Supporting Information for

Synthesis of Cyclotriveratrylene-Sucrose-Based Capsules

Łukasz Szyszka, Piotr Cmoch, Aleksandra Butkiewicz, Mykhaylo A. Potopnyk and Sławomir Jarosz

Institute of Organic Chemistry, Polish Academy of Sciences, ul. Kasprzaka 44/52, 01-224 Warsaw, Poland

Contents

1. General

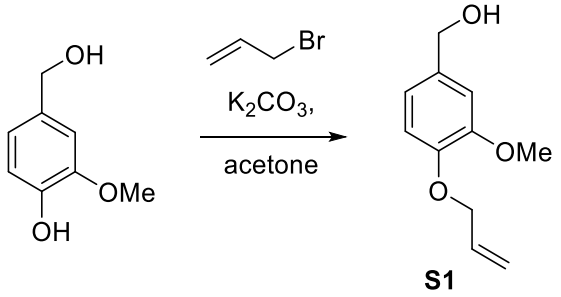
Commercially available reagents and solvents were used as received. TLC was performed on Merck silica gel 60 F_{254} plates. Compounds were purified using automatic flash chromatography system Knauer with UV and ELSD detection and Grace Resolv or Reveleris cartridges. The NMR spectra were recorded with Bruker Avance II 400 MHz (at 400 MHz and 100 MHz for ^{1}H and ^{13}C NMR spectra, respectively), Varian VNMRS 500 MHz (at 500 MHz and 125 MHz for ^{1}H and ^{13}C NMR spectra, respectively) or Varian VNMRS 600 MHz (at 600 MHz and 150 MHz for ^{1}H and ^{13}C NMR spectra, respectively) spectrometers for solutions in $CDCl_3$, acetone-d_6, CD_3OD or CD_3CN, and TMS as the internal standard at 298 K. All significant resonances were assigned by COSY (^{1}H-^{1}H), HSQC (^{1}H-^{13}C) and HMBC (^{1}H-^{13}C) correlations. Mass spectra were measured with Synapt G2-S HDMS (*Waters Inc*) mass spectrometer equipped with an electrospray ion source and q-TOF type mass analyzer. Optical rotations were measured with a Jasco P 2000 apparatus in $CHCl_3$ or MeOH with a sodium lamp at r.t. (c~1). Elemental analyses were obtained with a Perkin–Elmer 2400 CHN analyzer. The ECD and UV spectra of ***P*-8** and ***M*-8** were recorded at room temperature in MeCN (for UV-spectroscopy, Fluka) on a Jasco J-715 spectropolarimeter with concentrations of 7.0×10^{-5} M in 0.1 cm quartz cell. All spectra were recorded using a 100 nm/min scanning speed, a step size of 0.2 nm, a bandwidth of 1 nm, a response time of 0.5 s, and an accumulation of 5 scans. The baseline of the spectra was corrected by subtracting the spectrum of the pure solvent recorded under the same conditions.

2. Computational details

First, the conformational analysis of ***M*-8** and ***P*-8** was performed by using Conflex 7 program[1] with the MMFF94s force field and 5 kcal/mol energy window. Next, ten most stable conformers for each ***P*-8** and ***M*-8** molecules were optimized at the CAM-B3LYP/SVP/PCM (MeCN) level.[2] The stable structures were found by ascertaining that all the harmonic frequencies were real and the relative abundances were calculated on the ΔG values relative to the most stable conformer. The Electronic Absorption EA and ECD spectra were calculated for all conformers with a population higher than 1% taking into account the lowest 150 singlet states. Finally, the EA and ECD spectra were averaged taking into account the ΔG values at room temperature and plotted with Gaussian bandshape and 0.20 eV half-height width. All calculations were performed using the Gaussian 16 package of programs.[3]

3. Synthesis

3.1. Synthesis of 1-*O*-allyl-vanillyl alcohol (S1)

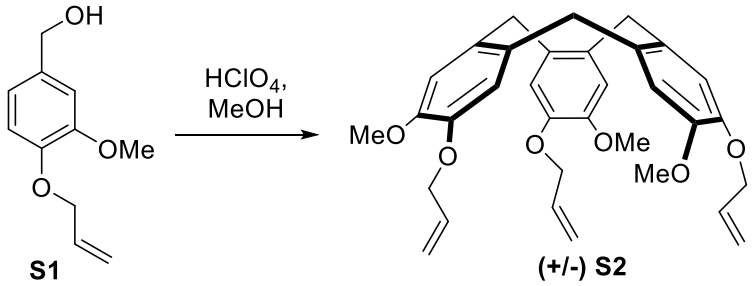


S1

1-*O*-allyl-vanillyl alcohol (**S1**) was prepared according to the literature procedure.[4] To the solution of vanillyl alcohol (5 g, 0.032 mol) in acetone (25 mL), K_2CO_3 (4.5 g, 0.032 mol)

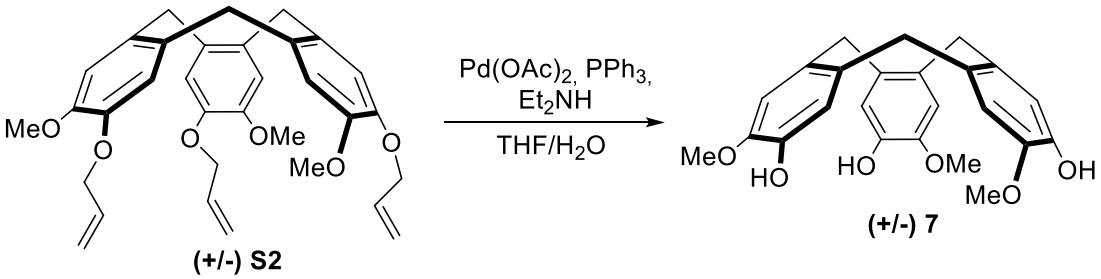
and allyl bromide (3.3 mL, 0.038 mol) were added. The mixture was stirred under reflux overnight. Afterwards, acetone was removed under vacuum and the residue was partitioned between CH_2Cl_2 (50 mL) and water (30 mL). The organic phase was then dried over Na_2SO_4 and concentrated. The crude product was purified by crystallization from methyl *tert*-butyl ether/hexanes obtaining **S1** (6 g, 0.031 mol, 95%) as white crystals. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 6.93 (s, 1H), 6.85 (s, 2H), 6.02–6.13 (m, 1H), 5.39 (dd, *J* = 1.5 Hz, 17.3 Hz, 1H), 5.28 (dd, *J* = 1.4 Hz, 10.5 Hz, 1H), 4.58–4.62 (m, 4H), 3.88 (s, 3H), 1.76 (s, OH) ppm. ^{13}C{H} NMR (100 MHz, $CDCl_3$) δ: 149.62, 147.54, 134.01, 133.31, 119.26, 117.89, 113.44, 110.88, 69.95, 65.24, 55.88 ppm. HRMS (ESI-TOF) calcd for $C_{11}H_{14}O_3Na$ $[M + Na]^+$: 217.0841, found: 217.0836. ^{1}H and ^{13}C NMR spectra were consistent with those previously reported in the literature.[4]

3.2. Synthesis of cyclotri-1-*O*-allyl-vanillyl alcohol (S2)



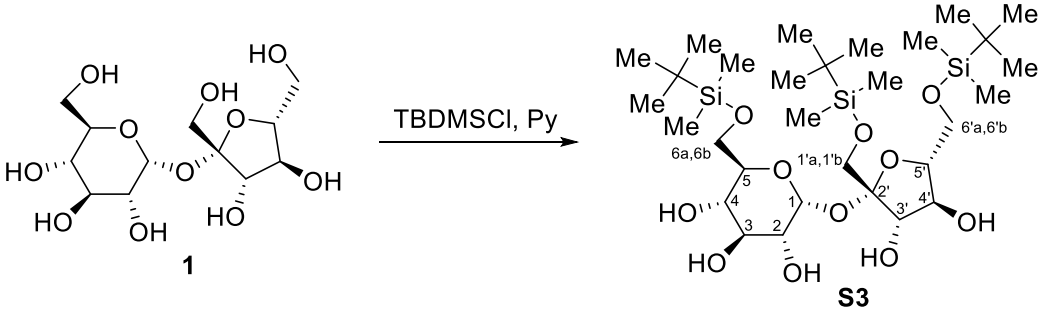
Racemic compound **S2** was prepared according to a modified literature procedure.[4] To the cooled to 0 °C solution of **S1** (11.1 g, 0.057 mol) in MeOH (66.6 mL), 65% aqueous $HClO_4$ (33.3 mL) was added dropwise, the reaction mixture was allowed to reach room temperature, and stirred for 20 h. Then it was diluted with CH_2Cl_2 (60 mL), cooled to 0 °C, and 50% aq. NaOH was carefully added dropwise as its color changed from pink to yellow. The layers were separated and the aqueous one was washed with CH_2Cl_2 (3× 30 mL). Combined organic phases were washed with water (80 mL), then brine (50 mL), dried over Na_2SO_4, and concentrated under reduced pressure. The resulting residue was suspended in Et_2O (50 mL) and stirred for 4h before being filtered off. The solid was washed with Et_2O (3 × 10 mL) and dried in high vacuum. Pure racemic compound **12** (5.22 g, 0.01 mol, 52 %) was obtained as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 6.85 (s, 3H), 6.79 (s, 3H), 6.01–6.11 (m, 3H), 5.37 (d, *J* = 17.2 Hz, 3H), 5.25 (d, *J* = 10.7 Hz, 3H), 4.74 (d, *J* = 13.7 Hz, 3H), 4.53–4.64 (m, 6H) 3.83 (s, 9H), 3.51 (d, *J* = 13.8 Hz, 3H) ppm. ^{13}C{H} NMR (100 MHz, $CDCl_3$) δ: 148.24, 146.79, 133.77, 132.36, 131.77, 117.47, 115.66, 113.69, 70.23, 56.13, 36.52 ppm. HRMS (ESI-TOF) calcd for $C_{33}H_{36}O_6Na$ $[M + Na]^+$: 551.2410, found: 551.2407. ^{1}H and ^{13}C NMR spectra were consistent with those previously reported in the literature.[4]

3.3. Cyclotriguaiacylene (7)



Racemic compound **7** was prepared according to a modified literature procedure.[5] This reaction was conducted under an argon atmosphere. To a solution of **S2** (9.0 g, 0.017 mol) in THF (225 mL) and H_2O (45 mL), $Pd(OAc)_2$ (572.5 mg, 2.55 mmol), PPh_3 (2.0 g, 7.65 mmol), and diethylamine (90 mL) were added, and the mixture was stirred for 4 h at 80 °C. After removal of solvents under vacuum, ethyl acetate (100 mL) was added, the dark insoluble residue was filtered and washed with ethyl acetate. The resulting filtrate was washed with water (100 mL) and then with brine (100 mL). Combined organic phases were dried over Na_2SO_4 and concentrated. The resulting yellow solid was washed with ether (3 × 50 mL) and recrystallized from dichloromethane/hexanes giving the desired product **7** (4.52 g, 0.011 mol, 65%) as off-white powder. ^{1}H NMR (500 MHz, acetone-d_6): δ = 6.99 (s, 3H), 6.93 (s, 3H), 4.74 (d, J = 13.6 Hz, 3H), 3.80 (s, 9H), 3.50 (d, J = 13.6 Hz, 3H) ppm. ^{13}C{H} NMR (125 MHz, acetone-d_6): δ = 146.81, 145.83, 133.86, 132.00, 117.15, 114.24, 56.54, 36.47 ppm. HRMS (ESI-TOF) calcd for $C_{24}H_{24}O_6Na$ $[M + Na]^+$: 431.1471, found: 431.1472. ^{1}H and ^{13}C NMR spectra were consistent with those previously reported in the literature.[5]

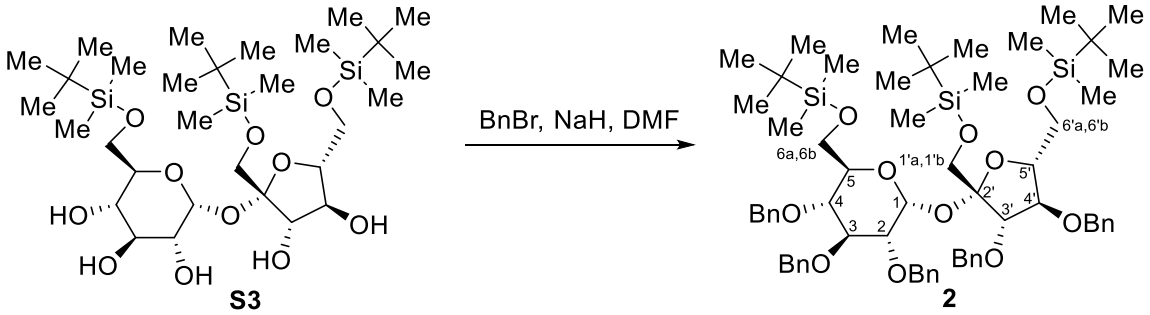
3.4. 1',6,6'-Tri-*O*-*tert*-butyldimethylsilylsucrose (S3)



Sucrose (**1**, 10 g, 0.029 mol) was dissolved in boiling pyridine (200 mL). After cooling to room temperature, a solution of *tert*-butyldimethylsilyl chloride (16.5 g, 0.109 mol) in pyridine (100 mL) was added dropwise during 30 min and the mixture was stirred for 24 h at 60 °C. Pyridine was evaporated and the products were isolated by column chromatography (hexanes/ethyl acetate = 1:2 to 100% ethyl acetate) to afford compound **S3** (13.0 g, 0.019 mol, 65 %) as a white solid. $[\alpha]_D$ = +50.4 (MeOH). ^{1}H NMR (600 MHz, CD_3OD): δ = 5.39 (d, $J_{1,2}$ = 3.9 Hz, 1H, H-1), 4.17 (d, $J_{3',4'}$ = 8.7 Hz, 1H, H-3'), 3.87–3.92 (m, 2H, H-4', H-6'a), 3.81–3.86 (m, 3H, H-6'b, H-6a, H-6b), 3.78 (m, 1H, H-5), 3.70 (d, $J_{1'a,1'b}$ = 11.2 Hz, 1H, H-1'a), 3.68 (m, 1H, H-5'), 3.66 (d, 1H, H-1'b), 3.61 (dd, $J_{3,2}$ = 9.8 Hz, $J_{3,4}$ = 9.0 Hz, 1H, H-3), 3.54 (dd, $J_{4,5}$ = 9.8 Hz, 1H, H-4), 3.32 (dd, 1H, H-2), 0.912 (s, 9H, ^{t}Bu), 0.909 (s, 9H, ^{t}Bu), 0.900 (s, 9H, ^{t}Bu), 0.81–0.95 (m, 18H, 6 × SiCH_3) ppm. ^{13}C{H} NMR (150 MHz, CD_3OD): δ

= 105.55 (C-2'), 93.25 (C-1), 83.86 (C-5'), 77.47 (C-3'), 75.80 (C-4'), 74.98 (C-3), 74.26 (C-5), 73.21 (C-2), 71.34 (C-4), 65.86 (C-6'), 64.27 (C-1'), 64.00 (C-6), 26.61 (triple intensity, 3C-^{t}Bu), 26.50 (triple intensity, 3C-^{t}Bu), 26.44 (triple intensity, 3C-^{t}Bu), 19.44 (C_{quat}, ^{t}Bu), 19.21 (C_{quat}, ^{t}Bu), 19.18 (C_{quat}, ^{t}Bu), -4.84, -4.84, -4.93, -4.97, -5.05, -5.22 (6 × *C*H_3-Si) ppm. HRMS (ESI-TOF) calcd for $C_{30}H_{64}O_{11}Si_3Na$ $[M + Na]^+$: 707.3654, found: 707.3632. Anal. calcd for $C_{30}H_{64}O_{11}Si_3$: C, 52.60; H, 9.42; found: C, 52.59; H, 9.27.

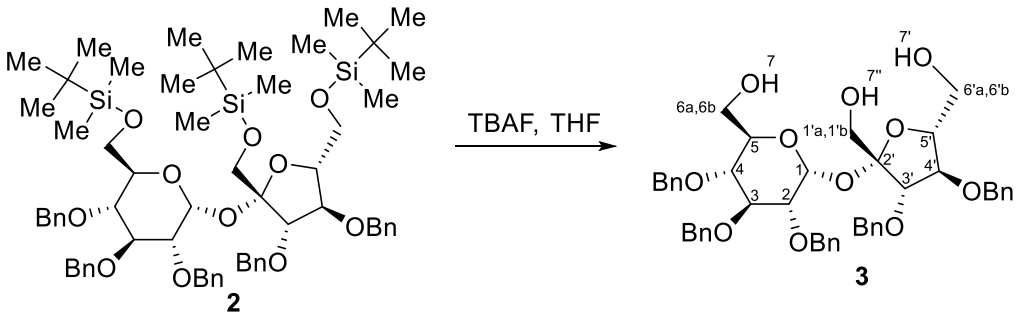
3.5. 1',6,6'-Tri-*O*-*tert*-butyldimethylsilyl-2,3,3',4,4'-penta-*O*-benzylsucrose (2)



Sodium hydride (60% dispersion in mineral oil, 6.47 g, 161.7 mmol) was added portionwise at 0–5 °C to a stirred solution of compound **S3** (10.55 g, 15.4 mmol) in DMF (385 mL) and the mixture was stirred at room temperature for 30 min. Benzyl bromide (19.2 mL, 161.7 mmol) was added dropwise during 20 min and the mixture was stirred overnight. Excess of hydride was decomposed by careful addition of methanol (20 mL) and the mixture was partitioned between saturated aq. NH_4Cl (200 mL) and diethyl ether (300 mL). The layers were separated and the aqueous one was extracted with diethyl ether (3 × 200 mL). Combined organic solutions were dried over Na_2SO_4, concentrated, and the resulting residue was purified by column chromatography (hexanes/CH_2Cl_2 = 4:1 to 1:1) to afford pure product **2** (9.6 g, 55 %) as a colorless oil. $[\alpha]_D$ = +30.3 ($CHCl_3$). ^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.37–7.53 (m, 25H, 25 × H-Ph), 6.06 (d, $J_{1,2}$ = 3.7 Hz, 1H, H-1), 5.07 (d, *J* = 10.7 Hz, 1H, benzylic H), 5.01 (d, *J* = 11.0 Hz, 1H, benzylic H), 4.93 (d, *J* = 10.7 Hz, 1H, benzylic H), 4.91 (d, *J* = 11.8 Hz, 1H, benzylic H), 4.90 (d, *J* = 11.1 Hz, 1H, benzylic H), 4.90 (d, *J* = 11.0 Hz, 1H, benzylic H), 4.84 (d, *J* = 11.0 Hz, 1H, benzylic H), 4.79 (d, *J* = 11.7 Hz, 1H, benzylic H), 4.74 (d, *J* = 11.0 Hz, 1H, benzylic H), 4.69 (d, *J* = 11.0 Hz, 1H, benzylic H), 4.65 (d, $J_{3',4'}$ = 8.2 Hz, 1H, H-3'), 4.46 (dd, $J_{4',3'}$ = 8.2 Hz, $J_{4',5'}$ = 8.0 Hz, 1H, H-4'), 4.10 (dd, $J_{3,2}$ = 9.6 Hz, $J_{3,4}$ = 9.1 Hz, 1H, H-3), 4.04–4.07 (m, 2H, H-5, H-6'a), 3.97–4.01 (m, 2H, H-5', H-6'b), 3.91 (d, $J_{1'a,1'b}$ = 11.1 Hz, 1H, H-1'a), 3.86 (dd, $J_{4,5}$ = 10.0 Hz, $J_{4,3}$ = 9.1 Hz, 1H, H-4), 3.78 (d, $J_{1'b,1'a}$ = 11.1 Hz, 1H, H-1'b), 3.73 (dd, $J_{6a,6b}$ = 11.7 Hz, $J_{6a,5}$ = 2.2 Hz, 1H, H-6a), 3.65 (dd, $J_{2,1}$ = 3.7 Hz, $J_{2,3}$ = 9.6 Hz, 1H, H-2), 3.59 (dd, $J_{6b,6a}$ = 10.7 Hz, 1H, H-6b), 1.05 (s, 9H, ^{t}Bu), 1.05 (s, 9H, ^{t}Bu), 1.02 (s, 9H, ^{t}Bu), 0.23 (s, 3H, SiCH_3), 0.21 (s, 3H, SiCH_3), 0.21 (s, 3H, SiCH_3), 0.20 (s, 3H, SiCH_3), 0.15 (s, 3H, SiCH_3), 0.14 (s, 3H, SiCH_3) ppm. ^{13}C{H} NMR (150 MHz, $CDCl_3$): δ = 139.26, 139.22, 138.83, 138.72, 138.30 (C_{quat}, 5 × C-Ph), 127.50–128.46 (m, 25 × C-Ph), 104.53 (C-2'), 88.94 (C-1), 83.17 (C-3'), 82.32 (C-3), 81.11 (C-4'), 80.72 (C-5'), 80.60 (C-2), 77.41 (C-4), 75.83, 74.86, 73.27, 72.79, 72.08 (5 × O<u>*C*</u>H_2Ph), 71.53 (C-5), 65.96 (C-1'), 63.57 (C-6'), 61.66 (C-6), 26.14 (triple intensity, 3C-^{t}Bu), 26.13 (triple intensity, 3C-^{t}Bu), 26.07 (triple intensity, 3C-^{t}Bu),18.52, 18.45, 18.43 (3 × C_{quat}, ^{t}Bu), -4.91, -5.04, -5.10, -5.24, -5.24, -5.28 (6 × Si*C*H_3) ppm. HRMS (ESI-TOF) calcd for $C_{65}H_{94}O_{11}Si_3Na$ $[M + Na]^+$:

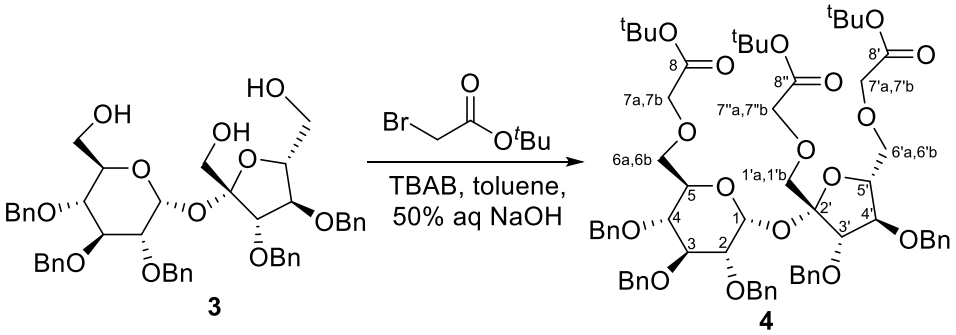
1157.6002, found: 1157.6008. Anal. calcd for $C_{67}H_{94}O_{12}Si_3$ ($C_{65}H_{94}O_{11}Si_3$+ H_2O): C, 67.83; H, 8.54; found: C, 67.89; H, 8.42.

3.6. 2,3,3',4,4'-Penta-*O*-benzylsucrose (3)



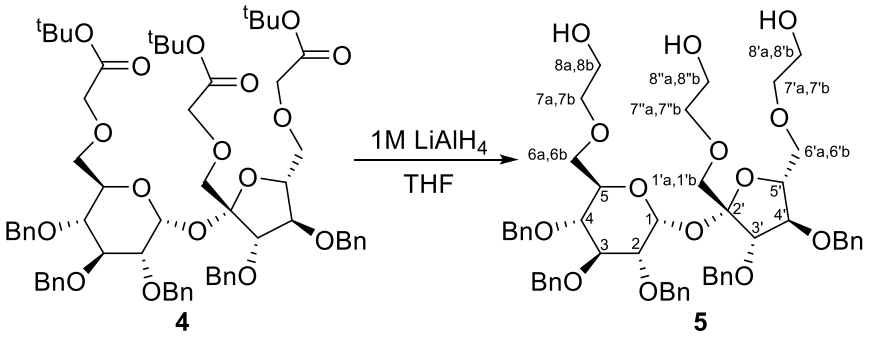
To a solution of **2** (7 g, 6.16 mmol) in THF (30 mL), a 1M TBAF solution in THF (27.7 mL) was added and the mixture was stirred for 24 h at 60 °C. The solvent was evaporated *in vacuo* and the residue was purified by column chromatography (hexanes/ethyl acetate = 4:1 to 1:2) to give pure triol **3** (3.8 g, 78 %) as a colorless oil. $[\alpha]_D$ = +18.8 ($CHCl_3$). ^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.22–7.42 (m, 25H, 25 × H-Ph), 5.25 (d, $J_{1,2}$ = 3.5 Hz, 1H, H-1), 4.92 (d, *J* = 11.7 Hz, 1H, benzylic H), 4.87 (d, *J* = 11.0 Hz, 1H, benzylic H), 4.83 (d, *J* = 11.5 Hz, 1H, benzylic H), 4.80 (s, 2H, benzylic H), 4.69 (d, *J* = 11.6 Hz, 1H, benzylic H), 4.64 (d, *J* = 11.1 Hz, 1H, benzylic H), 4.62 (d, *J* = 11.7 Hz, 1H, benzylic H), 4.56 (d, *J* = 11.7 Hz, 1H, benzylic H), 4.49 (d, *J* = 11.6 Hz, 1H, benzylic H), 4.11 (m, 1H, H-3'), 4.09 (m, 1H, H-4'), 4.07 (m, 1H, H-5), 4.02 (dd, $J_{3,2}$ = 9.4 Hz, $J_{3,4}$ = 9.4 Hz, 1H, H-3), 3.98 (dd, $J_{5',4'}$ = 9.2 Hz, $J_{5',6'a}$ = 4.5 Hz, 1H, H-5'), 3.89 (dd, $J_{7',6'a}$ = 10.9 Hz, $J_{7',6'b}$ = 3.3 Hz, 1H, H-7'), 3.83 (d, $J_{6'a,6'b}$ = 11.8 Hz, 1H, H-6a), 3.68 (dd, $J_{6b,6a}$ = 12.0 Hz, $J_{6b,5}$ = 3.5 Hz, 1H, H-6b), 3.61 (s, 2H, H-1'a, H-1'b), 3.55–3.59 (m, 2H, H-2, H-6'a), 3.49 (dd, $J_{4,5}$ = 9.6 Hz, $J_{4,3}$ = 9.4 Hz, 1H, H-4), 3.39 (dd, $J_{6'b,7'}$ = 10.9 Hz, $J_{6'b,6'a}$ = 11.3 Hz, 1H, H-6'b), 3.25 (s, 1H, H-7''), 2.63 (s, 1H, H-7) ppm. ^{13}C{H} NMR (150 MHz, $CDCl_3$): δ = 138.37, 138.35, 138.19, 137.81, 136.74 (C_{quat}, 5 × C-Ph), 127.72–128.91 (m, 25 × C-Ph), 106.05 (C-2'), 91.09 (C-1), 86.35 (C-3'), 82.33 (C-5'), 82.23 (C-4'), 81.99 (C-3), 78.83 (C-2), 77.77 (C-4), 75.69, 75.11, 75.11 (3 × O<u>*C*</u>H_2Ph), 73.87 (C-5), 72.89, 72.50 (2 × O<u>*C*</u>H_2Ph), 64.83 (C-6'), 61.71 (C-6), 60.94 (C-1') ppm. HRMS (ESI-TOF) calcd for $C_{47}H_{52}O_{11}Na$ $[M + Na]^+$: 815.3407, found: 815.3391. Anal. calcd for $C_{47}H_{52}O_{11}$: C, 71.19; H, 6.61; found: C, 70.98; H, 6.68.

3.7. 2,3,3',4,4'-Penta-*O*-benzyl-1',6,6'-tri-*O*-(2-*tert*-butoxy-2-oxoethyl)-sucrose (4)



To a solution of triol **3** (280 mg, 0.35 mmol) in toluene (8 mL), Bu_4NBr (22.8 mg, 0.07 mmol) was added followed by 50% aqueous NaOH (8 mL). Next, *tert*-butyl bromoacetate (0.31 mL, 2.12 mmol) was added and the mixture was vigorously stirred at room temperature for 24 h. The layers were separated and the aqueous one extracted with ether (3 × 15 mL). Combined organic solutions were washed with water (2 × 10 mL) and brine (10 mL), dried over Na_2SO_4, concentrated, and the residue was purified by flash chromatography (hexanes/ethyl acetate = 90:10) to afford pure product **4** (224 mg, 0.2 mmol, 56%) as a yellowish oil. $[\alpha]_D$ = +33.7 ($CHCl_3$). ^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.21–7.37 (m, 25H, 25 × H-Ph), 5.69 (d, $J_{1,2}$ = 3.6 Hz, 1H, H-1), 4.91 (d, J = 11.0 Hz, 1H, benzylic H), 4.86 (d, J = 10.8 Hz, 1H, benzylic H), 4.84 (d, J = 11.0 Hz, 1H, benzylic H), 4.77 (d, J = 11.0 Hz, 1H, benzylic H), 4.72 (d, J = 11.5 Hz, 1H, benzylic H), 4.70 (d, J = 12.2 Hz, 1H, benzylic H), 4.67 (d, J = 11.3 Hz, 1H, benzylic H), 4.62 (d, J = 11.8 Hz, 1H, benzylic H), 4.59 (d, J = 11.7 Hz, 1H, benzylic H), 4.58 (d, J = 11.7 Hz, 1H, benzylic H), 4.50 (d, $J_{3',4'}$ = 7.4 Hz, 1H, H-3'), 4.10–4.14 (m, 2H, H-4', H-5'), 4.06 (m, 1H, H-5), 4.04 (d, $J_{7''a,7''b}$ = 16.5 Hz, 1H, H-7''a), 4.03 (d, $J_{7'a,7'b}$ = 16.5 Hz, 1H, H-7'a), 3.96 (d, $J_{7'b,7'a}$ = 16.5 Hz, 1H, H-7'b), 3.94 (dd, $J_{3,4}$ = 9.8 Hz, $J_{3,2}$ = 9.7 Hz, 1H, H-3), 3.92 (d, $J_{7''b,7''a}$ = 16.5 Hz, 1H, H-7''b), 3.90 (d, $J_{1'a,1'b}$ = 11.1 Hz, 1H, H-1'a), 3.89 (d, $J_{7a,7b}$ = 16.4 Hz, 1H, H-7a), 3.85 (d, $J_{7b,7a}$ = 16.4 Hz, 1H, H-7b), 3.79 (dd, $J_{6'a,6'b}$ = 10.4 Hz, $J_{6'a,5'}$ = 6.1 Hz, 1H, H-6'a), 3.76 (dd, $J_{6'b,6'a}$ = 10.4 Hz, $J_{6'b,5'}$ = 3.6 Hz, 1H, H-6'b), 3.65 (dd, $J_{4,3}$ = 9.8 Hz, $J_{4,5}$ = 9.3 Hz, 1H, H-4), 3.61 (dd, $J_{6a,6b}$ = 10.8 Hz, $J_{6a,5}$ = 3.2 Hz, 1H, H-6a), 3.54 (dd, $J_{2,3}$ = 9.7 Hz, $J_{2,1}$ = 3.6 Hz, 1H, H-2), 3.52 (d, $J_{1'b,1'a}$ = 11.1 Hz, 1H, H-1'b), 3.47 (dd, $J_{6b,6a}$ = 10.8 Hz, $J_{6b,5}$ = 1.7 Hz, 1H, H-6b), 1.45 (s, 9H, 9 × -$CO_2C(C\underline{H}_3)_3$), 1.44 (s, 9H, 9 × -$CO_2C(C\underline{H}_3)_3$), 1.43 (s, 9H, 9 ×-$CO_2C(C\underline{H}_3)_3$) ppm. ^{13}C{H} NMR (150 MHz, $CDCl_3$): δ = 169.33, 169.29, 169.19 (C-8, C-8', C-8"), 138.96, 138.81, 138.39, 138.39, 138.32 (C_{quat}, 5 × C-Ph), 127.36–128.23 (m, 25 × C-Ph), 104.46 (C-2'), 89.96 (C-1), 83.85 (C-3'), 82.16 (C-5'), 81.91 (C-3), 81.42, 81.31, 81.19 (3 ×C_{quat}, $CO_2\underline{C}(CH_3)_3$), 79.59 (C-4'), 79.53 (C-2), 77.29 (C-4), 75.40, 74.70, 73.06 (3 × O$\underline{C}H_2$Ph), 72.62 (C-6'), 72.41 (C-1'), 72.40, 72.26 (2 × O$\underline{C}H_2$Ph), 70.54 (C-5), 69.72 (C-6), 69.09 (C-7''), 69.04 (C-7), 68.97 (C-7'), 28.10, 28.08, 28.08 (triple intensity, 9 × -$CO_2C(\underline{C}H_3)_3$) ppm. HRMS (ESI-TOF) calcd for $C_{65}H_{82}O_{17}Na$ $[M + Na]^+$: 1157.5450, found: 1157.5457. Anal. calcd for $C_{65}H_{82}O_{17}$: C, 68.76; H, 7.28; found: C, 68.76; H, 7.20.

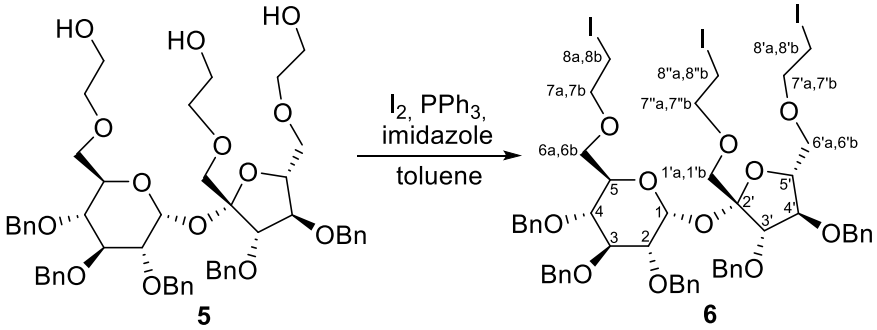
3.8. 2,3,3',4,4'-Penta-*O*-benzyl-1',6,6'-tri-O-(2-hydroxyethyl)-sucrose (5)



To the cooled to -78 °C solution of compound **4** (559 mg, 0.49 mmol) in dry THF (16 mL), 1M $LiAlH_4$ in THF (2.95 mL, 2.95 mmol) was added dropwise, the mixture was allowed to reach room temperature, and stirred additional 20 min at rt. Excess of hydride was carefully

decomposed with aqueous saturated Na_2SO_4 (5 mL) and then Celite was added. Next, the resulting residue was filtered and washed with ethyl acetate (3 × 10 mL). The organic solution was dried over Na_2SO_4, concentrated, and purified by flash chromatography (hexanes/ethyl acetate = 1:1 to 1:4) to give pure product **5** (408 mg, 0.44 mmol, 90%) as a yellowish oil. $[\alpha]_D$= +37.9 ($CHCl_3$). ^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.21–7.38 (m, 25H, 25 × H-Ph), 6.12 (d, $J_{1,2}$ = 3.9 Hz, 1H, H-1), 4.98 (d, J = 11.0 Hz, 1H, benzylic H), 4.82 (d, J = 11.1 Hz, 2H, 2 × benzylic H), 4.74 (d, J = 11.2 Hz, 2H, 2 × benzylic H), 4.69 (dd, $J_{4',5'}$ = 8.6 Hz, $J_{4',3'}$ = 8.5 Hz, 1H, H-4'), 4.66 (s, 2H, 2 × benzylic H), 4.61 (d, J = 11.8 Hz, 1H, benzylic H), 4.59 (d, J = 11.1 Hz, 1H, benzylic H), 4.52 (d, J = 11.2 Hz, 1H, benzylic H), 4.30 (d, $J_{3',4'}$ = 8.5 Hz, 1H, H-3'), 4.15 (m, 1H, H-5), 3.92 (dd, $J_{3,2}$ = 9.3 Hz, $J_{3,4}$ = 9.2 Hz, 1H, H-3), 3.84–3.94 (m, 2H, H-5', H-6'a), 3.62–3.71 (m, 5H, H-4, H-1'a, H-8''a, H-8''b, H-8a), 3.61 (m, 2H, H-7''a, H-7''b), 3.55 (d, $J_{1'b,1'a}$ = 10.8 Hz, 1H, H-1'b), 3.52 (m, 1H, H-8b), 3.46 (dd, $J_{2,3}$ = 9.6 Hz, $J_{2,1}$ = 3.9 Hz, 1H, H-2), 3.42 (m, 1H, H-8'b), 3.38 (m, 1H, H-6'b), 3.24–3.35 (m, 7H, H-8'b, H-6a, H-6b, H-7a, H-7b, H-7'a, H-7'b) ppm. ^{13}C{H} NMR (150 MHz, $CDCl_3$): δ = 139.08, 138.68, 138.02, 137.95, 137.65 (C_{quat}, 5 × C-Ph), 127.34–128.54 (m, 25 × C-Ph), 103.57 (C-2'), 88.05 (C-1), 83.74 (C-3'), 81.92 (C-3), 79.01 (C-5'), 78.92 (C-4'), 78.76 (C-2), 77.03 (C-4), 75.27, 74.69 (2 × O<u>*C*</u>H_2Ph), 74.52 (C-1'), 73.16, 73.08 (2 × O<u>*C*</u>H_2Ph), 73.04 (C-7''), 72.94 (C-7), 72.25 (C-7'), 72.02 (O<u>*C*</u>H_2Ph), 70.61 (C-5), 68.44 (C-6'), 68.40 (C-6), 61.62, 61.61, 61.57 (C-8, C-8', C-8'') ppm. HRMS (ESI-TOF) calcd for $C_{53}H_{64}O_{14}Na$ [M + Na]$^+$: 947.4194, found: 947.4183. Anal. calcd for $C_{53}H_{64}O_{14}$: C, 68.81; H, 6.97; found: C, 68.75; H, 6.95.

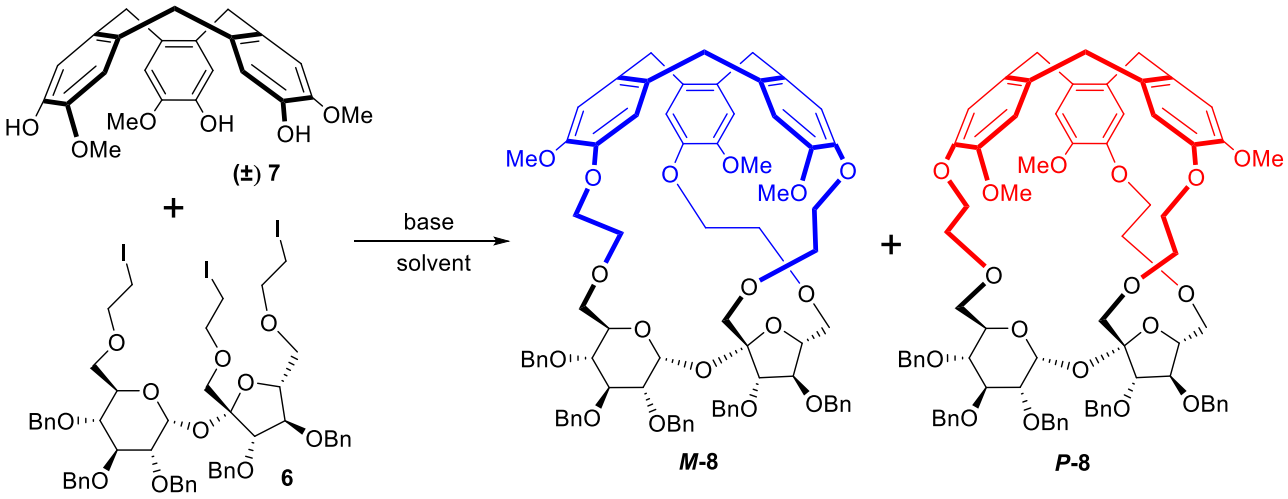
3.9. 2,3,3',4,4'-Penta-*O*-benzyl-1',6,6'-tri-O-(2-iodoethyl)-sucrose (6)



To a solution of triol **5** (702 mg, 0.759 mmol) in toluene (25 mL), PPh_3 (716 mg, 2.73 mmol) was added, the mixture was boiled under reflux for 15 min, and then cooled to 50 °C. Imidazole (310 mg, 4.55 mmol) was added, the mixture was allowed to reach room temperature, and the solution of iodine (693 mg, 2.73 mmol) in toluene (20 mL) was added dropwise during 20 min. After another 20 min, the excess of iodine was decomposed with saturated $Na_2S_2O_3$ (5 mL). Water (20 mL) was added, the phases were separated, the aqueous one was extracted with ethyl acetate (2 × 20 mL) and combined organic phases were washed with water (30 mL), brine (30 mL), dried over Na_2SO_4 and concentrated. The resulting residue was purified by flash chromatography (hexanes/ethyl acetate = 9:1) to afford compound **6** (810 mg, 0.64 mmol, 85%) as a colorless oil. $[\alpha]_D$ = +33.8 ($CHCl_3$). ^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.24–7.37 (m, 25H, 25 × H-Ph), 5.65 (d, $J_{1,2}$ = 3.5 Hz, 1H, H-1), 4.94 (d, J = 10.9 Hz, 1H, benzylic H), 4.90 (d, J = 11.1 Hz, 1H, benzylic H), 4.80 (d, J = 10.9 Hz, 1H, benzylic H), 4.79 (d, J = 11.4 Hz, 1H, benzylic H), 4.68 (d, J = 11.7Hz, 1H, benzylic H), 4.67 (d, J = 11.5 Hz, 1H, benzylic H), 4.66 (d, J = 11.8 Hz, 1H, benzylic H), 4.64 (d, J = 11.5

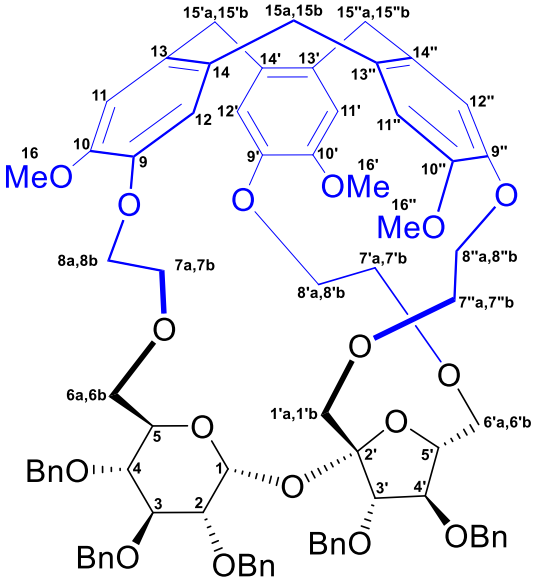
Hz, 1H, benzylic H), 4.63 (d, J = 11.8 Hz, 1H, benzylic H), 4.59 (d, J = 11.8 Hz, 1H, benzylic H), 4.45 (d, $J_{3',4'}$ = 7.3 Hz, 1H, H-3'), 4.12 (dd, $J_{4',3'}$ = 7.3 Hz, $J_{4',5'}$ = 7.3 Hz, 1H, H-4'), 4.07 (m, 1H, H-5'), 4.04 (m, 1H, H-5), 3.95 (dd, $J_{3,2}$ = 9.4 Hz, $J_{3,4}$ = 9.3 Hz, 1H, H-3), 3.65–3.73 (m, 7H, H-7a, H-7'a, H-7''a, H-7''b, H-6'a, H-6'b, H-1'a), 3.64 (m, 1H, H-4), 3.57 (m, 1H, H-6a), 3.51–3.56 (m, 3H, H-7b, H-7'b, H-2), 3.46 (d, $J_{1'b,1'a}$ = 11.0 Hz, 1H, H-1'b), 3.39 (dd, $J_{6b,6a}$ = 10.7 Hz, $J_{6b,5}$ = 1.4 Hz, 1H, H-6b), 3.08–3.22 (m, 6H, H-8a, H-8b, H-8'a, H-8'b, H-8''a, H-8''b) ppm. $^{13}C\{H\}$ NMR (150 MHz, $CDCl_3$): δ = 138.76, 138.59, 138.23, 138.16, 138.13 (C_{quat}, 5 × C-Ph), 127.53–128.38 (m, 25 × C-Ph), 104.38 (C-2'), 90.10 (C-1), 83.67 (C-3'), 82.18 (C-4'), 81.95 (C-3), 79.83 (C-2), 79.59 (C-5'), 77.39 (C-4), 75.54, 74.94, 73.13, 72.67, 72.53 (5 × O<u>C</u>H_2Ph), 72.16 (C-7'), 72.06 (C-7), 71.95 (C-7"), 71.81 (C-6'), 71.67 (C-1'), 70.63 (C-5), 69.25 (C-6), 2.82, 2.80, 2.73 (C-8, C-8', C-8'') ppm. HRMS (ESI-TOF) calcd for $C_{53}H_{61}O_{11}I_3Na$ $[M + Na]^+$: 1277.1246, found: 1277.1244. Anal. calcd for $C_{53}H_{61}O_{11}I_3$: C, 50.73; H, 4.90; found: C, 50.72; H, 5.01.

3.10. General procedure for the synthesis of compounds *M*-8 and *P*-8



To a solution (0.002 M, 160 mL or 0.001 M, 320 mL) of ***rac*-7** (130 mg, 0.319 mmol) in dry solvent (acetone/acetonitrile/propionitrile/DMF), cesium carbonate (623 mg, 1.91 mmol) was added and the mixture was stirred at room temperature for 30 min under an argon atmosphere. The solution of compound **6** (400 mg, 0.319 mmol) in appropriate dry solvent (10 mL) was added dropwise during 40 min, the mixture was stirred at required temperature for 48-96 h (for details see Table 1 of the main text). After cooling to rt., the mixture was filtered through Celite and the solvents were removed under vacuum. The residue was dissolved in CH_2Cl_2 (20 mL) and washed with water (2 × 10 mL). The aqueous phases were extracted with CH_2Cl_2 (2 × 20 mL) and the combined organic solutions were washed with brine (20 mL), dried over Na_2SO_4, and concentrated. The resulting residue was purified by flash chromatography (hexanes/ethyl acetate = 4:1 to 3:1) to afford pure compounds ***M*-8** and ***P*-8** as colorless solids.

3.10.1. Characterization of compound *M*-8

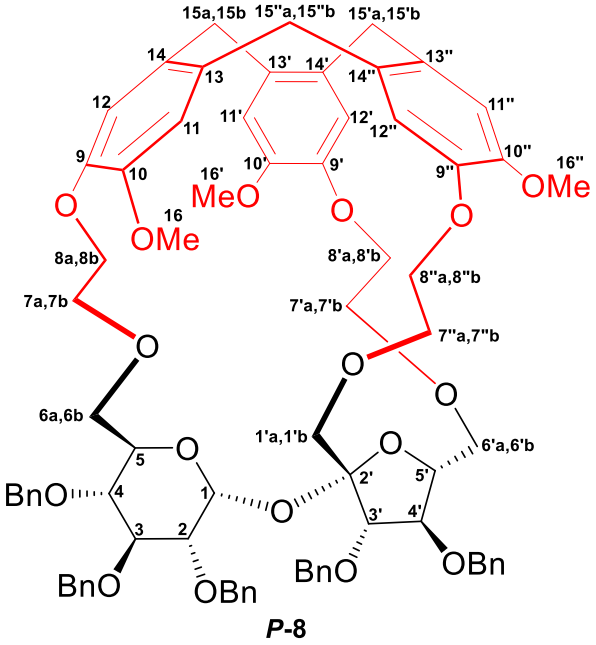


***M*-8**

$[\alpha]_D$= -60.7 ($CHCl_3$). ^{1}H NMR (600 MHz, CD_3CN): δ = 7.16–7.43 (m, 25H, 25 × H-Ph), 7.024 (s, 1H, H-12'), 7.009 (s, 1H, H-11), 6.972 (s, 1H, H-12), 6.963 (s, 1H, H-11'), 6.910 (s, 1H, H-11"), 6.837 (s, 1H, H-12"), 5.26 (d, $J_{1,2}$ = 3.1 Hz, 1H, H-1), 4.90 (d, *J*= 11.3 Hz, 1H, benzylic H), 4.75 (d, $J_{15"b,15"a}$ = 13.3 Hz, 1H, H-15"b), 4.74 (d, *J* = 11.3 Hz, 1H, benzylic H), 4.72 (d, *J* = 11.0 Hz, 1H, benzylic H), 4.72 (d, 1H, H-15'b), 4.69 (d, *J* = 11.2 Hz, 1H, benzylic H), 4.68 (d, $J_{15b,15a}$ = 13.7 Hz, 1H, H-15b), 4.65 (d, *J* = 11.8 Hz, 1H, benzylic H), 4.62 (d, *J* = 11.6 Hz, 1H, benzylic H), 4.59 (d, *J* = 11.0 Hz, 1H, benzylic H), 4.54 (d, *J* = 11.2 Hz, 1H, benzylic H), 4.49 (d, *J* = 11.8 Hz, 1H, benzylic H), 4.45 (d, *J* = 11.6 Hz, 1H, benzylic H), 4.37 (dt, $J_{8b,8a}$ = 13.0 Hz, $J_{8b,7}$ = 2.8 Hz, 1H, H-8b), 4.28 (dd, $J_{8"b,8"a}$ = 11.6 Hz, $J_{8"b,7"}$ = 7.0 Hz, 1H, H-8"b), 4.23 (m, 1H, H-8'b), 4.19 (m, 1H, H-8'a), 4.16 (m, 1H, H-8"a), 4.12 (m, 1H, H-8a), 3.97 (d, $J_{3',4'}$ = 6.6 Hz, 1H, H-3'), 3.97 (d, $J_{1'b,1'a}$ = 11.9 Hz, 1H, H-1'b), 3.94 (m, 1H, H-7"b), 3.79 (s, 3H, 3 × H-16"), 3.77 (dd, $J_{6a,6b}$ = 13.0 Hz, $J_{6a,5}$ = 2.4 Hz, 1H, H-6b), 3.74 (s, 3H, 3 × H-16), 3.74 (dd, $J_{7b,7a}$ = 13.3 Hz, $J_{7b,8}$ = 2.4 Hz, 1H, H-7b), 3.72 (s, 3H, 3 × H-16'), 3.72 (m, 1H, H-7"a), 3.65 (m, 1H, H-4'), 3.65 (m, 1H, H-3), 3.56 (m, 1H, H-7a), 3.53 (m, 1H, H-4), 3.52 (d, $J_{15"a,15"b}$ = 13.3 Hz, 1H, H-15"a), 3.50 (d, $J_{15'a,15'b}$ = 13.7 Hz ,1H, H-15'a), 3.49 (d, $J_{15a,15b}$ = 13.7 Hz, 1H, H-15a), 3.42 (d, $J_{1'a,1'b}$ = 11.9 Hz, 1H, H-1'a), 3.37 (dd, $J_{2,3}$ = 9.7 Hz, $J_{2,1}$ = 3.1 Hz, 1H, H-2), 3.36 (m, 1H, H-5'), 3.34 (m, 1H, H-5), 3.28 (m, 1H, H-7'b), 2.96 (dt, $J_{7'a,7'b}$ = 10.8 Hz, $J_{7'a,8}$ = 3.5 Hz, 1H, H-7'a), 2.89 (dd, $J_{6a,6b}$ = 13.0 Hz, $J_{6a,5}$ = 0.8 Hz, 1H, H-6a), 2.61 (dd, $J_{6'b,6'a}$ = 8.9 Hz, $J_{6'b,5'}$= 8.7 Hz, 1H, H-6'b), 1.59 (dd, $J_{6'a,6'b}$ = 8.9 Hz, $J_{6'a,5'}$ = 5.0 Hz, 1H, H-6'a) ppm. ^{13}C{H} NMR (150 MHz, CD_3CN): δ = 150.55 (C-10'), 149.75 (C-10), 148.06 (C-10"), 146.77 (C-9"), 145.60 (C-9), 145.03 (C-9'), 140.15, 140.00, 140.01, 139.87, 139.81 (C_{quat}, 5 × C-Ph), 135.15 (C-13'), 134.06 (C-13), 133.30 (C-14), 132.95 (C-14"), 131.91 (C-13"), 131.74 (C-14'), 128.21–129.33 (m, 25 ×C-Ph), 121.82 (C-12'), 117.41 (C-12), 114.96 (C-11), 114.14 (C-11'), 113.62 (C-12"), 113.04 (C-11"), 105.34 (C-2'), 91.64 (C-1), 86.59 (C-4'), 85.06 (C-3'), 82.22 (C-3), 81.81 (C-2), 80.54 (C-5'), 78.08 (C-4), 75.93, 75.34, 73.83 (3 × O<u>C</u>H_2Ph), 73.67 (C-6'), 73.22 (C-5), 72.47, 72.39 (2 × O<u>C</u>H_2Ph), 70.83 (C-1'), 70.76 (C-6), 70.65 (C-8"), 69.91 (C-7), 69.69 (C-8'), 69.21 (C-7"), 68.94 (C-8), 67.57 (C-7'), 56.89 (C-16), 56.39 (C-16'), 56.24 (C-16"), 36.32 (C-15"), 36.18 (C-15), 35.87 (C-15')

ppm. HRMS (ESI-TOF) calcd for $C_{77}H_{82}O_{17}Na$ $[M + Na]^+$: 1301.5450, found: 1301.5447. Anal. calcd for $C_{77}H_{82}O_{17}$: C, 72.28; H, 6.46; found: C, 72.26; H, 6.67.

3.10.2. Characterization of compound *P*-8

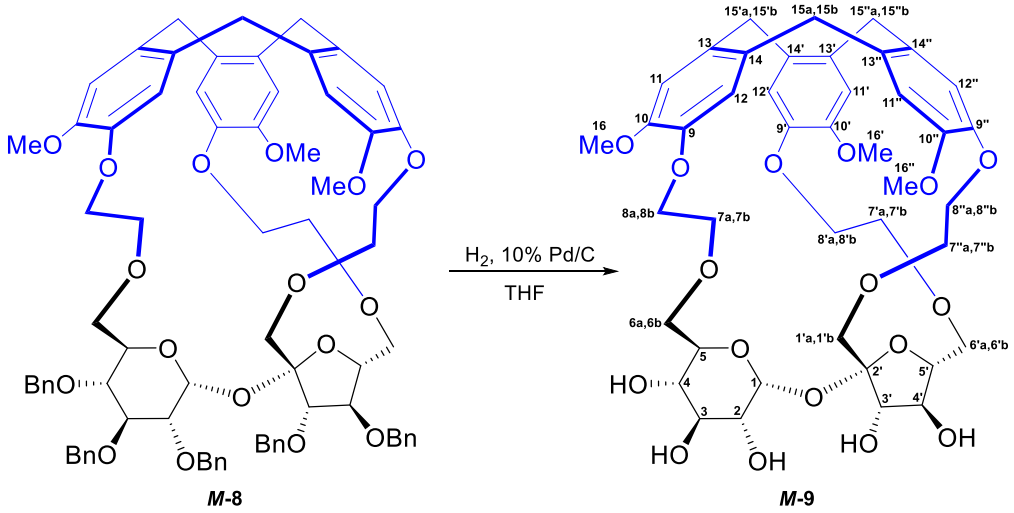


***P*-8**

$[\alpha]_D$= +101.4 ($CHCl_3$). ^{1}H NMR (600 MHz, CD_3CN): δ = 7.20–7.35 (m, 25H, 25 × H-Ph), 7.004 (s, 1H, H-11), 6.971 (s, 1H, H-12'), 6.919 (s, 1H, H-11"), 6.915 (s, 1H, H-11'), 6.902 (s, 1H, H-12), 6.896 (s, 1H, H-12"), 4.93 (d, $J_{1,2}$ = 3.5 Hz, 1H, H-1), 4.75 (d, $J_{15b,15a}$ = 13.3 Hz, 1H, H-15b), 4.74 (d, *J* = 11.3 Hz, 1H, benzylic H), 4.72 (d, *J* = 11.3 Hz, 1H, benzylic H), 4.70 (m, 1H, H-15'b), 4.66 (m, 2H, 2 × benzylic H), 4.65 (m, 1H, benzylic H), 4.65 (d, *J* = 11.3 Hz, 1H, benzylic H), 4.65 (d, $J_{15"b,15"a}$ = 13.5 Hz, 1H, H-15"b), 4.62 (d, *J*= 11.7 Hz, 1H, benzylic H), 4.55 (d, *J* = 11.3 Hz, 1H, benzylic H), 4.52 (d, *J*= 11.7 Hz, 1H, benzylic H), 4.47 (d, *J* = 11.3 Hz, 1H, benzylic H), 4.28 (ddd, $J_{8"b,8"a}$ = 12.3 Hz, $J_{8"b,7"a}$ = 6.1 Hz, $J_{8"b,7"b}$ = 1.5 Hz, 1H, H-8"b), 4.22 (m, 2H, H-8a, H-8b), 4.12 (d, $J_{3',4'}$ = 7.5 Hz, 1H, H-3'), 4.09 (ddd, $J_{8"a,8"b}$ = 12.3 Hz, $J_{8"a,7"a}$ = 6.2 Hz, $J_{8"a,7"b}$ = 2.0 Hz, 1H, H-8"a), 4.05 (m, 2H, H-8'a, H-8'b), 3.772 (s, 3H, 3 × H-16), 3.75 (m, 1H, H-7"b), 3.71 (dd, $J_{4'5'}$ = 7.6 Hz, $J_{4'3'}$ = 7.5 Hz, 1H, H-4'), 3.678 (s, 3H, 3 × H-16'), 3.653 (s, 3H, 3 × H-16"), 3.646 (m, 1H, H-3), 3.62 (m, 1H, H-7"a), 3.56 (m, 1H, H-7b), 3.49 (d, $J_{15a,15b}$ = 13.3 Hz, 1H, H-15a), 3.48 (d, $J_{15"a,15"b}$ = 13.5 Hz, 1H, H-15"a), 3.47 (m, 1H, H-7a), 3.47 (d, $J_{1'b,1'a}$ = 11.6 Hz, 1H, H-1'b), 3.46 (m, 1H, H-15'a), 3.456 (m, 1H, H-4), 3.436 (m, 1H, H-5), 3.42 (m, 1H, H-6b), 3.354 (dd, $J_{2,3}$ = 9.6 Hz, $J_{2,1}$ = 3.5 Hz, 1H, H-2), 3.32 (m, 1H, H-7'b), 3.21 (d, $J_{1'a,1'b}$ = 11.6 Hz, 1H, H-1'a), 3.20 (m, 1H, H-7'a), 3.14 (ddd, $J_{5',4'}$ = 7.6 Hz, $J_{5',6'a}$ = 6.6 Hz, $J_{5',6'b}$ = 4.5 Hz, 1H, H-5'), 2.47 (dd, $J_{6a,6b}$ = 11.6 Hz, $J_{6a,5}$ = 1.6 Hz, 1H, H-6a), 2.29 (dd, $J_{6'a,6'b}$ = 11.5 Hz, $J_{6'a,5'}$ = 6.6 Hz, 1H, H-6'a), 2.02 (dd, $J_{6'b,6'a}$ = 11.5 Hz, $J_{6'b,5'}$ = 4.5 Hz, 1H, H-6'b) ppm. ^{13}C{H} NMR (150 MHz, CD_3CN): δ = 150.39 (C-10'), 150.23 (C-10), 148.33 (C-10"), 146.47 (C-9"), 145.75 (C-9), 145.45 (C-9'), 140.15, 139.99, 139.92, 139.75, 139.68 (C_{quat}, 5 × C-Ph), 135.48 (C-13'), 134.01 (C-14), 133.88 (C-14"), 133.40 (C-13"), 132.47, 132.42 (C-13, C-14'), 128.31–129.29 (m, 25 × C-Ph), 122.32 (C-12'), 119.49 (C-12), 115.98 (C-11), 115.41 (C-12"), 113.92 (C-11'), 113.85 (C-11"), 104.22 (C-2'), 92.04 (C-1), 84.90 (C-3'), 84.61 (C-4'), 82.51 (C-3), 81.19 (C-2), 78.62 (C-5'), 78.17 (C-4), 75.83, 75.16, 73.90, 72.87 (4 × O<u>*C*</u>H_2Ph), 72.74 (C-

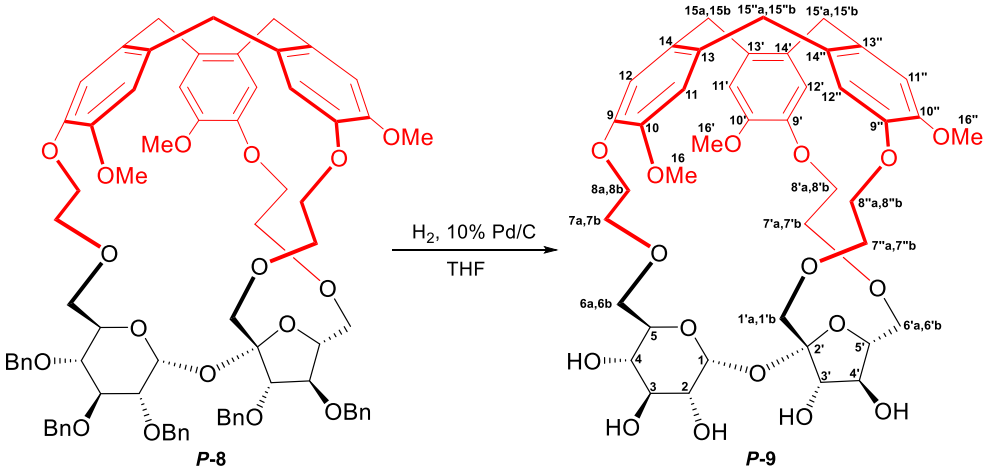
6'), 72.71 (O<u>*C*</u>H$_2$Ph), 71.83 (C-5), 70.63 (C-7'), 70.39 (C-1'), 70.17 (C-6), 69.96 (C-8'), 69.89 (C-7"), 69.46 (C-7), 68.09 (C-8), 66.94 (C-8"), 57.59 (C-16), 56.40 (C-16'), 56.11 (C-16"), 36.33 (C-15"), 36.20 (C-15), 35.95 (C-15') ppm. HRMS (ESI-TOF) calcd for $C_{77}H_{82}O_{17}Na$ $[M + Na]^+$: 1301.5450, found: 1301.5426. Anal. calcd for $C_{77}H_{82}O_{17}$: C, 72.28; H, 6.46; found: C, 72.30; H, 6.53.

