.45639
C 3.82353 -3.21892 -1.51399
N 5.05624 -2.93264 -2.16236
C 4.98393 -3.28240 -3.53960
O 3.57835 -3.03923 -0.34465
O 5.85636 -3.14820 -4.36209
C 6.20434 -2.36842 -1.52631
C 7.48771 -2.55720 -2.07088
C 8.60189 -1.96935 -1.47403
C 8.47493 -1.21416 -0.29970
C 7.19973 -1.06204 0.26345
C 6.07431 -1.61065 -0.34901
N 9.60484 -0.59318 0.29319
C 9.69653 0.76198 0.63071
C 10.99205 1.02836 1.15327
C 11.71427 -0.22592 1.13140
C 10.82722 -1.20232 0.59754
C 8.74439 1.77025 0.49831
C 9.07555 3.07324 0.92629
C 10.36765 3.34421 1.45102
C 11.31646 2.33350 1.55757
C 13.00611 -0.60365 1.52801
C 13.39458 -1.93535 1.39663
C 12.50023 -2.89327 0.88211
C 11.21033 -2.54480 0.47963
C 8.06003 4.06793 0.84505
C 7.07445 4.79272 0.75718
C -3.62365 -3.84999 3.75504
C -2.91963 -3.79352 2.55509
C -1.60429 -4.26243 2.45631
C -1.04978 -4.81158 3.63016
C -1.76310 -4.86364 4.83518
C -3.07196 -4.37295 4.91843
C -4.98394 -3.28250 3.53958
N -5.05626 -2.93267 2.16235
C -3.82355 -3.21895 1.51396
O -5.85637 -3.14832 4.36207
O -3.57838 -3.03922 0.34463
C -6.20435 -2.36842 1.52632
C -6.07432 -1.61062 0.34904
C -7.19974 -1.06200 -0.26341
C -8.47494 -1.21413 0.29975
C -8.60190 -1.96935 1.47406
C -7.48772 -2.55722 2.07089
N -9.60485 -0.59313 -0.29314
C -10.82722 -1.20229 -0.59753
C -11.71426 -0.22588 -1.13140
C -10.99205 1.02839 -1.15324
C -9.69654 0.76202 -0.63066
C -11.21031 -2.54477 -0.47964
C -12.50020 -2.89324 -0.88216
C -13.39455 -1.93533 -1.39669
C -13.00609 -0.60362 -1.52805
C -11.31645 2.33353 -1.55755
C -10.36764 3.34425 -1.45098
C -9.07555 3.07328 -0.92622
C -8.74440 1.77029 -0.49824
C -8.06003 4.06797 -0.84498
C -7.07445 4.79275 -0.75712
H 0.67748 -6.36987 -1.02750
H -0.67754 -6.36990 1.02734
H -1.50418 0.82954 1.54877
H -1.47513 3.28269 1.57019
H 1.47515 3.28269 -1.57009
H 1.50420 0.82955 -1.54868
H -2.77099 4.30743 -0.34385

```
H         -3.79116        8.51191       -0.42505
H         -1.39789        9.13405       -0.15970
H          1.39793        9.13405        0.15956
H          3.79120        8.51191        0.42494
H          2.77100        4.30743        0.34397
H          3.64425       -4.39860       -5.84786
H          1.28318       -5.28862       -5.71998
H          0.02428       -5.18772       -3.60026
H          7.61411       -3.12742       -2.98728
H          9.58228       -2.08815       -1.93848
H          7.08175       -0.50320        1.19312
H          5.09763       -1.47067        0.10598
H          7.75618        1.57709        0.08372
H         10.60367        4.35894        1.77575
H         12.30817        2.55547        1.95912
H         13.69623        0.13749        1.93891
H         14.39806       -2.24241        1.70031
H         12.81937       -3.93521        0.79751
H         10.52400       -3.29934        0.09315
H         -0.02430       -5.18786        3.60014
H         -1.28320       -5.28883        5.71985
H         -3.64426       -4.39880        5.84778
H         -5.09764       -1.47063       -0.10594
H         -7.08176       -0.50313       -1.19306
H         -9.58229       -2.08815        1.93850
H         -7.61412       -3.12746        2.98728
H        -10.52399       -3.29931       -0.09315
H        -12.81934       -3.93519       -0.79758
H        -14.39802       -2.24240       -1.70040
H        -13.69621        0.13752       -1.93895
H        -12.30816        2.55551       -1.95912
H        -10.60366        4.35898       -1.77571
H         -7.75620        1.57713       -0.08363

184
GBD4-B3LYP-def2svp-freq.out   Energy: -3443460.4961442
C          2.31582       -1.51879       -1.90214
C          1.45082       -1.44814       -0.81401
C          0.45910       -2.40932       -0.58693
C          0.38193       -3.44660       -1.53492
C          1.23945       -3.50677       -2.63780
C          2.24511       -2.54632       -2.85026
C          3.22797       -0.33865       -1.85183
N          2.88700        0.39450       -0.68201
C          1.81322       -0.24634       -0.00508
O          4.08637       -0.05005       -2.65092
O          1.30261        0.11463        1.02848
