Electronic Supplementary Material (ESI) for ChemComm.
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Supporting Information

Flow-chemistry Enabled Efficient Synthesis of β-peptides: Backbone Topology vs. Helix Formation

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Contents

Experimental methods

Peptide synthesis: Foldamers **1-4** were synthesized by means of continuous-flow solid-phase peptide synthesizer (CF-SPPS) involving 9H-fluoren-9-ylmethoxycarbonyl (Fmoc) technology. The peptide chains were elongated on Tentagel R RAM resin (0.20 mmol g^{-1}) and the syntheses were carried out manually on a 0.1 mmol scale. Couplings were performed with HATU/DIPEA {HATU = [2-(7-aza-1Hbenzotriazol-1-yl]- 1,1,3,3-tetramethyluronium hexafluorophosphate, DIPEA = N,Ndiisopropylethylamine} in dimethylformamide (2 mL, DMF) at 60 bar pressure, 70 °C temperature and 0.15 mL min^{-1} flow rate. For the deprotection step; a solution mixture (2mL) contains 2% DBU and 2% piperidine dissolved in DMF was used. The formed peptide sequences were cleaved from the resin with 95% trifluoroacetic acid (TFA), and 5% H_2O at room temperature for 3 h. TFA was then removed *in vacuo*, and the peptide was precipitated in dried diethylether. The resulting free peptide was filtered off, and dissolved in 10% aqueous acetic acid, and lyophilized. The crude peptides were analysed by HPLC-MS on a Phenomenex Luna 5 µ column (4.6 mm x 250 mm). The solvent system consisted of 0.1% AcOH in water (A), and 0.1% AcOH in 80% acetonitrile (B); the gradient was 5% – 50% B during 25 min or 5% – 80% B during 35 min, at a flow rate of 1 mL min^{-1}. The analysis was performed on a Dionex HPLC equipped with a Thermo LCQ Fleet mass spectrometer.

Synthesis of oligomer 5 via continuous-flow retro-Diels-Alder (CF-rDA) reaction: Solutions of β-peptide oligomers **1-4** (50 mg) dissolved in MeOH (50 mL) were loaded, respectively, into the flow reactor (Figure 1a). The system temperature was set to 150 °C (for **2** and **4**) and 230 °C (for **1** and **3**), the pressure to 10 bar and the flow rate to 1 mL min^{-1}. When the pressure and the temperature of the flow system were stable, the solutions were passed through the heated reactor coil within a residence time of 14 min and the flow output was collected. The solvent was evaporated, and the residue was dissolved in 10% aqueous acetic acid (10mL) and subsequently lyophilized. The oligomer **5** was afforded in good yields (from **1**: 85 %; from **2**: 94 %; from **3**: 79 %; from **4**: 92 %). The full reaction parameter optimization is shown only for **2** in Figure 1b. The peptide was analysed by HPLC-MS and purified by RP-HPLC techniques, using a Luna 10 µ column (10 mm x 250 mm). The solvent system used was as follows: 0.1% TFA in water (A), 0.1% TFA in 80% acetonitrile (B); the gradient was 0%→20% B during 15 min, then 20%→50% during 60 min, at a flow

rate of 4 mL.min^{-1}, with detection at 206 nm. The flow reactor used in these experiments, was equipped with a heated 304 stainless steel tubing coil with 14 mL internal volume [Supelco premium grade 304 empty stainless steel tubing; dimensions: length (L) x outer diameter (OD) x inner diameter (ID) = 100 ft x 1/16 in x 0.03 in; product reference number: 20553] and an adjustable back-pressure regulator (ThalesNano, BPR, 0-300 bar). The tube reactor was heated in a Heraeus oven to the desired temperature, as schematized in Figure 1a.