3.11. Compound *M*-9



To a solution of compound ***M*-8** (51 mg, 0.04 mmol) in THF (4 mL), 10% Pd/C (10.6 mg, 0.01 mmol) was added and the mixture was stirred under a hydrogen atmosphere in an autoclave for 24 h at room temperature. The mixture was filtered through Celite, washed with THF (20 mL), and concentrated under reduced pressure. The pure product ***M*-9** (32.5 mg, 98%) was obtained as a white solid without further purification. $[\alpha]_D$ = –43.7 ($CHCl_3$). ^{1}H NMR (500 MHz, CD_3OD): δ = 7.07 (s, 1H, H-11'), 7.04 (s, 1H, H-12), 7.03 (s, 1H, H-11), 7.01 (s, 1H, H-12'), 6.91 (s, 1H, H-11''), 6.89 (s, 1H, H-12''), 5.00 (d, $J_{1,2}$ = 3.6 Hz, 1H, H-1), 4.79 (d, $J_{15'b,15'a}$ = 13.3 Hz, 1H, H-15'b), 4.75 (d, $J_{15''b,15''a}$ = 13.5 Hz, 1H, H-15''b), 4.71 (d, $J_{15b,15a}$ = 13.3 Hz, 1H, H-15b), 4.40 (m, 1H, H-7a), 4.29 (m, 1H, H-8''a), 4.19–4.23 (m, 2H, H-8'a, H-8'b), 4.11–4.18 (m, 2H, H-7b, H-8''b), 3.96 (d, $J_{3',4'}$ = 8.3 Hz, 1H, H-3'), 3.92 (m, 1H, H-7"a), 3.82 (s, 3H, 3 × H-16'), 3.77 (s, 3H, 3 × H-16), 3.77 (s, 3H, 3 × H-16''), 3.70–3.78 (m, 3H, H-7"b, H-1'a, H-6a), 3.62–3.68 (m, 2H, H-4', H-8a), 3.46–3.60 (m, 6H, H-3, H-1'b, H-8b, H-15a, H-15'a, H-15"a), 3.30–3.38 (m, 2H, H-4, H-5'), 3.20–3.27 (m, 3H, H-2, H-5, H-7'a), 3.01 (m, 1H, H-7'b), 2.74–2.80 (m, 2H, H-6'a, H-6b), 1.73 (dd, $J_{6'b,6'a}$ = 9.2 Hz, $J_{6'b,5'}$ = 5.9 Hz, 1H, H-6') ppm. ^{13}C{H} NMR (125 MHz, CD_3OD): δ = 150.56 (C-10'), 149.84 (C-10), 148.70 (C-10"), 147.10 (C-9''), 145.99 (C-9), 144.97 (C-9'), 136.03 (C-13'), 134.87 (C-13), 134.10 (C-14), 133.48 (C-13''), 132.69 (C-14''), 132.63 (C-14'), 121.85 (C-11'), 117.96 (C-12), 115.12 (C-11), 114.44 (C-12''), 114.04 (C-12'), 113.51 (C-11"), 105.89 (C-2'), 94.33 (C-1), 80.69 (C-5'), 79.68 (C-4'), 78.15 (C-3'), 75.02 (C-6'), 74.51 (C-3), 73.75 (C-5), 73.45 (C-2), 71.38 (C-6), 71.23 (C-8''), 70.96 (C-8), 70.71 (C-4), 70.40 (C-8'), 70.22 (C-7''), 69.86 (C-1'), 69.45 (C-7), 67.96 (C-7'), 57.00 (C-16), 56.33 (C-16'), 56.06 (C-16''), 36.60 (C-15'), 36.50 (C-15), 36.14 (C-15'') ppm. HRMS (ESI-TOF) calcd for $C_{42}H_{52}O_{17}K$ $[M + K]^+$: 867.2842, found: 867.2832.

3.12. Compound *P*-9



Compound ***P*-9** was synthesized according to previously described procedure for compound ***M*-9**. Compound ***P*-8** (48 mg, 0.038 mmol), 10% Pd/C (10 mg, 0.009 mmol) in THF (4 mL) gave unprotected ***P*-9** (31 mg, 99%) as a white solid. $[\alpha]_D$ = +120.5 ($CHCl_3$). ^{1}H NMR (500 MHz, CD_3OD): δ = 7.05 (s, 1H, H-11'), 7.02 (s, 1H, H-12), 7.00 (s, 1H, H-12''), 6.98 (s, 2H, H-11, H-12'), 6.95 (s, 1H, H-11''), 4.80 (d, $J_{15b,15a}$ = 13.2 Hz, 1H, H-15b), 4.78 (d, $J_{15'b,15'a}$ = 13.4 Hz, 1H, H-15'b), 4.77 (d, $J_{1,2}$ = 3.6 Hz, 1H, H-1), 4.72 (d, $J_{15''b,15''a}$ = 13.4 Hz, 1H, H-15''b), 4.40 (m, 1H, H-8''a), 4.31 (m, 1H, H-8a), 4.22–4.28 (m, 2H, H-8b, H-8'a), 4.16–4.21 (m, 2H, H-8'b, H-8''b), 4.03 (d, $J_{3',4'}$ = 8.8 Hz, 1H, H-3'), 3.85 (s, 3H, 3 × H-16''), 3.832 (s, 3H, 3 × H-16), 3.828 (s, 3H, 3 × H-16'), 3.80 (m, 1H, H-7''a), 3.73 (m, 1H, H-7''b), 3.68 (dd, $J_{4',3'}$ = 8.8 Hz, $J_{4',5'}$ = 8.2 Hz, 1H, H-4'), 3.51–3.61 (m, 7H, H-15a, H-15'a, H-15"a, H-7'a, H-7a, H-7b, H-1'a), 3.49 (dd, $J_{6a,6b}$ = 12.2 Hz, $J_{6a,5}$ = 1.5 Hz, 1H, H-6a), 3.45 (dd, $J_{3,2}$ = 9.7 Hz, $J_{3,4}$ = 8.7 Hz, 1H, H-3), 3.37–3.41 (m, 2H, H-4, H-7'b), 3.35 (m, 1H, H-5), 3.27 (dd, $J_{2,3}$ = 9.7 Hz, $J_{2,1}$ = 3.6 Hz, 1H, H-2), 3.23 (d, $J_{1'b,1'a}$ = 12.0 Hz, 1H, H-1'b), 3.11 (ddd, $J_{5',4'}$ = 8.2 Hz, $J_{5',6'a}$ = 6.9 Hz, $J_{5',6'b}$ = 4.5 Hz, 1H, H-5'), 2.50 (dd, $J_{6'a,6'b}$ = 11.4 Hz, $J_{6'a,5'}$ = 6.9 Hz, 1H, H-6'a), 2.44 (dd, $J_{6b,6a}$ = 12.2 Hz, $J_{6b,5}$ = 1.8 Hz, 1H, H-6b), 2.15 (dd, $J_{6'b,6'a}$ = 11.4 Hz, $J_{6'b,5'}$ = 4.4 Hz, 1H, H-6'b) ppm. ^{13}C{H} NMR (125 MHz, CD_3OD): δ = 150.69 (C-10), 150.40 (C-10'), 148.66 (C-10"), 146.30 (C-9''), 145.93 (C-9'), 145.55 (C-9), 135.51 (C-13'), 134.98 (C-13), 134.46 (C-14), 134.11 (C-13''), 133.20 (C-14'), 132.96 (C-14"), 121.83 (C-11'), 120.69 (C-12'), 115.94 (C-11''), 115.22 (C-12), 114.42 (C-11), 114.22 (C-12"), 104.60 (C-2'), 94.63 (C-1), 79.65 (C-5'), 78.11 (C-3'), 77.54 (C-4'), 74.69(C-3), 73.63 (C-5), 73.35 (C-2), 73.17(C-6'), 71.28 (C-7), 71.17 (C-7'), 70.59 (C-4), 70.44 (C-7''), 70.44 (C-6), 70.41 (C-8'), 69.21 (C-8), 68.61 (C-1'), 67.58 (C-8''), 56.93 (C-16), 56.53 (C-16'), 56.25 (C-16''), 36.69 (C-15"), 36.53 (C-15), 36.37 (C-15') ppm. HRMS (ESI-TOF) calcd for $C_{42}H_{52}O_{17}K$ $[M + K]^+$: 867.2842, found: 867.2838.

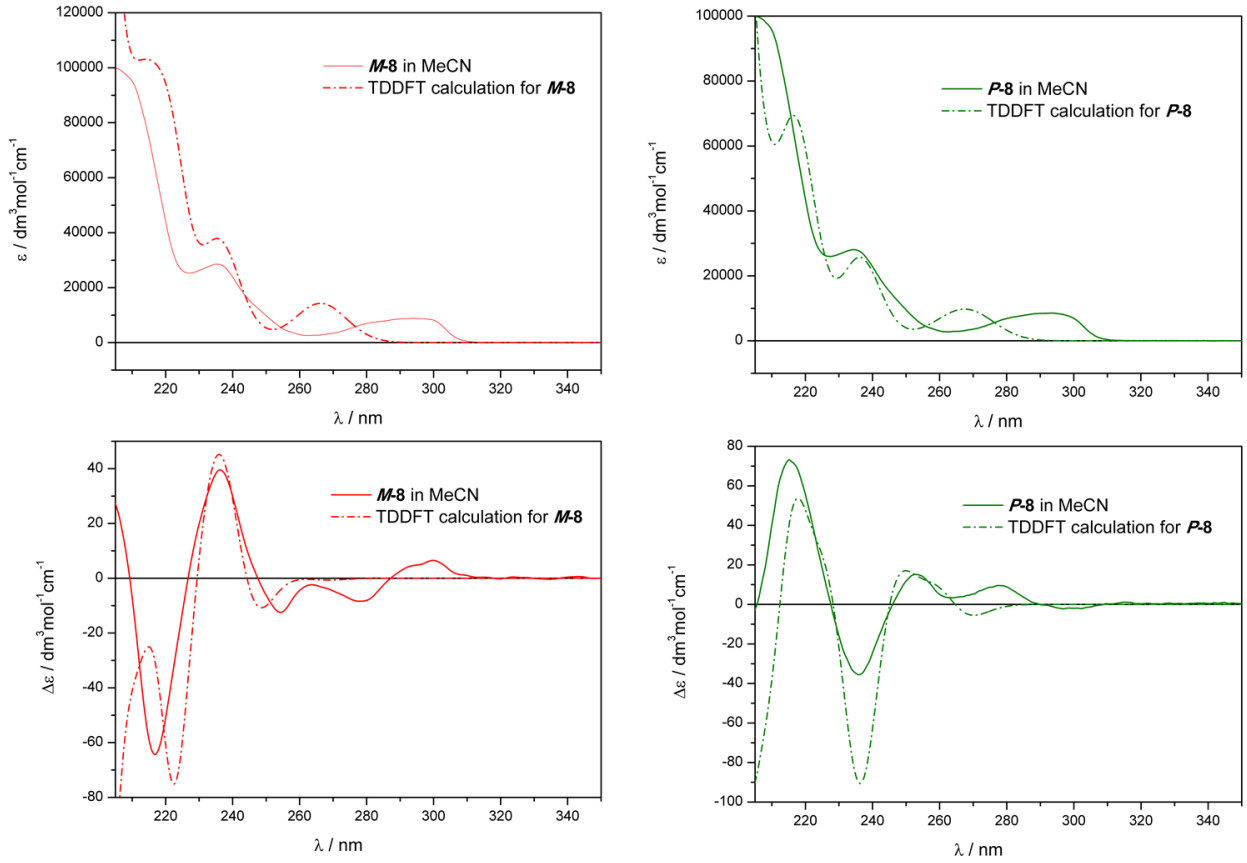


Figure S1. Comparison of experimental UV (top) and ECD (bottom) spectra of compounds ***M*-8** and ***P*-8** in MeCN solution with the simulated curves calculated at CAM-B3LYP/SVP/PCM(MeCN) level of theory.

Table S1. Calculated at CAM-B3LYP/SVP/PCM(CH_3CN) level of theory relative energies and conformer distribution at 25° C for *M*-8.

Conformer.	ΔG [kcal mol^{-1}]	Pop. [%]
***M*-8**(1)	0.00	43.7
***M*-8**(2)	0.46	20.2
***M*-8**(3)	0.60	15.8
***M*-8**(4)	0.99	8.2
***M*-8**(5)	1.13	6.4
***M*-8**(6)	1.21	5.7

Cartesian coordinates for individual conformers of compound *M*-8.

Compound ***M*-8**,conformer 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.595787	-1.927003	2.696787
2	6	0	-5.340892	-0.780099	2.396877
3	6	0	-4.904630	0.452196	2.911562
4	6	0	-3.731207	0.487324	3.676380
5	6	0	-2.970757	-0.651411	3.930932
6	6	0	-3.427503	-1.887920	3.445321
7	1	0	-4.923842	-2.905747	2.340691
8	1	0	-3.406022	1.437411	4.103947
9	6	0	-5.658107	1.756041	2.702008
10	1	0	-5.495160	2.383434	3.589458
11	1	0	-6.736388	1.564441	2.666166
12	6	0	-6.591441	-0.937961	1.551553
13	1	0	-7.364920	-0.238196	1.887228
14	1	0	-6.997691	-1.941890	1.739563
15	6	0	-5.222826	2.552703	1.483372
16	6	0	-5.901554	2.521284	0.253559
17	6	0	-4.083575	3.359474	1.598887
18	6	0	-5.393590	3.275126	-0.810570
19	6	0	-3.574474	4.091631	0.532995
20	1	0	-3.549300	3.425873	2.548824
21	6	0	-4.237010	4.034922	-0.701602
22	1	0	-5.904703	3.272759	-1.775505
23	6	0	-6.387888	-0.803912	0.050294
24	6	0	-5.834494	-1.885867	-0.643002
25	6	0	-6.723622	0.352012	-0.674026
26	6	0	-5.622683	-1.862440	-2.015862
27	1	0	-5.522431	-2.784413	-0.106766
28	6	0	-6.592837	0.333935	-2.066988
29	6	0	-6.064167	-0.752192	-2.751361
30	1	0	-6.895899	1.197165	-2.662738

31	6	0	-7.123982	1.658306	-0.016217
32	1	0	-7.792480	2.205657	-0.694985
33	1	0	-7.694240	1.485615	0.902511
34	8	0	-2.733233	-3.043992	3.661797
35	8	0	-1.831497	-0.637619	4.669046
36	8	0	-2.428254	4.812337	0.698880
37	8	0	-3.771491	4.745635	-1.774989
38	8	0	-5.940989	-0.687846	-4.109480
39	8	0	-4.999038	-2.925827	-2.608948
40	6	0	-6.719545	-1.619707	-4.843453
41	1	0	-6.528945	-1.430374	-5.907331
42	1	0	-6.442054	-2.657485	-4.602968
43	1	0	-7.793741	-1.477205	-4.640030
44	6	0	-2.685816	-3.501769	5.003909
45	1	0	-2.182937	-2.774868	5.657390
46	1	0	-3.701575	-3.697908	5.386444
47	1	0	-2.117945	-4.440655	5.000954
48	6	0	-2.562332	6.222865	0.612599
49	1	0	-1.560822	6.648660	0.750346
50	1	0	-2.955912	6.527938	-0.367627
51	1	0	-3.226633	6.601049	1.407738
52	6	0	-3.773963	-2.644644	-3.277799
53	1	0	-3.941833	-2.013886	-4.163876
54	1	0	-3.383396	-3.616221	-3.609182
55	6	0	-2.759502	-1.981666	-2.360345
56	1	0	-3.089083	-0.968617	-2.076300
57	1	0	-2.661473	-2.564966	-1.428609
58	6	0	-0.891744	0.410707	4.496744
59	1	0	-1.243308	1.114107	3.728633
60	1	0	-0.786275	0.975675	5.436860
61	6	0	0.454419	-0.184391	4.117059
62	1	0	1.173055	0.640563	3.949968
63	1	0	0.831685	-0.796270	4.948925
64	6	0	-3.021139	4.027410	-2.743641
65	1	0	-3.394905	2.994767	-2.837435
66	1	0	-3.169279	4.532024	-3.709045
67	6	0	-1.543487	4.021006	-2.397319
68	1	0	-1.387991	3.571241	-1.400678
69	1	0	-1.178044	5.063633	-2.341123
70	8	0	-1.540656	-1.922011	-3.066295
71	8	0	0.386171	-1.042825	3.007154
72	8	0	-0.865333	3.313126	-3.405702
73	6	0	2.438100	3.065281	-1.704466
74	6	0	1.181876	2.480954	-2.349716
75	6	0	1.994826	0.245623	-2.211756
76	6	0	3.296167	0.703345	-1.532449
77	6	0	3.099524	2.028066	-0.804079
78	1	0	0.461815	2.268631	-1.542223
79	1	0	3.150149	3.353944	-2.499335
80	1	0	2.189879	-0.604526	-2.876544

81	1	0	4.035405	0.871294	-2.335896
82	1	0	2.428171	1.862329	0.055197
83	8	0	1.502146	1.274018	-3.030624
84	8	0	1.077587	-0.096634	-1.215909
85	8	0	3.783775	-0.233290	-0.610144
86	8	0	4.339188	2.534617	-0.362491
87	8	0	2.053184	4.191087	-0.951552
88	6	0	4.621645	2.363460	1.008061
89	1	0	3.891824	2.920943	1.623578
90	1	0	4.531497	1.296733	1.277282
91	6	0	2.947936	5.278871	-0.961707
92	1	0	2.967229	5.747570	-1.964776
93	1	0	3.971056	4.928698	-0.748328
94	6	0	6.016263	2.843502	1.314180
95	6	0	6.336244	3.285161	2.601254
96	6	0	7.018001	2.818137	0.340971
97	6	0	7.633537	3.683622	2.913590
98	1	0	5.558688	3.320417	3.369118
99	6	0	8.315062	3.223025	0.650437
100	1	0	6.768709	2.485053	-0.667148
101	6	0	8.628374	3.654336	1.937640
102	1	0	7.867149	4.026684	3.924011
103	1	0	9.087684	3.200997	-0.121671
104	1	0	9.645091	3.971647	2.179538
105	6	0	2.545171	6.305785	0.065543
106	6	0	1.489658	6.088314	0.951592
107	6	0	3.262555	7.504386	0.148270
108	6	0	1.161968	7.050849	1.908036
109	1	0	0.921309	5.160552	0.884508
110	6	0	2.934798	8.464196	1.100087
111	1	0	4.090590	7.686464	-0.542552
112	6	0	1.881067	8.239832	1.986651
113	1	0	0.336086	6.865657	2.598938
114	1	0	3.505195	9.394370	1.151454
115	1	0	1.623083	8.991579	2.735707
116	6	0	0.535468	3.429266	-3.349047
117	1	0	0.816112	4.466900	-3.101060
118	1	0	0.926832	3.189888	-4.348714
119	6	0	0.066920	-1.074664	-1.430064
120	8	0	-0.837188	-0.915502	-0.384568
121	6	0	-0.329443	-1.536381	0.802050
122	6	0	0.760289	-2.525807	0.331421
123	6	0	0.614694	-2.481813	-1.188479
124	1	0	-1.151226	-2.102157	1.267048
125	1	0	1.765467	-2.166836	0.611480
126	1	0	-0.180343	-3.198105	-1.460792
127	6	0	-0.666274	-0.873287	-2.755976
128	1	0	-1.188319	0.099645	-2.713310
129	1	0	0.064195	-0.824125	-3.572838
130	8	0	1.763901	-2.733123	-1.938438

131	8	0	0.564892	-3.847196	0.764567
132	6	0	0.953712	-4.100915	2.105296
133	1	0	0.443765	-3.395124	2.780668
134	1	0	2.041184	-3.938771	2.216185
135	6	0	0.591848	-5.519325	2.447410
136	6	0	1.562366	-6.521062	2.500940
137	6	0	-0.745595	-5.858420	2.681319
138	6	0	1.208624	-7.839247	2.787698
139	1	0	2.609338	-6.265423	2.318022
140	6	0	-1.102414	-7.174155	2.962888
141	1	0	-1.509063	-5.076267	2.650585
142	6	0	-0.124852	-8.168224	3.017098
143	1	0	1.978894	-8.612564	2.829912
144	1	0	-2.149251	-7.427121	3.146073
145	1	0	-0.404399	-9.200111	3.241158
146	6	0	4.643339	-1.214633	-1.134316
147	1	0	4.137019	-1.792420	-1.926817
148	1	0	5.528645	-0.734401	-1.593608
149	6	0	5.091482	-2.160848	-0.049521
150	6	0	4.656335	-2.035110	1.270194
151	6	0	5.970364	-3.200606	-0.374468
152	6	0	5.089527	-2.933411	2.247030
153	1	0	3.971646	-1.228080	1.531012
154	6	0	6.402136	-4.096366	0.598258
155	1	0	6.318080	-3.310948	-1.405047
156	6	0	5.961597	-3.966317	1.916050
157	1	0	4.740480	-2.820981	3.276125
158	1	0	7.088173	-4.902094	0.327378
159	1	0	6.300995	-4.667969	2.681062
160	6	0	3.100393	-4.309300	-3.143479
161	6	0	2.851845	-3.695551	-4.374915
162	6	0	4.194878	-5.168678	-3.025913
163	6	0	3.681906	-3.937656	-5.466158
164	1	0	1.999238	-3.020939	-4.471852
165	6	0	5.022241	-5.419006	-4.119579
166	1	0	4.405748	-5.644655	-2.065075
167	6	0	4.768994	-4.802211	-5.342491
168	1	0	3.477501	-3.449926	-6.422000
169	1	0	5.874125	-6.094146	-4.012184
170	1	0	5.419497	-4.992692	-6.198902
171	6	0	2.178482	-4.083960	-1.973649
172	1	0	1.288348	-4.734663	-2.066236
173	1	0	2.678941	-4.364959	-1.031912
174	6	0	0.114633	-0.447517	1.765355
175	1	0	-0.706720	0.285767	1.828850
176	1	0	1.002868	0.076290	1.369605

Compound ***M*-8**, conformer 2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.652068	-1.541195	3.282535
2	6	0	-5.566789	-0.686133	2.664773
3	6	0	-5.353962	0.701301	2.754023
4	6	0	-4.246448	1.155975	3.477561
5	6	0	-3.325255	0.296730	4.074612
6	6	0	-3.526868	-1.088878	3.968019
7	1	0	-4.797646	-2.622563	3.246479
8	1	0	-4.087870	2.230251	3.595147
9	6	0	-6.266730	1.730191	2.107133
10	1	0	-6.234800	2.643896	2.716810
11	1	0	-7.307130	1.386696	2.136394
12	6	0	-6.760753	-1.309600	1.963385
13	1	0	-7.629344	-0.646291	2.039238
14	1	0	-7.032285	-2.219048	2.517689
15	6	0	-5.871411	2.100680	0.686308
16	6	0	-6.453165	1.526213	-0.456687
17	6	0	-4.865321	3.060603	0.514129
18	6	0	-5.978271	1.911611	-1.715275
19	6	0	-4.389828	3.429574	-0.738663
20	1	0	-4.413170	3.545636	1.381744
21	6	0	-4.946789	2.825924	-1.875384
22	1	0	-6.416111	1.483151	-2.619208
23	6	0	-6.536351	-1.708791	0.514786
24	6	0	-5.868729	-2.909814	0.253333
25	6	0	-6.961108	-0.928373	-0.573142
26	6	0	-5.617534	-3.357858	-1.037356
27	1	0	-5.499042	-3.526989	1.074510
28	6	0	-6.776176	-1.424206	-1.868324
29	6	0	-6.123623	-2.624220	-2.120729
30	1	0	-7.139548	-0.864628	-2.732562
31	6	0	-7.540065	0.464170	-0.415514
32	1	0	-8.235159	0.650881	-1.245800
33	1	0	-8.132163	0.545253	0.502064
34	8	0	-2.686973	-2.039326	4.449503
35	8	0	-2.267978	0.771907	4.793321
36	8	0	-3.374519	4.336197	-0.834659
37	8	0	-4.505674	3.162525	-3.126865
38	8	0	-5.954446	-3.031698	-3.412679
39	8	0	-4.896629	-4.507760	-1.212587
40	6	0	-6.623426	-4.229547	-3.774692
41	1	0	-6.404532	-4.412205	-4.834297
42	1	0	-6.272873	-5.085108	-3.177503
43	1	0	-7.713268	-4.122220	-3.646535
44	6	0	-2.051204	-1.880680	5.705970
45	1	0	-1.133506	-1.286710	5.619180
46	1	0	-2.723797	-1.403415	6.435256
47	1	0	-1.803971	-2.891738	6.057637

48	6	0	-3.702844	5.568780	-1.459473
49	1	0	-4.049068	5.413324	-2.490937
50	1	0	-4.481510	6.099872	-0.886790
51	1	0	-2.789180	6.175100	-1.468353
52	6	0	-3.658233	-4.371099	-1.901384
53	1	0	-3.817982	-4.036622	-2.937839
54	1	0	-3.212971	-5.374946	-1.923157
55	6	0	-2.715143	-3.413651	-1.191432
56	1	0	-3.115340	-2.387145	-1.210012
57	1	0	-2.613379	-3.703306	-0.131368
58	6	0	-1.357746	1.668720	4.178387
59	1	0	-1.715651	1.945154	3.175530
60	1	0	-1.300006	2.594907	4.772440
61	6	0	0.025754	1.040924	4.122884
62	1	0	0.715999	1.746671	3.622119
63	1	0	0.393425	0.877155	5.145908
64	6	0	-3.630148	2.244553	-3.764083
65	1	0	-3.927154	1.205710	-3.544939
66	1	0	-3.727806	2.405600	-4.846882
67	6	0	-2.190339	2.476474	-3.344825
68	1	0	-1.900385	3.514453	-3.593557
69	1	0	-2.089493	2.366283	-2.250114
70	8	0	-1.475364	-3.472205	-1.861225
71	8	0	0.044534	-0.220152	3.498606
72	8	0	-1.384669	1.556948	-4.038827
73	6	0	1.742110	2.209664	-2.156140
74	6	0	0.637263	1.287317	-2.674140
75	6	0	1.731980	-0.666002	-1.852447
76	6	0	2.938529	0.150478	-1.357928
77	6	0	2.490445	1.561636	-0.996829
78	1	0	-0.129558	1.221489	-1.884665
79	1	0	2.459621	2.411863	-2.972695
80	1	0	2.053118	-1.647779	-2.221095
81	1	0	3.645394	0.217619	-2.203488
82	1	0	1.789697	1.498435	-0.148367
83	8	0	1.148610	-0.011205	-2.949219
84	8	0	0.825467	-0.794847	-0.796604
85	8	0	3.568855	-0.408762	-0.235597
86	8	0	3.590068	2.373446	-0.651840
87	8	0	1.123249	3.401201	-1.730698
88	6	0	3.757365	2.609081	0.725029
89	1	0	2.859879	3.108949	1.136632
90	1	0	3.869093	1.650524	1.261654
91	6	0	1.835426	4.596029	-1.959069
92	1	0	1.787727	4.863283	-3.033552
93	1	0	2.897779	4.464132	-1.703052
94	6	0	4.967167	3.473351	0.973763
95	6	0	5.234018	3.915408	2.274544
96	6	0	5.838737	3.836546	-0.053700
97	6	0	6.349900	4.701425	2.542425

98	1	0	4.556155	3.641203	3.087821
99	6	0	6.957414	4.627050	0.214279
100	1	0	5.634808	3.492120	-1.067466
101	6	0	7.217707	5.061130	1.510609
102	1	0	6.543628	5.038520	3.563227
103	1	0	7.629817	4.904674	-0.600843
104	1	0	8.093285	5.679608	1.719495
105	6	0	1.261479	5.718356	-1.131935
106	6	0	0.024829	5.605962	-0.494578
107	6	0	1.983987	6.909368	-1.001569
108	6	0	-0.475834	6.664913	0.263773
109	1	0	-0.550247	4.684976	-0.592082
110	6	0	1.480719	7.968132	-0.252036
111	1	0	2.957585	7.005957	-1.490158
112	6	0	0.246836	7.848336	0.387354
113	1	0	-1.442133	6.558217	0.762207
114	1	0	2.058612	8.890480	-0.159555
115	1	0	-0.147099	8.675394	0.982045
116	6	0	-0.005954	1.817068	-3.949657
117	1	0	0.174852	2.902781	-4.028913
118	1	0	0.479111	1.320561	-4.802850
119	6	0	-0.025031	-1.927302	-0.646595
120	8	0	-0.967859	-1.563269	0.309330
121	6	0	-0.383276	-1.638168	1.619559
122	6	0	0.900291	-2.486572	1.453055
123	6	0	0.721154	-3.063981	0.049733
124	1	0	-1.085237	-2.165109	2.284183
125	1	0	1.792690	-1.840702	1.448980
126	1	0	0.033317	-3.925575	0.118031
127	6	0	-0.736134	-2.287139	-1.947709
128	1	0	-1.366946	-1.428706	-2.240803
129	1	0	0.011092	-2.438458	-2.737161
130	8	0	1.880470	-3.425808	-0.636211
131	8	0	1.034835	-3.530636	2.382491
132	6	0	1.552327	-3.155988	3.652542
133	1	0	1.426292	-4.044691	4.286888
134	1	0	0.955425	-2.334353	4.078412
135	6	0	3.010024	-2.758936	3.599867
136	6	0	3.392747	-1.419965	3.711328
137	6	0	3.999380	-3.727537	3.396292
138	6	0	4.735465	-1.052953	3.619683
139	1	0	2.622452	-0.660258	3.863016
140	6	0	5.340380	-3.365807	3.304135
141	1	0	3.713196	-4.779651	3.316026
142	6	0	5.711287	-2.024941	3.413810
143	1	0	5.019230	-0.001620	3.706678
144	1	0	6.102561	-4.133027	3.150334
145	1	0	6.763182	-1.740001	3.341535
146	6	0	4.469147	-1.471459	-0.487459
147	1	0	4.707638	-1.881305	0.506653

148	1	0	3.976230	-2.276808	-1.050439
149	6	0	5.746949	-1.059637	-1.183823
150	6	0	6.347847	-1.920791	-2.105805
151	6	0	6.371669	0.155279	-0.888862
152	6	0	7.557102	-1.581851	-2.711175
153	1	0	5.864640	-2.870187	-2.352269
154	6	0	7.574369	0.500175	-1.499824
155	1	0	5.899796	0.842233	-0.185700
156	6	0	8.173703	-0.369422	-2.410493
157	1	0	8.015132	-2.266911	-3.428299
158	1	0	8.046906	1.456012	-1.261457
159	1	0	9.118072	-0.099581	-2.888446
160	6	0	3.511157	-5.060161	-1.246263
161	6	0	3.280961	-4.937160	-2.620280
162	6	0	4.733467	-5.574427	-0.809653
163	6	0	4.254801	-5.321415	-3.537581
164	1	0	2.329123	-4.530944	-2.968329
165	6	0	5.707156	-5.968270	-1.726639
166	1	0	4.929088	-5.662092	0.262062
167	6	0	5.471033	-5.840673	-3.093119
168	1	0	4.063393	-5.218095	-4.608033
169	1	0	6.658678	-6.368392	-1.369710
170	1	0	6.234419	-6.143462	-3.813100
171	6	0	2.450124	-4.663563	-0.254277
172	1	0	1.653944	-5.432134	-0.221888
173	1	0	2.876349	-4.600415	0.758861
174	6	0	-0.220311	-0.212179	2.119448
175	1	0	-1.164986	0.309120	1.891703
176	1	0	0.586035	0.299923	1.564679

Compound ***M*-8**, conformer 3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.790290	2.492733	3.347959
2	1	0	-3.941692	1.830806	4.214046
3	1	0	-3.411525	3.458645	3.708333
4	6	0	-2.771663	1.876471	2.402636
5	1	0	-3.082731	0.865071	2.092822
6	1	0	-2.693933	2.487837	1.487054
7	6	0	-0.927831	-0.250745	-4.535584
8	1	0	-1.266592	-0.983089	-3.789065
9	1	0	-0.827357	-0.782029	-5.495732
10	6	0	0.417667	0.340682	-4.148043
11	1	0	1.143884	-0.484330	-4.018514
12	1	0	0.781931	0.985052	-4.960984
13	6	0	-2.933370	-4.090642	2.591201
14	1	0	-3.303455	-3.056255	2.676874

15	1	0	-3.110127	-4.595542	3.551918
16	6	0	-1.446874	-4.090502	2.285171
17	1	0	-1.263346	-3.652859	1.287827
18	1	0	-1.081225	-5.134271	2.250198
19	8	0	-1.545798	1.823146	3.096807
20	8	0	0.355033	1.158039	-3.007122
21	8	0	-0.797067	-3.373572	3.305786
22	6	0	2.528041	-3.063038	1.655851
23	6	0	1.253908	-2.506441	2.290062
24	6	0	2.024218	-0.253560	2.176158
25	6	0	3.330279	-0.681938	1.485501
26	6	0	3.159859	-2.008493	0.754306
27	1	0	0.539727	-2.298423	1.476162
28	1	0	3.243794	-3.323795	2.457561
29	1	0	2.210336	0.589443	2.852386
30	1	0	4.077761	-0.837209	2.283917
31	1	0	2.478839	-1.857026	-0.100105
32	8	0	1.549261	-1.299367	2.983033
33	8	0	1.096763	0.092186	1.190379
34	8	0	3.792928	0.268719	0.564667
35	8	0	4.408143	-2.483022	0.301925
36	8	0	2.184466	-4.204177	0.906396
37	6	0	4.664526	-2.319582	-1.074554
38	1	0	3.915444	-2.869319	-1.673394
39	1	0	4.581700	-1.252334	-1.345605
40	6	0	3.120441	-5.270842	0.949698
41	1	0	3.189878	-5.657428	1.983702
42	1	0	4.116468	-4.909893	0.654159
43	6	0	6.045748	-2.820521	-1.405997
44	6	0	6.322433	-3.319181	-2.682235
45	6	0	7.078159	-2.760559	-0.466452
46	6	0	7.607509	-3.739427	-3.017798
47	1	0	5.520801	-3.381258	-3.423136
48	6	0	8.362319	-3.186816	-0.798740
49	1	0	6.862991	-2.383497	0.534130
50	6	0	8.632520	-3.674778	-2.075797
51	1	0	7.807272	-4.126933	-4.019349
52	1	0	9.159191	-3.137020	-0.053048
53	1	0	9.639432	-4.008806	-2.335485
54	6	0	2.659209	-6.359025	0.020021
55	6	0	3.261084	-6.535776	-1.227652
56	6	0	1.593119	-7.190141	0.378250
57	6	0	2.811232	-7.524842	-2.101171
58	1	0	4.095485	-5.892122	-1.518136
59	6	0	1.138499	-8.177169	-0.491944
60	1	0	1.117263	-7.063957	1.354146
61	6	0	1.747783	-8.346253	-1.735474
62	1	0	3.294171	-7.653652	-3.072302
63	1	0	0.308177	-8.822821	-0.197357
64	1	0	1.394505	-9.122677	-2.417615

65	6	0	0.606468	-3.468810	3.274697
66	1	0	0.907477	-4.501024	3.028942
67	1	0	0.975528	-3.226728	4.282134
68	6	0	0.070296	1.046878	1.433545
69	8	0	-0.836567	0.899467	0.388617
70	6	0	-0.351685	1.566248	-0.782398
71	6	0	0.724846	2.559880	-0.291475
72	6	0	0.591328	2.470084	1.227348
73	1	0	-1.187827	2.131689	-1.221640
74	1	0	1.733700	2.225799	-0.589087
75	1	0	-0.214428	3.163678	1.525665
76	6	0	-0.653683	0.798716	2.756912
77	1	0	-1.157733	-0.182405	2.692161
78	1	0	0.080884	0.742525	3.569551
79	8	0	1.742033	2.721990	1.975117
80	8	0	0.504923	3.889854	-0.684763
81	6	0	0.876799	4.189100	-2.020804
82	1	0	0.362849	3.502669	-2.712888
83	1	0	1.963694	4.036741	-2.149632
84	6	0	0.503359	5.615809	-2.312343
85	6	0	1.468908	6.622847	-2.354694
86	6	0	-0.839554	5.955967	-2.510708
87	6	0	1.104833	7.947342	-2.595984
88	1	0	2.520135	6.366460	-2.199283
89	6	0	-1.206628	7.277801	-2.746725
90	1	0	-1.599117	5.169779	-2.488709
91	6	0	-0.233968	8.277204	-2.790345
92	1	0	1.871283	8.724848	-2.630051
93	1	0	-2.257708	7.531515	-2.902530
94	1	0	-0.521555	9.313993	-2.978768
95	6	0	4.635488	1.264601	1.088822
96	1	0	4.125245	1.822704	1.892756
97	1	0	5.537032	0.800685	1.533241
98	6	0	5.048785	2.231751	0.008719
99	6	0	4.605600	2.105406	-1.308260
100	6	0	5.902353	3.291938	0.335185
101	6	0	5.006177	3.023083	-2.280972
102	1	0	3.940082	1.282704	-1.569714
103	6	0	6.301670	4.206945	-0.633474
104	1	0	6.255799	3.402958	1.363733
105	6	0	5.853355	4.076082	-1.948590
106	1	0	4.651107	2.910099	-3.307942
107	1	0	6.968233	5.028512	-0.361538
108	1	0	6.167274	4.792892	-2.710430
109	6	0	3.076261	4.281710	3.202564
110	6	0	2.870972	3.621693	4.417984
111	6	0	4.153592	5.162594	3.086028
112	6	0	3.726882	3.839122	5.494304
113	1	0	2.031898	2.930172	4.514086
114	6	0	5.006806	5.388170	4.165177

115	1	0	4.330609	5.675151	2.137237
116	6	0	4.796885	4.724966	5.371874
117	1	0	3.556372	3.315155	6.437529
118	1	0	5.844903	6.080498	4.058756
119	1	0	5.467742	4.896014	6.216603
120	6	0	2.127642	4.079839	2.050057
121	1	0	1.226086	4.705902	2.190878
122	1	0	2.595656	4.407159	1.106716
123	6	0	0.102609	0.516932	-1.783963
124	1	0	-0.706893	-0.227528	-1.866265
125	1	0	1.002352	-0.004759	-1.411811
126	6	0	-4.034005	-3.312406	-1.724911
127	6	0	-5.197104	-2.546392	-1.577272
128	6	0	-5.867453	-2.574532	-0.342991
129	6	0	-5.332593	-3.351296	0.691355
130	6	0	-4.153862	-4.071171	0.551364
131	6	0	-3.494318	-4.060888	-0.685973
132	1	0	-3.501076	-3.328027	-2.677739
133	1	0	-5.837609	-3.396246	1.658476
134	6	0	-7.104351	-1.745922	-0.034046
135	1	0	-7.756730	-2.328358	0.631084
136	1	0	-7.685590	-1.551922	-0.941553
137	6	0	-5.660086	-1.720519	-2.765830
138	1	0	-6.741014	-1.549013	-2.713862
139	1	0	-5.494780	-2.316110	-3.674557
140	6	0	-6.720146	-0.456091	0.665297
141	6	0	-6.407818	0.729453	-0.020855
142	6	0	-6.577128	-0.484281	2.056961
143	6	0	-5.863613	1.794418	0.705242
144	6	0	-6.057535	0.584815	2.774380
145	1	0	-6.862224	-1.372131	2.624770
146	6	0	-5.638326	1.726208	2.074383
147	1	0	-5.569438	2.715614	0.198160
148	6	0	-4.929214	-0.398687	-2.937004
149	6	0	-3.759868	-0.389640	-3.708682
150	6	0	-5.378906	0.807094	-2.373906
151	6	0	-3.014912	0.767397	-3.922299
152	1	0	-3.424297	-1.318569	-4.172847
153	6	0	-4.650921	1.974525	-2.634529
154	6	0	-3.485574	1.978655	-3.388622
155	1	0	-4.989540	2.934813	-2.240060
156	6	0	-6.625569	0.914152	-1.514862
157	1	0	-7.049282	1.917510	-1.663497
158	1	0	-7.390240	0.214387	-1.870106
159	8	0	-2.318215	-4.723075	-0.878343
160	8	0	-3.658960	-4.801420	1.598045
161	8	0	-5.921279	0.475246	4.128374
162	8	0	-5.024714	2.777578	2.698370
163	8	0	-2.806009	3.150340	-3.564022
164	8	0	-1.876840	0.795955	-4.661583

165	6	0	-2.773064	3.659661	-4.887867
166	1	0	-2.215211	4.603873	-4.852890
167	1	0	-2.267077	2.963841	-5.572146
168	1	0	-3.793576	3.859049	-5.255794
169	6	0	-2.381836	-6.139968	-0.847546
170	1	0	-2.763295	-6.502706	0.118013
171	1	0	-3.023594	-6.520162	-1.660185
172	1	0	-1.359554	-6.510727	-0.995212
173	6	0	-6.706475	1.369952	4.900514
174	1	0	-6.446885	2.419315	4.692448
175	1	0	-7.780364	1.217953	4.702383
176	1	0	-6.502677	1.148065	5.955621

Compound ***M*-8**, conformer 4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.038976	1.813632	-3.489743
2	1	0	4.078171	1.127670	-4.349209
3	1	0	3.826878	2.825872	-3.859518
4	6	0	2.933685	1.385657	-2.538146
5	1	0	3.069963	0.338548	-2.221806
6	1	0	2.968440	2.007067	-1.627212
7	6	0	0.935346	-0.101158	4.570199
8	1	0	1.162010	-0.926837	3.880827
9	1	0	0.717723	-0.543979	5.555210
10	6	0	-0.277032	0.682372	4.096888
11	1	0	-1.133265	-0.012212	4.001616
12	1	0	-0.539763	1.439326	4.849918
13	6	0	1.281189	-3.884915	-1.808525
14	1	0	0.377989	-4.071576	-1.205396
15	1	0	1.592235	-2.839871	-1.644056
16	6	0	1.017912	-4.098182	-3.291224
17	1	0	1.968500	-3.992519	-3.833811
18	1	0	0.645293	-5.125541	-3.461390
19	8	0	1.709852	1.537821	-3.222811
20	8	0	-0.050831	1.388142	2.903813
21	8	0	0.132166	-3.147275	-3.828497
22	6	0	-2.900044	-2.725738	-1.645816
23	6	0	-1.642496	-2.287363	-2.394952
24	6	0	-2.140660	0.029079	-2.153875
25	6	0	-3.428307	-0.277602	-1.369654
26	6	0	-3.338783	-1.633727	-0.675877
27	1	0	-0.833458	-2.187845	-1.655011
28	1	0	-3.713227	-2.900007	-2.374236
29	1	0	-2.275637	0.911964	-2.789533
30	1	0	-4.247691	-0.334008	-2.108802
31	1	0	-2.577274	-1.573999	0.119997

32	8	0	-1.858793	-1.033472	-3.026579
33	8	0	-1.111276	0.230802	-1.229728
34	8	0	-3.715887	0.691751	-0.398269
35	8	0	-4.585809	-1.997426	-0.128212
36	8	0	-2.598000	-3.912237	-0.947259
37	6	0	-4.740468	-1.775038	1.255114
38	1	0	-3.991006	-2.356101	1.823777
39	1	0	-4.568773	-0.709136	1.484236
40	6	0	-3.623966	-4.894671	-0.931112
41	1	0	-3.839837	-5.224693	-1.963339
42	1	0	-4.544116	-4.460033	-0.512143
43	6	0	-6.126995	-2.170587	1.691265
44	6	0	-7.203477	-2.127653	0.802051
45	6	0	-6.360575	-2.550544	3.016308
46	6	0	-8.488542	-2.454535	1.230899
47	1	0	-7.022852	-1.841802	-0.234757
48	6	0	-7.645361	-2.871111	3.447573
49	1	0	-5.525059	-2.598056	3.720000
50	6	0	-8.714910	-2.824625	2.554838
51	1	0	-9.320391	-2.419412	0.523524
52	1	0	-7.810977	-3.166506	4.486093
53	1	0	-9.722260	-3.080829	2.890234
54	6	0	-3.167439	-6.062565	-0.101638
55	6	0	-2.549344	-7.165051	-0.696501
56	6	0	-3.320252	-6.043885	1.288053
57	6	0	-2.098236	-8.232027	0.078323
58	1	0	-2.425299	-7.190450	-1.782239
59	6	0	-2.868887	-7.106368	2.066777
60	1	0	-3.807081	-5.188466	1.763359
61	6	0	-2.257111	-8.204027	1.462192
62	1	0	-1.622089	-9.090087	-0.401140
63	1	0	-2.999087	-7.080930	3.150883
64	1	0	-1.906604	-9.040125	2.071300
65	6	0	-1.221813	-3.282504	-3.461888
66	1	0	-1.427643	-4.303004	-3.101332
67	1	0	-1.837901	-3.101389	-4.357387
68	6	0	0.023762	1.035660	-1.523719
69	8	0	0.941132	0.771776	-0.510785
70	6	0	0.643009	1.547472	0.653950
71	6	0	-0.282092	2.690728	0.184736
72	6	0	-0.280359	2.524039	-1.332968
73	1	0	1.586611	1.978839	1.021985
74	1	0	-1.306387	2.550688	0.571325
75	1	0	0.588621	3.086405	-1.717722
76	6	0	0.659836	0.679864	-2.868616
77	1	0	0.986597	-0.374452	-2.831787
78	1	0	-0.095314	0.764567	-3.660316
79	8	0	-1.439978	2.913594	-2.005292
80	8	0	0.190334	3.978160	0.489255
81	6	0	0.000222	4.391404	1.833578

82	1	0	0.476109	3.671582	2.517811
83	1	0	-1.079639	4.409260	2.068363
84	6	0	0.603660	5.758447	1.997188
85	6	0	-0.182648	6.909330	1.914545
86	6	0	1.983143	5.892364	2.187660
87	6	0	0.394431	8.173643	2.023956
88	1	0	-1.261495	6.813707	1.766077
89	6	0	2.563003	7.153993	2.294067
90	1	0	2.601063	4.993351	2.262347
91	6	0	1.769085	8.297852	2.212160
92	1	0	-0.232652	9.065825	1.961407
93	1	0	3.640867	7.246911	2.445602
94	1	0	2.223203	9.287541	2.298517
95	6	0	-4.433506	1.813050	-0.851179
96	1	0	-3.887604	2.319899	-1.665813
97	1	0	-5.412470	1.497148	-1.259645
98	6	0	-4.648113	2.794010	0.273277
99	6	0	-4.078013	2.611668	1.533815
100	6	0	-5.431000	3.931423	0.044327
101	6	0	-4.284336	3.550267	2.546352
102	1	0	-3.468320	1.727552	1.720117
103	6	0	-5.635906	4.867709	1.052559
104	1	0	-5.883690	4.085769	-0.938775
105	6	0	-5.061242	4.680561	2.310394
106	1	0	-3.831852	3.392619	3.528140
107	1	0	-6.250068	5.749635	0.857026
108	1	0	-5.222822	5.413977	3.103319
109	6	0	-2.688297	4.602506	-3.142574
110	6	0	-2.673098	3.937747	-4.373117
111	6	0	-3.674941	5.561277	-2.905313
112	6	0	-3.625523	4.227854	-5.345621
113	1	0	-1.906053	3.184474	-4.563903
114	6	0	-4.625505	5.859246	-3.881176
115	1	0	-3.703881	6.078368	-1.943067
116	6	0	-4.604259	5.191674	-5.102998
117	1	0	-3.603277	3.700223	-6.301828
118	1	0	-5.390966	6.612271	-3.681096
119	1	0	-5.351009	5.419898	-5.866643
120	6	0	-1.636744	4.310691	-2.105086
121	1	0	-0.680984	4.791557	-2.387789
122	1	0	-1.929981	4.735810	-1.130961
123	6	0	0.073530	0.633451	1.726593
124	1	0	0.767078	-0.216114	1.848002
125	1	0	-0.903055	0.229726	1.403694
126	6	0	3.300489	-3.644439	1.933943
127	6	0	4.600680	-3.174120	1.707591
128	6	0	5.167624	-3.348786	0.435672
129	6	0	4.385540	-3.932308	-0.568976
130	6	0	3.072246	-4.322433	-0.357223
131	6	0	2.524431	-4.206607	0.929522

132	1	0	2.843427	-3.552942	2.921049
133	1	0	4.780749	-4.047350	-1.579771
134	6	0	6.543958	-2.830817	0.044739
135	1	0	7.021544	-3.569249	-0.614172
136	1	0	7.192954	-2.735297	0.921473
137	6	0	5.292074	-2.438778	2.841966
138	1	0	6.380667	-2.479175	2.728120
139	1	0	5.065698	-2.961191	3.782024
140	6	0	6.417977	-1.517088	-0.702448
141	6	0	6.350517	-0.268457	-0.059967
142	6	0	6.250429	-1.567945	-2.090291
143	6	0	5.994753	0.850879	-0.820580
144	6	0	5.925411	-0.447576	-2.843297
145	1	0	6.356137	-2.513396	-2.625991
146	6	0	5.730470	0.774796	-2.183438
147	1	0	5.887183	1.829132	-0.347370
148	6	0	4.823944	-0.998858	2.977702
149	6	0	3.700764	-0.749734	3.776022
150	6	0	5.446290	0.080236	2.328559
151	6	0	3.160860	0.523879	3.932483
152	1	0	3.227712	-1.582231	4.299295
153	6	0	4.938803	1.367191	2.547247
154	6	0	3.816413	1.609571	3.328394
155	1	0	5.422497	2.234116	2.092352
156	6	0	6.652437	-0.073698	1.419501
157	1	0	7.257701	0.839460	1.510775
158	1	0	7.291810	-0.888935	1.776702
159	8	0	1.238220	-4.565357	1.202111
160	8	0	2.325926	-4.767329	-1.414227
161	8	0	5.752108	-0.578598	-4.191248
162	8	0	5.303996	1.896533	-2.839878
163	8	0	3.357269	2.889168	3.458657
164	8	0	2.051256	0.770301	4.676496
165	6	0	3.426031	3.446986	4.761423
166	1	0	3.046598	4.474032	4.688739
167	1	0	2.808196	2.880421	5.472535
168	1	0	4.468422	3.473868	5.120838
169	6	0	0.912200	-5.936368	1.033499
170	1	0	1.521403	-6.567132	1.702242
171	1	0	-0.146174	-6.049818	1.298361
172	1	0	1.062844	-6.262776	-0.006299
173	6	0	6.678588	0.127712	-5.001010
174	1	0	6.620106	1.213711	-4.830040
175	1	0	7.708534	-0.213102	-4.804473
176	1	0	6.423337	-0.089203	-6.045917

Compound ***M*-8**, conformer 5

Center	Atomic	Atomic	Coordinates (Angstroms)		

Number	Number	Type	X	Y	Z
1	6	0	-4.660058	-1.273441	2.852401
2	6	0	-5.292521	-0.070090	2.515628
3	6	0	-4.728086	1.130521	2.978046
4	6	0	-3.539810	1.076030	3.717330
5	6	0	-2.883827	-0.120428	3.994379
6	6	0	-3.475624	-1.323623	3.575376
7	1	0	-5.091943	-2.227503	2.543075
8	1	0	-3.109838	2.004027	4.097796
9	6	0	-5.333571	2.499731	2.709167
10	1	0	-5.098355	3.149297	3.563862
11	1	0	-6.426346	2.433349	2.671811
12	6	0	-6.564521	-0.135548	1.689315
13	1	0	-7.249906	0.665575	1.988455
14	1	0	-7.078055	-1.074050	1.942003
15	6	0	-4.788328	3.150028	1.450087
16	6	0	-5.437349	3.094346	0.206698
17	6	0	-3.543702	3.789668	1.530398
18	6	0	-4.775462	3.607876	-0.915328
19	6	0	-2.893925	4.297646	0.413751
20	1	0	-3.034450	3.888894	2.491047
21	6	0	-3.507908	4.163505	-0.840869
22	1	0	-5.230835	3.539674	-1.904828
23	6	0	-6.378349	-0.115213	0.178647
24	6	0	-5.984148	-1.294931	-0.462255
25	6	0	-6.588632	1.031634	-0.606387
26	6	0	-5.816233	-1.375716	-1.840128
27	1	0	-5.766901	-2.193796	0.118568
28	6	0	-6.516764	0.915891	-1.998455
29	6	0	-6.151796	-0.265826	-2.629526
30	1	0	-6.734392	1.774250	-2.637175
31	6	0	-6.780285	2.415401	-0.018128
32	1	0	-7.362118	3.023091	-0.725056
33	1	0	-7.362260	2.381239	0.908636
34	8	0	-2.898801	-2.535658	3.826679
35	8	0	-1.718150	-0.180797	4.689588
36	8	0	-1.661393	4.868001	0.553103
37	8	0	-2.866811	4.531213	-1.992688
38	8	0	-6.077099	-0.296813	-3.992350
39	8	0	-5.340339	-2.537238	-2.384132
40	6	0	-6.989815	-1.169983	-4.638623
41	1	0	-6.822064	-1.068678	-5.718252
42	1	0	-6.827351	-2.217579	-4.341807
43	1	0	-8.030369	-0.887357	-4.408573
44	6	0	-2.837065	-2.927959	5.188851
45	1	0	-2.228919	-2.228473	5.779699
46	1	0	-3.848764	-2.992445	5.623398
47	1	0	-2.373835	-3.922365	5.213296
48	6	0	-1.574594	6.240809	0.198587

49	1	0	-2.261768	6.845066	0.813464
50	1	0	-0.543320	6.556470	0.397112
51	1	0	-1.807691	6.396444	-0.865231
52	6	0	-4.127238	-2.440574	-3.125358
53	1	0	-4.273907	-1.869144	-4.054195
54	1	0	-3.854816	-3.471644	-3.388047
55	6	0	-3.009404	-1.816049	-2.306855
56	1	0	-3.223878	-0.755746	-2.094943
57	1	0	-2.929809	-2.331195	-1.334595
58	6	0	-0.683446	0.745904	4.396510
59	1	0	-1.014925	1.453394	3.623261
60	1	0	-0.445862	1.331445	5.298944
61	6	0	0.559212	-0.005880	3.949482
62	1	0	1.347706	0.729774	3.700385
63	1	0	0.928282	-0.627156	4.778172
64	6	0	-1.763972	3.695760	-2.326106
65	1	0	-0.876988	3.988705	-1.741798
66	1	0	-2.004807	2.647106	-2.083738
67	6	0	-1.506575	3.809828	-3.819704
68	1	0	-1.196799	4.841250	-4.071417
69	1	0	-2.444036	3.601213	-4.355446
70	8	0	-1.820110	-1.935792	-3.055776
71	8	0	0.322266	-0.888213	2.882650
72	8	0	-0.558390	2.874840	-4.272191
73	6	0	2.493758	2.821993	-2.079259
74	6	0	1.266568	2.240029	-2.781483
75	6	0	1.943924	-0.007167	-2.381103
76	6	0	3.236096	0.446870	-1.684379
77	6	0	3.056542	1.829480	-1.064591
78	1	0	0.469651	2.145384	-2.027956
79	1	0	3.275769	3.034884	-2.831881
80	1	0	2.109695	-0.931827	-2.946218
81	1	0	4.014814	0.524571	-2.464114
82	1	0	2.331609	1.753174	-0.236999
83	8	0	1.557324	0.959665	-3.322368
84	8	0	0.972077	-0.187351	-1.393152
85	8	0	3.644211	-0.437220	-0.675058
86	8	0	4.287280	2.327797	-0.590895
87	8	0	2.076128	4.010716	-1.450666
88	6	0	4.525496	2.180345	0.792454
89	1	0	3.781122	2.755401	1.372161
90	1	0	4.421117	1.119696	1.077378
91	6	0	3.039673	5.018264	-1.226560
92	1	0	2.837546	5.860888	-1.914134
93	1	0	4.048849	4.644616	-1.449211
94	6	0	5.912711	2.659280	1.131226
95	6	0	6.951683	2.577223	0.200893
96	6	0	6.188180	3.157870	2.407758
97	6	0	8.240715	2.982019	0.542002
98	1	0	6.738439	2.199455	-0.799801

99	6	0	7.477563	3.555856	2.752559
100	1	0	5.381127	3.240401	3.140659
101	6	0	8.509290	3.469680	1.819317
102	1	0	9.042515	2.915197	-0.197095
103	1	0	7.675881	3.943774	3.754276
104	1	0	9.519842	3.786684	2.086203
105	6	0	3.003917	5.521751	0.197355
106	6	0	1.944081	5.222703	1.055168
107	6	0	4.045187	6.329554	0.666069
108	6	0	1.927634	5.721599	2.358311
109	1	0	1.124694	4.597790	0.698634
110	6	0	4.028982	6.827924	1.965413
111	1	0	4.883548	6.567524	0.005436
112	6	0	2.968017	6.524277	2.818671
113	1	0	1.089436	5.480097	3.016248
114	1	0	4.852591	7.453605	2.316757
115	1	0	2.954463	6.912984	3.839255
116	6	0	0.781689	3.126482	-3.916184
117	1	0	0.918803	4.181205	-3.629365
118	1	0	1.413095	2.923157	-4.796351
119	6	0	-0.098083	-1.112670	-1.525957
120	8	0	-0.974315	-0.815721	-0.486232
121	6	0	-0.514775	-1.405969	0.734137
122	6	0	0.474873	-2.518729	0.325949
123	6	0	0.350617	-2.538288	-1.196055
124	1	0	-1.382449	-1.862398	1.234278
125	1	0	1.507469	-2.249395	0.607205
126	1	0	-0.489668	-3.210868	-1.443289
127	6	0	-0.835282	-0.959423	-2.856130
128	1	0	-1.254754	0.061470	-2.903561
129	1	0	-0.117864	-1.062540	-3.680425
130	8	0	1.489202	-2.910147	-1.912385
131	8	0	0.142727	-3.792791	0.815755
132	6	0	0.456673	-4.013689	2.181980
133	1	0	-0.029459	-3.247543	2.806501
134	1	0	1.547643	-3.922521	2.333051
135	6	0	-0.020348	-5.387960	2.560802
136	6	0	0.854227	-6.476151	2.579925
137	6	0	-1.371709	-5.599394	2.854918
138	6	0	0.391902	-7.754150	2.890838
139	1	0	1.911784	-6.319795	2.351477
140	6	0	-1.837204	-6.875244	3.162344
141	1	0	-2.058396	-4.748410	2.850521
142	6	0	-0.955521	-7.955947	3.180650
143	1	0	1.087519	-8.596188	2.905939
144	1	0	-2.893915	-7.028492	3.393118
145	1	0	-1.319867	-8.956393	3.424610
146	6	0	4.453999	-1.507155	-1.094935
147	1	0	3.931075	-2.116716	-1.852310
148	1	0	5.377179	-1.119869	-1.567138

149	6	0	4.817795	-2.387493	0.073725
150	6	0	4.328932	-2.152820	1.359402
151	6	0	5.667177	-3.479980	-0.136531
152	6	0	4.680453	-2.995838	2.415139
153	1	0	3.666448	-1.304619	1.531763
154	6	0	6.017369	-4.320725	0.914894
155	1	0	6.056567	-3.675552	-1.139195
156	6	0	5.523553	-4.081562	2.198022
157	1	0	4.289865	-2.798161	3.416070
158	1	0	6.681557	-5.168677	0.733116
159	1	0	5.798860	-4.739928	3.024756
160	6	0	2.779875	-4.626038	-2.962614
161	6	0	2.627610	-4.081892	-4.241796
162	6	0	3.828921	-5.517369	-2.728604
163	6	0	3.507033	-4.423955	-5.265255
164	1	0	1.811390	-3.381958	-4.430503
165	6	0	4.705902	-5.867658	-3.754308
166	1	0	3.965116	-5.939497	-1.729891
167	6	0	4.548289	-5.320110	-5.025100
168	1	0	3.377792	-3.990065	-6.259385
169	1	0	5.521345	-6.566728	-3.555847
170	1	0	5.237569	-5.589004	-5.828507
171	6	0	1.805449	-4.287243	-1.865396
172	1	0	0.877006	-4.876624	-1.989241
173	1	0	2.224604	-4.559849	-0.882525
174	6	0	0.046990	-0.314619	1.631123
175	1	0	-0.709927	0.485356	1.697824
176	1	0	0.957998	0.117558	1.180351

Compound ***M*-8**, conformer 6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.134797	-4.404015	3.341042
2	1	0	0.678850	-4.144646	4.261765
3	1	0	-0.883885	-4.712379	3.612071
4	6	0	0.064351	-3.191007	2.427700
5	1	0	1.072848	-2.802414	2.208208
6	1	0	-0.391275	-3.476738	1.463905
7	6	0	0.933055	-0.340542	-4.465530
8	1	0	1.667209	-0.146576	-3.670613
9	1	0	1.322597	0.112520	-5.391263
10	6	0	-0.410913	0.285102	-4.131918
11	1	0	-0.266197	1.370656	-3.974375
12	1	0	-1.094823	0.157012	-4.983123
13	6	0	4.701709	0.456170	2.943033
14	1	0	4.143382	-0.491294	3.017575
15	1	0	5.125396	0.680221	3.932453

16	6	0	3.774285	1.583897	2.527085
17	1	0	3.368195	1.393672	1.517983
18	1	0	4.352146	2.525529	2.471253
19	8	0	-0.701739	-2.216465	3.098266
20	8	0	-1.045784	-0.314928	-3.031807
21	8	0	2.756941	1.685214	3.493090
22	6	0	0.448397	4.070735	1.764199
23	6	0	0.843892	2.724477	2.371650
24	6	0	-1.358318	1.844208	2.191618
25	6	0	-1.873629	3.130616	1.525012
26	6	0	-0.753724	3.911662	0.837540
27	1	0	1.171028	2.066650	1.549370
28	1	0	0.167288	4.759894	2.581568
29	1	0	-2.135598	1.422176	2.840548
30	1	0	-2.261765	3.772028	2.336276
31	1	0	-0.417826	3.353139	-0.052813
32	8	0	-0.275301	2.145764	3.030122
33	8	0	-0.993697	0.934376	1.196582
34	8	0	-2.883128	2.874788	0.584798
35	8	0	-1.197049	5.202799	0.480015
36	8	0	1.556483	4.572496	1.056520
37	6	0	-1.756726	5.365465	-0.816583
38	1	0	-2.439842	4.535626	-1.041364
39	1	0	-2.353423	6.287538	-0.757470
40	6	0	1.807340	5.949484	1.202741
41	1	0	2.015778	6.187924	2.263986
42	1	0	0.916036	6.528394	0.910396
43	6	0	-0.720492	5.503633	-1.906577
44	6	0	-0.491034	4.469006	-2.816557
45	6	0	0.032371	6.677454	-2.022771
46	6	0	0.470372	4.599119	-3.818663
47	1	0	-1.080776	3.551275	-2.745521
48	6	0	0.992239	6.812558	-3.020663
49	1	0	-0.143928	7.499621	-1.324275
50	6	0	1.214893	5.770831	-3.921526
51	1	0	0.636199	3.782030	-4.524510
52	1	0	1.570688	7.735747	-3.098589
53	1	0	1.967041	5.876178	-4.706431
54	6	0	2.982973	6.367351	0.358194
55	6	0	3.658121	5.466259	-0.465142
56	6	0	3.401254	7.702251	0.387518
57	6	0	4.728569	5.895249	-1.251292
58	1	0	3.336676	4.424909	-0.488920
59	6	0	4.470159	8.129342	-0.393704
60	1	0	2.879824	8.417449	1.030026
61	6	0	5.138609	7.224988	-1.219508
62	1	0	5.243556	5.181797	-1.899018
63	1	0	4.783947	9.175104	-0.359336
64	1	0	5.976298	7.558399	-1.835870
65	6	0	1.969799	2.846421	3.386212

66	1	0	2.604669	3.707833	3.119869
67	1	0	1.521016	3.032497	4.373330
68	6	0	-1.046266	-0.470114	1.421865
69	8	0	-0.276562	-1.045141	0.415144
70	6	0	-1.027507	-1.118591	-0.801784
71	6	0	-2.510465	-0.954943	-0.398681
72	6	0	-2.446203	-1.009202	1.126288
73	1	0	-0.881902	-2.122266	-1.230435
74	1	0	-2.897605	0.029067	-0.714733
75	1	0	-2.459664	-2.075228	1.412722
76	6	0	-0.463847	-0.873870	2.777400
77	1	0	0.615162	-0.636769	2.770572
78	1	0	-0.930491	-0.278525	3.571151
79	8	0	-3.431760	-0.313888	1.826696
80	8	0	-3.349180	-1.987236	-0.847655
81	6	0	-3.721744	-1.908528	-2.214551
82	1	0	-2.819681	-1.873746	-2.845929
83	1	0	-4.289184	-0.976963	-2.392824
84	6	0	-4.558126	-3.112117	-2.548520
85	6	0	-5.951988	-3.037090	-2.577922
86	6	0	-3.940169	-4.343974	-2.789821
87	6	0	-6.719054	-4.169529	-2.848251
88	1	0	-6.442817	-2.078568	-2.389730
89	6	0	-4.703803	-5.477443	-3.056361
90	1	0	-2.848483	-4.405987	-2.775969
91	6	0	-6.095798	-5.392259	-3.086175
92	1	0	-7.808637	-4.096241	-2.872070
93	1	0	-4.210998	-6.433773	-3.246059
94	1	0	-6.694826	-6.280717	-3.298234
95	6	0	-4.194729	2.838639	1.090454
96	1	0	-4.291126	2.057268	1.863837
97	1	0	-4.443276	3.805685	1.567985
98	6	0	-5.179361	2.554872	-0.015426
99	6	0	-4.768128	2.282928	-1.320894
100	6	0	-6.548543	2.553715	0.274878
101	6	0	-5.707334	2.011378	-2.317305
102	1	0	-3.703475	2.285776	-1.554701
103	6	0	-7.485090	2.282136	-0.717222
104	1	0	-6.884470	2.765615	1.293401
105	6	0	-7.067002	2.008112	-2.020152
106	1	0	-5.369266	1.802113	-3.334888
107	1	0	-8.549857	2.285487	-0.473328
108	1	0	-7.801469	1.796607	-2.800261
109	6	0	-5.522965	-0.390965	2.984909
110	6	0	-4.931014	-0.202025	4.237609
111	6	0	-6.885842	-0.126717	2.835270
112	6	0	-5.688230	0.241884	5.318125
113	1	0	-3.865330	-0.404728	4.359275
114	6	0	-7.647796	0.310109	3.918051
115	1	0	-7.356517	-0.258918	1.857990

116	6	0	-7.050273	0.497695	5.162044
117	1	0	-5.212816	0.387127	6.290837
118	1	0	-8.712975	0.512324	3.785509
119	1	0	-7.644408	0.845286	6.010026
120	6	0	-4.712576	-0.912310	1.826870
121	1	0	-4.600732	-2.009621	1.911219
122	1	0	-5.235210	-0.719483	0.875016
123	6	0	-0.470676	-0.089418	-1.771405
124	1	0	0.624960	-0.215508	-1.788078
125	1	0	-0.685115	0.932060	-1.408992
126	6	0	5.104844	-0.838981	-1.361355
127	6	0	5.226513	-2.228183	-1.228904
128	6	0	5.585958	-2.755094	0.022901
129	6	0	5.777223	-1.871133	1.091282
130	6	0	5.607188	-0.499493	0.963527
131	6	0	5.280211	0.031345	-0.292554
132	1	0	4.852509	-0.396935	-2.327345
133	1	0	6.060156	-2.253032	2.074353
134	6	0	5.709319	-4.243457	0.309133
135	1	0	6.529096	-4.393704	1.025086
136	1	0	5.986106	-4.796692	-0.594407
137	6	0	4.959750	-3.086497	-2.454045
138	1	0	5.507575	-4.032618	-2.382294
139	1	0	5.376192	-2.565456	-3.327474
140	6	0	4.425966	-4.776554	0.915752
141	6	0	3.355881	-5.265425	0.147804
142	6	0	4.269173	-4.679827	2.302702
143	6	0	2.140930	-5.526181	0.790987
144	6	0	3.068190	-4.964924	2.937922
145	1	0	5.100000	-4.356067	2.932651
146	6	0	1.964441	-5.337910	2.156251
147	1	0	1.274168	-5.864228	0.219207
148	6	0	3.489834	-3.356478	-2.733403
149	6	0	2.797811	-2.447604	-3.544113
150	6	0	2.806123	-4.480256	-2.239360
151	6	0	1.452387	-2.607733	-3.866658
152	1	0	3.333010	-1.589332	-3.954312
153	6	0	1.467326	-4.658936	-2.608387
154	6	0	0.781432	-3.752065	-3.405081
155	1	0	0.916118	-5.539236	-2.271157
156	6	0	3.451135	-5.525604	-1.348022
157	1	0	2.954098	-6.485836	-1.545888
158	1	0	4.498767	-5.670751	-1.634741
159	8	0	5.092968	1.369855	-0.476365
160	8	0	5.790995	0.324767	2.040986
161	8	0	2.980997	-4.822010	4.292789
162	8	0	0.722614	-5.529466	2.696852
163	8	0	-0.534648	-3.976649	-3.693322
164	8	0	0.766966	-1.737041	-4.651457
165	6	0	-0.838289	-4.249570	-5.052113

166	1	0	-1.918993	-4.431841	-5.106913
167	1	0	-0.579659	-3.399052	-5.698664
168	1	0	-0.304467	-5.150201	-5.399113
169	6	0	6.249442	2.181983	-0.346857
170	1	0	6.709374	2.067882	0.645280
171	1	0	6.990524	1.933800	-1.125163
172	1	0	5.927569	3.222499	-0.477255
173	6	0	2.727216	-6.012147	5.022416
174	1	0	1.761840	-6.460876	4.742113
175	1	0	3.529415	-6.750219	4.857229
176	1	0	2.705624	-5.739315	6.085004

Table S2. Calculated at CAM-B3LYP/SVP/PCM(CH_3CN) level of theory relative energies and conformer distribution at 25° C for *P*-8.