C          3.52868        1.60220       -0.25602
C          4.76619        1.99075       -0.80419
C          5.37544        3.17956       -0.40730
C          4.79544        3.99721        0.57174
C          3.57455        3.59931        1.13342
C          2.93736        2.43111        0.71654
N          5.42981        5.20009        0.98164
C          6.76089        5.32919        1.38855
C          7.02776        6.69254        1.70118
C          5.79958        7.41907        1.46916
C          4.83917        6.46622        1.02465
C          7.73675        4.34527        1.52537
C          9.02399        4.72600        1.95951
C          9.29863        6.08631        2.26674
C          8.31087        7.05657        2.14391
C          5.42671        8.76949        1.57897
C          4.13197        9.15566        1.25236
C          3.18138        8.20130        0.79869
C          3.54453        6.84332        0.67747
C         10.01147        3.70471        2.05182
C         10.73950        2.71758        2.05505
C          1.84264        8.55302        0.46699
C          0.66068        8.68338        0.16631
C         -1.45121       -1.44803        0.81446
C         -2.31594       -1.51836        1.90283
C         -2.24510       -2.54570        2.85114
C         -1.23953       -3.50623        2.63872
C         -0.38216       -3.44630        1.53571
C         -0.45950       -2.40924        0.58749
C         -1.81393       -0.24656        0.00516
N         -2.88741        0.39449        0.68228
C         -3.22800       -0.33813        1.85251
O         -1.30387        0.11408       -1.02878
O         -4.08594       -0.04897        2.65189
C         -3.52916        1.60200        0.25603
C         -4.76774        1.98947        0.80247
C         -5.37697        3.17824        0.40543
C         -4.79593        3.99677       -0.57228
C         -3.57399        3.59981       -1.13238
C         -2.93677        2.43176       -0.71511
N         -5.43025        5.19958       -0.98237
C         -6.76118        5.32860       -1.38987
C         -7.02811        6.69199       -1.70226
C         -5.80015        7.41866       -1.46947
C         -4.83980        6.46586       -1.02476
C         -7.73687        4.34462       -1.52743
C         -9.02401        4.72532       -1.96190
C         -9.29869        6.08567       -2.26889
C         -8.31106        7.05600       -2.14544
C         -5.42750        8.76918       -1.57876
C         -4.13299        9.15552       -1.25144
C         -3.18245        8.20122       -0.79757
C         -3.54542        6.84315       -0.67680
C        -10.01139        3.70396       -2.05452
C        -10.73911        2.71659       -2.05795
C          5.32580       -2.93043       -5.08117
C          4.52611       -2.84769       -3.94439
C          3.14391       -2.64428       -4.03565
C          2.61308       -2.55154       -5.33798
C          3.42388       -2.63289       -6.47808
C          4.80715       -2.81966       -6.36584
C          6.73706       -3.15260       -4.65907
N          6.71988       -3.23400       -3.23838
C          5.39766       -3.05163       -2.74874
O          7.70498       -3.25056       -5.37249
O          5.06159       -3.07415       -1.58816
C          7.86953       -3.46486       -2.42232
C          9.00658       -4.10212       -2.95165
C         10.14071       -4.29277       -2.16348
C         10.15965       -3.89210       -0.82008
C          9.01134       -3.29063       -0.28520
C          7.88799       -3.05791       -1.07647
N         11.32007       -4.06755       -0.02225
C         12.05292       -5.24926        0.13496
C         13.16139       -4.99962        0.99180
C         13.09097       -3.60471        1.37188
C         11.94307       -3.06458        0.72912
C         11.80600       -6.52868       -0.37968
C         12.69486       -7.55041       -0.04317
C         13.80514       -7.31495        0.78994
C         14.04026       -6.04514        1.31314
C         13.88117       -2.77361        2.18243
C         13.52813       -1.43973        2.35364
