Supporting Information

Synthesis and Supramolecular Assembly of MRI Active Biogenic Amine Host Polymers

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1. General information

All metathesis reactions were conducted under nitrogen atmosphere using *Schlenk*-technique or under argon using a glovebox. CD_3OD, $CDCl_3$, THF-d_8, CD_2Cl_2 (Eurisotop), dopamine • HCl (**12**), **G2**, other reagents and solvents (Aldrich), were used as received.

Dimethyl 4-oxo-1,4-dihydropyridine-2,6-dicarboxylate (**3**)[1] bicyclo[2.2.1]hept-5-en-2-ylmethanol (**4**)[2], bicyclo[2.2.1]hept-5-ene-2,2-diyldimethanol (**9**)[3], bicyclo[2.2.1]hept-5-en-2-ylmethyl 4-methylbenzenesulfonate[4], tetraethylene glycol ditosylate[5], **G3**[6] and Tos-4[7] were synthetized according to literature resources.

NMR spectra were obtained on a Varian Unity INOVA spectrometer operating at an equivalent ^{1}H frequency of 500 MHz. Notation for the ^{1}H NMR spectral splitting patterns includes singlet (s), doublet (d), triplet (t), broad (br) and multiplet/overlapping peaks (m). Signals are given as δ values in ppm, coupling constants (*J*) are expressed in Hertz.

Solid-state NMR magic angle spinning (MAS) spectra of samples were recorded on Varian NMR System spectrometer operating at an equivalent ^{1}H frequency of 600 MHz with a Chemagnetics 3.2 mm narrow-bore triple resonance with T3 probe in double resonance mode. The spinning rate of the rotor was 10 kHz in all cases. Adamantane was used as external chemical shift reference (38.55 and 29.50 ppm). The 90° pulse lengths were 3.0 μs for carbon and 2.4 μs for the proton channel. Cross polarization techniques were used to record solid-state $^{13}C\{^1H\}$ NMR spectra with SPINAL-64 decoupling at 18 °C with a recycle delay of 10 s which is 5 times larger than T_{1H}.

GPC measurements were carried out using Waters 2695 separation unit and Waters 2414 RI detectors (Waters, Milford, USA) at 35 °C column and detector temperature. The sample compartment was used at 25 °C. Column bank contained four columns (4.6*300 mm): Styragel HR 0.5, Styragel HR 1, Styragel HR 2 and Styragel HR 4 (Waters, Milford, USA). The third order calibration curve was used, and the calibration standards were Polystyrenes in the 500-310000 Da molecular weight range. The eluent was HPLC grade THF (VWR International, Leuven, Belgium). The flow rate was 0.5 ml/min. For the calculations of the molecular weights, Millennium^{32} Chromatography Manager was used. The concentration of the samples was 5 mg/mL, and the volumes of injections were in the range of 10-50 μL.

The Matrix-Assisted Laser Desorption/Ionization Time-of-Flight Mass Spectrometric (MALDI-TOF MS) measurements were performed with an AutoFlex Speed mass spectrometer equipped with a time-of-flight (TOF) mass analyzer. In all cases, 19.5 kV (IonSource 1) and 18.3 kV (IonSource 2) acceleration voltages were used with pulsed ion extraction (PIE^{TM}). The

positive ions were detected in the linear mode. A Bruker smartbeam^{TM}-II solid phase laser (355 nm, ≥ 100 μJ/pulse) operating at 500 Hz was used to produce laser desorption, and 5000 shots were summed. The MALDI-TOF MS spectra were externally calibrated using polyethylene glycol (PEG) standard (Mn = 1450 g/mol, Sigma-Aldrich, Taufkirchen, Germany).

Samples for MALDI-TOF MS were prepared with 2,5-dihydroxybenzoic acid (DHB) (Sigma-Aldrich, Taufkirchen, Germany) matrix dissolved in tetrahydrofuran (VWR International, Leuven, Belgium) at a concentration of 20 mg/mL. The concentrations of the analyte solutions were 5 mg/mL, and sodium trifluoroacetate (NaTFA) (Sigma-Aldrich, Taufkirchen, Germany) was dissolved in THF at a concentration of 5 mg/mL (used as the cationization agent to promote ionization). The solutions were mixed in a 10:2:1 (v/v) ratio (matrix/analyte/cationization agent). A volume of 0.5 μL of the solution was deposited onto a metal sample plate and allowed to air-dry.

The glass transition temperature (T_g) was determined by a Setaram DSC92 differential scanning calorimeter from -140 °C to 130 °C. The samples, with an average mass of 30-40 mg were pressed in 120 μL aluminum pans and sealed with pierced lids. On each sample, at least three measurements were performed, with two different scanning rates (two measurements with 20 °C/min, and one measurement with 10 °C/min), during the measurement, the calorimeter was purged with high purity nitrogen (flow rate 20 mL/min). Calcined α-alumina powder was used as reference material. The calorimeter was calibrated with high purity metals (5 different metals, with at least 3 different scanning rates). The data obtained from the first measurement was not evaluated (the thermal history of the sample is removed). Thermal stability was investigated by simultaneous thermogravimetry-differential scanning calorimetry (TG-DSC) on a Setaram LabsysEvo system. The measurements were performed under pyrolytic conditions in a flowing (80 mL/min) high purity argon (99.999%) atmosphere, in 25-500 °C temperature range, with a scanning rate of 10 °C/min. An average of 10-15 mg sample was placed in 100 μL aluminum pan; the samples were used “as received”. The measurements were blank corrected. All measurement results were evaluated with Calisto Processing software.

GC-MS analyses were carried out using a Shimadzu GC-MS-QP2010 instrument equipped with a Rxi-5Sil MS column coupled with a quadrupole mass filter with pre-rods.

HRMS and MS-MS analyses were performed on a Thermo Velos Pro Orbitrap Elite (Thermo Fisher Scientific) system. The ionization method was ESI operated in positive ion mode. The protonated molecular ion peaks were fragmented by CID at a normalized collision energy of 35%. For the CID experiment helium was used as the collision gas. The samples were dissolved in methanol. Data acquisition and analysis were accomplished with Xcalibur software

version 2.0 (Thermo Fisher Scientific). In cases of fluorinated samples **10** and **11**, HRMS analyses were performed on a Thermo Q Exactive GC Orbitrap (Thermo Fisher Scientific) system. The ionization method was EI operated in positive ion mode. Electron energy was set at 70 eV. Data acquisition and analysis were accomplished with Xcalibur software version 2.0 (Thermo Fisher Scientific).

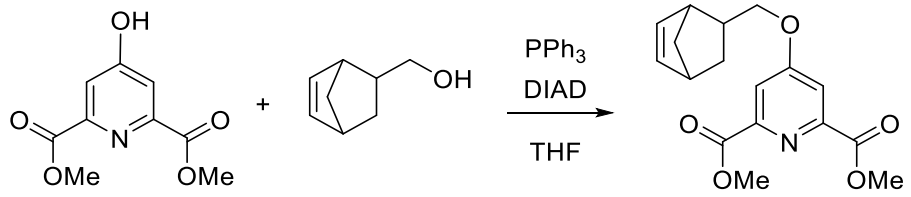
TLC was performed on Merck Kieselgel 60 F_{254} plates or Merck Aluminium oxide 60 F_{254} plates and spots were visualized by UV light or by exposing it with iodine or the aqueous solution of $(NH_4)_6Mo_7O_{24}$, $Ce(SO_4)_2$ and sulfuric acid.

Flash column chromatography was performed by a CombiFlash Rf 150 apparatus using gradient elution in normal (silica or alumina column; hexane–ethyl acetate, dichloromethane–methanol or dichloromethane–ethanol as eluent) phase mode. Sample loadings were performed in the case of silica flash chromatography by drying the sample onto a silica cartridge.

In some cases, gradient elution preparative HPLC was applied (Armen) on a Gemini 250x50.00 mm; 10 µm, C18, 110A column using 10 ml of TFA in 5 l water and acetonitrile as the two solvents.

2. Synthesis of norbornene functionalized pyridino-18-crown-6 ether (7).

2.1. Synthesis of dimethyl 4-(bicyclo[2.2.1]hept-5-en-2-ylmethoxy)pyridine-2,6-dicarboxylate (5) by *Mitsunobu* reaction



3 **4** **5**

Chelidamic acid dimethyl ester (dimethyl 4-oxo-1,4-dihydropyridine-2,6-dicarboxylate, **3**, 10.3 g, 48.8 mmol), 5-norbornene-2-methanol (bicyclo[2.2.1]hept-5-en-2-ylmethanol, **4**, 9.09 g, 73.2 mmol, 1.5 equivalent of **3**) and triphenylphosphine (25.6 g, 97.6 mmol, 2.0 equivalent of **3**) were dissolved in pure and dry THF (310 mL) and cooled to 0 °C. Then DIAD (diisopropyl-diazene-1,2-dicarboxylate, 14.4 mL, 73.2 mmol, 1.5 equivalent of **3**) was added dropwise in nitrogen atmosphere. The reaction mixture was allowed to warm to room temperature and stirred for additional 12 hours. Then the solvent was removed under reduced pressure, and the

crude product (65.9 g) was dissolved in 40 mL of ethyl acetate at 50 °C. 80 ml hexane was added and the solution was cooled down to -10 °C. In 20 hours the formed solid precipitate (triphenylphosphine oxide) was filtered off, and the filtrate was concentrated by vacuum. The crude product (45 g) was purified by flash chromatography (eluent: hexane and ethyl acetate from 0% to 40% using gradient elution). **5** (9.44 g, 61%) was obtained as a white solid containing a mixture of *endo* (74%) and *exo* (26%) isomers. Pure *endo* isomer can be achieved by multiple chromatography (eluent: hexane and ethyl acetate from 10% to 30%).Mixture of *endo* and *exo* isomers in a ratio of 74/26 of **5**.

endo isomer of **5**

^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.75 (s, 2H, Ar), 6.19 (dd, 1H, *J*= 5.7 Hz, 3.0 Hz, CH=), 5.92 (dd, 1H, *J*=5.7 Hz, 3.0 Hz, CH=), 3.99 (s, 6H, OCH_3), 3.86 (dd, 1H, J_1=9.2 Hz, J_2=6.6 Hz, OCH_aH_b), 3.72 (t, 1H, *J*=9.3 Hz, OCH_aH_b), 3.01 (bs, 1H, C*H*-CH=), 2.86 (bs, 1H, C*H*-CH=), 2.58 (m, 1H, J_1=9.3 Hz, J_2=4.0 Hz, C*H*-CH_2O), 1.93 (ddd, 1H, J_1=11.8 Hz, J_2=9.3 Hz, J_3=4.0 Hz, CH_aH_b-CH-CH_2O), 1.49 (ddd, 1H, J_1=8.3 Hz, J_2=4.0 Hz, J_3=2.0 Hz =CH-CH-CH_aH_b-CH-CH=), 1.31 (bd, 1H, *J*=8.3 Hz, =CH-CH-CH_aH_b-CH-CH=), 0.64 (ddd, 1H J_1=11.8 Hz, J_2=4.4 Hz, J_3=2.6 Hz, CH_aH_b-CH-CH_2O). ^{13}C{^{1}H} NMR (125 MHz, CDCl3) δ: 167.20, 165.35, 149.85, 138.17, 132.08, 114.63, 72.63, 53.28, 49.59, 43.94, 42.35, 38.11, 29.06. HRMS (ESI) m/z: [M + H] + Calcd for $C_{17}H_{20}O_5N$ 318.13360; Found 318.13247. HR-ESI-MS-MS (CID=35%; rel. int. %): 252(2); 212(100); 107(2).

exo isomer of **5**

^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.80 (s, 2H, Ar), 6.16-6.13 (m, 1H, CH=), 6.12-6.09 (m, 1H, CH=), 4.19 (dd, *J*= 9.0 Hz, 6.3 Hz, 1H, OCH_aH_b), 4.11 (q, *J*= 9.0 Hz, 1H, OCH_aH_b), 4.00 (s, 6H, OCH_3), 2.89(bs, 1 H, C*H*-CH=), 2.85(bs, 1H, C*H*-CH=), 2.58 (m, 1H, C*H*-CH_2O) 1.98-1.91 (m, 1H, CH_aH_b-CH-CH_2O), 1.71 (bs, 1H, =CH-CH-CH_aH_b-CH-CH=), 1.42-1.22 (m, 2H, =CH-CH-CH_aH_b-CH-CH=, CH_aH_b-CH-CH_2O).

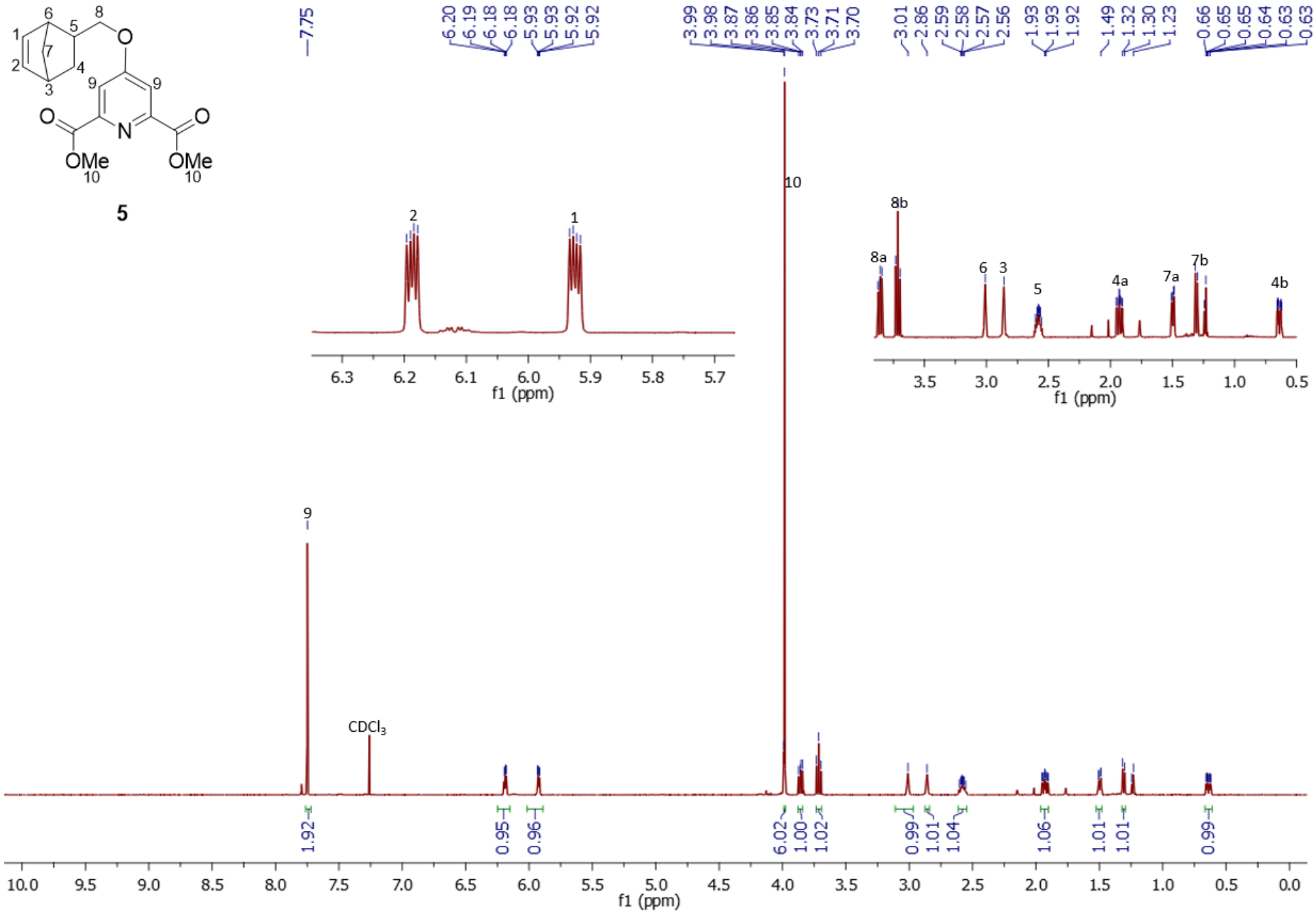


Figure S1. ^{1}H NMR spectrum of *endo* isomer of **5** ($CDCl_3$).

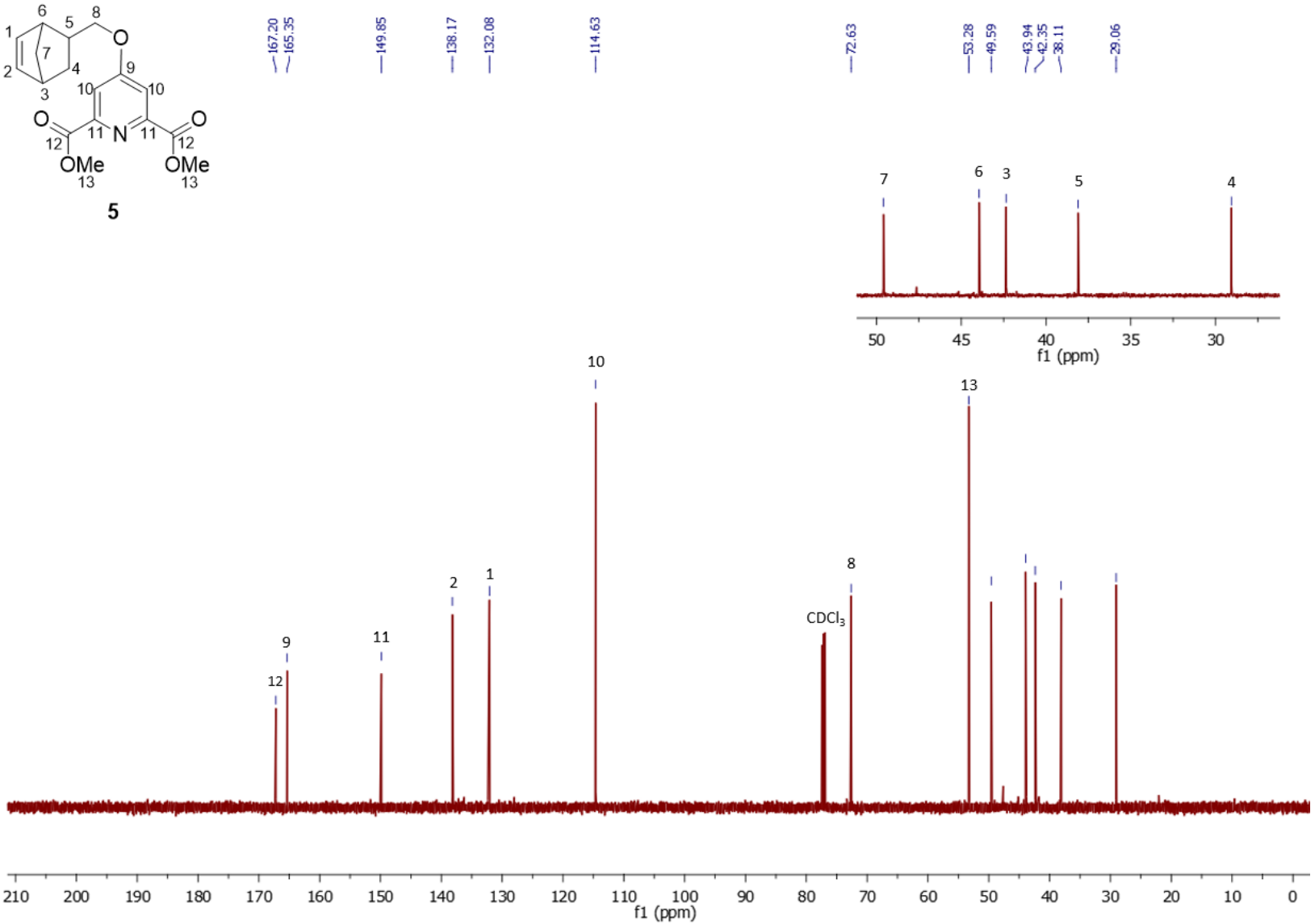
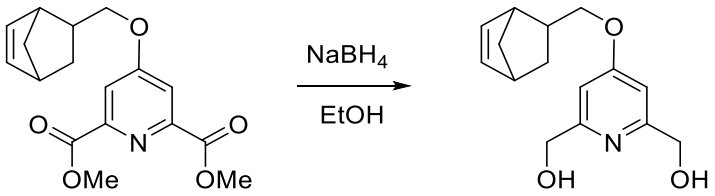


Figure S2. $^{13}C\{^{1}H\}$ NMR spectrum of *endo* isomer of **5** ($CDCl_3$).

2.2. Synthesis of (4-(bicyclo[2.2.1]hept-5-en-2-ylmethoxy)pyridine-2,6-diyl)dimethanol (6)



5 **6**

To an ethanolic suspension of **5** (0.50 g, 1.58 mmol) (5.0 ml) sodium borohydride (0.276 g, 7.30 mmol) was gradually added at 0 °C. The mixture was stirred at 0 °C for 1 hour then at room temperature for additional 2 hours and finally at reflux temperature for 14 hours. The solvent was evaporated by vacuum giving a waxy solid. Acetone (7 ml) was added, and the mixture was refluxed for 1 hour. When the solvent was evaporated, aqueous potassium carbonate solution (2 g in 5 ml water) was added, and the resulting mixture was refluxed for 2 hours. The mixture was concentrated, and 2 ml of brine was added. The mixture was extracted with chloroform (5×10 ml). The combined organic phase was dried over anhydrous sodium sulfate, and the solvent was evaporated under reduced pressure to give a pale yellow solid (0.466 g). This crude product was purified by column-chromatography (eluent: DCM/MeOH = 4/1) to give a white solid (**6**, 0.336 g, 81%).

endo isomer of **6**

^{1}H NMR (500 MHz, $CDCl_3$) δ: 6.67 (s, 2H, 2×Py-H), 6.18 (dd, 1H, J_1=5.7 Hz, J_2=3.0 Hz, CH=), 5.93 (dd, 1H, J_1=5.7 Hz, J_2=3.0 Hz, CH=), 4.67 (s, 4H, 2×CH_2OH), 3.76 (dd, 1H, J_1=9.0 Hz, J_2=6.4 Hz, Ar-OCH_aH$_b$), 3.60 (t, 1H, J= 9.0 Hz, Ar-OCH$_a$$H_b$), 3.00 (s, 1H, C$H$-CH=), 2.86 (s, 1H, C$H$-CH=), 2.56 (m, 1H, C$H$-CH$_2$O), 1.92 (ddd, 1H, J_1=11.7 Hz, J_2=9.3 Hz, J_3=3.8 Hz, CH_aH$_b$-CH-CH$_2$O), 1.49 (dd, 1H, J_1=11.7 Hz, J_2=9.3 Hz, =CH-CH-CH_aH$_b$-CH-CH=), 1.31 (dd, 1H, J_1=11.7 Hz, J_2=9.3 Hz, =CH-CH-CH$_a$$H_b$-CH-CH=), 0.62 (ddd, 1H, J_1=11.7 Hz, J_2=4.3 Hz, J_3=2.6 Hz, CH$_a$$H_b$-CH-CH$_2$O). ^{13}C{^{1}H} NMR (125 MHz, CDCl3) δ: 166.77, 160.46, 138.01, 132.23, 105.80, 71.81, 64.62, 49.60, 43.99, 42.39, 38.22, 29.12. HRMS (ESI) m/z: [M + H] + Calcd for $C_{15}H_{20}O_3N$ 262.14377; Found 262.14307. HR-ESI-MS-MS (CID=35%; rel. int. %): 196(33); 156(100).

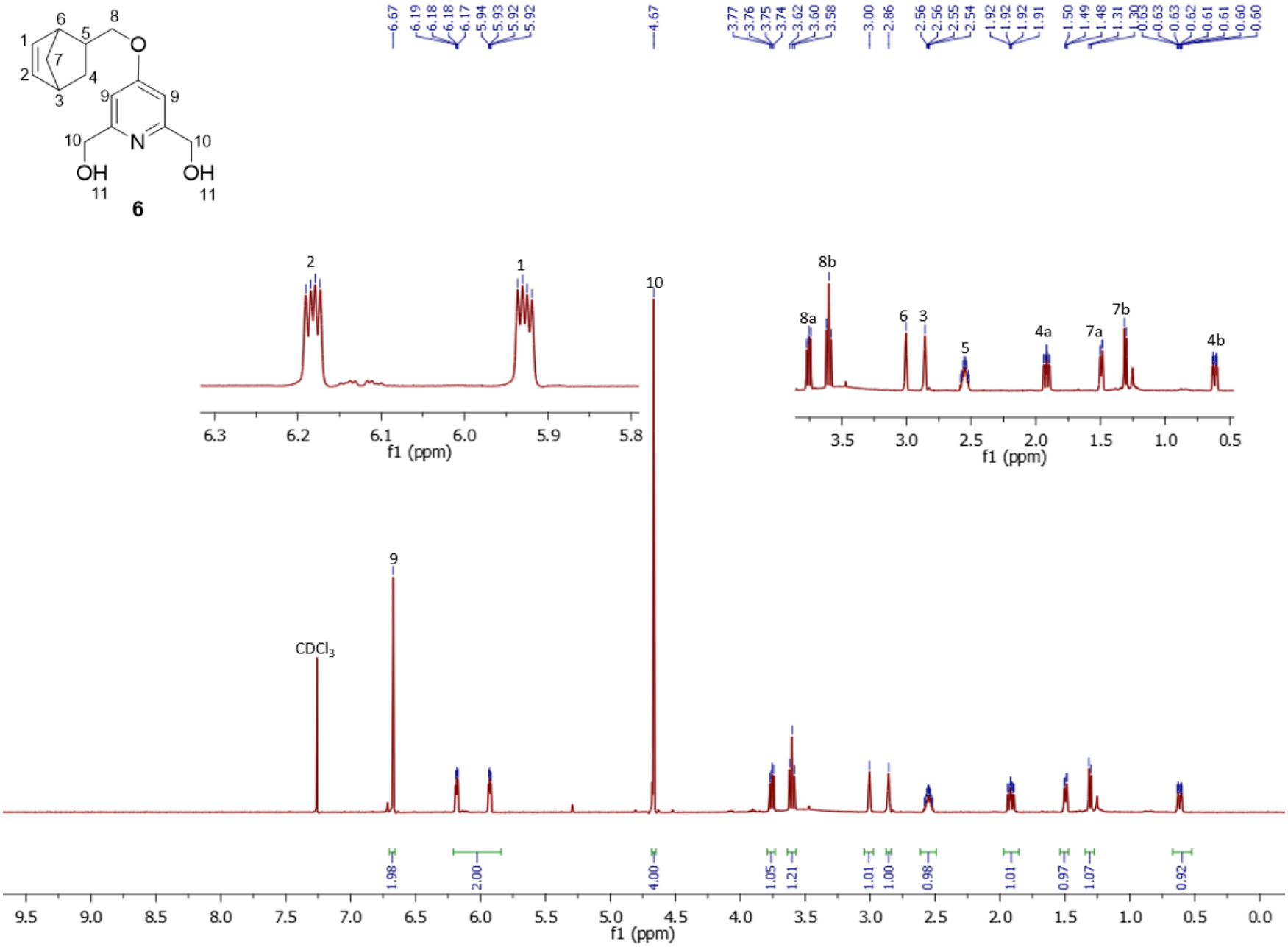


Figure S3. ^{1}H NMR spectrum of *endo* isomer of **6** ($CDCl_3$).

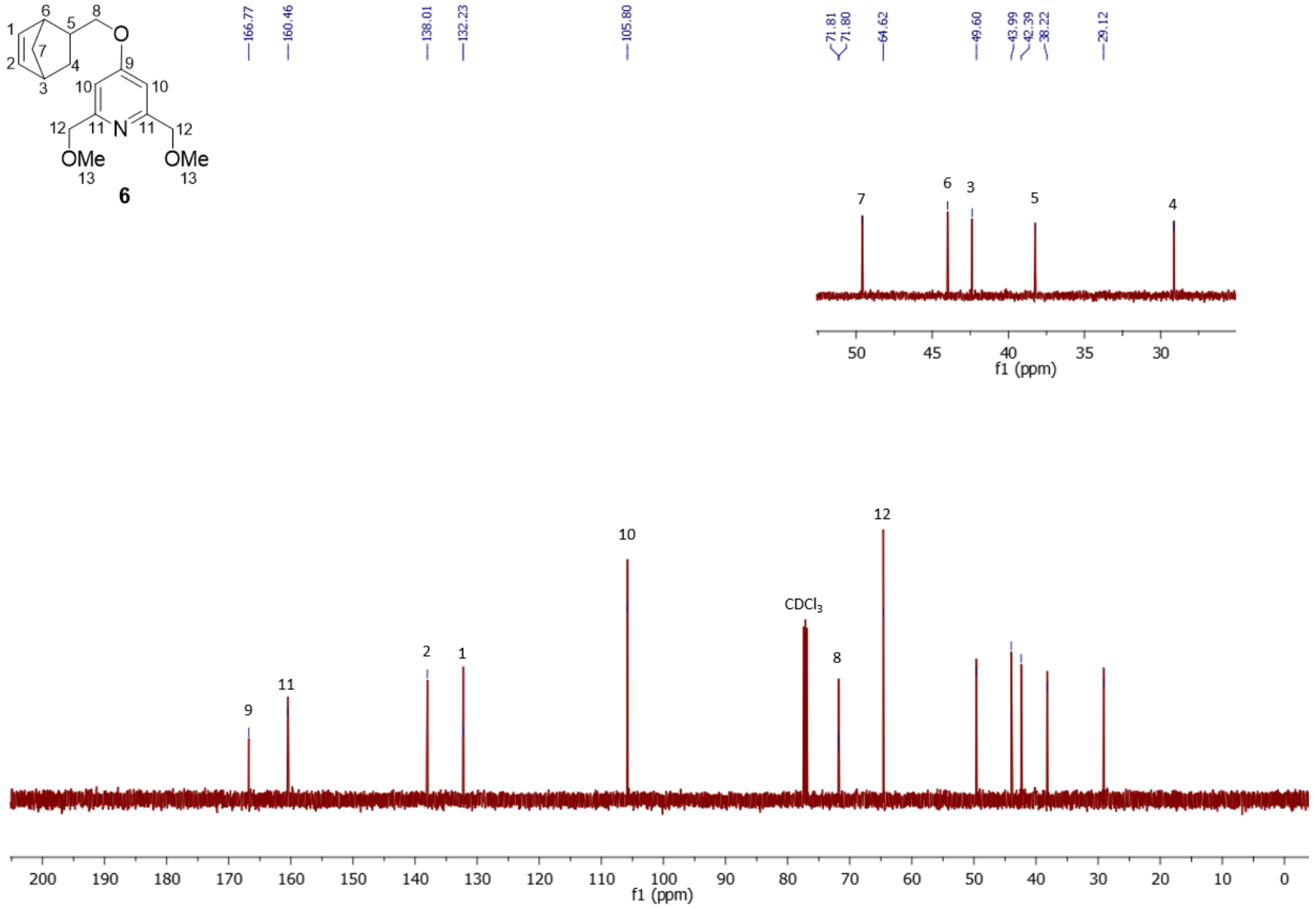
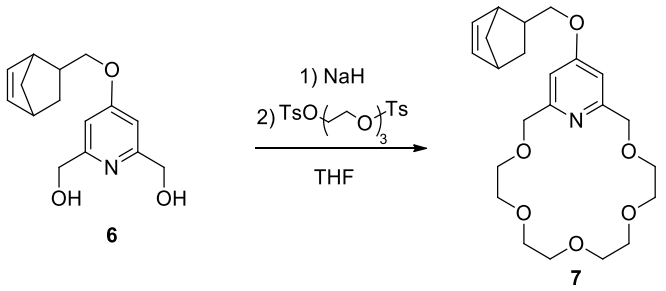


Figure S4. $^{13}C\{^{1}H\}$ NMR spectrum of *endo* isomer of **6** ($CDCl_3$).

2.3. Synthesis of 1^4-(bicyclo[2.2.1]hept-5-en-2-ylmethoxy)-3,6,9,12,15-pentaoxa-1(2,6)-pyridinecyclohexadecaphane (7)



A THF (30 mL) solution of **6** (1.73 g, 6.63 mmol) was added dropwise to a 5 mL THF suspension of sodium hydride (0.48 g, 21.0 mmol, 80% dispersion in mineral oil) in nitrogen atmosphere at 0 °C. Then the mixture was stirred at 0 °C for 10 minutes, later on at room temperature for 30 minutes and finally at reflux temperature for 4 hours. The mixture was cooled to -60 °C, and a THF solution (30 mL) of tetraethylene glycol ditosylate (3.50 g, 6.96 mmol) was added. The mixture was stirred at -60 °C for 20 minutes and at room temperature for 7 days. The solvent was evaporated under reduced pressure, and the residue was dissolved in a mixture of dichloromethane (100 mL) and ice cold water (50 mL). The mixture was stirred for 5 minutes, the phases were separated, and the aqueous phase was extracted with dichloromethane (3×100 mL). The combined organic phase was dried over anhydrous magnesium sulfate, and the solvent was evaporated under reduced pressure. This residue (4.00 g) was purified by flash chromatography on alumina (eluent: dichloromethane and ethanol from 0 to 5% using gradient elution) to give 1.41 g (60%) of **7** as a colorless oil. Purity: 85% (^{1}H NMR).

Further purification was made by preparative HPLC using water (5% TFA) and acetonitrile eluent. The TFA salt was liberated to **7** by dissolving in dichloromethane (50 mL), followed by the addition of tetramethyl ammonium hydroxide solution (10 m/m%) in water (10 mL). The phases were separated; the aqueous phase was washed with dichloromethane (3×50 mL); the organic phases were combined. The solvent was evaporated under reduced pressure to give 0.99 g (42%) of **7** as colorless oil.

R_f = 0.75 (alumina TLC, eluent: 5% MeOH in dichloromethane, using iodine to visualization).

TFA salt of **7**

^{1}H NMR (500 MHz, $CDCl_3$) δ: 9.60 (bs, 1 H, HN), 7.15 (s, 2H, Ar), 6.18 (dd, 1H, J= 5.6 Hz, 3.0 Hz, CH=), 5.90 (dd, 1H, J= 5.6 Hz, 2.8 Hz, CH=), 4.73 (s, 4H, 2×ArCH_2), 3.99 (dd, 1H, J=

9.4 Hz, 6.9 Hz, Ar-OCH_aH$_b$), 3.88-3.81 (m, 5H, Ar-OCH$_a$$H_b$, 1×OC$H_2CH_2$O), 3.72-3.58 (m, 12H, 3×OCH_2CH_2O), 2.98 (bs, 1H, C*H*-CH=), 2.84 (bs, 1H, C*H*-CH=), 2.60-2.55 (m, 1H, C*H*-CH$_2$O), 1.90 (ddd, 1H, J= 12.1 Hz, 9.2 Hz, 3.7 Hz, OCH$_2$CHCH_aH$_b$), 1.47 (dd, 1H, J= 8.3 Hz, 1.5 Hz, CHCH_aH$_b$CH), 1.29 (d, 1H, J= 8.3 Hz, CHCH$_a$$H_b$CH), 0.64 (ddd, 1H J= 11.9 Hz, 4.0 Hz, 2.7 Hz, OCH$_2$CHCH$_a$$H_b$). ^{13}C{^{1}H} NMR (125 MHz, CDCl$_3$): 171.21, 154.03, 138.41, 131.77, 110.75, 74.66, 70.58, 70.56, 69.95, 69.86, 69.17, 49.51, 43.83, 42.32, 37.82, 28.74.