Conformer	ΔG [kcal mol^{-1}]	Pop. [%]
***P*-8**(1)	0.00	52.7
***P*-8**(2)	0.38	28.0
***P*-8**(3)	1.17	7.3
***P*-8**(4)	1.27	6.2
***P*-8**(5)	1.69	3.1
***P*-8**(6)	1.73	2.7

Cartesian coordinates for individual conformers of compound *P*-8.

Compound ***P*-8**, conformer 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.775853	-0.352682	4.666314
2	6	0	1.271063	4.526839	2.002037
3	1	0	2.320184	4.816751	2.149278
4	1	0	0.773500	4.555417	2.986014
5	6	0	1.206385	3.126222	1.417288
6	1	0	0.162404	2.776913	1.363632
7	1	0	1.591161	3.149010	0.382966
8	6	0	-2.548915	-1.070968	4.651204
9	1	0	-2.255197	-1.306527	5.686447
10	1	0	-1.747803	-0.456058	4.216946
11	6	0	-2.717988	-2.362020	3.878419
12	1	0	-1.792720	-2.960520	3.989249
13	1	0	-3.547698	-2.938246	4.313787
14	6	0	-2.847029	0.530449	-3.810268
15	1	0	-2.582311	0.693196	-4.864837
16	1	0	-2.250198	1.223848	-3.195488
17	6	0	-2.555989	-0.897364	-3.387874
18	1	0	-3.025305	-1.087945	-2.414779
19	1	0	-2.992413	-1.605884	-4.117115
20	8	0	1.970797	2.276419	2.239702
21	8	0	-3.033585	-2.179637	2.520873
22	8	0	-1.156781	-1.067978	-3.316952
23	6	0	3.237587	0.267923	0.537699
24	6	0	1.804149	0.121088	1.051885
25	6	0	0.943578	-0.148346	-1.150854
26	6	0	2.316506	0.117693	-1.784044
27	6	0	3.418615	-0.352429	-0.842234
28	1	0	1.630659	-0.940624	1.297178
29	1	0	3.470664	1.342691	0.459083
30	1	0	0.133929	0.253694	-1.770129

31	1	0	2.406808	1.212600	-1.888422
32	1	0	3.353616	-1.448778	-0.744828
33	8	0	0.867214	0.534274	0.069655
34	8	0	0.787987	-1.534329	-0.977389
35	8	0	2.490714	-0.508048	-3.028192
36	8	0	4.696507	0.014077	-1.312924
37	8	0	4.095061	-0.349985	1.471472
38	6	0	1.850032	0.103482	-4.141024
39	1	0	2.124407	-0.527614	-4.998993
40	6	0	5.403643	-0.991635	-1.999151
41	1	0	5.590231	-1.853151	-1.330718
42	1	0	4.799782	-1.362472	-2.845349
43	6	0	5.249745	0.390779	1.835073
44	1	0	4.942997	1.358076	2.270834
45	1	0	5.859905	0.592272	0.940650
46	6	0	6.716798	-0.455622	-2.507750
47	6	0	7.746942	-1.343067	-2.835674
48	6	0	6.921486	0.913200	-2.694473
49	6	0	8.952717	-0.873826	-3.349189
50	1	0	7.603223	-2.416528	-2.684819
51	6	0	8.131264	1.384572	-3.203383
52	1	0	6.123466	1.608174	-2.432390
53	6	0	9.149441	0.494205	-3.534901
54	1	0	9.747122	-1.580431	-3.599940
55	1	0	8.278054	2.458458	-3.340841
56	1	0	10.096706	0.864190	-3.933247
57	6	0	6.032029	-0.409198	2.839313
58	6	0	5.757140	-0.300215	4.205107
59	6	0	7.003542	-1.320762	2.417430
60	6	0	6.440493	-1.083698	5.132413
61	1	0	4.999223	0.410187	4.545479
62	6	0	7.689271	-2.106664	3.340722
63	1	0	7.226441	-1.412587	1.351173
64	6	0	7.407826	-1.989942	4.700906
65	1	0	6.218616	-0.985569	6.197347
66	1	0	8.448490	-2.812882	2.997549
67	1	0	7.946176	-2.603677	5.426494
68	6	0	1.559848	0.933053	2.313417
69	1	0	2.138143	0.478792	3.129054
70	1	0	0.485645	0.866689	2.566865
71	6	0	-0.475506	-2.102877	-1.197153
72	8	0	-1.480740	-1.304749	-0.614516
73	6	0	-2.304548	-2.033540	0.286776
74	6	0	-2.010525	-3.508317	0.000663
75	6	0	-0.553714	-3.474280	-0.471296
76	1	0	-3.354108	-1.787692	0.065574
77	1	0	-2.107827	-4.125530	0.908610
78	1	0	-0.355949	-4.307441	-1.166126
79	6	0	-0.750635	-2.265551	-2.701985
80	1	0	0.183644	-2.598227	-3.177819

81	1	0	-1.514848	-3.046001	-2.840049
82	8	0	0.271141	-3.559465	0.655279
83	8	0	-2.793773	-4.033875	-1.043314
84	6	0	-2.016643	-1.626046	1.722674
85	1	0	-2.002889	-0.522837	1.775830
86	1	0	-1.023792	-1.999381	2.027845
87	6	0	-4.150741	-4.252998	-0.731234
88	1	0	-4.716469	-3.304822	-0.738911
89	1	0	-4.230447	-4.669031	0.291986
90	1	0	0.755059	0.054109	-4.034093
91	6	0	2.286229	1.528256	-4.390710
92	6	0	3.629217	1.823787	-4.650713
93	6	0	1.363072	2.574574	-4.352596
94	6	0	4.036729	3.135771	-4.870015
95	1	0	4.362853	1.014390	-4.676688
96	6	0	1.766567	3.891443	-4.573737
97	1	0	0.313206	2.358232	-4.138839
98	6	0	3.104620	4.174292	-4.833156
99	1	0	5.088242	3.351632	-5.072654
100	1	0	1.030492	4.696826	-4.530961
101	1	0	3.424812	5.204324	-5.005305
102	6	0	2.201101	-4.391430	1.770874
103	6	0	3.225034	-3.588675	2.277980
104	6	0	1.746290	-5.471857	2.534879
105	6	0	3.792733	-3.865700	3.522259
106	1	0	3.581598	-2.726623	1.709718
107	6	0	2.307386	-5.748099	3.777752
108	1	0	0.944108	-6.104706	2.146459
109	6	0	3.335418	-4.945075	4.273416
110	1	0	4.593835	-3.228206	3.903944
111	1	0	1.945561	-6.596799	4.362590
112	1	0	3.779244	-5.163277	5.247405
113	6	0	1.567402	-4.094693	0.438829
114	1	0	2.182716	-3.387002	-0.135823
115	1	0	1.477028	-5.023784	-0.153353
116	6	0	-4.767182	-5.214178	-1.716337
117	6	0	-3.987685	-6.131559	-2.423241
118	6	0	-6.152962	-5.218736	-1.903211
119	6	0	-4.582855	-7.036136	-3.301070
120	1	0	-2.906192	-6.127323	-2.283720
121	6	0	-6.749322	-6.126653	-2.774572
122	1	0	-6.773882	-4.502614	-1.358102
123	6	0	-5.964478	-7.038579	-3.478660
124	1	0	-3.960245	-7.746063	-3.850479
125	1	0	-7.833235	-6.117672	-2.909164
126	1	0	-6.429756	-7.747703	-4.166738
127	6	0	-1.613296	5.240706	1.672895
128	6	0	-2.943792	5.013337	1.300696
129	6	0	-3.250185	4.894995	-0.064635
130	6	0	-2.215873	5.041764	-0.997088

131	6	0	-0.892657	5.238106	-0.622910
132	6	0	-0.584371	5.321356	0.743461
133	1	0	-1.361554	5.341274	2.730029
134	1	0	-2.424710	4.979020	-2.066889
135	6	0	-4.642317	4.585958	-0.587040
136	1	0	-4.779741	5.129489	-1.532204
137	1	0	-5.405443	4.973989	0.096348
138	6	0	-3.973210	4.865178	2.408675
139	1	0	-4.967837	5.153579	2.052167
140	1	0	-3.720176	5.576807	3.207145
141	6	0	-4.877958	3.109279	-0.859571
142	6	0	-5.456084	2.229089	0.072911
143	6	0	-4.489785	2.601161	-2.103450
144	6	0	-5.641959	0.891906	-0.294414
145	6	0	-4.639190	1.262300	-2.446276
146	1	0	-4.050561	3.263667	-2.852448
147	6	0	-5.241214	0.391062	-1.528018
148	1	0	-6.115758	0.192223	0.397009
149	6	0	-3.999433	3.469030	3.004784
150	6	0	-3.090672	3.190200	4.038942
151	6	0	-4.847191	2.452377	2.547633
152	6	0	-2.985149	1.927768	4.609841
153	1	0	-2.463295	3.998357	4.412914
154	6	0	-4.722784	1.177432	3.120280
155	6	0	-3.806994	0.893296	4.119172
156	1	0	-5.355642	0.354012	2.783982
157	6	0	-5.893736	2.653689	1.463416
158	1	0	-6.775853	2.056824	1.734809
159	1	0	-6.231084	3.696120	1.452919
160	8	0	0.722056	5.485415	1.111031
161	8	0	0.071580	5.284443	-1.585060
162	6	0	0.795573	6.497750	-1.703693
163	1	0	1.505537	6.365203	-2.529931
164	1	0	0.119938	7.336089	-1.944033
165	1	0	1.349109	6.728126	-0.782512
166	8	0	-4.233081	0.819756	-3.678103
167	8	0	-5.407455	-0.938989	-1.789489
168	6	0	-6.310215	-1.266248	-2.835719
169	1	0	-6.321732	-2.360314	-2.917055
170	1	0	-7.327163	-0.912776	-2.597232
171	1	0	-5.986270	-0.831738	-3.791982
172	8	0	-2.151919	1.605210	5.625170
173	6	0	-1.260882	2.580190	6.114450
174	1	0	-0.672868	2.100450	6.905883
175	1	0	-0.578177	2.937261	5.325430
176	1	0	-1.797173	3.443795	6.540805

Compound ***P*-8**, conformer 2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.477254	-2.852515	-2.202090
2	6	0	-4.900208	-3.399695	-0.981080
3	6	0	-4.242477	-4.540171	-0.503601
4	6	0	-3.219373	-5.116022	-1.275053
5	6	0	-2.816639	-4.573774	-2.489294
6	6	0	-3.449158	-3.401344	-2.948516
7	1	0	-4.953249	-1.955957	-2.603354
8	1	0	-2.740872	-6.024138	-0.910386
9	6	0	-4.538628	-5.171746	0.845168
10	1	0	-4.372536	-6.255104	0.764307
11	1	0	-5.594040	-5.047022	1.109783
12	6	0	-6.047466	-2.720244	-0.251044
13	1	0	-6.584082	-3.447253	0.368664
14	1	0	-6.769889	-2.381398	-1.006934
15	6	0	-3.641759	-4.635132	1.948183
16	6	0	-4.014299	-3.591117	2.810931
17	6	0	-2.360736	-5.186932	2.075807
18	6	0	-3.095113	-3.158359	3.774340
19	6	0	-1.438371	-4.716214	3.000940
20	1	0	-2.058507	-6.008074	1.422914
21	6	0	-1.814457	-3.686114	3.875040
22	1	0	-3.359853	-2.360588	4.471031
23	6	0	-5.649198	-1.514696	0.581628
24	6	0	-5.604027	-0.265772	-0.047064
25	6	0	-5.332361	-1.591006	1.949926
26	6	0	-5.224330	0.894780	0.618276
27	1	0	-5.872978	-0.170351	-1.100917
28	6	0	-4.967354	-0.416857	2.616399
29	6	0	-4.889179	0.815184	1.976889
30	1	0	-4.733783	-0.442833	3.683014
31	6	0	-5.358165	-2.885814	2.744552
32	1	0	-5.665643	-2.644991	3.771692
33	1	0	-6.127362	-3.559279	2.351232
34	8	0	-3.115863	-2.850998	-4.148543
35	8	0	-1.856014	-5.090205	-3.288439
36	6	0	-1.151444	-6.231822	-2.859192
37	1	0	-0.416463	-6.460496	-3.640068
38	1	0	-0.621835	-6.048079	-1.909543
39	1	0	-1.820777	-7.098535	-2.732529
40	8	0	-0.175480	-5.234162	3.094766
41	8	0	-0.941386	-3.154305	4.776251
42	6	0	-0.524176	-4.003826	5.831649
43	1	0	-1.387182	-4.335538	6.433434
44	1	0	0.013995	-4.883782	5.450822
45	1	0	0.147811	-3.415587	6.469757
46	8	0	-4.526122	1.932056	2.682951
47	8	0	-5.152798	2.066101	-0.080872

48	6	0	-6.072094	3.080762	0.296737
49	1	0	-5.879270	3.943995	-0.352449
50	1	0	-7.110183	2.741288	0.144935
51	1	0	-5.932323	3.373771	1.346947
52	6	0	0.669927	-5.071269	1.966644
53	1	0	1.617585	-5.564127	2.222932
54	1	0	0.255675	-5.576540	1.077353
55	6	0	0.919171	-3.603942	1.660042
56	1	0	-0.010017	-3.118048	1.324091
57	1	0	1.238420	-3.085928	2.581083
58	6	0	-1.786917	-2.375954	-4.320830
59	1	0	-1.330881	-2.887670	-5.183256
60	1	0	-1.175575	-2.614395	-3.438194
61	6	0	-1.800706	-0.884400	-4.581427
62	1	0	-0.772398	-0.562385	-4.836973
63	1	0	-2.445398	-0.675964	-5.448082
64	6	0	-3.129412	2.137277	2.858356
65	1	0	-2.994793	2.645112	3.824372
66	1	0	-2.603413	1.170149	2.902677
67	6	0	-2.564007	2.966482	1.720139
68	1	0	-2.902020	2.541018	0.767720
69	1	0	-2.939724	4.005236	1.780024
70	8	0	1.909158	-3.526515	0.659335
71	8	0	-2.311527	-0.121462	-3.516885
72	8	0	-1.153898	2.950457	1.809692
73	6	0	3.250664	-0.949616	0.881956
74	6	0	1.949722	-1.125173	0.094590
75	6	0	0.884786	0.632983	1.272842
76	6	0	2.106811	0.857508	2.172113
77	6	0	3.386651	0.466689	1.435886
78	1	0	2.002696	-0.506735	-0.817104
79	1	0	3.234364	-1.645819	1.738592
80	1	0	-0.046524	0.824154	1.816901
81	1	0	2.002488	0.182216	3.040032
82	1	0	3.534729	1.158734	0.591169
83	8	0	0.839005	-0.708164	0.873948
84	8	0	0.993515	1.488630	0.163454
85	8	0	2.198755	2.190673	2.606907
86	8	0	4.501778	0.491414	2.298888
87	8	0	4.307859	-1.281619	0.017850
88	6	0	1.539112	2.466264	3.833586
89	1	0	0.460126	2.264780	3.738357
90	6	0	5.230115	1.711378	2.362283
91	1	0	4.535615	2.561080	2.410366
92	1	0	5.783315	1.670913	3.312035
93	6	0	5.423334	-1.963755	0.565746
94	1	0	5.114945	-2.486198	1.486516
95	1	0	6.210750	-1.245827	0.838591
96	6	0	6.199990	1.884276	1.216879
97	6	0	7.412275	1.185178	1.205283

98	6	0	5.903318	2.724866	0.140767
99	6	0	8.299892	1.313055	0.140763
100	1	0	7.665749	0.537678	2.048814
101	6	0	6.788112	2.855360	-0.929610
102	1	0	4.970356	3.294465	0.142899
103	6	0	7.986705	2.147006	-0.933109
104	1	0	9.244586	0.764601	0.150064
105	1	0	6.539868	3.516451	-1.762806
106	1	0	8.682500	2.249511	-1.768717
107	6	0	5.941644	-2.959874	-0.438154
108	6	0	5.210966	-4.122540	-0.711173
109	6	0	7.133157	-2.732632	-1.128054
110	6	0	5.667500	-5.038805	-1.653450
111	1	0	4.273521	-4.302327	-0.177190
112	6	0	7.594466	-3.650623	-2.072402
113	1	0	7.707367	-1.825265	-0.923402
114	6	0	6.862024	-4.804690	-2.336558
115	1	0	5.091267	-5.944408	-1.856486
116	1	0	8.529909	-3.461433	-2.603688
117	1	0	7.221255	-5.525259	-3.074694
118	6	0	1.723172	-2.560639	-0.347137
119	1	0	2.452218	-2.794656	-1.133156
120	1	0	0.708018	-2.634684	-0.777895
121	6	0	-0.148090	2.161404	-0.289356
122	8	0	-1.242559	1.274061	-0.362696
123	6	0	-1.835747	1.244630	-1.655834
124	6	0	-1.285358	2.475631	-2.380598
125	6	0	0.096630	2.648372	-1.744264
126	1	0	-2.927089	1.312696	-1.532399
127	1	0	-1.191965	2.301399	-3.464771
128	1	0	0.402491	3.707512	-1.767803
129	6	0	-0.493732	3.344469	0.630878
130	1	0	0.450032	3.829548	0.917963
131	1	0	-1.108037	4.064487	0.068321
132	8	0	1.002084	1.850904	-2.453054
133	8	0	-2.031709	3.641255	-2.127960
134	6	0	-1.513917	-0.064505	-2.359296
135	1	0	-1.732388	-0.896922	-1.667114
136	1	0	-0.441041	-0.097427	-2.613629
137	6	0	-3.275345	3.716072	-2.786349
138	1	0	-4.016127	3.049981	-2.310268
139	1	0	-3.158101	3.373648	-3.833143
140	1	0	1.946308	1.808835	4.622756
141	6	0	1.758331	3.909754	4.195920
142	6	0	2.933798	4.309212	4.838659
143	6	0	0.805612	4.876877	3.864203
144	6	0	3.154089	5.649409	5.146165
145	1	0	3.683014	3.558972	5.104721
146	6	0	1.022576	6.218766	4.172450
147	1	0	-0.109979	4.562897	3.356811

148	6	0	2.197242	6.607421	4.813238
149	1	0	4.075056	5.948346	5.651692
150	1	0	0.269431	6.965603	3.911165
151	1	0	2.367213	7.658622	5.056678
152	6	0	3.136794	1.451753	-3.419246
153	6	0	2.931241	1.660931	-4.787536
154	6	0	4.045610	0.471494	-3.014600
155	6	0	3.622616	0.909572	-5.732527
156	1	0	2.220559	2.425023	-5.112851
157	6	0	4.743098	-0.280475	-3.960785
158	1	0	4.209215	0.275163	-1.952419
159	6	0	4.533658	-0.063557	-5.319732
160	1	0	3.454662	1.085276	-6.797475
161	1	0	5.450820	-1.043416	-3.628092
162	1	0	5.079441	-0.652227	-6.060497
163	6	0	2.360259	2.258687	-2.413953
164	1	0	2.773291	2.122197	-1.404033
165	1	0	2.419131	3.334450	-2.662382
166	6	0	-3.790487	5.133226	-2.773274
167	6	0	-2.923433	6.220971	-2.653635
168	6	0	-5.159864	5.373412	-2.922798
169	6	0	-3.416663	7.524334	-2.682250
170	1	0	-1.855450	6.037224	-2.531843
171	6	0	-5.652888	6.675357	-2.958813
172	1	0	-5.849768	4.530003	-3.013331
173	6	0	-4.781473	7.756544	-2.836871
174	1	0	-2.727042	8.365885	-2.583815
175	1	0	-6.725247	6.846258	-3.076701
176	1	0	-5.166939	8.778160	-2.859367

Compound ***P*-8**, conformer 3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.986901	-0.726446	2.492356
2	6	0	4.862443	-2.123736	2.462103
3	6	0	3.988988	-2.731129	3.372698
4	6	0	3.298526	-1.930941	4.298207
5	6	0	3.435143	-0.548258	4.325677
6	6	0	4.286354	0.065627	3.385203
7	1	0	5.649467	-0.212659	1.793611
8	1	0	2.648635	-2.417259	5.024659
9	6	0	3.707759	-4.223422	3.389757
10	1	0	3.517044	-4.526608	4.428870
11	1	0	4.589971	-4.787183	3.068295
12	6	0	5.675765	-2.893634	1.434703
13	1	0	5.886728	-3.905414	1.798265
14	1	0	6.653041	-2.399464	1.341099

15	6	0	2.495785	-4.604458	2.556225
16	6	0	2.576467	-5.059119	1.229814
17	6	0	1.231335	-4.450679	3.137359
18	6	0	1.388173	-5.362694	0.554057
19	6	0	0.056496	-4.696167	2.438729
20	1	0	1.153577	-4.106752	4.170159
21	6	0	0.134399	-5.176300	1.122717
22	1	0	1.416479	-5.736651	-0.471331
23	6	0	5.050410	-2.950780	0.052208
24	6	0	5.302198	-1.891479	-0.825957
25	6	0	4.233712	-4.008524	-0.386171
26	6	0	4.748822	-1.825740	-2.099637
27	1	0	5.951949	-1.068076	-0.523109
28	6	0	3.699278	-3.946656	-1.677236
29	6	0	3.924048	-2.873453	-2.531988
30	1	0	3.077003	-4.762571	-2.051236
31	6	0	3.885435	-5.212011	0.474057
32	1	0	3.797399	-6.085971	-0.186293
33	1	0	4.705040	-5.438279	1.164797
34	8	0	4.490322	1.411960	3.396760
35	8	0	2.816686	0.273876	5.203352
36	6	0	1.900612	-0.272970	6.123059
37	1	0	1.506351	0.564656	6.710606
38	1	0	1.064721	-0.777534	5.610363
39	1	0	2.387224	-0.990052	6.804374
40	8	0	-1.177348	-4.487754	2.990500
41	8	0	-0.978513	-5.404288	0.370104
42	6	0	-1.846897	-6.434869	0.810186
43	1	0	-2.669166	-6.488752	0.085297
44	1	0	-1.324505	-7.406364	0.830982
45	1	0	-2.255018	-6.219199	1.807770
46	8	0	3.370635	-2.868457	-3.785640
47	8	0	4.989895	-0.722350	-2.867980
48	6	0	5.743592	-0.929216	-4.052816
49	1	0	5.847957	0.048784	-4.539490
50	1	0	6.746663	-1.319849	-3.813704
51	1	0	5.232949	-1.624866	-4.734008
52	6	0	-1.457260	-3.181045	3.469489
53	1	0	-2.480400	-3.216866	3.867425
54	1	0	-0.784119	-2.899198	4.296484
55	6	0	-1.369795	-2.158453	2.350299
56	1	0	-0.333168	-2.079040	1.985453
57	1	0	-1.983790	-2.498712	1.498656
58	6	0	3.375683	2.263856	3.166489
59	1	0	3.283051	2.965716	4.010461
60	1	0	2.445517	1.679048	3.124734
61	6	0	3.575678	3.052994	1.889690
62	1	0	2.762874	3.801003	1.809512
63	1	0	4.530358	3.596522	1.944802
64	6	0	2.018874	-2.433942	-3.873333

65	1	0	1.554035	-2.981770	-4.705841
66	1	0	1.474201	-2.686516	-2.949255
67	6	0	1.958380	-0.935341	-4.101889
68	1	0	2.613359	-0.439693	-3.375088
69	1	0	2.330730	-0.689933	-5.114697
70	8	0	-1.811725	-0.916878	2.847687
71	8	0	3.639137	2.261643	0.728870
72	8	0	0.621439	-0.507030	-3.954987
73	6	0	-3.122439	0.457045	0.630718
74	6	0	-1.608647	0.515960	0.847353
75	6	0	-1.171385	-0.238085	-1.363212
76	6	0	-2.662232	-0.453321	-1.651356
77	6	0	-3.484428	0.550164	-0.848930
78	1	0	-1.258816	1.532282	0.601389
79	1	0	-3.492401	-0.513684	1.005553
80	1	0	-0.547957	-0.983575	-1.869961
81	1	0	-2.914295	-1.465091	-1.289780
82	1	0	-3.248307	1.565316	-1.209241
83	8	0	-0.945992	-0.417800	0.008223
84	8	0	-0.837639	1.058162	-1.778003
85	8	0	-2.992878	-0.323447	-3.009521
86	8	0	-4.866156	0.297325	-0.971861
87	8	0	-3.686778	1.502646	1.381920
88	6	0	-2.631893	-1.408030	-3.852898
89	1	0	-2.982836	-1.111343	-4.852396
90	6	0	-5.548209	1.080361	-1.921468
91	1	0	-5.500377	2.150003	-1.641200
92	1	0	-5.063763	0.982101	-2.907849
93	6	0	-5.003904	1.329268	1.871770
94	1	0	-5.259995	0.256779	1.868161
95	1	0	-5.729638	1.836442	1.215249
96	6	0	-6.989471	0.650696	-2.019413
97	6	0	-7.421514	-0.577197	-1.515044
98	6	0	-7.916638	1.483924	-2.654410
99	6	0	-8.754816	-0.966025	-1.645807
100	1	0	-6.702128	-1.224701	-1.013708
101	6	0	-9.245815	1.094735	-2.789413
102	1	0	-7.592812	2.451981	-3.046730
103	6	0	-9.670647	-0.134110	-2.284071
104	1	0	-9.078891	-1.928603	-1.243148
105	1	0	-9.957180	1.757383	-3.287565
106	1	0	-10.714498	-0.438966	-2.385717
107	6	0	-5.097784	1.873462	3.274430
108	6	0	-4.346528	1.286499	4.300354
109	6	0	-5.917087	2.961500	3.575309
110	6	0	-4.418273	1.780197	5.598770
111	1	0	-3.699753	0.434834	4.071478
112	6	0	-5.993427	3.456982	4.877930
113	1	0	-6.504558	3.428415	2.780419
114	6	0	-5.243434	2.867805	5.891298

115	1	0	-3.829716	1.313287	6.391902
116	1	0	-6.640158	4.309104	5.098713
117	1	0	-5.300125	3.253943	6.911478
118	6	0	-1.216995	0.229922	2.287047
119	1	0	-1.542761	1.075989	2.905180
120	1	0	-0.114984	0.159816	2.339418
121	6	0	0.430332	1.302507	-2.314947
122	8	0	1.420779	0.609614	-1.590143
123	6	0	2.480257	1.459551	-1.164707
124	6	0	2.289045	2.772516	-1.929264
125	6	0	0.771005	2.803717	-2.162963
126	1	0	3.433264	0.980301	-1.435355
127	1	0	2.616208	3.634386	-1.326952
128	1	0	0.534463	3.364093	-3.083520
129	6	0	0.476720	0.882363	-3.795325
130	1	0	-0.474539	1.185923	-4.256453
131	1	0	1.298546	1.417726	-4.294978
132	8	0	0.096529	3.341038	-1.060878
133	8	0	2.924227	2.774424	-3.187672
134	6	0	2.441195	1.630665	0.345793
135	1	0	2.335683	0.634331	0.810399
136	1	0	1.563653	2.237549	0.627414
137	6	0	4.332887	2.919746	-3.167963
138	1	0	4.643746	2.802638	-4.216604
139	1	0	4.806554	2.103961	-2.596504
140	1	0	-1.536356	-1.510954	-3.909079
141	6	0	-3.261427	-2.723771	-3.457741
142	6	0	-4.651933	-2.839098	-3.348943
143	6	0	-2.470527	-3.840974	-3.185579
144	6	0	-5.235939	-4.046368	-2.979386
145	1	0	-5.280830	-1.968541	-3.550089
146	6	0	-3.052062	-5.054641	-2.817875
147	1	0	-1.382705	-3.759601	-3.254970
148	6	0	-4.436263	-5.159441	-2.714142
149	1	0	-6.322704	-4.122004	-2.898370
150	1	0	-2.417087	-5.916806	-2.603100
151	1	0	-4.895027	-6.107408	-2.424347
152	6	0	-0.751788	5.210812	0.160569
153	6	0	-0.346794	6.367119	0.831151
154	6	0	-1.860591	4.506604	0.640173
155	6	0	-1.040521	6.818433	1.953242
156	1	0	0.524798	6.921624	0.473689
157	6	0	-2.545913	4.946859	1.768999
158	1	0	-2.188455	3.598326	0.134596
159	6	0	-2.140458	6.107464	2.427191
160	1	0	-0.711265	7.725237	2.465491
161	1	0	-3.397897	4.369860	2.135082
162	1	0	-2.678837	6.453865	3.312177
163	6	0	-0.018090	4.747733	-1.070668
164	1	0	-0.563909	5.061033	-1.982305

165	1	0	0.975530	5.228543	-1.113646
166	6	0	4.788689	4.259771	-2.638518
167	6	0	4.296885	5.441542	-3.203573
168	6	0	5.700120	4.343062	-1.585130
169	6	0	4.714947	6.680677	-2.728442
170	1	0	3.576141	5.384127	-4.022920
171	6	0	6.126606	5.583630	-1.110855
172	1	0	6.071304	3.425380	-1.122567
173	6	0	5.634679	6.754358	-1.681433
174	1	0	4.325259	7.596348	-3.178887
175	1	0	6.841737	5.633887	-0.286791
176	1	0	5.964766	7.726840	-1.309598

Compound ***P*-8**, conformer 4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.828283	0.592454	-5.032082
2	6	0	-1.233508	4.982686	-0.535253
3	1	0	-2.251598	5.387012	-0.454389
4	1	0	-0.881344	5.159059	-1.565714
5	6	0	-1.244145	3.494497	-0.232241
6	1	0	-0.244083	3.061894	-0.395951
7	1	0	-1.489127	3.342598	0.833271
8	6	0	1.554521	-0.032073	-4.935885
9	1	0	1.064728	-0.008101	-5.922297
10	1	0	0.908036	0.518049	-4.236993
11	6	0	1.718498	-1.472858	-4.499932
12	1	0	0.731189	-1.971304	-4.557955
13	1	0	2.397711	-1.985778	-5.196822
14	6	0	3.386207	-0.502414	3.465341
15	1	0	3.317082	-0.563437	4.560926
16	1	0	2.759608	0.339412	3.128271
17	6	0	2.900999	-1.784231	2.814527
18	1	0	3.185320	-1.778614	1.755053
19	1	0	3.384992	-2.658963	3.288890
20	8	0	-2.190454	2.879549	-1.075455
21	8	0	2.278488	-1.624341	-3.219528
22	8	0	1.499675	-1.859197	2.962978
23	6	0	-3.306554	0.648107	0.429894
24	6	0	-2.013972	0.517961	-0.379640
25	6	0	-0.814353	-0.311567	1.492111
26	6	0	-2.022908	-0.131304	2.419990
27	6	0	-3.319812	-0.295537	1.629806
28	1	0	-2.000143	-0.473326	-0.863477
29	1	0	-3.373094	1.680016	0.815889
30	1	0	0.125662	-0.118791	2.020908
31	1	0	-1.986455	0.908583	2.787462

32	1	0	-3.382944	-1.331885	1.260678
33	8	0	-0.880677	0.638077	0.465460
34	8	0	-0.832242	-1.620770	0.981548
35	8	0	-2.023038	-1.028601	3.500538
36	8	0	-4.449256	0.020608	2.412776
37	8	0	-4.374077	0.400610	-0.449937
38	6	0	-1.163582	-0.708816	4.585791
39	1	0	-1.312577	-1.525566	5.307620
40	6	0	-5.057036	-1.056252	3.114551
41	1	0	-4.286912	-1.661436	3.612030
42	1	0	-5.674496	-0.582888	3.891777
43	6	0	-5.557162	1.164891	-0.288302
44	1	0	-5.318147	2.098239	0.247647
45	1	0	-6.286156	0.609935	0.320268
46	6	0	-5.924726	-1.927748	2.236783
47	6	0	-7.193829	-1.492337	1.838780
48	6	0	-5.475451	-3.173309	1.790281
49	6	0	-7.988032	-2.275144	1.005773
50	1	0	-7.567036	-0.528981	2.196186
51	6	0	-6.266736	-3.961618	0.954843
52	1	0	-4.494901	-3.537558	2.107887
53	6	0	-7.523119	-3.512025	0.557755
54	1	0	-8.978467	-1.922868	0.708594
55	1	0	-5.899422	-4.932440	0.615005
56	1	0	-8.145600	-4.127974	-0.094918
57	6	0	-6.134974	1.486124	-1.641883
58	6	0	-5.507865	2.429660	-2.464466
59	6	0	-7.278275	0.836311	-2.108938
60	6	0	-6.018128	2.716995	-3.726629
61	1	0	-4.608109	2.937724	-2.105911
62	6	0	-7.793373	1.123532	-3.373623
63	1	0	-7.771985	0.095655	-1.474427
64	6	0	-7.163683	2.063999	-4.184292
65	1	0	-5.522622	3.457320	-4.358909
66	1	0	-8.690224	0.608996	-3.725802
67	1	0	-7.565248	2.291280	-5.174343
68	6	0	-1.908305	1.560926	-1.479423
69	1	0	-2.643305	1.316045	-2.256431
70	1	0	-0.896521	1.497236	-1.920281
71	6	0	0.383886	-2.300061	0.822654
72	8	0	1.355417	-1.444470	0.263778
73	6	0	1.942732	-1.980490	-0.915520
74	6	0	1.546031	-3.459113	-0.928842
75	6	0	0.196154	-3.449144	-0.205242
76	1	0	3.034154	-1.863094	-0.837211
77	1	0	1.430517	-3.839796	-1.956710
78	1	0	0.020619	-4.414664	0.297855
79	6	0	0.884893	-2.845110	2.170992
80	1	0	0.012498	-3.231460	2.718194
81	1	0	1.581315	-3.676599	1.981832

82	8	0	-0.800194	-3.191662	-1.153275
83	8	0	2.428283	-4.272682	-0.194414
84	6	0	1.471836	-1.215471	-2.142217
85	1	0	1.571506	-0.134587	-1.938284
86	1	0	0.407873	-1.434578	-2.336159
87	6	0	3.685325	-4.495866	-0.791765
88	1	0	4.338096	-3.612139	-0.681876
89	1	0	3.551339	-4.666074	-1.877855
90	1	0	-0.109030	-0.742684	4.270137
91	6	0	-1.472861	0.617079	5.241543
92	6	0	-0.490257	1.601671	5.357060
93	6	0	-2.752793	0.879249	5.743176
94	6	0	-0.772547	2.822948	5.969468
95	1	0	0.509574	1.413240	4.957532
96	6	0	-3.039752	2.097379	6.350584
97	1	0	-3.530454	0.117157	5.652794
98	6	0	-2.048327	3.073078	6.467058
99	1	0	0.007999	3.582642	6.049901
100	1	0	-4.042287	2.288865	6.739826
101	1	0	-2.273603	4.028864	6.945349
102	6	0	-2.956478	-3.575732	-2.077717
103	6	0	-3.958772	-2.610059	-2.194644
104	6	0	-2.732058	-4.451403	-3.145821
105	6	0	-4.728317	-2.526422	-3.355622
106	1	0	-4.140923	-1.902561	-1.382227
107	6	0	-3.496023	-4.367634	-4.305525
108	1	0	-1.948557	-5.209114	-3.063336
109	6	0	-4.499384	-3.403724	-4.411920
110	1	0	-5.508518	-1.765383	-3.431738
111	1	0	-3.312227	-5.059622	-5.130489
112	1	0	-5.101950	-3.338494	-5.320667
113	6	0	-2.100852	-3.666436	-0.843022
114	1	0	-2.538358	-3.078986	-0.022880
115	1	0	-2.028531	-4.717118	-0.506922
116	6	0	4.354616	-5.696069	-0.170759
117	6	0	3.611273	-6.707948	0.439701
118	6	0	5.745388	-5.824778	-0.236818
119	6	0	4.246848	-7.827268	0.974482
120	1	0	2.526939	-6.607894	0.497818
121	6	0	6.380877	-6.945999	0.290867
122	1	0	6.339199	-5.037291	-0.708758
123	6	0	5.632378	-7.951551	0.900624
124	1	0	3.652913	-8.609691	1.452541
125	1	0	7.468133	-7.031726	0.230957
126	1	0	6.129437	-8.828956	1.320010
127	6	0	1.737385	5.454359	-0.572881
128	6	0	3.078984	5.060897	-0.493180
129	6	0	3.570471	4.589303	0.735009
130	6	0	2.701853	4.549873	1.832523
131	6	0	1.362562	4.906457	1.739982

132	6	0	0.869445	5.359001	0.507014
133	1	0	1.343245	5.833862	-1.517384
134	1	0	3.057008	4.203944	2.805252
135	6	0	4.991805	4.091657	0.934049
136	1	0	5.319804	4.392609	1.938781
137	1	0	5.674327	4.586832	0.234832
138	6	0	3.910961	5.120303	-1.763397
139	1	0	4.971612	5.254053	-1.525530
140	1	0	3.611776	6.014470	-2.328095
141	6	0	5.131936	2.582072	0.830095
142	6	0	5.468616	1.914450	-0.361270
143	6	0	4.906516	1.819669	1.980623
144	6	0	5.582859	0.520365	-0.338337
145	6	0	4.984922	0.431639	1.987330
146	1	0	4.659864	2.311978	2.923850
147	6	0	5.341427	-0.232405	0.805587
148	1	0	5.870330	-0.023024	-1.240625
149	6	0	3.706181	3.904119	-2.649567
150	6	0	2.626439	3.933910	-3.547635
151	6	0	4.503991	2.755357	-2.577997
152	6	0	2.304152	2.847577	-4.351785
153	1	0	2.036143	4.846352	-3.621694
154	6	0	4.161133	1.658293	-3.382950
155	6	0	3.078183	1.674718	-4.245076
156	1	0	4.747927	0.738484	-3.347078
157	6	0	5.721305	2.630084	-1.676191
158	1	0	6.486678	2.063176	-2.224770
159	1	0	6.157877	3.617954	-1.491546
160	8	0	-0.452624	5.696187	0.411077
161	8	0	0.554609	4.749053	2.826093
162	6	0	-0.015037	5.925783	3.374410
163	1	0	-0.613075	5.615566	4.240818
164	1	0	0.771220	6.621383	3.713590
165	1	0	-0.663837	6.435388	2.647934
166	8	0	4.750957	-0.263013	3.145230
167	8	0	5.418947	-1.593993	0.731781
168	6	0	6.446977	-2.208176	1.495023
169	1	0	6.365358	-3.289581	1.328674
170	1	0	7.439567	-1.866356	1.157510
171	1	0	6.330387	-1.993069	2.566642
172	8	0	1.296443	2.823667	-5.253281
173	6	0	0.452716	3.945921	-5.365508
174	1	0	-0.294269	3.702996	-6.130529
175	1	0	-0.063324	4.161740	-4.415113
176	1	0	1.009777	4.843226	-5.681393

Compound ***P*-8**, conformer 5

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	8	0	-3.963527	-0.447300	4.519839
2	6	0	1.187363	4.478969	2.193778
3	1	0	2.219932	4.785307	2.409319
4	1	0	0.639951	4.442854	3.150721
5	6	0	1.189101	3.110313	1.534810
6	1	0	0.159347	2.735969	1.417858
7	1	0	1.615929	3.198047	0.520628
8	6	0	-2.711758	-1.126147	4.534810
9	1	0	-2.448241	-1.378426	5.574807
10	1	0	-1.918506	-0.473260	4.143093
11	6	0	-2.813812	-2.404461	3.730119
12	1	0	-1.876077	-2.977995	3.863738
13	1	0	-3.641539	-3.012413	4.124071
14	6	0	-2.701745	0.628491	-3.906869
15	1	0	-2.402904	0.810839	-4.949001
16	1	0	-2.129398	1.313736	-3.260489
17	6	0	-2.419066	-0.805208	-3.499729
18	1	0	-2.920108	-1.013976	-2.546277
19	1	0	-2.828731	-1.502229	-4.255142
20	8	0	1.944803	2.239326	2.343460
21	8	0	-3.085152	-2.201798	2.366568
22	8	0	-1.022700	-0.973285	-3.384845
23	6	0	3.256344	0.280788	0.617332
24	6	0	1.812236	0.117299	1.095920
25	6	0	1.000874	-0.095013	-1.130678
26	6	0	2.386535	0.186764	-1.727338
27	6	0	3.468832	-0.304151	-0.773436
28	1	0	1.634894	-0.950982	1.307534
29	1	0	3.487322	1.357915	0.571230
30	1	0	0.205055	0.321295	-1.758277
31	1	0	2.477826	1.283625	-1.806934
32	1	0	3.403292	-1.402646	-0.704959
33	8	0	0.896983	0.556928	0.104429
34	8	0	0.843494	-1.484741	-0.993372
35	8	0	2.585295	-0.412841	-2.981034
36	8	0	4.755955	0.074523	-1.208046
37	8	0	4.095559	-0.358730	1.553192
38	6	0	1.995988	0.244509	-4.093580
39	1	0	2.257230	-0.384248	-4.957914
40	6	0	5.480100	-0.915923	-1.896860
41	1	0	5.640199	-1.795669	-1.245149
42	1	0	4.903567	-1.262849	-2.771858
43	6	0	5.235427	0.378498	1.966908
44	1	0	4.911674	1.333011	2.418119
45	1	0	5.868941	0.605248	1.094875
46	6	0	6.813422	-0.377316	-2.347706
47	6	0	7.815163	-1.266898	-2.750861
48	6	0	7.068307	0.994291	-2.402287

49	6	0	9.042643	-0.795618	-3.206629
50	1	0	7.631099	-2.343897	-2.705399
51	6	0	8.300383	1.467285	-2.854316
52	1	0	6.291499	1.689606	-2.084017
53	6	0	9.290216	0.576097	-3.259665
54	1	0	9.814122	-1.503772	-3.517421
55	1	0	8.486405	2.543353	-2.888315
56	1	0	10.254635	0.947238	-3.613243
57	6	0	5.994201	-0.442750	2.972019
58	6	0	5.696616	-0.353308	4.334365
59	6	0	6.965984	-1.355151	2.552290
60	6	0	6.357979	-1.156769	5.260672
61	1	0	4.938185	0.357362	4.672986
62	6	0	7.629518	-2.161032	3.474420
63	1	0	7.206564	-1.431746	1.488684
64	6	0	7.325542	-2.063670	4.831369
65	1	0	6.118453	-1.073752	6.323064
66	1	0	8.389157	-2.867696	3.133085
67	1	0	7.846592	-2.693106	5.556142
68	6	0	1.538863	0.893127	2.373791
69	1	0	2.103631	0.419275	3.187832
70	1	0	0.460565	0.814743	2.605193
71	6	0	-0.410881	-2.050186	-1.265535
72	8	0	-1.436168	-1.264058	-0.701144
73	6	0	-2.287214	-2.009986	0.159482
74	6	0	-1.982032	-3.478940	-0.144333
75	6	0	-0.510945	-3.434915	-0.568271
76	1	0	-3.329601	-1.761529	-0.090688
77	1	0	-2.107932	-4.113135	0.748232
78	1	0	-0.289357	-4.255046	-1.271354
79	6	0	-0.635275	-2.182937	-2.781595
80	1	0	0.315008	-2.504618	-3.232511
81	1	0	-1.393149	-2.961291	-2.960830
82	8	0	0.276768	-3.539542	0.583016
83	8	0	-2.730432	-3.985449	-1.222695
84	6	0	-2.046822	-1.627651	1.611051
85	1	0	-2.041598	-0.525540	1.684196
86	1	0	-1.062080	-2.001168	1.941022
87	6	0	-4.098317	-4.204410	-0.961038
88	1	0	-4.663146	-3.256166	-0.991224
89	1	0	-4.215863	-4.618964	0.059087
90	1	0	0.897561	0.242425	-4.011914
91	6	0	2.503930	1.650977	-4.312123
92	6	0	1.615856	2.722439	-4.418272
93	6	0	3.877169	1.900443	-4.411922
94	6	0	2.085032	4.019046	-4.631091
95	1	0	0.541546	2.542066	-4.327720
96	6	0	4.349427	3.192536	-4.618253
97	1	0	4.581700	1.071167	-4.317754
98	6	0	3.453082	4.256616	-4.731144

99	1	0	1.376245	4.846223	-4.710896
100	1	0	5.424393	3.372189	-4.692895
101	1	0	3.823827	5.270928	-4.894712
102	6	0	2.169747	-4.388688	1.747314
103	6	0	3.186339	-3.602239	2.293107
104	6	0	1.681341	-5.472295	2.485687
105	6	0	3.714378	-3.898725	3.550355
106	1	0	3.567730	-2.737719	1.745104
107	6	0	2.202650	-5.767727	3.741364
108	1	0	0.884262	-6.092106	2.066962
109	6	0	3.224030	-4.981156	4.275777
110	1	0	4.510406	-3.273877	3.962416
111	1	0	1.814845	-6.618628	4.306008
112	1	0	3.636622	-5.214510	5.259934
113	6	0	1.579245	-4.071809	0.400141
114	1	0	2.212757	-3.355946	-0.143849
115	1	0	1.507932	-4.991930	-0.208506
116	6	0	-4.677777	-5.167511	-1.966574
117	6	0	-3.872933	-6.088396	-2.639722
118	6	0	-6.055257	-5.170704	-2.206967
119	6	0	-4.435111	-6.995383	-3.536564
120	1	0	-2.797598	-6.084888	-2.458713
121	6	0	-6.618933	-6.081013	-3.097411
122	1	0	-6.695701	-4.451727	-1.688905
123	6	0	-5.808888	-6.996661	-3.767255
124	1	0	-3.792829	-7.708149	-4.058993
125	1	0	-7.696825	-6.071002	-3.273802
126	1	0	-6.248315	-7.707748	-4.470147
127	6	0	-1.701583	5.211190	1.768399
128	6	0	-3.012103	4.989450	1.327009
129	6	0	-3.249389	4.884526	-0.052959
130	6	0	-2.167459	5.024763	-0.930514
131	6	0	-0.864356	5.210580	-0.487703
132	6	0	-0.627139	5.296959	0.892487
133	1	0	-1.502775	5.304566	2.837695
134	1	0	-2.320704	4.963559	-2.009712
135	6	0	-4.615860	4.596541	-0.649867
136	1	0	-4.704277	5.163780	-1.586870
137	1	0	-5.409849	4.972349	0.004532
138	6	0	-4.096296	4.828443	2.379697
139	1	0	-5.072008	5.124165	1.979345
140	1	0	-3.882206	5.525746	3.201611
141	6	0	-4.843005	3.128669	-0.969370
142	6	0	-5.456210	2.226738	-0.081311
143	6	0	-4.408455	2.651265	-2.209866
144	6	0	-5.626500	0.898609	-0.486787
145	6	0	-4.544181	1.321175	-2.590283
146	1	0	-3.942791	3.332054	-2.925785
147	6	0	-5.178775	0.427804	-1.716258
148	1	0	-6.126468	0.182597	0.168531

149	6	0	-4.150023	3.422903	2.950890
150	6	0	-3.314212	3.124229	4.033439
151	6	0	-4.963287	2.402687	2.427649
152	6	0	-3.232194	1.851802	4.581501
153	1	0	-2.700286	3.903439	4.489733
154	6	0	-4.862579	1.117655	2.974341
155	6	0	-4.000523	0.819756	4.022236
156	1	0	-5.462654	0.296698	2.577473
157	6	0	-5.955856	2.622817	1.296658
158	1	0	-6.848244	2.020195	1.515969
159	1	0	-6.293835	3.664947	1.291284
160	8	0	0.657242	5.470776	1.327966
161	8	0	0.149647	5.241582	-1.397616
162	6	0	0.876505	6.454067	-1.503977
163	1	0	1.630469	6.305105	-2.287552
164	1	0	0.213433	7.284814	-1.799487
165	1	0	1.378427	6.706972	-0.559244
166	8	0	-4.093145	0.908745	-3.816598
167	8	0	-5.333604	-0.895387	-2.016075
168	6	0	-6.195967	-1.197790	-3.103217
169	1	0	-6.203130	-2.289638	-3.210726
170	1	0	-7.221542	-0.850352	-2.894800
171	1	0	-5.836702	-0.740643	-4.036040
172	8	0	-2.393219	1.619012	5.634235
173	6	0	-3.031390	1.366666	6.875448
174	1	0	-2.240755	1.191797	7.616086
175	1	0	-3.633735	2.234776	7.190982
176	1	0	-3.681726	0.479432	6.821603

Compound ***P*-8**, conformer 6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.947255	-0.497412	4.525941
2	6	0	1.178825	4.471493	2.207108
3	1	0	2.211780	4.778689	2.419474
4	1	0	0.636097	4.429728	3.166398
5	6	0	1.180356	3.105824	1.541718
6	1	0	0.150709	2.730559	1.426175
7	1	0	1.604331	3.198504	0.526783
8	6	0	-2.694045	-1.173798	4.532705
9	1	0	-2.429397	-1.436109	5.569917
10	1	0	-1.902421	-0.515287	4.147234
11	6	0	-2.793934	-2.443956	3.715037
12	1	0	-1.855057	-3.017049	3.842283
13	1	0	-3.620336	-3.057537	4.102999
14	6	0	-2.705949	0.646422	-3.892301
15	1	0	-2.407835	0.838644	-4.932874

16	1	0	-2.134650	1.326872	-3.239937
17	6	0	-2.419924	-0.790388	-3.498560
18	1	0	-2.916316	-1.008072	-2.544696
19	1	0	-2.831966	-1.481392	-4.258157
20	8	0	1.939461	2.232484	2.344522
21	8	0	-3.066270	-2.227587	2.353788
22	8	0	-1.022763	-0.957306	-3.391456
23	6	0	3.262856	0.284800	0.614572
24	6	0	1.817722	0.115460	1.087421
25	6	0	1.014513	-0.088633	-1.143166
26	6	0	2.402087	0.198162	-1.733892
27	6	0	3.481860	-0.294271	-0.777647
28	1	0	1.641915	-0.954179	1.293530
29	1	0	3.490532	1.362847	0.573217
30	1	0	0.219711	0.329585	-1.770888
31	1	0	2.491214	1.295712	-1.807376
32	1	0	3.418978	-1.393205	-0.713738
33	8	0	0.905480	0.557727	0.094431
34	8	0	0.858834	-1.479383	-1.013688
35	8	0	2.608914	-0.394879	-2.989104
36	8	0	4.769950	0.089786	-1.204712
37	8	0	4.101156	-0.355360	1.550782
38	6	0	1.997947	0.246243	-4.101225
39	1	0	2.286322	-0.367768	-4.967132
40	6	0	5.498168	-0.894177	-1.900002
41	1	0	5.670173	-1.773610	-1.251223
42	1	0	4.918082	-1.243008	-2.771811
43	6	0	5.239930	0.382666	1.966354
44	1	0	4.914298	1.333742	2.423525
45	1	0	5.870750	0.616022	1.094200
46	6	0	6.822574	-0.341340	-2.359043
47	6	0	7.033394	1.033078	-2.488376
48	6	0	7.858400	-1.218002	-2.698190
49	6	0	8.254906	1.520788	-2.952059
50	1	0	6.230654	1.719193	-2.217605
51	6	0	9.075892	-0.732273	-3.166510
52	1	0	7.709714	-2.296147	-2.592124
53	6	0	9.278781	0.641474	-3.295073
54	1	0	8.406294	2.598825	-3.044784
55	1	0	9.874527	-1.430614	-3.426803
56	1	0	10.235165	1.024231	-3.657984
57	6	0	6.003028	-0.442034	2.965312
58	6	0	5.703083	-0.366198	4.327988
59	6	0	6.981441	-1.344284	2.539142
60	6	0	6.368529	-1.173141	5.248284
61	1	0	4.939546	0.336562	4.671610
62	6	0	7.649185	-2.153545	3.455294
63	1	0	7.223920	-1.410158	1.475246
64	6	0	7.342728	-2.069866	4.812574
65	1	0	6.127069	-1.100830	6.311021

66	1	0	8.414009	-2.852154	3.108989
67	1	0	7.867002	-2.701987	5.532669
68	6	0	1.537845	0.884835	2.367767
69	1	0	2.101745	0.409207	3.181380
70	1	0	0.459122	0.802014	2.595584
71	6	0	-0.396487	-2.044853	-1.281860
72	8	0	-1.419639	-1.263670	-0.706901
73	6	0	-2.268844	-2.017573	0.148677
74	6	0	-1.960878	-3.483981	-0.164952
75	6	0	-0.491014	-3.433695	-0.592456
76	1	0	-3.311942	-1.769702	-0.099217
77	1	0	-2.082454	-4.123669	0.724273
78	1	0	-0.268911	-4.249211	-1.300703
79	6	0	-0.629804	-2.169725	-2.797274
80	1	0	0.318059	-2.487741	-3.255932
81	1	0	-1.387552	-2.948163	-2.976299
82	8	0	0.299769	-3.542411	0.556352
83	8	0	-2.711353	-3.986396	-1.243766
84	6	0	-2.028889	-1.645550	1.602997
85	1	0	-2.025650	-0.544046	1.684927
86	1	0	-1.043481	-2.019965	1.929983
87	6	0	-4.077773	-4.210584	-0.978759
88	1	0	-4.645209	-3.263694	-1.001647
89	1	0	-4.190726	-4.631167	0.039403
90	1	0	0.900391	0.203058	-4.020933
91	6	0	2.451351	1.672333	-4.310063
92	6	0	3.806617	1.964176	-4.500999
93	6	0	1.531454	2.722138	-4.307362
94	6	0	4.229759	3.276142	-4.687962
95	1	0	4.537172	1.151742	-4.497371
96	6	0	1.950722	4.038993	-4.498168
97	1	0	0.471613	2.508278	-4.146752
98	6	0	3.301083	4.318328	-4.688708
99	1	0	5.290946	3.489002	-4.836026
100	1	0	1.217184	4.848006	-4.488084
101	1	0	3.633228	5.348342	-4.836405
102	6	0	2.195759	-4.396809	1.711959
103	6	0	3.208386	-3.609424	2.263790
104	6	0	1.713548	-5.489066	2.441578
105	6	0	3.738636	-3.913461	3.518281
106	1	0	3.584844	-2.738357	1.722785
107	6	0	2.237064	-5.792081	3.694539
108	1	0	0.919638	-6.109727	2.018110
109	6	0	3.254469	-5.004488	4.234951
110	1	0	4.531518	-3.287806	3.935144
111	1	0	1.854126	-6.649704	4.252290
112	1	0	3.668837	-5.243786	5.216933
113	6	0	1.602686	-4.071765	0.367864
114	1	0	2.234314	-3.351475	-0.172461
115	1	0	1.531609	-4.987929	-0.246711

116	6	0	-4.658047	-5.169529	-1.987779
117	6	0	-3.853036	-6.084276	-2.669039
118	6	0	-6.036360	-5.175176	-2.223346
119	6	0	-4.415862	-6.987650	-3.569126
120	1	0	-2.777080	-6.078827	-2.491788
121	6	0	-6.600639	-6.081909	-3.117039
122	1	0	-6.676951	-4.460987	-1.698882
123	6	0	-5.790428	-6.991422	-3.795004
124	1	0	-3.773449	-7.695597	-4.097908
125	1	0	-7.679169	-6.073894	-3.289597
126	1	0	-6.230372	-7.699659	-4.500445
127	6	0	-1.711467	5.189064	1.800654
128	6	0	-3.023665	4.967682	1.364427
129	6	0	-3.269182	4.880978	-0.015371
130	6	0	-2.194533	5.045365	-0.897741
131	6	0	-0.889889	5.234819	-0.460815
132	6	0	-0.643326	5.295305	0.919222
133	1	0	-1.506386	5.265985	2.870042
134	1	0	-2.355103	5.002358	-1.976772
135	6	0	-4.636700	4.587296	-0.606871
136	1	0	-4.734580	5.159990	-1.539588
137	1	0	-5.429912	4.952651	0.054377
138	6	0	-4.101200	4.791996	2.421659
139	1	0	-5.080117	5.087430	2.028987
140	1	0	-3.885426	5.483635	3.247928
141	6	0	-4.854864	3.119732	-0.935050
142	6	0	-5.460854	2.207996	-0.052033
143	6	0	-4.419571	2.653136	-2.179494
144	6	0	-5.624888	0.881855	-0.466601
145	6	0	-4.548841	1.325030	-2.568937
146	1	0	-3.958558	3.341292	-2.891376
147	6	0	-5.177418	0.422215	-1.700257
148	1	0	-6.119552	0.158569	0.184723
149	6	0	-4.147629	3.382297	2.982626
150	6	0	-3.306458	3.078280	4.059475
151	6	0	-4.961172	2.363968	2.456241
152	6	0	-3.219646	1.802482	4.598882
153	1	0	-2.692339	3.855775	4.518440
154	6	0	-4.855768	1.075618	2.994139
155	6	0	-3.988495	0.772607	4.036326
156	1	0	-5.456248	0.256147	2.594834
157	6	0	-5.958441	2.590116	1.330603
158	1	0	-6.847644	1.981872	1.547270
159	1	0	-6.300648	3.630867	1.335520
160	8	0	0.643385	5.466530	1.348379
161	8	0	0.116822	5.295302	-1.377411
162	6	0	0.836842	6.514130	-1.455882
163	1	0	1.586046	6.390378	-2.248230
164	1	0	0.167419	7.348965	-1.724246
165	1	0	1.344155	6.743876	-0.508237

166	8	0	-4.097708	0.923445	-3.798842
167	8	0	-5.326466	-0.899479	-2.009520
168	6	0	-6.189987	-1.197888	-3.096869
169	1	0	-6.192241	-2.288927	-3.212502
170	1	0	-7.216684	-0.856877	-2.883452
171	1	0	-5.835095	-0.732097	-4.027095
172	8	0	-2.375882	1.564630	5.646672
173	6	0	-3.008481	1.303831	6.888997
174	1	0	-2.214505	1.125457	7.625212
175	1	0	-3.610612	2.169192	7.212386
176	1	0	-3.657888	0.416085	6.832440

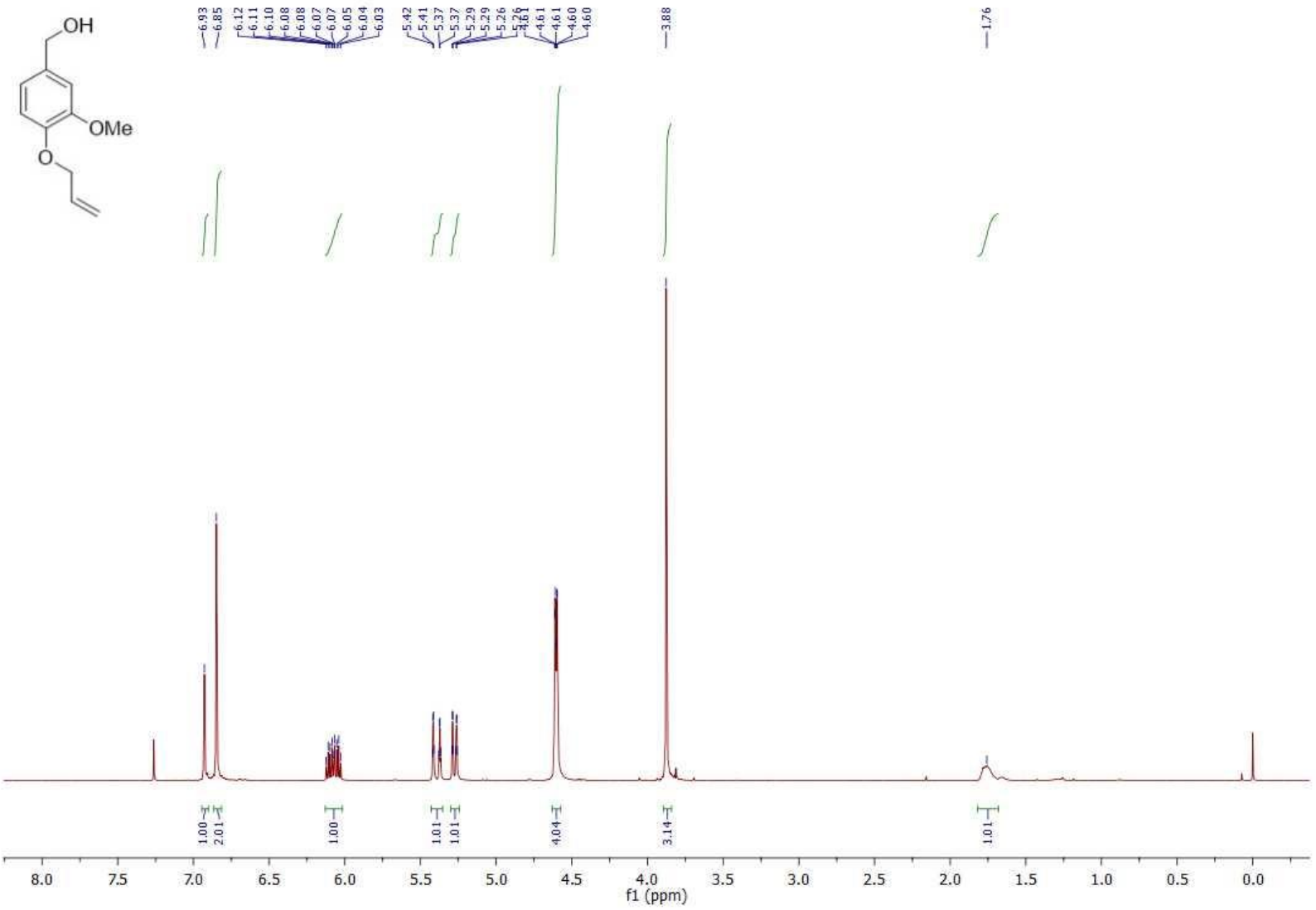


Figure S2. ^{1}H NMR spectrum of compound **S1.**

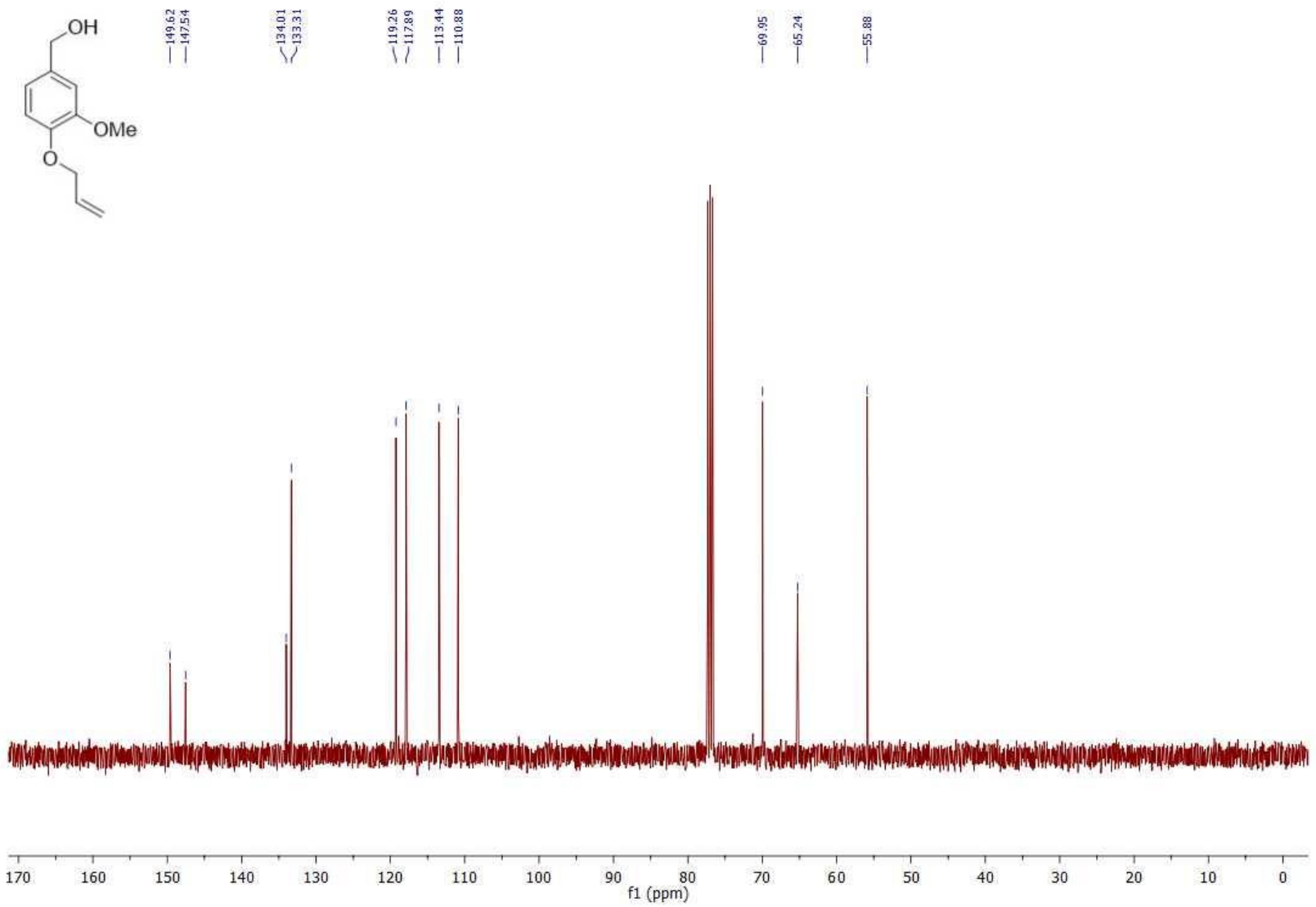


Figure S3. ^{13}C NMR spectrum of compound **S1**.