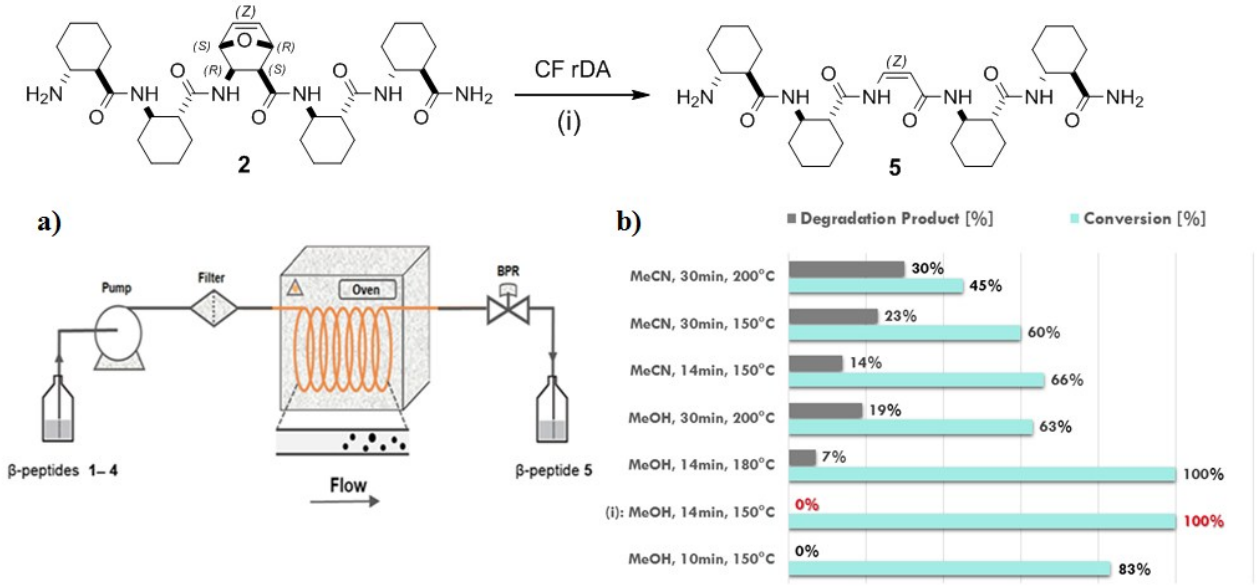
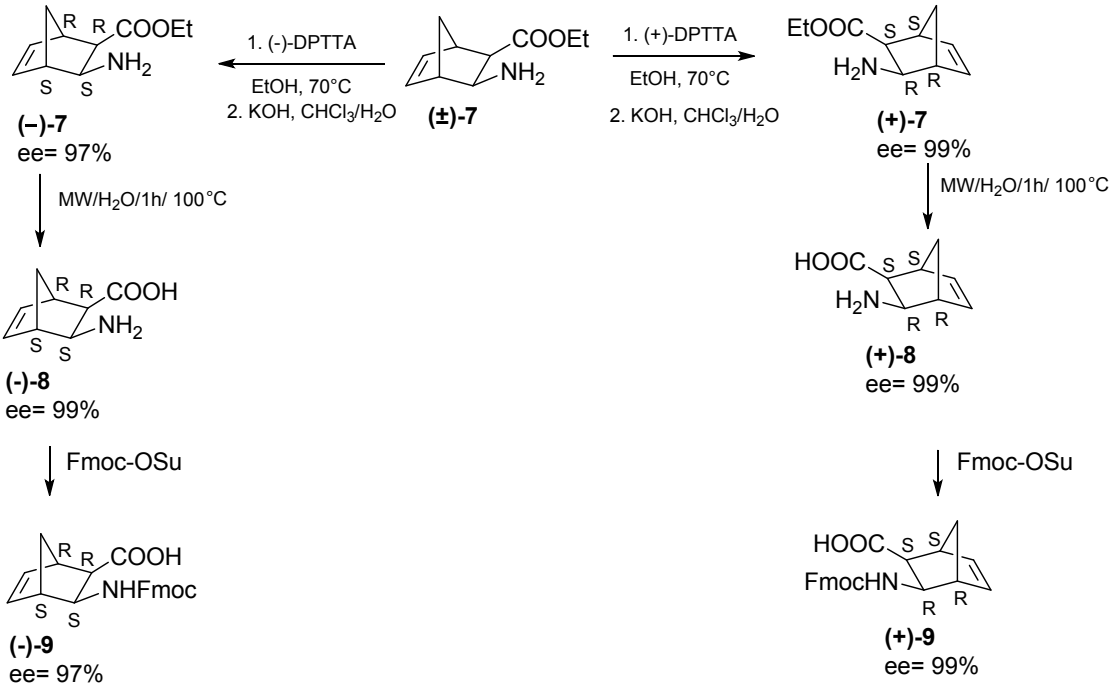