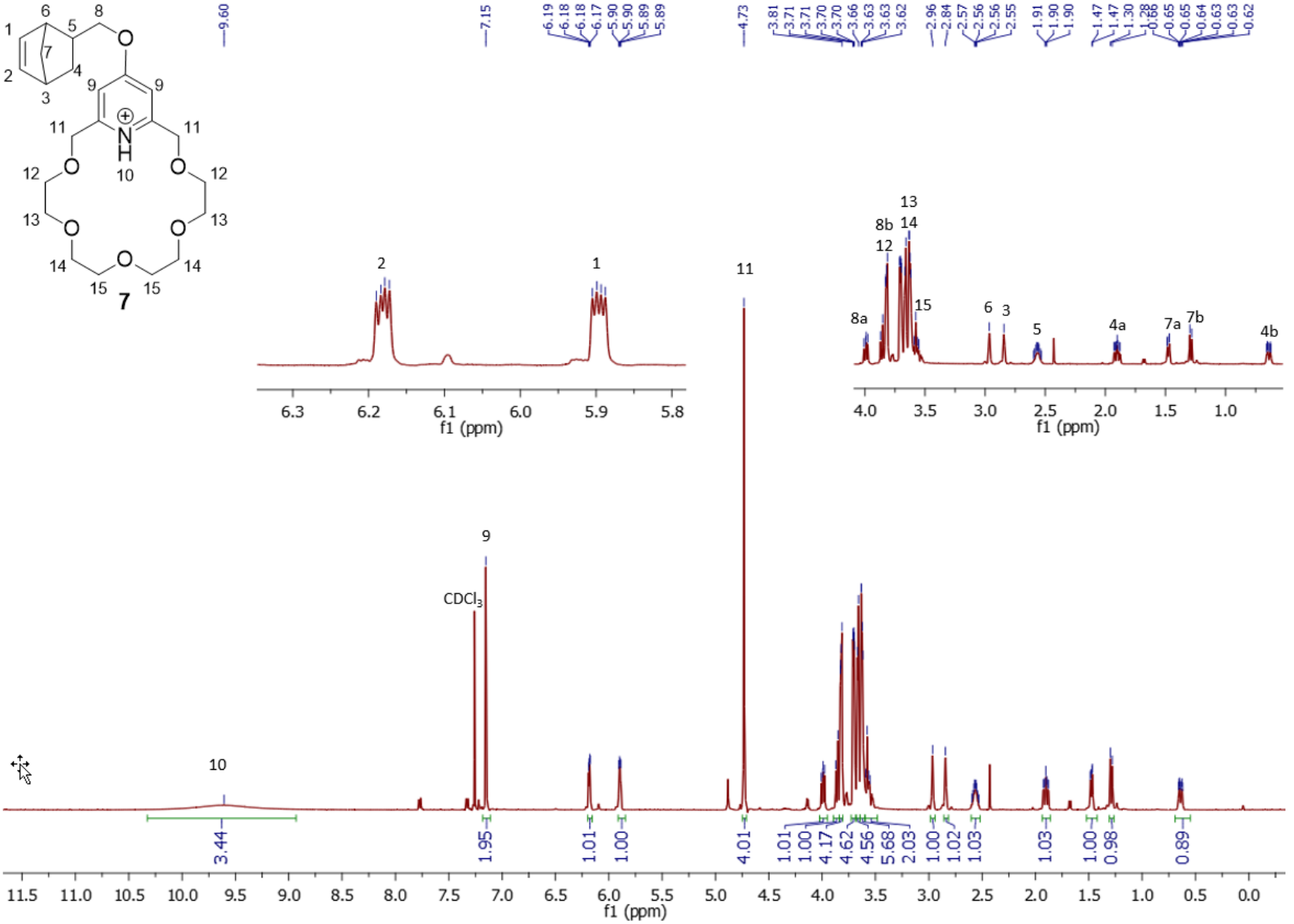


Figure S5. ^{1}H NMR spectrum of TFA salt of *endo* isomer of **7** in CDCl3.

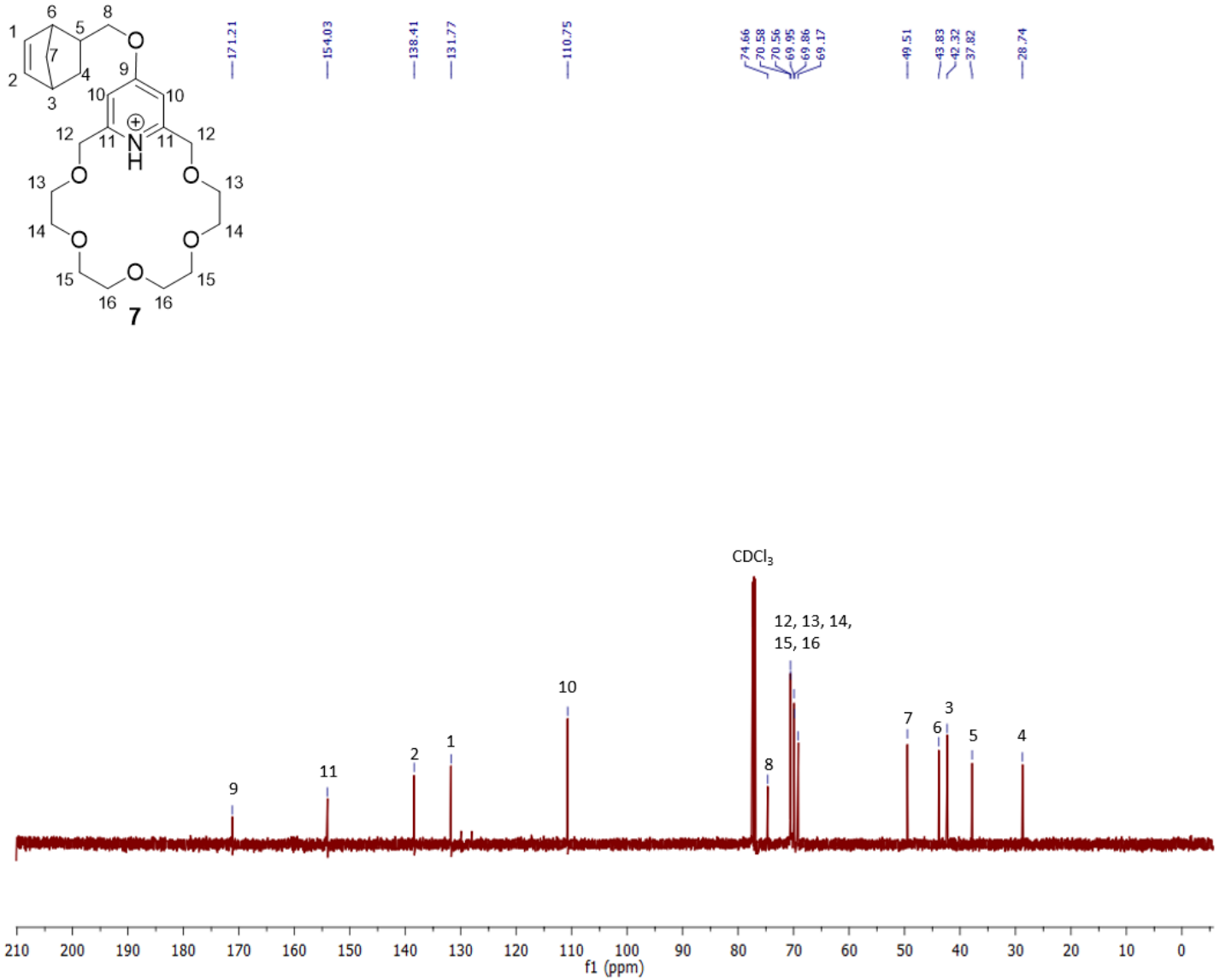


Figure S6. $^{13}C\{^{1}H\}$ NMR spectrum of TFA salt of *endo* isomer of **7** in $CDCl_3$.

Non-TFA salt of **7**

^{1}H NMR (500 MHz, CD_2Cl_2) δ: 6.73 (s, 2H, Ar), 6.19 (dd, 1H, *J*= 5.5 Hz, 2.9 Hz, CH=), 5.95 (dd, 1H, *J*= 5.5 Hz, 2.7 Hz, CH=), 4.58 (s, 4H, 2×ArCH_2), 3.78 (dd, 1H, *J*= 9.2 Hz, 6.6 Hz, Ar-OCH_aH$_b$), 3.70-3.51 (m, 17H, Ar-OCH$_a$$H_b$, 4×OC$H_2CH_2$O), 3.01 (bs, 1H, C*H*-CH=), 2.85 (bs, 1H, C*H*-CH=), 2.59-2.51 (m, 1H, C*H*-CH_2O), 1.92 (ddd, 1H, *J*= 12.2 Hz, 9.0 Hz, 3.5 Hz, OCH$_2$CHCH_aH$_b$), 1.47 (dd, 1H, *J*= 8.3 Hz, 1.7 Hz, CHCH_aH$_b$CH), 1.33 (m, 1H, HCH$_a$$H_b$CH), 0.64 (ddd, 1H, *J*= 11.9 Hz, 4.0 Hz, 2.8 Hz, OCH$_2$CHCH$_a$$H_b$). ^{13}C{^{1}H} NMR (125 MHz, CD_2Cl_2): 166.89, 160.11, 138.30, 132.71, 107.97, 74.30, 72.11, 71.30, 71.00, 70.80, 70.07, 49.95, 44.53, 42.94, 38.74, 29.50. HRMS (ESI) m/z: [M + H] + Calcd for $C_{23}H_{34}O_6N$ 420.23806; Found 420.23677. HR-ESI-MS-MS (CID=35%; rel. int. %): 367(7); 354(100); 314(60).

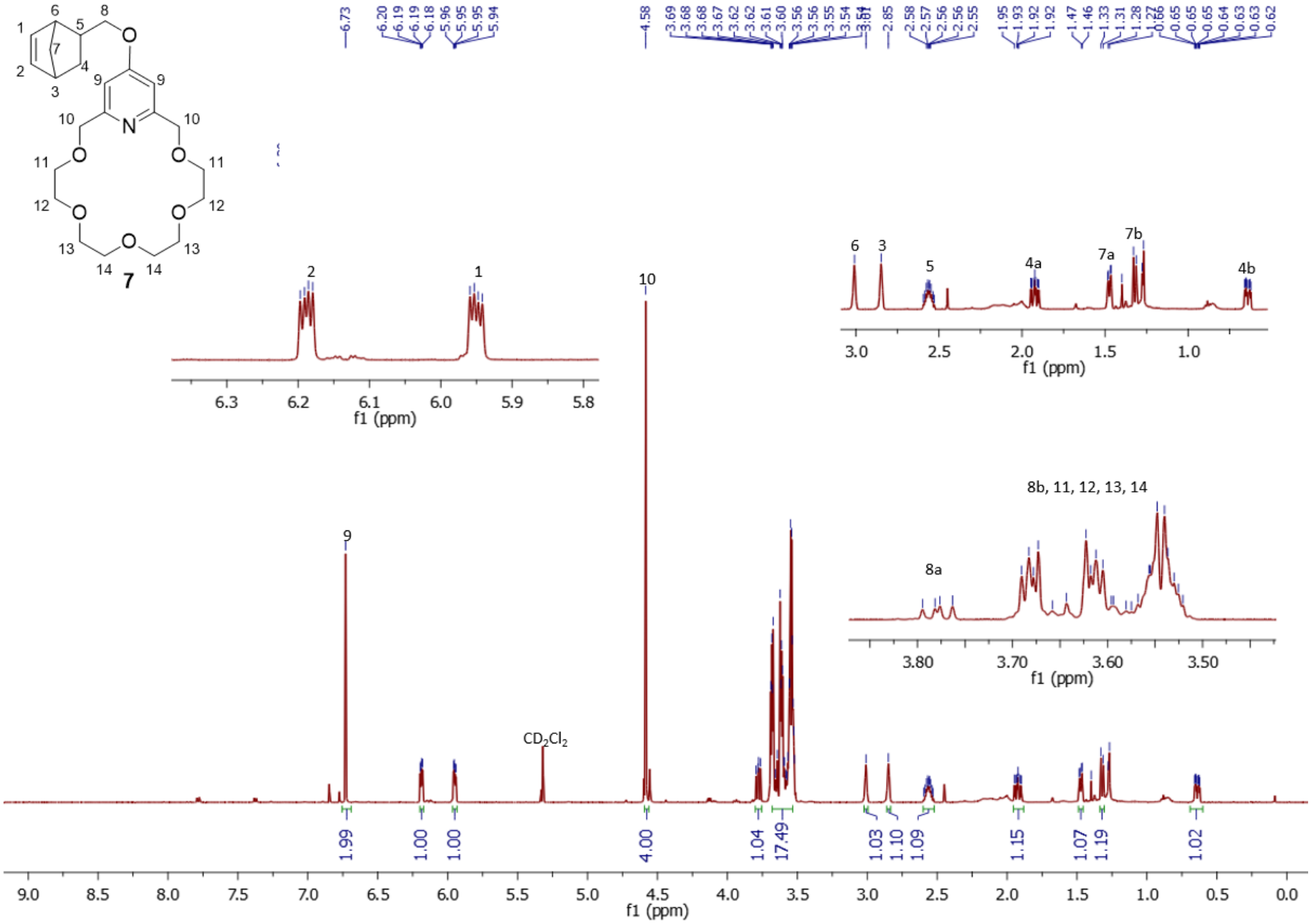


Figure S7. ^{1}H NMR spectrum of *endo* isomer of **7** in CD_2Cl_2.

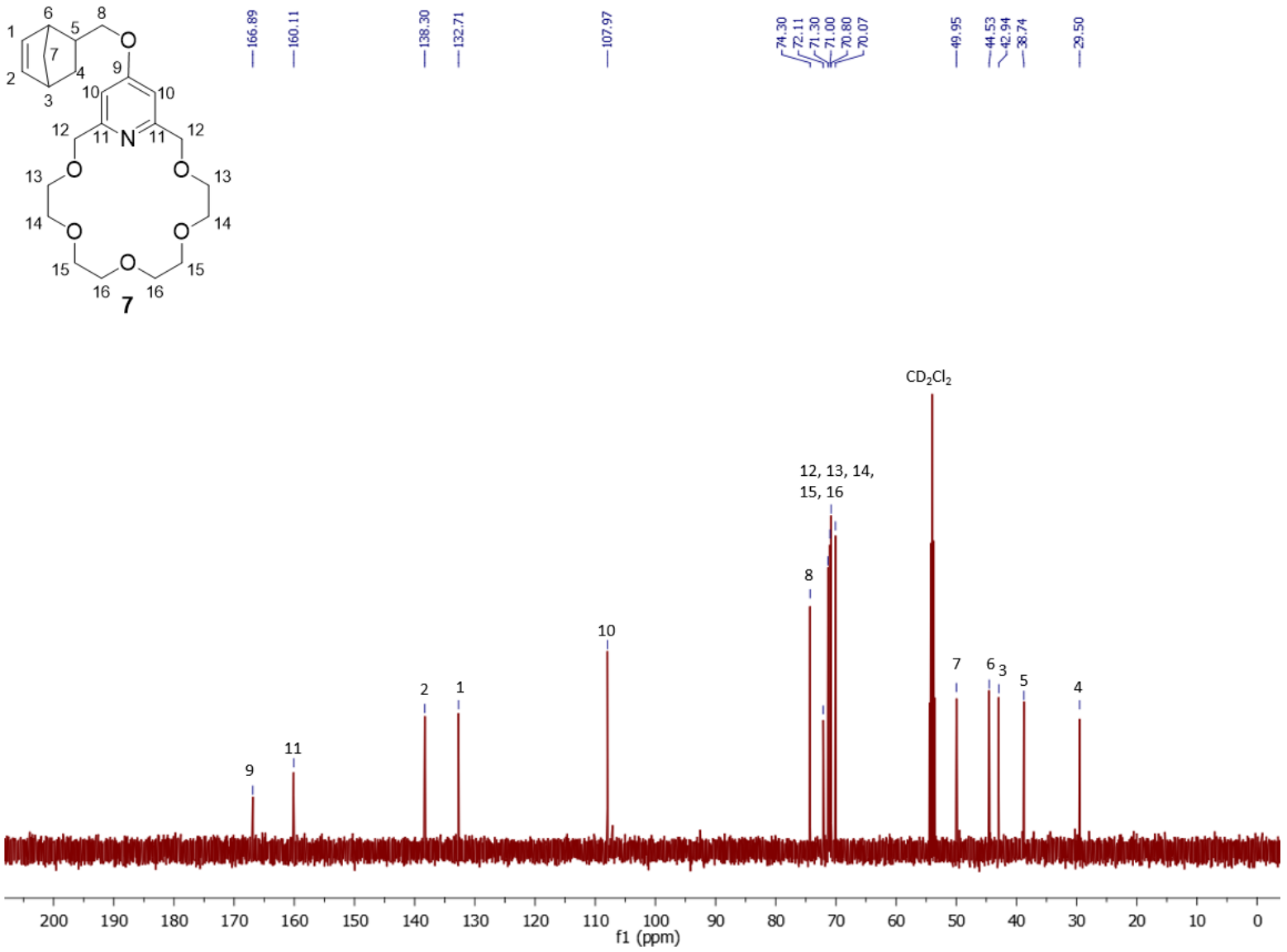
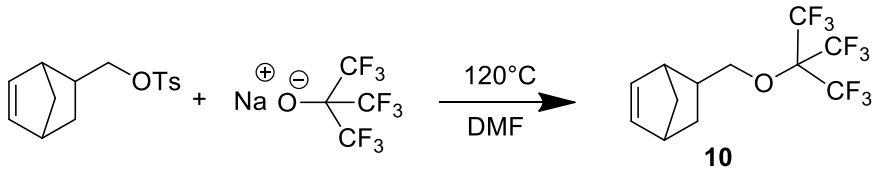


Figure S8. $^{13}C\{^{1}H\}$ NMR spectrum of *endo* isomer of **7** in CD_2Cl_2.

3. Synthesis of fluorinated norbornene derivatives 10 and 11

3.1. 5-(((1,1,1,3,3,3-hexafluoro-2-(trifluoromethyl)propan-2-yl)oxy)methyl) bicyclo[2.2.1]hept-2-ene (10)



10

A *Schlenk*-tube was charged with bicyclo[2.2.1]hept-5-en-2-ylmethyl 4-methylbenzenesulfonate[4] (5.7 g, 20.5 mmol), sodium 1,1,1,3,3,3-hexafluoro-2-(trifluoromethyl)propan-2-olate[7] (10.6 g, 41.0 mmol) in *N*,*N*-dimethyl formamide (32 mL) and fitted to a condenser. The solution was heated overnight at 120 °C then cooled down to room temperature. The reaction mixture was diluted with water (70 mL) and extracted with diethyl ether (3 × 20 mL). The combined organic phase was dried over Na_2SO_4 and the solvent was evaporated under reduced pressure (400 mbar). The crude product (4.6 g, pale yellow oil) was filtered trough a silica plug (washed with pentane) than concentrated under vacuum (400 mbar) to give **10** as a mixture of *endo* (81%) and *exo* (19%) isomers (4.20 g, 60%) as a colorless oil. Mixture of *endo* and *exo* isomers in a ratio of 74/26 of **5**.

<u>*endo* isomer of **10**</u>

^{1}H NMR (500 MHz, $CDCl_3$) δ: 6.18 (dd, 1H, J_1=5.7 Hz, J_2=3.1 Hz, CH=), 5.93 (dd, 1H, J_1=5.7 Hz, J_2=3.1 Hz, CH), 3.78 (t, 1H, J= 7.5 Hz, OCH_aH$_b$), 3.56 (t, 1H, J= 7.5 Hz, OCH$_a$$H_b$), 2.97 (bs, 1H, C*H*-CH=), 2.83 (bs, 1H, C*H*-CH=), 2.43 (m, 1H, C*H*-CH$_2$O), 1.84 (ddd, 1H, J_1=11.8 Hz, J_2=9.3 Hz, J_3=3.7 Hz, CH_aH$_b$-CH-CH$_2$O), 1.48 (m, 1H, =CH-CH-CH_aH$_b$), 1.28 (m, 1H, =CH-CH-CH$_a$$H_b$,), 0.51 (ddd, 1H, J_1=11.8 Hz, J_2=4.6 Hz, J_3=2.6 Hz, CH$_a$$H_b$-CH-CH$_2$O). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$) δ: 138.08, 132.15, 73.01, 49.47, 43.68, 42.26, 39.01, 28.59. ^{19}F NMR (125 MHz, $CDCl_3$) δ: -70.83 (s, 9F. HRMS (HR-EI-MS) m/z: [M] + Calcd for $C_{12}H_{11}OF_9$ 342,06662; Found 342.06618.

<u>*exo* isomer of **10**</u>

^{1}H NMR (500 MHz, $CDCl_3$) δ: 6.12 (dd, 0.19H, J_1=5.6 Hz, J_2=3.0 Hz, CH= *exo*), 6.09 (dd, 0.19H, J_1=5.6 Hz, J_2=3.0 Hz, CH= *exo*), 4.06 (t, 0.19H, J= 7.5 Hz, OCH_aH$_b$ *exo*), 3.89 (t, 0.19H, J= 7.5 Hz, OCH$_a$$H_b$ *exo*), 2.85 (bs, 0.19H, C*H*-CH= *exo*), 2.78 (bs, 0.19H, C*H*-CH= *exo*), 1.76 (m, 0.19H, C*H*-CH$_2$O *exo*), 1.38 (m, 0.19H, =CH-CH-CH_aH$_b$ *exo*), 1,28 (m, 2H, =CH-CH-CH$_a$$H_b$, C$H_aH_b$-CH-CH$_2$O), 1.14 (m, 0.2H, CH$_a$$H_b$-CH-CH$_2$O *exo*). ^{13}C{^{1}H} NMR (125 MHz,

$CDCl_3$) δ: 137.17, 136.37, 121.82, 119.48, 73.73, 45.06, 43.33, 41.69, 39.23, 29.22. ^{19}F NMR (125 MHz, $CDCl_3$) δ: -70.72 (s, 9F). HRMS (HR-EI-MS) m/z: [M] + Calcd for $C_{12}H_{11}OF_9$ 342,06662; Found 342.06618.

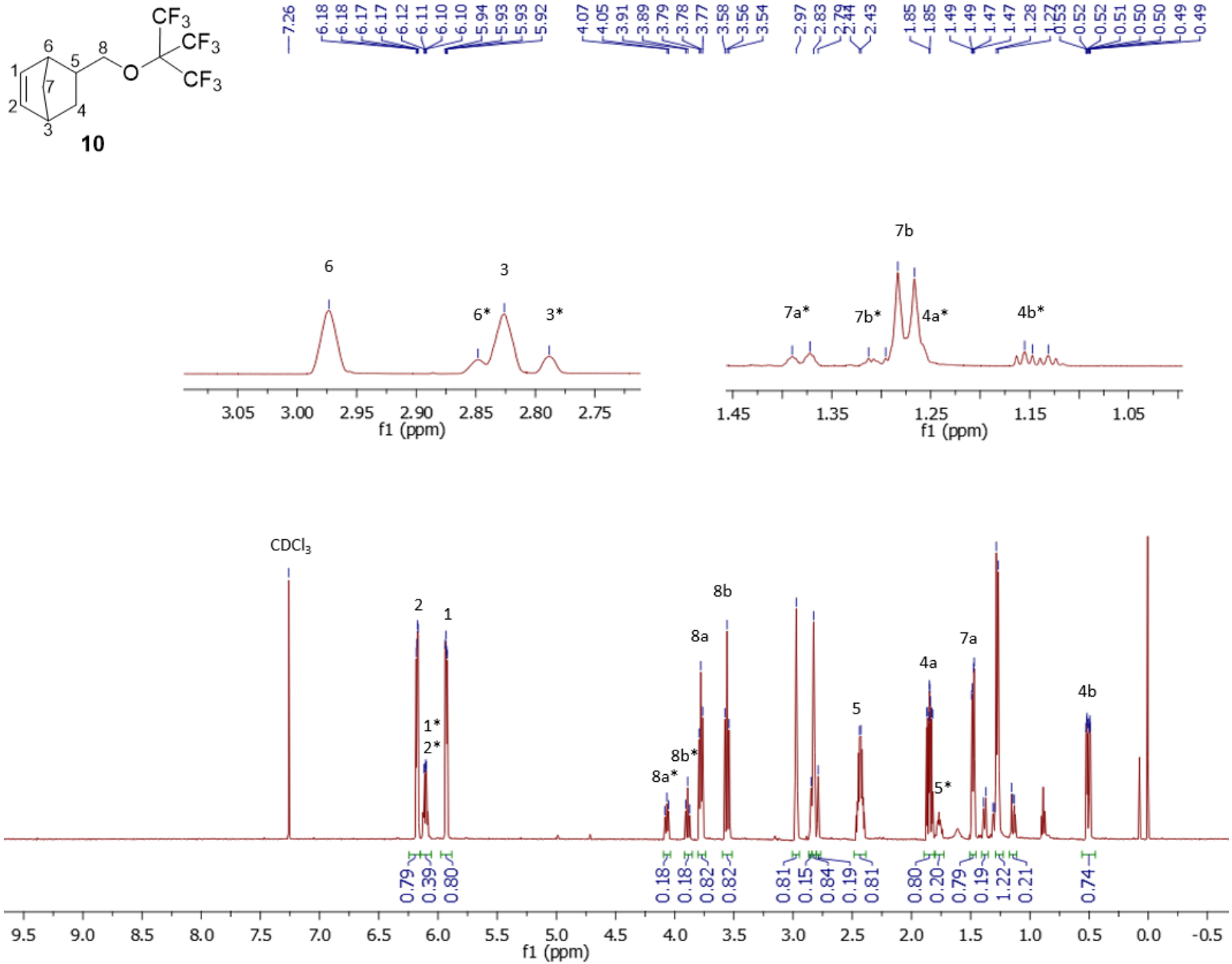


Figure S9. ^{1}H NMR spectrum of **10** in $CDCl_3$. (* peaks of the ~19% *exo* isomer)

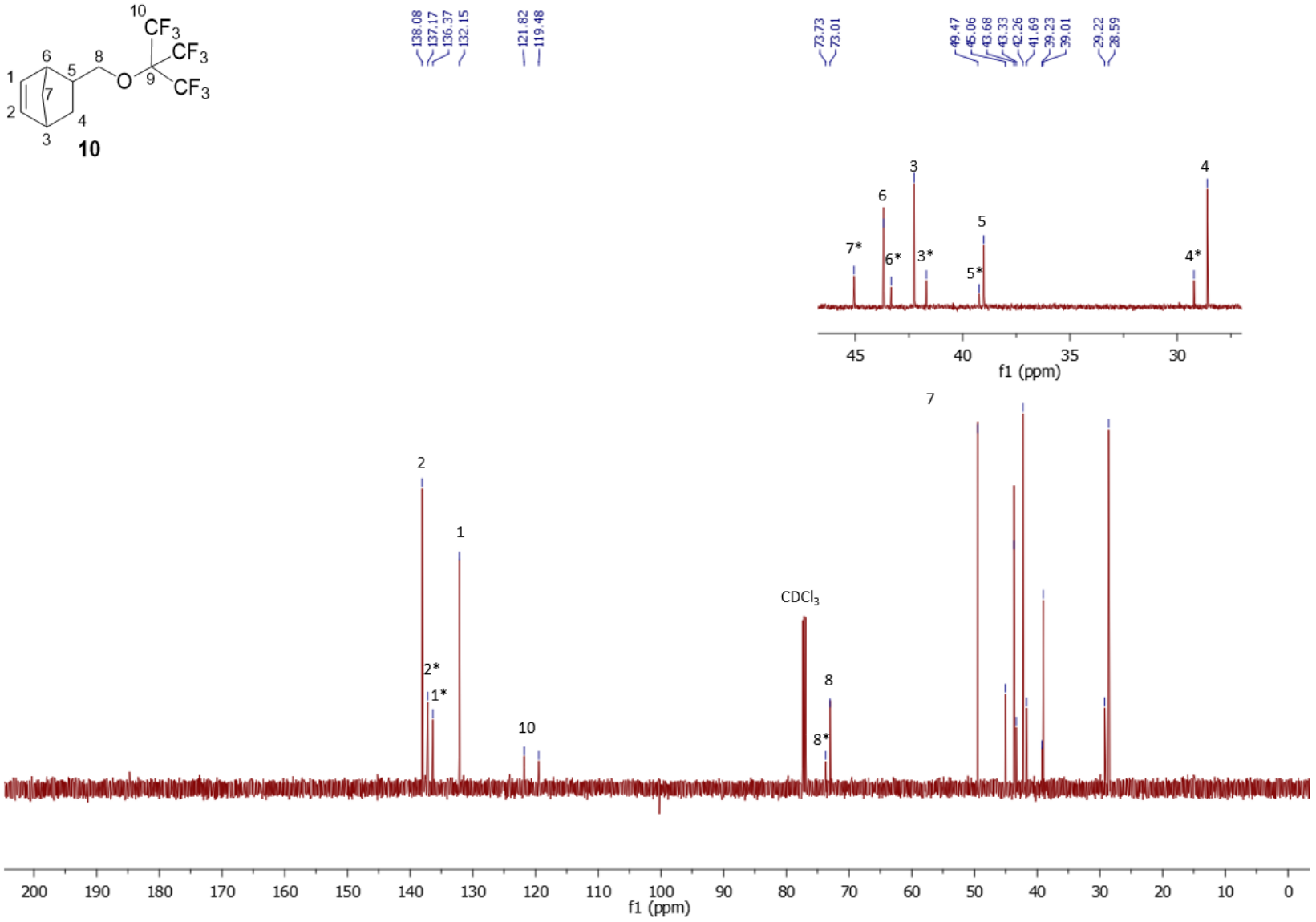


Figure S10. $^{13}C\{^{1}H\}$ NMR spectrum of **10** in $CDCl_3$. (* peaks of the ~19% *exo* isomer)

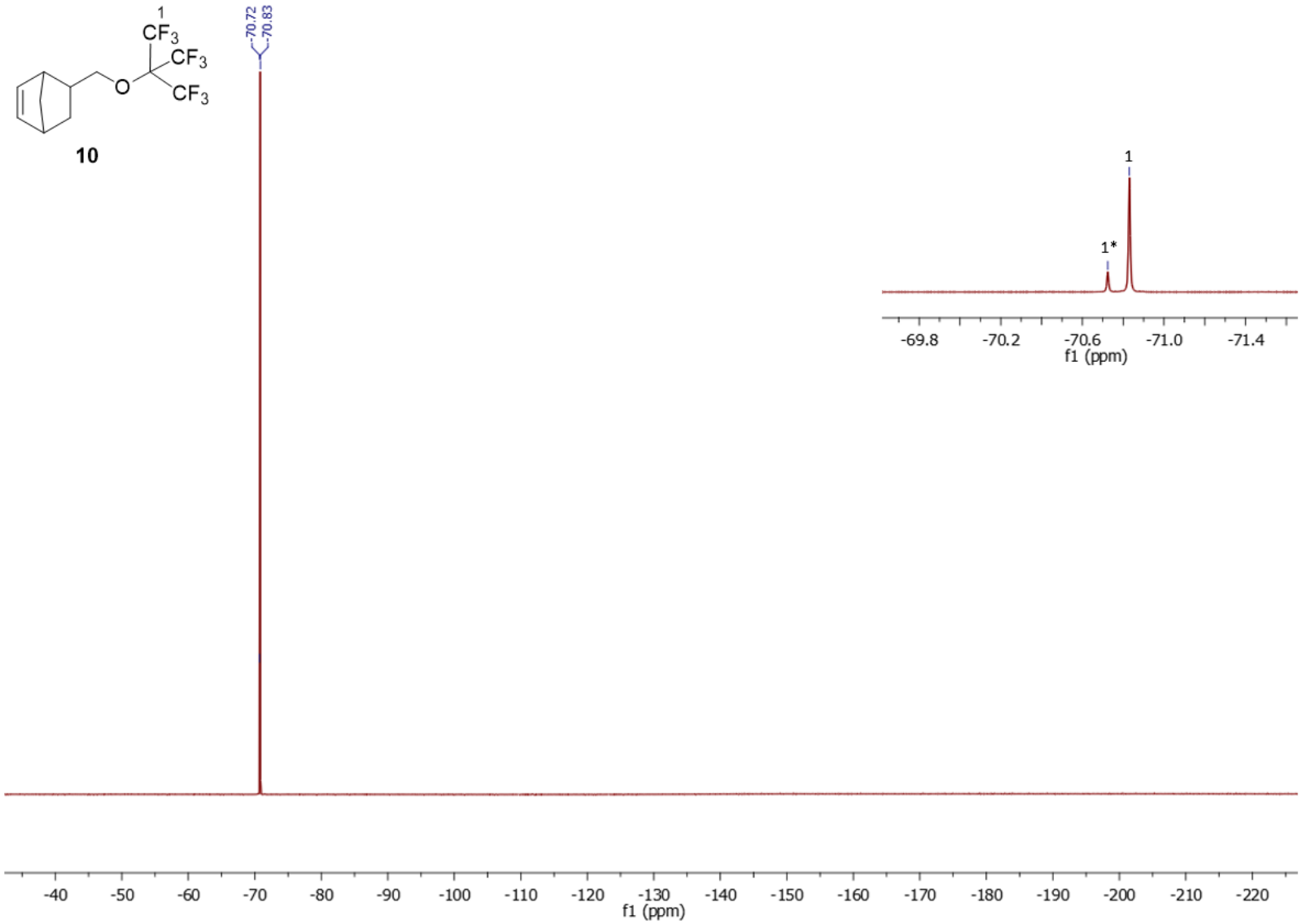
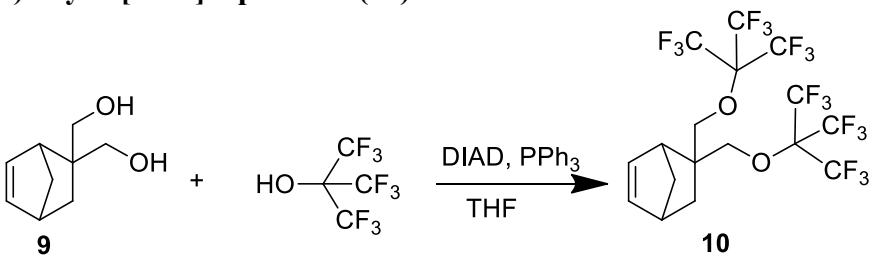


Figure S11. ^{19}F NMR spectrum of **10** in $CDCl_3$. (* peaks of the ~19% *exo* isomer)

5,5-bis(((1,1,1,3,3,3-hexafluoro-2-(trifluoromethyl)propan-2-yl)oxy)methyl)bicyclo[2.2.1]hept-2-ene (11)



9 **10**

A *Schlenk*-tube was charged with bicyclo[2.2.1]hept-5-ene-2,2-diyl)dimethanol[3] (3.0 g, 19.5 mmol), THF (80 mL), triphenylphosphine (15.3 g, 58.4 mmol) and cooled down to 0 °C. Then diisopropyl-azodicarboxylate (11.5 mL, 58.4 mmol) in THF (20 mL) was added dropwise under nitrogen. The reaction mixture was allowed to warm to room temperature and stirred for 20 minutes. Then nonafluoro-*tert*-butanol (8.14 mL, 58.4 mmol) was added and the solution was stirred for additional 30 hours. The solvent was evaporated under reduced pressure to give a pale yellow oil (10 g). The crude product was purified by distillation (5 mbar, 65 °C) to give **11** (3.11 g, 27%) as a colourless oil.

^{1}H NMR (500 MHz, $CDCl_3$) δ: 6.25 (bs, 1H, CH=), 6.06 (bs, 1H, CH=), 4.23 (d, 1H, *J*= 8.3 Hz, OCH_aH$_b$), 4.05 (d, 1H, *J*= 8.3 Hz, OCH$_a$$H_b$), 3.91 (d, 1H, *J*= 7.9 Hz, OCH_aH$_b$), 3.78 (d, 1H, *J*= 7.9 Hz, OCH$_a$$H_b$), 2.90 (1H, bs, C*H*-CH=), 2.74 (1H, bs, C*H*-CH=), 1.60-1.46 (m, 3H, CH-CH_2-CH, CH_aH$_b$-C), 0.86 (d, 1H, CH$_a$$H_b$-C). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$) δ: 138.56, 133.78, 121.65, 119.32, 71.83, 70.72, 48.43, 47.43, 45.71, 42.45, 32.42. ^{19}F NMR (125 MHz, $CDCl_3$) δ: -69.12, -69.23. HRMS (HR-EI-MS) m/z: [M] + Calcd for $C_{17}H_{12}O_2F_{18}$ 590.05499; Found 590.05721

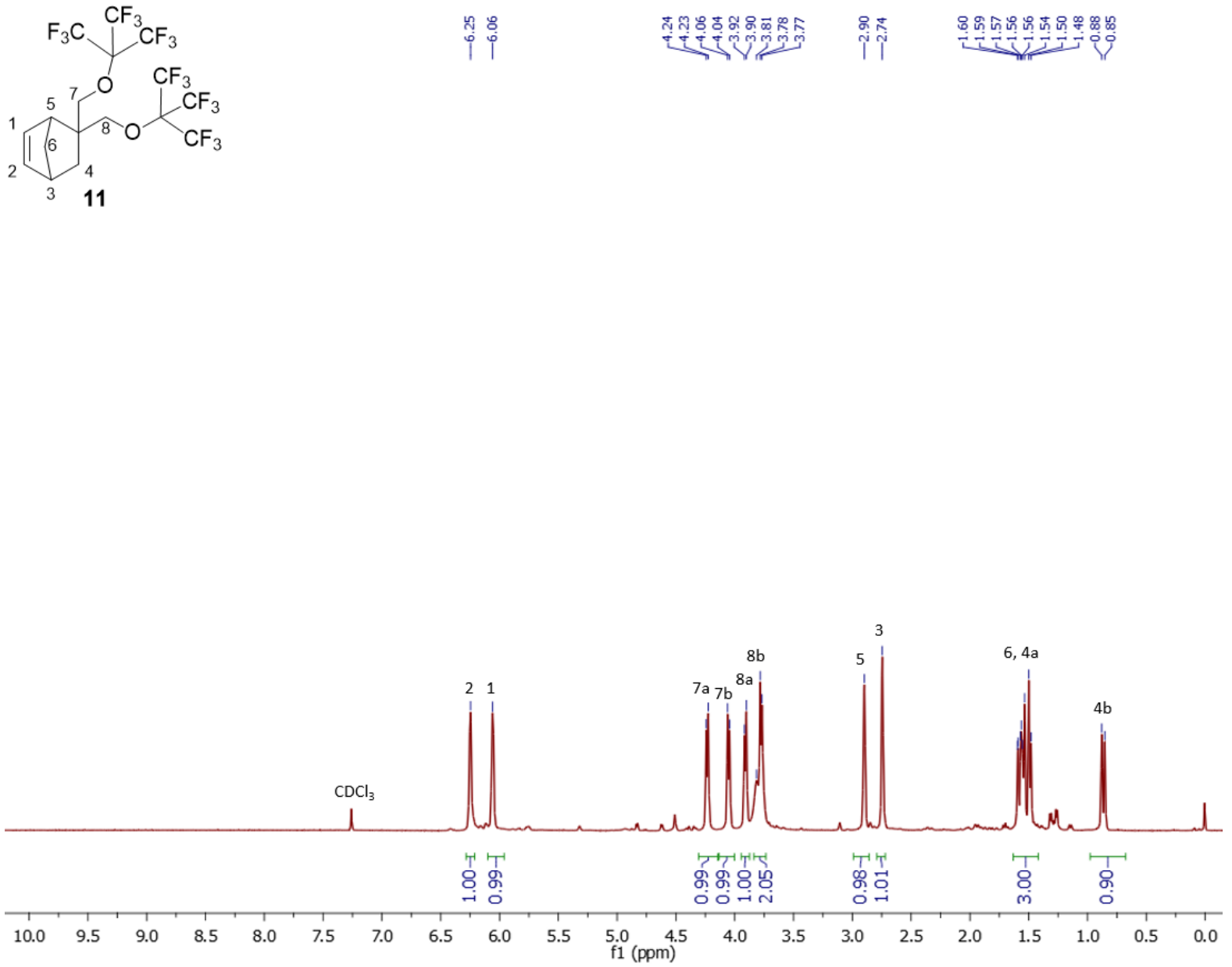


Figure S12. ^{1}H NMR spectrum of **11** ($CDCl_3$).