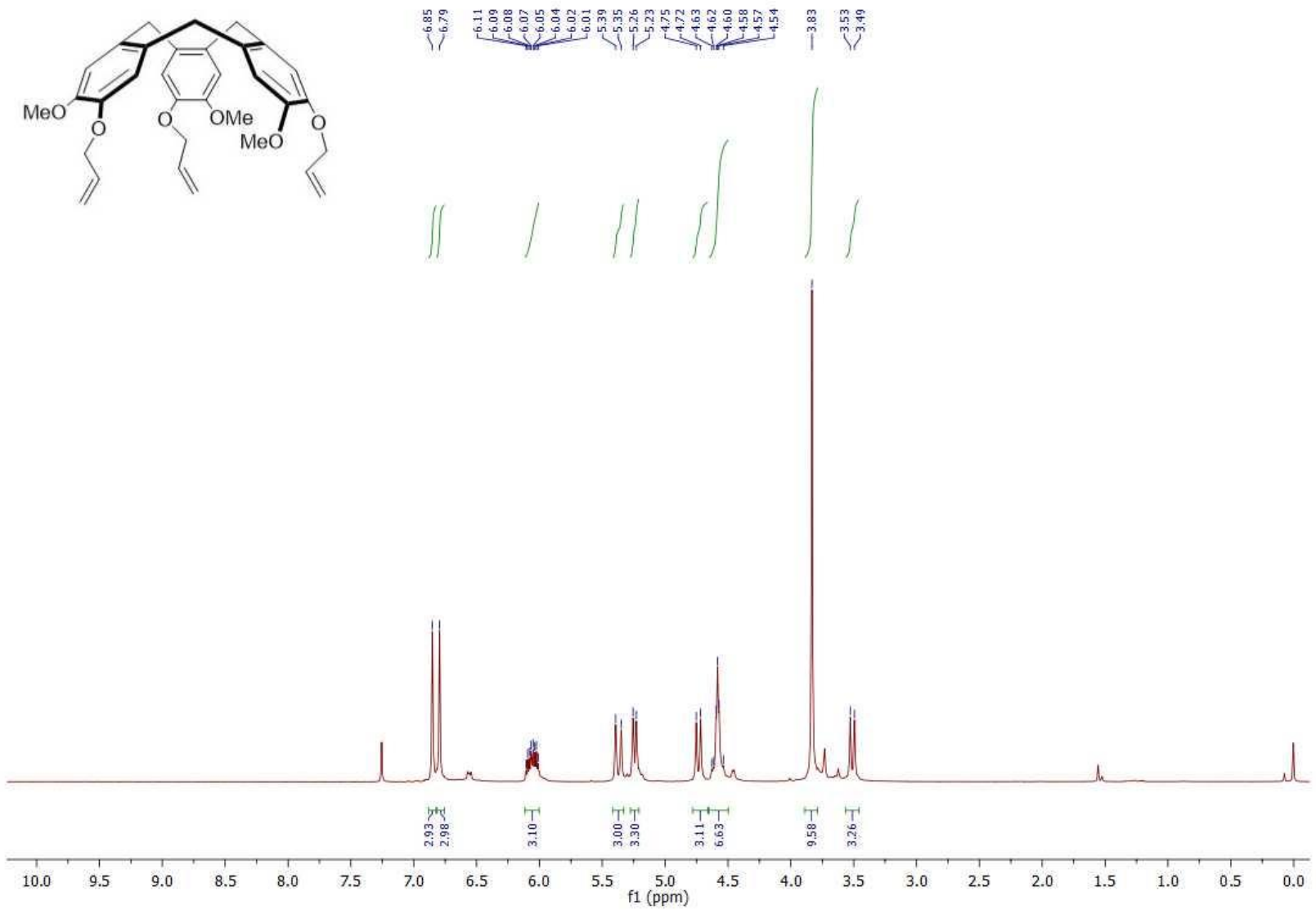


Figure S4. ^{1}H NMR spectrum of compound ***rac*-S2.**

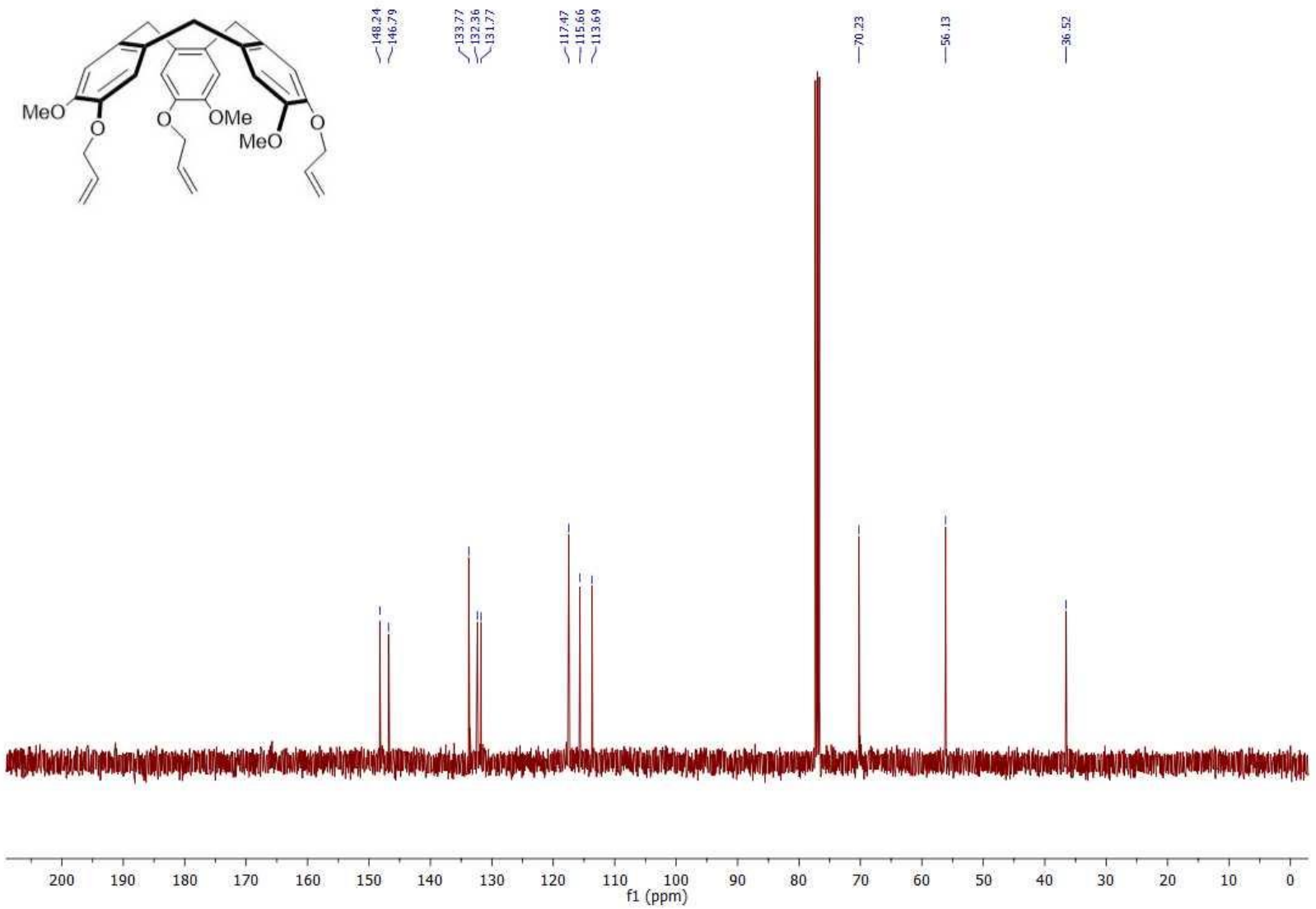


Figure S5. ^{13}C NMR spectrum of compound ***rac*-S2**.

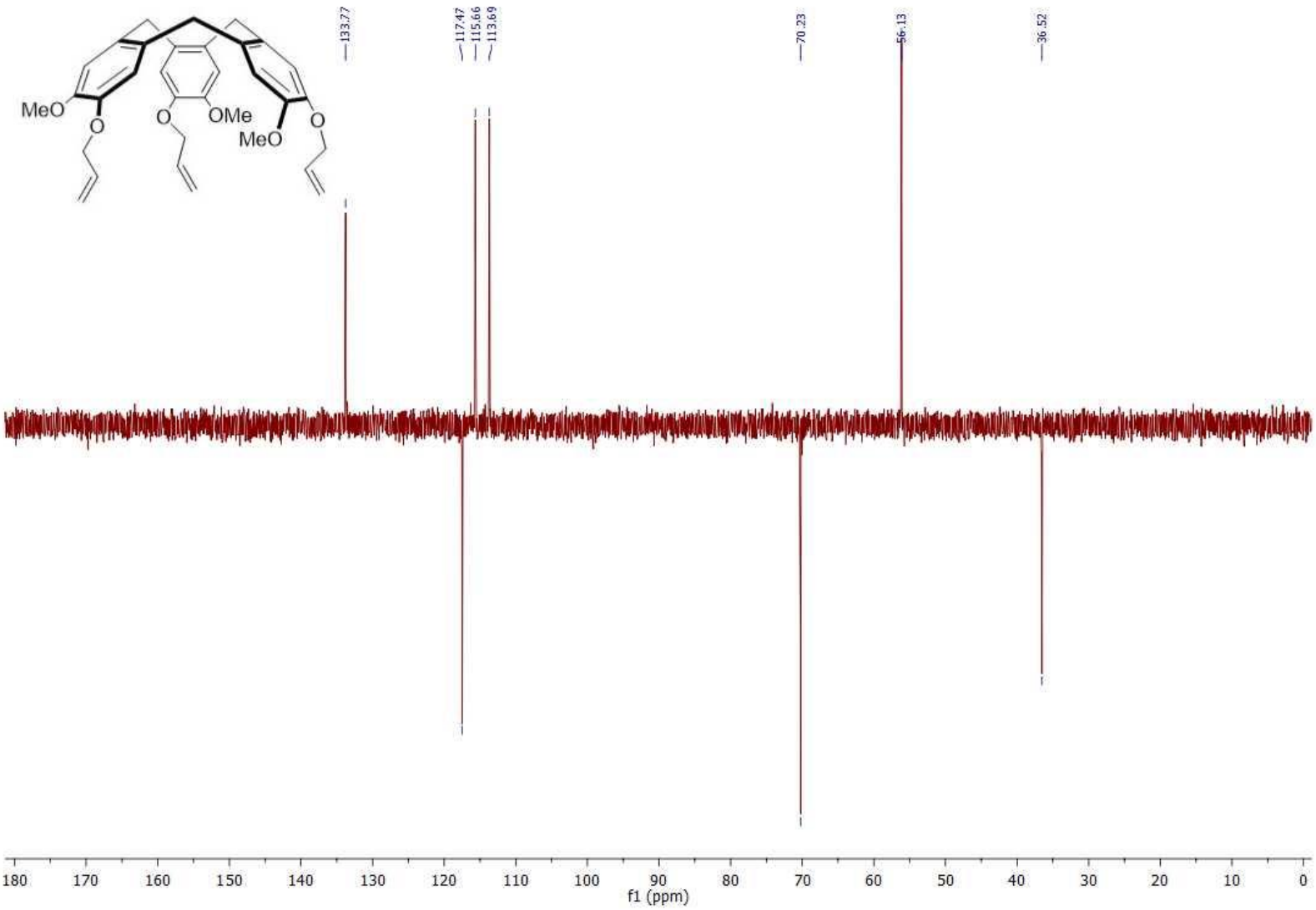


Figure S6. DEPT ^{13}C NMR spectrum of compound ***rac*-S2**.

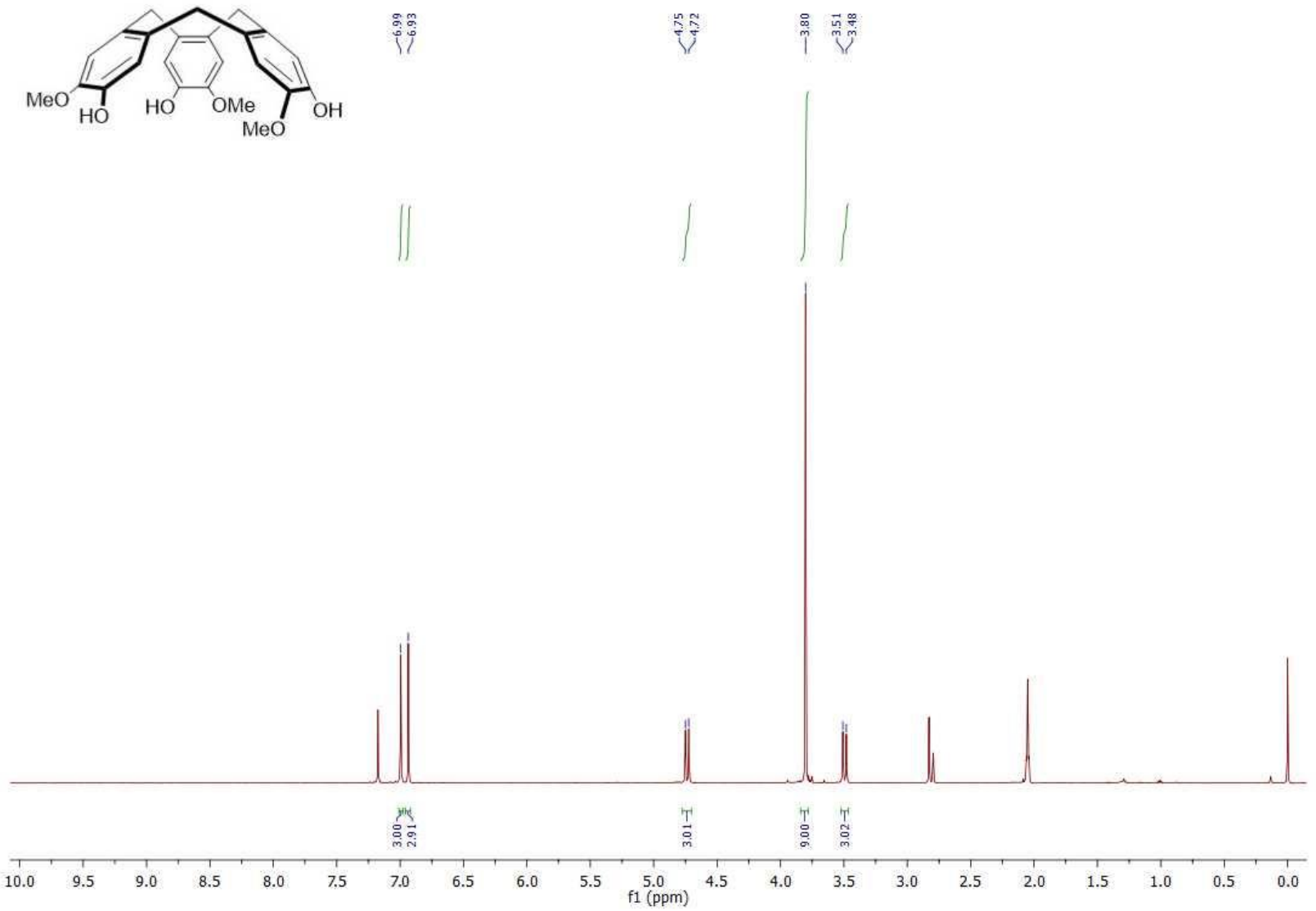


Figure S7. ^{1}H NMR spectrum of compound ***rac*-7.**

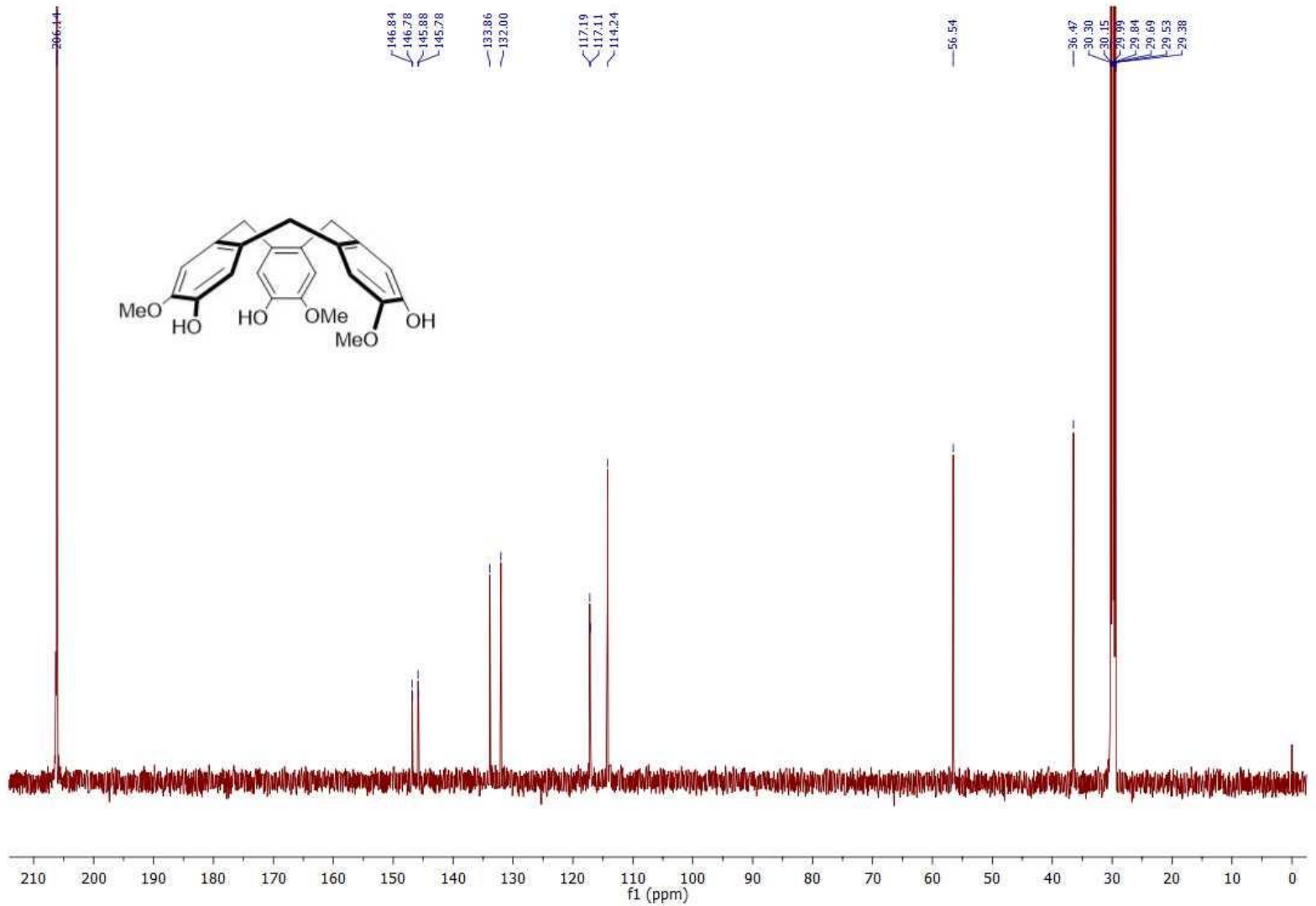


Figure S8. ^{13}C NMR spectrum of compound ***rac*-7**.

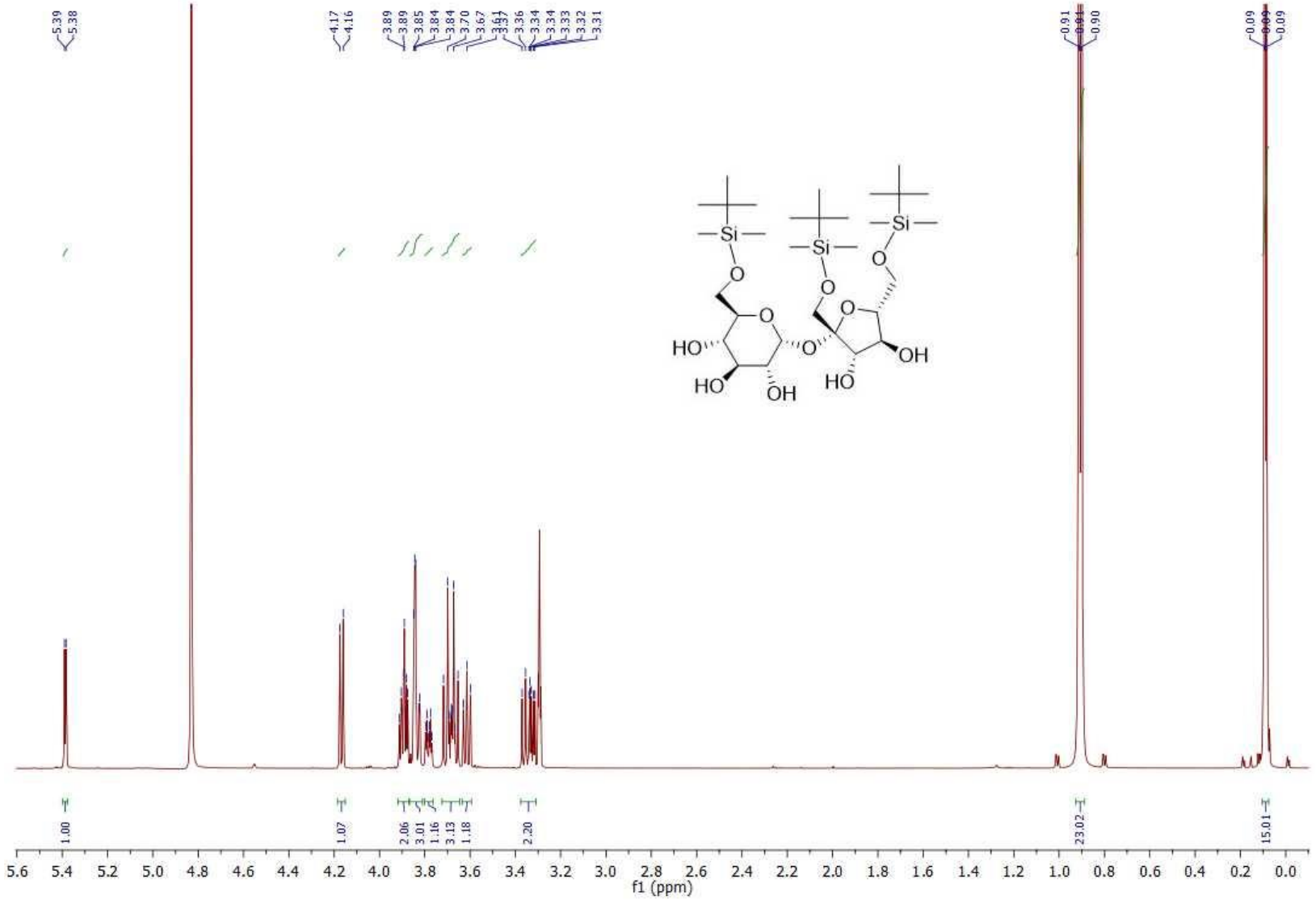


Figure S9. ^{1}H NMR spectrum of compound **S3.**

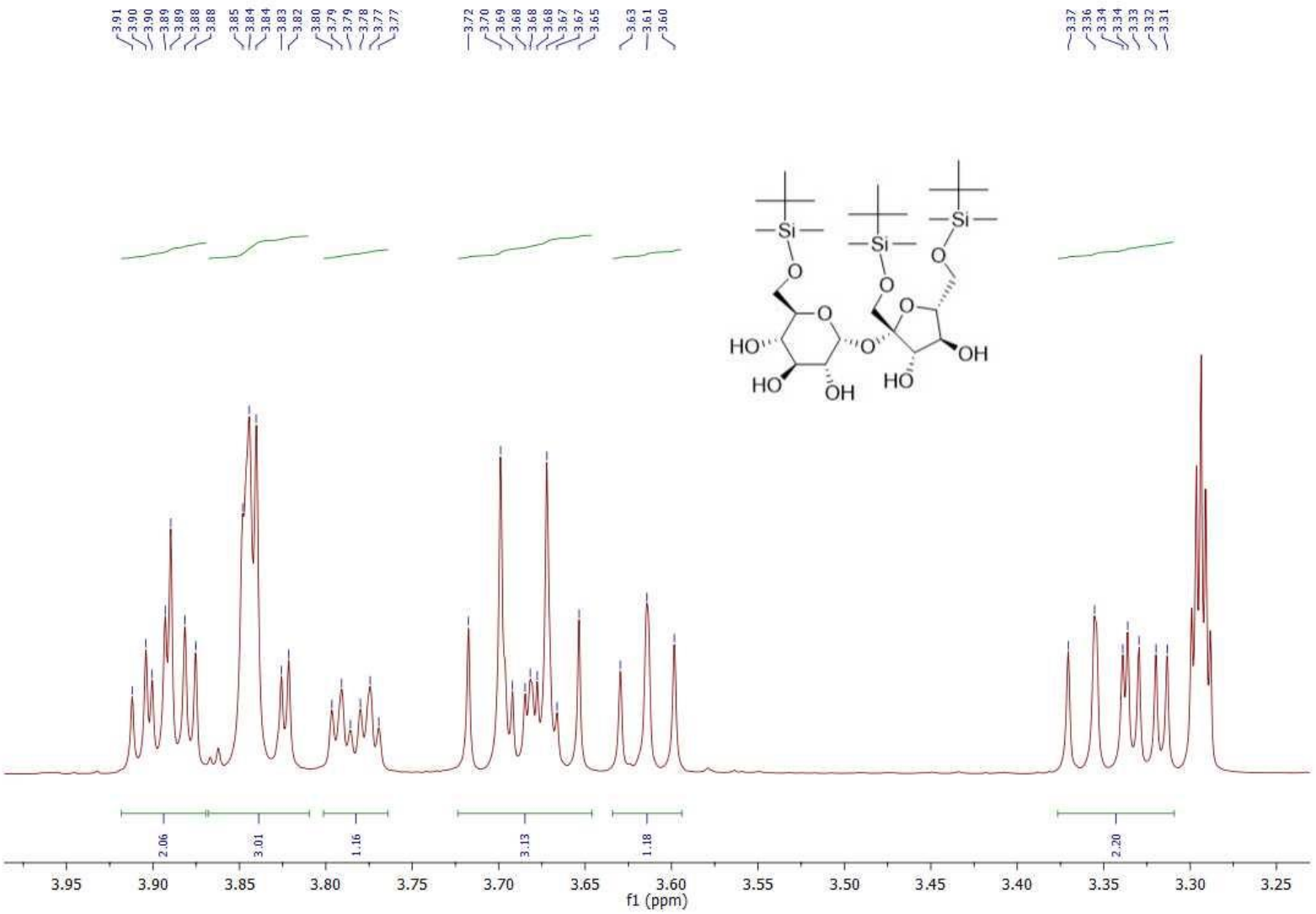


Figure S10. ^{1}H NMR spectrum of compound **S3** (aliphatic part).

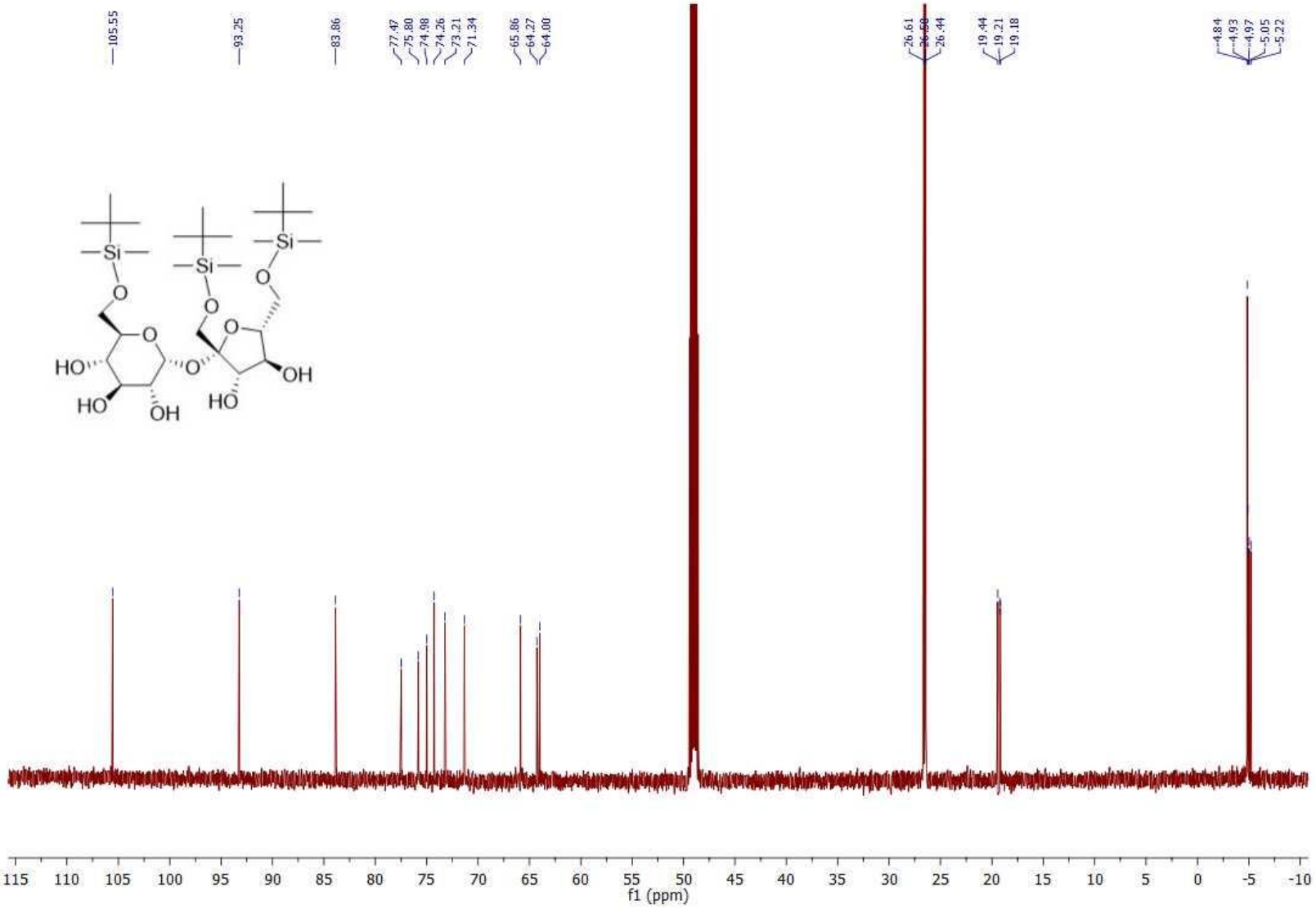


Figure S11. ^{13}C NMR spectrum of compound **S3.**

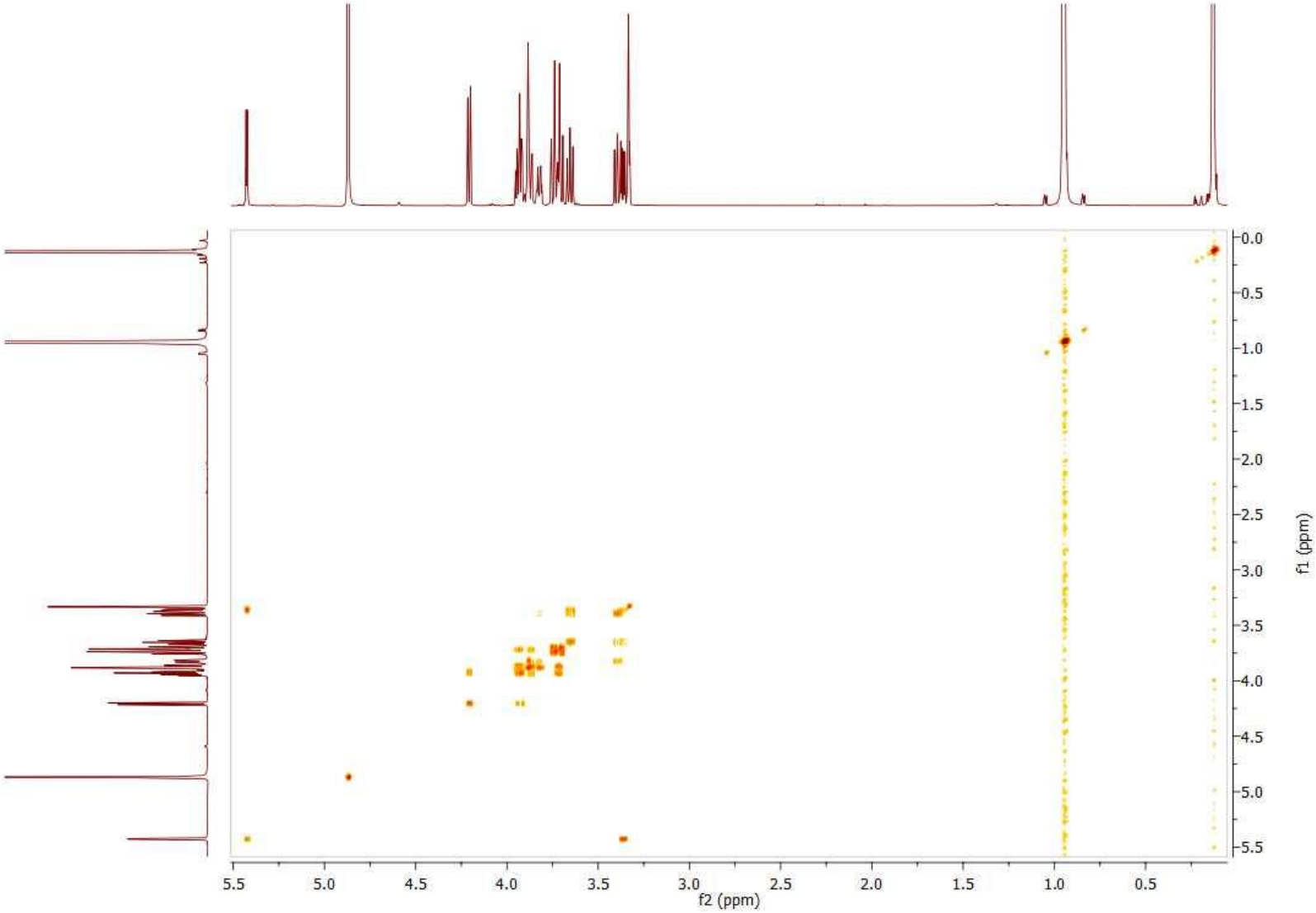


Figure S12. ^{1}H–^{1}H COSY spectrum of compound **S3**.

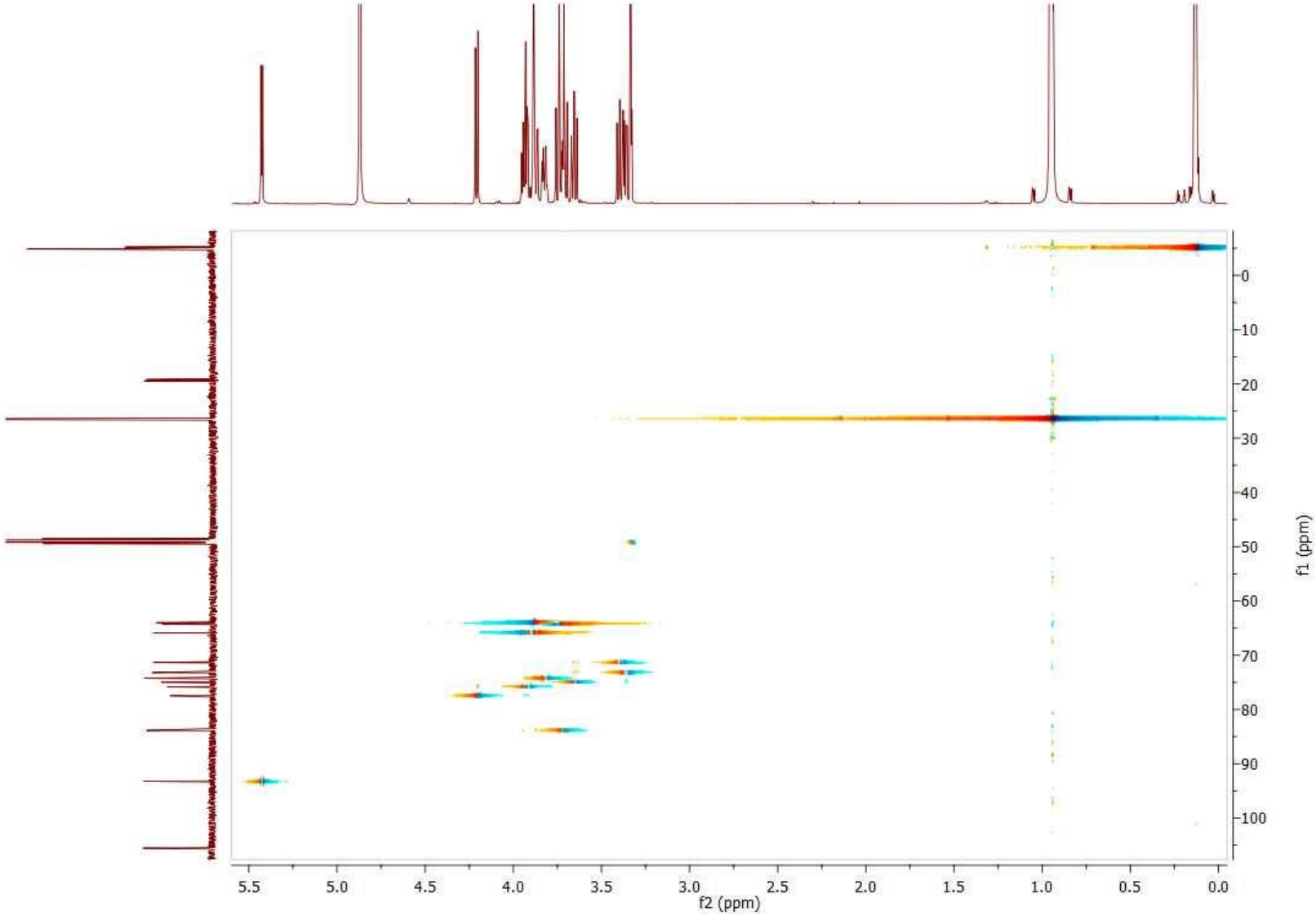


Figure S13. ^{1}H–^{13}C HSQC spectrum of compound **S3**.

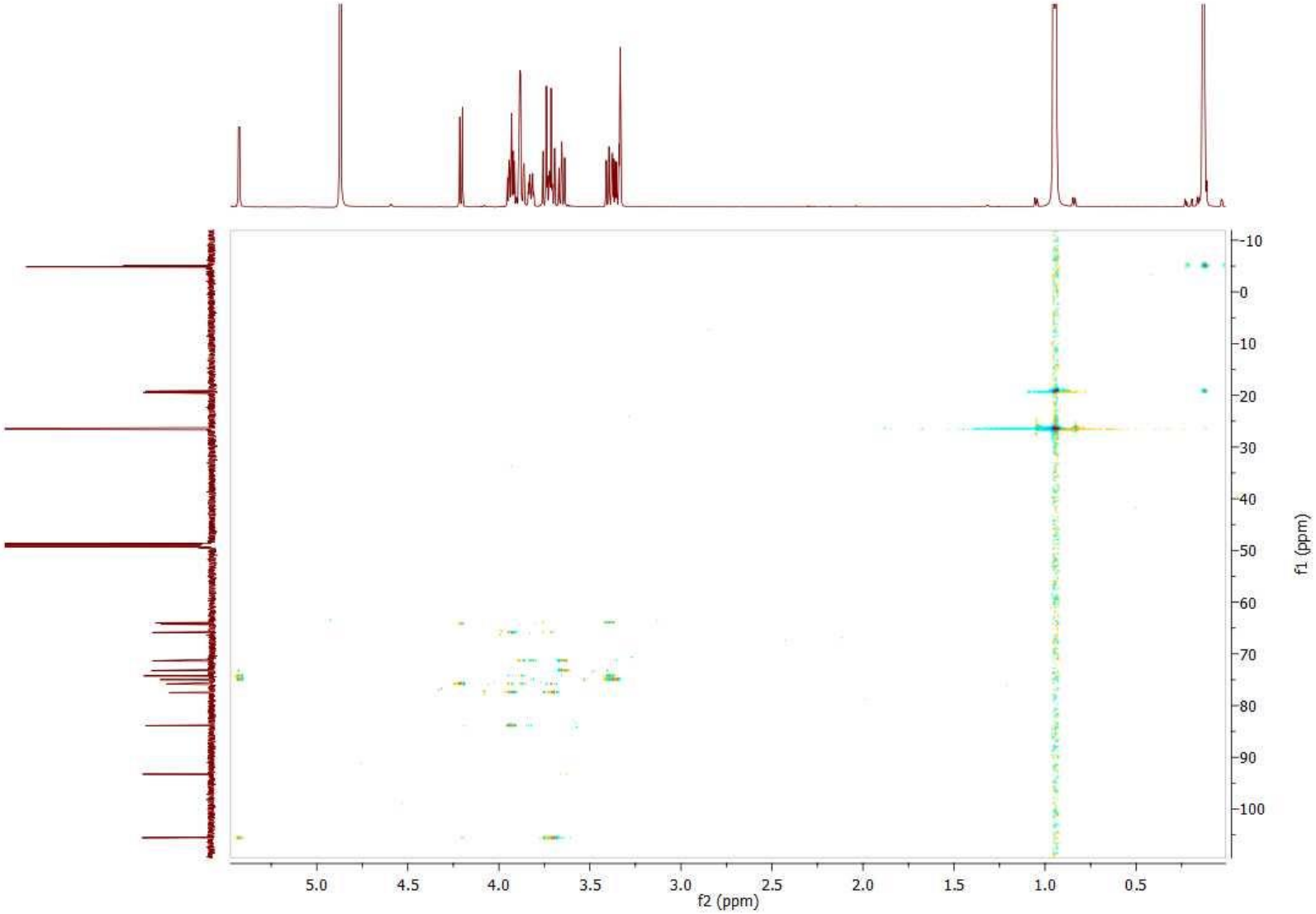


Figure S14. $^{1}H–^{13}C$ HMBC spectrum of compound **S3**.

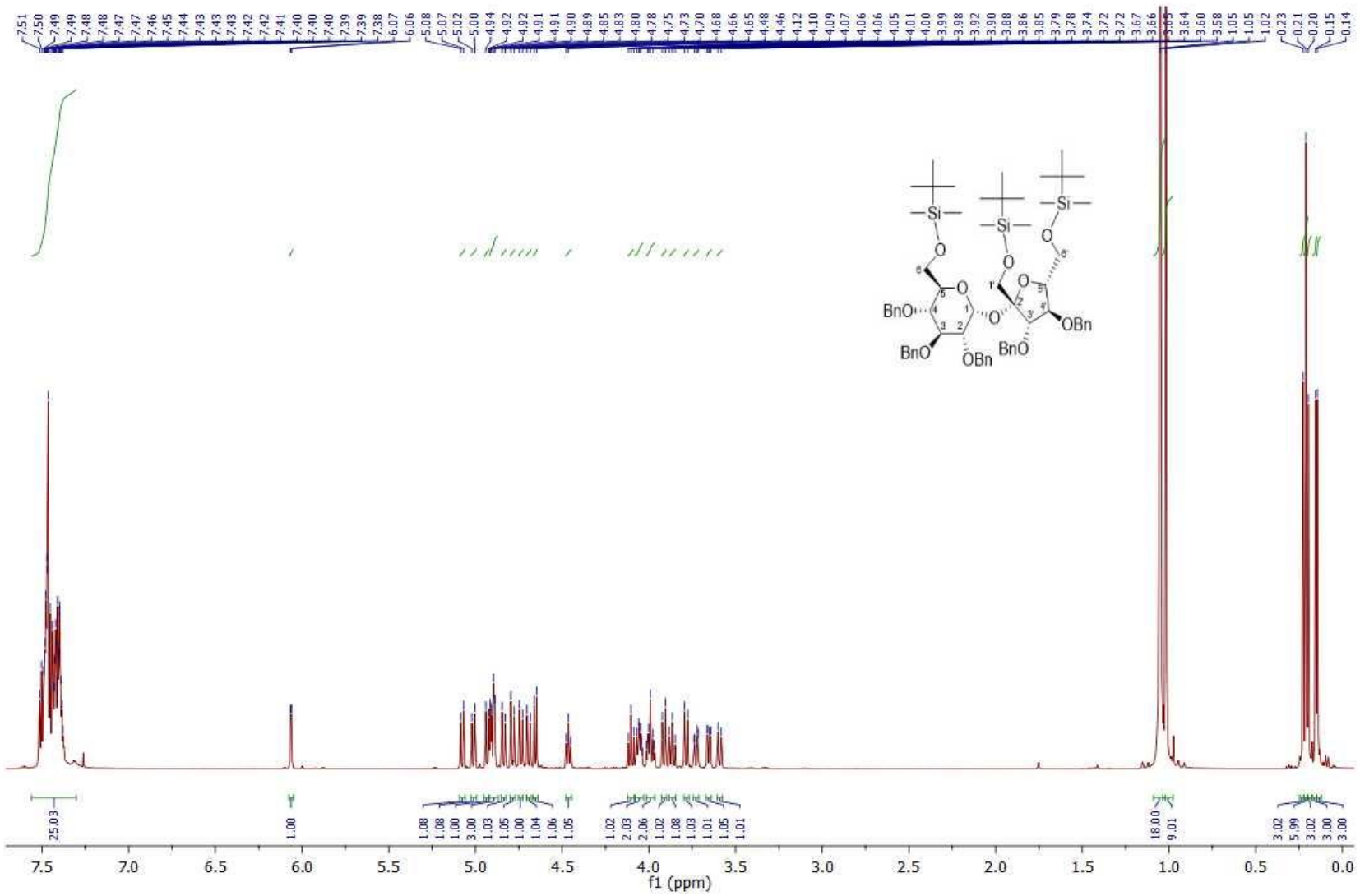


Figure S15. ^{1}H NMR spectrum of compound **2.**

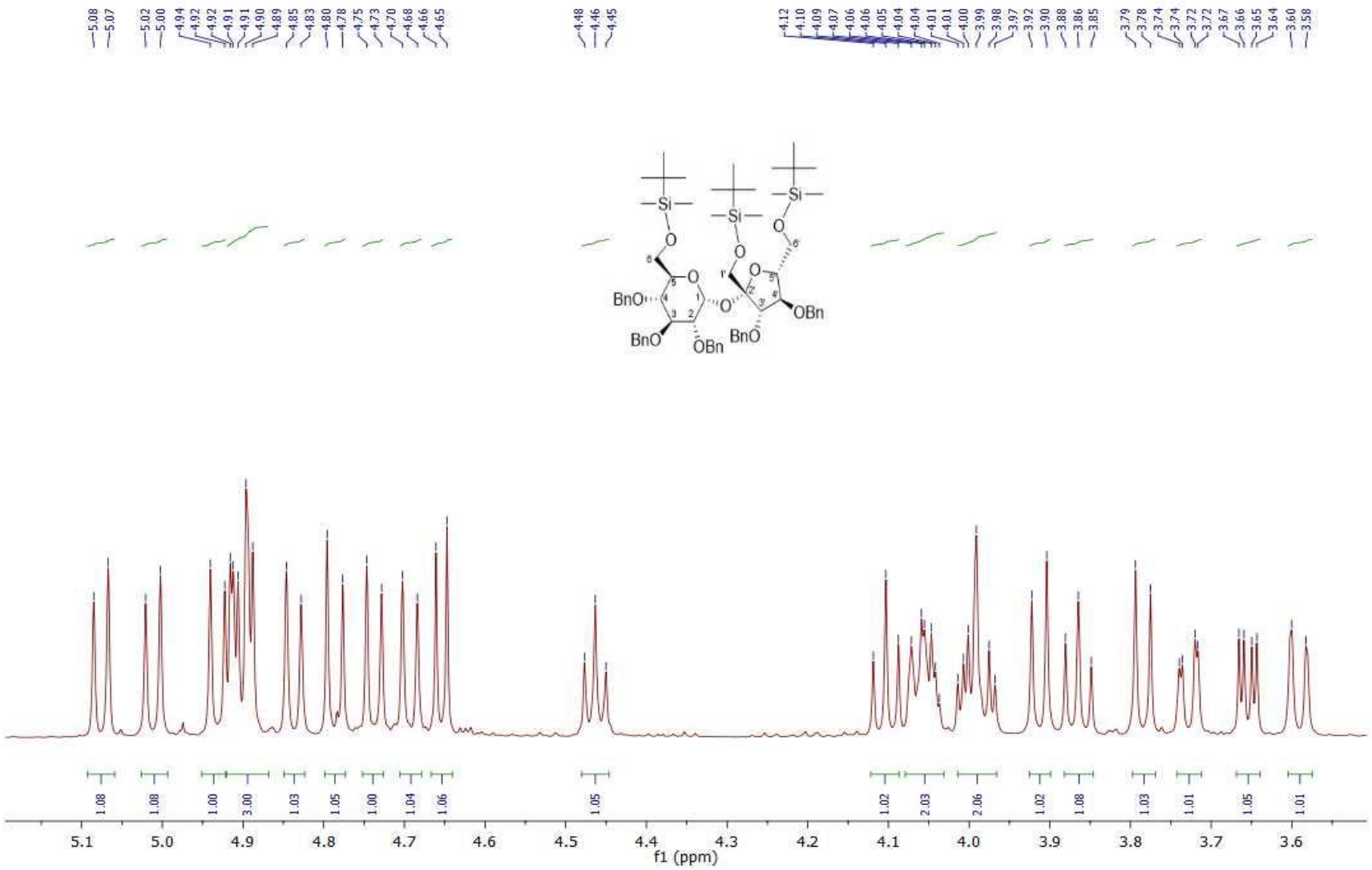


Figure S16. ^{1}H NMR spectrum of compound **2** (aliphatic part).

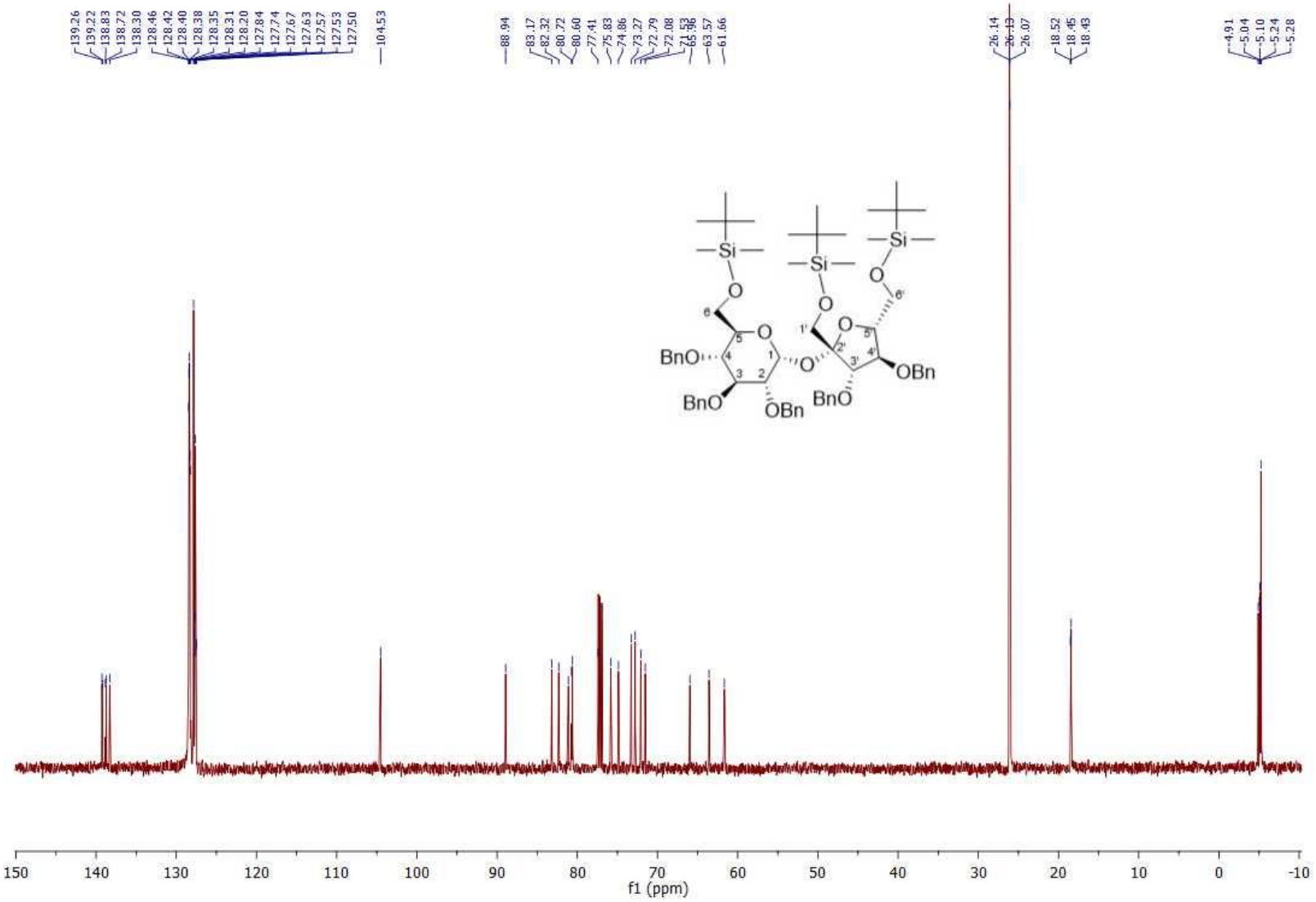


Figure S17. ^{13}C NMR spectrum of compound **2**.

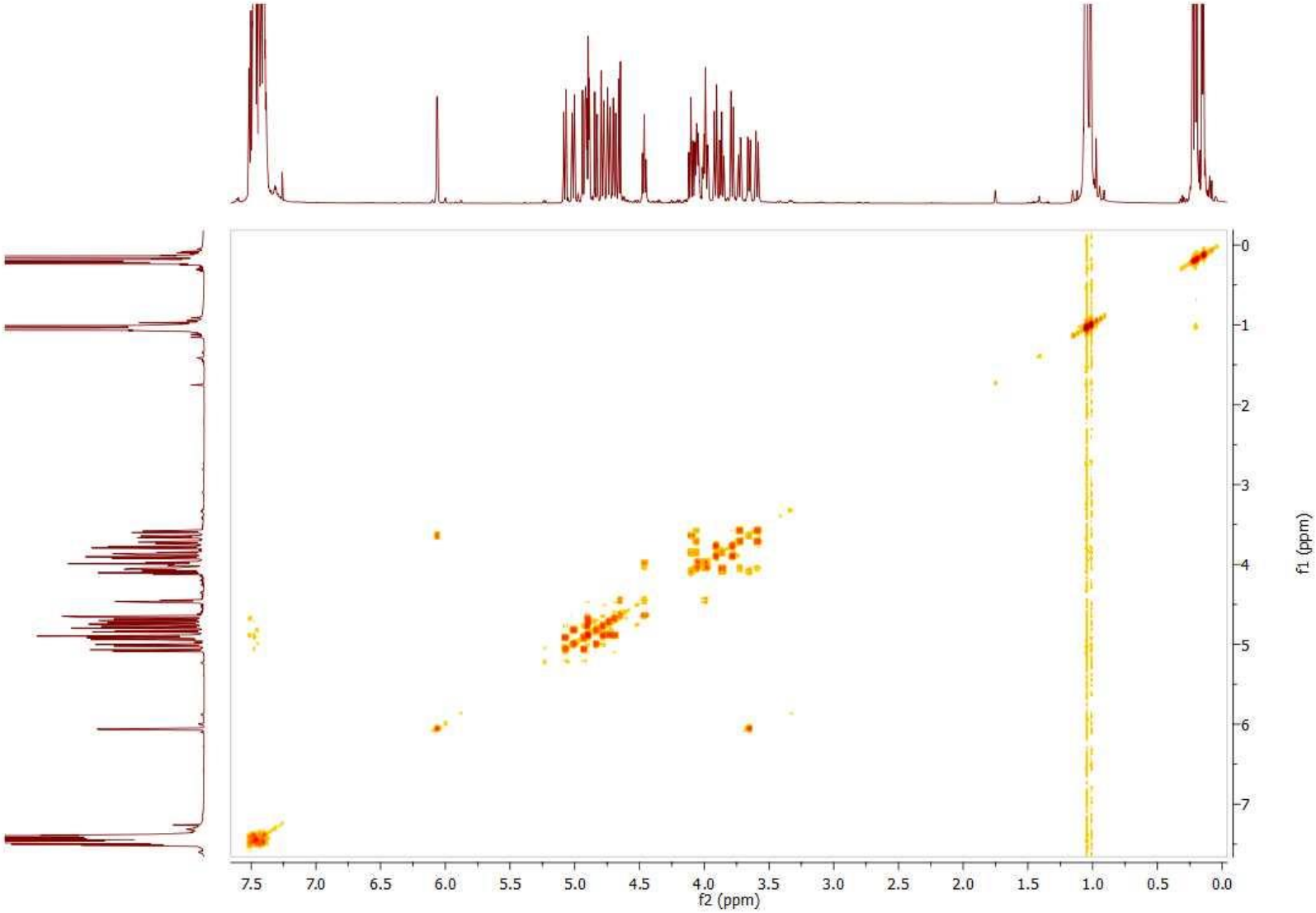


Figure S18. ^{1}H–^{1}H COSY spectrum of compound **2**.