C         12.38159       -0.90457        1.70766
C         11.59134       -1.72442        0.87455
C         11.95771        0.44163        1.89620
C         11.43997        1.54912        1.99528
C         -1.84385        8.55299       -0.46537
C         -0.66197        8.68337       -0.16435
C         -4.52611       -2.84675        3.94523
C         -5.32589       -2.92932        5.08196
C         -4.80731       -2.81844        6.36665
C         -3.42404       -2.63173        6.47896
C         -2.61315       -2.55055        5.33891
C         -3.14390       -2.64342        4.03655
C         -5.39759       -3.05077        2.74955
N         -6.71985       -3.23309        3.23912
C         -6.73713       -3.15149        4.65980
O         -5.06148       -3.07332        1.58898
O         -7.70509       -3.24938        5.37317
C         -7.86942       -3.46411        2.42298
C         -9.00655       -4.10124        2.95233
C        -10.14054       -4.29215        2.16403
C        -10.15928       -3.89190        0.82051
C         -9.01092       -3.29053        0.28564
C         -7.88770       -3.05754        1.07702
N        -11.31953       -4.06774        0.02251
C        -12.05213       -5.24962       -0.13454
C        -13.16029       -5.00049       -0.99193
C        -13.08991       -3.60572       -1.37254
C        -11.94236       -3.06516       -0.72952
C        -11.80525       -6.52880        0.38071
C        -12.69383       -7.55079        0.04426
C        -13.80380       -7.31582       -0.78940
C        -14.03888       -6.04626       -1.31321
C        -13.87989       -2.77507       -2.18376
C        -13.52697       -1.44121       -2.35536
C        -12.38079       -0.90561       -1.70909
C        -11.59078       -1.72500       -0.87532
C        -11.95704        0.44057       -1.89801
C        -11.43966        1.54824       -1.99702
H         -0.37889       -4.22091       -1.41099
H          1.13791       -4.33328       -3.34516
H          5.24000        1.38294       -1.56841
H          6.31511        3.47677       -0.87582
H          3.11334        4.20693        1.91387
H          1.99311        2.14966        1.17265
H          7.53075        3.29886        1.30431
H         10.30095        6.35972        2.60047
H          8.53462        8.09752        2.38944
H          6.14977        9.51507        1.91837
H          3.82985       10.20054        1.34016
H          2.81439        6.12010        0.31649
H         -1.13792       -4.33262        3.34622
H          0.37868       -4.22060        1.41188
H         -5.24243        1.38096        1.56560
H         -6.31744        3.47473        0.87281
H         -3.11195        4.20804       -1.91186
H         -1.99165        2.15106       -1.16994
H         -7.53088        3.29815       -1.30665
H        -10.30092        6.35907       -2.60291
H         -8.53481        8.09699       -2.39080
H         -6.15054        9.51470       -1.91831
H         -3.83102       10.20046       -1.33889
H         -2.81531        6.12004       -0.31556
H          1.53884       -2.39079       -5.45729
H          2.96443       -2.54338       -7.46531
H          5.45791       -2.88182       -7.24021
H          9.02421       -4.41282       -3.99290
H         11.02856       -4.74806       -2.60557
H          8.99374       -2.99616        0.76528
H          7.01454       -2.58463       -0.63653
H         10.94360       -6.72723       -1.01727
H         12.52076       -8.55589       -0.43474
H         14.48268       -8.13729        1.03113
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H	-5.45813	-2.88046	7.24099
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H	-1.53891	-2.38987	5.45826
H	-9.02433	-4.41163	3.99366
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H	-7.01420	-2.58436	0.63707
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H	-14.48113	-8.13836	-1.03053
H	-14.89398	-5.86683	-1.96969
H	-14.76609	-3.17389	-2.68339
H	-14.12496	-0.79028	-2.99532
H	-10.72333	-1.30030	-0.37231

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