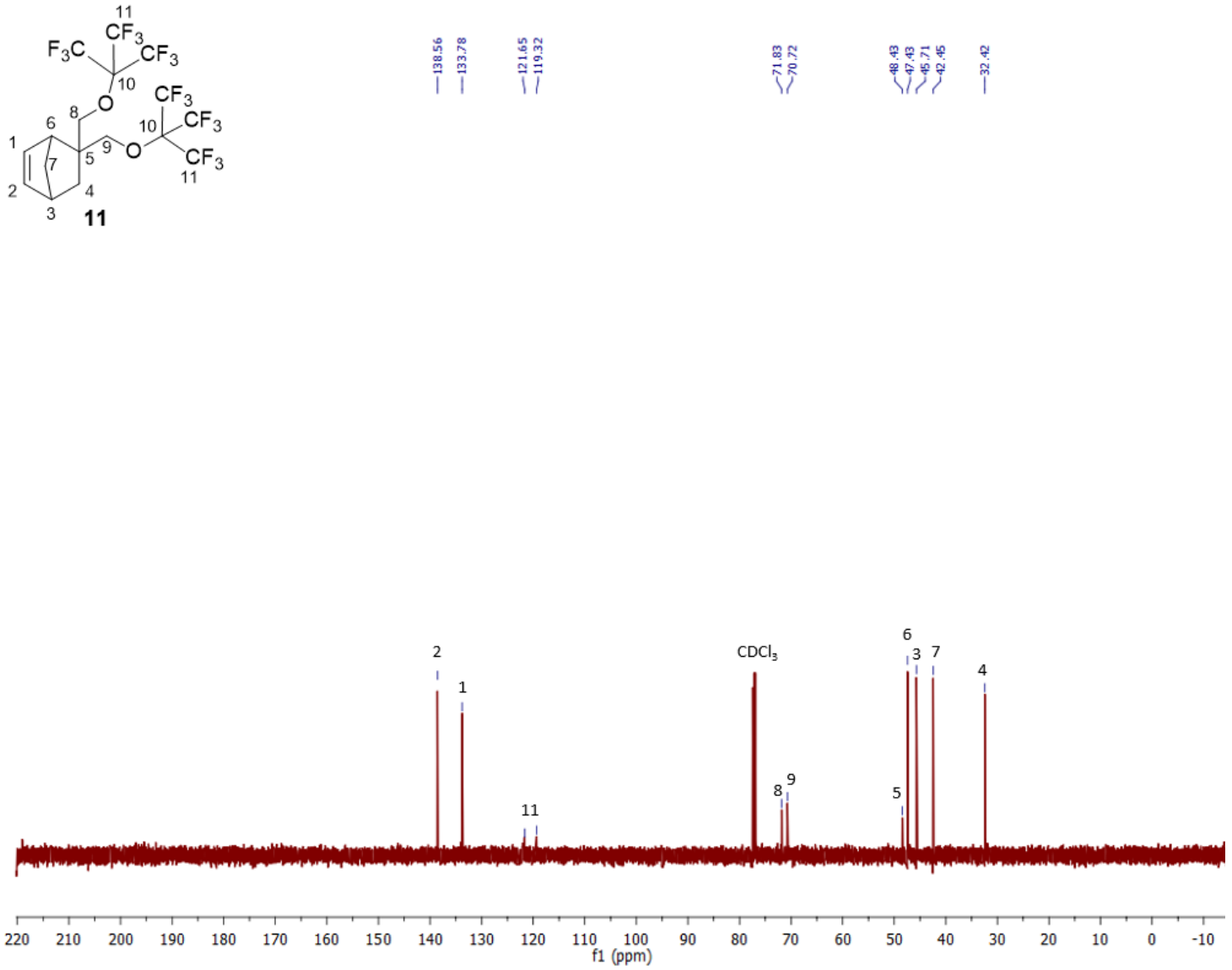


Figure S13. $^{13}C\{^{1}H\}$ NMR spectrum of **11** ($CDCl_3$).

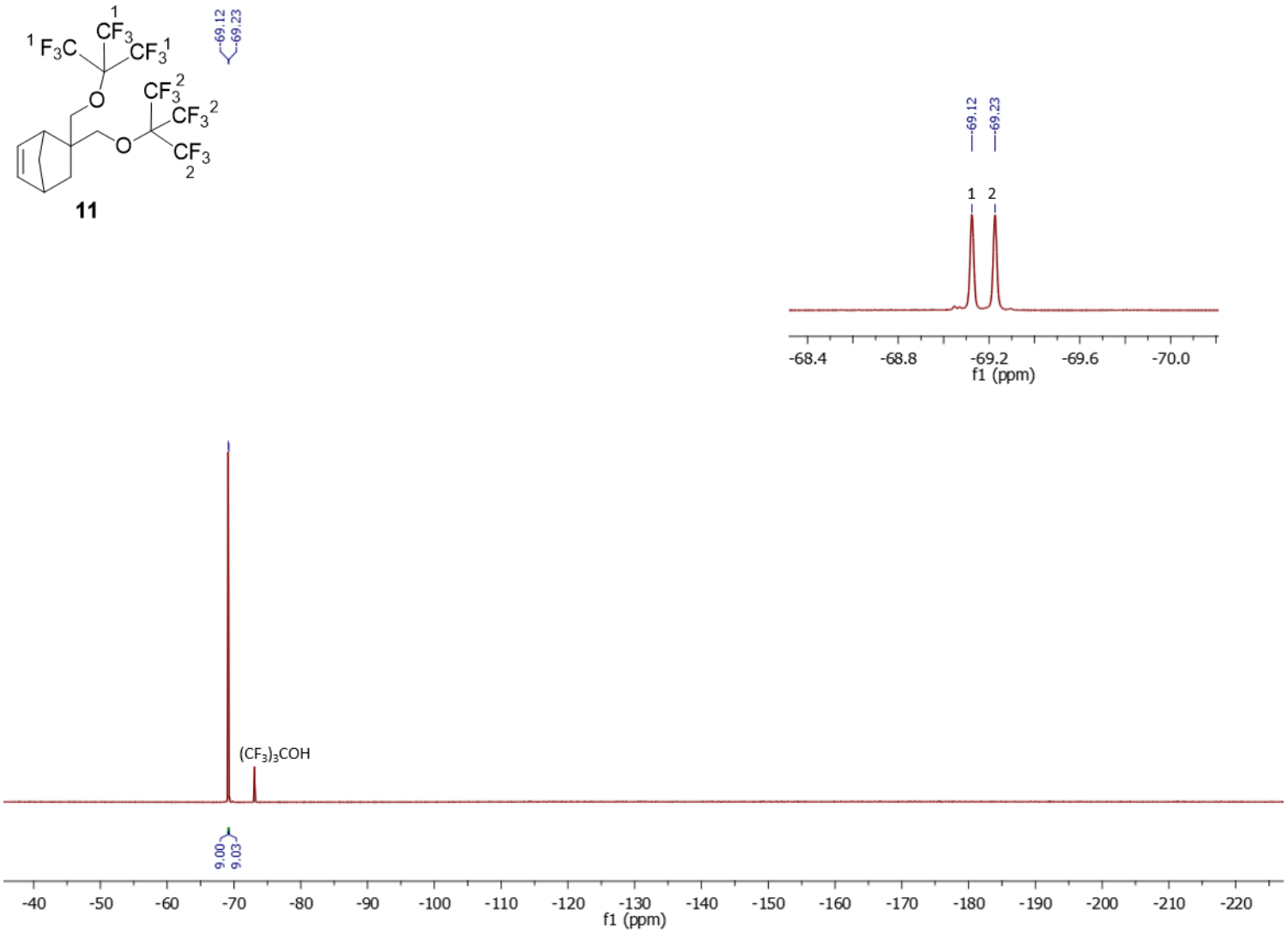
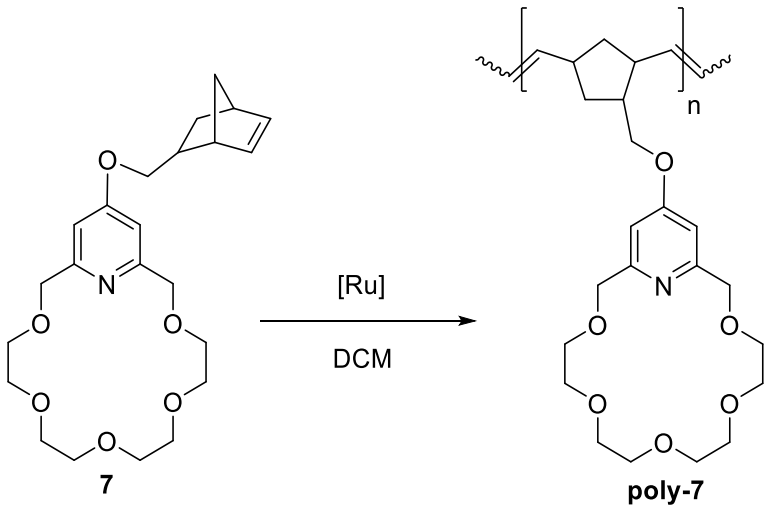


Figure S14. ^{19}F NMR spectrum of **11** ($CDCl_3$).

4. Homopolymer synthesis

4.1. Polymerization of crown ether 7



In a glovebox a vial was charged with crown ether **7** (50 mg, 119 mmol, 10 mg/mL) and DCM (4.7 mL). Then DCM solution (0.3 mL) of **G2** (2.0 mg, 2.3 mmol, 2 mol% of 7) or **G3** (2.1 mg, 2.3 mmol, 2 mol% of 7) was added. The reaction mixture was stirred for 2 hours at 30 °C. The solution was transparent. The vial was removed from the glovebox, ethyl vinyl ether (0.1 mL) was added, and the mixture was stirred for additional 30 minutes. The solvent was evaporated under reduced pressure to give 50 mg (99%) of **poly-7** (**G2**) or 46.5 mg (93%) of **poly-7** (**G3**) as a vaxy solid. NMR measurements showed characteristic broad signals.

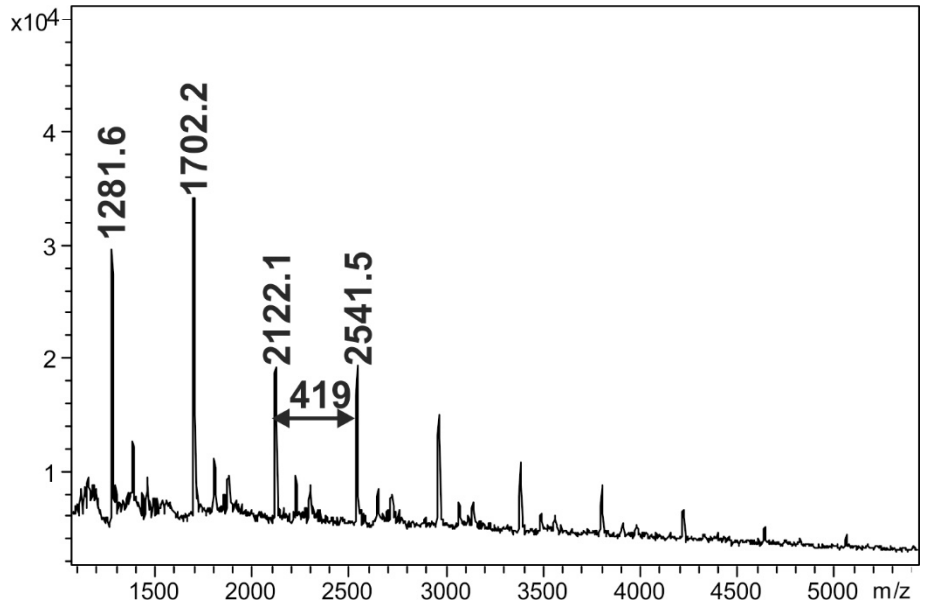
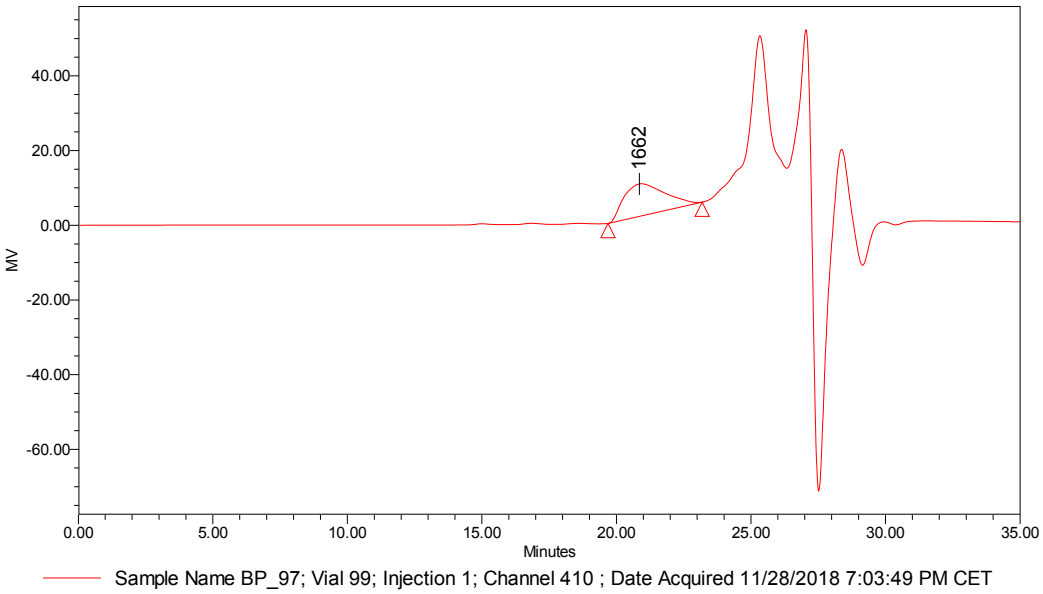


Figure S15. MALDI-TOF MS spectrum of **poly-7** (**G2**) polymer, 7 (m/z: 419), (Linear mode, DHB/NaTFA)

GPC Report



GPC Sample Results

	Sample Name	Inj	RT (min)	Mn	Mw	MP	Poly-dispersity
1	BP_97	1	20.850	1303	1525	1662	1.170

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Figure S16. GPC chromatogram of **poly-7** (**G3**) polymer.

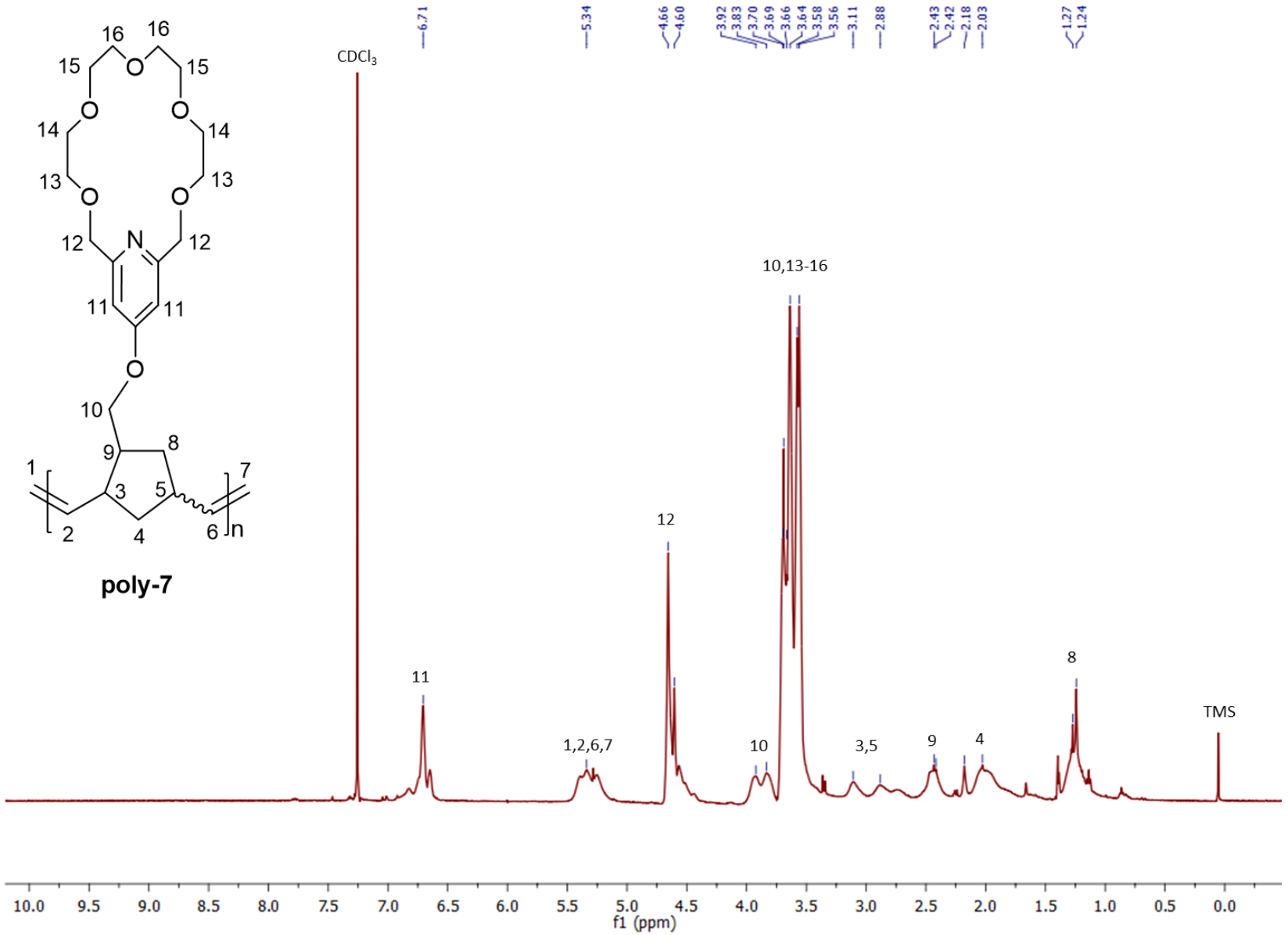


Figure S17. ^{1}H NMR spectrum of **poly-7** prepared by **G2** ($CDCl_3$).

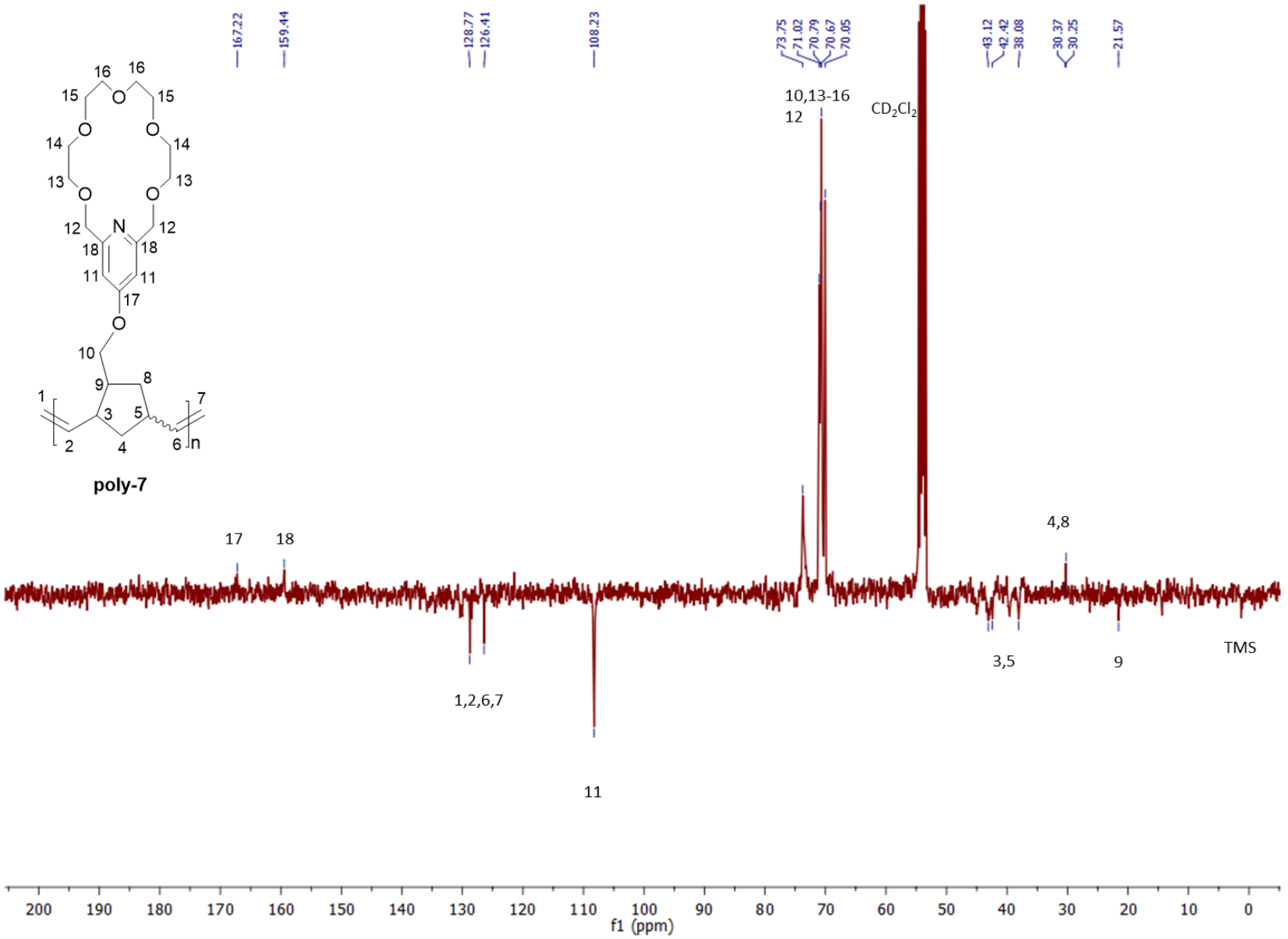


Figure S18. DEPT-Q NMR spectrum of **poly-7** prepared by **G2** (CD_2Cl_2).

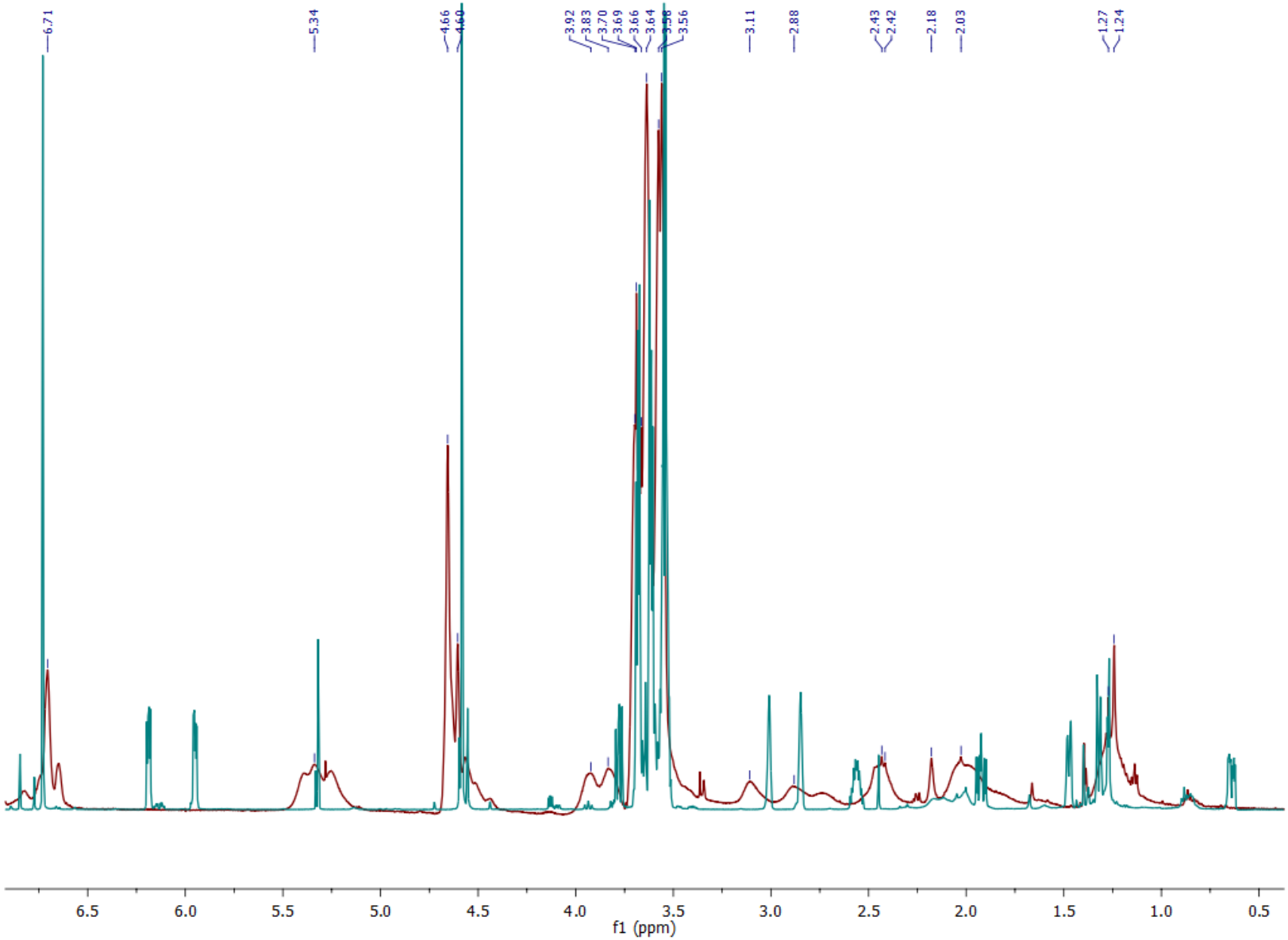


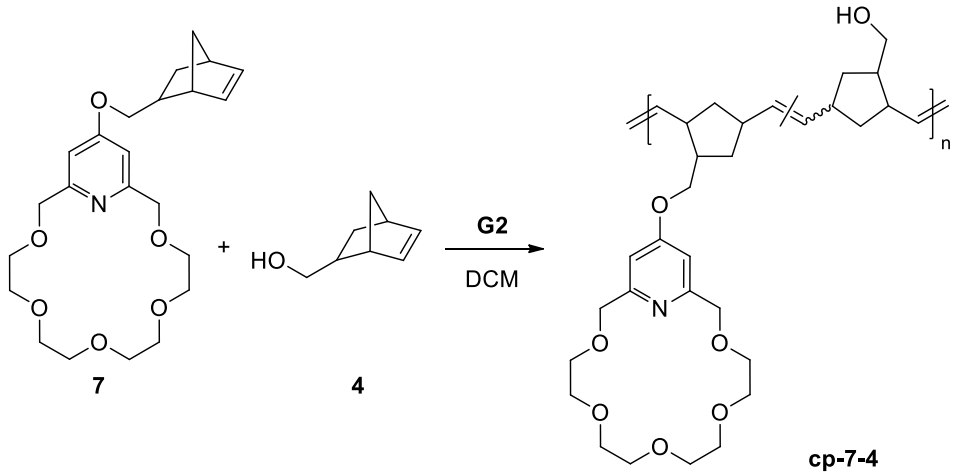
Figure S19. Superimposed ^{1}H NMR spectra of **7** monomer (blue) and **poly-7** (dark red) (CD_2Cl_2).

5. Synthesis of copolymers 7 and 8-11

5.1. The general method for copolymerization of crown ether 7 and other norbornenes

In a glovebox a vial was charged with 50 mg of the corresponding norbornene monomers [crown ether **7** (20-40 mg) and norbornene **8**, **9**, **10** or **11** (10-30 mg, 1 or 5 equivalent of **7**)] and DCM (4.7 mL, 10 mg/mL). Then DCM (0.3 mL) solution of catalyst (**G2** or **G3** (2 mol% / norbornene units)) was added. The mixture was stirred for 2 hours at 30 °C. The vial was removed from the glovebox, ethyl vinyl ether (0.1 mL) was added, and the solution was stirred for 30 minutes. After the removal of the solvent a solid glue-like product was obtained.

5.2. Copolymerization of crown ether 7 and norbornene-methanol (4)



7 4 cp-7-4

In a glovebox crown ether **7** (50.0 mg, 0.119 mmol), norbornene-methanol **4** (14.8 mg, 0.119 mmol, 1 equivalent of **7**) were measured into a vial, dissolved in DCM (6.0 mL). **G2** catalyst (4.1 mg, 0.0048 mmol (2 mol% / norbornene monomers)) in DCM (0.5 mL) was added to the solution, and the mixture was stirred for 2 hours at 30 °C. The vial was removed from the glovebox, ethyl vinyl ether (0.1 mL) was added, and the solution was stirred for 30 minutes. After the removal of the solvent 60 mg (92%) brownish solid product was obtained.

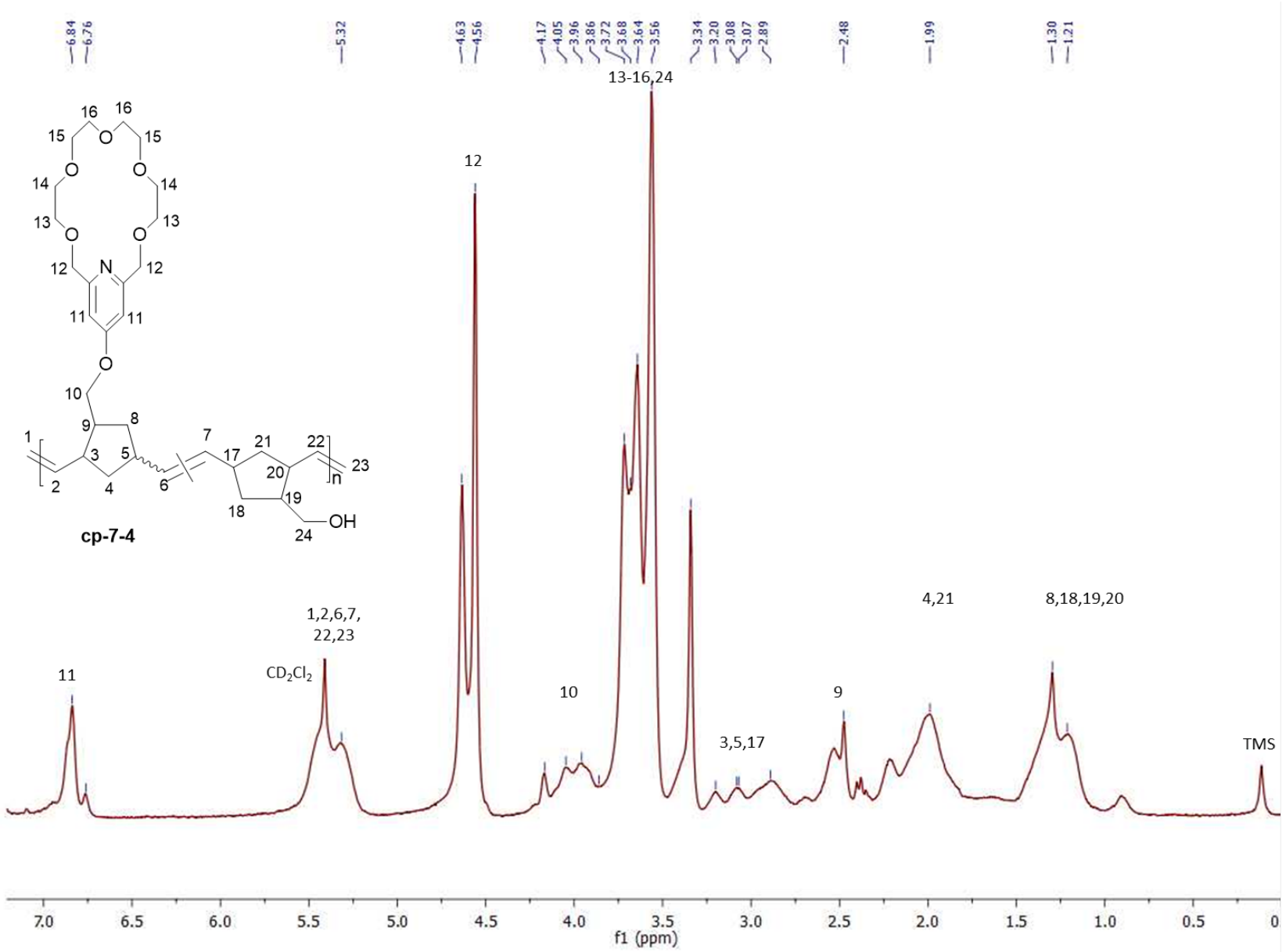


Figure S20. ^{1}H NMR spectrum of **cp-7-4** (**1/1** equivalent, **G2**) (1 : 1 mixture of MeOD and CD_2Cl_2).

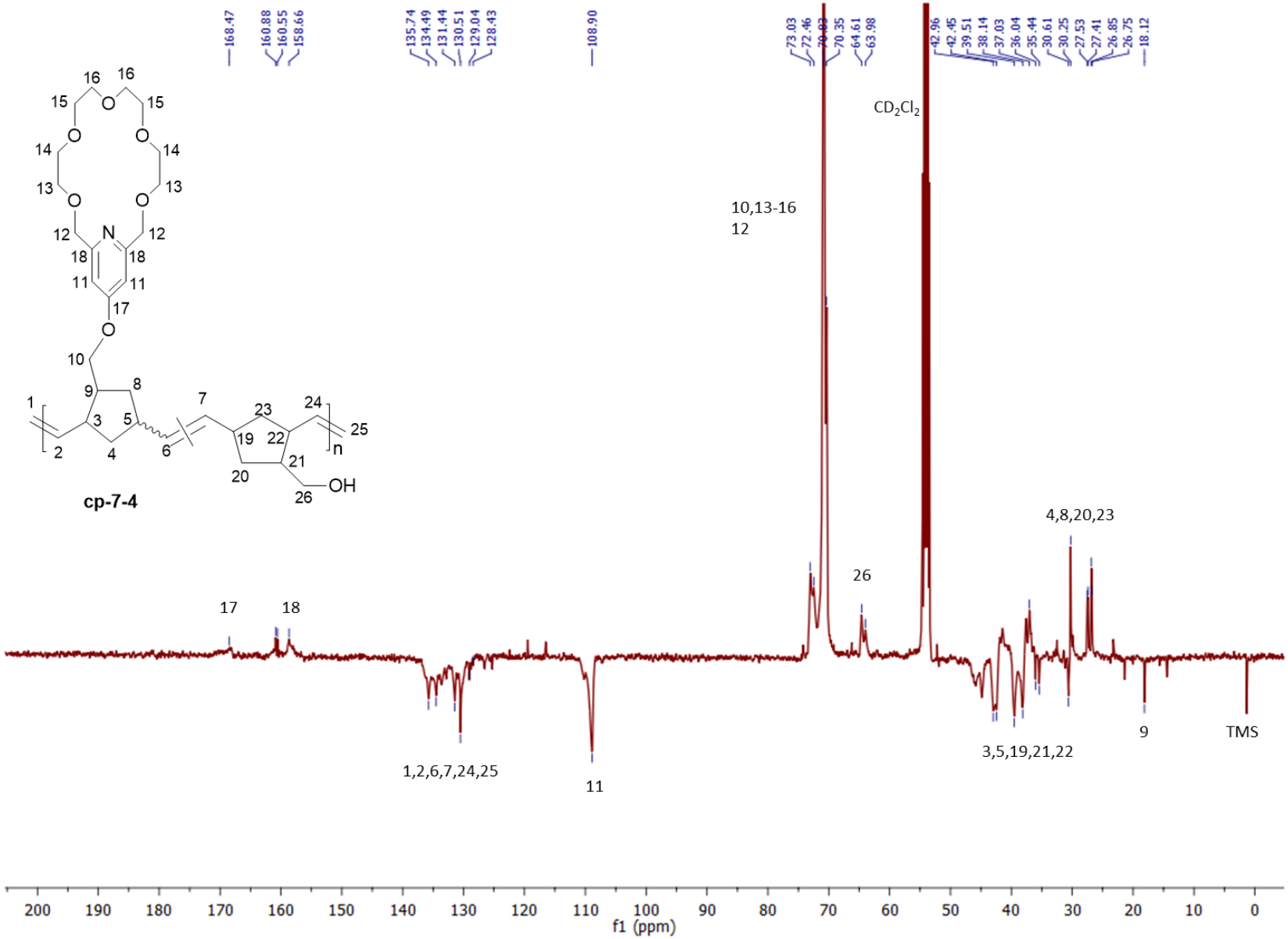


Figure S21. DEPT-Q NMR spectrum of **cp-7-4** (**1/1** equivalent, **G2**) (CD_2Cl_2).