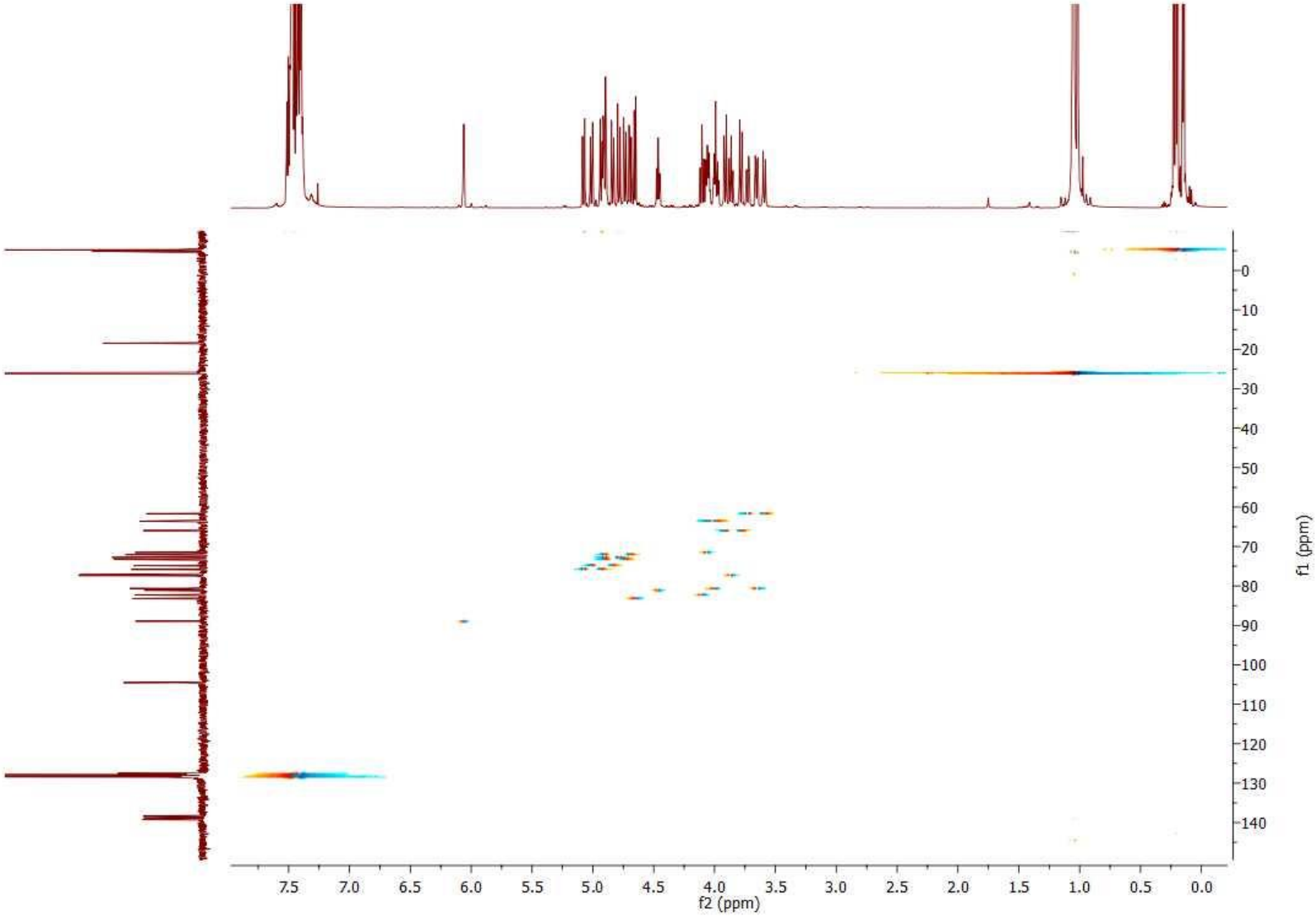


Figure S19. $^{1}H–^{13}C$ HSQC spectrum of compound **2**.

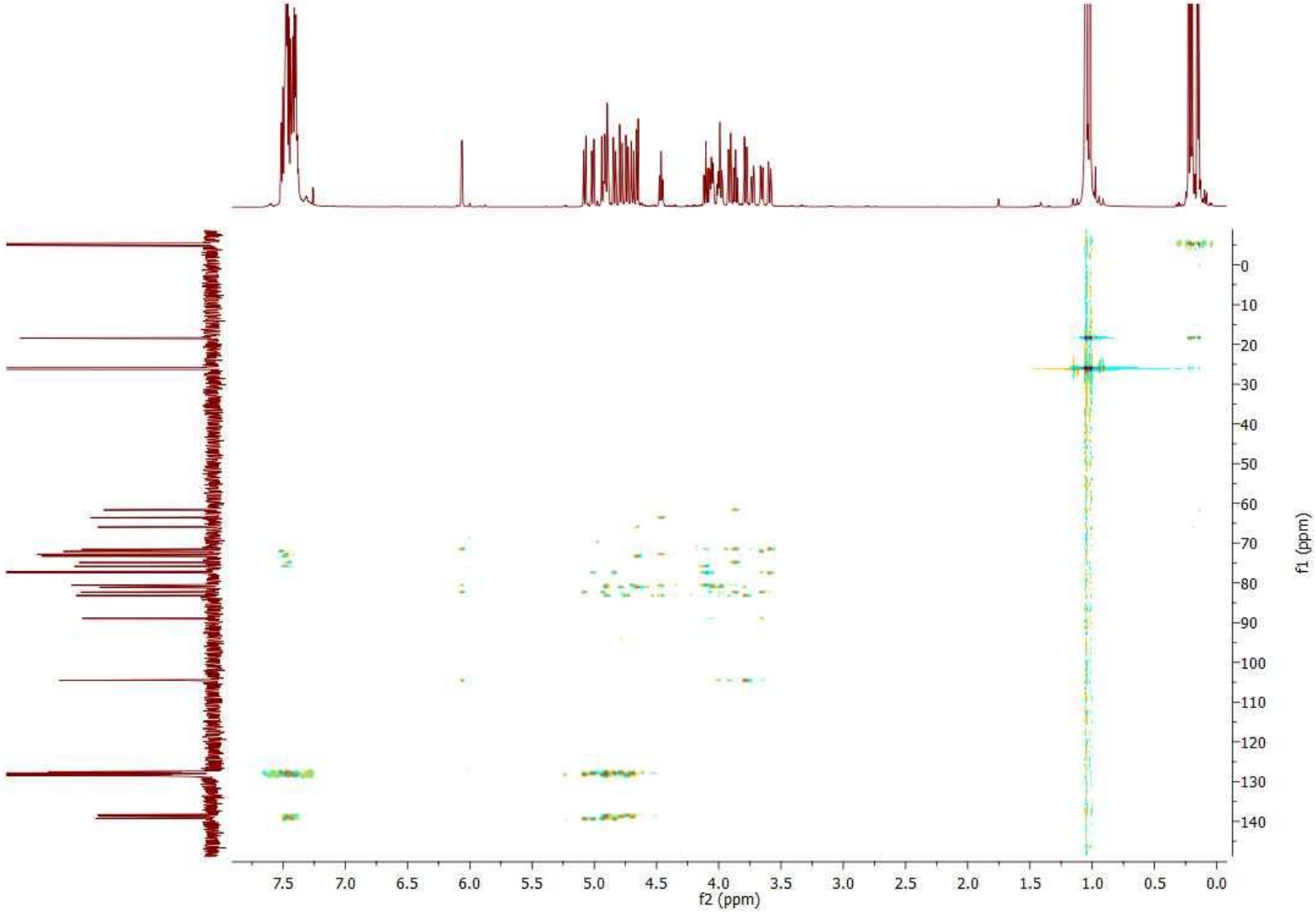


Figure S20. ^{1}H–^{13}C HMBC spectrum of compound **2**.

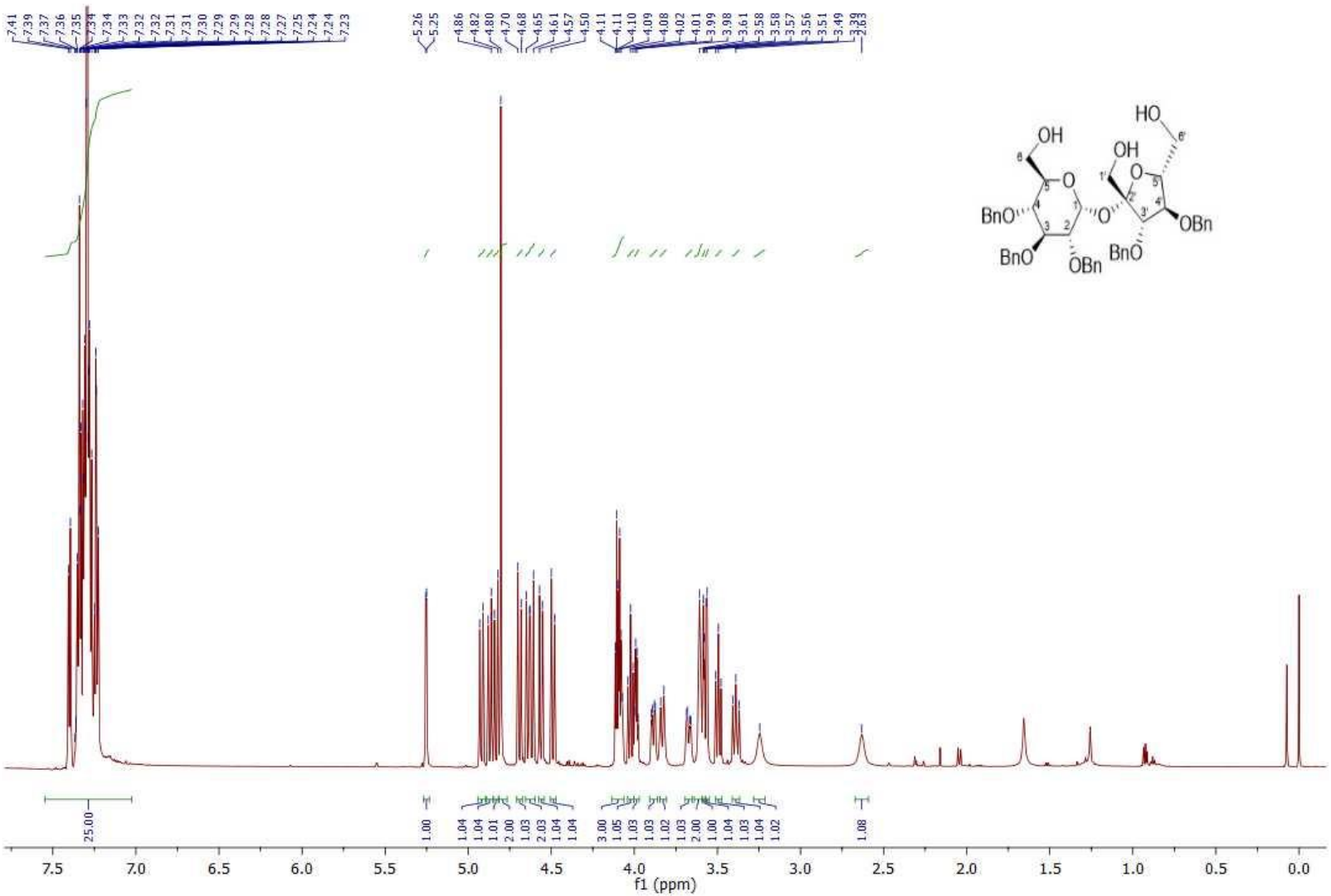


Figure S21. ^{1}H NMR spectrum of compound **3.**

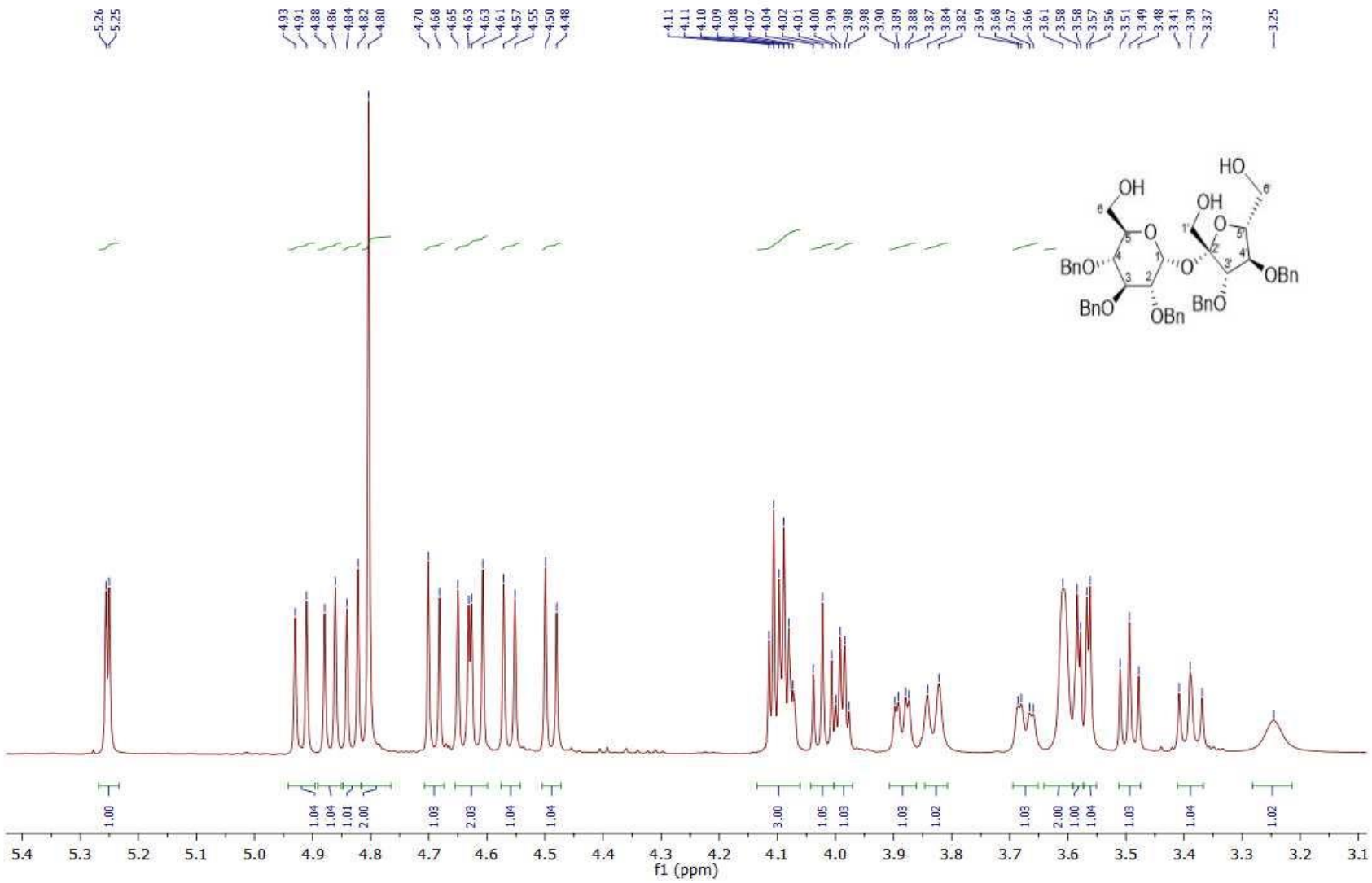


Figure S22. ^{1}H NMR spectrum of compound **3** (aliphatic part).

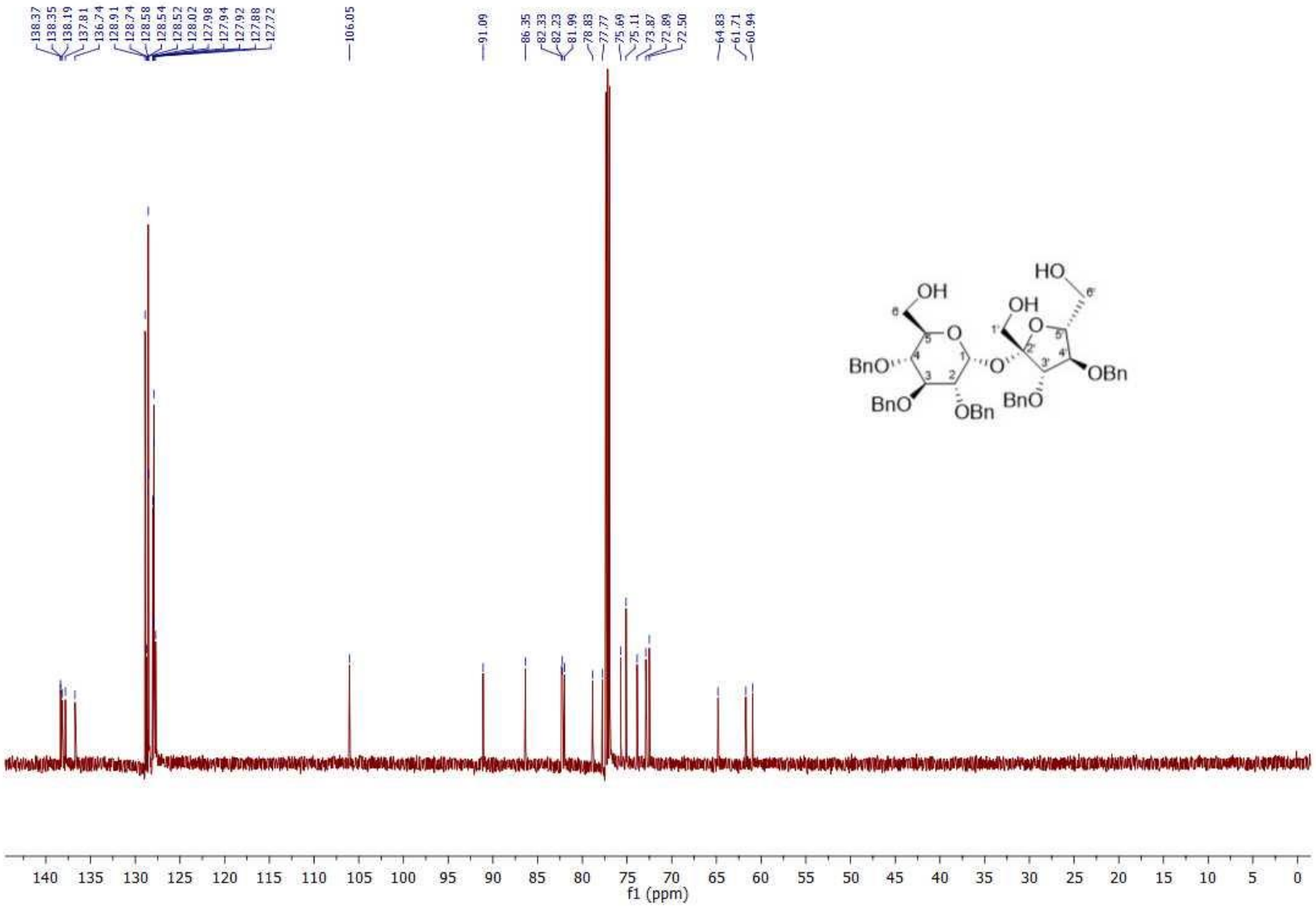


Figure S23. ^{13}C NMR spectrum of compound **3**.

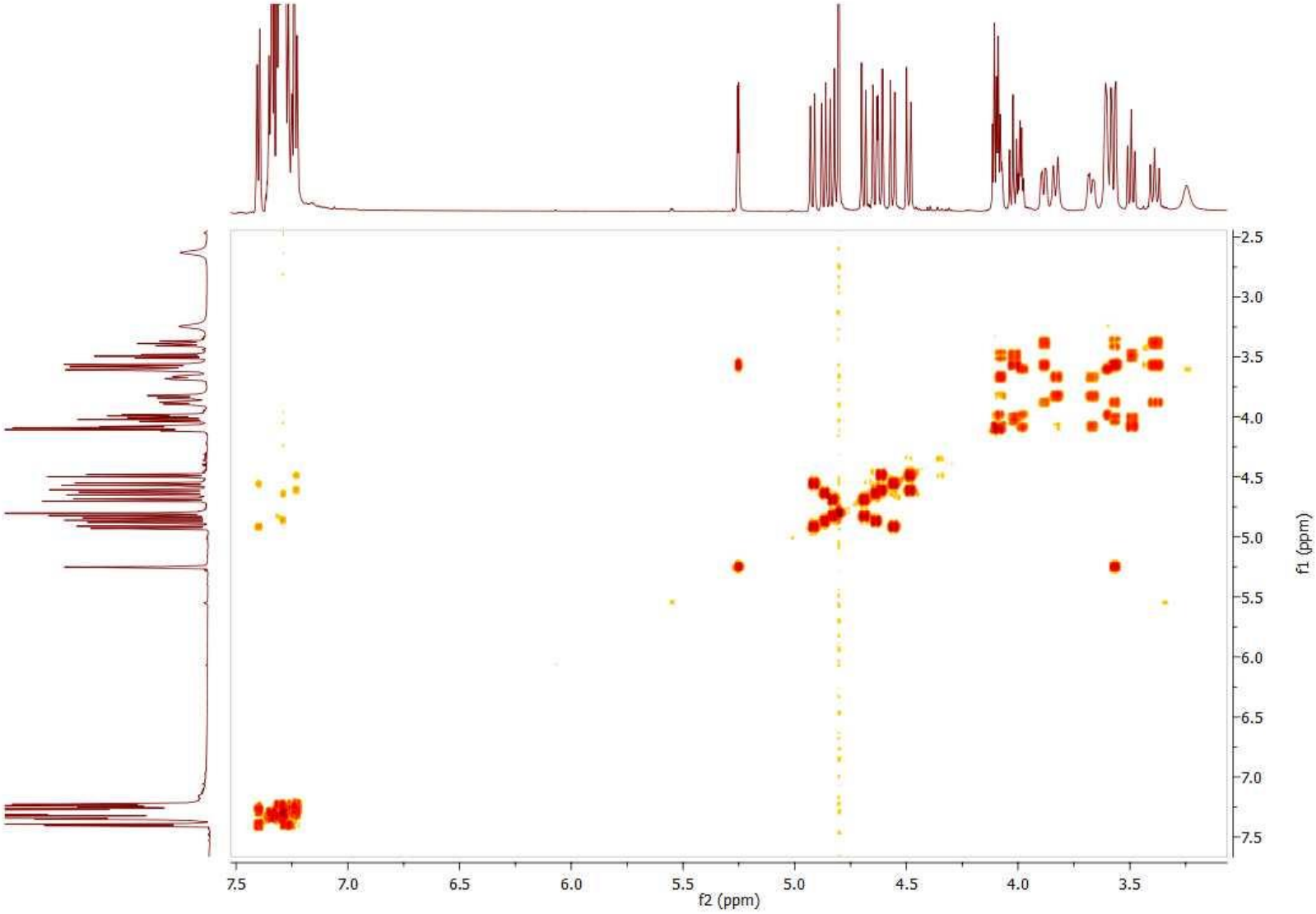


Figure S24. ^{1}H–^{1}H COSY spectrum of compound **3**.

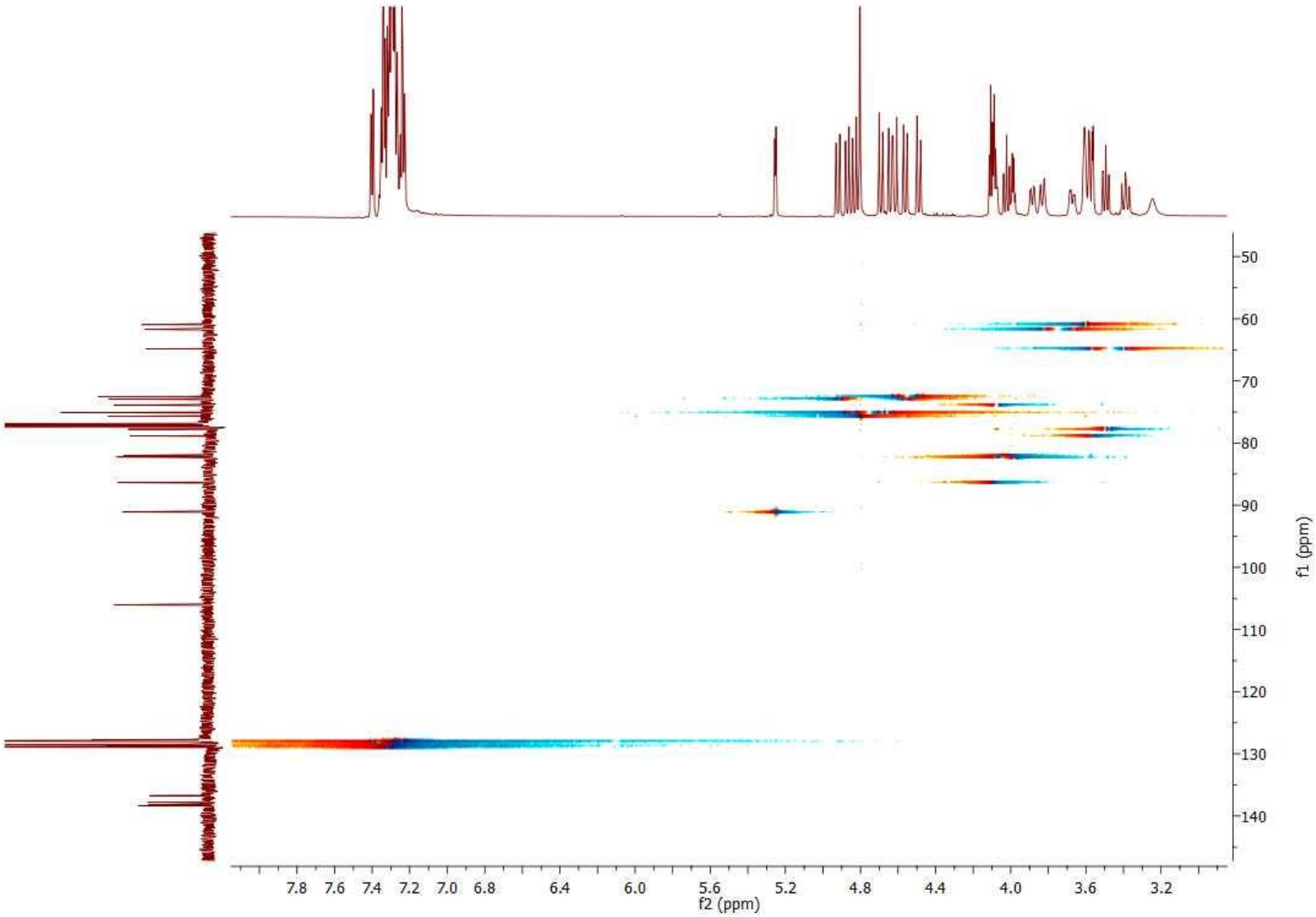


Figure S25. $^{1}H–^{13}C$ HSQC spectrum of compound **3**.

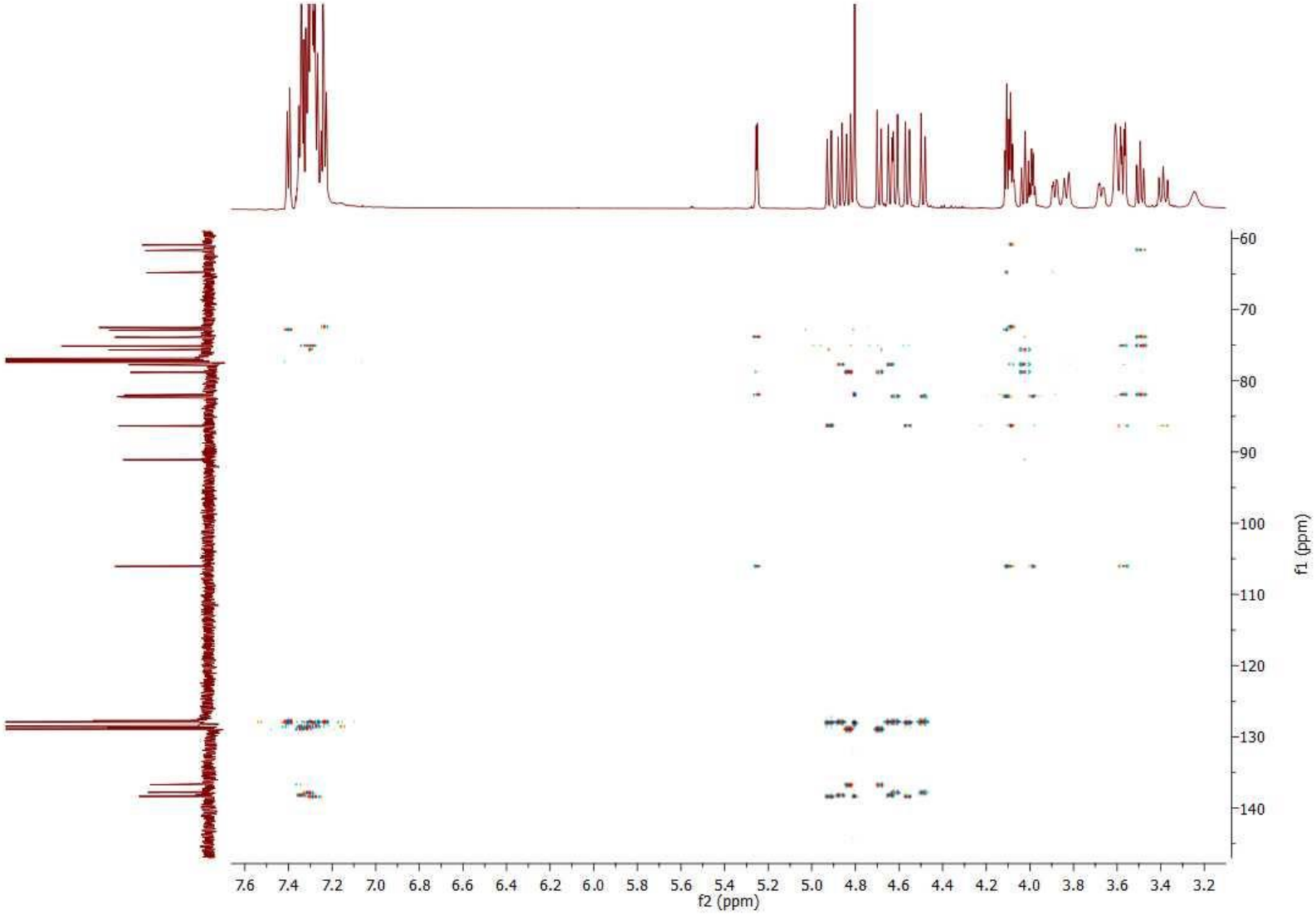


Figure S26. ^{1}H–^{13}C HMBC spectrum of compound **3**.

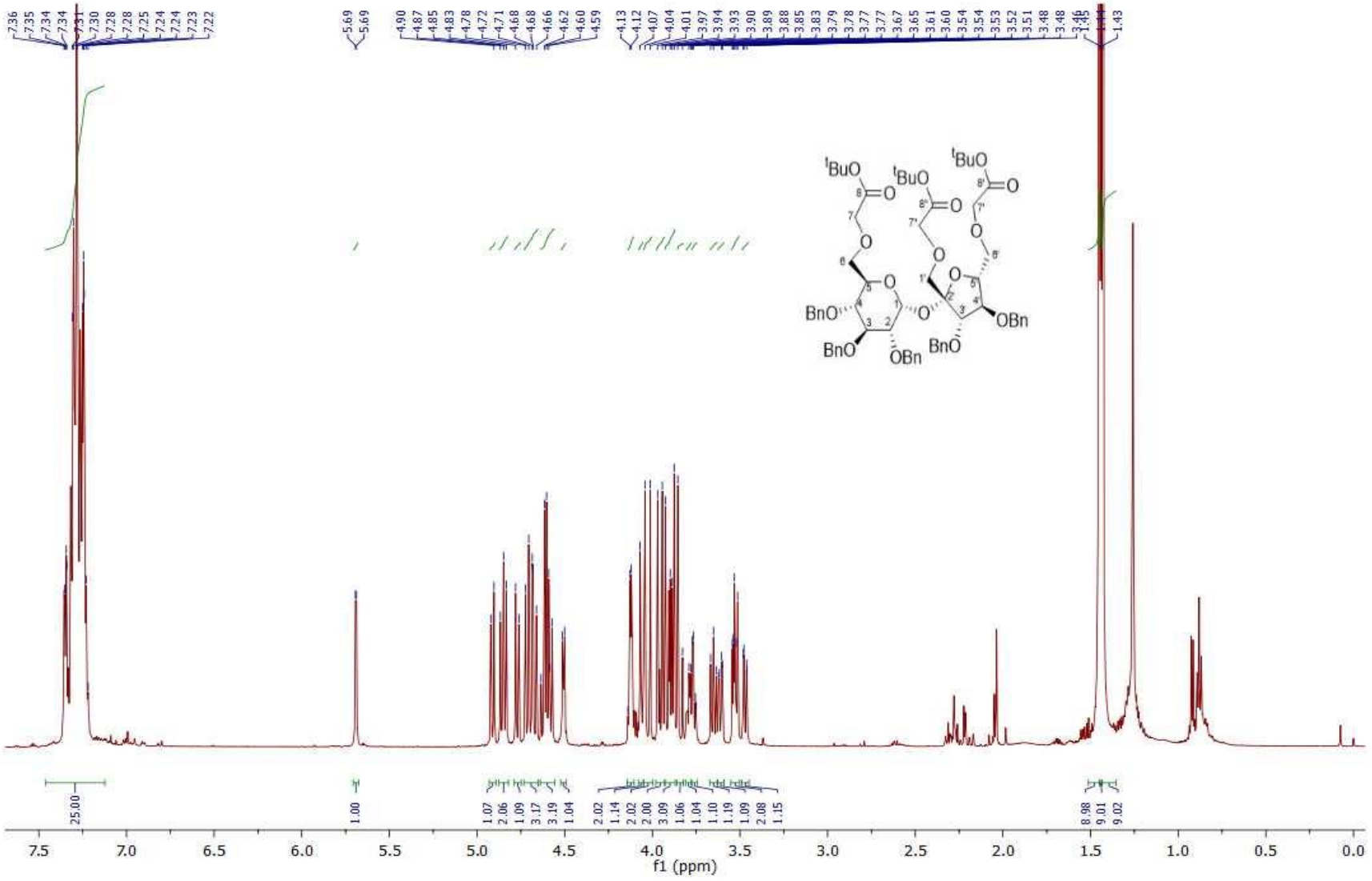


Figure S27. ^{1}H NMR spectrum of compound **4.**

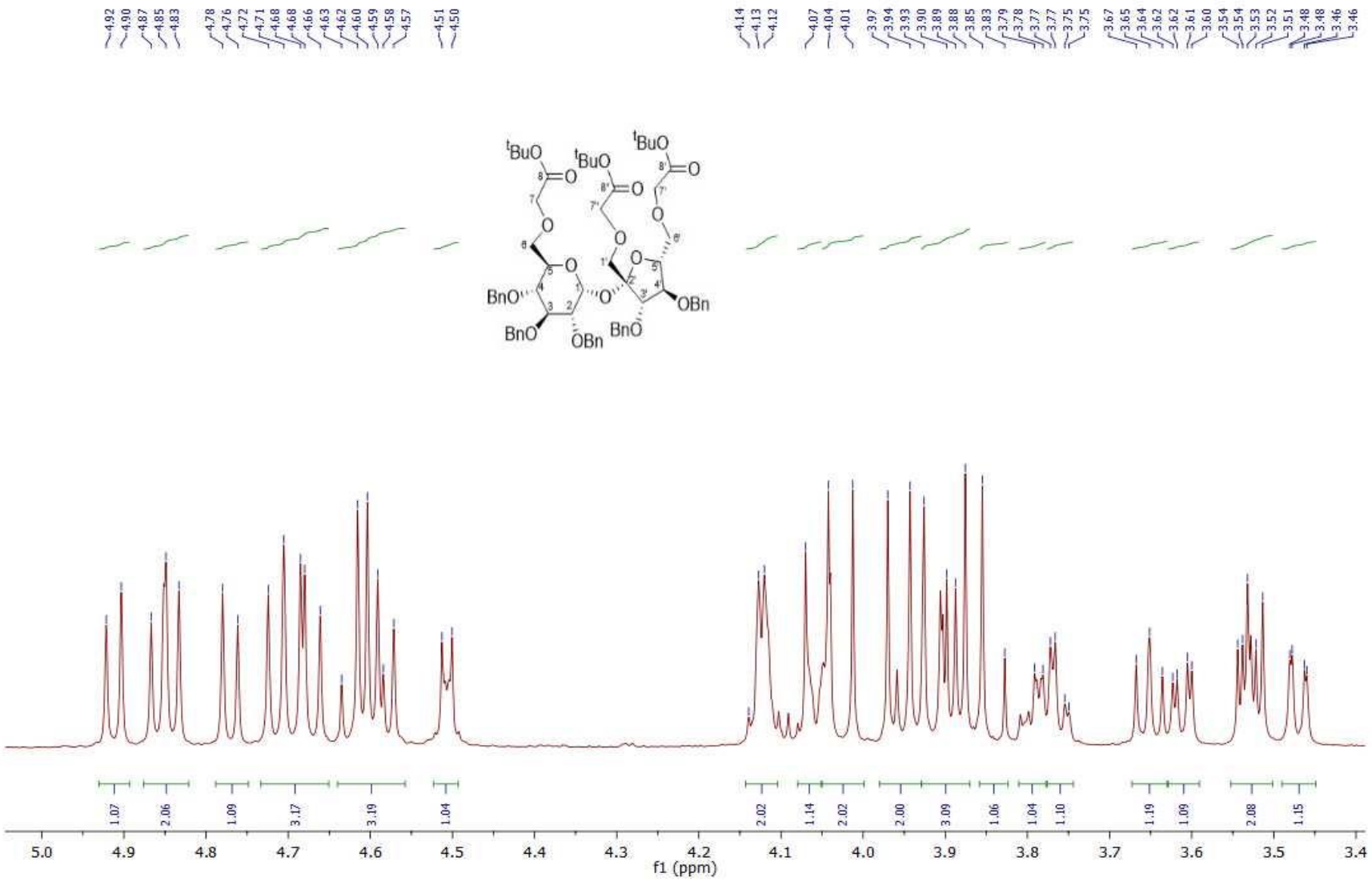


Figure S28. ^{1}H NMR spectrum of compound **4** (aliphatic part).

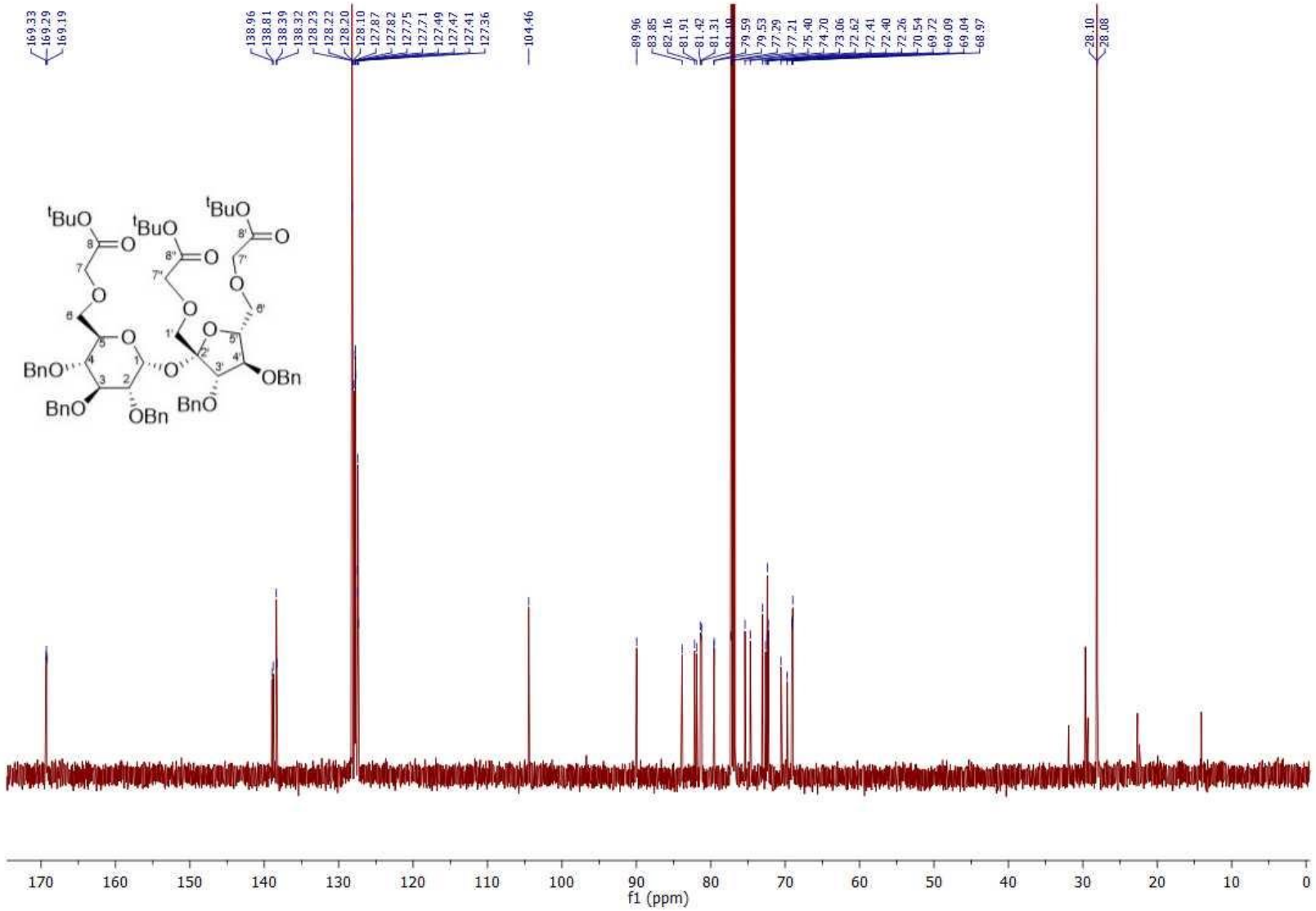


Figure S29. ^{13}C NMR spectrum of compound **4**.

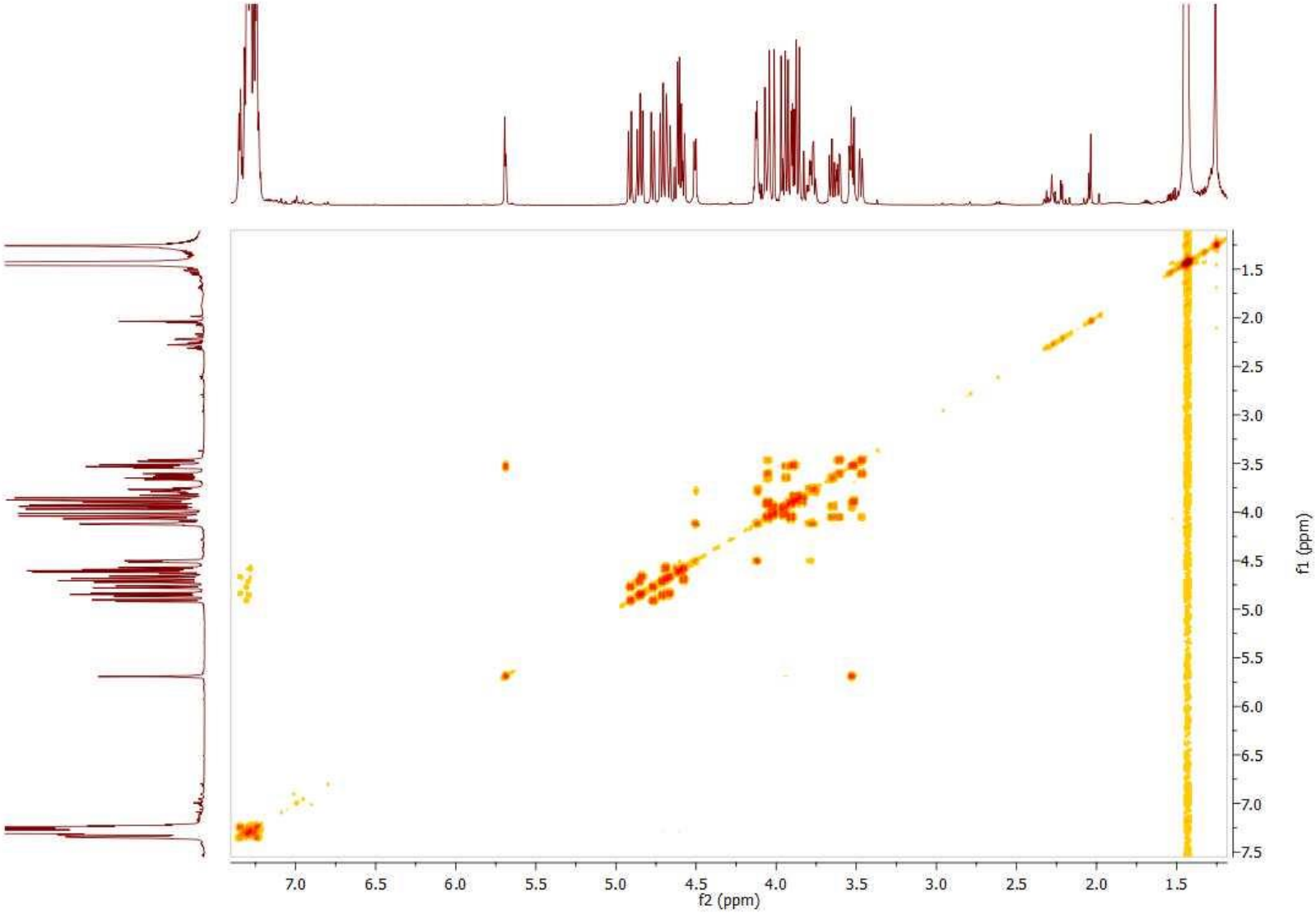


Figure S30. ^{1}H–^{1}H COSY spectrum of compound **4**.

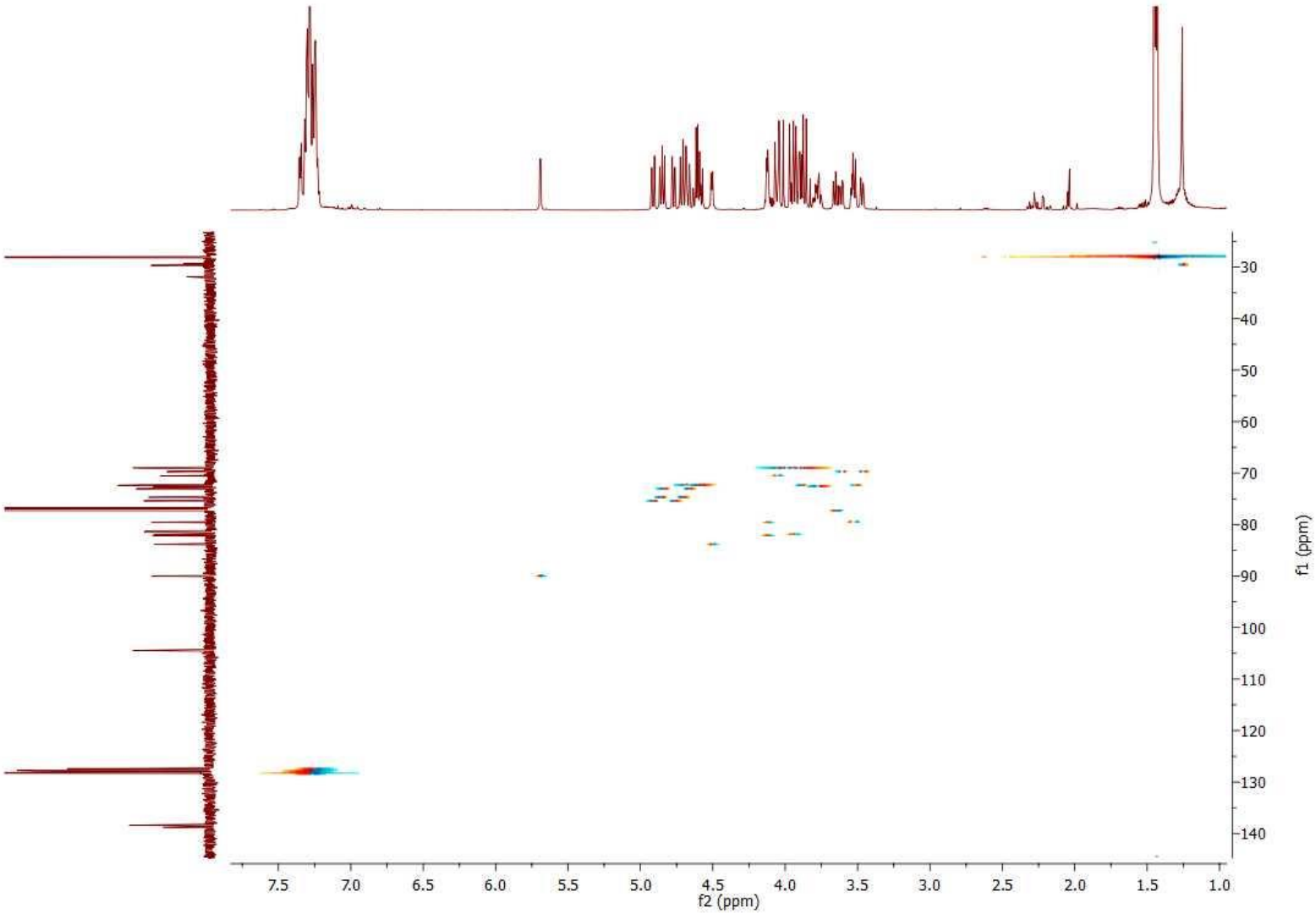


Figure S31. $^{1}H–^{13}C$ HSQC spectrum of compound **4**.

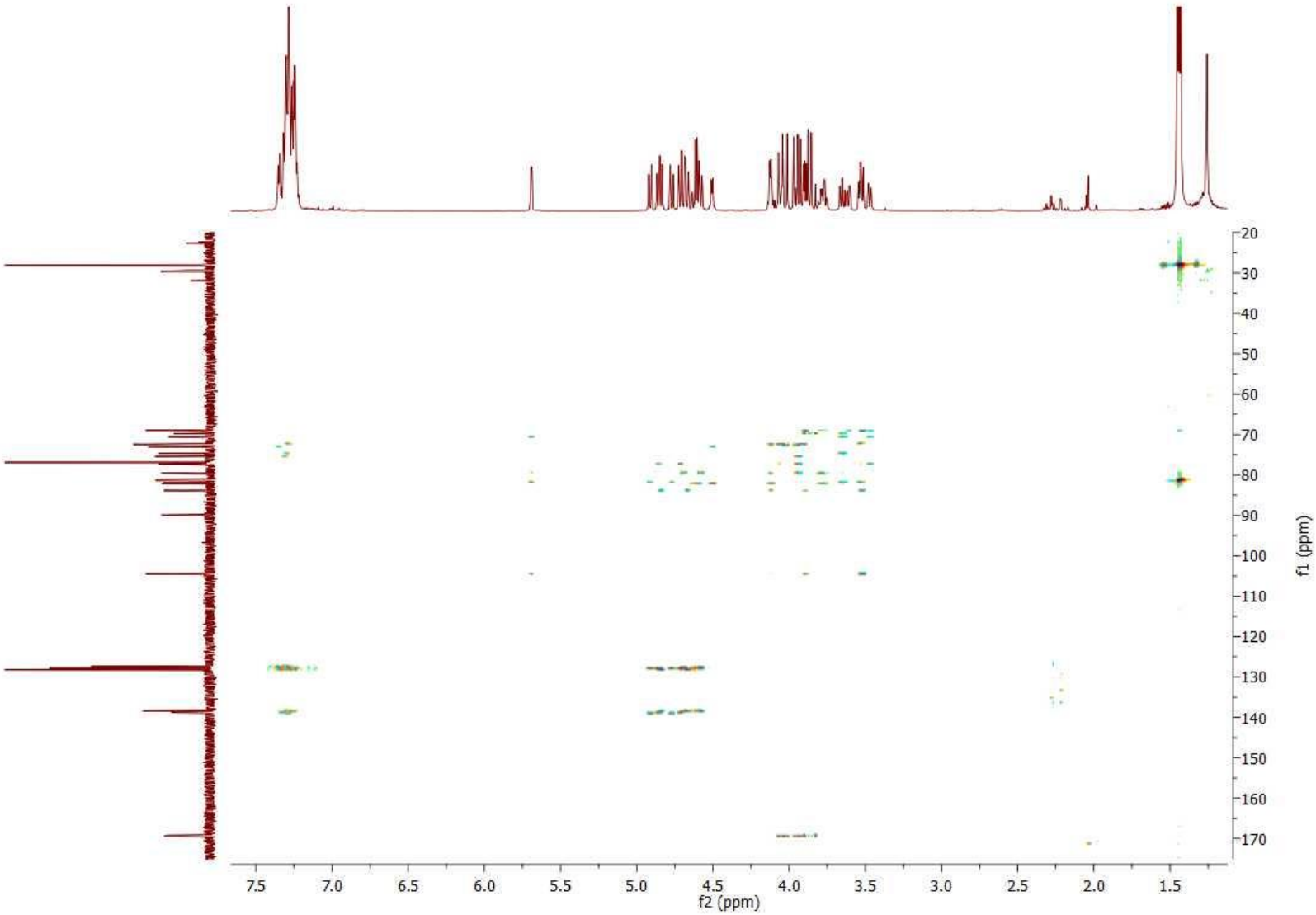


Figure S32. ^{1}H–^{13}C HMBC spectrum of compound **4**.

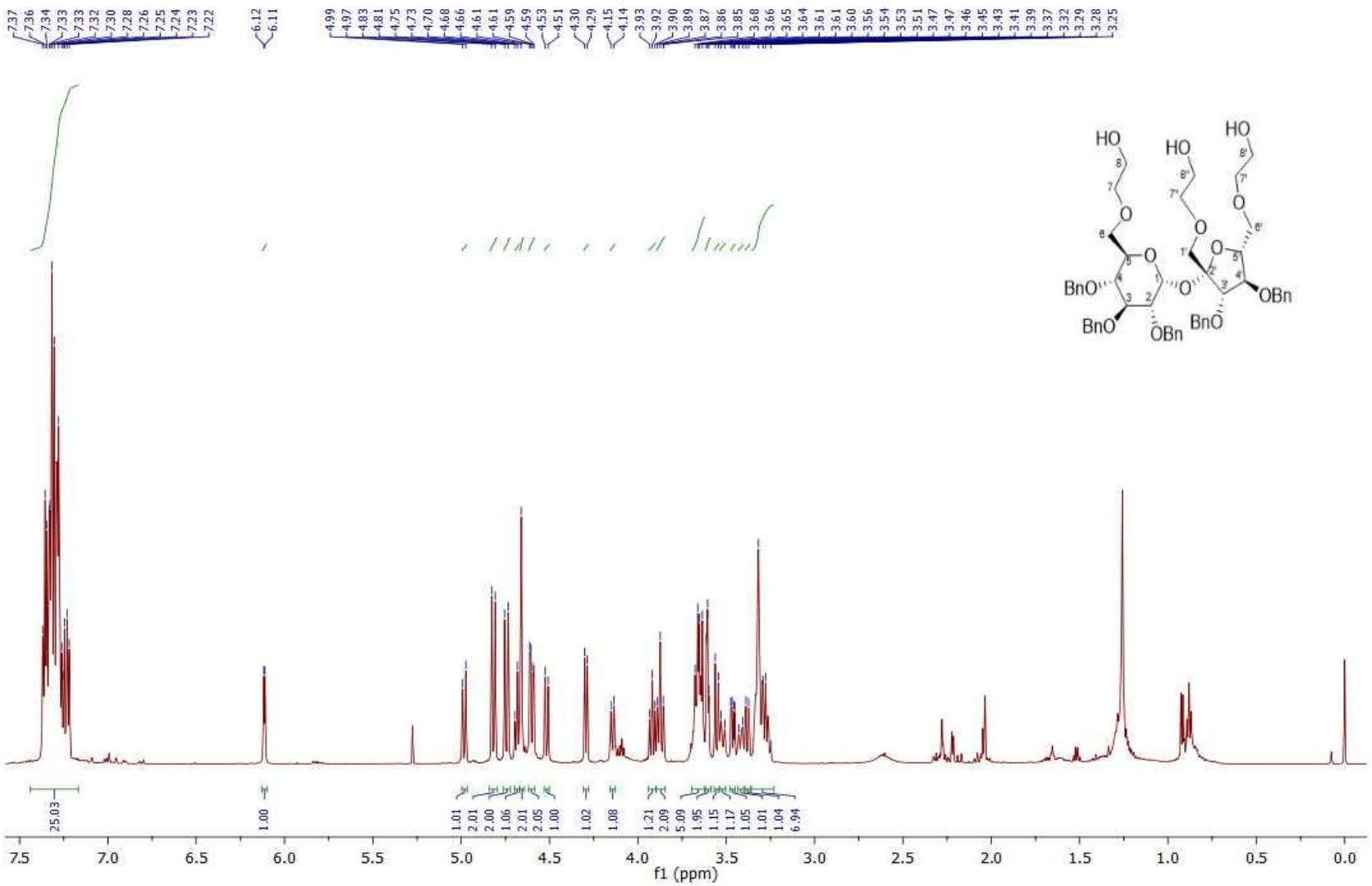


Figure S33. ^{1}H NMR spectrum of compound **5**.

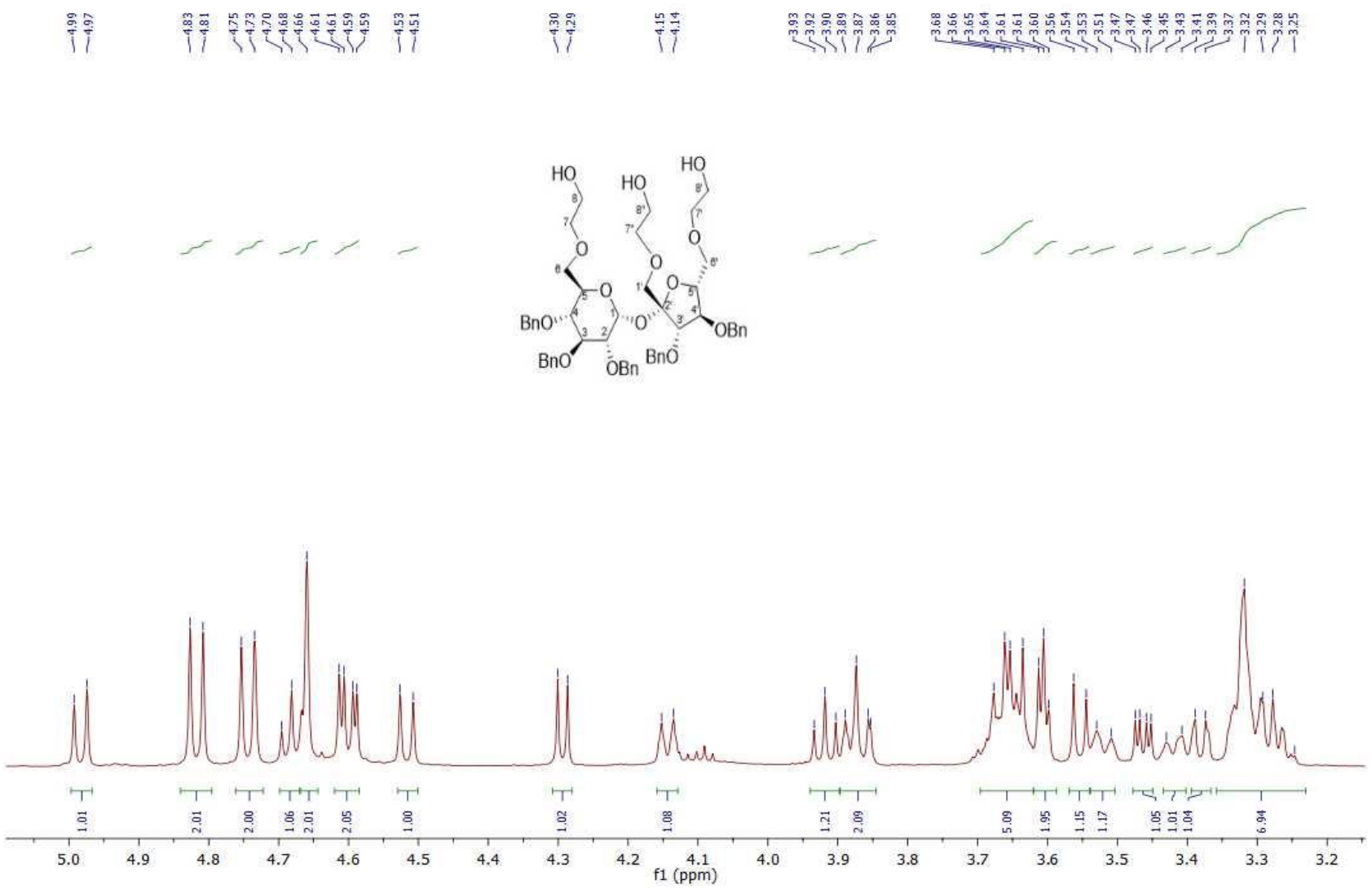


Figure S34. ^{1}H NMR spectrum of compound **5** (aliphatic part).

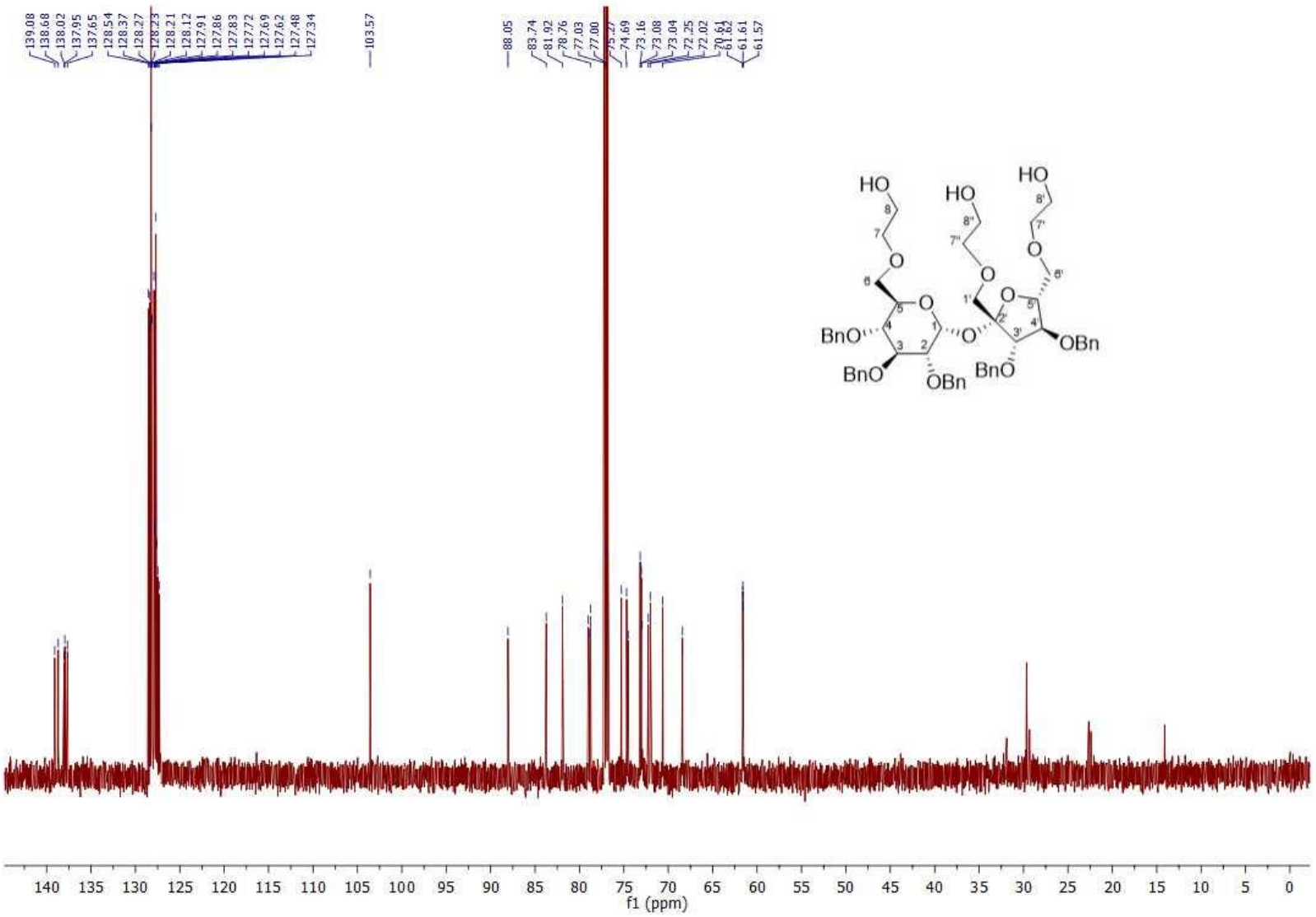


Figure S35. ^{13}C NMR spectrum of compound **5**.

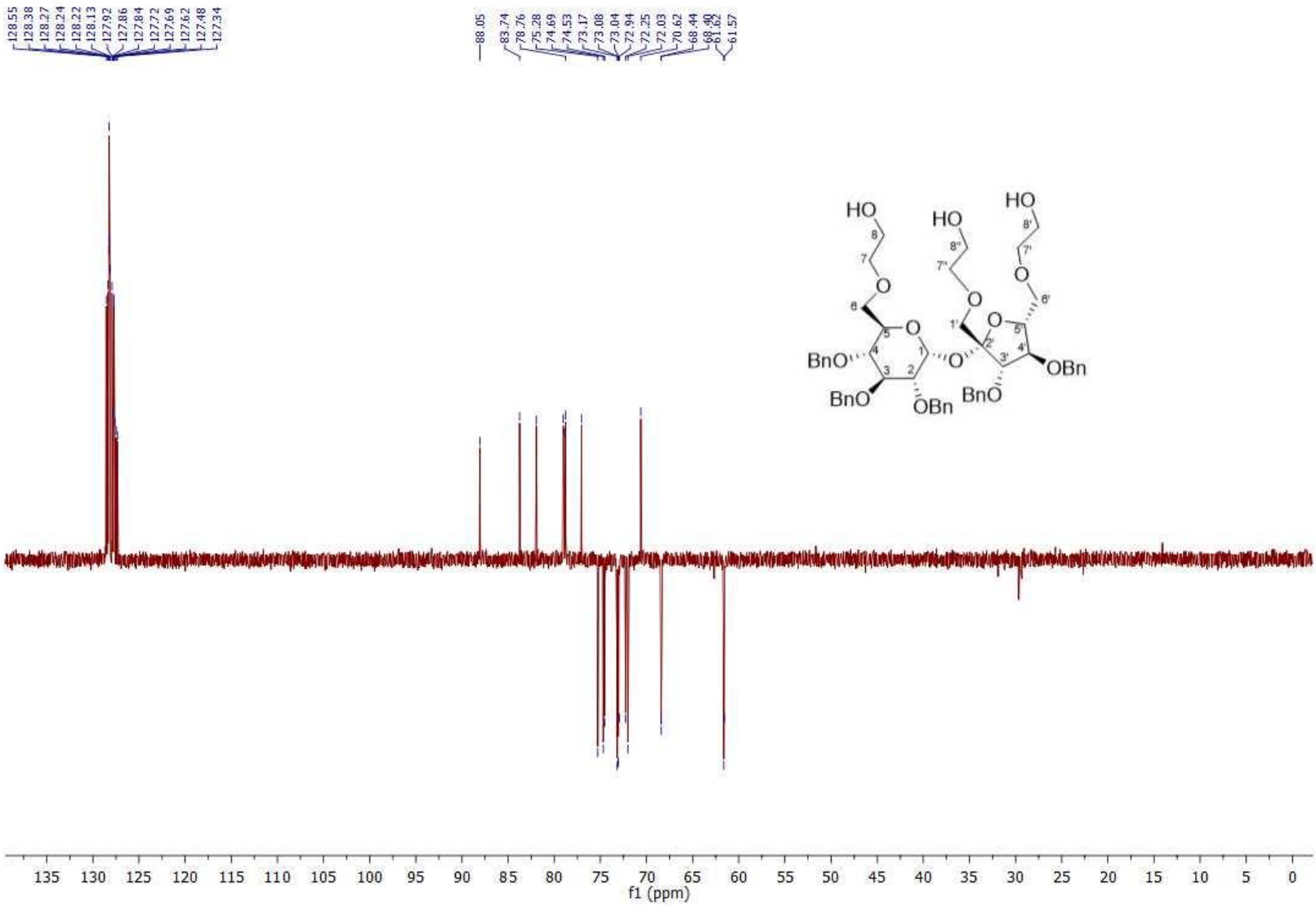


Figure S36. DEPT^{13}C NMR spectrum of compound **5**.

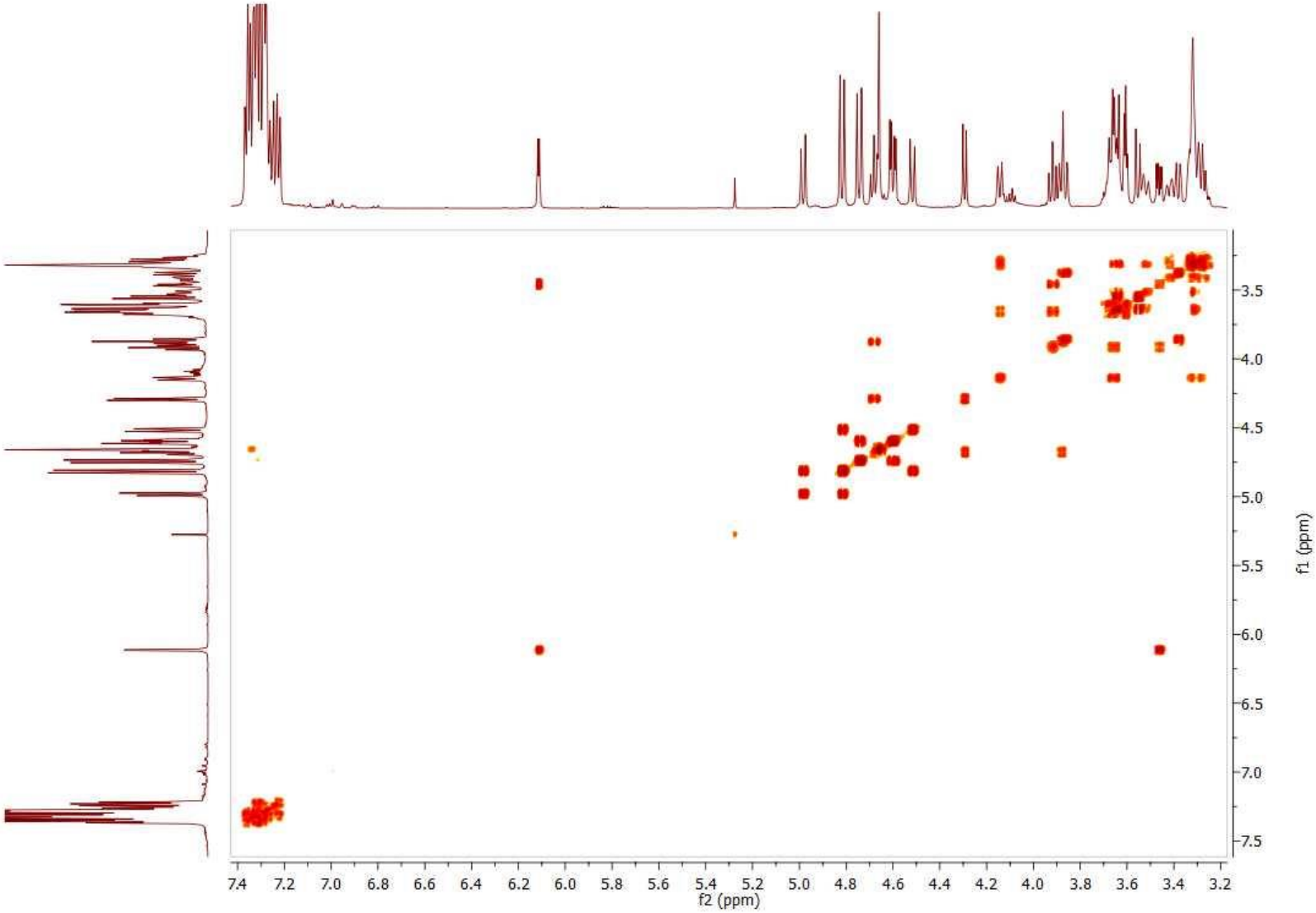


Figure S37. ^{1}H–^{1}H COSY spectrum of compound **5**.

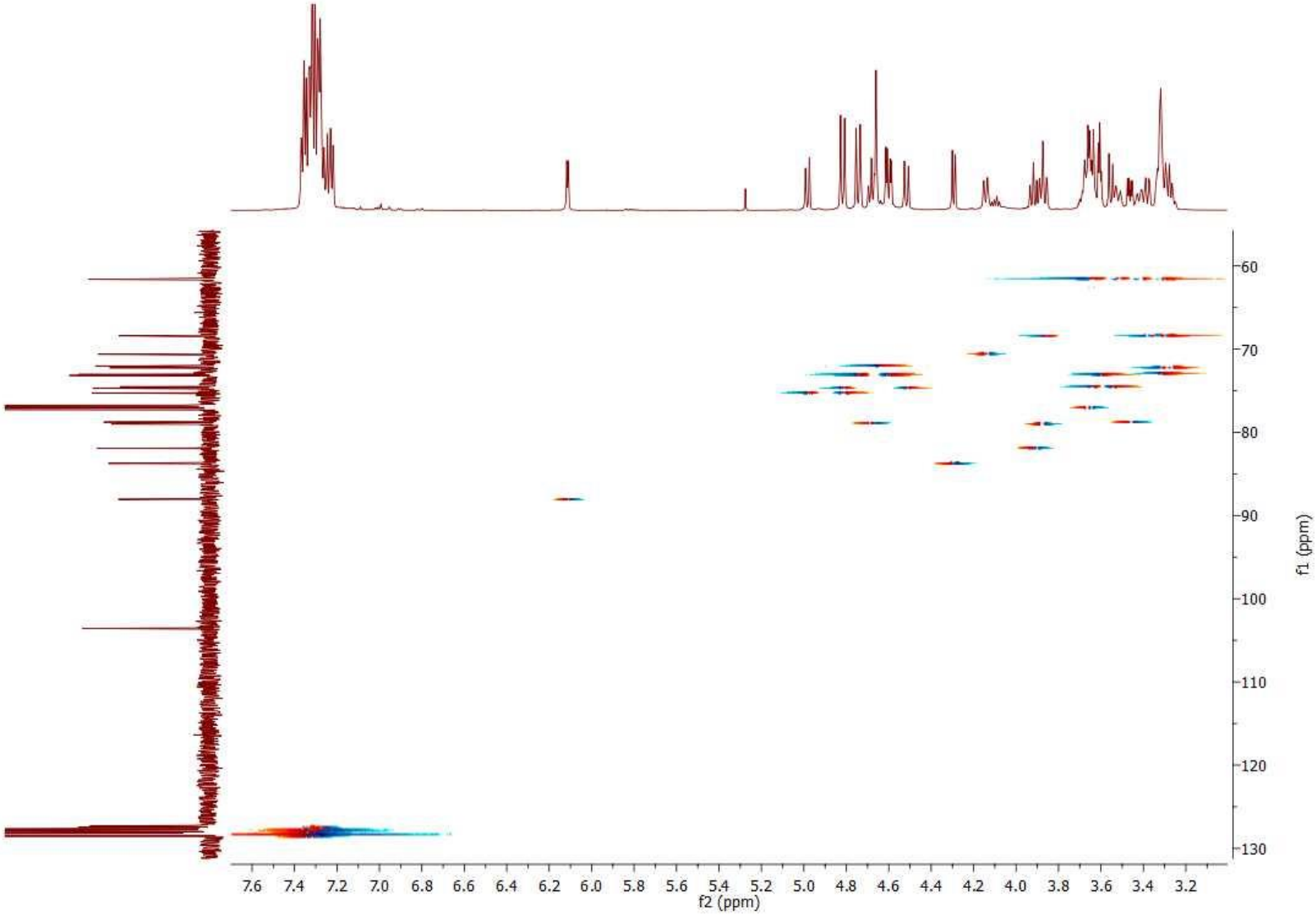


Figure S38. ^{1}H–^{13}C HSQC spectrum of compound **5**.

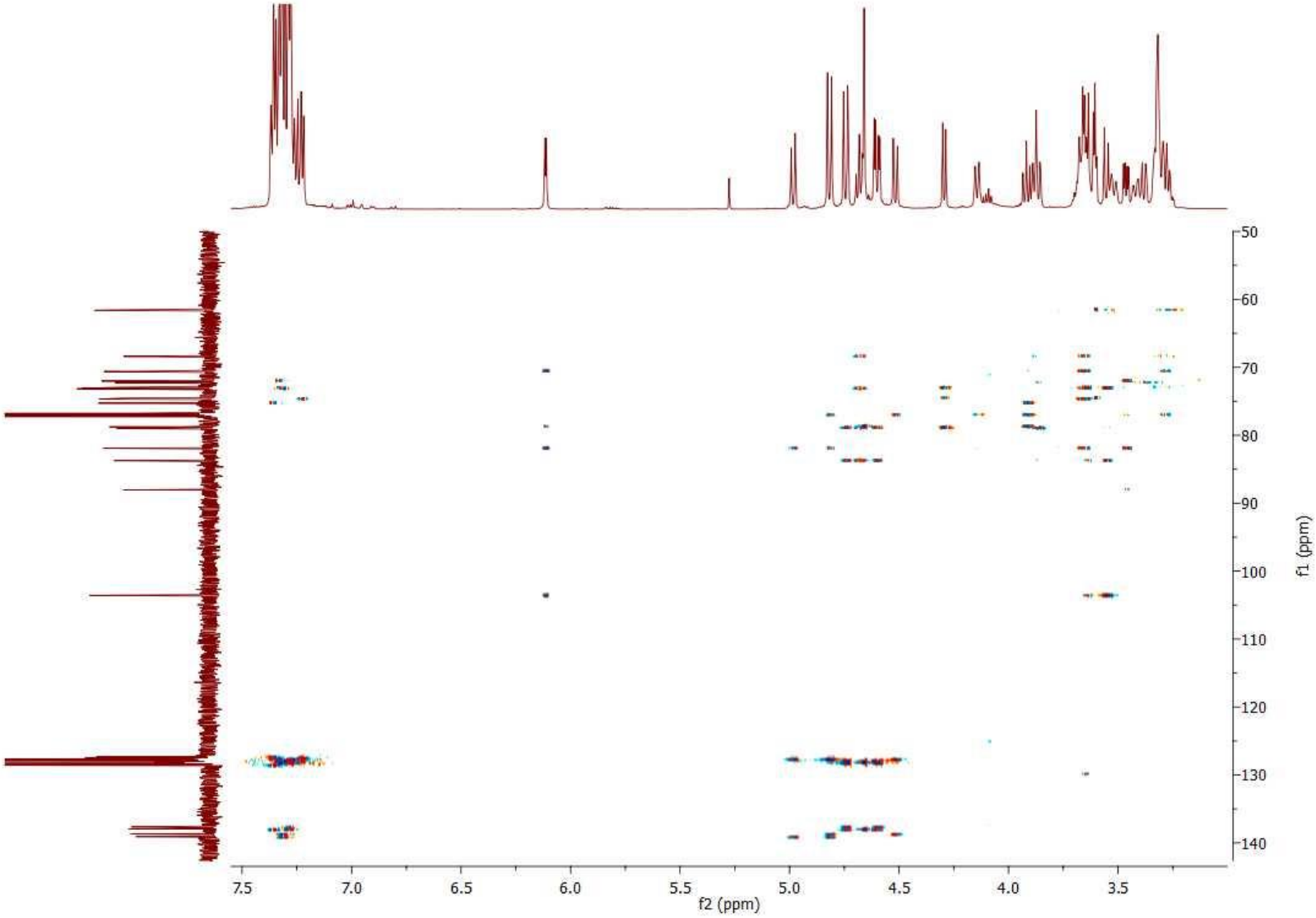


Figure S39. ^{1}H–^{13}C HMBC spectrum of compound **5**.

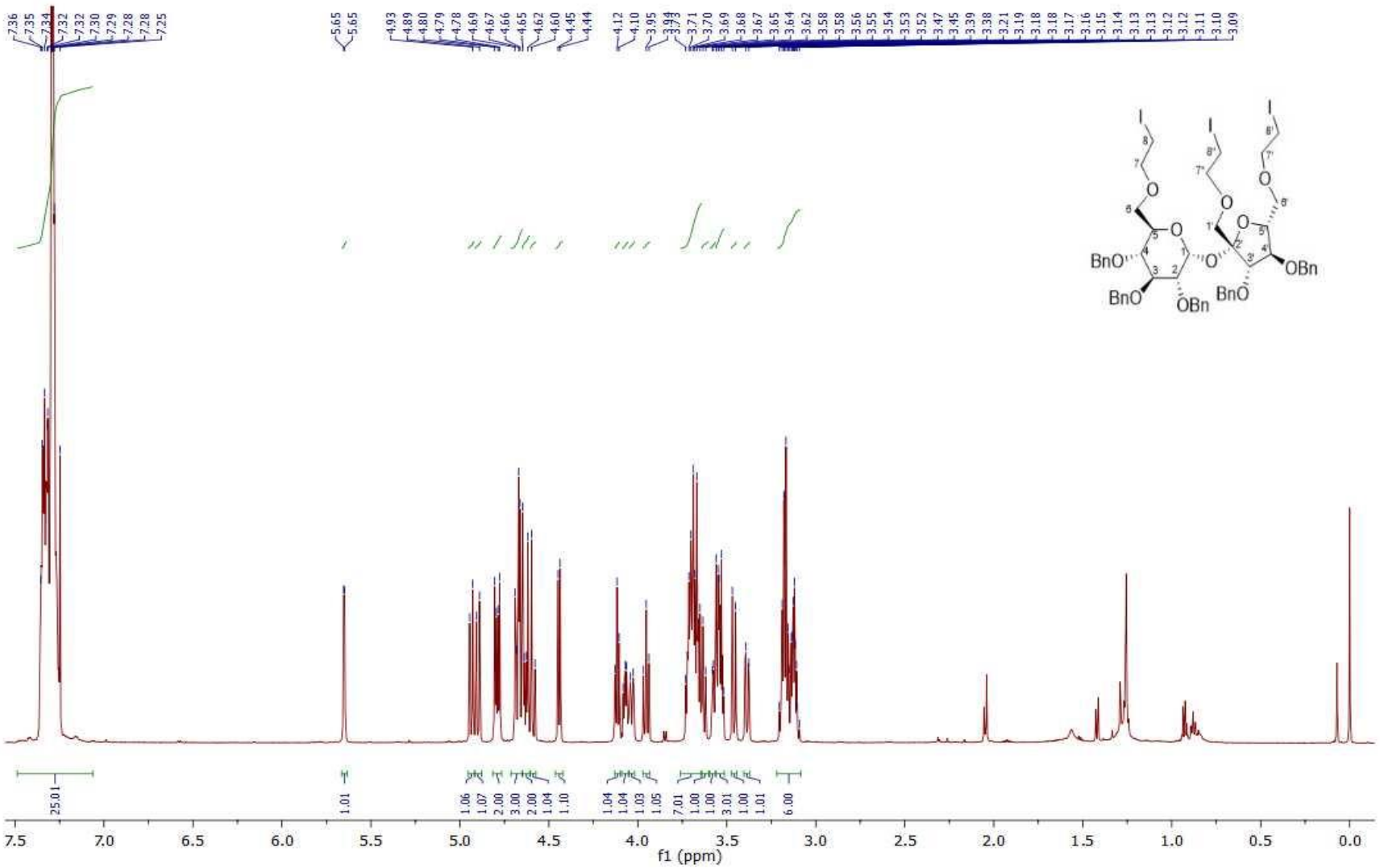


Figure S40. ^{1}H NMR spectrum of compound **6**.

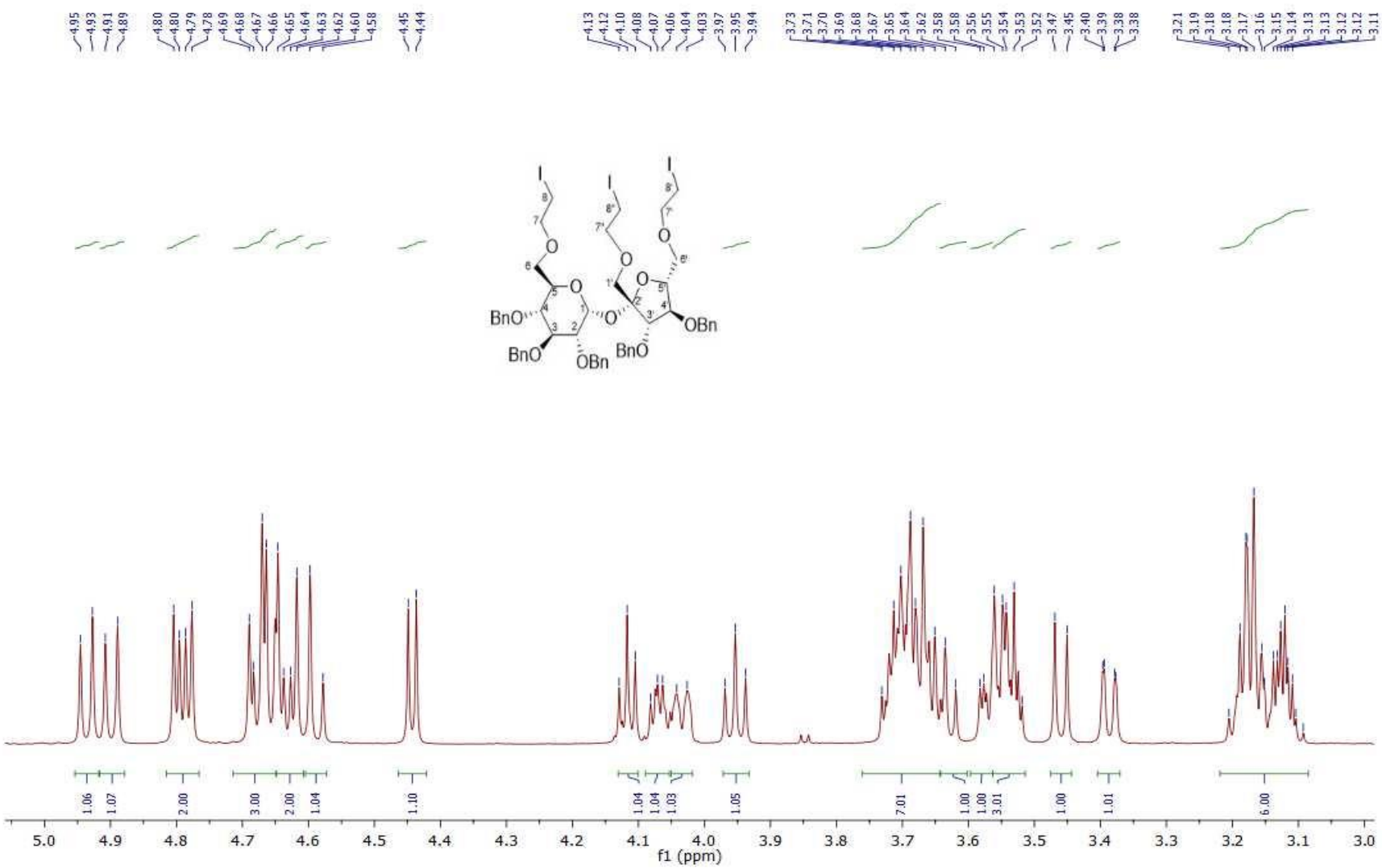


Figure S41. ^{1}H NMR spectrum of compound **6** (aliphatic part).

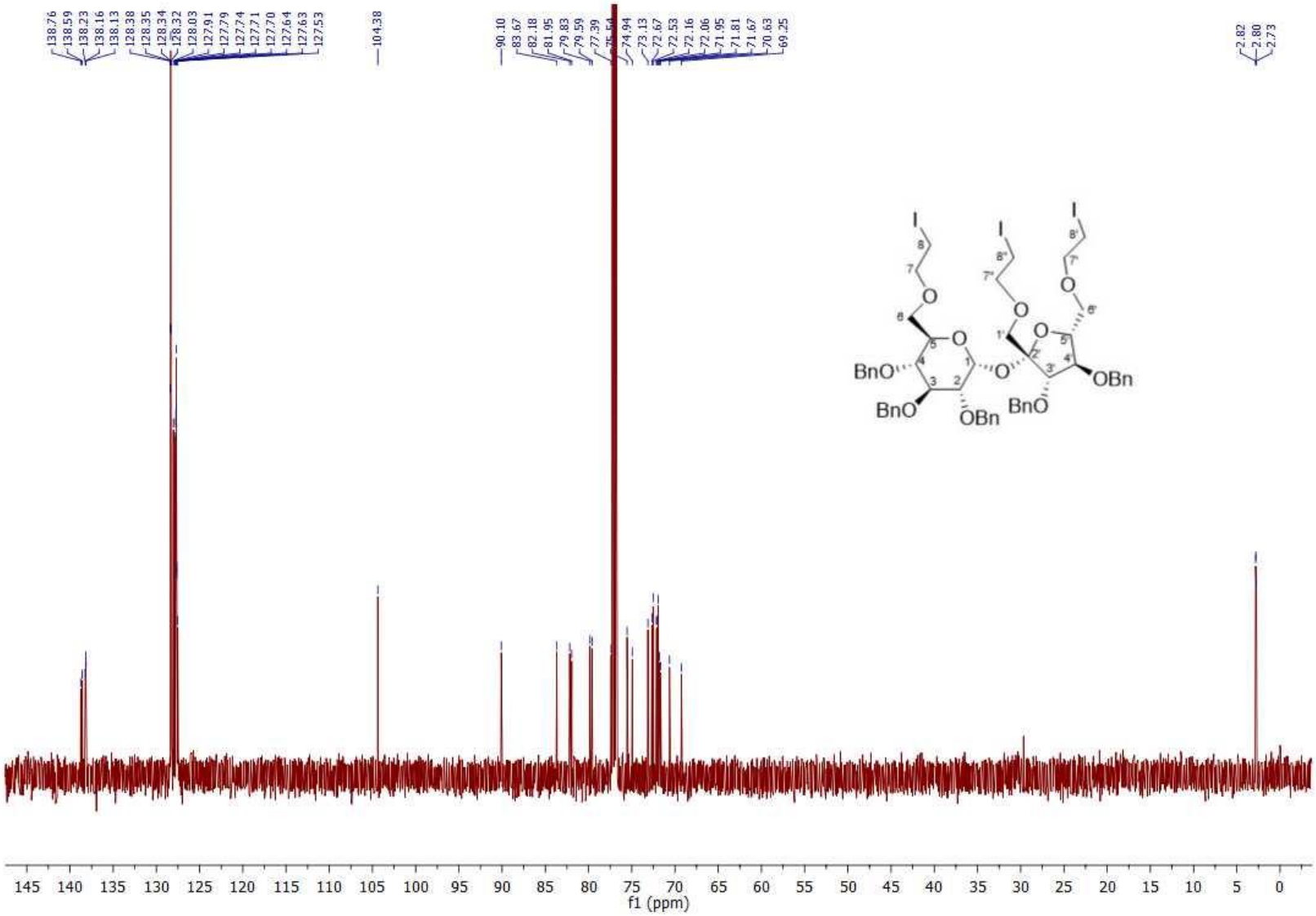


Figure S42. ^{13}C NMR spectrum of compound **6**.

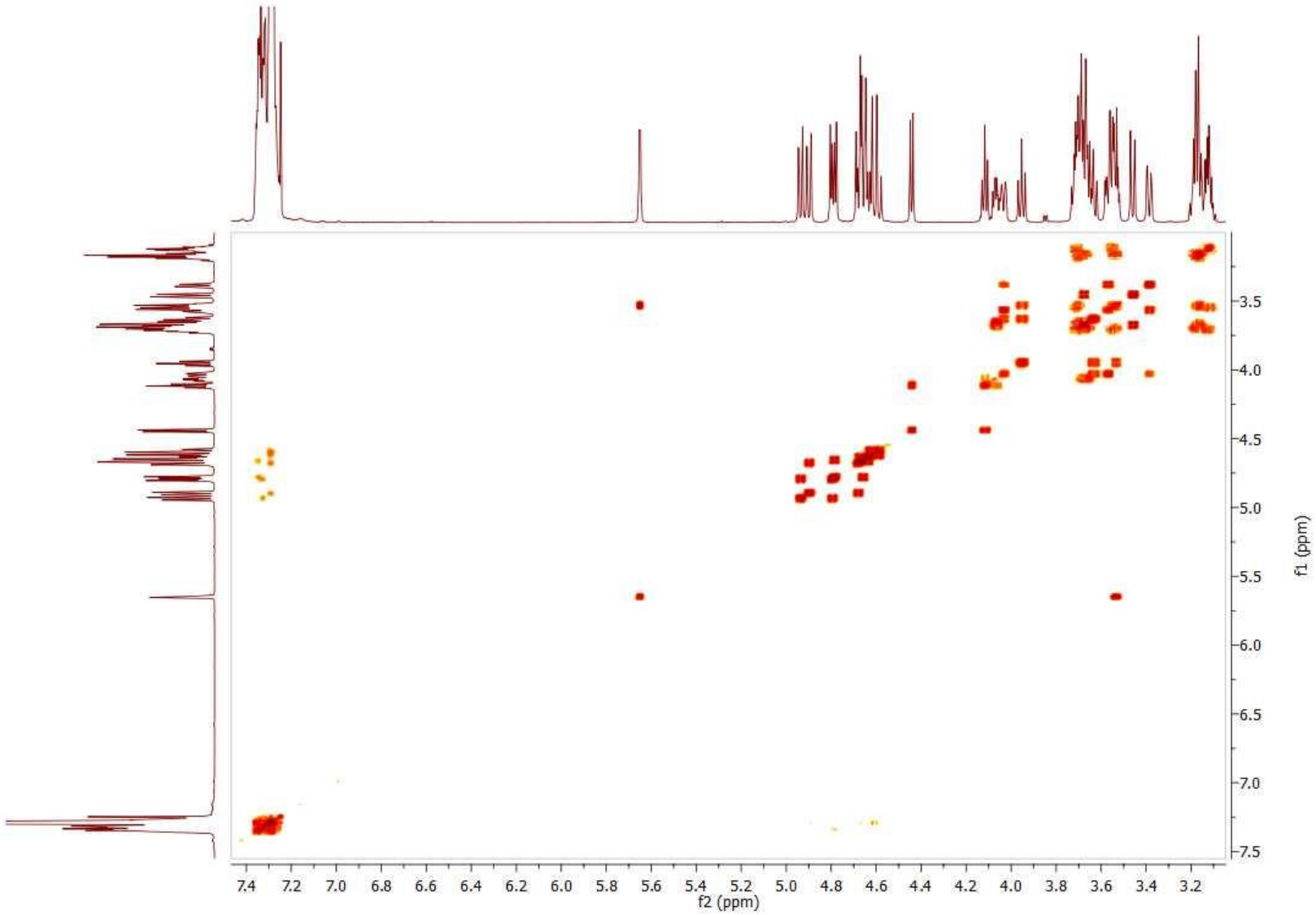


Figure S43. ^{1}H–^{1}H COSY spectrum of compound **6**.

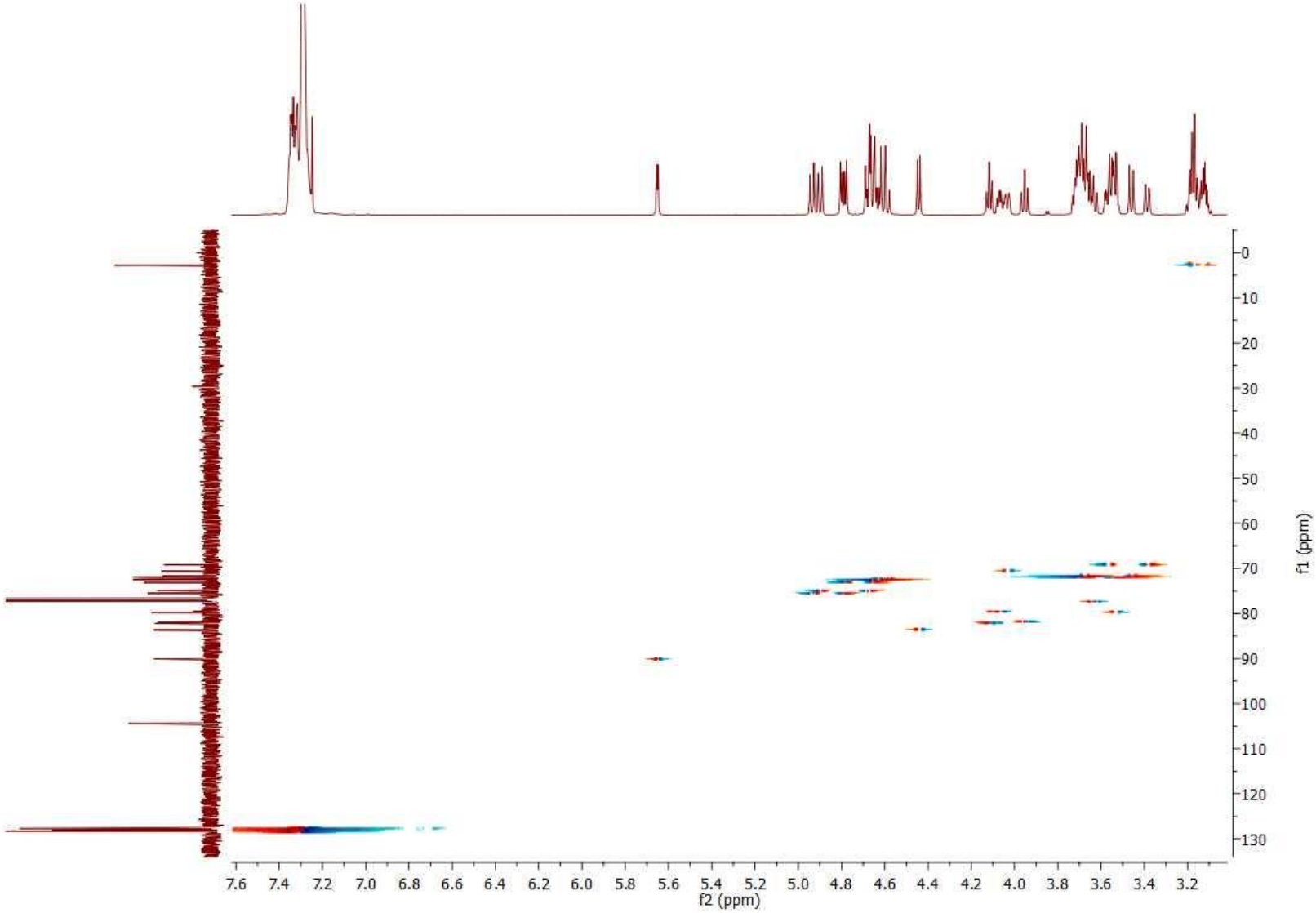


Figure S44. $^{1}H–^{13}C$ HSQC spectrum of compound **6**.

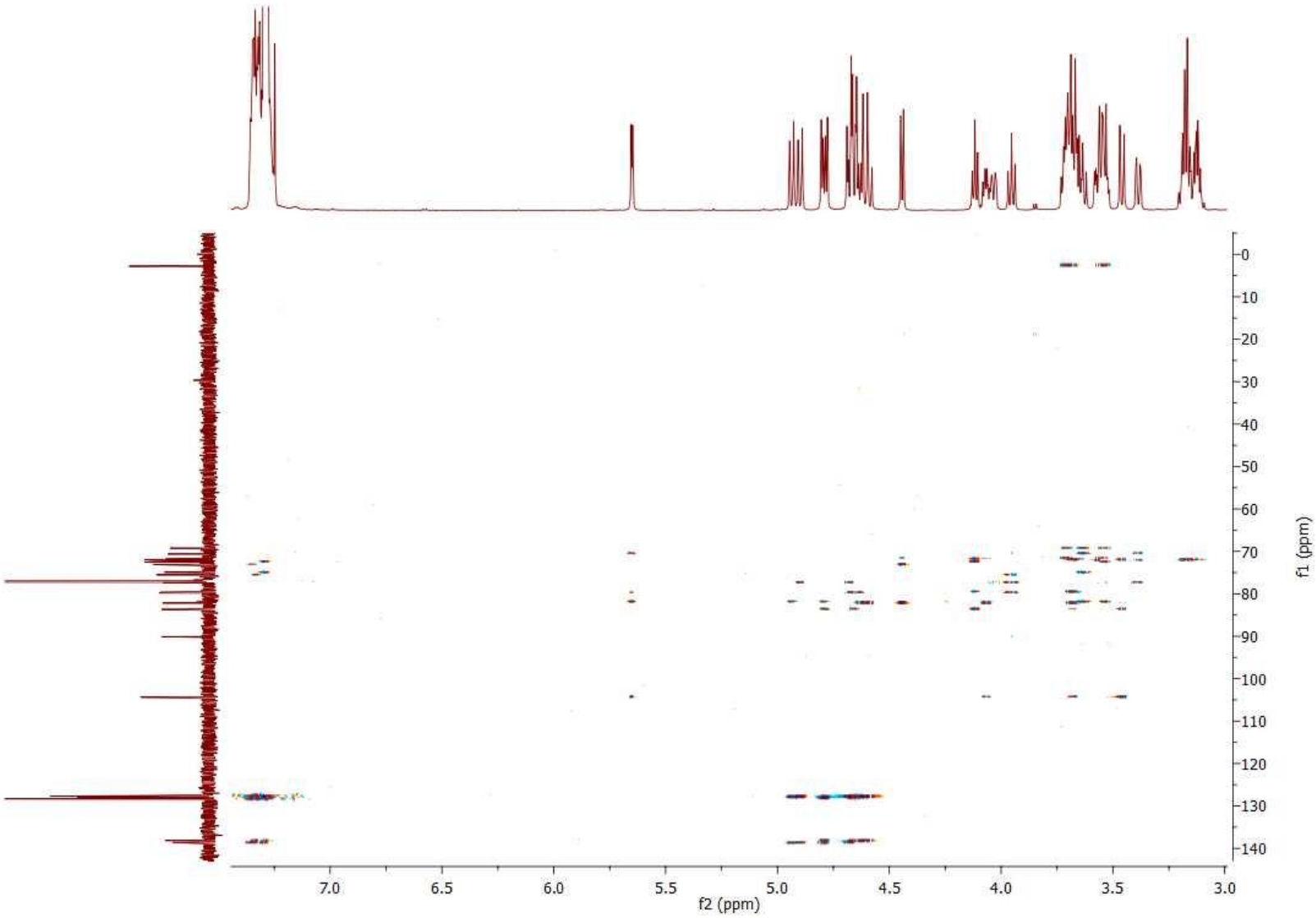


Figure S45. ^{1}H–^{13}C HMBC spectrum of compound **6**.

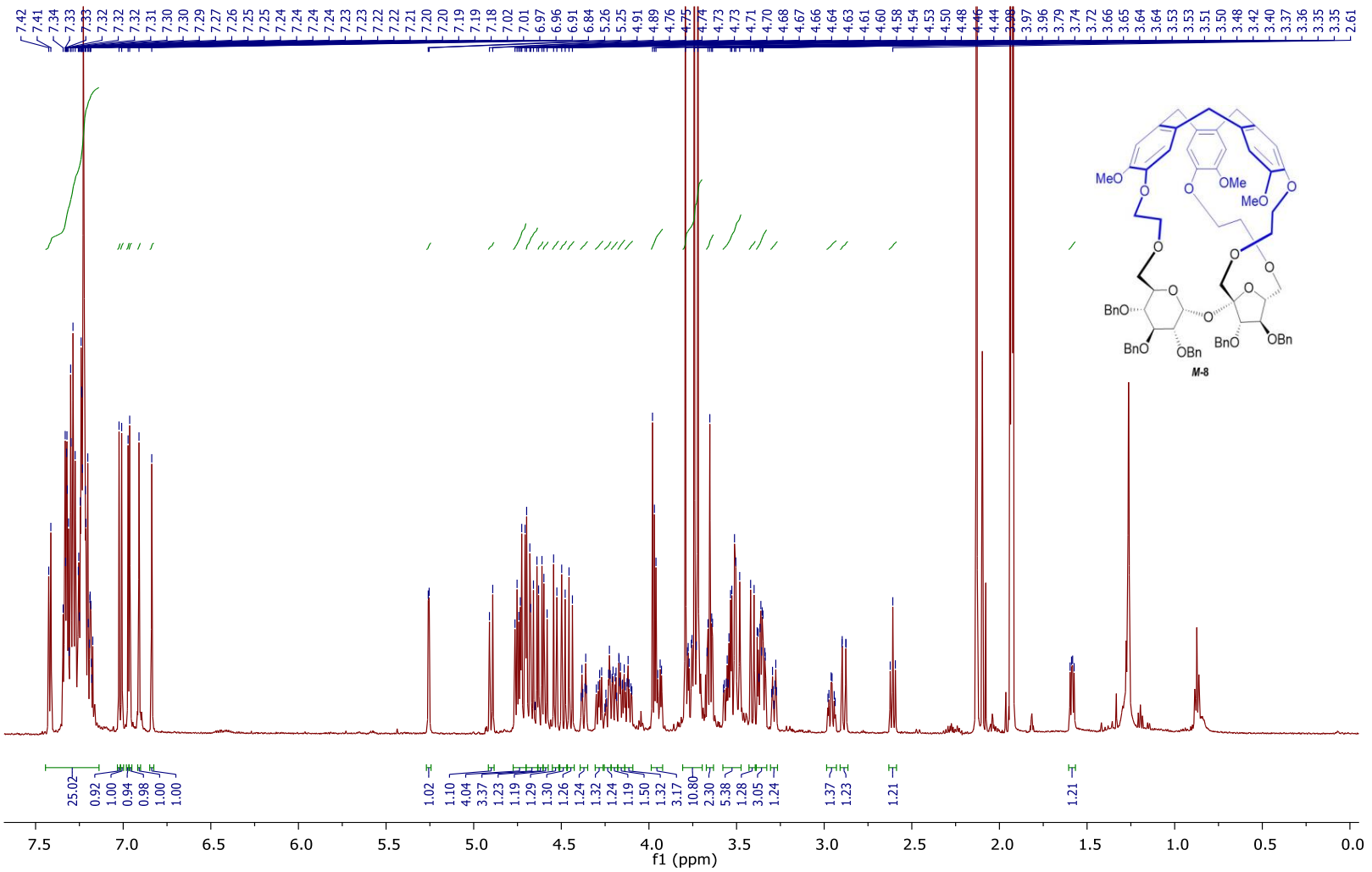


Figure S46. ^{1}H NMR spectrum of compound ***M*-8.**

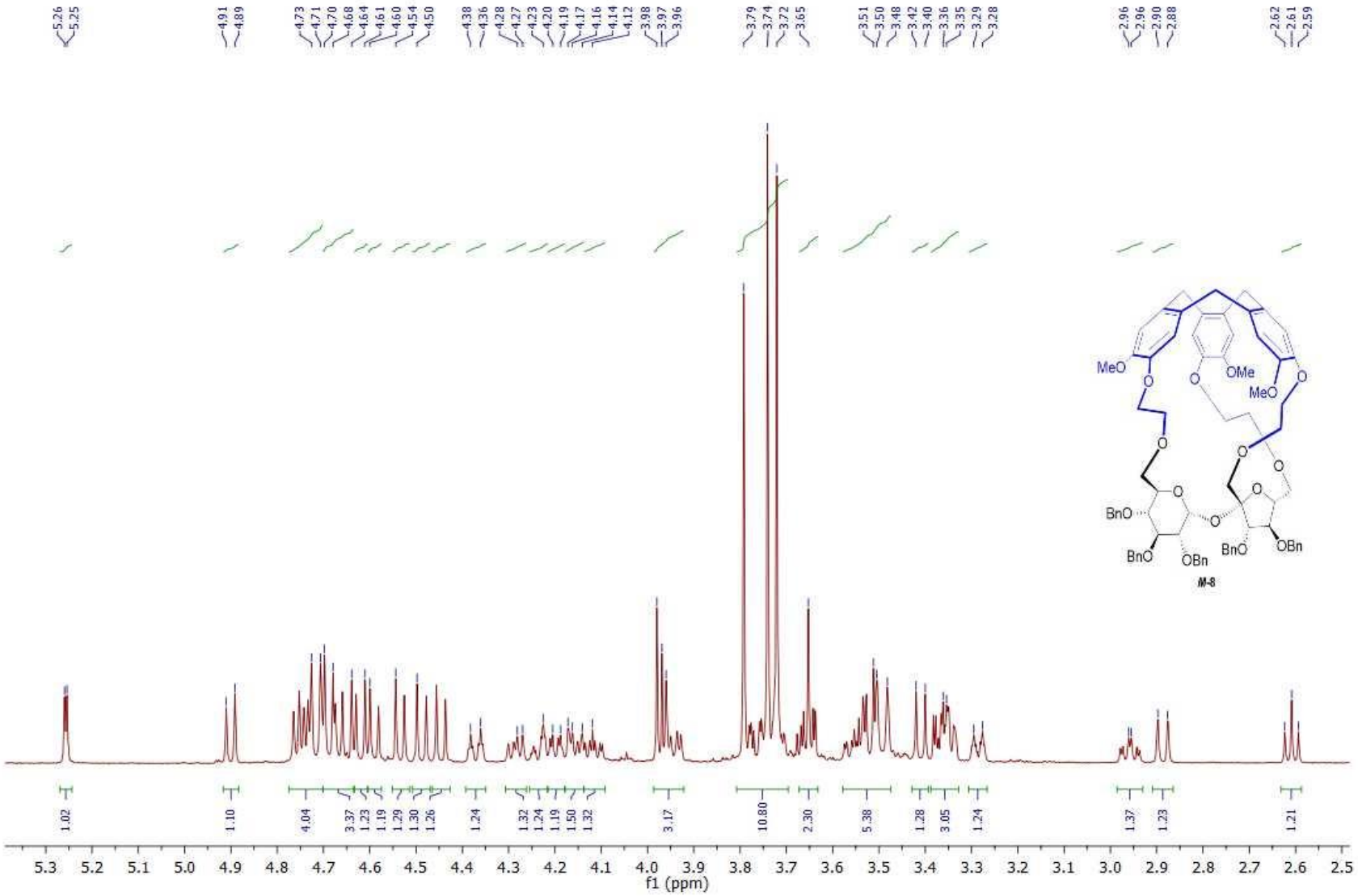


Figure S47. ^{1}H NMR spectrum of compound ***M*-8** (aliphatic part).

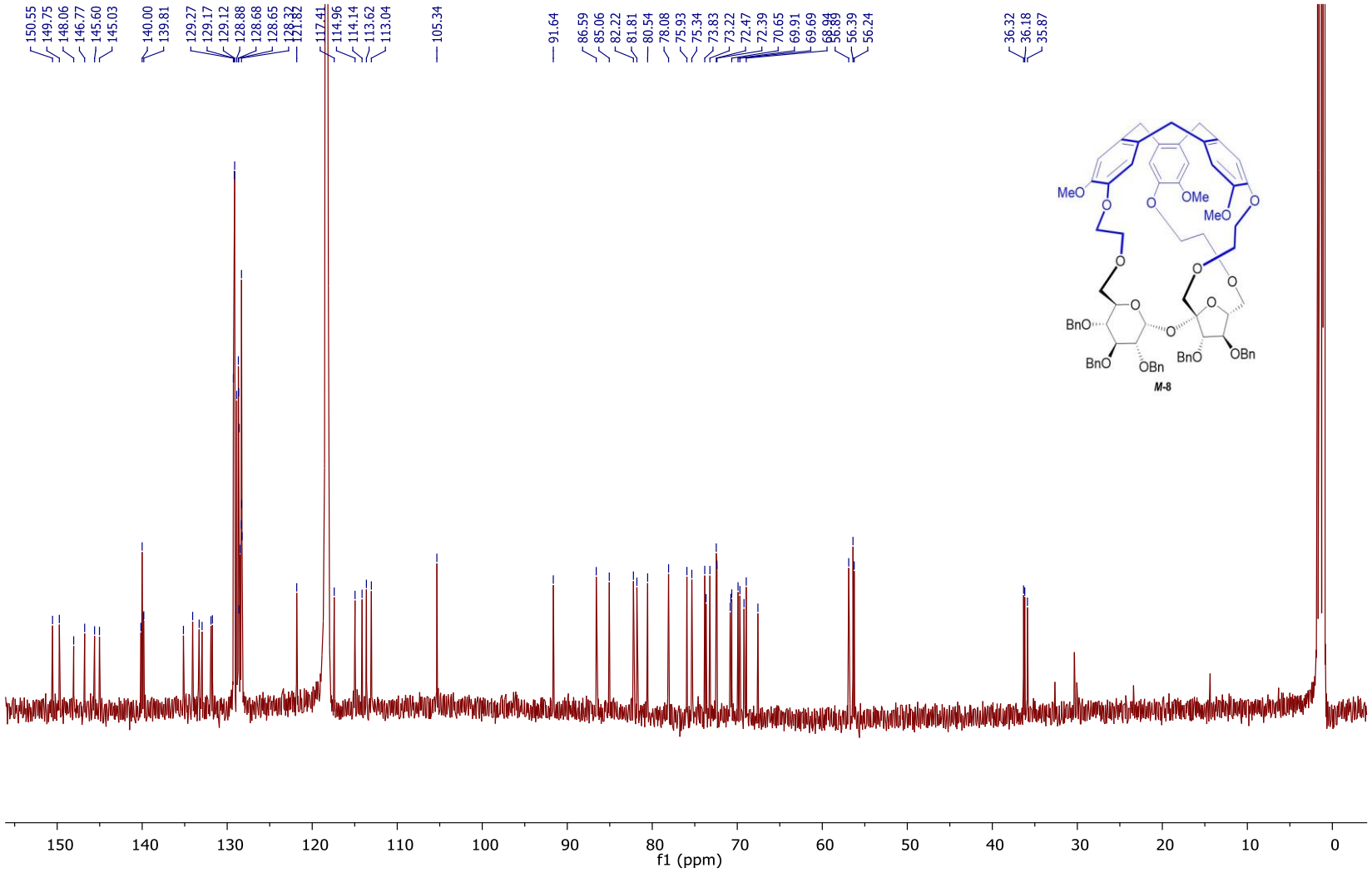


Figure S48. ^{13}C NMR spectrum of compound ***M*-8**.

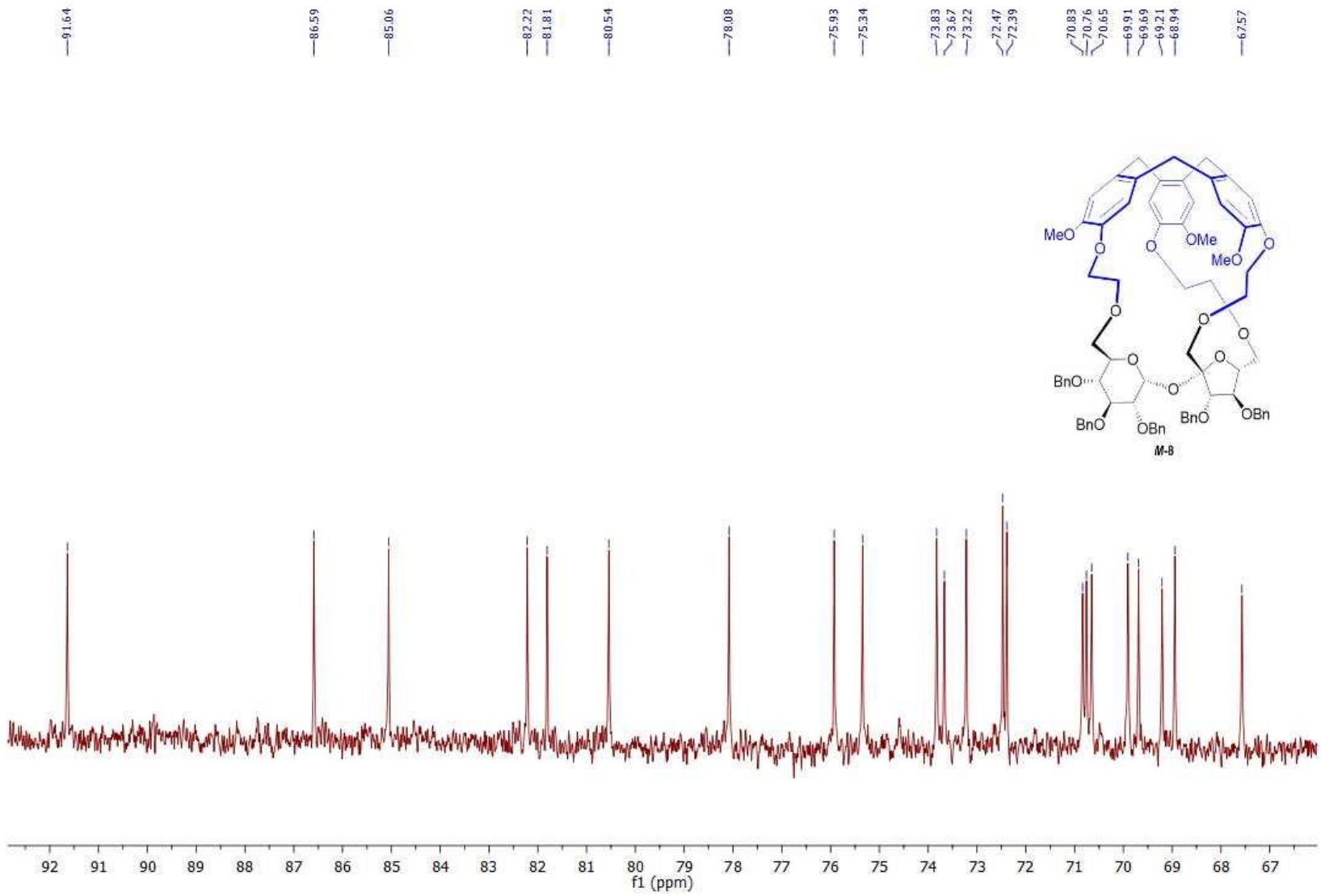


Figure S49. ^{13}C NMR spectrum of compound ***M*-8** (aliphatic part).

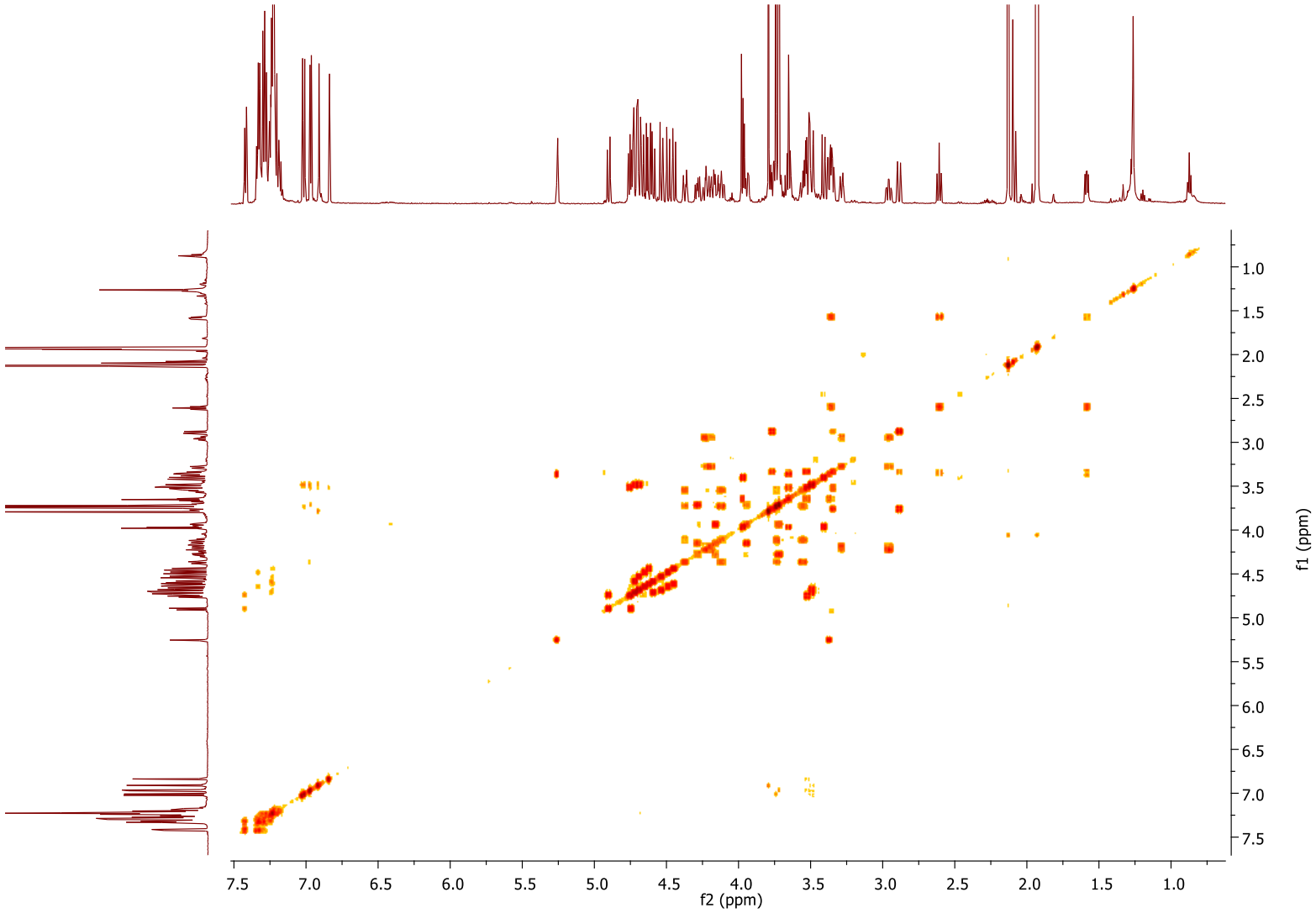


Figure S50. ^{1}H–^{1}H COSY spectrum of compound ***M*-8**.

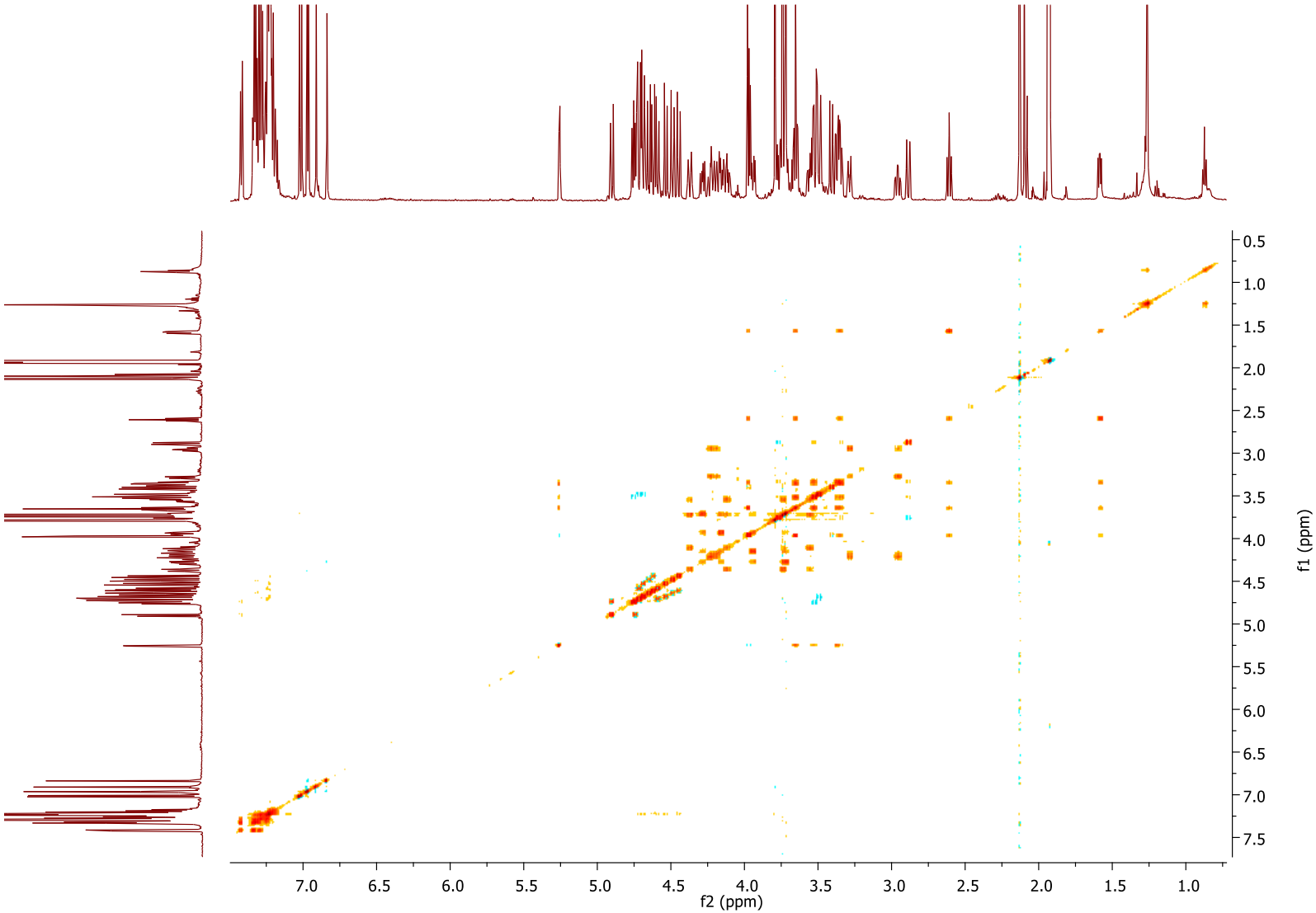


Figure S51. ^{1}H–^{1}H TOCSY spectrum of compound ***M*-8**.