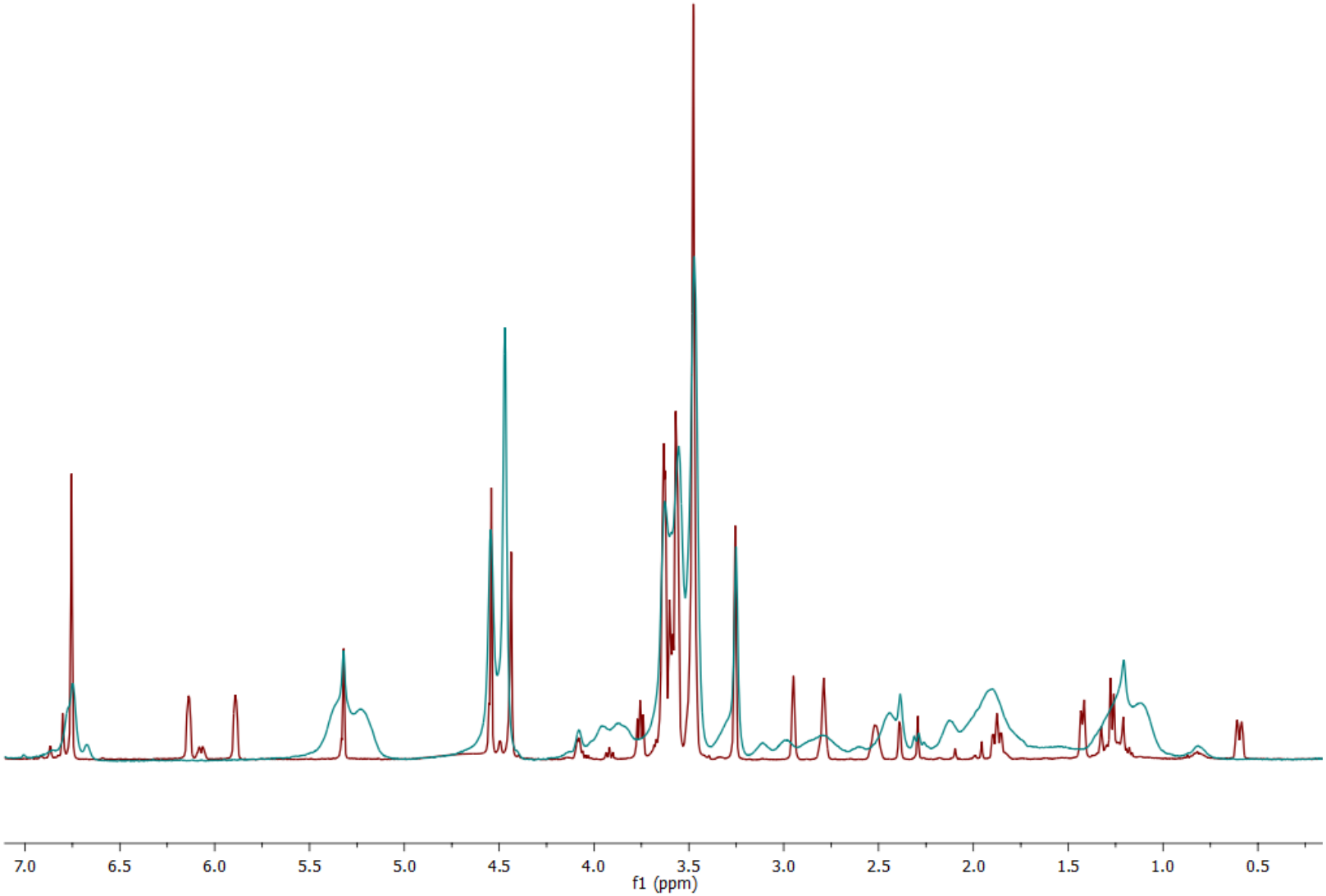
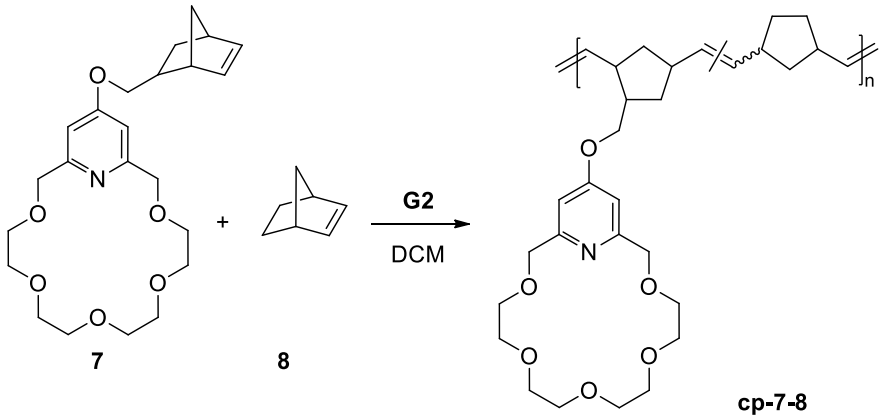


Figure S22. Stacked ^{1}H NMR spectra of **7** (red) and **cp-7-4** (**1/1** equivalent, **G2**) (blue) (MeOD : CD_2Cl_2 = 1 : 1).

5.3. Copolymerization of crown ether 7 and norbornene (8)



In a glovebox a vial was charged with DCM (4.7 mL), crown ether **7** (40.8 mg, 0.0973 mmol) and norbornene (**8**, 9.2 mg, 0.0973 mmol, 1 equivalent of **7**). DCM (0.3 mL) solution of **G2** (3.3 mg, 0.0039 mmol (2 mol% / norbornene monomers)) or **G3** (3.5 mg) in DCM (0.3 mL) was added. The mixture was stirred for 2 hours at 30 °C. The vial was removed from the glovebox, ethyl vinyl ether (0.1 mL) was added, and the solution was stirred for 30 minutes. After the removal of the solvent 49 mg (98%) **cp-7-8** (1/1 equivalent, **G2**) or 47.5 mg (95%) **cp-7-8** (1/1 equivalent, **G3**) brownish product was obtained.

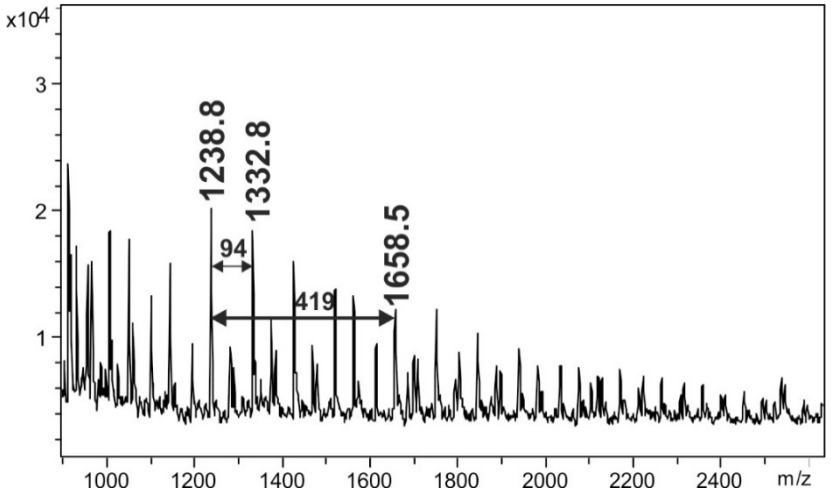
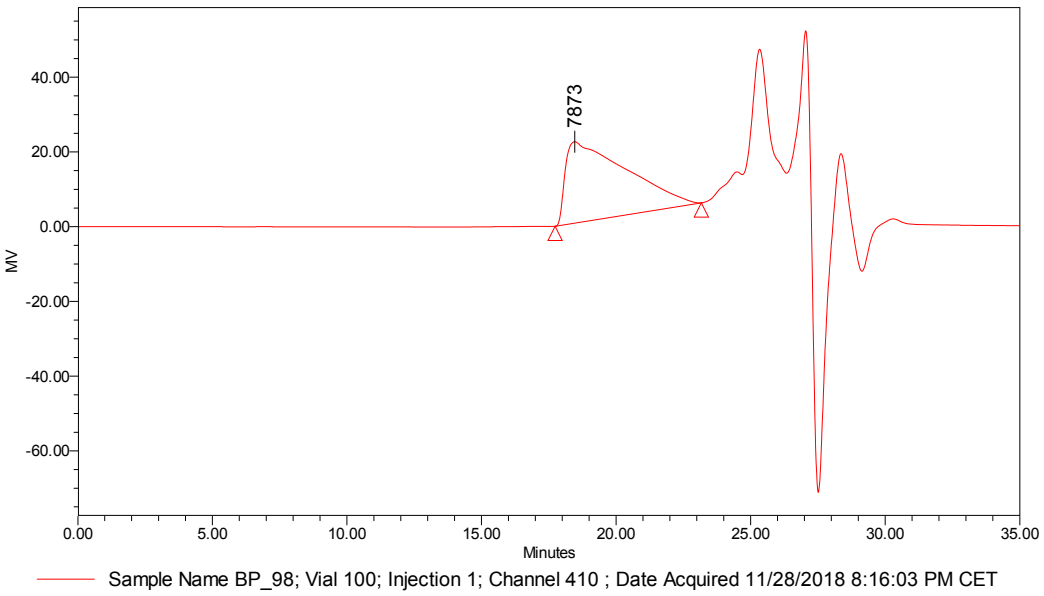


Figure S23. MALDI-TOF MS spectrum of **cp-7-8** (1/1 equivalent, **G3**) copolymer, **7** (m/z: 419), **8** (m/z: 94) (**7**/**8** = 1/1) (Linear mode, DHB/NaTFA)

GPC Report



GPC Sample Results

	Sample Name	Inj	RT (min)	Mn	Mw	MP	Poly-dispersity
1	BP_98	1	18.462	2676	4491	7873	1.678

Reported by User: System
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Figure S24. GPC chromatogram of **poly-7-8** (**7**/**8** = 1/1, **G3**) polymer.

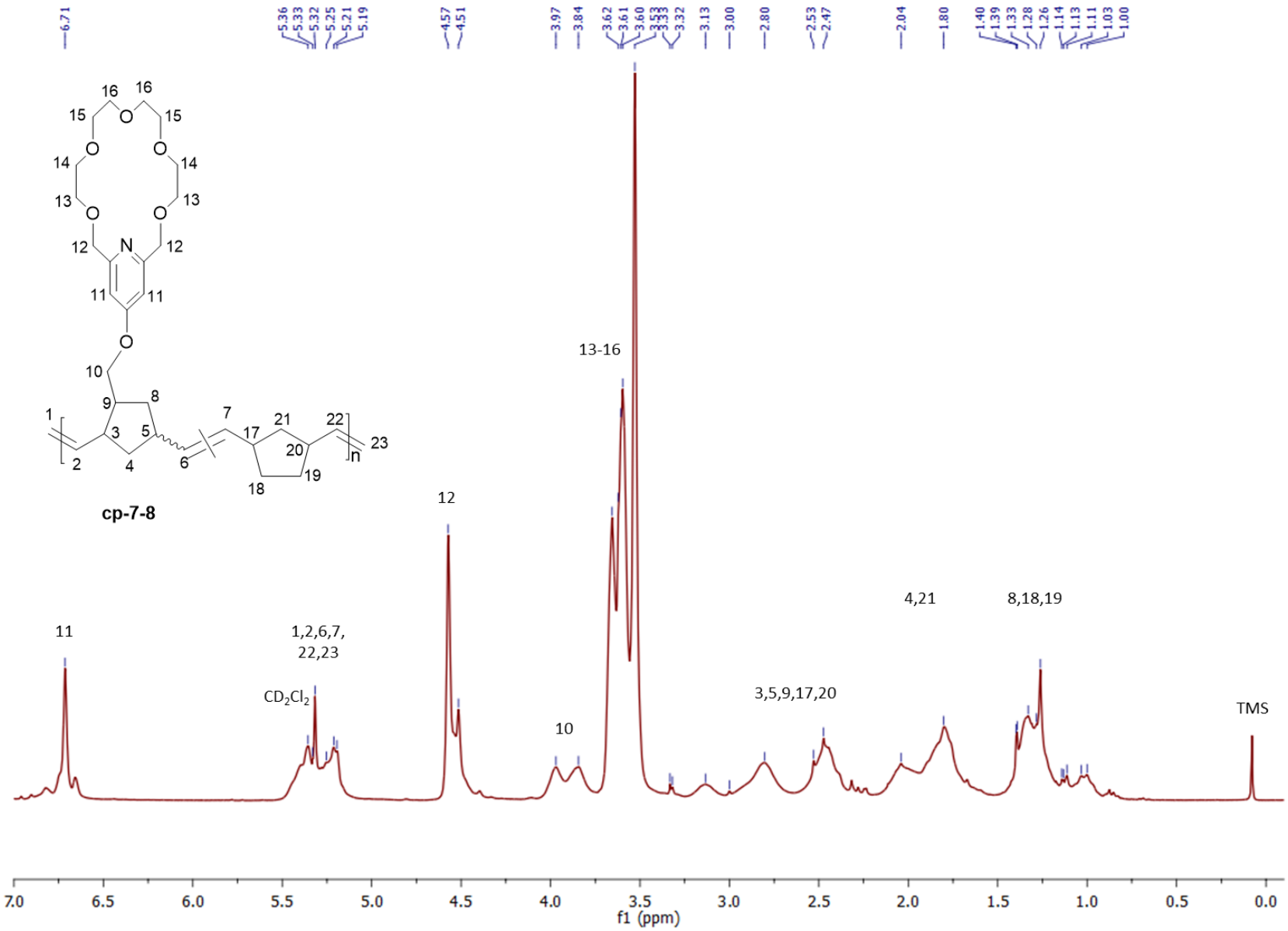


Figure S25. ^{1}H NMR spectrum of **cp-7-8** (1/1 equivalent, **G2**) (CD_2Cl_2).

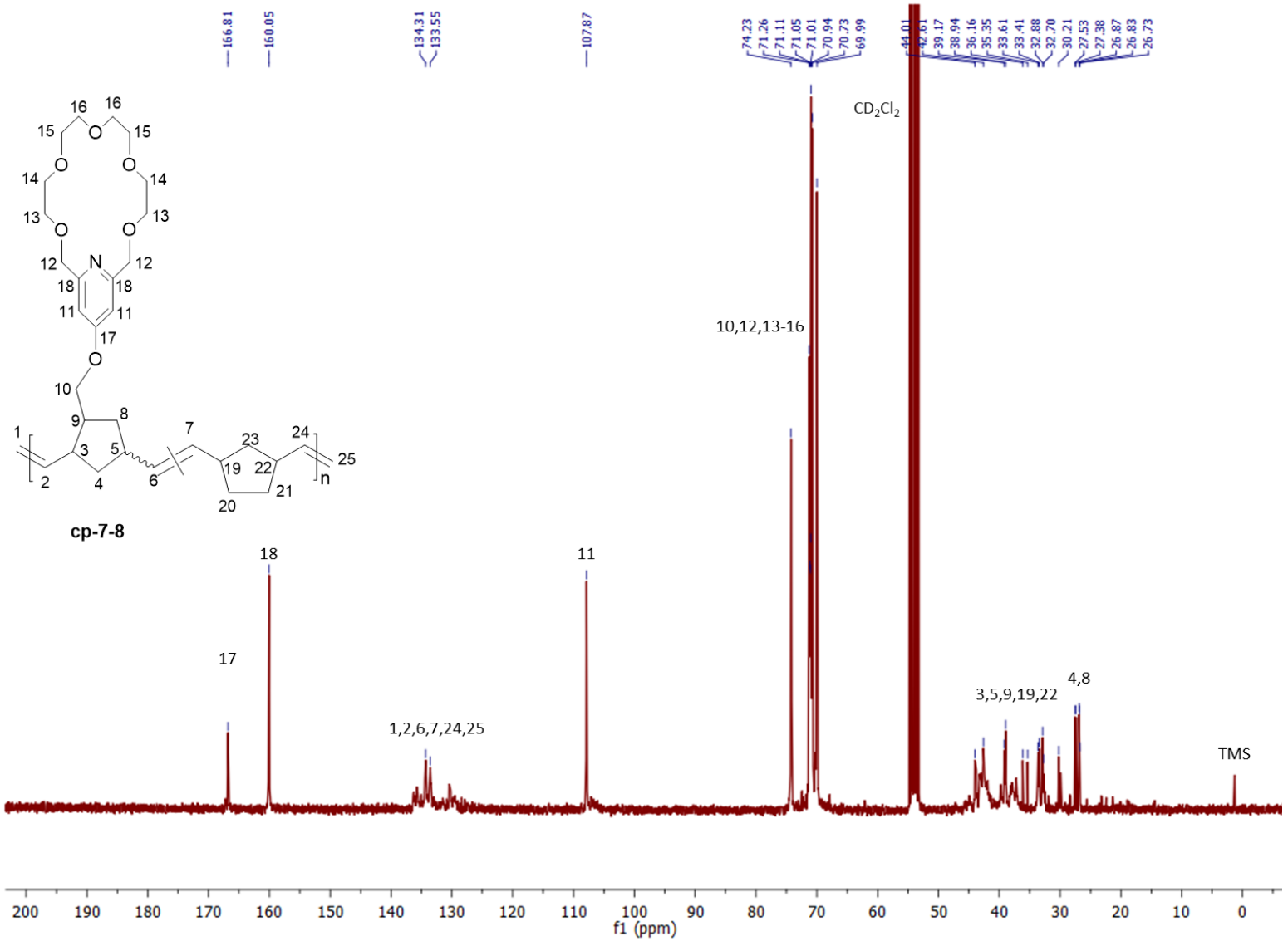


Figure S26. $^{13}C\{^{1}H\}$ NMR spectrum of **cp-7-8** (1/1 equivalent, **G2**) (CD_2Cl_2).

CP-7-8 (1/5 equivalent)

In a glovebox a vial was charged with DCM (2.2 mL), crown ether **7** (13.2 mg, 0.0315 mmol) and norbornene (**8**, 14.8 mg, 0.1573 mmol, 5 equivalent of **7**). DCM (0.3 mL) solution of **G2** (3.2 mg, 0.0038 mmol (2 mol% / norbornene monomers)) or **G3** (3.3 mg) was added. The mixture was stirred for 2 hours at 30 °C. The vial was removed from the glovebox, ethyl vinyl ether (0.1 mL) was added, and the solution was stirred for 30 minutes. After the removal of the solvent 27.2 mg (97%) **cp-7-8** (1/5 equivalent, **G2**) or 25.5 mg (91%) **cp-7-8** (1/5 equivalent, **G3**) brownish product was obtained.

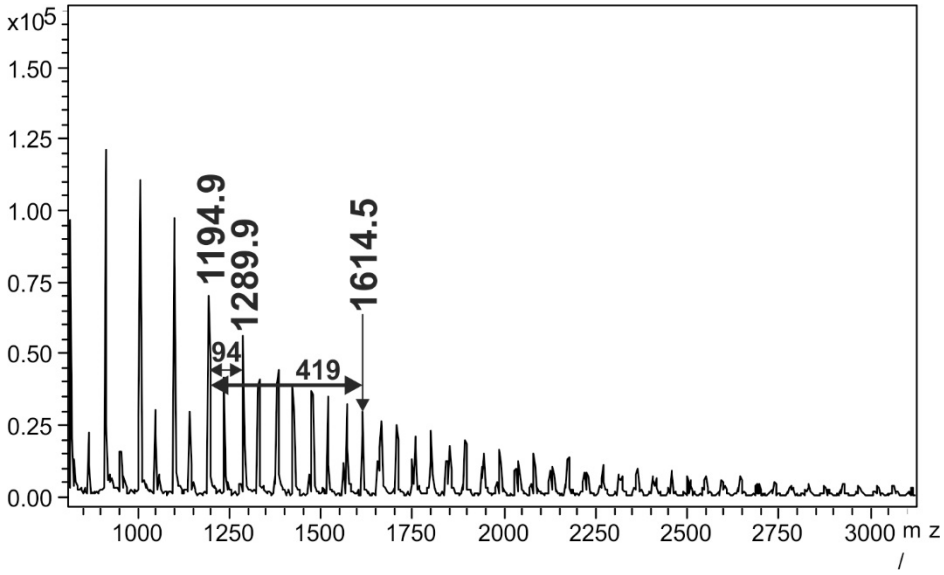
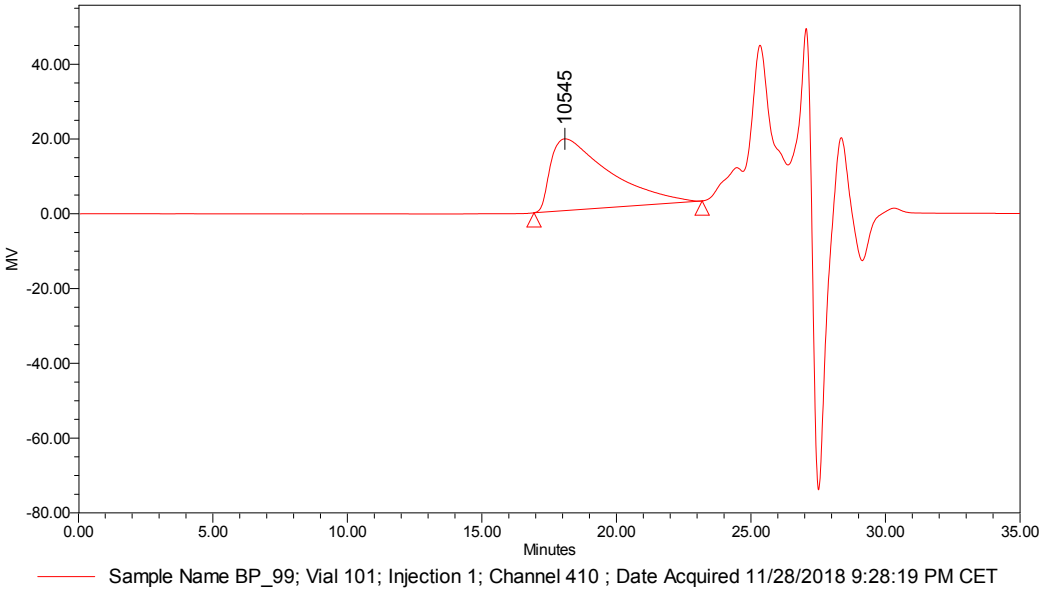


Figure S27. MALDI-TOF MS spectrum of **cp-7-8** (1/5 equivalent, **G3**) copolymer, **7** (m/z: 419), **8** (m/z: 94) (**7**/**8** = 1/5) (Linear mode, DHB/NaTFA)

GPC Report



GPC Sample Results

	Sample Name	Inj	RT (min)	Mn	Mw	MP	Poly-dispersity
1	BP_99	1	18.084	3834	7185	10545	1.874

Reported by User: System
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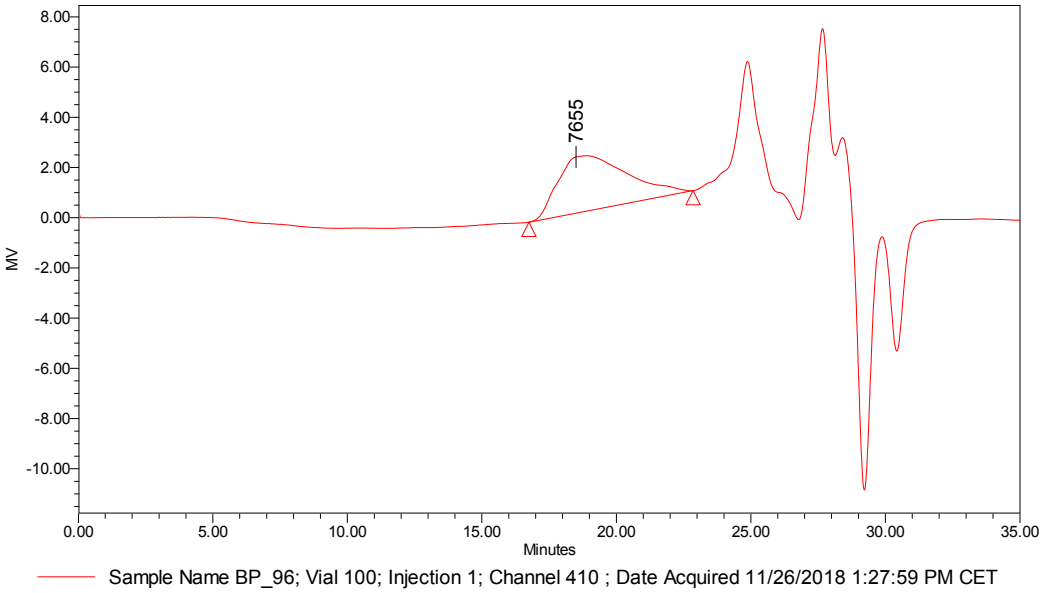
Figure S28. GPC chromatogram of **cp-7-8** (1/5 equivalent, **G3**) copolymer

GPC Report



GPC Sample Results

	Sample Name	Inj	RT (min)	Mn	Mw	MP	Poly-dispersity
1	BP_96	1	18.500	3311	5966	7655	1.802

Reported by User: System
Report Method: GPC_reportdisp
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Project Name: 2016THF
Date Printed: 4/3/2019

Figure S29. GPC chromatogram of **cp-7-8** (1/5 equivalent, **G2**) copolymer

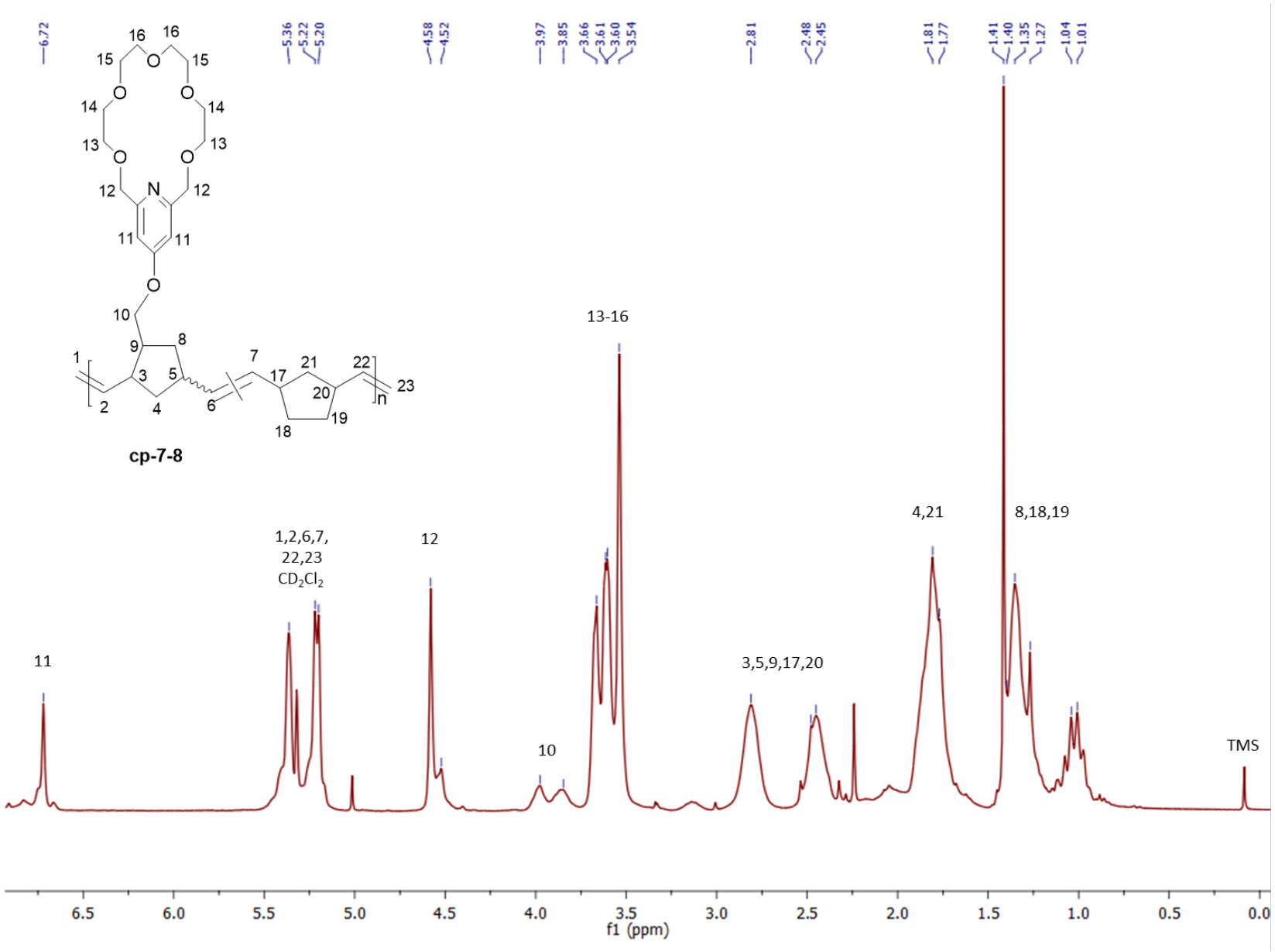


Figure S30. ^{1}H NMR spectrum of **cp-7-8** (1/5 equivalent, **G2**) (CD_2Cl_2).

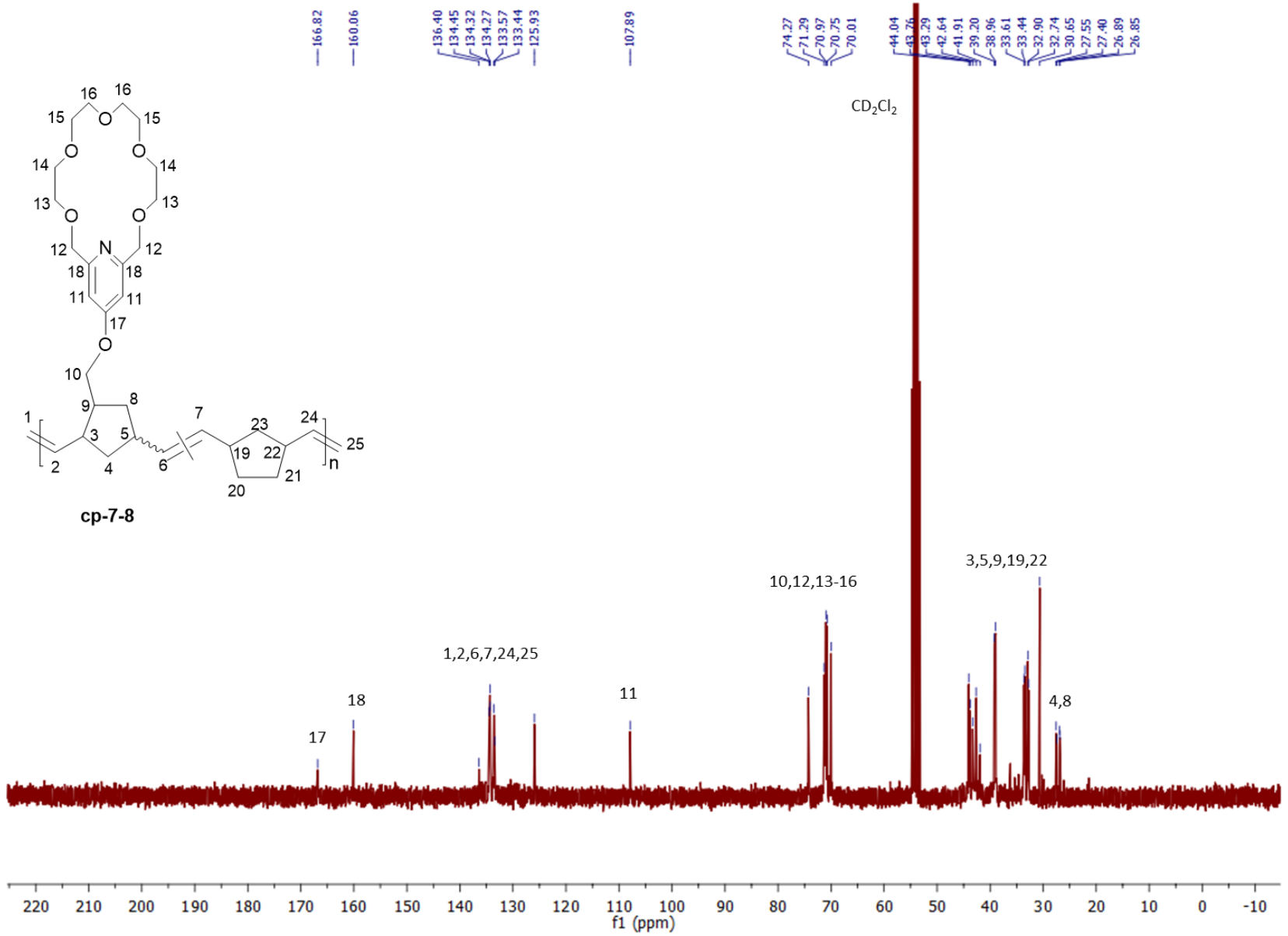


Figure S31. $^{13}C\{^{1}H\}$ NMR spectrum of **cp-7-8** (1/5 equivalent, **G2**) (CD_2Cl_2).

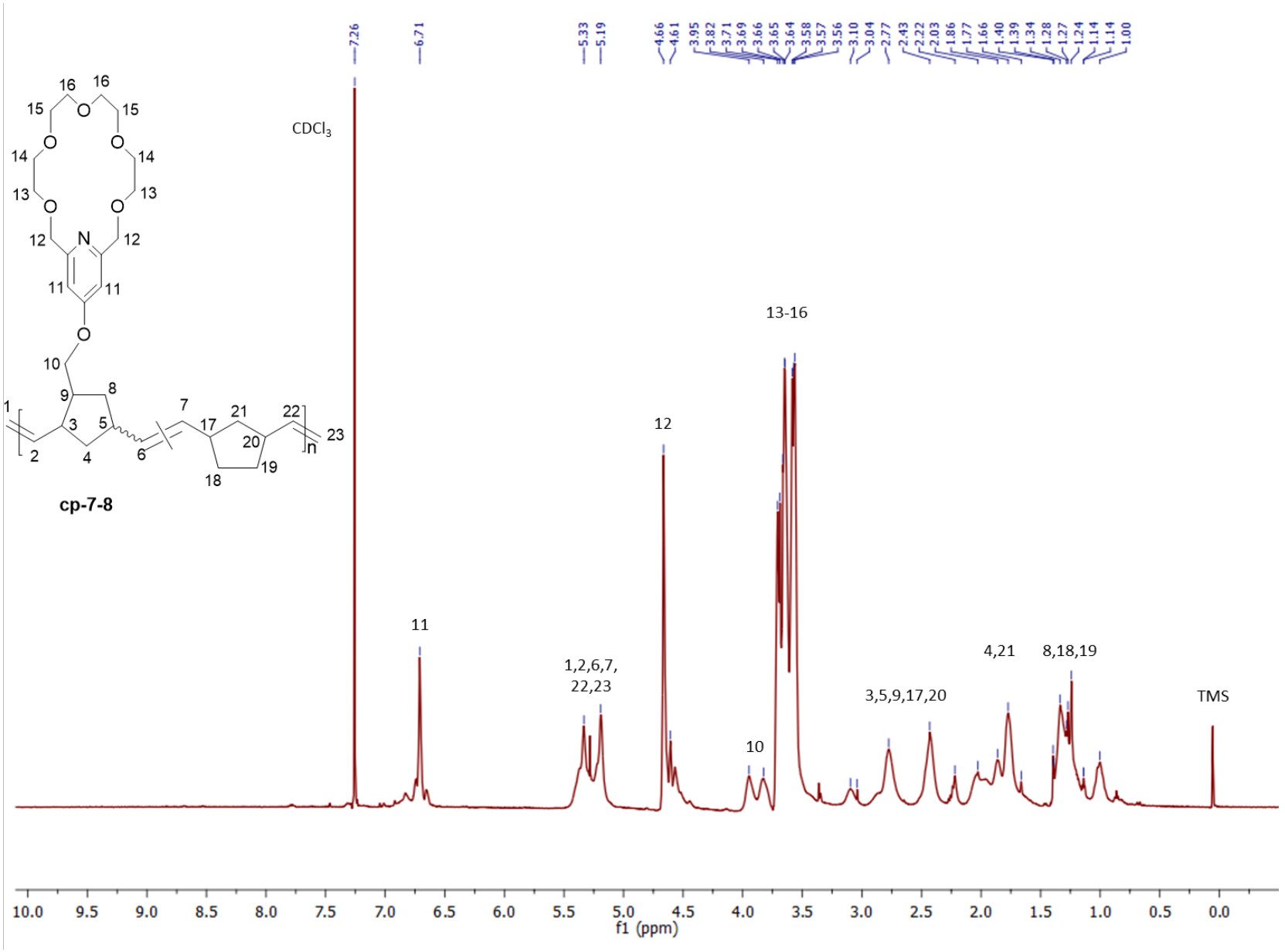


Figure S32. ^{1}H NMR spectrum of **cp-7-8** (1/1 equivalent, **G3**) ($CDCl_3$).