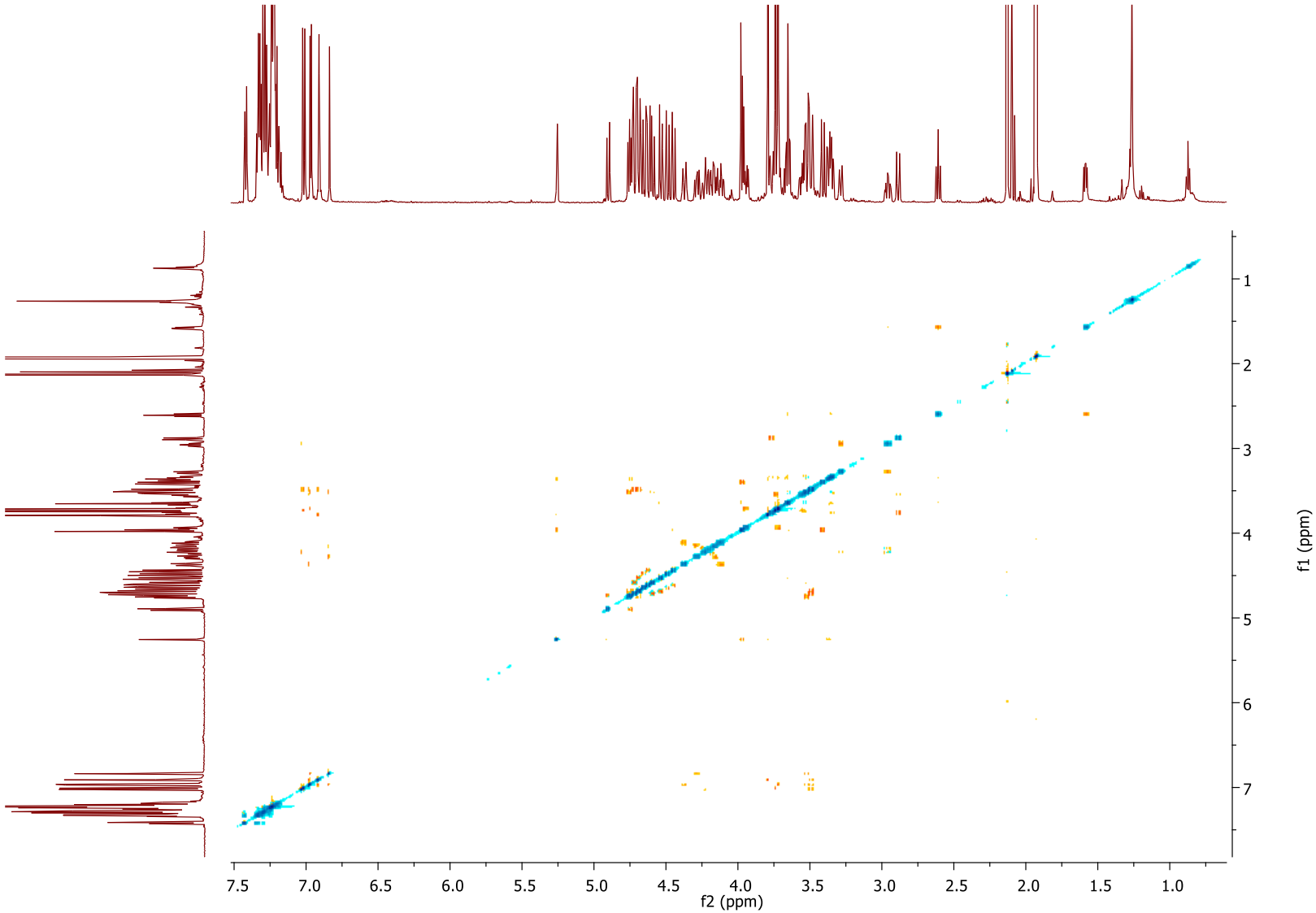


Figure S52. ^{1}H–^{1}H ROESY spectrum of compound ***M*-8**.

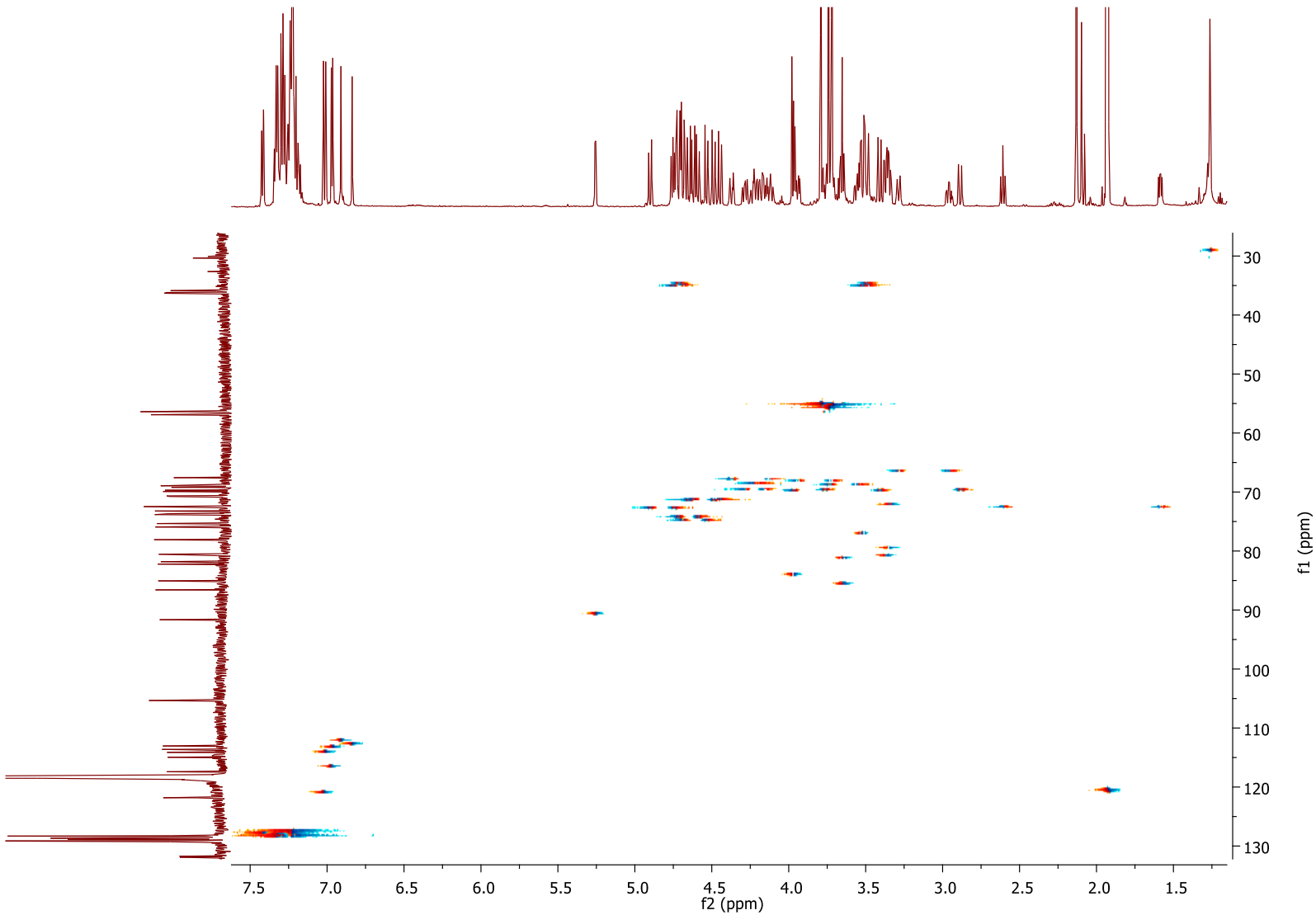


Figure S53. ^{1}H–^{13}C HSQC spectrum of compound ***M*-8**.

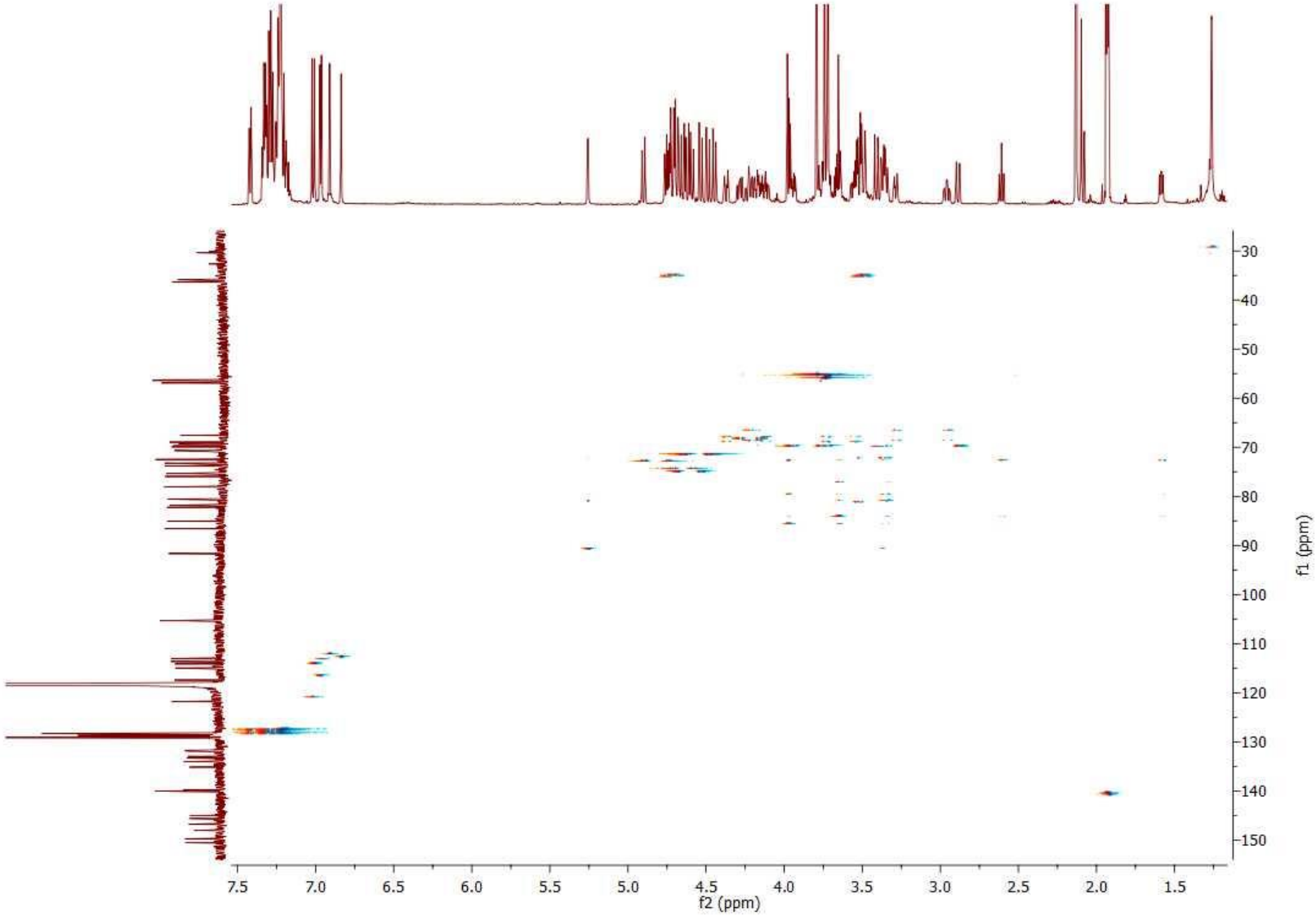


Figure S54. ^{1}H–^{13}C HSQCTOCSY spectrum of compound ***M*-8**.

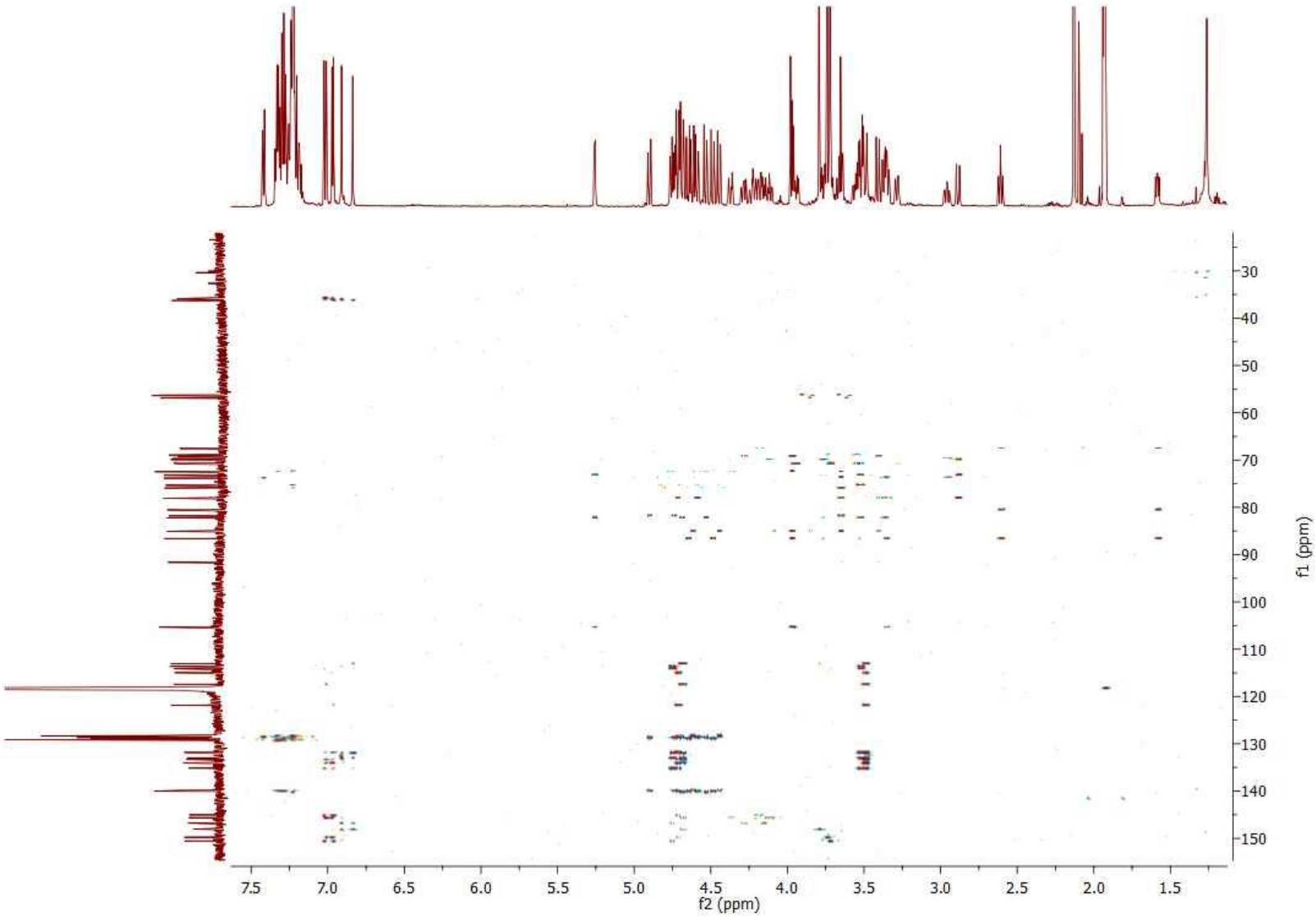


Figure S55. $^{1}H–^{13}C$ HMBC spectrum of compound ***M*-8**.

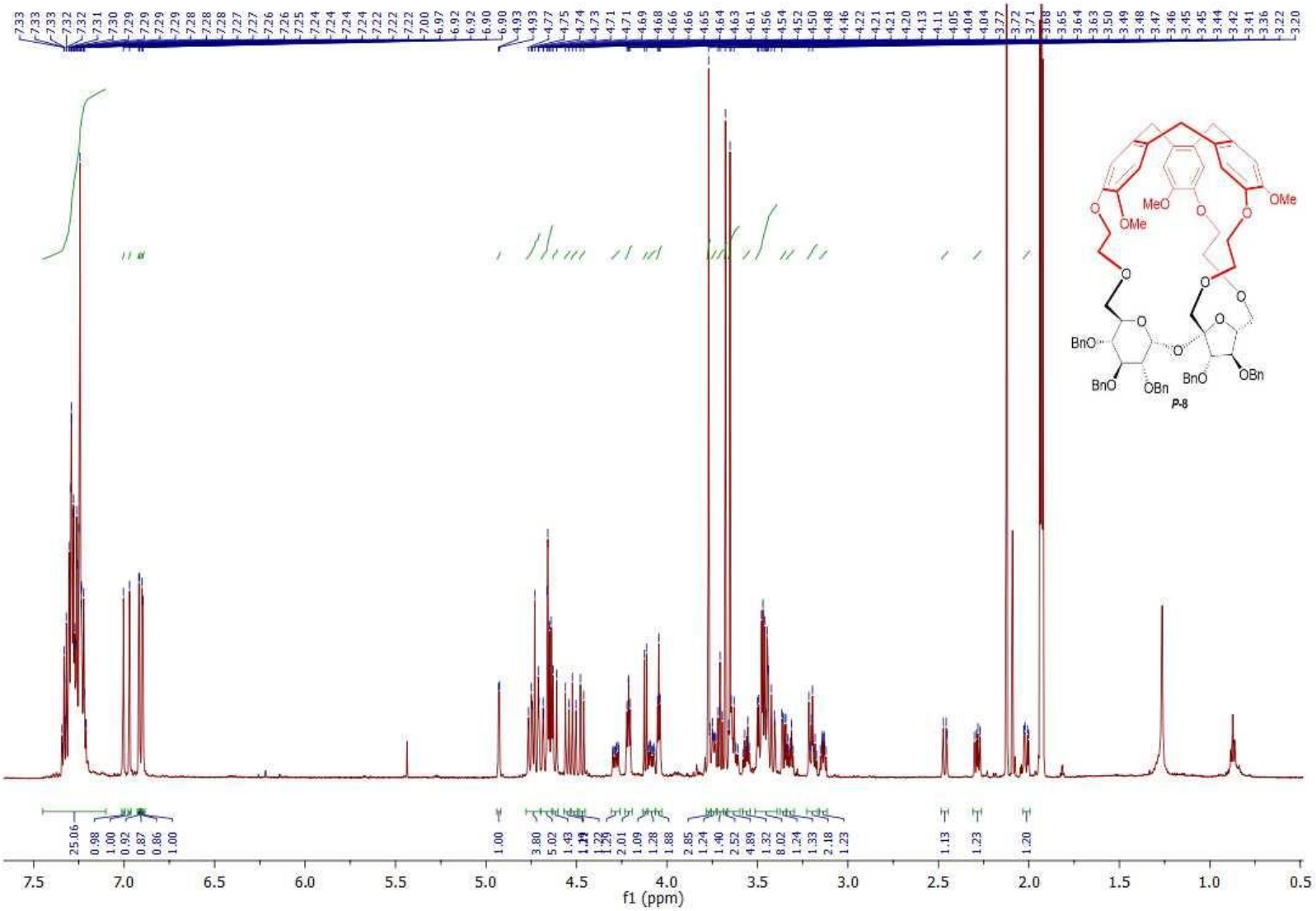


Figure S56. ^{1}H NMR spectrum of compound ***P*-8.**

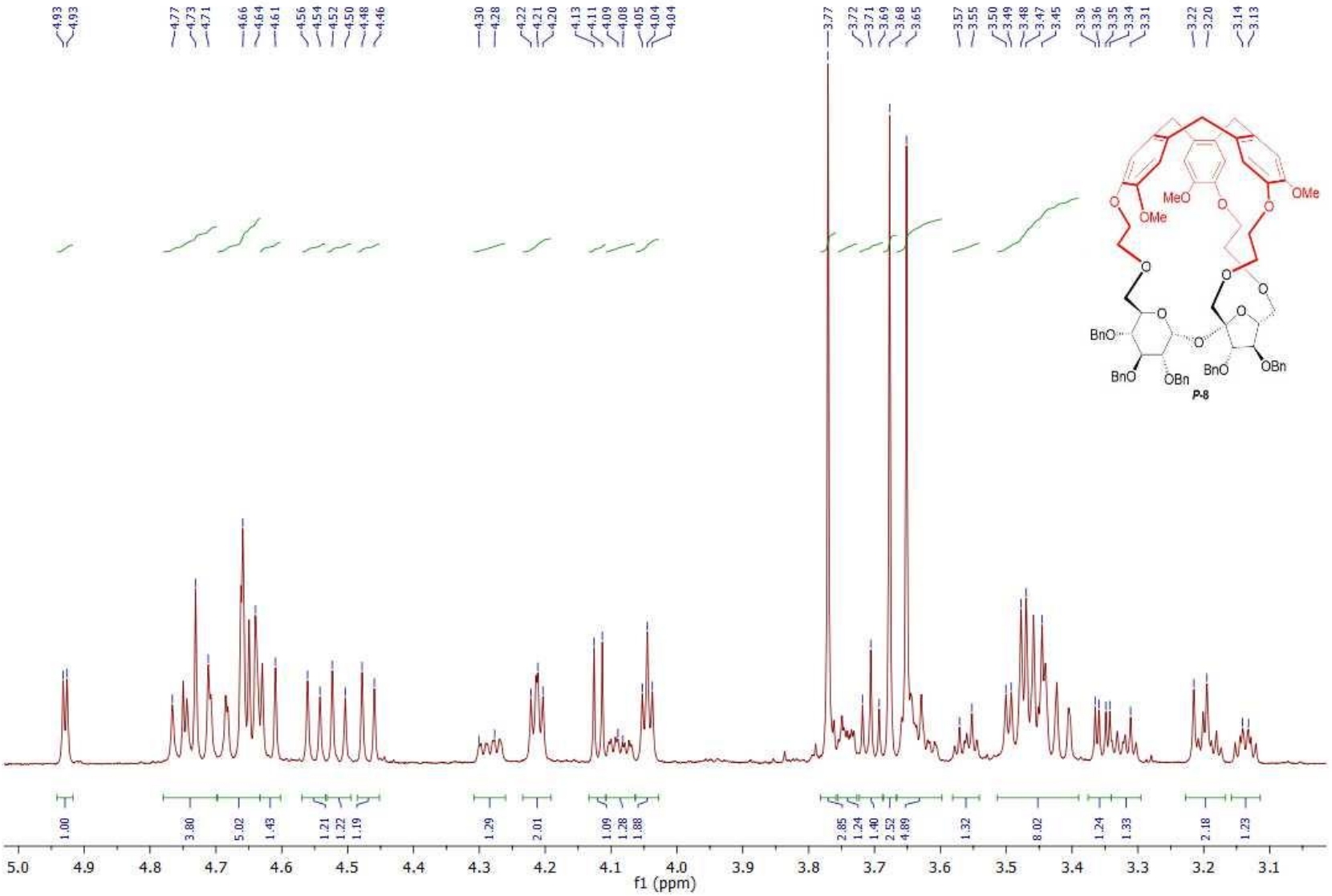


Figure S57. ^{1}H NMR spectrum of compound ***P*-8** (aliphatic part).

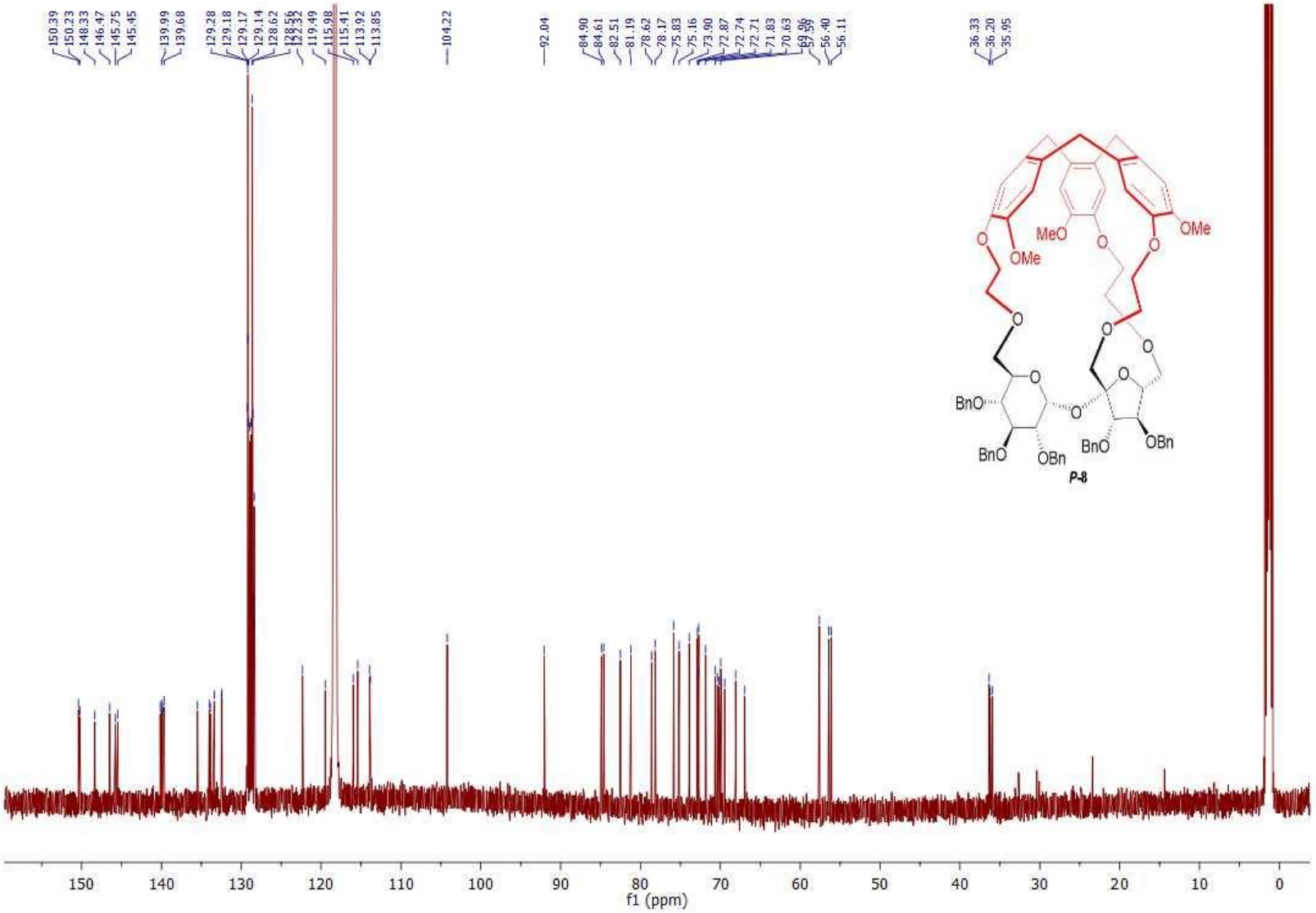


Figure S58. ^{13}C NMR spectrum of compound ***P*-8**.

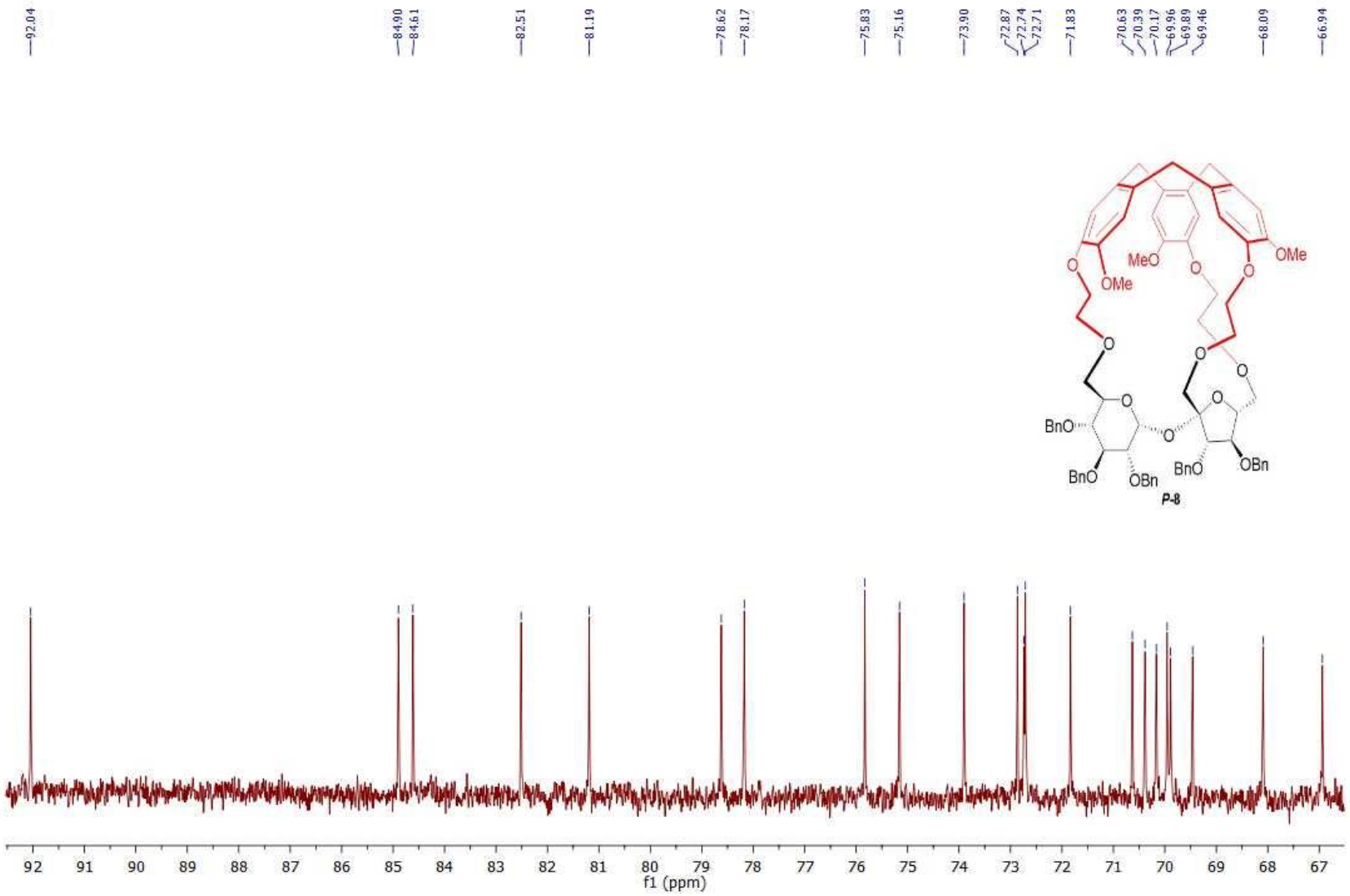


Figure S59. ^{13}C NMR spectrum of compound ***P*-8** (aliphatic part).

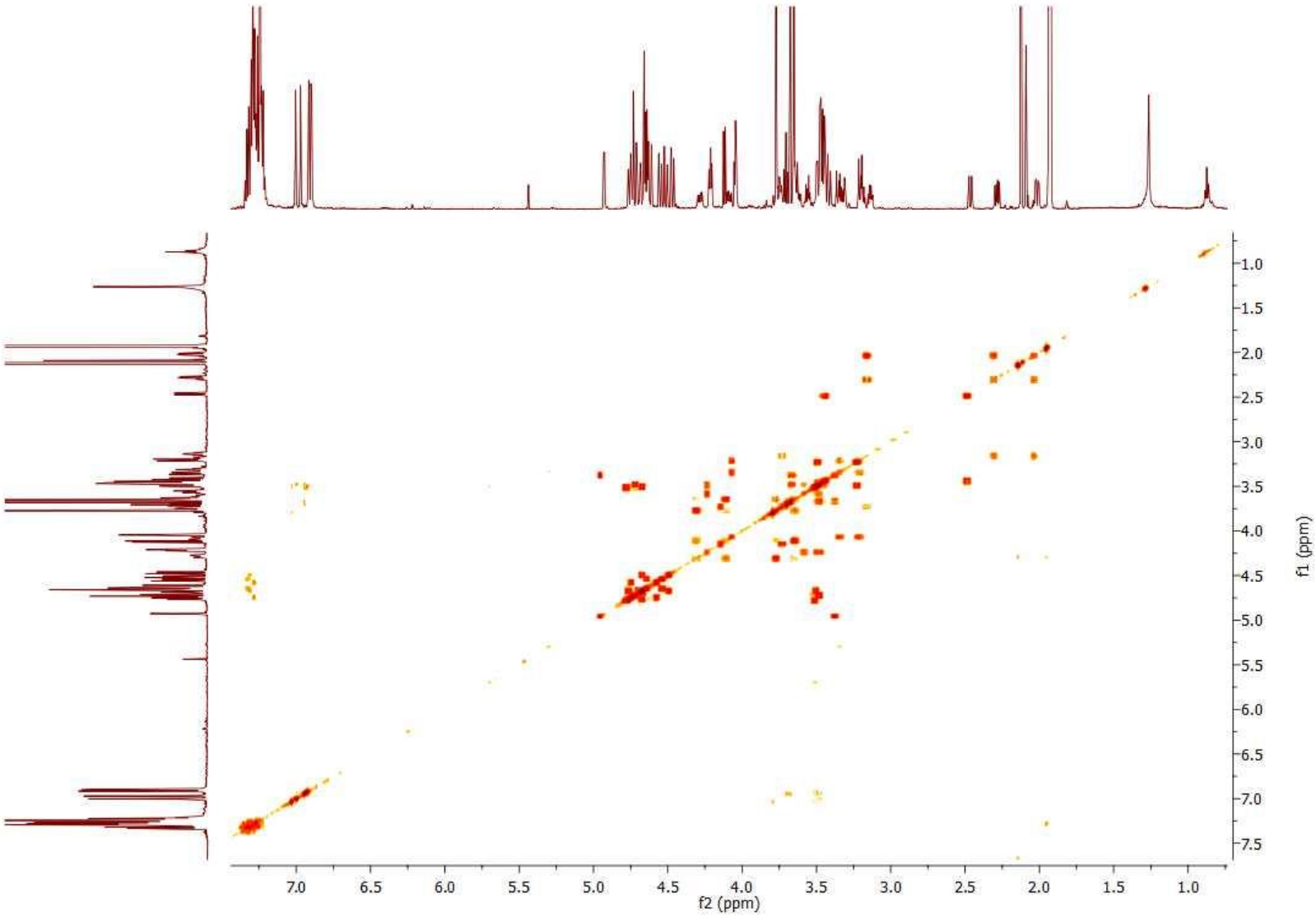


Figure S60. ^{1}H–^{1}H COSY spectrum of compound ***P*-8**.

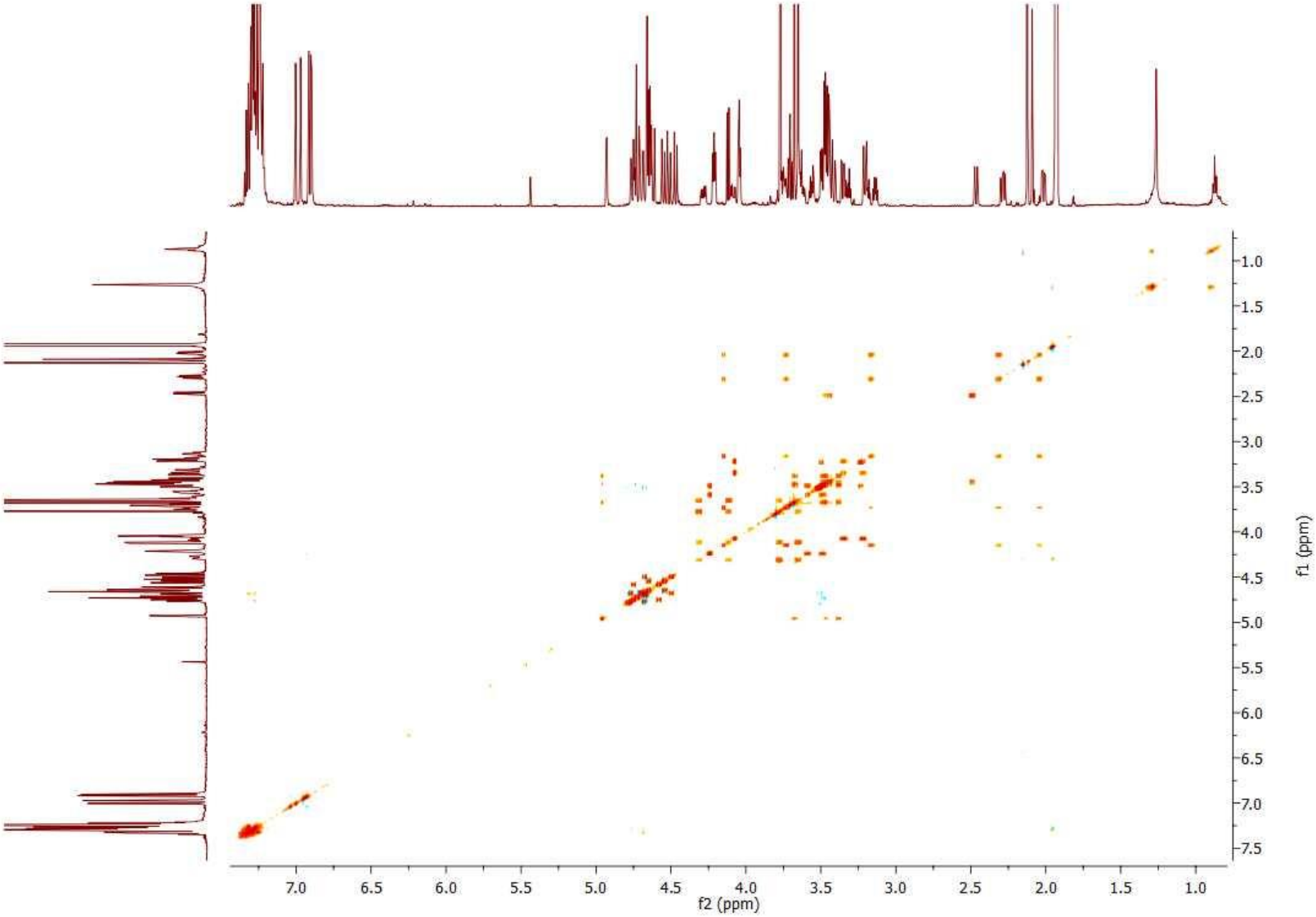


Figure S61. ^{1}H–^{1}H TOCSY spectrum of compound ***P*-8**.

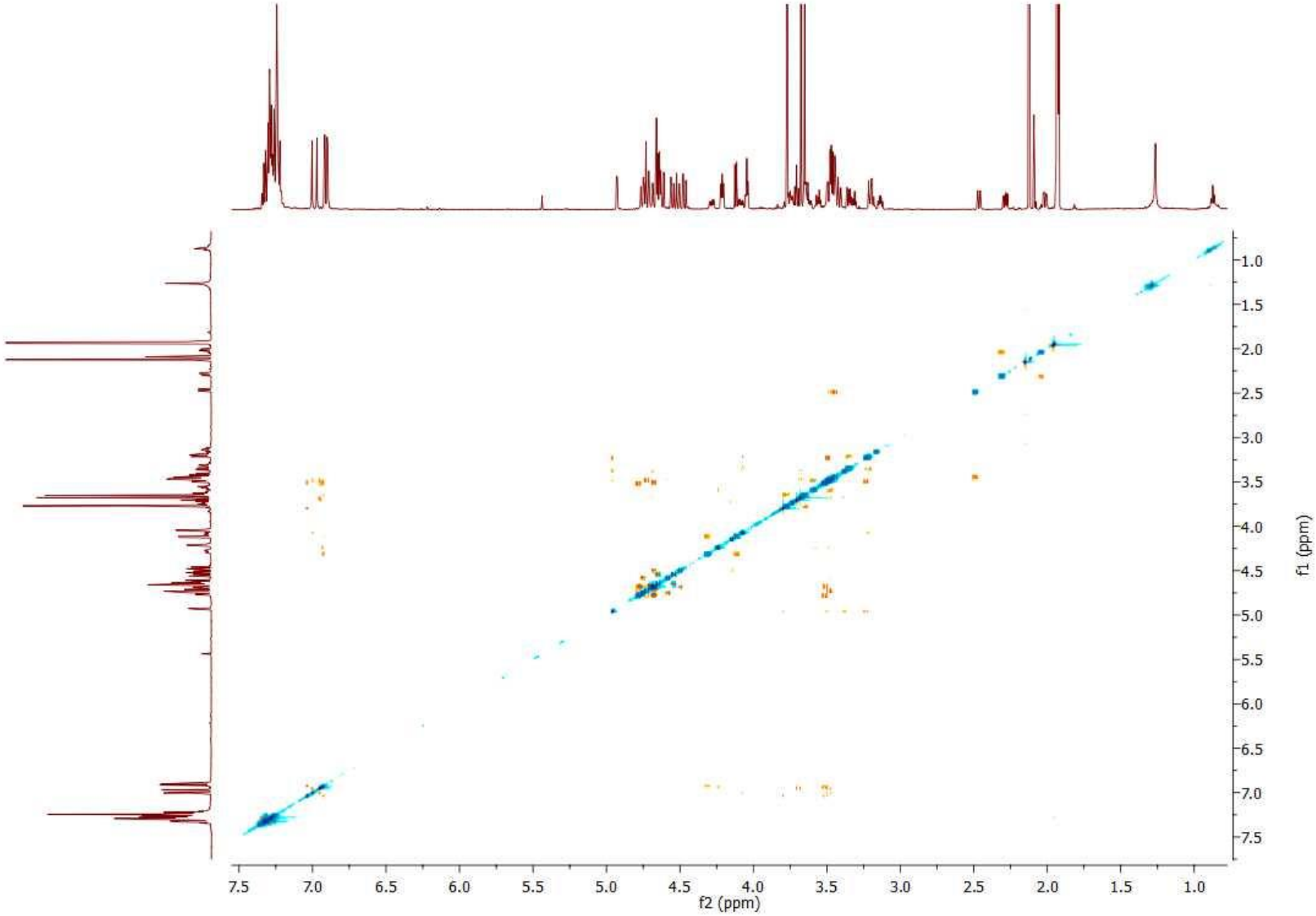


Figure S62. ^{1}H–^{1}H ROESY spectrum of compound ***P*-8**.

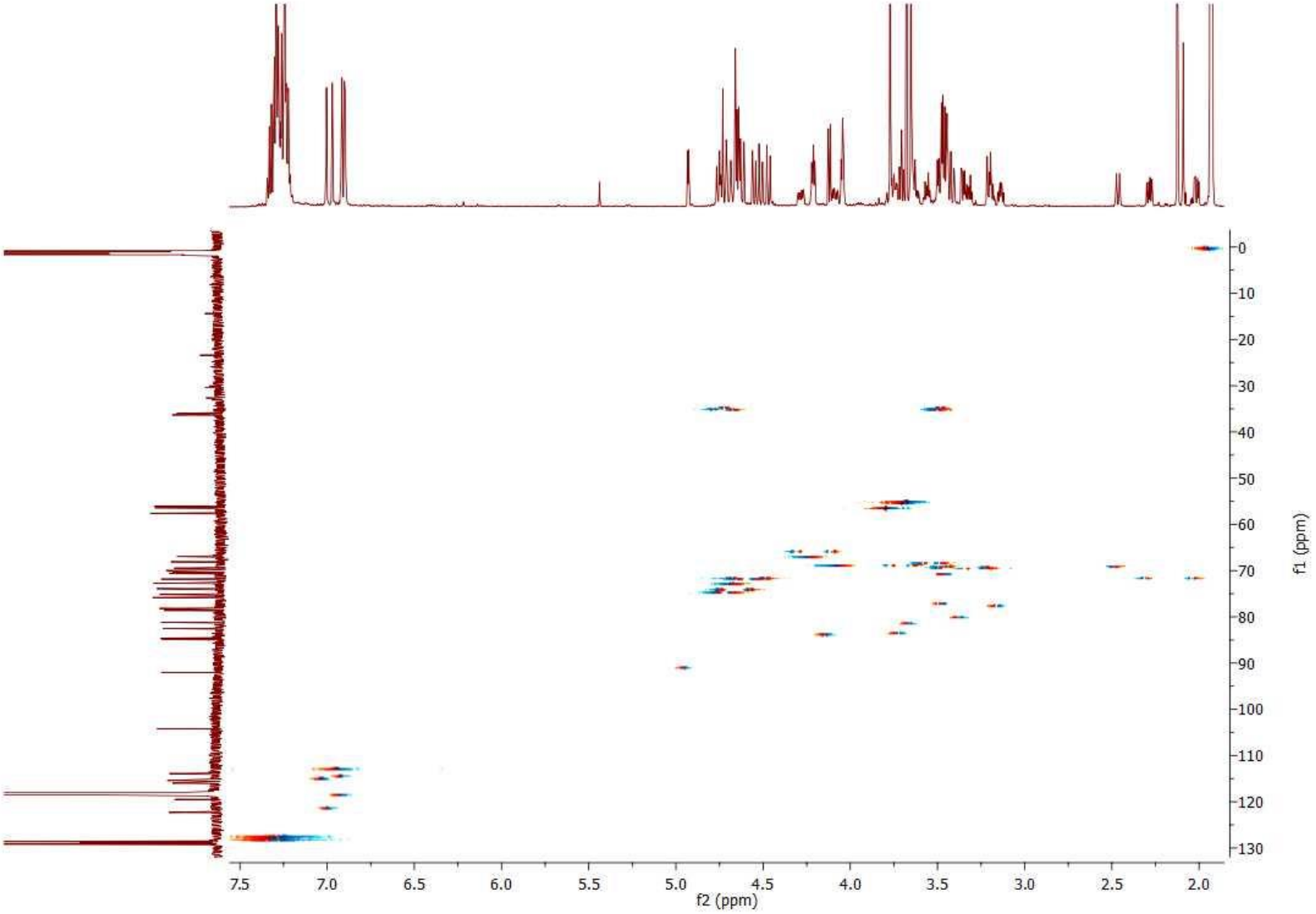


Figure S63. ^{1}H–^{13}C HSQC spectrum of compound ***P*-8**.

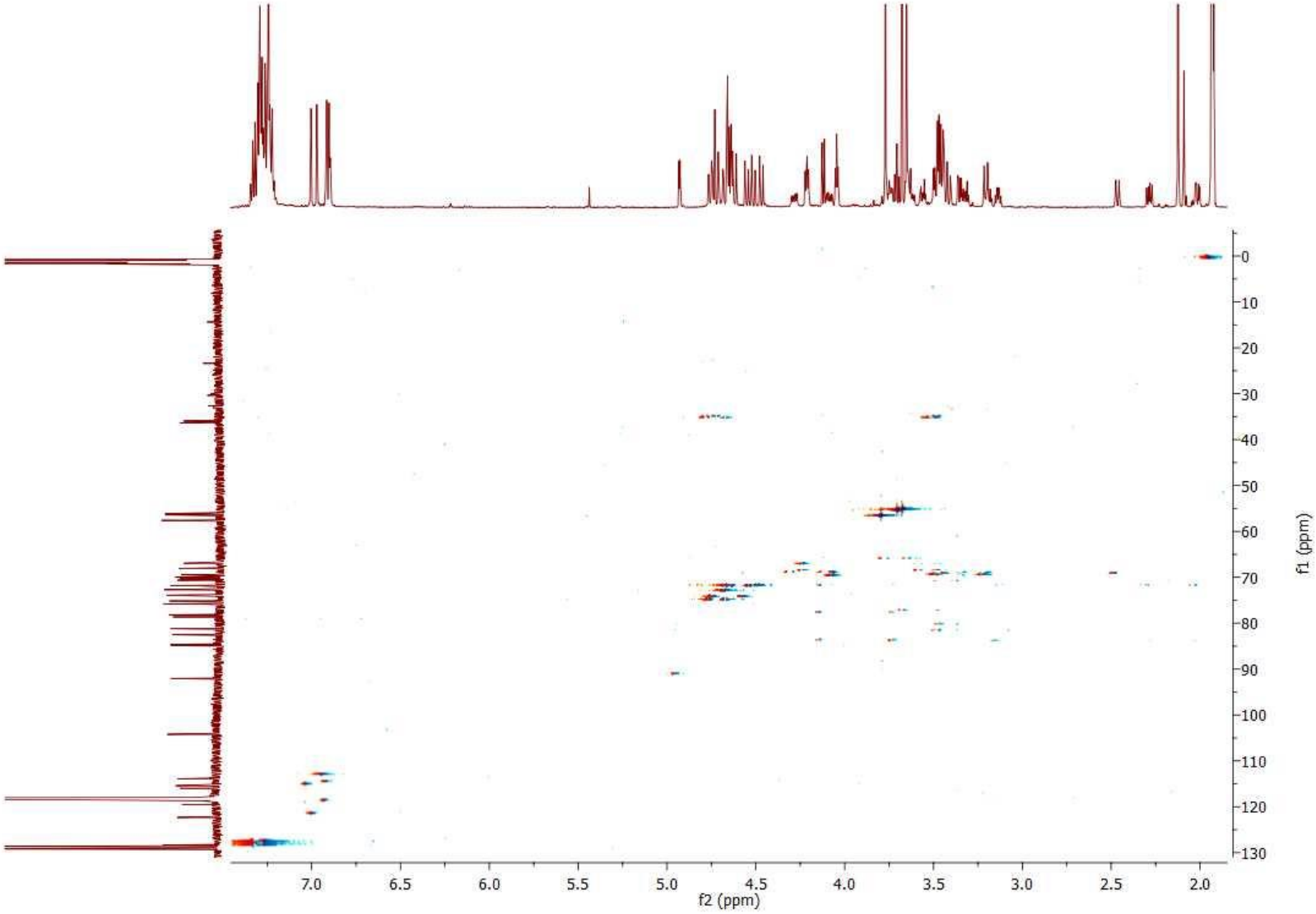


Figure S64. ^{1}H–^{13}C HSQC TOCSY spectrum of compound ***P*-8**.

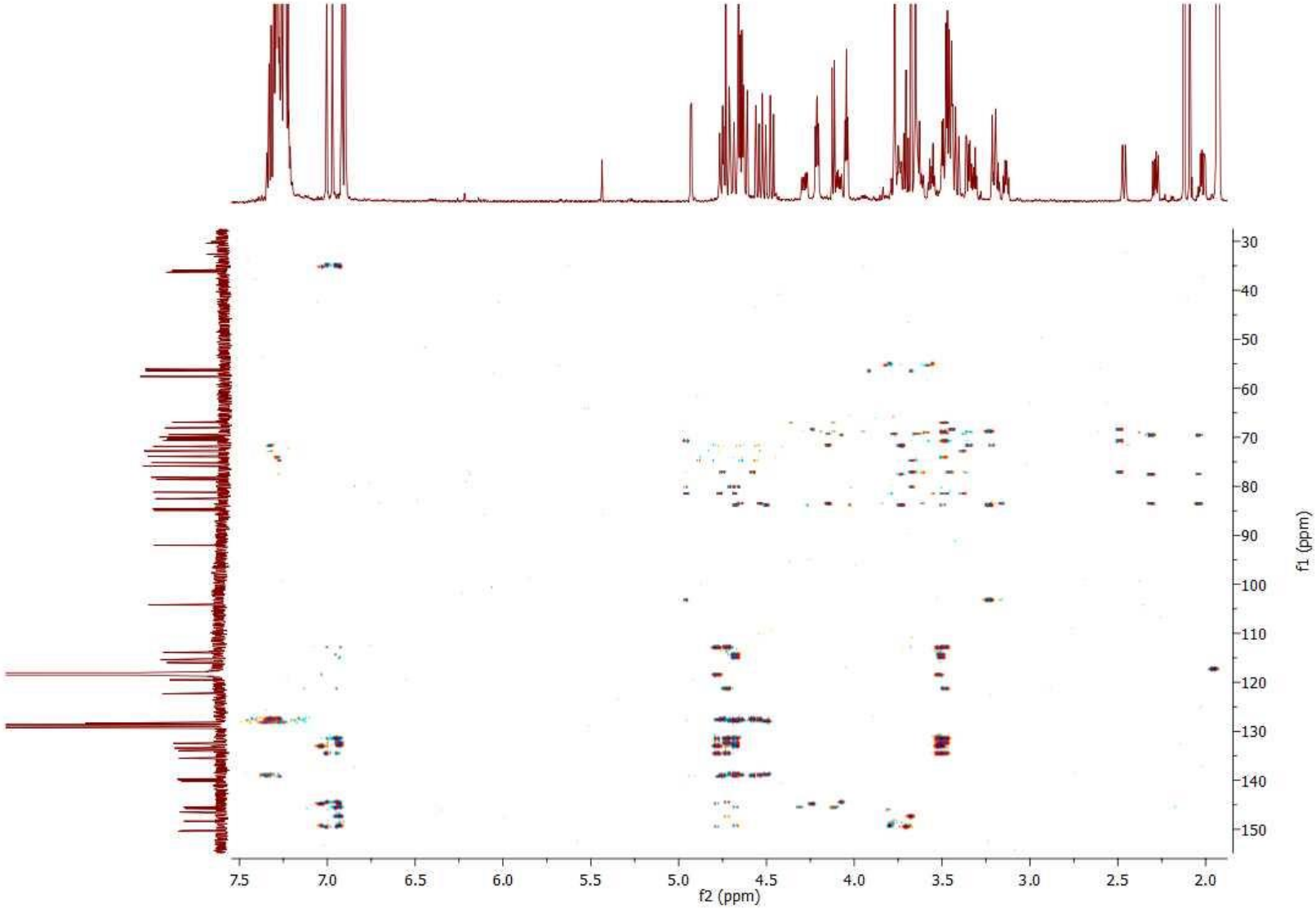


Figure S65. ^{1}H–^{13}C HMBC spectrum of compound ***P*-8**.

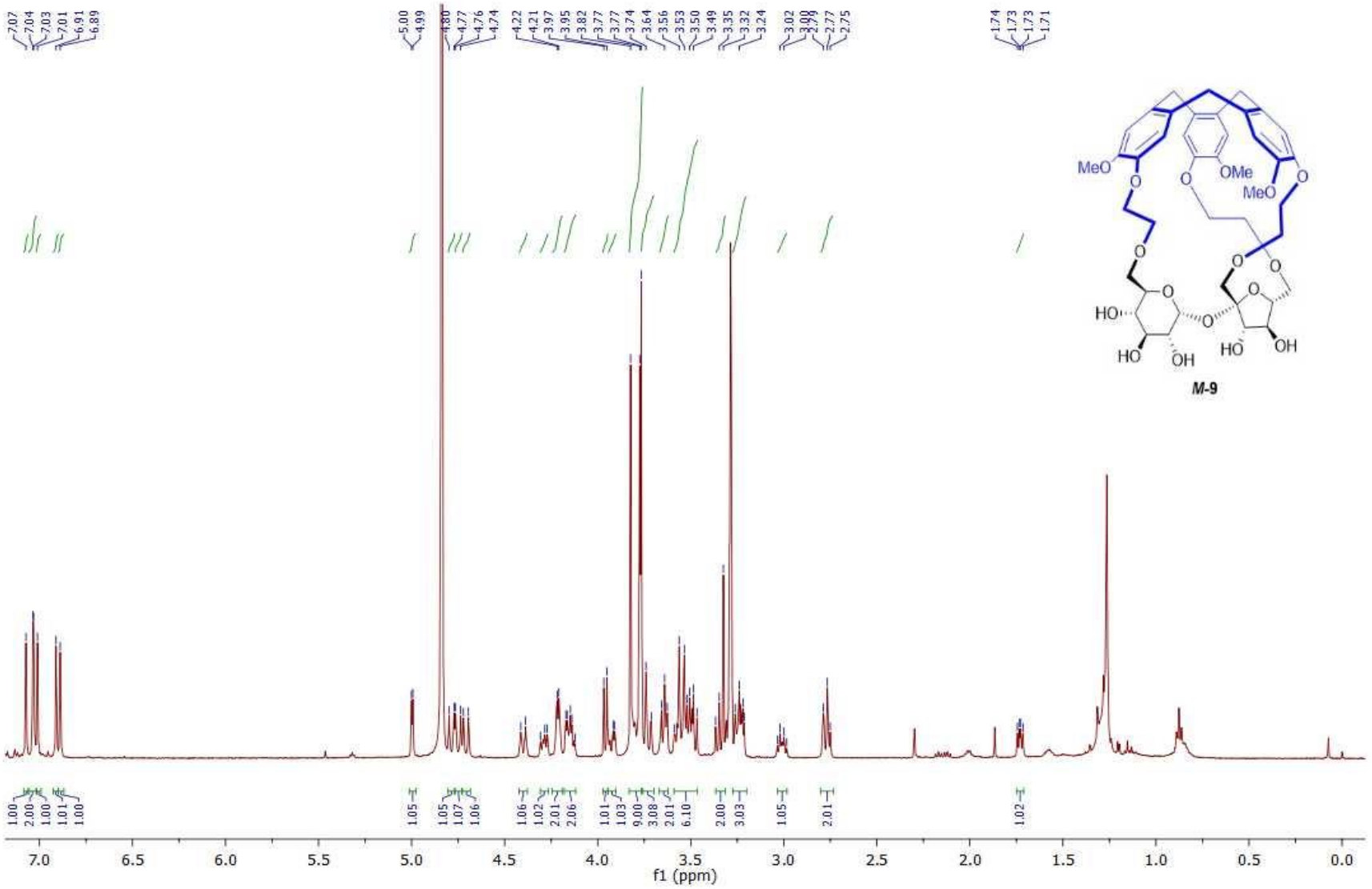


Figure S66. ^{1}H NMR spectrum of compound ***M*-9.**

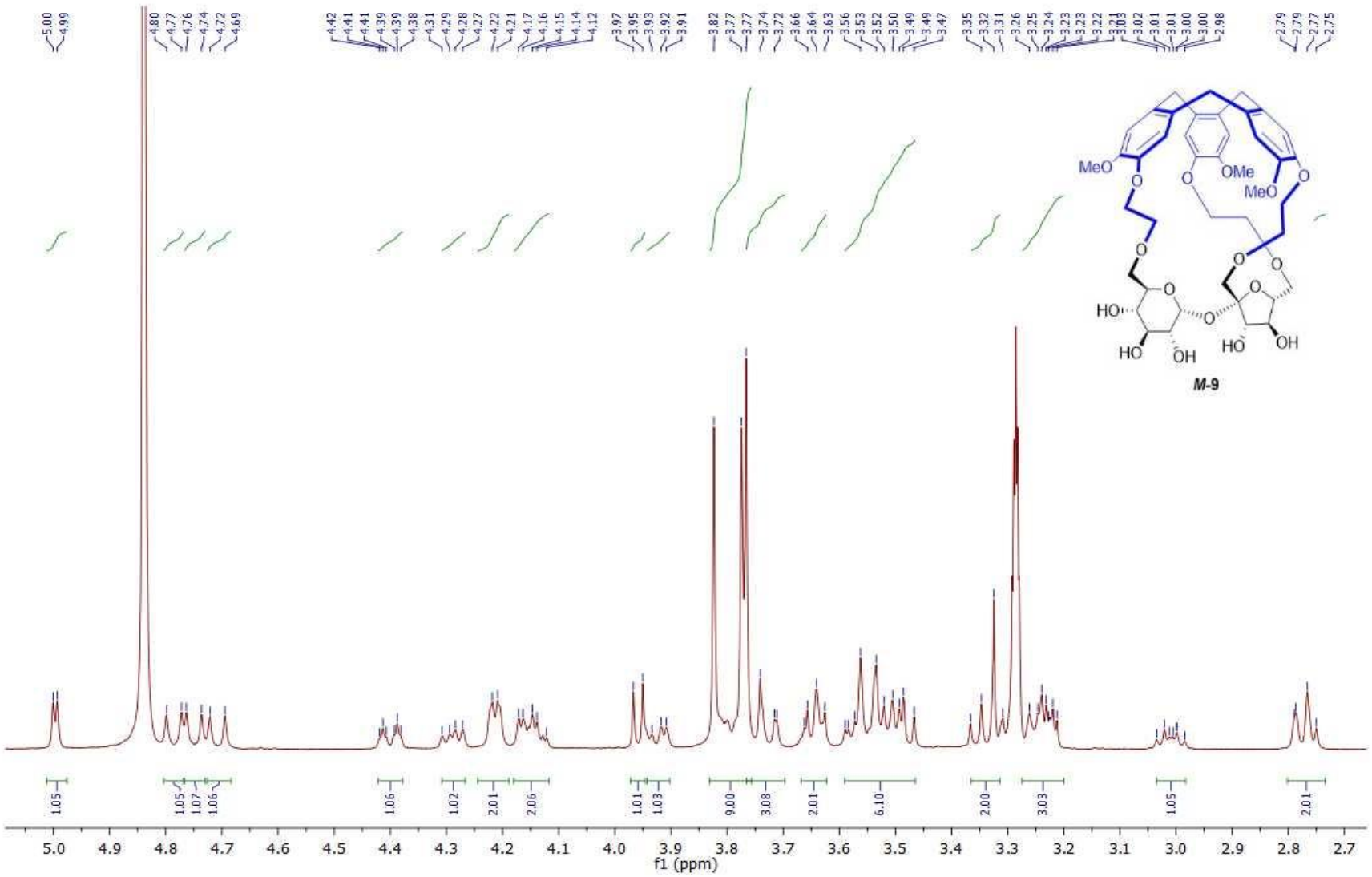


Figure S67. ^{1}H NMR spectrum of compound ***M*-9** (aliphatic part).

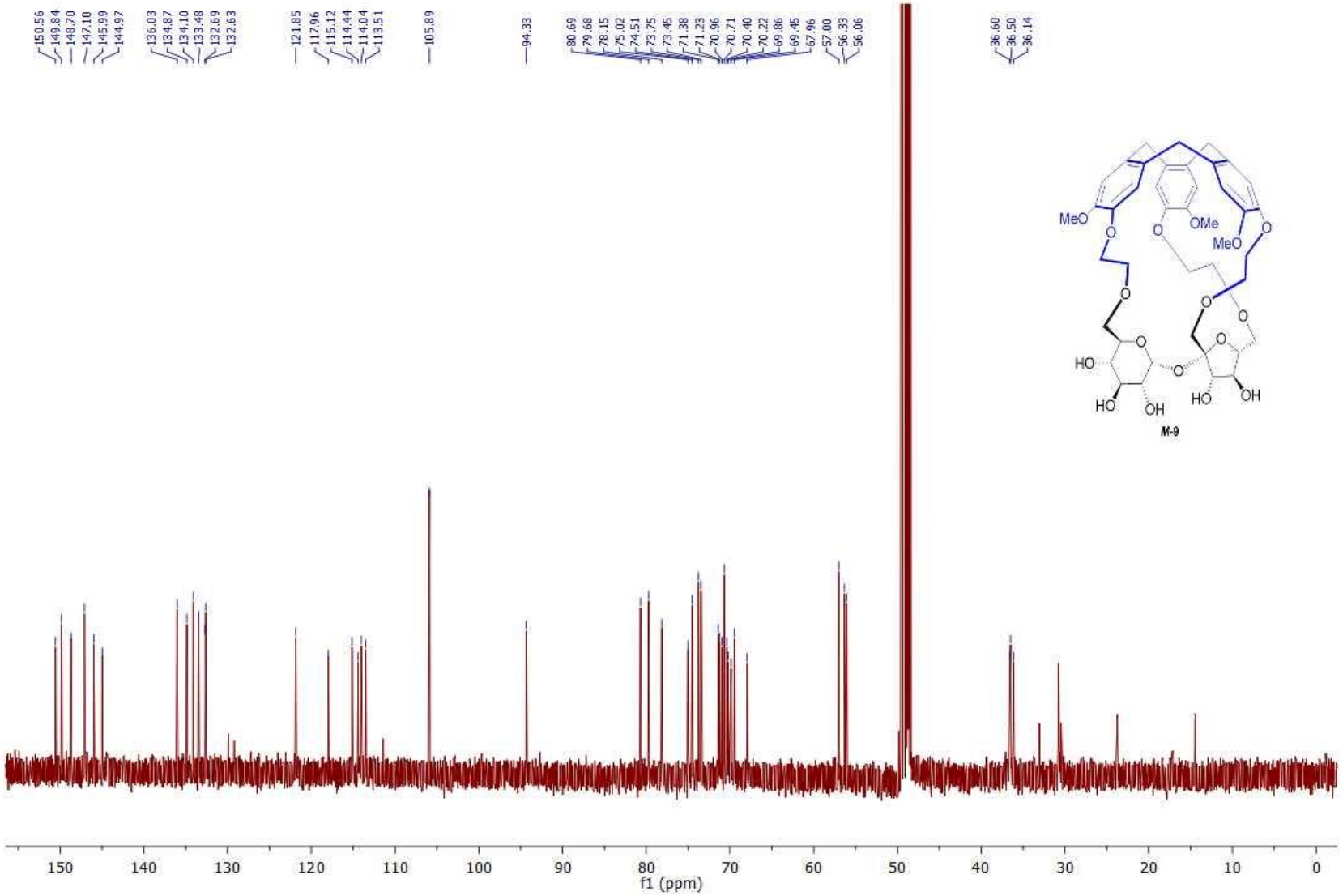


Figure S68. ^{13}C NMR spectrum of compound ***M*-9**.

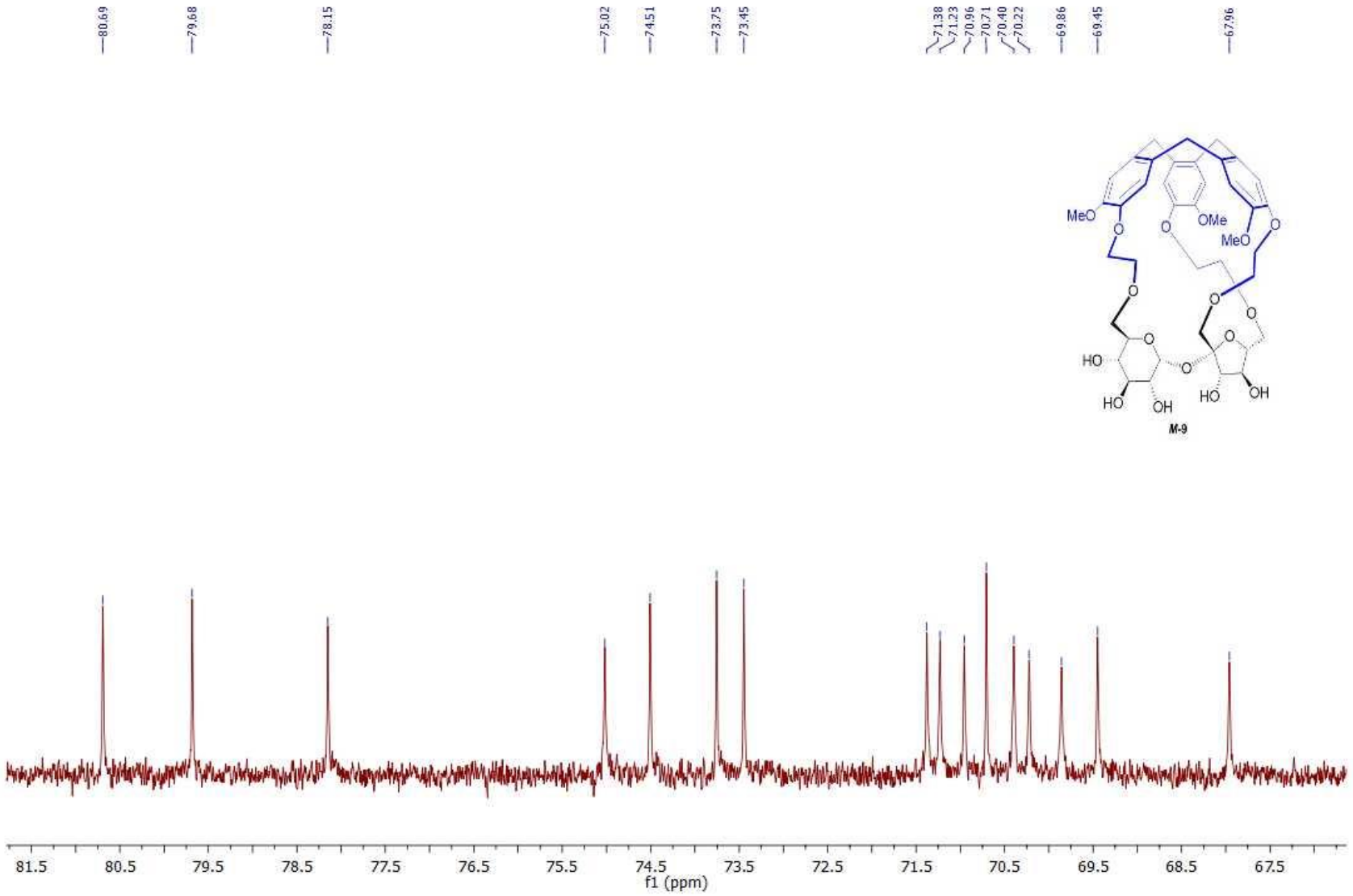


Figure S69. ^{13}C NMR spectrum of compound ***M*-9** (aliphatic part).

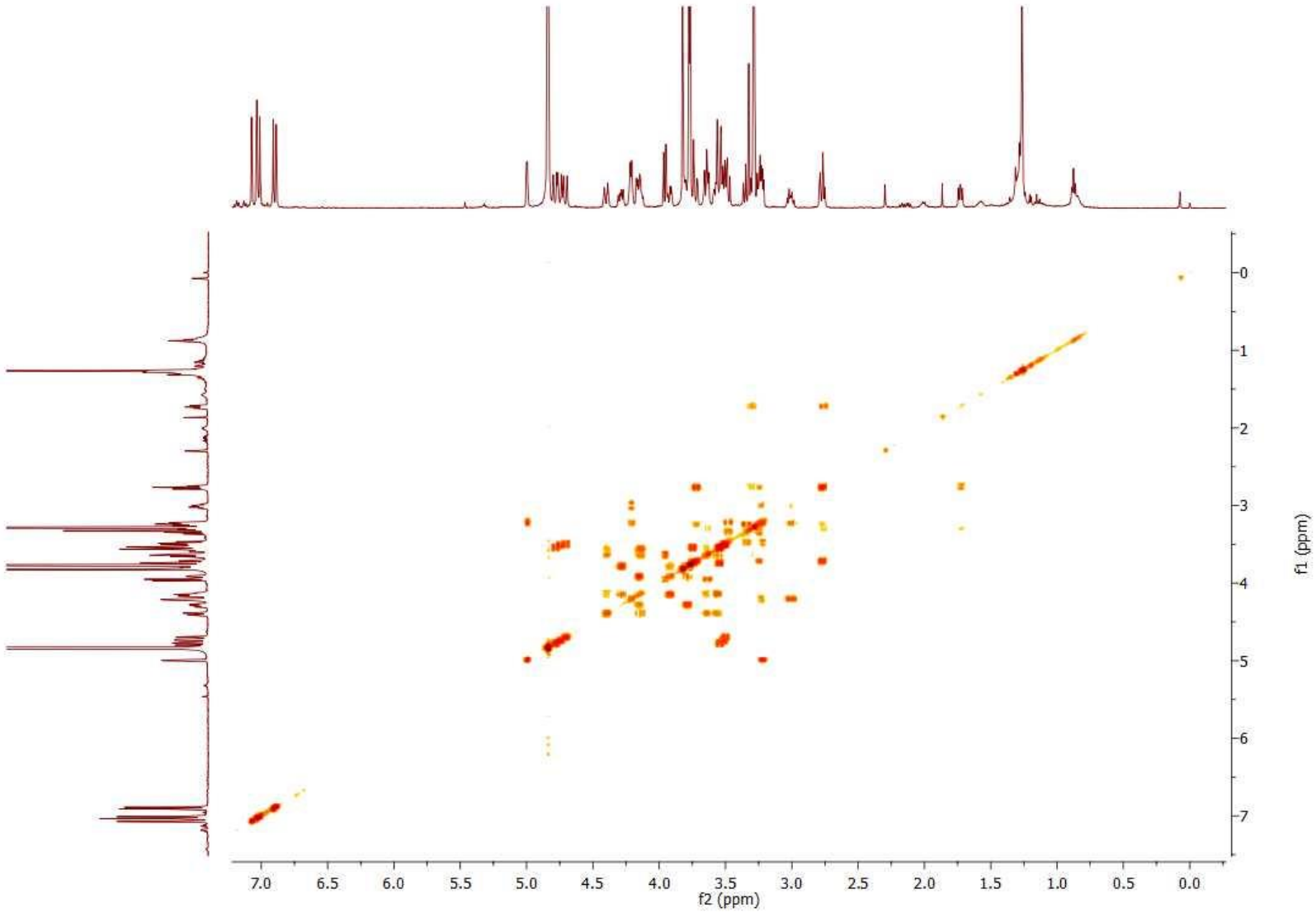


Figure S70. ^{1}H–^{1}H COSY spectrum of compound ***M*-9**.

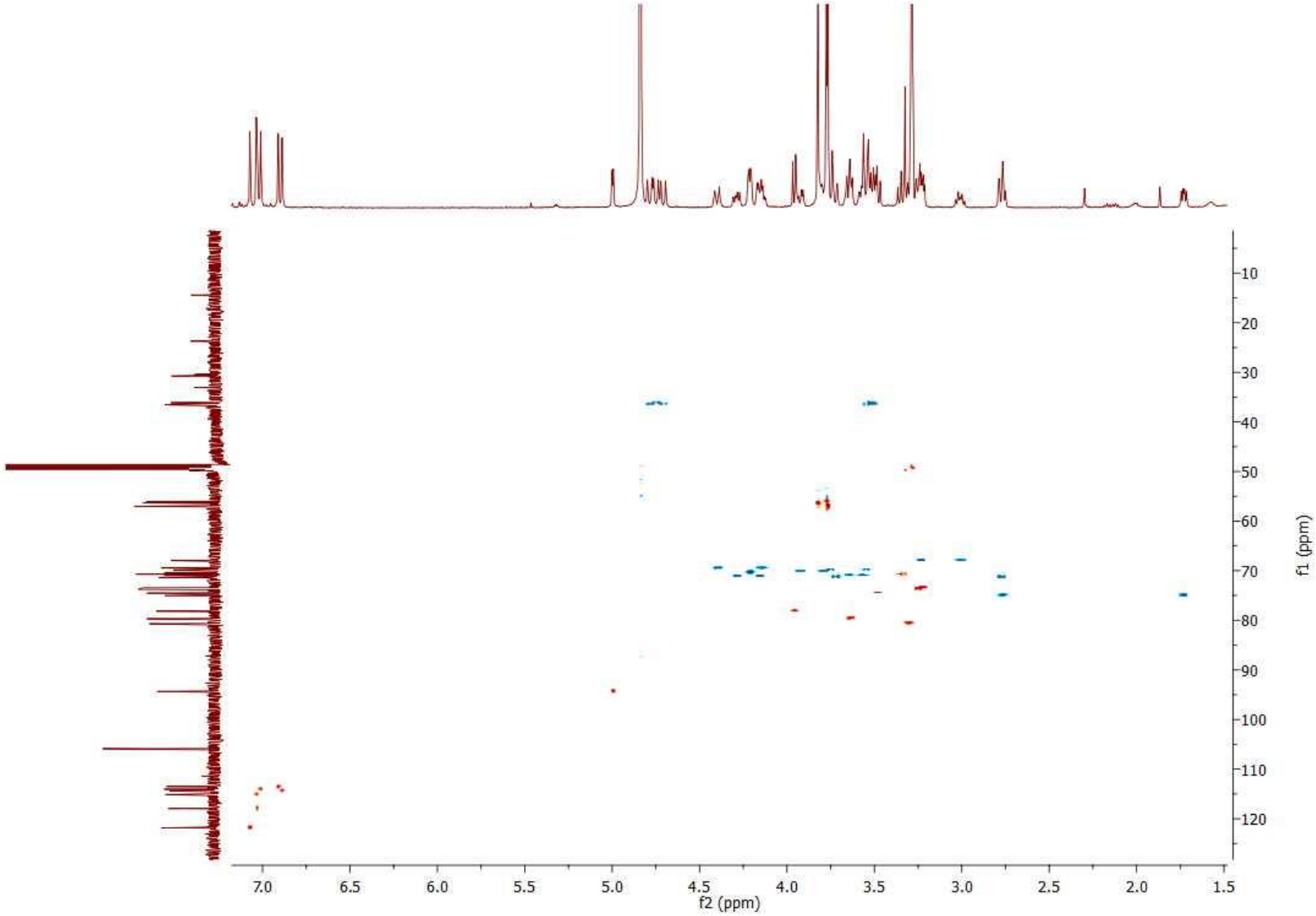


Figure S71. ^{1}H–^{13}C HSQC spectrum of compound ***M*-9**.

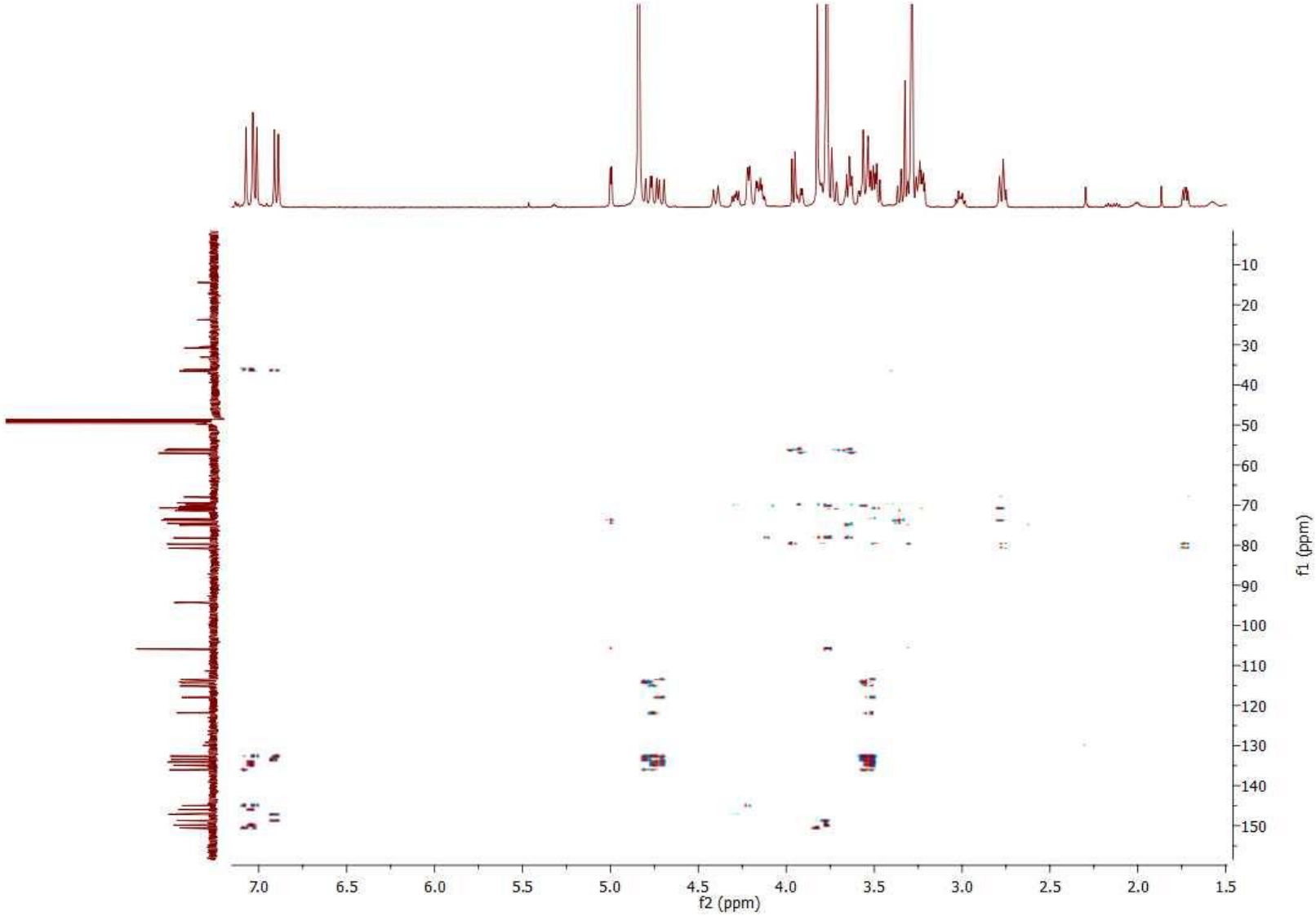


Figure S72. ^{1}H–^{13}C HMBC spectrum of compound ***M*-9**.

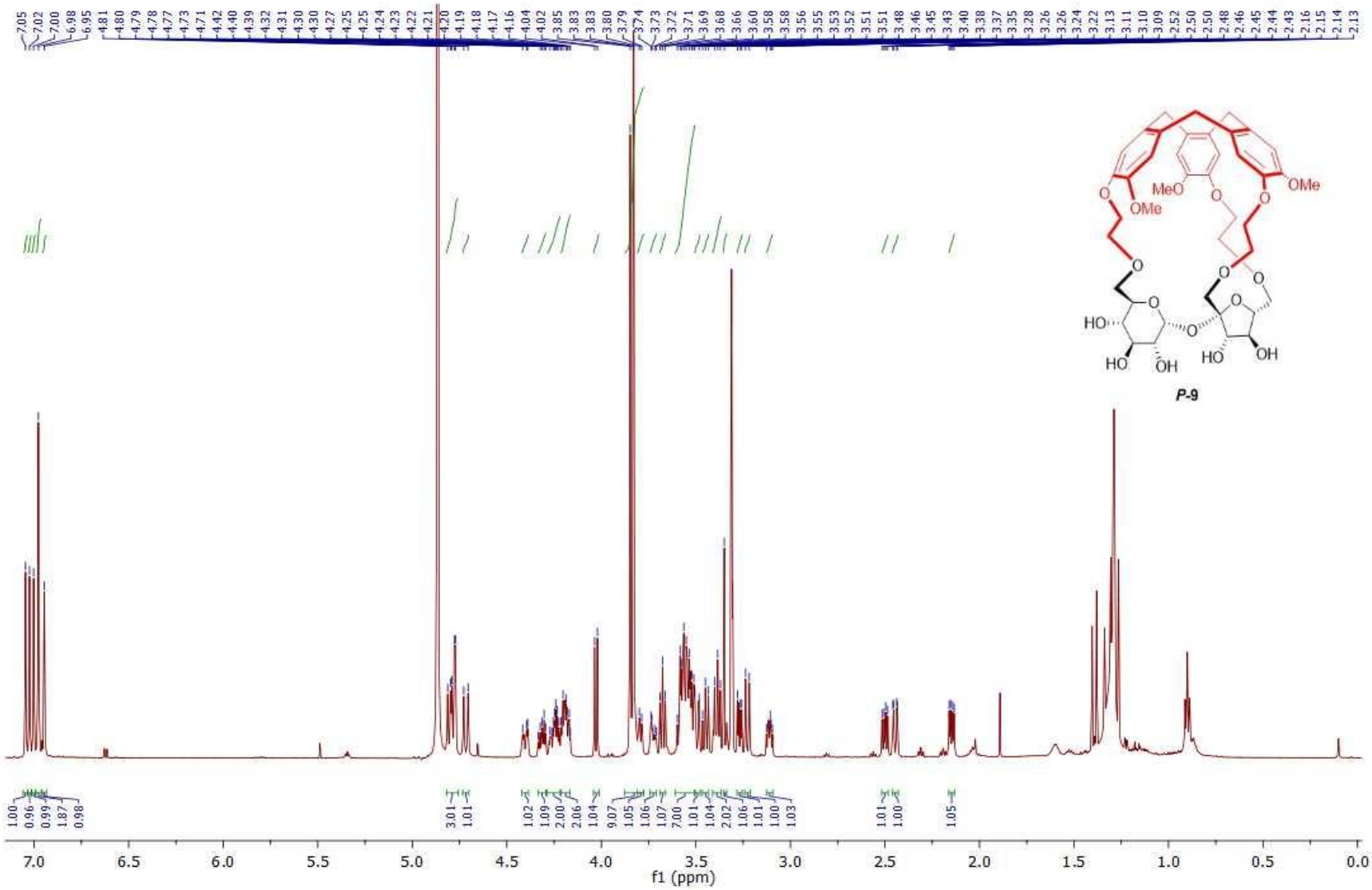


Figure S73. ^{1}H NMR spectrum of compound ***P*-9.**

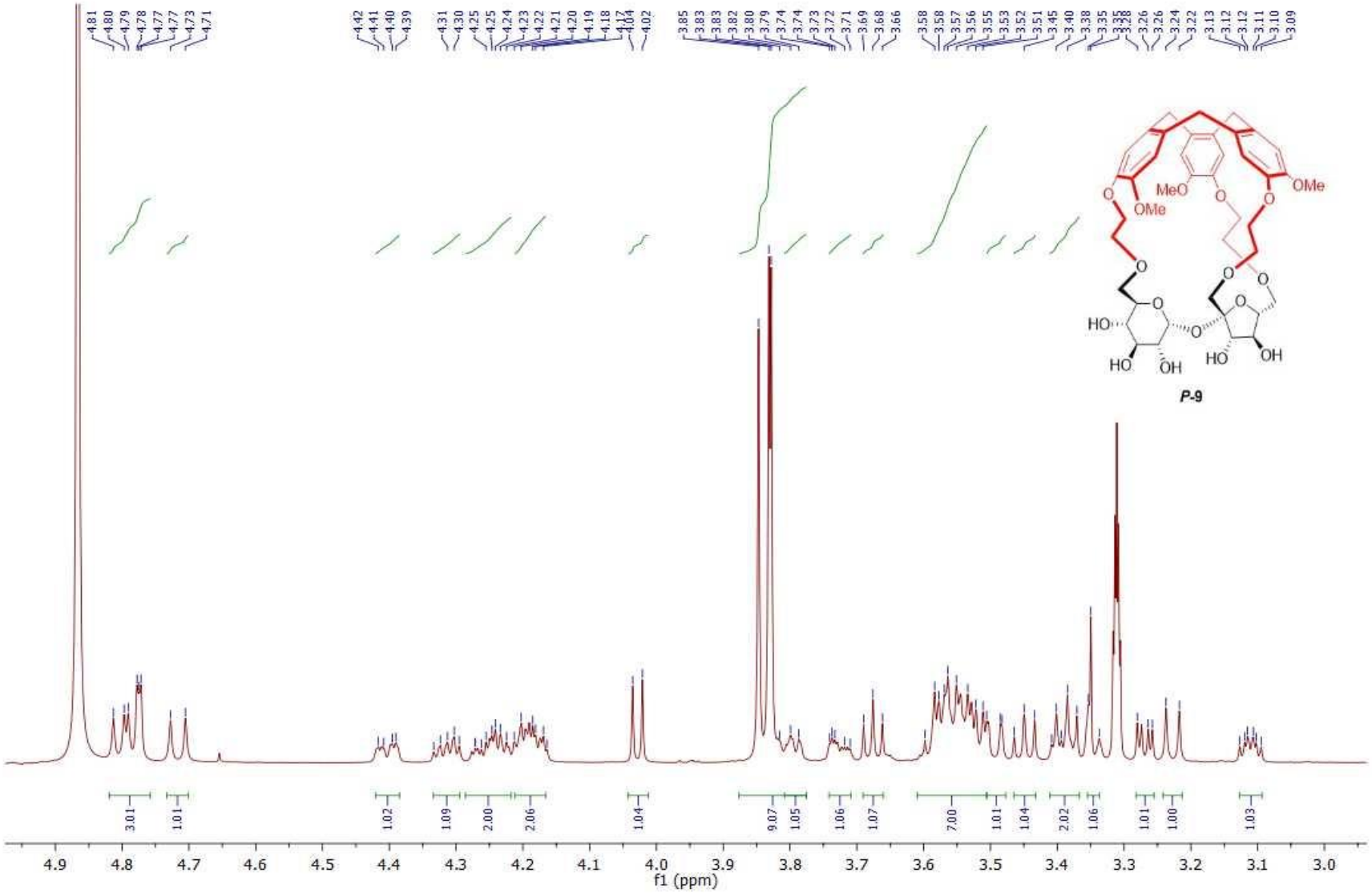


Figure S74. ^{1}H NMR spectrum of compound ***P*-9** (aliphatic part).

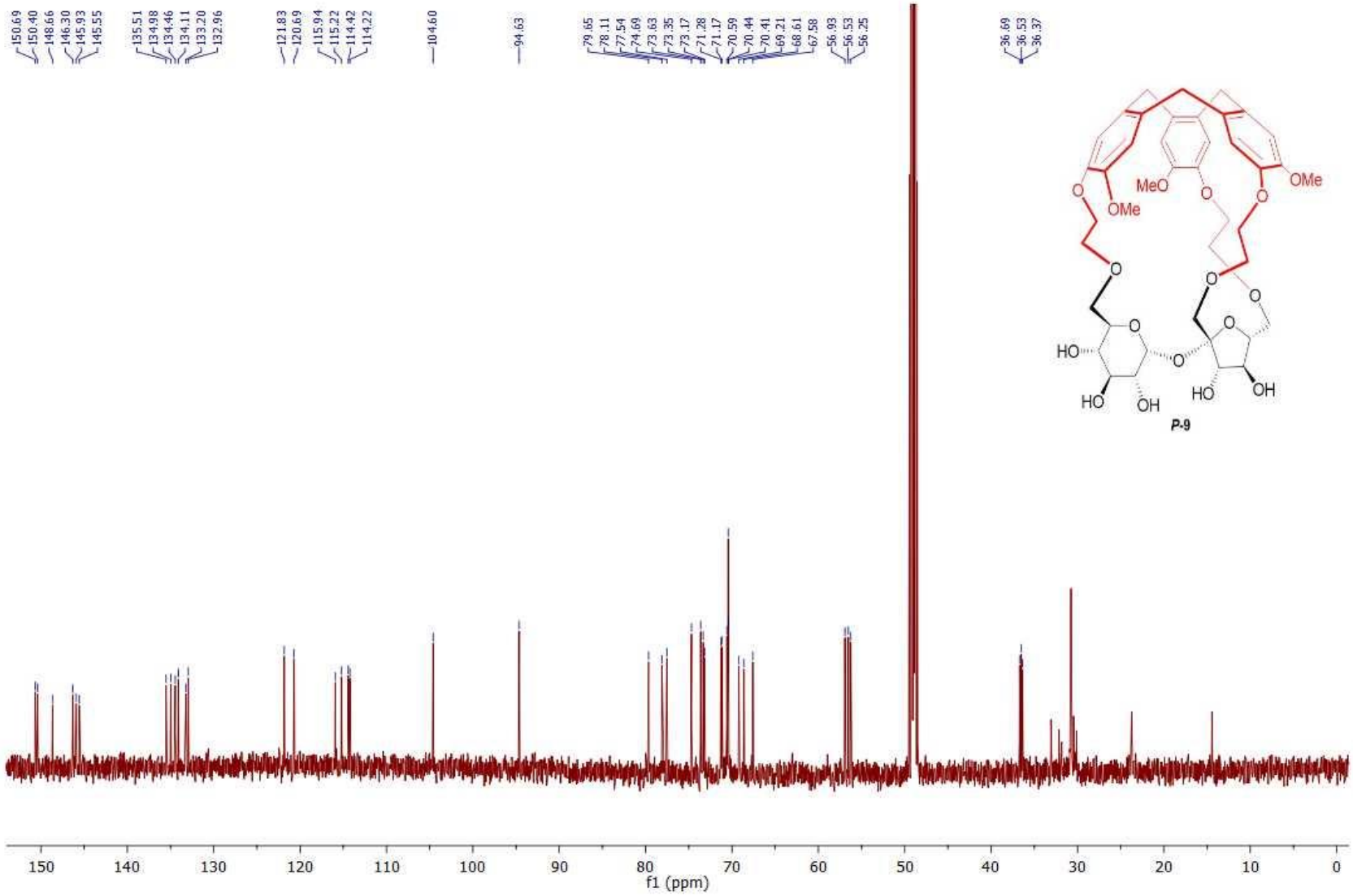


Figure S75. ^{13}C NMR spectrum of compound ***P*-9**.

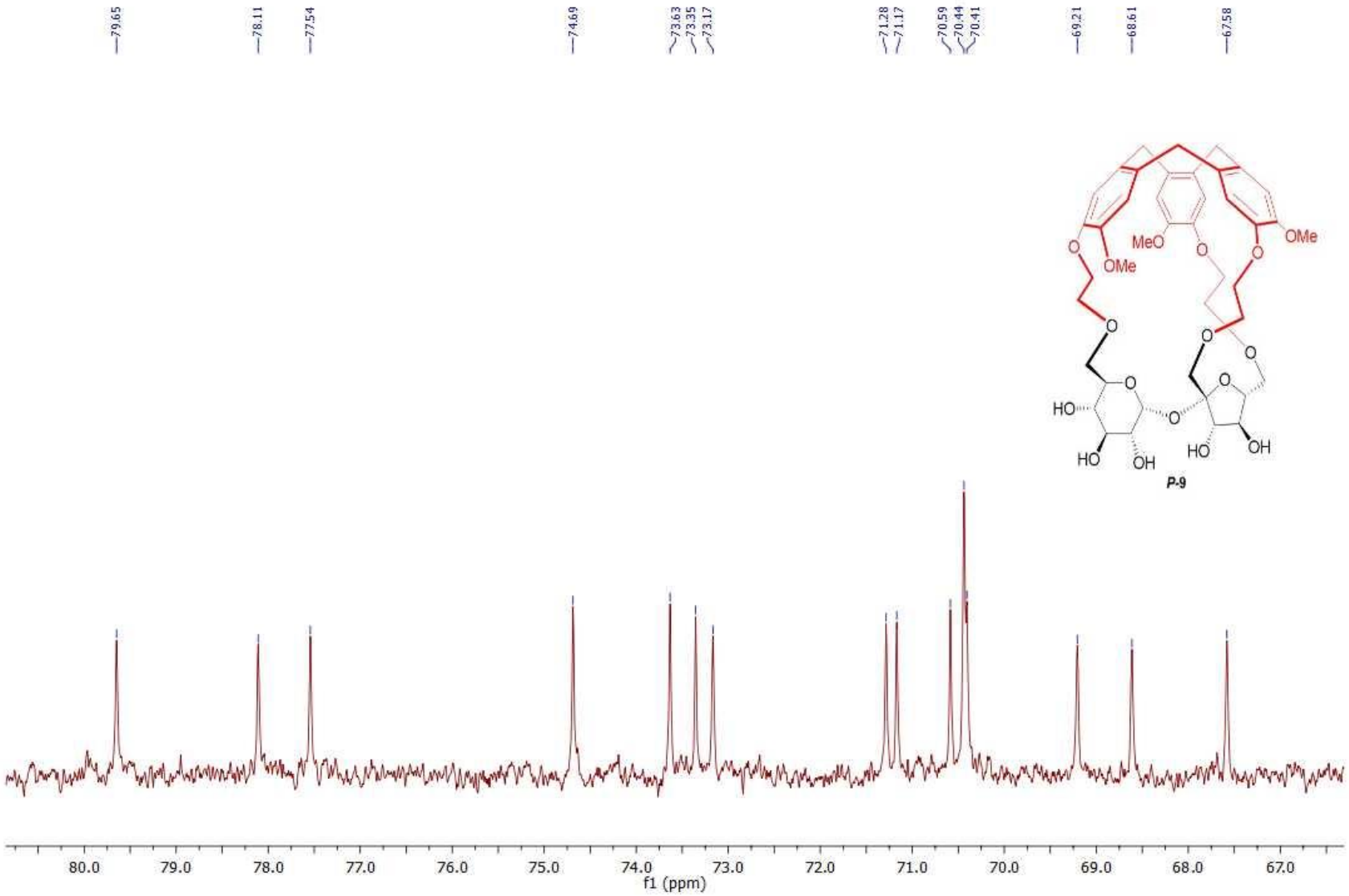


Figure S76. ^{13}C NMR spectrum of compound ***P*-9** (aliphatic part).

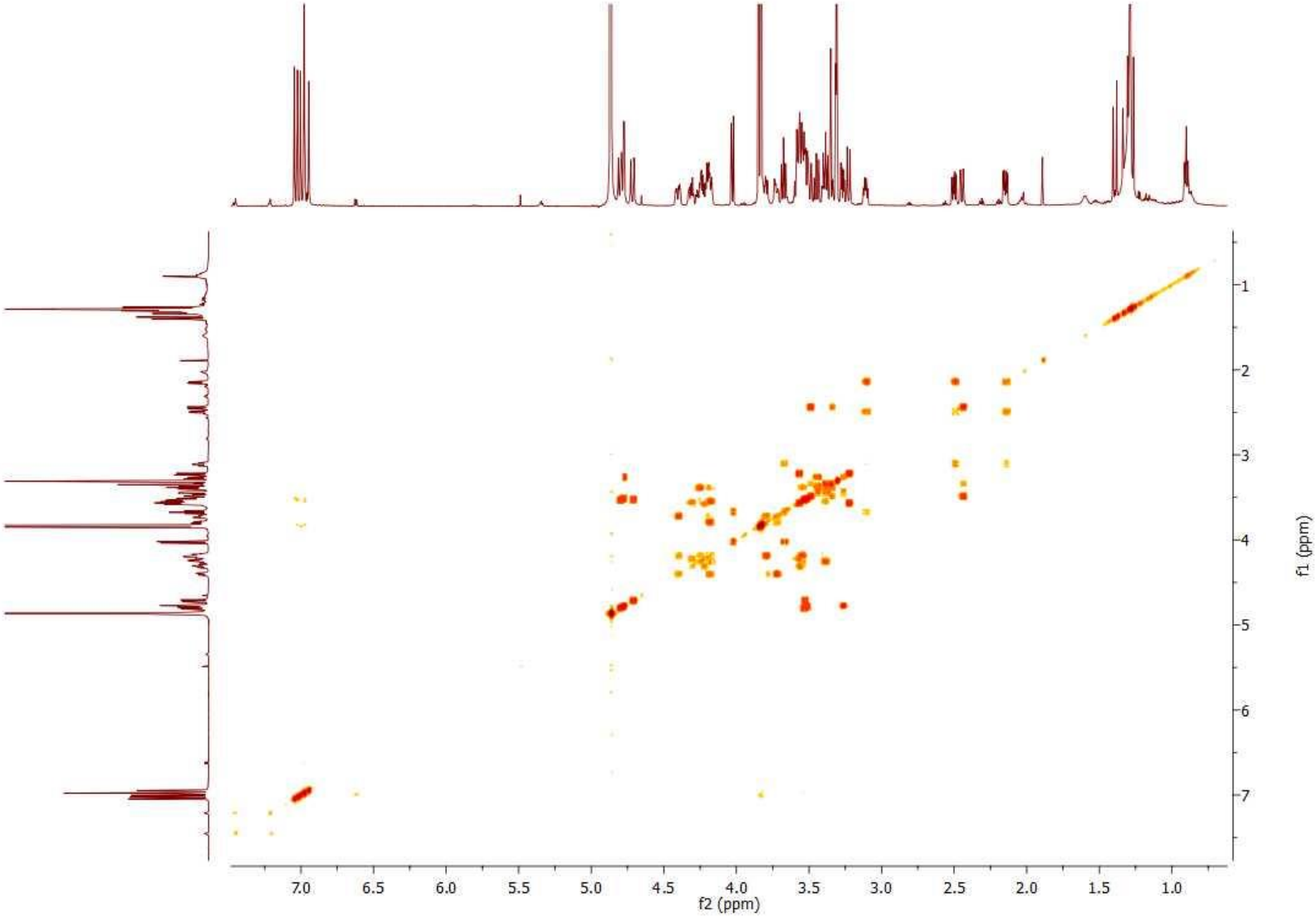


Figure S77. ^{1}H–^{1}H COSY spectrum of compound ***P*-9**.

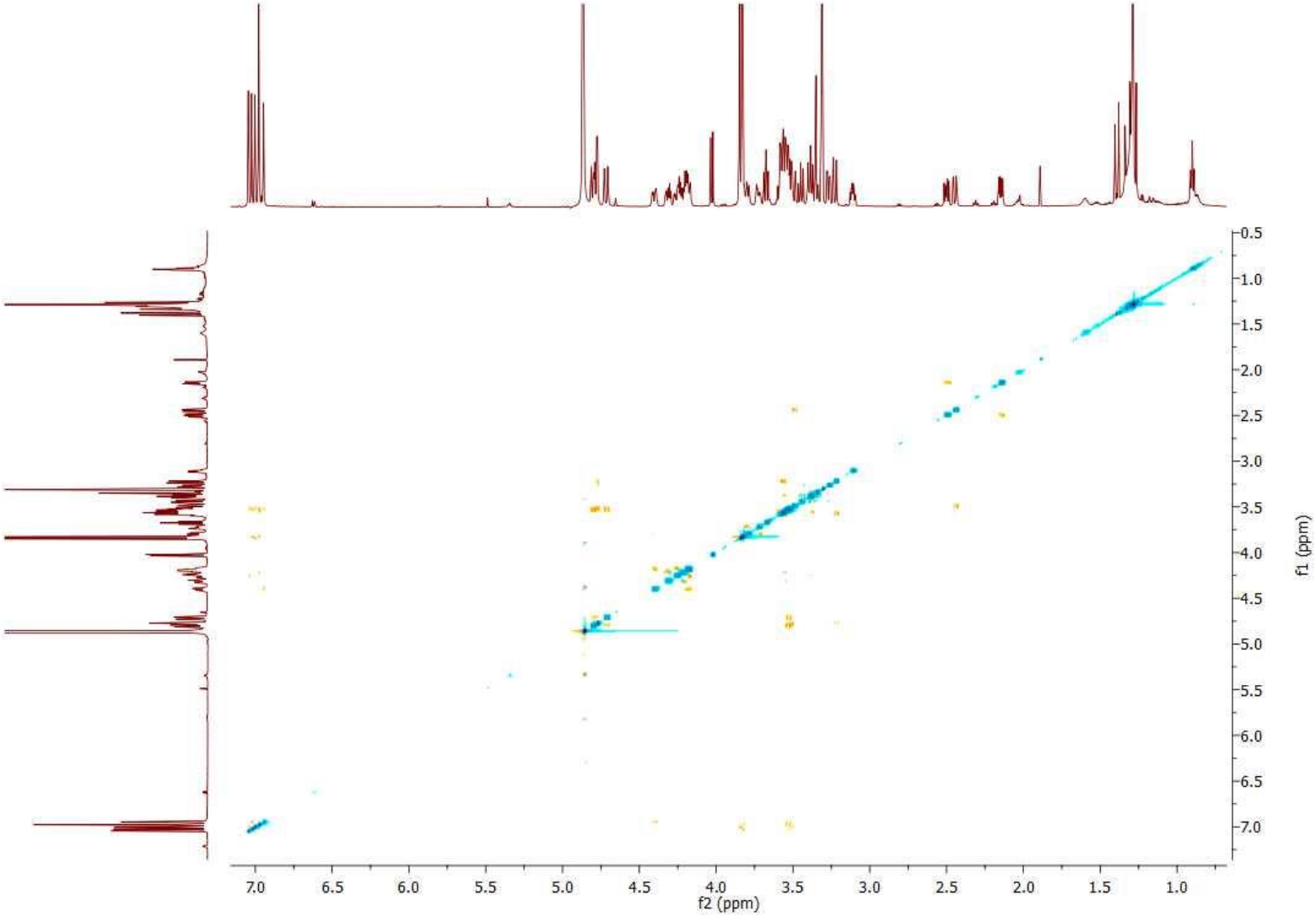


Figure S78. ^{1}H–^{1}H ROESY spectrum of compound ***P*-9**.

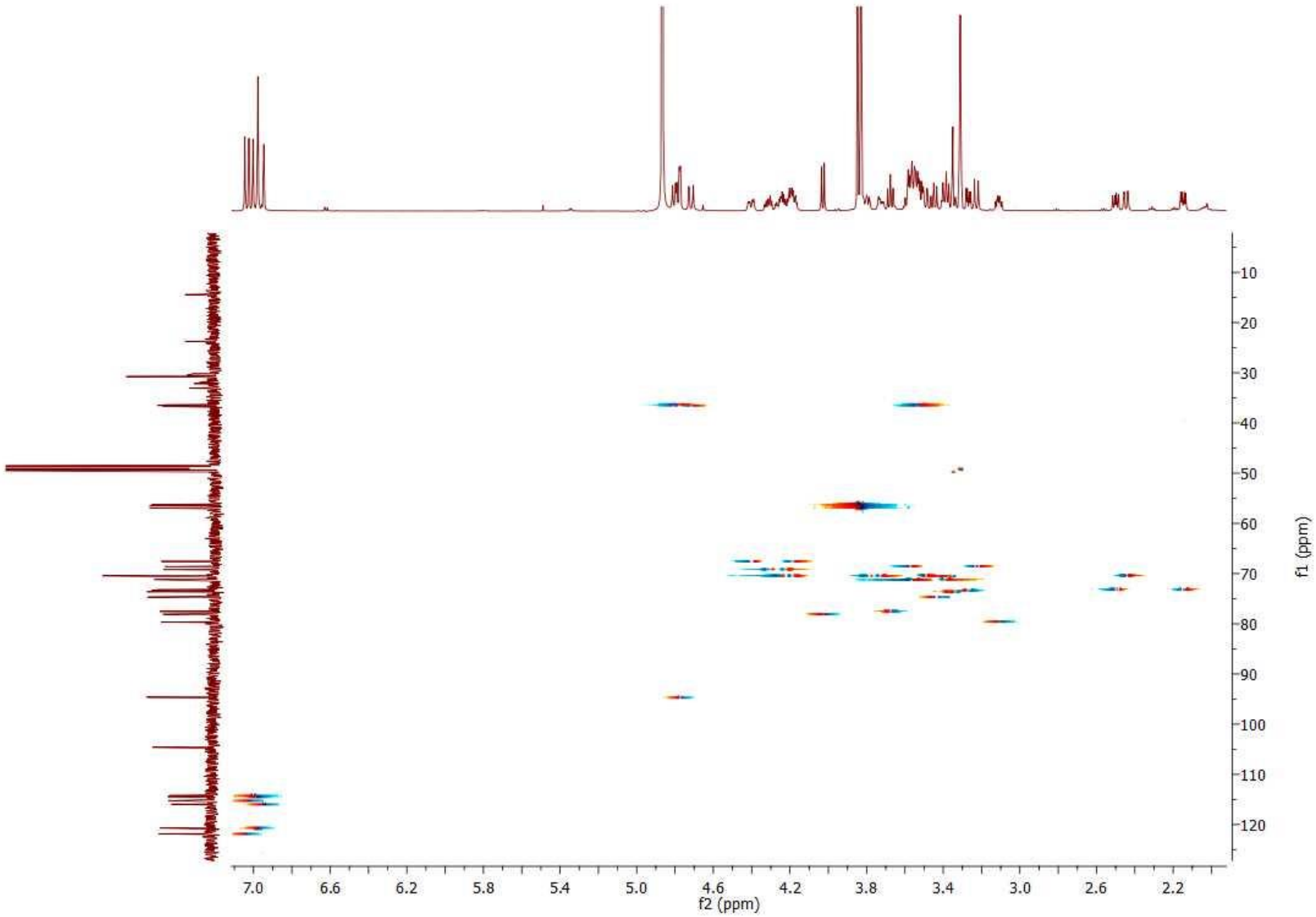


Figure S79. ^{1}H–^{13}C HSQC spectrum of compound ***P*-9**.

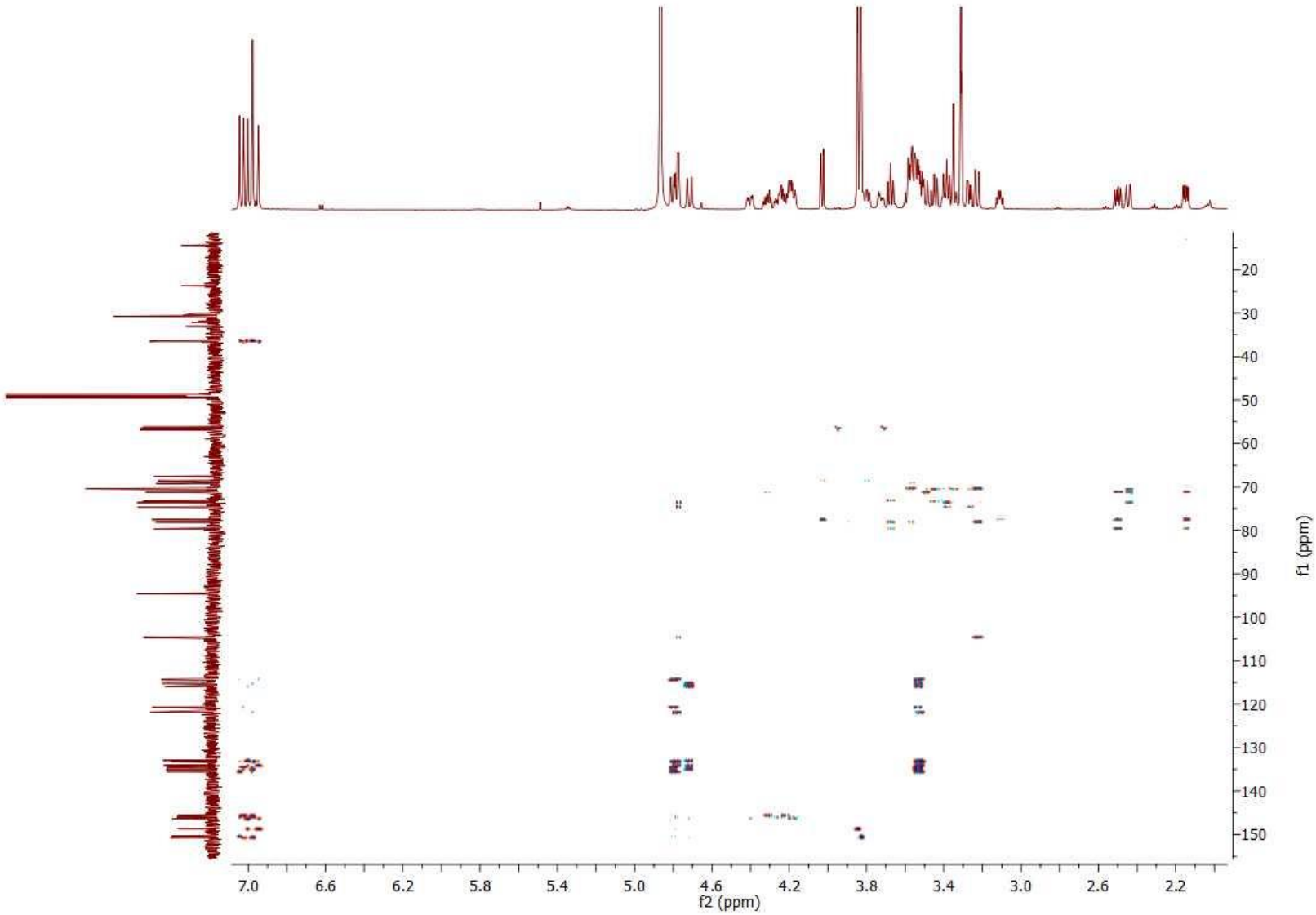


Figure S80. ^{1}H–^{13}C HMBC spectrum of compound ***P*-9**.

Elements Used:
C: 0-100 H: 0-100 O: 17-17 Na: 1-1

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	O	Na
1301.5447	1301.5450	-0.3	-0.2	36.5	C77 H82 O17 Na	296.4	n/a	n/a	77	82	17	1

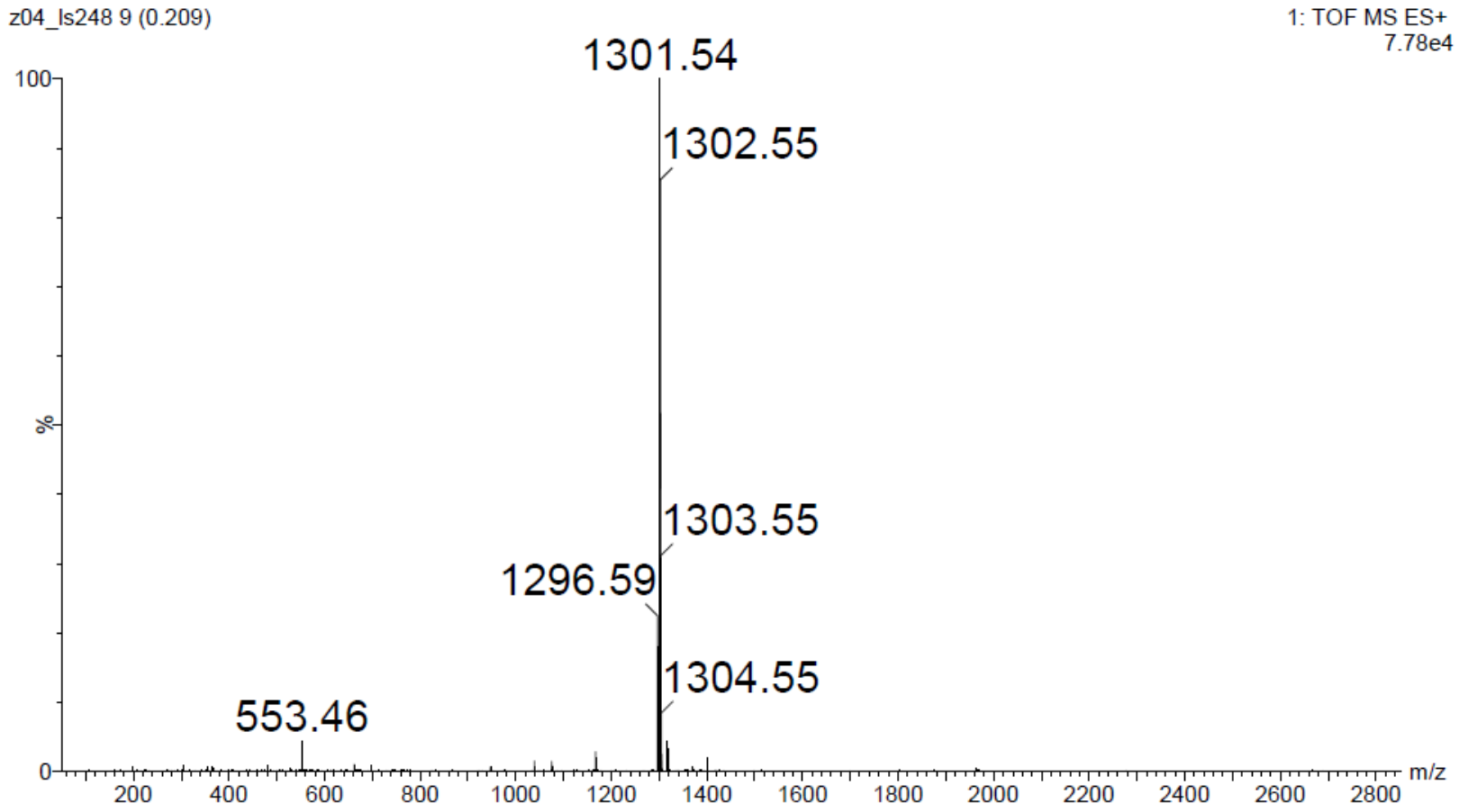


Figure S81. HRMS spectrum of compound ***M*-8**.

Elements Used:
C: 0-100 H: 0-100 O: 17-17 Na: 1-1

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	O	Na
1301.5426	1301.5450	-2.4	-1.8	36.5	C77 H82 O17 Na	315.3	n/a	n/a	77	82	17	1

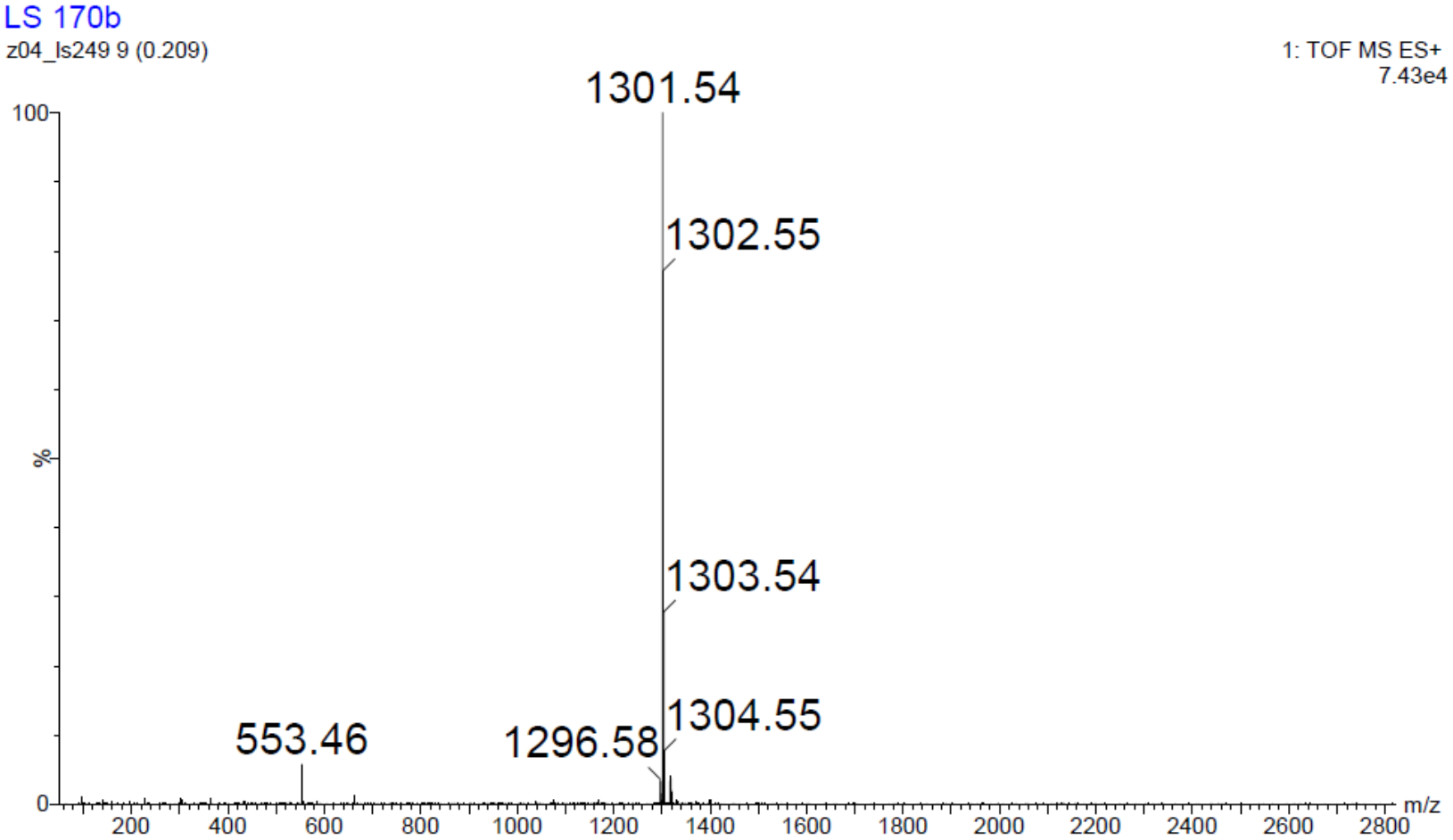


Figure S82. HRMS spectrum of compound ***P*-8**.

Elements Used:
C: 0-150 H: 0-150 O: 15-17 K: 1-1

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	O	K
867.2832	867.2842	-1.0	-1.2	16.5	C42 H52 O17 K	273.4	n/a	n/a	42	52	17	1

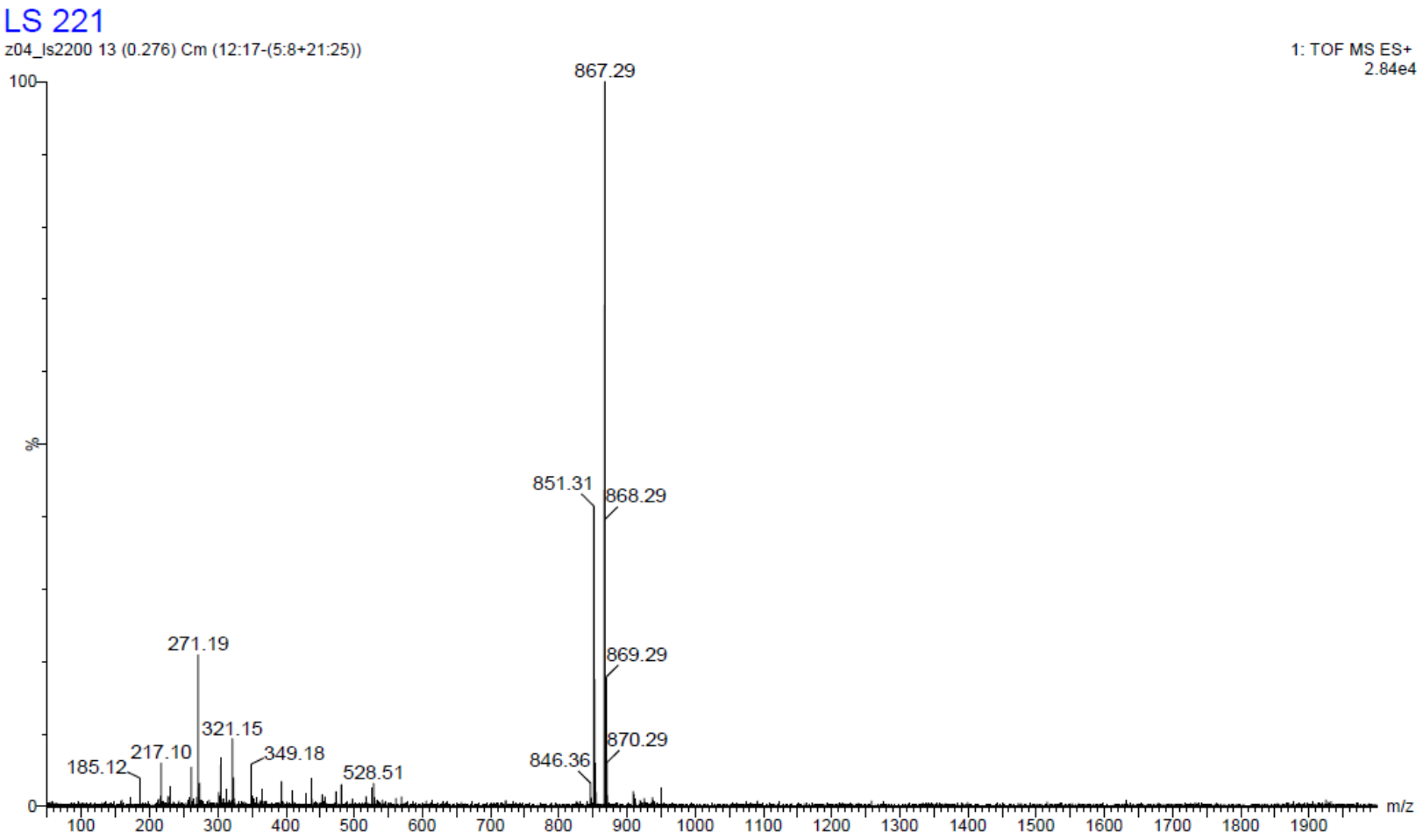


Figure S83. HRMS spectrum of compound ***M*-9**.

Elements Used:
C: 0-100 H: 0-100 O: 17-17 K: 1-1

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	O	K
867.2838	867.2842	-0.4	-0.5	16.5	C42 H52 O17 K	398.0	n/a	n/a	42	52	17	1

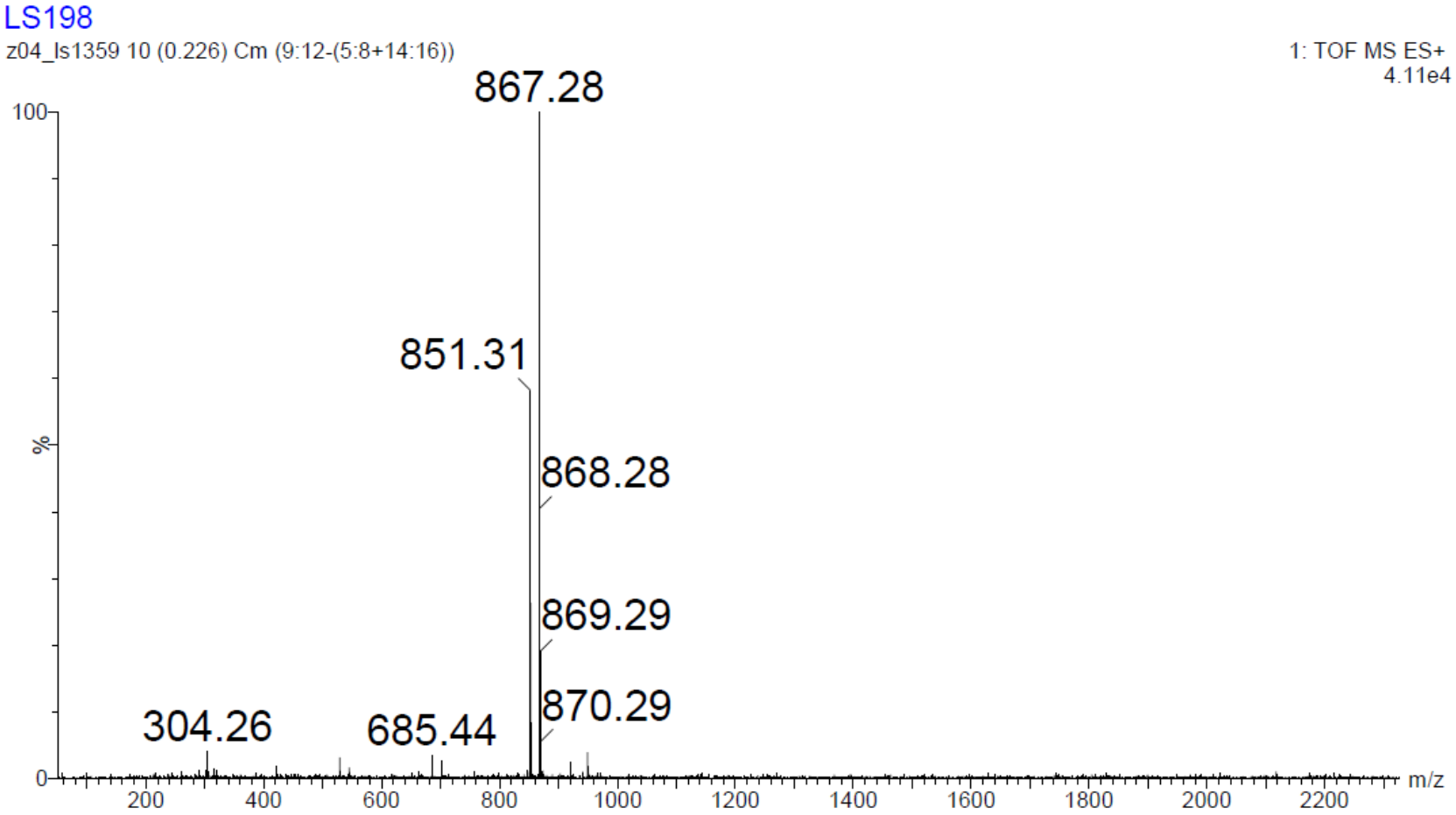


Figure S84. HRMS spectrum of compound ***P*-9**.

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