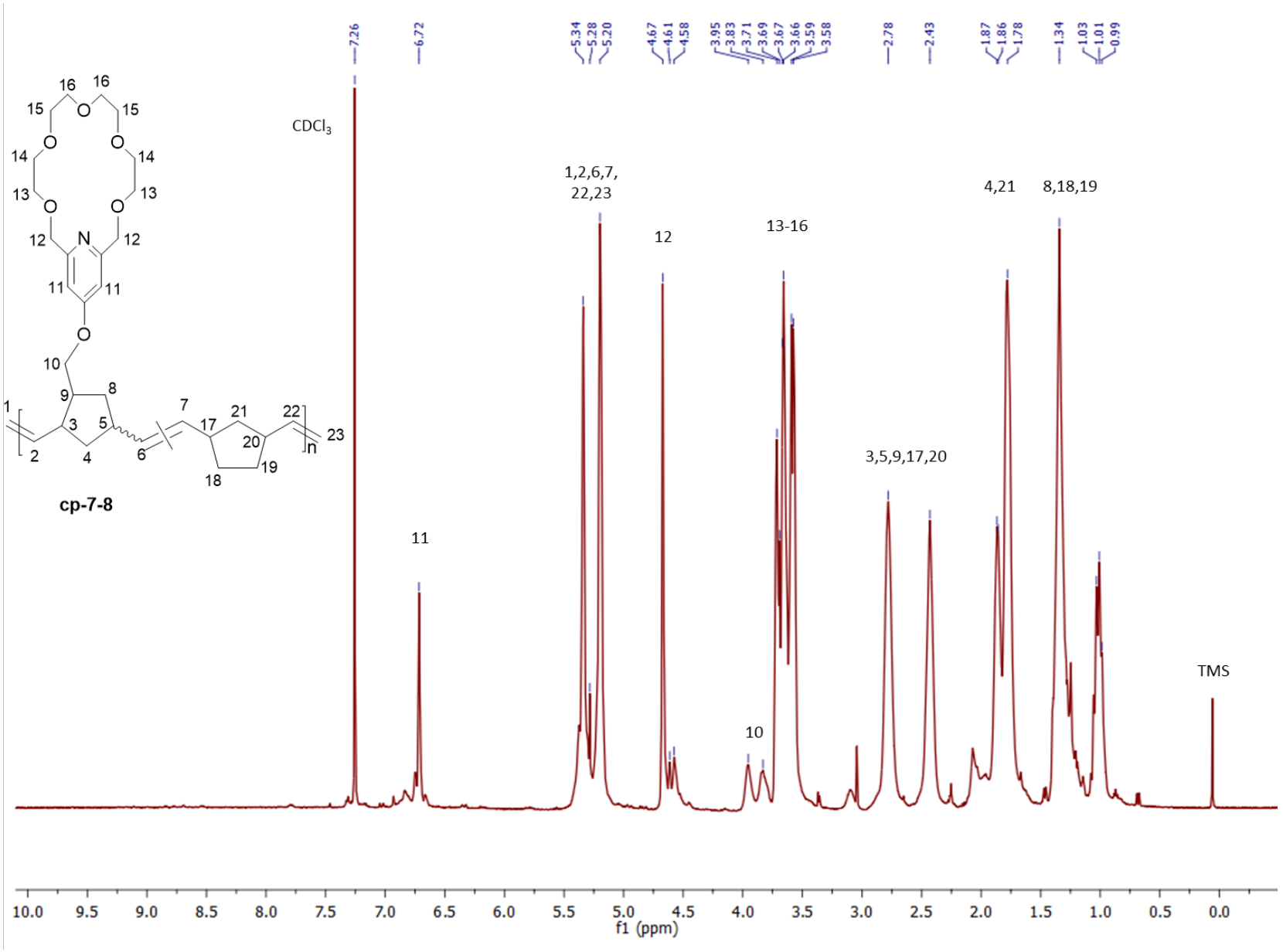


Figure S33. ^{1}H NMR spectrum of **cp-7-8** (1/5 equivalent, **G3**) ($CDCl_3$).

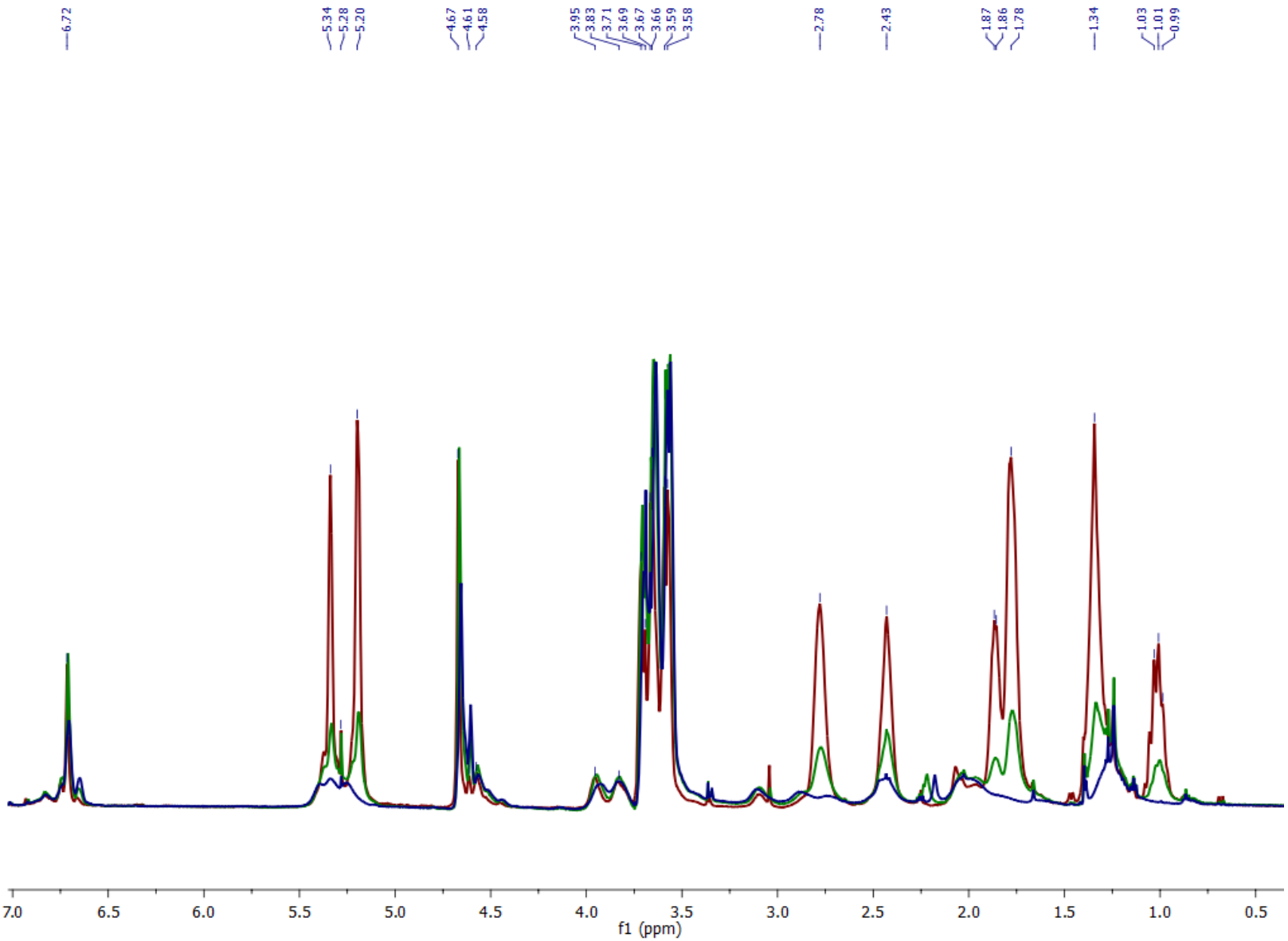
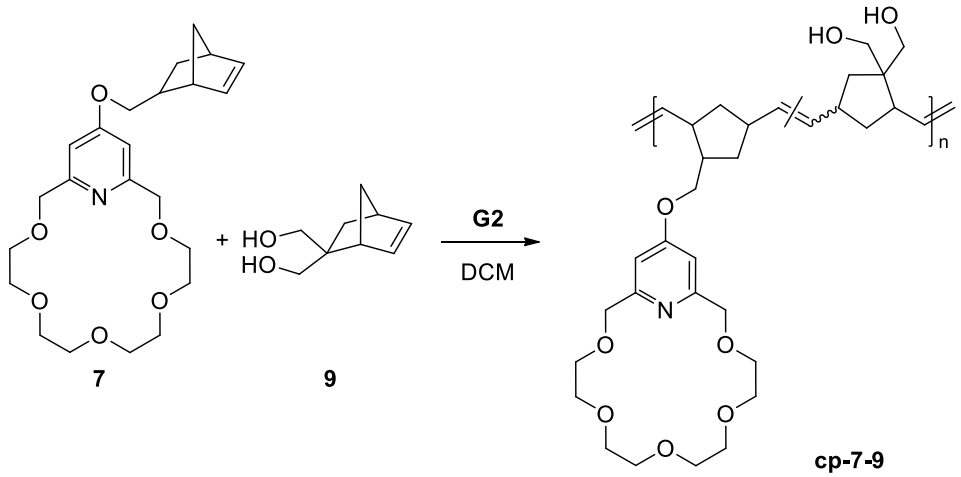


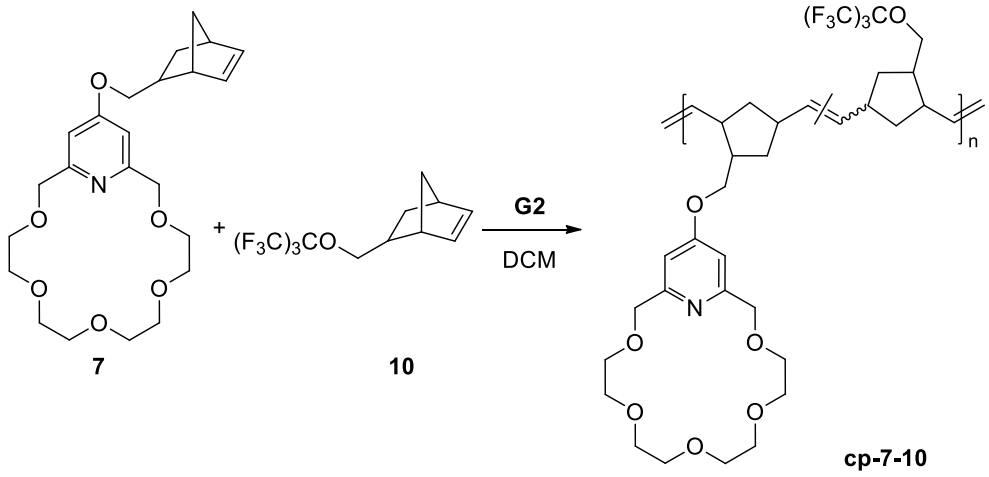
Figure S34. Superimposed ^{1}H NMR spectra of **poly-7** (blue), **cp-7-8** (1/1 equivalent) (green), **cp-7-8** (1/5 equivalent (red), prepared by **G3** ($CDCl_3$).

5.4. Copolymerization of crown ether 7 and norbornene-dimethanol 9



In a glovebox a vial was charged with DCM (2.3 mL), crown ether **7** (9.0 mg, 0.0021 mmol), **9** dimethanol (16.5 mg, 0.107 mmol, 5 equivalent of **7**). DCM (0.2 mL) solution of **G2** catalyst (2.2 mg, 0.0026 mmol (2 mol% / norbornene monomers)) was added. The mixture was stirred for 2 hours at 30 °C. The solid precipitate was formed. The vial was removed from the glovebox, ethyl vinyl ether (0.1 mL) was added, and the solution was stirred for 30 minutes. After the removal of the solvent 23 mg (90%) brownish product was obtained which was non-soluble in THF, DCM, chloroform, toluene, methanol, ethanol or 2-propanol.

5.5. Copolymerization of crown ether 7 and norborneneylmethyl-perfluoro-*tert*-butyl ether (10)



CP-7-10 (1/1 equivalent, G2)

In a glovebox a vial was charged with DCM (9.7 mL), crown ether **7** (55.0 mg, 0.131 mmol) and norbornene **10** (44.9 mg, 0.131 mmol, 1 equivalent of **7**). DCM (0.3 mL) solution of **G2** catalyst (4.6 mg, 0.0052 mmol (2 mol% / norbornene monomers)) was added. The mixture was stirred for 2 hours at 30 °C. The vial was removed from the glovebox, ethyl vinyl ether (0.1 mL) was added, and the solution was stirred for 30 minutes. After the removal of the solvent 95.9 mg (96%) brownish product was obtained.

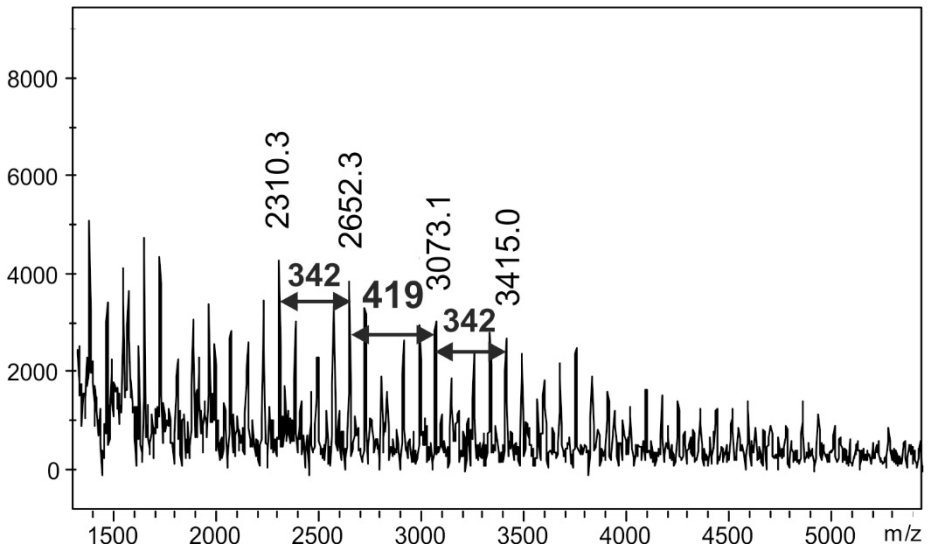


Figure S35. MALDI-TOF MS spectrum of **cp-7-10** (1/5 equivalent, **G2**) copolymer, **7** (m/z: 419), **10** (m/z: 342) (**7**/**10** = 1/5) (Linear mode, DHB/NaTFA)

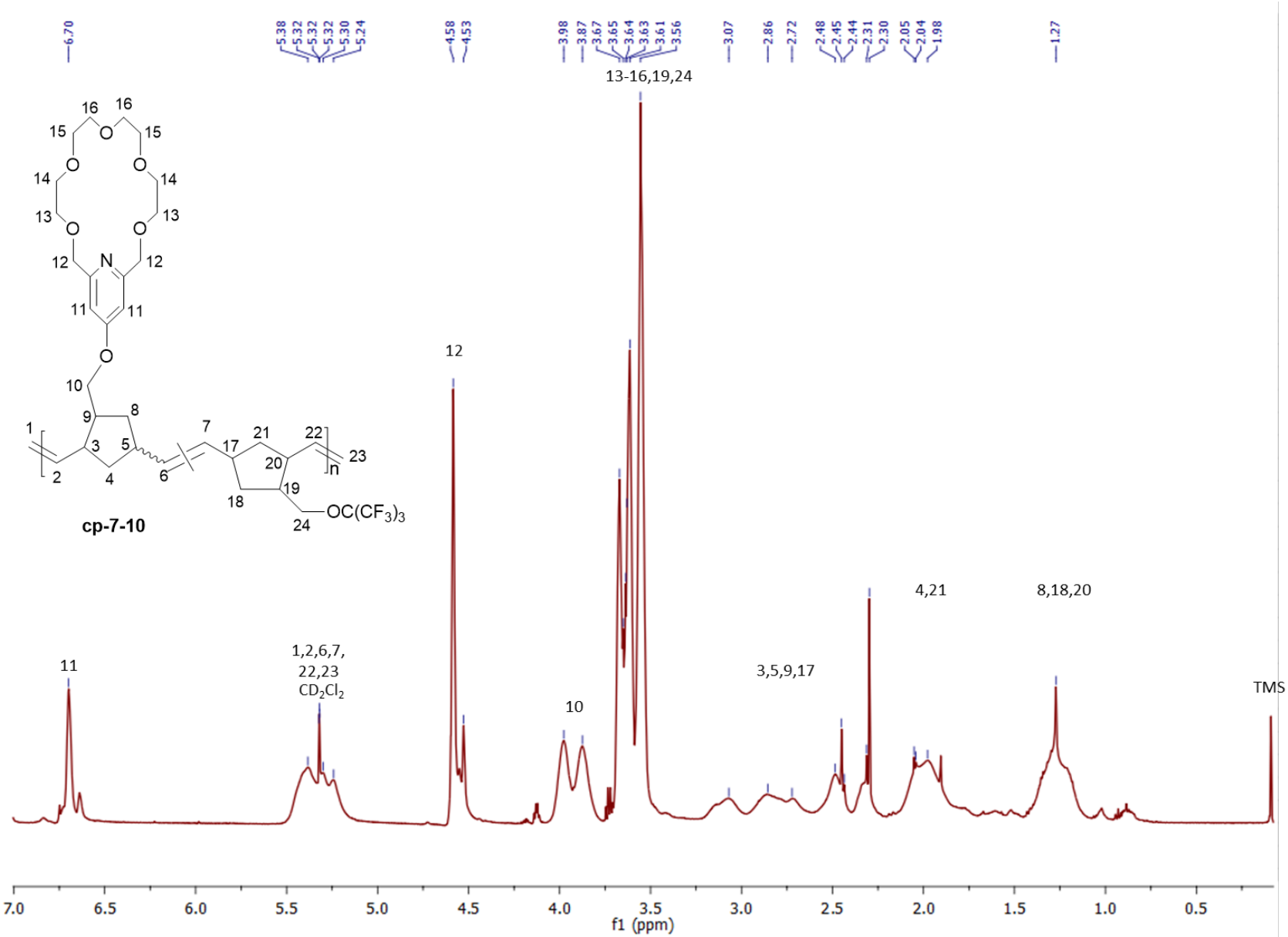


Figure S36. ^{1}H NMR spectrum of **cp-7-10** (1/1 equivalent, **G2**) (CD_2Cl_2).

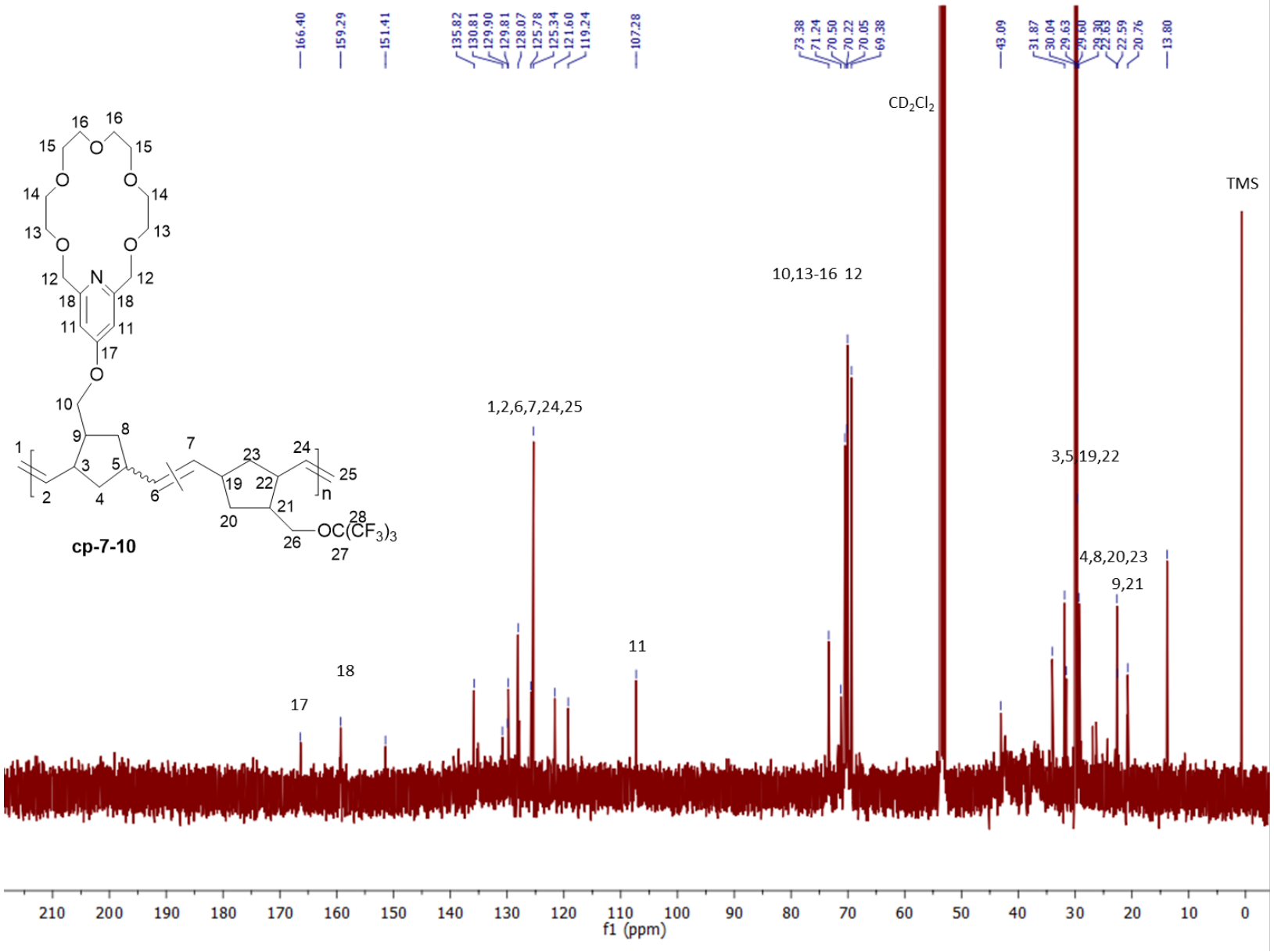


Figure S37. $^{13}C\{^{1}H\}$ NMR spectrum of **cp-7-10** (1/1 equivalent, **G2**) (CD_2Cl_2).

CP-7-10 (1/5 equivalent, G2)

In a glovebox a vial was charged with DCM (4.7 mL), crown ether **7** (10.0 mg, 0.0238 mmol) and norbornene ether **10** (40.8 mg, 0.1192 mmol, 5 equivalent of **7**). DCM (0.3 mL) solution of **G2** catalyst (2.43 mg, 0.0029 mmol (2 mol% / norbornene monomers)) was added. The mixture was stirred for 2 hours at 30 °C. The vial was removed from the glovebox, ethyl vinyl ether (0.1 mL) was added, and the solution was stirred for 30 minutes. After the removal of the solvent 48.3 mg (95%) brownish product was obtained.

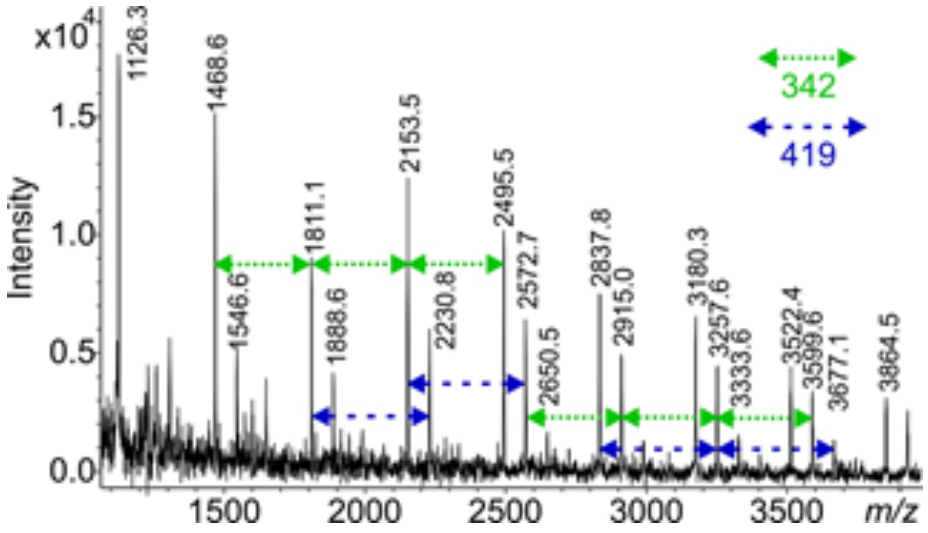
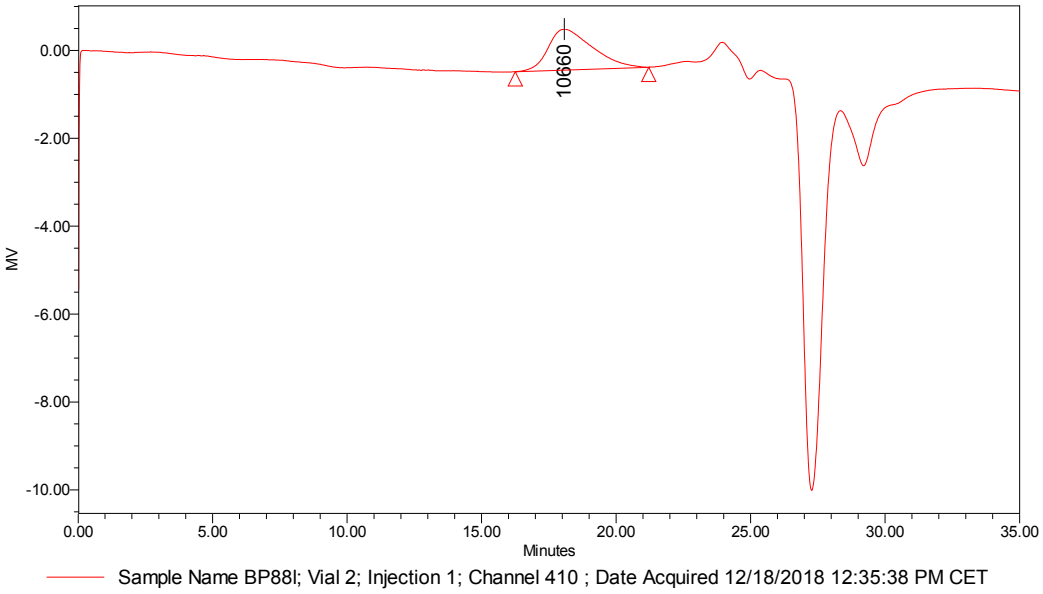


Figure S38. MALDI-TOF MS spectrum of **cp-7-10** (1/5 equivalent, **G2**) copolymer **7** (m/z: 419), **10** (m/z: 342) (**7**/**10** = 1/5) (Linear mode, DHB/NaTFA)

GPC Report



GPC Sample Results

	Sample Name	Inj	RT (min)	Mn	Mw	MP	Poly-dispersity
1	BP88I	1	18.071	6905	9845	10660	1.426

Reported by User: System
Report Method: GPC_reportdisp
Page: 1 of 1

Project Name: 2016THF
Date Printed: 4/3/2019

Figure S39. GPC chromatogram of **cp-7-10** (1/5 equivalent, **G2**) copolymer

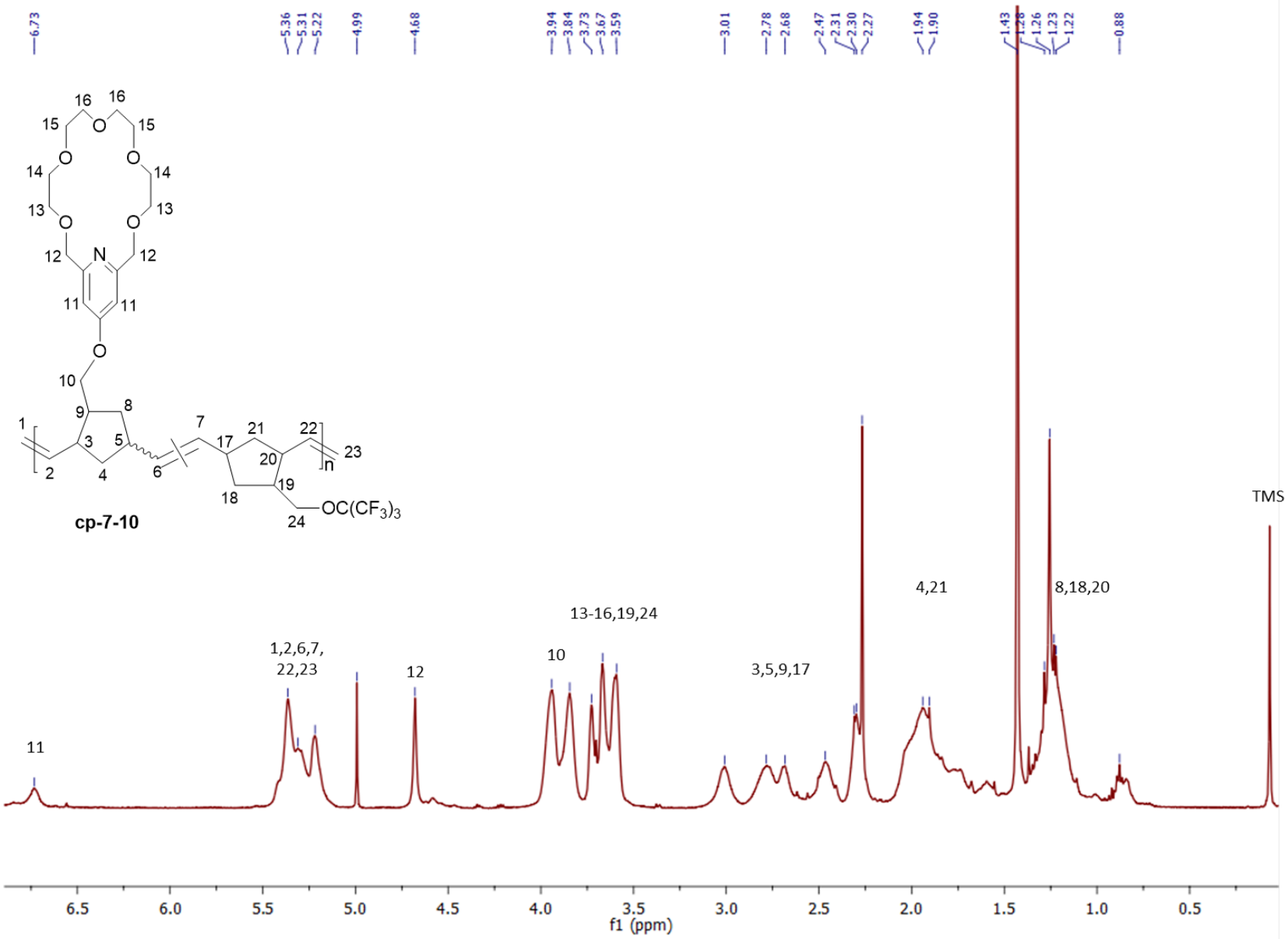


Figure S40. ^{1}H NMR spectrum of **cp-7-10** (1/5 equivalent, **G2**) (CD_2Cl_2).

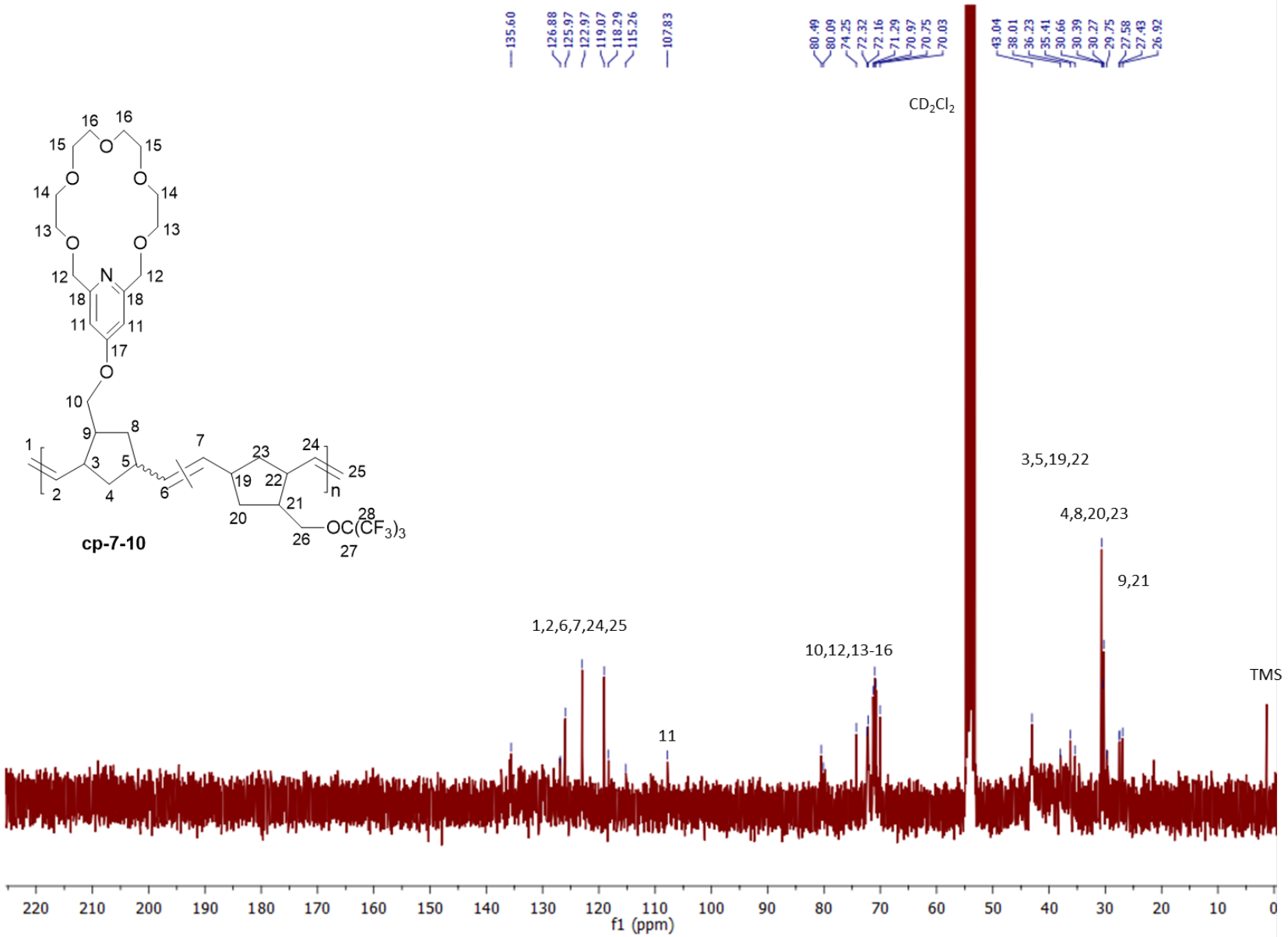


Figure S41. $^{13}C\{^{1}H\}$ NMR spectrum of **cp-7-10** (1/5 equivalent, **G2**) in CD_2Cl_2.

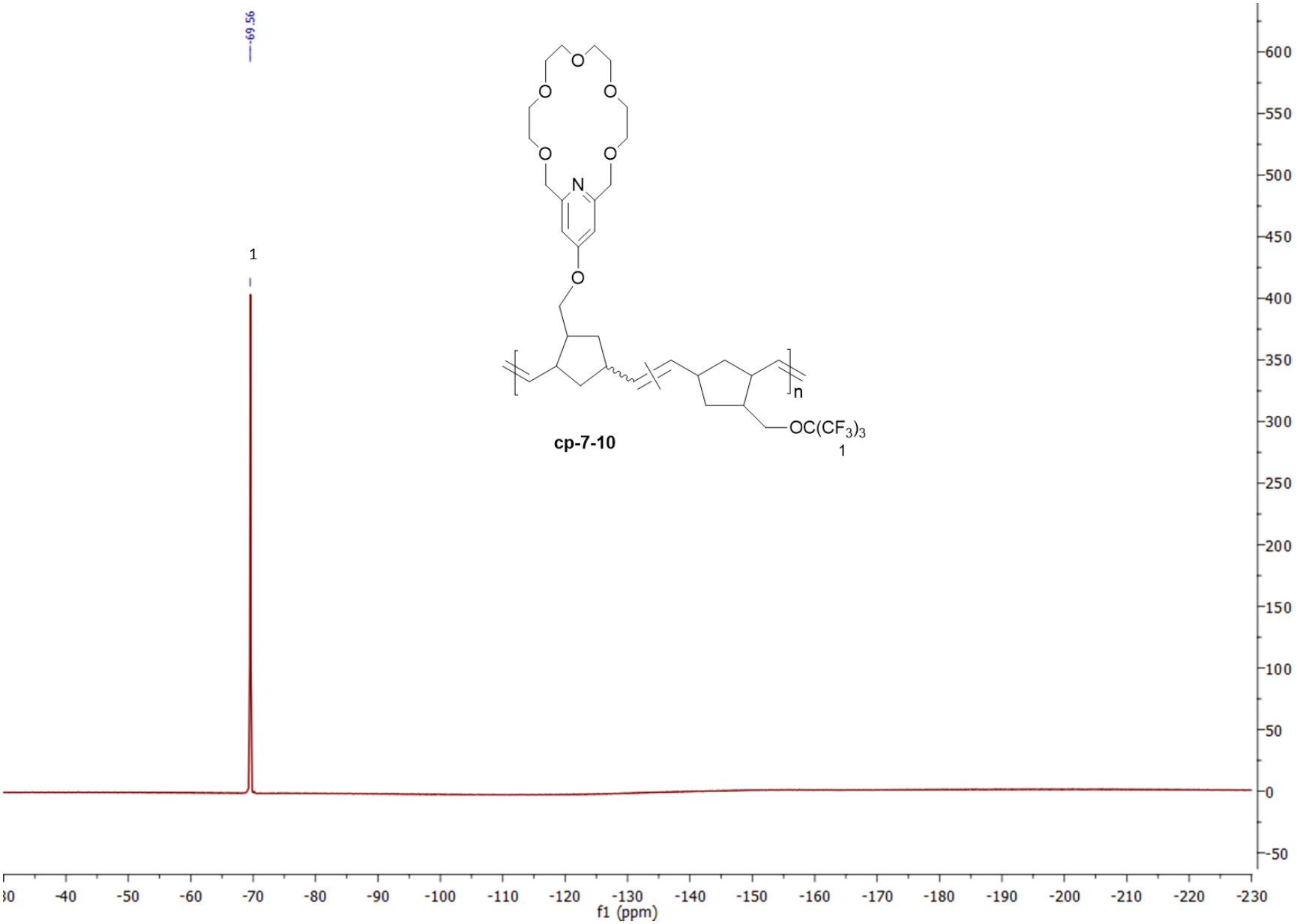
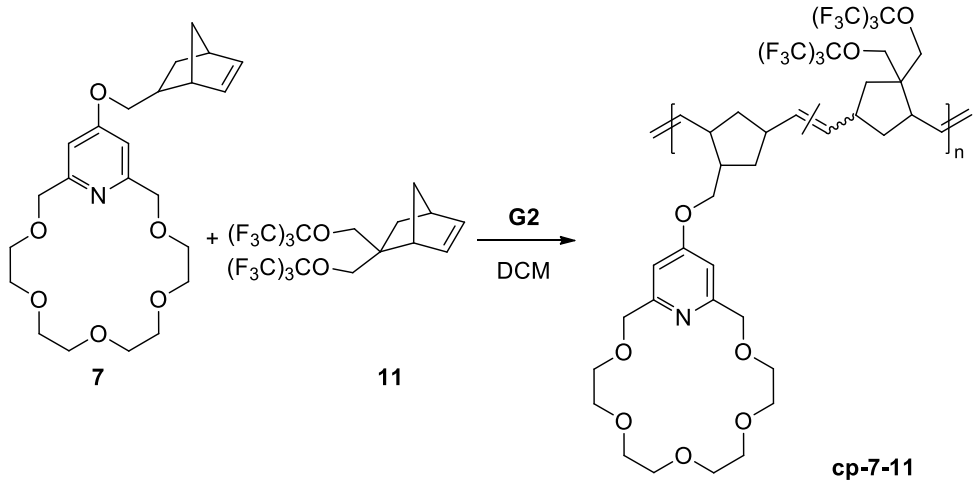


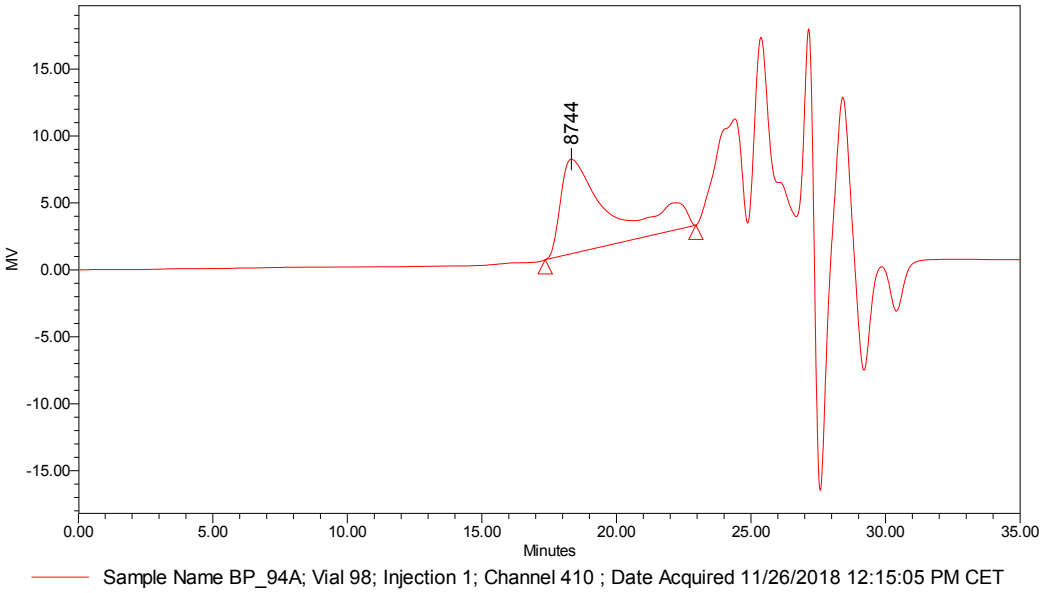
Figure S42. ^{19}F NMR spectrum of **cp-7-10** (1/5 equivalent, **G2**) in CD_2Cl_2.

5.6. Copolymerization of crown ether 7 and bis(perfluoro-*tert*-butyloxymethyl)norbornene (11)



In a glovebox a vial was charged with DCM (4.7 mL), crown ether **7** (6.3 mg, 0.0150 mmol) and norbornene **11** (44.3 mg, 0.0751 mmol, 5 equivalent of **7**). DCM (0.3 mL) solution of **G2** catalyst (1.53 mg, 0.0018 mmol (2 mol% / norbornene monomers)) was added. The mixture was stirred for 2 hours at 30 °C. The vial was removed from the glovebox, ethyl vinyl ether (0.1 mL) was added, and the solution was stirred for 30 minutes. After the removal of the solvent 49 mg (97%) brownish product was obtained.

GPC Report



GPC Sample Results

	Sample Name	Inj	RT (min)	Mn	Mw	MP	Poly-dispersity
1	BP_94A	1	18.324	2592	5589	8744	2.156

Reported by User: System
Report Method: GPC_reportdisp
Page: 1 of 1

Project Name: 2016THF
Date Printed: 4/3/2019

Figure S43. GPC chromatogram of **cp-7-11** (1/5 equivalent, **G2**) copolymer

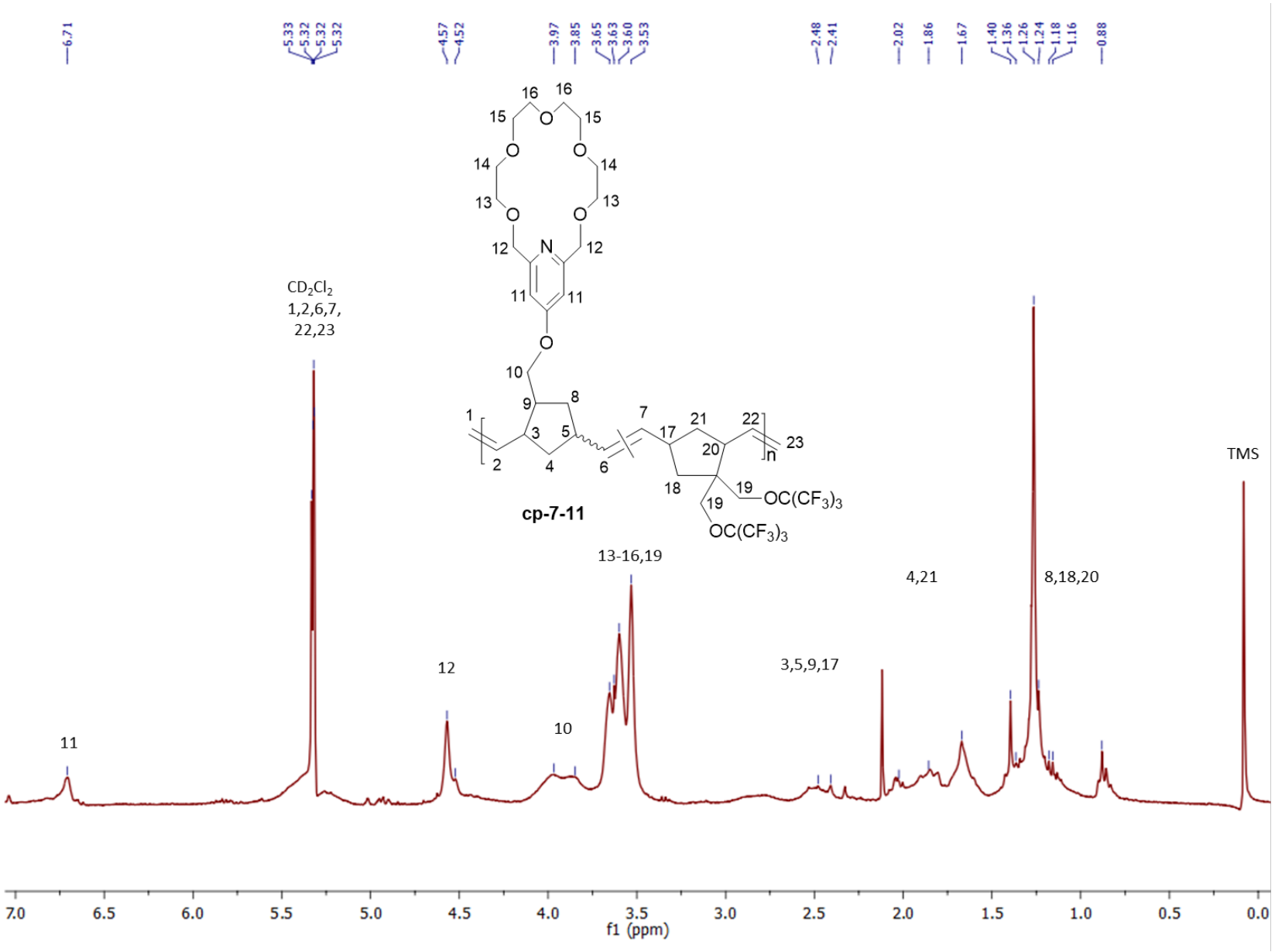


Figure S44. ^{1}H NMR spectrum of **cp-7-11** (1/5 equivalent, **G2**) (CD_2Cl_2).

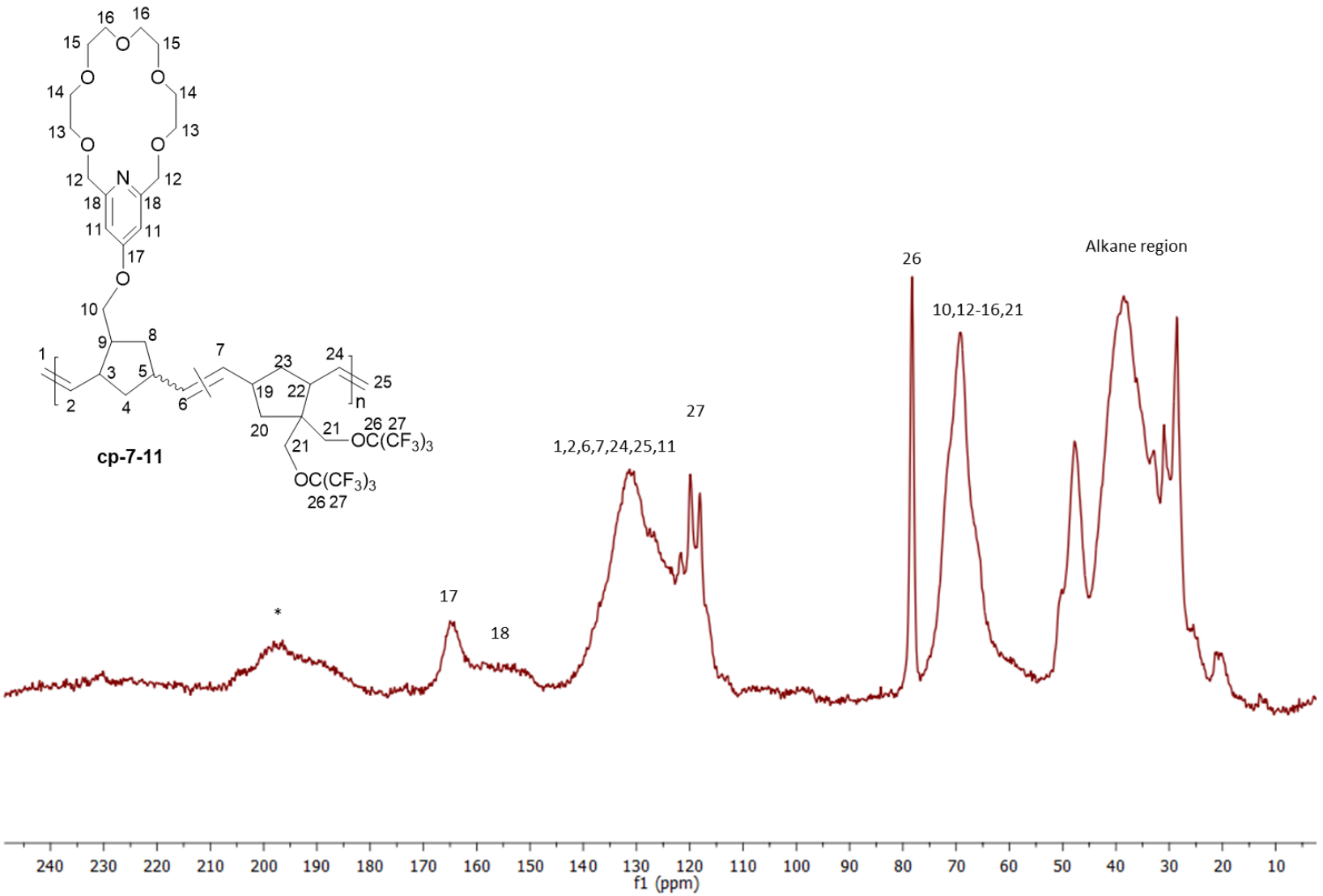


Figure S45. Solid state ^{13}C NMR spectrum of **cp-7-11** (1/5 equivalent, **G2**) (* spinning side band)

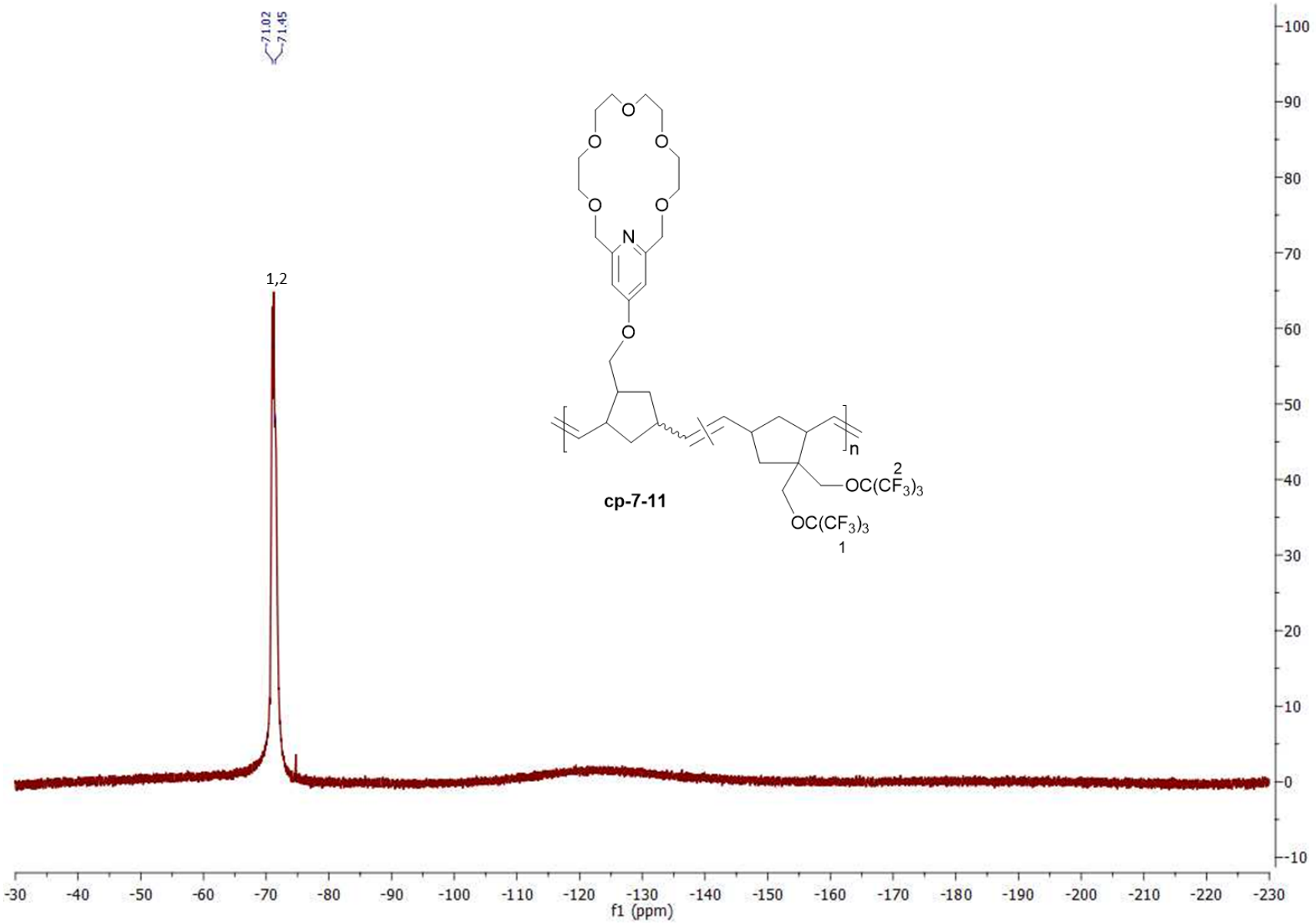


Figure S46. ^{19}F NMR spectrum of **cp-7-11** (1/5 equivalent, **G2**) in CD_2Cl_2.

6. Complexation of biogenic amines with norbornene functionalized pyridino-18-crown-6 ether (7) monomer and its polymers

Crown ether **7** (2.5 mg, 0.00596 mmol) was measured to a vial, dissolved in the mixture of CD_2Cl_2 (0.3 mL) and CD_3OD (0.3 mL) 1 equivalent of dopamine hydrochloride (**12**, 1.30 mg, 0.00596 mmol) or L-alanine-L-Lysine hydrochloride (**13**, 1.51 mg, 0.00596 mmol) was added to a sample. The mixture was placed into an NMR tube, ^1H NMR measurements were carried out.

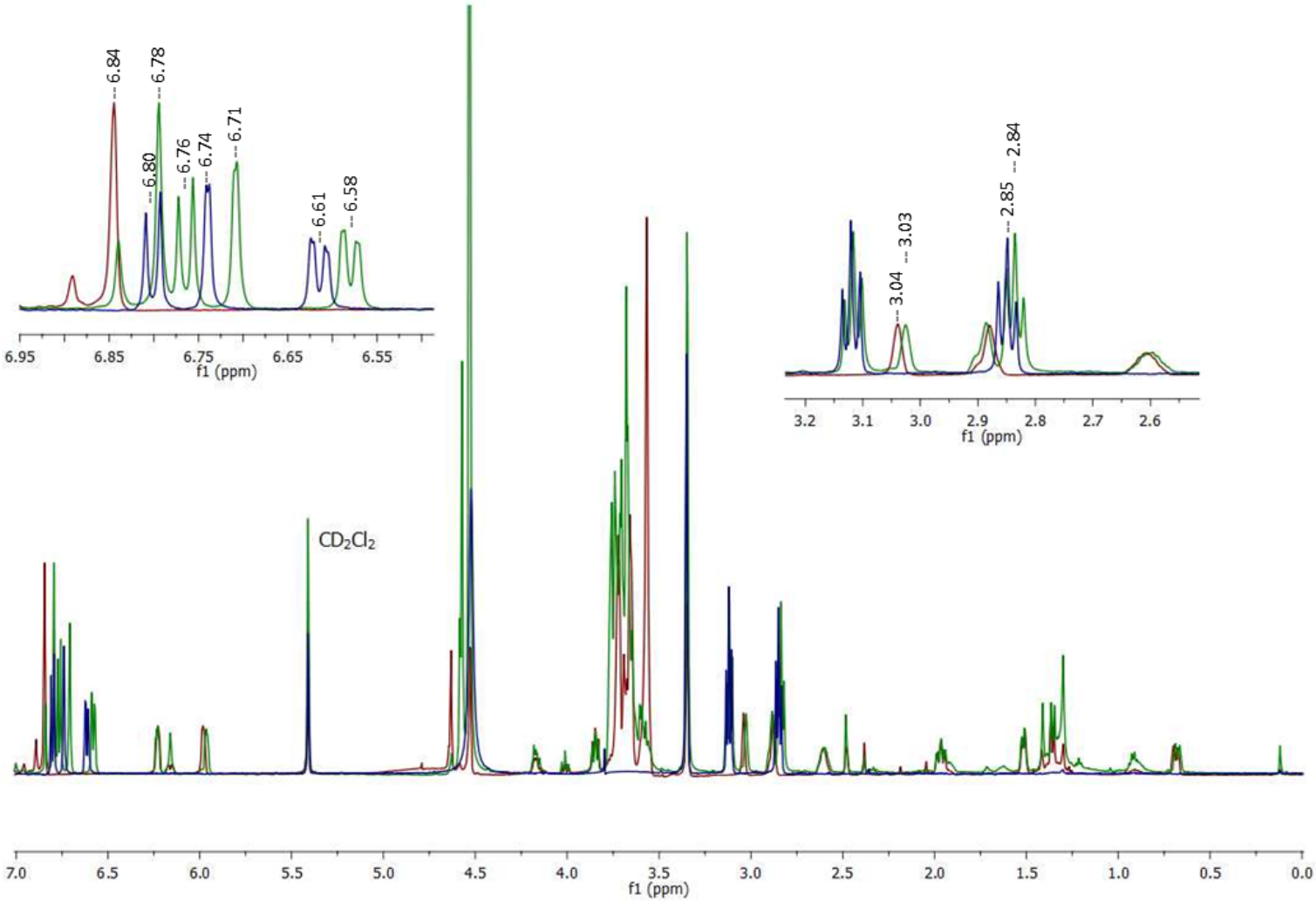


Figure S47. Superimposed ^{1}H NMR spectra of **7** (marine), **12** (blue) and the complex of **7** and **12** (green) (1/1 mixture of CD_3OD and CD_2Cl_2, [**7**] = [**12**] = 0.01 mmol/mL).

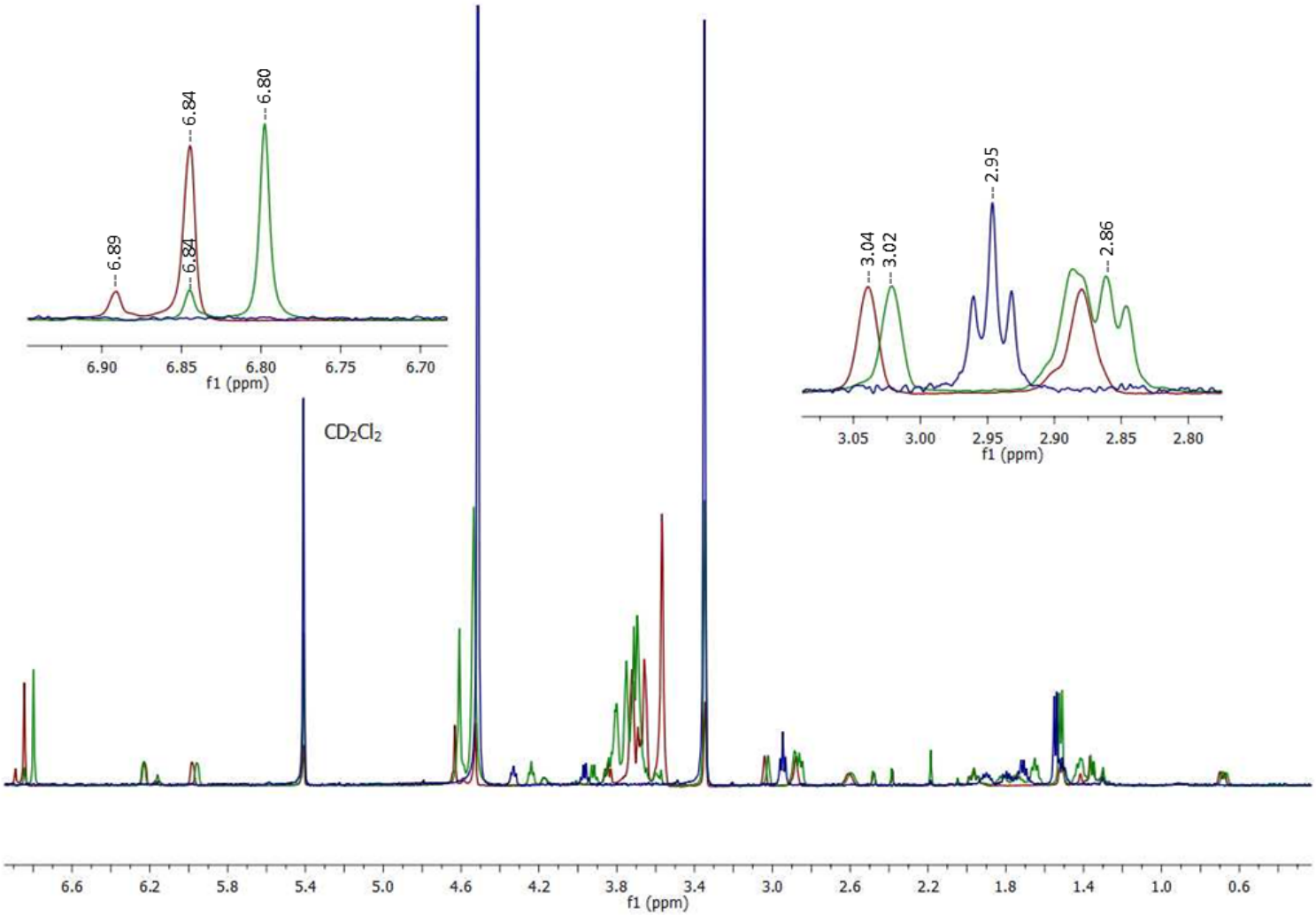


Figure S48. Superimposed ^{1}H NMR spectra of **7** (marine), **13** (blue) and the complex of **7** and **13** (green) (1/1 mixture of CD_3OD and CD_2Cl_2, [**7**] = [**13**] = 0.01 mmol/mL).

6.1. ^{1}H NMR investigation of poly-7 and cp-7-10 with dopamine hydrochloride (12) and 13

Polymer [**poly-7** or **cp-7-10**, 0.00596 mmol)] was measured to a vial, dissolved in the mixture of CD_2Cl_2 (0.3 mL) and CD_3OD (0.3 mL) 1 equivalent [per crown ether unit (**7**)] of **12** or **13** (0.00596 mmol) was added to a sample. The mixture was placed into an NMR tube, ^{1}H NMR measurements were carried out.

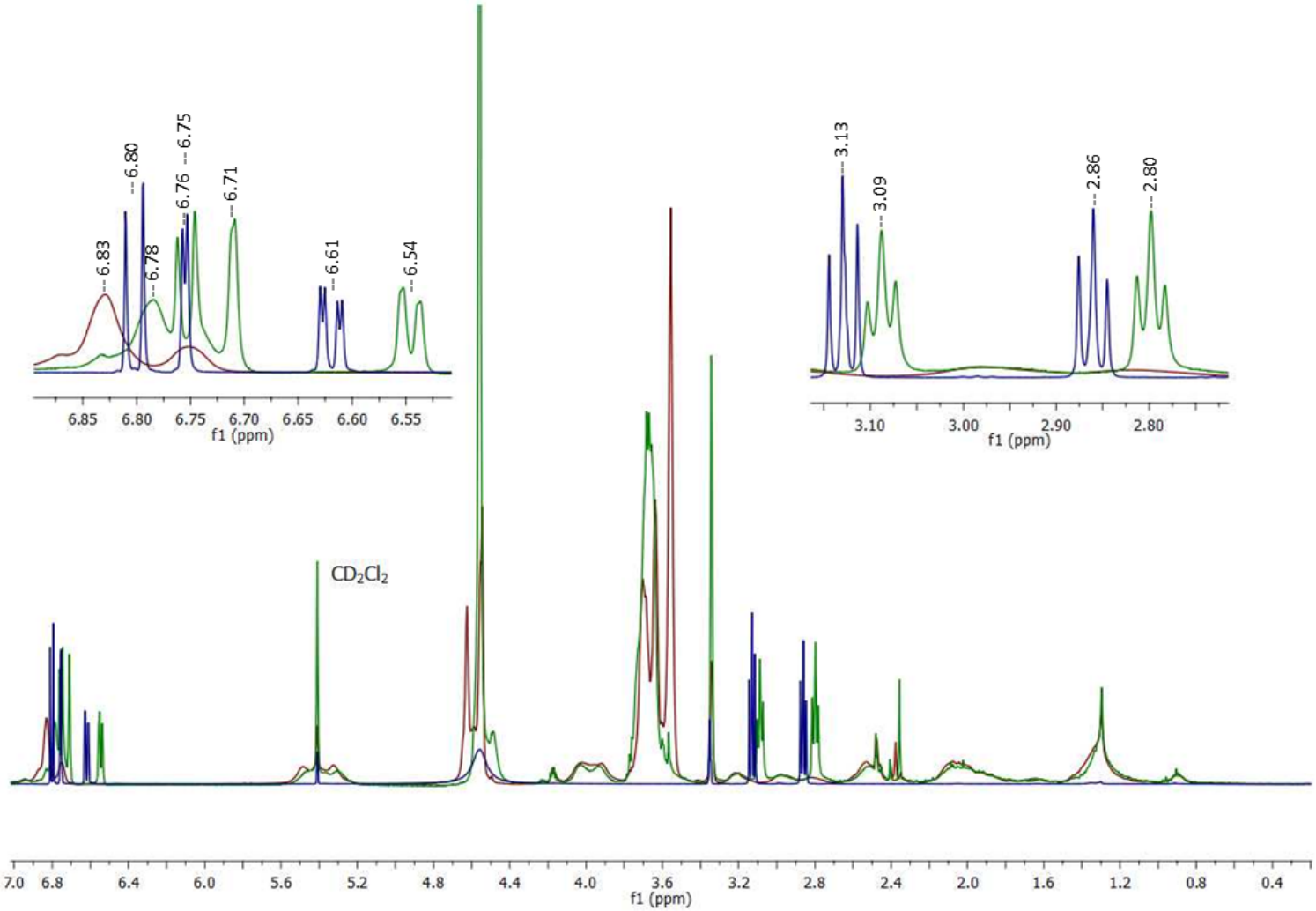


Figure S49. Superimposed ^{1}H NMR spectra of **poly-7** (marine), **12** (blue) and the complex of **poly-7** and **12** (green) (1/1 mixture of CD_3OD and CD_2Cl_2, [**poly-7**] = [**12**] = 0.01 mmol/mL).

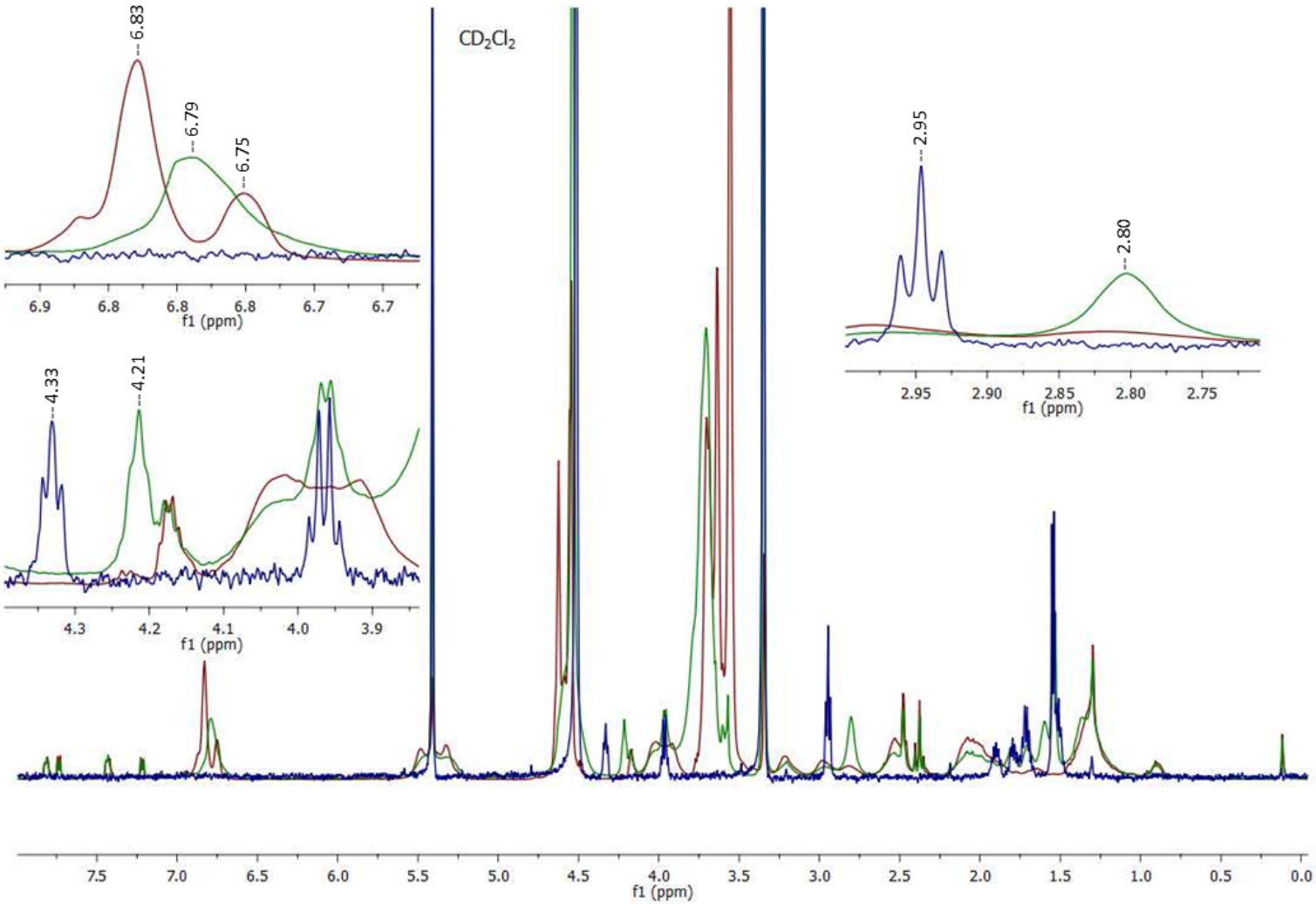


Figure S50. Superimposed ^{1}H NMR spectra of **poly-7** (marine), L-alanine-L-lysine hydrochloride (**13**) (blue) and their complex (green) (1/1 mixture of CD_3OD and CD_2Cl_2, [**poly-7**] = [**13**] = 0.01 mmol/mL).

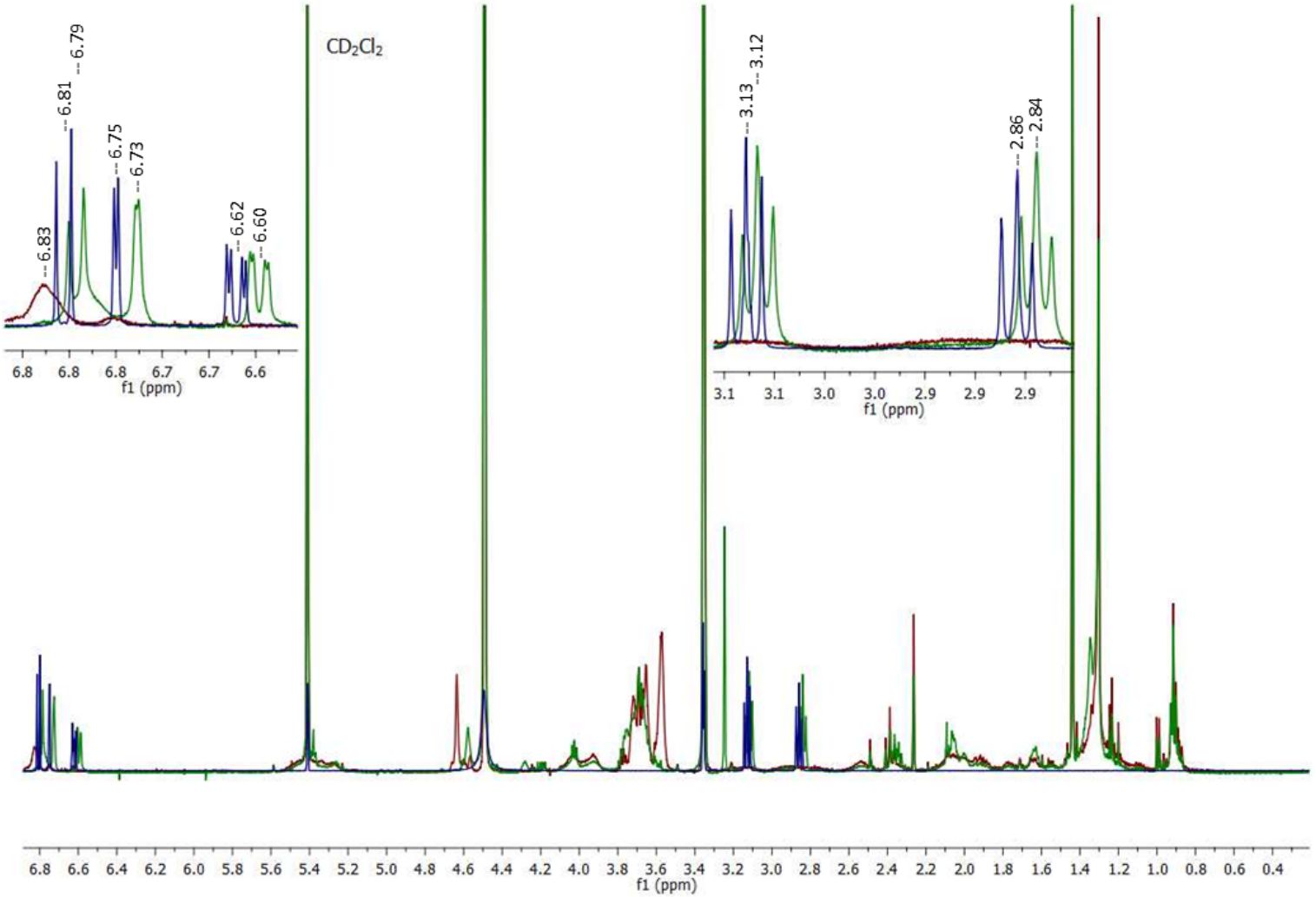


Figure S51. Superimposed ^{1}H NMR spectra of **cp-7-10** (marine), **12** (blue) and their complex (green) (1/1 mixture of CD_3OD and CD_2Cl_2, [**cp-7-10**] = [**12**] = 0.01 mmol/mL).

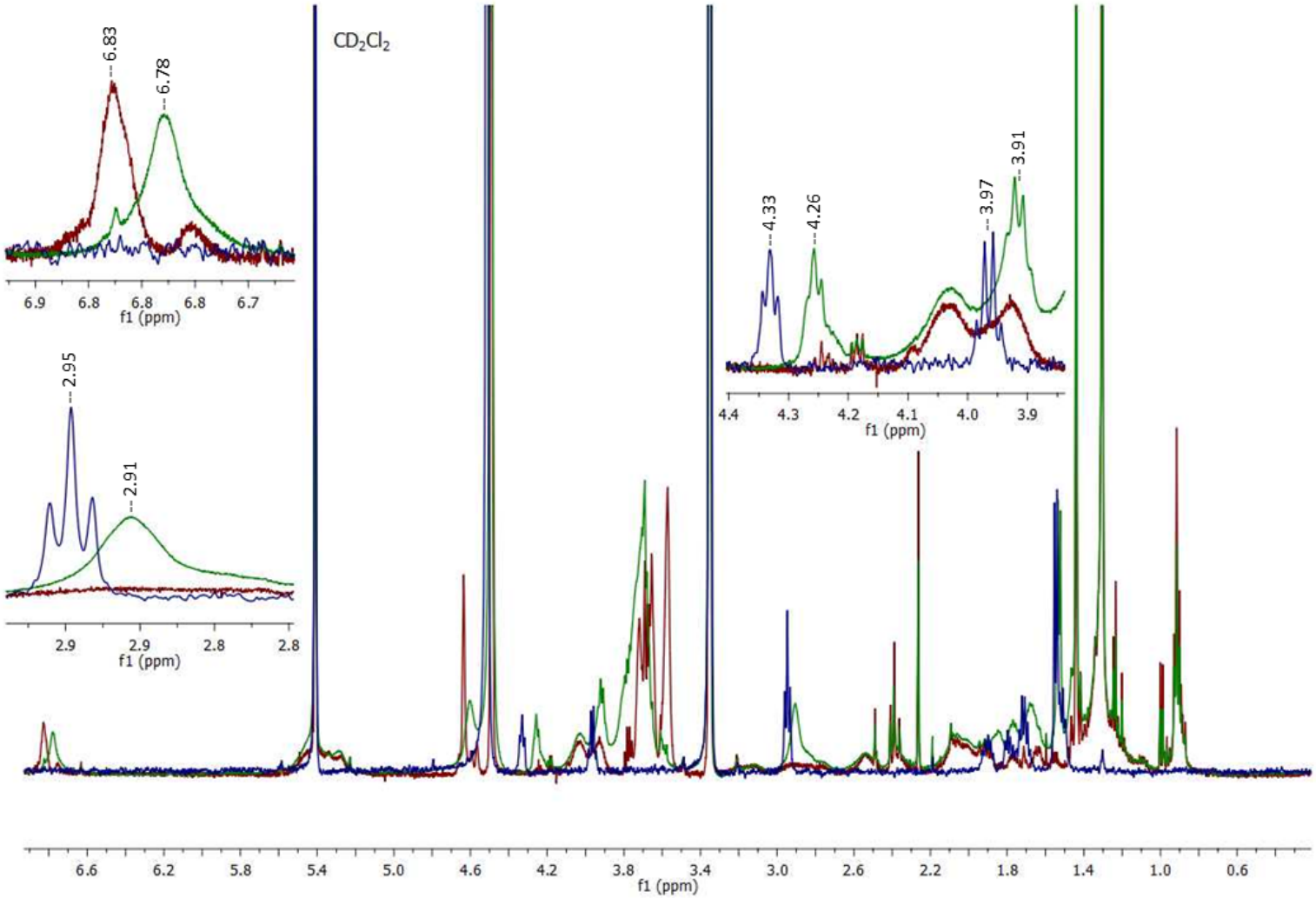


Figure S52. Superimposed ^{1}H NMR spectra of **cp-7-10** (marine), L-alanine-L-lysine hydrochloride (**13**, blue) and their complex (green) (1/1 mixture of CD_3OD and CD_2Cl_2, [**cp-7-10**] = [**13**] = 0.01 mmol/mL).

7. Optimized geometries

Structure: 7 : norbornene functionalized pyridino crown-ether

CHARGE:0 SPIN MULTIPLICITY: 1

O	-0.353636	2.803941	1.411326
O	0.497597	4.193889	-1.047018
O	0.212976	-0.090425	1.873508
O	2.427706	-2.107811	1.212509
O	4.198749	-1.940102	-1.146526
C	-0.231169	4.756928	0.032149
H	0.459148	5.216577	0.760924
H	-0.856850	5.551701	-0.398265
C	-1.132678	3.767901	0.730473
H	-1.793491	3.271934	-0.006978
H	-1.777090	4.313891	1.446110
C	-1.180227	1.867895	2.073877
H	-1.810031	2.388969	2.818953
H	-1.854070	1.369212	1.350642
C	-0.350555	0.835215	2.789870
H	-1.013520	0.301072	3.494689
H	0.445265	1.328275	3.378289
C	0.610942	-1.271890	2.551671
H	1.416657	-1.052384	3.276376
H	-0.252339	-1.674363	3.112577
C	1.079508	-2.326678	1.581665
H	0.429982	-2.330397	0.683920
H	0.988730	-3.312174	2.073606
C	2.947012	-3.224508	0.515863
H	3.066799	-4.082054	1.205496
H	2.253044	-3.534664	-0.287802
C	4.287708	-2.874207	-0.081904
H	4.729673	-3.787095	-0.506001
H	4.963991	-2.494272	0.703842
C	1.687097	3.517558	-0.696128
H	2.508252	3.915694	-1.314609
H	1.952366	3.699712	0.358393
C	4.149678	-0.581392	-0.766415
H	4.443287	-0.454422	0.289244
H	4.880232	-0.026885	-1.377964
C	2.798415	0.062921	-0.966109
C	1.621637	2.024644	-0.922541
C	1.676507	-0.667371	-1.325469
C	0.457541	0.007747	-1.445222
H	1.722900	-1.744135	-1.478685
C	0.428050	1.392628	-1.269461
H	-0.478762	1.981335	-1.381780
N	2.785110	1.389574	-0.763519
O	-0.628077	-0.749993	-1.712322
C	-1.909416	-0.113815	-1.669510
H	-2.017483	0.562784	-2.533897
H	-1.986831	0.483704	-0.746058
C	-2.962739	-1.199816	-1.685007
C	-2.812991	-2.249039	-0.531029
C	-4.392705	-0.638638	-1.454859
H	-2.906854	-1.732634	-2.645930
C	-4.244349	-2.814756	-0.503873
H	-1.991355	-2.957821	-0.681452
C	-4.891047	-1.447361	-0.216461
H	-4.392928	0.444565	-1.260112
H	-5.038734	-0.826223	-2.323491
H	-4.399205	-3.541011	0.305896
H	-4.556900	-3.245428	-1.467165
H	-5.976312	-1.420605	-0.068199
C	-2.800300	-1.461319	0.767105
H	-1.903168	-1.210685	1.336511
C	-4.040224	-0.983113	0.953271
H	-4.366845	-0.282385	1.724002

Structure: 7-12 : pyridino crown-ether+ dopaminium ion complex (PERPENDICULAR)

CHARGE:1 SPIN MULTIPLICITY: 1

O	2.880019	-1.743333	2.637091	H	-8.358099	2.648387	0.986952
O	0.215567	-0.852351	2.279989	H	-9.804314	-0.103884	-1.272109
O	4.016190	-3.121148	0.417547	H	-9.277421	1.621741	-1.250241
O	2.970992	-2.720405	-2.186090	H	-10.091608	0.842345	1.206955
O	0.352195	-1.644134	-2.366053	C	-7.674625	-1.036484	0.022680
C	0.898868	-0.745850	3.519329	H	-7.002203	-1.893759	-0.036359
H	1.414331	0.230216	3.585436	C	-8.569200	-0.773904	0.986853
H	0.182335	-0.813193	4.357144	H	-8.776789	-1.372479	1.875363
C	1.888299	-1.873818	3.644603	C	3.246923	2.244679	0.210967
H	1.373769	-2.845738	3.540347	C	2.652255	3.219593	-0.591716
H	2.356626	-1.829958	4.643004	C	4.590035	2.400803	0.581028
C	3.906309	-2.719134	2.753524	C	3.379749	4.335425	-1.015825
H	4.515811	-2.516611	3.650759	H	1.606943	3.113664	-0.889726
H	3.459902	-3.724697	2.849026	C	5.320111	3.507232	0.163163
C	4.774408	-2.666572	1.523604	H	5.089123	1.658469	1.208580
H	5.655129	-3.315058	1.678577	C	4.709992	4.483338	-0.643473
H	5.132359	-1.633824	1.349319	H	2.916211	5.103413	-1.639134
C	4.795896	-3.247707	-0.757611	O	5.503808	5.534673	-1.002619
H	5.243612	-2.273979	-1.030935	H	5.002554	6.144223	-1.567962
H	5.614302	-3.972665	-0.599137	O	6.621869	3.639211	0.541232
C	3.908884	-3.738223	-1.871987	H	6.969137	4.461278	0.155718
H	3.381228	-4.656614	-1.557614				
H	4.523257	-3.971693	-2.758751				
C	2.042296	-3.114041	-3.183689				
H	2.577309	-3.419017	-4.099770				
H	1.440214	-3.969097	-2.827111				
C	1.151226	-1.942454	-3.499711				
H	0.510403	-2.197103	-4.362387				
H	1.766180	-1.064842	-3.772628				
C	-0.826747	0.095013	2.198041				
H	-1.566715	-0.074553	2.999437				
H	-0.422177	1.117266	2.334854				
C	-0.491370	-0.538325	-2.618126				
H	0.120029	0.360931	-2.829117				
H	-1.123322	-0.727331	-3.502830				
C	-1.365716	-0.261472	-1.421213				
C	-1.514343	0.031040	0.855832				
C	-2.700972	0.057973	-1.599204				
C	-3.473869	0.386459	-0.475781				
H	-3.160128	0.056102	-2.587789				
C	-2.867793	0.366890	0.781871				
H	-3.415194	0.598888	1.693821				
N	1.883540	-1.296051	-0.001334				
H	0.866822	-1.045237	-0.019016				
H	2.073708	-2.052723	-0.674432				
H	2.147746	-1.607334	0.947711				
N	-0.772437	-0.276562	-0.212077				
O	-4.761901	0.689172	-0.700523				
C	-5.586072	1.027894	0.423852				
H	-5.158732	1.904035	0.938668				
H	-5.608409	0.179985	1.128434				
C	2.678237	-0.113665	-0.384413				
H	3.734305	-0.416190	-0.441340				
H	2.351262	0.194175	-1.388902				
C	2.481962	1.013450	0.625000				
H	1.407570	1.243684	0.695536				
H	2.820482	0.664187	1.612308				
C	-6.968128	1.335256	-0.105908				
C	-7.641238	0.167133	-0.902477				
C	-7.990988	1.613735	1.028862				
H	-6.892359	2.205609	-0.774690				
C	-9.110970	0.620882	-0.823888				
H	-7.212666	0.006445	-1.897677				
C	-9.140887	0.606869	0.716058				
H	-7.565349	1.445266	2.029519				

Structure: 7-12 : pyridino crown-ether+dopaminium ion complex (FOLDED)

CHARGE:1 SPIN MULTIPLICITY: 1

O	3.917992	-2.452020	-1.068781	H	-7.129537	-1.347775	1.010030
O	1.099674	-1.967779	-0.830081	H	-8.740478	1.742755	-0.610565
O	5.707690	-0.260967	-0.935071	H	-8.120641	1.085423	0.951416
O	4.825848	2.254182	0.026919	H	-8.957576	-0.916741	-0.660534
O	2.084414	2.770964	-0.244721	C	-6.654965	0.954952	-2.063390
C	1.673803	-3.229388	-1.142093	H	-6.030351	1.351624	-2.865258
H	1.856464	-3.724778	-0.176668	C	-7.526330	-0.061478	-2.143165
H	0.960700	-3.838164	-1.722776	H	-7.759082	-0.663698	-3.022961
C	2.978029	-3.117046	-1.894562	C	1.006604	-0.475466	2.379247
H	2.850310	-2.567391	-2.845465	C	1.018034	-1.869985	2.298251
H	3.332322	-4.135545	-2.138140	C	-0.229989	0.184961	2.393247
C	5.218490	-2.475165	-1.628981	C	-0.177169	-2.589662	2.197929
H	5.610426	-3.507702	-1.649615	H	1.962864	-2.417156	2.297857
H	5.194998	-2.091485	-2.665326	C	-1.422428	-0.523734	2.312457
C	6.124958	-1.610760	-0.794973	H	-0.280685	1.273433	2.469726
H	7.164400	-1.720793	-1.149492	C	-1.395480	-1.922048	2.192913
H	6.083513	-1.916556	0.266496	H	-0.170189	-3.679171	2.116427
C	6.561478	0.644789	-0.252518	O	-2.616410	-2.524923	2.077359
H	6.542892	0.444132	0.834228	H	-2.502932	-3.487864	2.029547
H	7.598573	0.521703	-0.610119	O	-2.610626	0.142033	2.340099
C	6.106149	2.049887	-0.542039	H	-3.328210	-0.514209	2.364716
H	6.064355	2.208753	-1.635216				
H	6.835105	2.762605	-0.116420				
C	4.328143	3.548229	-0.258554				
H	5.003330	4.321411	0.150073				
H	4.256013	3.692739	-1.352023				
C	2.967127	3.701870	0.364907				
H	2.609465	4.732029	0.196660				
H	3.012824	3.520259	1.454718				
C	0.350971	-1.382586	-1.890204				
H	1.016393	-1.062590	-2.709781				
H	-0.374407	-2.114159	-2.281039				
C	0.738507	3.016862	0.100071				
H	0.631754	3.085152	1.199762				
H	0.407952	3.982990	-0.322131				
C	-0.151337	1.904627	-0.402564				
C	-0.358368	-0.184352	-1.313217				
C	-1.526070	2.012814	-0.211145				
C	-2.336872	0.933635	-0.562558				
H	-1.968874	2.896969	0.250134				
C	-1.737187	-0.200317	-1.128665				
H	-2.312675	-1.077908	-1.417888				
N	3.050120	0.024013	0.142845				
H	2.666065	0.964696	-0.061533				
H	3.897052	-0.110778	-0.436909				
H	2.344116	-0.676617	-0.145444				
N	0.432335	0.838737	-0.958490				
O	-3.654509	1.048943	-0.314708				
C	-4.453346	-0.137209	-0.405555				
H	-3.976958	-0.938721	0.184294				
H	-4.516277	-0.463447	-1.457107				
C	3.415458	-0.107906	1.572617				
H	3.703120	-1.153778	1.742960				
H	4.293241	0.528021	1.736666				
C	2.280853	0.337147	2.482891				
H	2.664437	0.303769	3.515269				
H	2.051082	1.393647	2.266243				
C	-5.821316	0.197380	0.143314				
C	-6.563065	1.357722	-0.602146				
C	-6.819241	-0.985589	0.020219				
H	-5.700930	0.490397	1.197555				
C	-8.005461	1.073333	-0.143029				
H	-6.150370	2.350930	-0.394494				
C	-8.024537	-0.347642	-0.737330				
H	-6.396041	-1.836365	-0.534737				

Structure: 7-13 : pyridino crown-ether+diamid.H^+ ion complex (Lysine coord.)

CHARGE:1 SPIN MULTIPLICITY: 1

O	-3.260590	-2.971564	-2.085666	C	7.915530	-2.491163	0.456424
O	-0.770723	-1.485256	-2.177647	H	8.070167	-3.507155	0.089409
O	-4.705883	-3.036762	0.365402	N	1.023568	2.403497	-1.240025
O	-4.056257	-1.176180	2.425803	C	-0.388592	2.564238	-1.681562
O	-1.323451	-0.439898	2.452535	C	-0.595173	4.074428	-1.813131
C	-1.359525	-2.179583	-3.270811	O	0.074999	4.656686	-2.670385
H	-2.044555	-1.466557	-3.753161	H	1.652405	2.950613	-1.845450
H	-0.585950	-2.472873	-4.000027	H	-0.999801	2.117425	-0.895995
C	-2.143808	-3.402499	-2.848644	C	-0.598084	1.872780	-3.016698
H	-1.524021	-4.099949	-2.256426	H	0.077935	2.295467	-3.772828
H	-2.488522	-3.934290	-3.753334	H	-1.633703	2.021889	-3.353069
C	-4.129502	-4.031658	-1.715430	H	-0.414991	0.793594	-2.910998
H	-4.553162	-4.503898	-2.618491	H	1.071538	2.760182	-0.263226
H	-3.574761	-4.797828	-1.144402	H	1.322096	1.419314	-1.274402
C	-5.243369	-3.464868	-0.873293	N	-1.492095	4.725397	-1.054896
H	-6.009299	-4.244091	-0.710197	C	-2.150691	4.369438	0.202727
H	-5.718915	-2.617840	-1.401627	C	-1.257403	3.628699	1.230911
C	-5.677878	-2.422253	1.192924	O	-0.028964	3.484460	0.983288
H	-6.026221	-1.474722	0.740447	C	-3.552298	3.765677	0.023475
H	-6.551865	-3.086294	1.317215	C	-3.636111	2.419441	-0.690104
C	-5.069896	-2.164104	2.547212	C	-3.158079	1.215358	0.120910
H	-4.635691	-3.099315	2.943246	C	-3.186176	-0.043167	-0.727984
H	-5.852047	-1.816611	3.243961	H	-2.313944	5.340999	0.693788
C	-3.314964	-1.013356	3.626778	H	-4.148273	4.499560	-0.540121
H	-3.985812	-0.691339	4.442065	H	-3.999679	3.688132	1.024935
H	-2.853806	-1.976123	3.911263	H	-3.084289	2.473907	-1.645176
C	-2.243744	0.027003	3.427696	H	-4.686733	2.243679	-0.972684
H	-1.730749	0.180695	4.393987	H	-3.799448	1.080140	1.006769
H	-2.674964	0.992932	3.111131	H	-2.134230	1.354973	0.507758
C	0.478266	-2.020654	-1.789013	H	-2.619101	0.100116	-1.659600
H	0.361197	-3.055886	-1.417885	H	-4.216589	-0.322726	-0.992942
H	1.169408	-2.047013	-2.648004	H	-1.528690	5.715416	-1.292680
C	-0.151047	0.348364	2.431266	O	-1.843207	3.279487	2.277829
H	-0.396982	1.414494	2.277303				
H	0.378114	0.269873	3.398288				
C	0.775088	-0.113343	1.334169				
C	1.074381	-1.186549	-0.681232				
C	2.133485	0.159411	1.441423				
C	2.992737	-0.260478	0.420739				
H	2.538676	0.679714	2.309946				
C	2.448894	-0.951609	-0.671067				
H	3.063267	-1.312714	-1.493932				
N	-2.574844	-1.183570	-0.017360				
H	-1.549866	-1.026797	0.140398				
H	-3.034303	-1.324346	0.897451				
H	-2.702640	-2.031377	-0.590594				
N	0.244988	-0.765223	0.285180				
O	4.294408	0.027860	0.567057				
C	5.207661	-0.418379	-0.446087				
H	4.934062	0.039264	-1.411093				
H	5.138193	-1.514474	-0.541473				
C	6.595270	0.005259	-0.021786				
C	7.056740	-0.554289	1.366150				
C	7.695044	-0.515090	-0.986917				
H	6.618079	1.104152	0.027595				
C	8.578951	-0.371044	1.219904				
H	6.567866	-0.074269	2.220804				
C	8.671037	-1.266701	-0.029800				
H	7.292418	-1.184096	-1.762338				
H	8.207333	0.316462	-1.489972				
H	9.139227	-0.771442	2.075845				
H	8.871997	0.671965	1.026452				
H	9.665729	-1.447094	-0.452076				
C	6.953021	-2.067320	1.288786				
H	6.161360	-2.667138	1.740493				

Structure: 7-13 : pyridino crown-ether+diamid.H^+ ion complex (N-terminal coord.)

CHARGE:1 SPIN MULTIPLICITY: 1

O	-2.286429	0.793901	2.355799	H	-7.158262	-2.791693	0.145484
O	0.249140	-0.296784	1.830402	H	-8.794076	-3.208874	0.314062
O	-2.841497	3.349081	1.419073	H	-8.347686	-2.288072	-0.978267
O	-1.282102	4.467540	-0.680750	C	-2.054182	1.267674	-0.923698
O	1.125126	3.160140	-1.247284	C	-2.393050	-0.194347	-0.662826
C	-0.728592	-0.989929	2.590702	H	-2.928961	1.902433	-0.732698
H	-1.350032	-1.612977	1.924436	C	-1.564505	1.437141	-2.354069
H	-0.240854	-1.644420	3.335520	H	-1.296904	2.487071	-2.535268
C	-1.598536	0.002248	3.312206	H	-0.686567	0.796679	-2.525627
H	-0.992646	0.651707	3.969447	H	-2.357906	1.147318	-3.056533
H	-2.325019	-0.550507	3.932624	N	-3.700680	-0.490144	-0.686366
C	-3.295144	1.597132	2.945460	C	-4.226865	-1.831422	-0.487396
H	-4.090774	0.954266	3.360017	C	-4.809917	-1.942351	0.947176
H	-2.863718	2.203914	3.761527	O	-5.966456	-2.442320	1.092459
C	-3.872197	2.497644	1.886050	C	-5.214887	-2.217548	-1.581448
H	-4.698228	3.088024	2.320391	C	-5.425078	-3.737032	-1.651979
H	-4.277442	1.889559	1.054470	C	-6.778745	-4.147925	-2.242422
C	-3.318859	4.369118	0.561742	C	-7.866343	-4.310462	-1.192819
H	-3.810033	3.932592	-0.328496	H	-3.355459	-2.503043	-0.521048
H	-4.059391	4.997693	1.087798	H	-6.162128	-1.682985	-1.405236
C	-2.152616	5.226096	0.146812	H	-4.834214	-1.860220	-2.549968
H	-1.609488	5.572324	1.044318	H	-5.329312	-4.173723	-0.644233
H	-2.519251	6.109610	-0.403763	H	-4.611300	-4.168620	-2.253366
C	-0.095146	5.181576	-0.992870	H	-6.696749	-5.120487	-2.748794
H	-0.344587	6.136406	-1.487354	H	-7.099794	-3.420841	-3.007318
H	0.462897	5.402596	-0.065296	H	-7.598982	-5.102952	-0.481444
C	0.750443	4.350237	-1.919622	H	-8.831466	-4.560951	-1.649579
H	1.647337	4.929113	-2.203460	H	-4.363321	0.279606	-0.740377
H	0.192263	4.110810	-2.843570	O	-4.088927	-1.536953	1.878052
C	1.916991	2.330524	-2.073447	C	1.100331	-1.213684	1.175925
H	1.313754	1.952904	-2.921045	H	1.667349	-1.807184	1.914343
H	2.761669	2.902096	-2.494447	H	0.497748	-1.913220	0.568225
C	2.451294	1.168084	-1.274827	O	-1.490108	-1.021413	-0.523084
C	2.064374	-0.493453	0.266773				
C	3.761896	0.758599	-1.459896				
C	4.234598	-0.346905	-0.740472				
H	4.429677	1.283043	-2.143543				
C	3.367735	-0.980213	0.152554				
H	3.676902	-1.830247	0.758092				
N	-0.993931	1.675959	0.020021				
H	-0.081986	1.180205	-0.164561				
H	-0.843811	2.692342	-0.085592				
H	-1.292314	1.479529	0.992064				
N	1.602372	0.549406	-0.432359				
O	5.510595	-0.704628	-0.955034				
C	6.035842	-1.817362	-0.217956				
H	5.437410	-2.716662	-0.438206				
H	5.969155	-1.604040	0.861866				
C	7.472284	-2.006703	-0.649440				
C	8.396766	-0.763774	-0.419638				
C	8.191416	-3.124955	0.152890				
H	7.478082	-2.242802	-1.724051				
C	9.771223	-1.456532	-0.474679				
H	8.214658	0.058108	-1.120568				
C	9.458499	-2.399579	0.702358				
H	7.568632	-3.525371	0.966964				
H	8.474614	-3.962145	-0.499782				
H	10.602223	-0.769613	-0.263637				
H	9.948454	-1.990136	-1.420744				
H	10.254348	-3.074164	1.036830				
C	8.319183	-0.423004	1.058102				
H	7.747362	0.402964	1.483918				
C	8.952372	-1.398524	1.726162				
H	9.002939	-1.532030	2.808039				
N	-8.055340	-3.074601	-0.385881				

Structure: all-*trans* H-(7-10)$_4$-H

CHARGE:0 SPIN MULTIPLICITY: 1

O	12.7198	-8.7607	2.8417	H	4.6024	-7.3762	2.6514	H	-2.0131	-0.1920	0.1450	C	-17.2341	-1.6371	-2.9826
O	13.6061	-7.7292	-0.1125	C	2.4191	-8.0580	1.3370	C	-5.5179	-0.2029	-3.1597	C	-18.0655	-3.6497	-1.7994
O	11.5256	-9.3217	6.1677	H	2.5145	-7.1952	0.6546	H	-4.8781	-1.0540	-3.4734	C	-17.7981	-2.6228	-4.0255
O	8.9384	-7.6047	5.2653	H	3.2479	-8.7670	1.1447	H	-5.1407	0.7207	-3.6606	H	-18.0174	-0.8567	-2.7901
O	7.2503	-6.5748	2.7227	C	1.0615	-8.7433	1.2404	C	-5.5208	-0.0170	-1.6620	C	-18.6832	-3.5982	-3.2185
C	14.1496	-8.4874	0.9918	H	0.7831	-9.2548	2.1807	C	-4.1639	0.2358	0.2402	H	-17.5515	-4.6101	-1.6229
H	13.8575	-9.5527	0.9126	H	1.0465	-9.4788	0.4060	C	-6.6826	0.1542	-0.9106	H	-18.8536	-3.5981	-1.0285
H	15.2416	-8.3960	0.8004	C	-0.5671	-7.0532	1.9235	C	-6.5459	0.3633	0.4793	H	-16.9876	-3.1603	-4.5487
C	13.7664	-7.8844	2.3360	H	-1.0975	-7.7564	2.5954	H	-7.6677	0.1455	-1.3750	H	-18.3688	-2.1049	-4.8126
H	13.3840	-6.8518	2.2507	H	0.2235	-6.5354	2.4942	C	-5.2781	0.3995	1.0741	H	-19.7122	-3.1696	-3.1431
H	14.6087	-7.8995	3.0547	C	-1.5300	-6.0835	1.2525	H	-5.1472	0.5615	2.1448	C	-15.9781	-0.9477	-3.4300
C	12.0957	-8.2921	4.0646	H	-2.3174	-5.7512	1.9644	N	-4.2680	0.0129	-1.1015	C	-18.7814	-4.9733	-3.8691
H	12.8188	-7.7391	4.6923	H	-2.0046	-6.5114	0.3499	O	-7.7331	0.5280	1.1195	H	-19.4271	-5.6474	-3.2918
H	11.2737	-7.6128	3.7800	C	4.2936	-3.3937	-1.7637	C	-7.7496	0.7584	2.5780	H	-19.2097	-4.9112	-4.8781
C	11.6186	-9.5744	4.7507	H	4.4397	-2.5938	-2.5268	H	-6.8349	1.2926	2.8928	H	-17.8077	-5.4666	-3.9682
H	12.3787	-10.3808	4.6863	H	4.2240	-4.3682	-2.2871	H	-7.7676	-0.2542	3.0227	O	-14.5608	5.1897	-1.4611
H	10.6657	-9.9547	4.3445	C	-0.0766	-4.8777	-0.2795	C	-9.0173	1.5543	2.8777	C	-13.5668	4.5258	-2.3330
C	10.2127	-9.0024	6.6774	H	0.3577	-5.8900	-0.4180	C	-8.9074	3.0872	2.6323	H	-12.5425	4.7370	-1.9926
H	9.4655	-9.7128	6.2753	H	-0.7570	-4.6668	-1.1330	C	-10.2522	1.0585	2.0989	H	-13.7173	4.9177	-3.3544
H	10.3480	-9.1940	7.7648	C	0.9798	-3.8115	-0.1557	C	-10.3338	3.5396	2.2437	C	-13.9870	3.0664	-2.1629
C	9.8338	-7.5522	6.4114	C	3.0889	-3.0953	-0.9004	H	-8.6140	3.5763	3.5938	C	-12.8017	2.1441	-1.7616
H	10.7039	-6.9183	6.1618	C	0.8182	-2.6716	0.6300	C	-11.1113	2.2977	1.7498	C	-14.5531	2.4428	-3.4524
H	9.2967	-7.1034	7.2699	C	1.8558	-1.7151	0.6248	H	-9.9580	0.5068	1.1870	H	-14.7784	3.0222	-1.3660
C	8.3245	-6.3265	4.9424	H	-0.0895	-2.5005	1.2210	H	-10.8301	0.3345	2.6993	C	-13.1859	0.7382	-2.2805
H	8.0797	-5.7765	5.8724	C	3.0083	-1.9157	-0.1462	H	-10.3126	4.3431	1.4878	H	-11.8822	2.4828	-2.3019
H	9.0541	-5.7349	4.3603	H	3.8197	-1.1884	-0.1747	H	-10.8420	3.9806	3.1208	C	-14.3118	0.9196	-3.3305
C	7.0700	-6.6764	4.1542	N	2.1022	-4.0358	-0.9124	H	-12.0803	2.2378	2.3023	H	-15.6192	2.6899	-3.5933
H	6.2650	-5.9253	4.3167	O	1.6193	-0.6447	1.4340	C	-7.9238	3.4568	1.5559	H	-14.0377	2.8359	-4.3490
H	6.6903	-7.6859	4.4044	C	2.4663	0.5566	1.2758	C	-11.3664	2.3547	0.2673	H	-13.5109	0.0790	-1.4551
C	12.2339	-7.9954	-0.4581	H	2.4972	0.8138	0.2023	O	-2.9614	8.0039	2.1109	H	-12.3102	0.2357	-2.7254
H	12.2089	-7.7840	-1.5525	H	3.4780	0.3109	1.6435	C	-3.1653	7.2774	0.8384	H	-13.9674	0.5255	-4.3165
H	11.9869	-9.0645	-0.3050	C	1.7564	1.5951	2.1426	H	-2.2011	7.0035	0.3852	C	-12.5657	2.1367	-0.2784
C	8.1506	-7.5284	2.1257	C	2.4367	2.9979	2.0931	H	-3.7251	7.9504	0.1652	C	-15.5610	0.2030	-2.8937
H	8.4490	-8.3193	2.8431	C	0.2900	1.8186	1.7295	C	-3.9798	6.0802	1.3285	H	-15.4287	-1.4419	-4.2331
H	7.5470	-8.0033	1.3186	C	1.2852	4.0344	2.1576	C	-3.3959	4.7278	0.8339	H	-16.1095	0.6906	-2.0844
C	9.3457	-6.8105	1.5466	H	3.0783	3.1045	3.0017	C	-5.4375	6.1002	0.8292	H	-13.4466	1.9193	0.3295
C	11.3132	-7.0537	0.2843	C	-0.0502	3.2549	2.1868	H	-3.9847	6.0948	2.4521	H	-10.4859	2.5713	-0.3419
C	9.5320	-5.4331	1.6522	H	0.1612	1.7022	0.6379	C	-4.6017	3.7613	0.7911	H	-2.6013	4.0989	2.7851
C	10.6670	-4.8701	1.0302	H	-0.3764	1.0731	2.1952	H	-3.0086	4.8599	-0.2074	H	-0.8098	3.9747	0.2510
H	8.8234	-4.7994	2.1870	H	1.3273	4.7324	1.3027	C	-5.8849	4.6248	0.6988	H	18.6637	-3.5027	-3.9738
C	11.5702	-5.6755	0.3263	H	1.3860	4.6664	3.0569	H	-6.0871	6.6778	1.5090	H	17.3733	-4.6059	-3.5049
H	12.4444	-5.2641	-0.1781	H	-0.4130	3.2181	3.2442	H	-5.5187	6.6035	-0.1528	C	-14.3775	6.5003	-0.9891
N	10.2290	-7.6258	0.8811	C	3.2642	3.2063	0.8542	H	-4.6239	3.1117	1.6852	C	-1.9694	8.9909	2.2444
O	10.7685	-3.5244	1.2093	C	-1.1006	3.8599	1.2980	H	-4.5235	3.0789	-0.0722	C	10.0969	7.1341	0.9236
C	11.8148	-2.7757	0.4856	O	8.9059	6.4103	0.7449	H	-6.3499	4.4812	-0.3067	C	19.9697	1.0987	-4.4509
H	11.5602	-2.8139	-0.5876	C	8.7058	5.5234	-0.4211	C	-2.3148	4.2047	1.7357	C	-13.2572	6.5247	0.1037
H	12.7941	-3.2535	0.6651	H	9.6408	5.0172	-0.7032	C	-6.8627	4.2377	1.7755	C	-14.1118	7.5421	-2.1241
C	11.7186	-1.3869	1.1120	H	8.3572	6.1655	-1.2499	H	-8.1472	3.0436	0.5706	C	-15.8022	6.7059	-0.3522
C	12.8233	-0.4159	0.5996	C	7.6414	4.5669	0.1169	H	-6.6360	4.6357	2.7671	C	-2.3699	9.5183	3.6723
C	10.3820	-0.6747	0.8352	C	7.8617	3.1175	-0.4034	O	-14.6500	-6.7090	2.4698	C	-2.0782	10.1242	1.1736
C	12.2024	0.9991	0.7176	C	6.2095	4.9432	-0.3039	O	-11.9395	-5.2685	1.4854	C	-0.5499	8.3310	2.2620
H	13.7104	-0.4937	1.2727	H	7.6964	4.5736	1.2380	O	-16.1869	-6.8333	-0.1887	C	10.4201	8.0748	-0.2825
C	10.6894	0.8326	1.0007	C	6.4541	2.4817	-0.4859	O	-15.8190	-9.6280	-1.4011	C	11.2816	6.1653	1.2558
H	10.0117	-0.8997	-0.1812	H	8.2899	3.1615	-1.4360	O	-13.6687	-8.6746	-3.5827	C	9.6674	7.9615	2.1924
H	9.5896	-1.0055	1.5264	C	5.4115	3.6200	-0.3564	C	-12.2503	-6.6107	1.9630	C	21.1512	0.0743	-4.3774
H	12.3865	1.5947	-0.1940	H	5.7612	5.6747	0.3896	H	-12.5737	-7.2526	1.1257	C	19.7455	1.6356	-5.9020
H	12.6856	1.5642	1.5339	H	6.1963	5.4295	-1.2976	H	-11.3235	-7.0285	2.4011	C	20.1727	2.2788	-3.4284
H	10.4972	1.1217	2.0639	H	6.3092	1.7134	0.2950	C	-13.3428	-6.4128	3.0066	F	-16.7719	6.3709	-1.2082
C	13.2274	-0.6939	-0.8229	H	6.3292	1.9464	-1.4435	H	-13.3265	-5.3957	3.4424	F	-16.0161	5.9331	0.7173
C	9.8286	1.6520	0.0805	H	4.7574	3.6256	-1.2615	H	-13.2643	-7.1625	3.8244	F	-16.0933	7.9446	0.0494
O	18.8043	0.5546	-3.8856	C	8.7642	2.3364	0.5081	C	-15.2230	-5.6693	1.6274	F	-13.4173	7.4650	1.0434
C	18.0674	-0.5501	-4.5339	C	4.5800	3.4316	0.8843	H	-15.3952	-4.7687	2.2467	F	-13.1984	5.3712	0.7783
H	18.7591	-1.2965	-4.9527	H	2.7065	3.1675	-0.0842	H	-14.5172	-5.4293	0.8115	F	-12.0113	6.7180	-0.3419
H	17.4517	-0.1078	-5.3365	H	5.1387	3.4800	1.8217	C	-16.5219	-6.2691	1.1116	F	-12.9279	7.4299	-2.7365
C	17.2525	-1.0884	-3.3578	H	8.4756	2.3513	1.5626	H	-17.3058	-5.5029	0.9555	F	-15.0061	7.4828	-3.1175
C	16.7373	-2.5275	-3.6469	H	10.1197	1.6304	-0.9719	H	-16.9162	-7.0575	1.7815	F	-14.1472	8.8154	-1.7103
C	15.9955	-0.2502	-3.0545	O	-3.2400	-2.8971	0.9706	C	-17.1410	-7.8318	-0.6502	F	-1.7639	9.7611	-0.0746
H	17.9056	-1.1037	-2.4492	O	-2.6759	-0.0399	2.1426	H	-17.3121	-8.5819	0.1466	F	-3.3099	10.6361	1.0712
C	15.4653	-2.6634	-2.7832	O	-6.6980	-4.0911	0.6799	H	-18.0977	-7.3240	-0.8785	F	-1.2901	11.1796	1.4161
H	16.4514	-2.6030	-4.7250	O	-7.3517	-3.1306	-2.2511	C	-16.5010	-8.4384	-1.8891	F	-1.7491	10.6255	4.0840
C	14.8884	-1.2381	-2.6084	O	-6.8524	-0.3339	-3.6799	H	-15.7749	-7.7575	-2.3702	F	-2.1597	8.6212	4.6409
H	16.2046	0.5135	-2.2854	C	-2.1478	-1.3598	2.4033	H	-17.2561	-8.7549	-2.6348	F	-3.6751	9.7929	3.7448
H	15.6597	0.3150	-3.9427	H	-1.2993	-1.5882	1.7201	C	-14.9193	-10.2458	-2.3462	F	0.3596	8.9892	2.9919
H	15.6973	-3.1243	-1.8058	H	-1.7565	-1.2410	3.4388	H	-14.8079	-11.2668	-1.9202	F	-0.5811	7.0992	2.7833
H	14.7308	-3.3367	-3.2554	C	-3.2320	-2.4247	2.3500	H	-15.3925	-10.3173	-3.3441	F	0.0396	8.1757	1.0719
H	14.0092	-1.1188	-3.2871	H	-4.2300	-2.0283	2.6144	C	-13.5862	-9.5118	-2.3913	F	9.3865	8.8469	-0.6372
C	17.7751	-3.5975	-3.3367	H	-2.9995	-3.2838	3.0090	H	-12.7307	-10.2029	-2.5182	F	10.7713	7.4530	-1.4135
C	14.4794	-0.9875	-1.1825	C	-4.2878	-3.8412	0.6657	H	-13.4154	-8.8859	-1.4982	F	11.4234	8.9311	-0.0527
H	12.4174	-0.6222	-1.5518	H	-3.9541	-4.2516	-0.3083	C	-11.2013	-5.2177	0.2481	F	10.4971	8.9380	2.5647
H	15.2895	-1.0598	-0.4532	H	-4.3087	-4.6554	1.4139	H	-10.7334	-4.2082	0.2816	F	9.5080	7.2038	3.2820
H	18.1206	-3.5658	-2.2958	C	-5.6367	-3.1210	0.5767	H	-10.3994	-5.9812	0.2335	F	8.4815	8.5510	2.0157
O	4.3004	-5.3792	1.2124	H	-5.7386	-2.5259	-0.3466	C	-12.6003	-7.7183	-3.7181	F	11.9753	5.7046	0.2093
O	5.5084	-3.3169	-0.9955	H	-5.8211	-2.4710	1.4578	H	-11.6191	-8.2018	-3.5444	F	10.8612	5.0645	1.8898
O	2.5168	-7.5989	2.7137	C	-7.0641	-4.7540	-0.5528	H	-12.6672	-7.4268	-4.7901	F	12.2171	6.6876	2.0590
O	0.0305	-7.8153	0.8376	H	-6.1717	-4.9706	-1.1673	C	-12.8550	-6.5432	-2.8004	F	19.0256	2.9275	-3.2086
O	-0.8747	-4.8312	0.9321	H	-7.4919	-5.7115	-0.1839	C	-12.1711	-5.3409	-0.9069	F	21.0527	3.2184	-3.7799
C	5.9044	-4.5157	-0.2883	C	-8.1066	-3.9340	-1.3005	C	-13.9585	-5.7091	-2.9930	F	18.6763	2.4337	-6.0056
H	5.5566	-5.4243	-0.8146	H	-8.6770	-3.2618	-0.6338	C	-14.1490	-4.6512	-2.0796	F	19.5487	0.6954	-6.8329
H	7.0127	-4.4612	-0.3546	H	-8.8138	-4.5785	-1.8585	H	-14.6544	-5.8618	-3.8181	F	21.2901	-0.7348	-5.4332
C	5.4294	-4.4629	1.1575	C	-8.1920	-2.2829	-3.0815	C	-13.2366	-4.4371	-1.0384	F	21.0309	-0.7537	-3.3338
H	5.1008	-3.4513	1.4577	H	-8.9679	-2.9054	-3.5697	H	-13.3402	-3.6061	-0.3399	F	22.3598	0.6333	-4.2352
H	6.2030	-4.8164	1.8686	H	-8.6880	-1.5297	-2.4422	N	-11.9716	-6.3781	-1.7677	F	20.7615	2.3635	-6.3824
C	3.6143	-5.4202	2.4896	C	-7.2512	-1.6607	-4.1035	O	-15.2747	-3.9187	-2.3111	F	20.5667	1.8700	-2.2183
H	4.0374	-4.6870	3.2011	H	-7.7813	-1.4525	-5.0592	C	-15.6684	-2.9041	-1.3105	H	-17.4075	-1.8059	-0.8132
H	2.5714	-5.1275	2.2609	H	-6.3708	-2.2963	-4.3143	H	-14.9308	-2.0837	-1.3688	H	-9.2109	1.4131	3.9761
C	3.7079	-6.8455	3.0248	C	-2.7511	0.3583	0.7613	H	-15.6337	-3.3745	-0.3095	H	1.7780	1.2377	3.2032
H	3.7016	-6.8705	4.1359	H	-2.4561	1.4354	0.7885	C	-17.0874	-2.4607	-1.6669	H	11.8404	-1.4974	2.2201

Structure: all-*trans* H-((7-12 complex)-10)$_4$-H cooligomer, CHARGE:4 SPIN MULTIPLICITY: 1

O	-8.8270	1.1468	-0.9367	H	12.1447	-2.4141	-4.1519	C	5.1600	-2.0246	1.6966	C	-10.0333	4.4449	5.1547	C	5.1591	9.5232	-2.6910
C	-9.7116	0.0194	-0.5758	C	10.7645	-0.0541	-3.2486	C	7.6195	-2.4569	0.9993	H	-10.7285	5.2928	4.9685	C	4.3742	9.3521	-0.4863
H	-10.7211	0.4526	-0.4523	H	12.4206	1.1927	-2.5014	C	7.0828	-0.8139	2.9346	H	-10.6101	3.5575	5.4827	N	5.7196	12.8598	-0.9172
H	-9.3773	-0.4356	0.3712	H	12.4511	0.9416	-4.2367	F	4.9482	-2.8268	2.7414	C	-8.9494	4.7995	6.1617	H	6.1271	12.1773	-1.6023
C	-9.5972	-0.9093	-1.7851	H	10.6636	-1.5175	-1.6092	F	4.2351	-1.0647	1.7901	H	-8.0792	4.1175	6.1216	H	6.4920	13.2085	-0.2983
C	-8.4797	-1.9873	-1.6726	H	9.9957	-2.1178	-3.1241	F	4.7948	-2.7409	0.6285	H	-9.3448	4.8144	7.1970	H	5.0450	12.3337	-0.3107
C	-10.8919	-1.7329	-1.9491	H	10.3762	-0.0744	-4.2972	F	8.9139	-2.1763	1.1823	C	-7.4069	6.6206	6.6036	N	5.1907	9.9596	-1.3957
H	-9.4150	-0.2796	-2.6901	C	12.6334	-3.1569	-2.1906	F	7.4795	-3.6909	1.5005	H	-7.6497	6.5087	7.6790	C	5.0395	14.0122	-1.6295
C	-9.1415	-3.2120	-0.9998	C	9.8863	0.8111	-2.3883	F	7.4917	-2.6067	-0.3232	H	-6.5135	6.0118	6.3672	H	4.6801	14.7498	-0.8695
H	-8.2006	-2.2730	-2.7196	H	12.4873	-2.9735	-1.1235	F	8.2933	-0.2459	2.9154	C	-7.2433	8.0811	6.2142	H	5.7959	14.5572	-2.2493
C	-10.6708	-3.0766	-1.2133	O	2.7260	6.8630	-2.6535	F	7.1575	-1.7116	3.9255	H	-6.7965	8.6777	7.0342	C	3.8960	13.5229	-2.5154
H	-11.7851	-1.1981	-1.5831	C	1.7982	6.1562	-1.7479	F	6.2742	0.1432	3.4047	H	-8.1948	8.5492	5.8974	H	3.5515	14.3800	-3.1486
H	-11.0850	-1.9161	-3.0235	H	1.0841	6.9016	-1.3496	C	11.9757	-11.0298	-2.4370	C	-6.0664	9.3845	4.5305	H	4.2714	12.7825	-3.2593
H	-8.8913	-3.2666	0.0745	H	2.3791	5.7127	-0.9208	C	10.7614	-10.9256	-3.4337	H	-6.9361	9.6609	3.9055	C	2.7240	12.9775	-1.7510
H	-8.7635	-4.1524	-1.4352	C	1.1244	5.1395	-2.6669	C	13.1161	-11.9305	-3.0219	H	-5.9550	10.1268	5.3458	C	2.0995	13.7453	-0.7567
H	-11.0300	-3.9108	-1.8622	C	1.9642	3.8810	-3.0421	C	11.5090	-11.5153	-1.0254	C	-4.7780	9.2550	3.7304	C	2.2458	11.6902	-2.0482
C	-7.2580	-1.5241	-0.9347	C	-0.1759	4.6225	-2.0200	F	9.9547	-11.9866	-3.4928	H	-4.0126	8.6599	4.2609	C	1.0129	13.2417	-0.0369
C	-11.3902	-3.0995	0.1082	H	0.8711	5.6633	-3.6257	F	9.9706	-9.8938	-3.1241	H	-4.3548	10.2545	3.4952	H	2.4620	14.7530	-0.5359
H	-7.3648	-1.4726	0.1518	C	1.0078	2.6665	-2.9303	F	11.1330	-10.6976	-4.6972	C	-4.3833	7.4592	2.1260	C	1.1579	11.1851	-1.3347
O	-17.9267	-5.6518	0.5187	H	2.2778	3.9952	-4.1098	F	14.0118	-12.3874	-2.1397	H	-3.3047	7.7008	2.0550	H	2.7079	11.0836	-2.8297
C	-18.9849	-5.5012	1.5402	C	-0.4024	3.2159	-2.6135	F	12.6859	-13.0342	-3.6469	H	-4.5387	6.7171	2.9329	C	0.5424	11.9598	-0.3228
H	-19.9184	-5.2519	1.0016	H	-0.0869	4.5826	-0.9173	F	13.8469	-11.2823	-3.9352	C	-4.9573	6.9985	0.7949	H	0.5343	13.8406	0.7430
H	-18.7140	-4.6811	2.2250	H	-1.0277	5.2925	-2.2252	F	12.4744	-11.5996	-0.1033	H	-4.1697	6.6458	0.1006	O	-0.5215	11.3618	0.3188
C	-19.0279	-6.8831	2.1936	H	1.3445	1.9634	-2.1473	F	10.9456	-12.7301	-1.0237	H	-5.5641	7.7773	0.2941	H	-0.8836	11.9499	1.0557
C	-18.0306	-7.1042	3.3755	H	1.0025	2.0829	-3.8666	F	10.5918	-10.7142	-0.4709	C	-8.7093	3.0104	3.6863	O	0.7309	9.9203	-1.6683
C	-20.4423	-7.1560	2.7550	H	-0.9710	3.3188	-3.5708	O	-18.0000	1.4960	-3.8273	H	-7.8159	3.0700	4.3422	H	-0.0491	9.6265	-1.0985
H	-18.7891	-7.6375	1.4011	C	3.1753	3.6606	-2.1802	O	-18.8424	-0.7518	-2.2369	H	-9.3195	2.1388	3.9961	C	15.9641	-1.2419	0.1969
C	-18.8934	-7.2105	4.6518	O	6.3080	-0.4276	0.6107	O	-15.5194	1.3486	-5.4996	C	-6.2619	5.1217	-0.0074	C	16.0164	-1.8028	-1.0890
H	-17.5427	-8.0985	3.2035	C	7.3013	0.5898	0.2141	O	-14.0123	-1.1031	-6.1281	H	-6.8145	5.7922	-0.7020	H	15.1919	-0.5269	0.4804
C	-20.2634	-7.7368	4.1758	H	8.3000	0.1412	0.0902	O	-14.6726	-2.8164	-3.6245	H	-5.3635	4.7273	-0.5316	C	17.0305	-2.7186	-1.4341
H	-21.0526	-6.2342	2.7837	H	7.3205	1.3605	1.0035	C	-19.5819	0.4801	-2.4048	C	-7.1474	4.0031	0.4769	H	17.0759	-3.1415	-2.4393
H	-20.9987	-7.8535	2.1061	C	6.7127	1.0841	-1.1084	H	-20.1444	0.2658	-3.3400	C	-8.3346	2.9791	2.2240	O	19.8978	-1.1039	4.8155
H	-18.9976	-6.2305	5.1503	C	7.7485	1.9809	-1.8530	H	-20.2935	0.6124	-1.5661	N	-7.9927	6.6805	3.0251	O	18.2133	-0.3523	2.6012
H	-18.4338	-7.8784	5.3983	C	5.4444	1.9421	-0.9317	C	-18.6703	1.6895	-2.5506	H	-7.3344	6.3692	2.2691	O	21.5822	-3.5710	4.6192
H	-20.2175	-8.8511	4.1055	H	6.4635	0.1963	-1.7415	H	-17.9132	1.7660	-1.7481	H	-7.4206	6.9957	3.8450	O	22.1936	-5.0681	2.1426
C	-16.9694	-6.0499	3.5047	C	6.8925	2.9894	-2.6454	H	-19.2506	2.6328	-2.5866	H	-8.5456	5.8430	3.3300	O	19.7206	-4.4199	0.4347
C	-21.4009	-7.3563	5.1162	H	8.3576	2.5440	-1.1016	C	-17.0248	2.5341	-4.1263	N	-7.5072	3.9761	1.7957	C	18.3918	0.4115	3.8169
H	-22.3660	-7.7348	4.7555	C	5.6044	3.2028	-1.8190	H	-17.4888	3.5314	-3.9928	C	-8.9002	7.7944	2.5429	H	19.2982	1.0046	3.5647
H	-21.2503	-7.7740	6.1200	H	4.5464	1.3616	-1.2080	H	-16.1743	2.4317	-3.4261	H	-9.5814	8.0967	3.3766	H	17.5311	1.0937	3.9643
H	-21.5082	-6.2714	5.2351	H	5.2876	2.2345	0.1214	C	-16.6288	2.2901	-5.5739	H	-8.2799	8.6969	2.3102	C	18.6067	-0.4718	5.0367
O	-10.3420	-5.8696	4.0246	H	6.6610	2.6063	-3.6569	H	-16.2762	3.2181	-6.0662	C	-9.6846	7.3758	1.3024	H	17.8322	-1.2526	5.1537
C	-11.0344	-4.6369	3.5991	H	7.4323	3.9372	-2.8082	H	-17.4466	1.8473	-6.1736	H	-10.1940	8.2838	0.8889	H	18.6535	0.1271	5.9680
H	-10.3750	-4.0136	2.9751	H	5.7523	4.0903	-1.1524	C	-15.0110	0.9532	-6.8072	H	-8.9842	7.0747	0.4886	C	20.2482	-2.0672	5.8487
H	-11.3360	-4.0905	4.5089	C	8.6423	1.1553	-2.7330	H	-15.7546	0.2872	-7.2843	C	-10.7166	6.3137	1.5506	H	20.1516	-1.5933	6.8455
C	-12.2118	-5.2209	2.8153	C	4.3979	3.4580	-2.6801	H	-14.8668	1.8519	-7.4385	C	-11.6576	6.4535	2.5822	H	19.5522	-2.9252	5.7845
C	-12.8150	-4.1462	1.8626	H	2.9818	3.6434	-1.1049	C	-13.6884	0.2558	-6.5260	C	-10.7533	5.1841	0.7162	C	21.6876	-2.4546	5.5493
C	-13.3701	-5.7003	3.7146	H	4.5840	3.4681	-3.7568	H	-13.0983	0.7746	-5.7485	C	-12.6261	5.4725	2.8091	H	22.2191	-2.7959	6.4601
H	-11.8396	-6.0875	2.2120	H	8.1992	0.8420	-3.6812	H	-13.0751	0.1682	-7.4465	H	-11.6402	7.3407	3.2215	H	22.2637	-1.6378	5.0752
C	-14.3071	-4.5230	1.7491	H	10.3327	1.1305	-1.4432	C	-13.2186	-1.5936	-5.0122	C	-11.7282	4.2086	0.9308	C	22.8752	-4.1024	4.2061
H	-12.7393	-3.1413	2.3500	O	12.3516	-9.6761	-2.4521	H	-12.1536	-1.6051	-5.3163	H	-10.0371	5.0623	-0.0995	H	23.3598	-3.3654	3.5379
C	-14.6818	-5.1271	3.1228	C	13.4063	-9.1509	-1.5612	H	-13.3480	-0.9168	-4.1454	C	-12.6606	4.3464	1.9857	H	23.5123	-4.2636	5.0978
H	-13.3907	-6.8042	3.7603	H	14.2515	-9.8524	-1.4944	C	-13.7513	-2.9922	-4.7429	H	-13.3511	5.5812	3.6208	C	22.5573	-5.4154	3.5060
H	-13.2472	-5.3715	4.7617	H	12.9519	-9.0012	-0.5662	H	-12.9458	-3.6956	-4.4553	O	-13.5631	3.3119	2.1208	H	21.7440	-5.9718	4.0079
H	-14.4746	-5.2490	0.9328	C	13.7725	-7.8470	-2.2719	H	-14.3144	-3.4117	-5.5986	H	-14.2188	3.4917	2.8684	H	23.4527	-6.0663	3.4363
H	-14.9289	-3.6456	1.5068	C	15.1540	-7.3252	-1.7799	C	-18.1760	-0.8933	-0.9508	O	-11.7198	3.1272	0.0788	C	21.1406	-5.9017	1.5865
H	-15.0392	-4.3024	3.7881	C	12.7647	-6.7082	-2.0132	H	-17.3754	-0.1304	-0.8627	H	-12.5299	2.5404	0.2147	H	21.5116	-6.9433	1.5203
C	-12.1202	-4.1344	0.5320	H	13.8215	-8.0423	-3.3726	H	-18.9117	-0.7335	-0.1381	C	3.5113	8.2994	-0.8164	H	20.2551	-5.8713	2.2508
C	-15.7435	-6.1820	2.9900	C	15.0695	-5.7934	-1.9429	C	-15.0568	-4.0752	-3.0139	C	3.5052	7.8621	-2.1506	C	20.8573	-5.3092	0.2150
H	-17.2665	-5.1559	4.0587	H	15.2706	-7.5650	-0.6943	H	-15.4446	-4.7648	-3.7963	H	2.8788	7.8411	-0.0564	H	20.5837	-6.0897	-0.5219
H	-15.4420	-7.0730	2.4351	C	13.5834	-5.4217	-1.7355	H	-14.1527	-4.5311	-2.5535	C	4.3349	8.4720	-3.1100	H	21.6994	-4.7105	-0.1808
H	-12.2462	-5.0391	-0.0662	H	12.0866	-6.5856	-2.8764	C	-16.1159	-3.7945	-1.9804	H	4.3253	8.1321	-4.1477	C	16.9585	-1.0836	2.5188
H	-11.2650	-2.1964	0.7116	H	12.1065	-6.9289	-1.1544	C	-17.6200	-2.2972	-0.9783	O	5.4759	13.4425	1.9842	H	16.9484	-1.8888	3.2827
C	-18.1112	-3.2821	-0.1128	H	15.4264	-5.4821	-2.9414	N	-16.9274	-1.1004	-4.5318	O	3.9264	11.2394	0.8230	H	16.1172	-0.3913	2.7199
C	-17.5579	-4.5687	-0.2171	H	15.7194	-5.2754	-1.2187	H	-16.2029	-1.7738	-4.1781	O	7.9197	14.2829	0.4729	C	19.0864	-4.0036	-0.8025
H	-18.8898	-3.0486	0.6129	H	13.4348	-5.1319	-0.6663	H	-16.4588	-0.1777	-4.7043	O	8.4085	13.6439	-2.4290	H	19.8382	-3.5037	-1.4527
C	-16.5458	-4.8423	-1.1582	C	13.1613	-4.2983	-2.6410	H	-17.6304	-0.9623	-3.7677	O	6.9565	11.0764	-3.0066	H	18.7067	-4.9072	-1.3274
H	-16.1231	-5.8454	-1.2405	H	13.3157	-4.4837	-3.7067	N	-16.6377	-2.5336	-1.8956	C	3.6981	11.8961	2.0915	C	17.9695	-3.0547	-0.4525
O	-0.8317	-2.5358	-1.0753	C	-1.1439	2.3160	-1.6654	C	-17.5847	-1.6094	-5.7995	H	3.0888	12.7713	1.7768	C	16.9424	-1.6410	1.1157
C	-1.2401	-1.2497	-0.4759	H	-0.8075	2.3636	-0.6260	H	-18.3230	-0.8503	-6.1577	H	3.0930	11.2439	2.7517	N	20.5761	-2.1764	2.1868
H	-0.4373	-0.5020	-0.5618	C	-9.0177	-5.8462	4.4943	H	-16.8089	-1.6880	-6.6036	C	4.9963	12.3133	2.7659	H	20.2531	-2.9045	1.5013
H	-1.4782	-1.4417	0.5851	C	-8.9271	-7.3454	4.9647	C	-18.2422	-2.9699	-5.5812	H	5.7647	11.5176	2.7636	H	20.7593	-2.6507	3.1049
C	-2.4627	-0.8959	-1.3250	C	-8.0280	-5.5616	3.3140	H	-18.5553	-3.3719	-6.5784	H	4.8256	12.6423	3.8102	H	19.7857	-1.5045	2.3289
C	-2.8555	0.5946	-1.0972	C	-8.8090	-4.8629	5.6910	H	-17.4867	-3.7084	-5.2253	C	6.7307	13.9883	2.4806	N	17.9297	-2.5318	0.8107
C	-3.7129	-1.7321	-0.9807	F	-7.7498	-4.2748	3.0798	C	-19.4372	-2.9372	-4.6718	H	6.5520	14.4393	3.4766	C	21.8251	-1.4678	1.6988
H	-2.2070	-1.0554	-2.4026	F	-6.8249	-6.1344	3.4469	C	-20.4956	-2.0465	-4.9075	H	7.4749	13.1745	2.5780	H	22.1410	-0.7179	2.4653
C	-4.3865	0.6285	-1.2887	F	-8.8664	-3.5645	5.3738	C	-19.4989	-3.8284	-3.5879	C	7.1392	15.0295	1.4507	H	22.6610	-2.2103	1.6311
H	-2.6259	0.8761	-0.0380	F	-7.6309	-4.9981	6.3128	C	-21.6056	-2.0102	-4.0592	H	7.7753	15.8203	1.8947	C	21.6026	-0.8126	0.3369
C	-4.8921	-0.7449	-0.7925	F	-9.7215	-5.0099	6.6581	H	-20.4613	-1.3704	-5.7662	H	6.2734	15.4978	0.9445	H	22.5883	-0.4342	-0.0357
H	-3.9174	-2.4650	-1.7815	F	-7.8293	-7.6845	5.6430	C	-20.6113	-3.8040	-2.7457	C	8.4774	15.1161	-0.5839	H	21.3130	-1.5809	-0.4171
H	-3.5700	-2.3331	-0.0652	F	-9.9515	-7.6726	5.7574	H	-18.6951	-4.5439	-3.4004	H	7.6502	15.5763	-1.1573	C	20.6182	0.3217	0.3605
H	-4.6540	0.7962	-2.3480	F	-8.9946	-8.2152	3.9519	C	-21.6610	-2.8827	-2.9718	H	9.0957	15.9147	-0.1289	C	20.7965	1.4077	1.2312
H	-4.8463	1.4597	-0.7294	F	-8.4991	-6.0221	2.1499	H	-22.4235	-1.3070	-4.2406	C	9.3159	14.1593	-1.4162	C	19.5187	0.2954	-0.5126
H	-5.1158	-0.6675	0.3006	C	0.4562	-3.0606	-0.8778	O	-22.6958	-2.9267	-2.0614	H	9.7290	13.3281	-0.8123	C	19.8765	2.4590	1.2653
C	-2.1336	1.5046	-2.0481	C	0.2273	-4.4660	-1.5507	H	-23.4065	-2.2439	-2.2830	H	10.1464	14.6784	-1.9339	H	21.6648	1.4389	1.8955
C	-6.1140	-1.1971	-1.5418	C	1.5158	-2.2193	-1.6666	O	-20.6223	-4.7087	-1.7096	C	8.8862	12.4292	-3.0694	C	18.6014	1.3464	-0.4870
H	-5.9987	-1.2462	-2.6270	C	0.8309	-3.2094	0.6331	H	-21.4982	-4.6951	-1.2079	H	9.7632	12.6855	-3.6964	H	19.3744	-0.5308	-1.2123
H	-2.4681	1.4499	-3.0867	F	1.2105	-5.3552	-1.3997	C	-8.8272	1.9795	1.3765	H	9.1929	11.6957	-2.2990	C	18.7716	2.4246	0.4130
O	15.1600	-1.5215	-2.1080	F	-0.8679	-5.0624	-1.0704	C	-8.4353	2.0219	0.0283	C	7.7159	11.9391	-3.9068	H	20.0138	3.2982	1.9528
C	14.0039	-0.6380	-1.8484	F	0.0210	-4.3925	-2.8685	H	-9.4853	1.1985	1.7580	H	8.0586	11.3613	-4.7877	O	17.7884	3.3908	0.3729
H	14.4092	0.3846	-1.7346	F	2.0556	-1.1925	-0.9996	C	-7.5861	3.0425	-0.4416	H	7.0519	12.7590	-4.2415	H	17.9639	4.1227	1.0464
H	13.5007	-0.9520	-0.9190	F	2.5736	-2.9196	-2.0944	H	-7.2870	3.0753	-1.4909	C	4.4402	9.8823	0.9263	O	17.5430	1.2657	-1.3635
C	13.1460	-0.8046	-3.1042	F	0.9982	-1.6674	-2.7686	O	-8.5242	6.1435	5.8015	H	5.4808	9.9109	1.3103	H	16.9922	2.1116	-1.3646
C	12.1981	-2.0416	-3.0958	F	1.0662	-2.0606	1.2768	O	-9.5047	4.2207	3.8259	H	3.8126	9.3047	1.6337	C	16.3184	-7.9350	-2.5482
C	12.2329	0.4315	-3.2813	F	1.9317	-3.9399	0.8550	O	-6.3147	8.0637	5.0917	C	6.0228	10.2181	-3.7109	H	16.3737	-9.0227	-2.4128
H	13.8363	-0.8972	-3.9801	F	-0.1219	-3.8059	1.3580	O	-5.1079	8.6809	2.4395	H	5.3981	10.8280	-4.4012	H	16.2580	-7.7498	-3.6282
C	10.8067	-1.5004	-2.7044	C	6.6038	-1.4103	1.5708	O	-5.8316	5.8851	1.1491	H	6.6075	9.4885	-4.3130	H	17.2799	-7.5250	-2.2116

8. Determination of the log*K* for the formation of complex 7-12 via NMR titration

Solutions of pyridino-18-crown-6 ether (**7**) and dopamine.HCl (**12**) having the same concentration ($c_0 = 0.0143$M) were mixed in various volume ratios and NMR spectra of the mixtures were measured. Complex stability constants were determined using the method described in ref. [8] following the chemical shift of the methylene protons next to the pyridine-ring of the pyridino-18-crown-6 ether.

Chemical equation of complex formation (see Table 1 for notations of concentrations):

$$\mathbf{7} + \mathbf{12} \rightleftharpoons \mathbf{7\text{-}12}$$

Table S1. Concentration balances in the equilibrium of complexation between dopamine.HCl (**12**) and pyridino-18-crown-6 (**7**) solutions ($c_0 = 0.0050$M) during NMR titration.

	pyridino-18-crown-6 ether (7)	**dopamine.HCl (12)**	**complex 7-12**
initial	$c_{7,0} = \frac{c_0 V_7}{V_7 + V_{12}}$	$c_{12,0} = \frac{c_0 V_{12}}{V_7 + V_{12}}$	0
change	$-x$	$-x$	$+x$
equilibrium	$c_{7,0} - x$	$c_{12,0} - x$	x

The equilibrium constant is calculated as:

$$K = \frac{c_{7\text{-}12}}{c_7 c_{12}} = \frac{x}{(c_{7,0} - x)(c_{12,0} - x)}$$

After rearranging, one arrives at the following quadratic equation:

$$Kx^2 - [K\overbrace{(c_{7,0} + c_{12,0})}^{c_0} + 1]x + Kc_{7,0}c_{12,0} = 0.$$

Dividing the previous equation by K and taking into account that $c_{7,0} + c_{12,0} = c_0$:

$$x^2 - [c_0 + K^{-1}]x + c_{7,0}c_{12,0} = 0.$$

The appropriate root of the quadratic equation, where $x < \min(c_{7,0}, c_{12,0})$, is:

$$x = \frac{[c_0 + K^{-1}] - \sqrt{[c_0 + K^{-1}]^2 - 4c_{7,0}c_{12,0}}}{2}$$

The δ_x chemical shift corresponding to the x complex concentration can be calculated by linear interpolation from the mole fractions and NMR chemical shifts of the crown ether in the free $(x_7; \delta_7)$ and complex forms $(x_{7\text{-}12} = 1 - x_7; \delta_{7\text{-}12})$:

$$\delta_x^{\text{calc}} = x_7\delta_7 + x_{7\text{-}12}\delta_{7\text{-}12} = \frac{c_7\delta_7 + c_{7\text{-}12}\delta_{7\text{-}12}}{c_7 + c_{7\text{-}12}}$$

The sum of square deviation of the experimental NMR shift (δ_x^{exp}) and calculated δ_x^{calc} NMR shift along the titration curve (i.e. for all x_i values) was minimized by optimizing the value of K, δ_7 and $\delta_{7\text{-}12}$:

$$\min_{K,\delta_7,\delta_{7\text{-}12}} \sum_i \left(\delta_{x_i}^{\text{calc}}(K, \delta_7, \delta_{7\text{-}12}) - \delta_{x_i}^{\text{exp}}\right)^2$$

The measured and fitted chemical shift values are shown on Figure S53 and in Table S1.

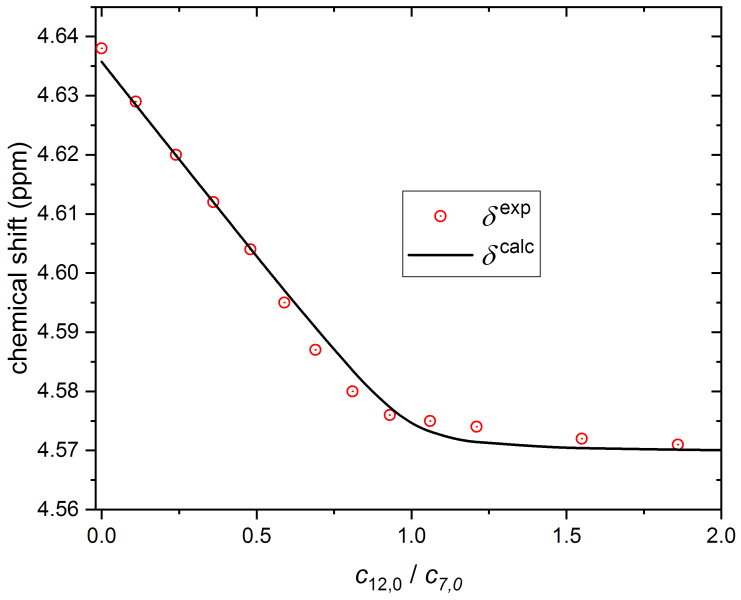


Figure S53.
The experimental values and fitted theoretical curve of chemical shifts for methylene protons next to the pyridine-ring within the crown ether as a function of the mixing ratios of the dopamine. HCl (**12**) and pyridino-18-crown-6 ether (**7**). The sum of concetrations in the mixture was constant: $c_{12,0} + c_{7,0} = 0.0143\text{M}$.

Table S2. The experimental and fitted chemical shift values for methylene protons next to the pyridine-ring within the crown ether as a function of the mixing ratios of the dopamine. HCl (**12**) and pyridino-18-crown-6 ether (**7**). The sum of concetrations in the mixture was constant: $c_{12,0} + c_{7,0} = 0.0143\text{M}$.

$\frac{c_{12,0}}{c_{7,0}} = \frac{V_{12,0}}{V_{7,0}}$	$\delta_{x_i}^{\text{exp}}$/ppm	$\delta_{x_i}^{\text{calc}}$/ppm
0	4.638	4.636
0.11	4.629	4.628
0.24	4.620	4.620
0.36	4.612	4.612
0.48	4.604	4.604
0.59	4.595	4.597
0.69	4.587	4.591
0.81	4.580	4.584
0.93	4.576	4.577
1.06	4.575	4.573
1.21	4.574	4.571
1.55	4.572	4.570
1.86	4.571	4.570
2.54	4.571	4.570

The optimized $\log K$ value and its 95% confidence interval (±2.2σ for 14-3=11 degrees of freedom from Student's t-distribution) are:

$$\boxed{\log K = 4.3 \pm 0.6}$$

Izatt et al. found $\log K$ values of 3.62 and 3.29 for similar complexes[9] shown on Figure S54 [R=Me; (R) and (S) enantiomers of PhEt]. Their values are somewhat lower which can be explained by the presence of the extra methyl groups which hinder complexation both sterically and by reducing the conformational flexibility of the crown ether ring.

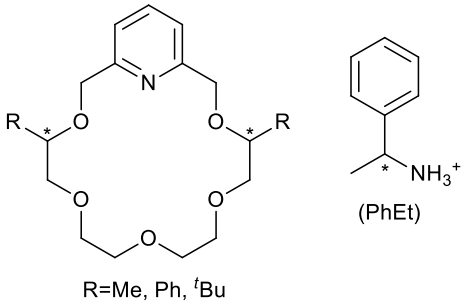


Figure S54. Complexation of molecules investigated by Izatt et al.[9]

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