Figure S1. *Synthesis of oligomer **5**: (a) illustration of CF rDA flow reactor; (b) reaction parameter optimization for the CF rDA reaction of **2**.*

Synthesis of oligomer 6: hydrogenation reaction was performed in an H-Cube® (ThalesNano) flow reactor apparatus. The flow system was washed with MeOH for 10 min before starting the reaction. Oligomer **5** (20 mg) was dissolved in MeOH (20 mL) and saturated on a 10% Pd/charcoal catalyst, the temperature was set to 50 °C, the pressure to 50 bar with a flow rate of 1 mL min^{-1}. The flow output was collected and after evaporation of the solvent the resulting peptide was dissolved in 10% aqueous acetic acid, and lyophilized. The oligomer **6** was obtained in a good yield (95%). The peptide **6** was analysed by HPLC-MS and the purity was determined by HPLC analysis.

Synthesis of Fmoc-*diexo*-ABHEC enantiomers: Fmoc protected *diexo*-3-aminobicyclo[2.2.1]hept-5-ene-2-carboxylic acid (Fmoc-*diexo*-ABHEC) **(–)-9** and **(+)-9** were synthesized started from the enantiomeric esters **(–)-7** and **(+)-7**, as illustrated in Scheme 1. The starting enantiomeric esters **(–)-7** and **(+)-7** were obtained from the racemic esters **(±)-7** by diastereomeric salt formation with *O*,*O'*-di-*p*-toluoyl-tartaric

acid (DPTTA), as previously described.[1] The enantiomeric amino esters **(–)-7** (ee >97%) and **(+)-7** (ee >99%) were hydrolyzed with water under microwave irradiation to furnish amino acids **(–)-8** and **(+)-8**, which were then reacted with (Fluorenylmethoxycarbonyl)hydroxysuccinimide ester (Fmoc OSu), affording the *N*-Fmoc-protected amino acids **(–)-9** and **(+)-9** in high yields.



Scheme S1. Synthesis of the enantiomeric Fmoc-*diexo*-ABHEC **(–)-9** and **(+)-9**

Melting points of synthesized compounds were measured with a Hinotex-X4 micro melting point apparatus and are uncorrected, **(–)-9** white crystals (72 % yield) m.p. 98–100 °C, **(+)-9** white crystals (68 % yield) m.p. 99–101 °C. Optical rotations for **(–)-9** and **(+)-9** were recorded with a Perkin-Elmer 341 polarimeter. **(–)-9**, $[\alpha]_D^{20}$ = –26.1 (c = 1, EtOH); **(+)-9**, $[\alpha]_D^{20}$ = +26.1. The corresponding *ee* values, after derivatization with diazomethane/MeOH, were 97 % **[(–)-9]** and 99 % **[(+)-9]**. Analysis of these compounds was carried out using an HPLC instrument equipped with a Phenomenex IA column with a solvent mixture of *n*-hexane/*i*PrOH, 80:20, flow rate 0.3 mL min^{-1}, detection at 254 nm; for **(–)-9**: t_R = 32.70 min (antipode: 33.75 min) and, for **(+)-9**: t_R = 33.75 min (antipode: 32.70 min).

HPLC method separation of diatoremeric β-peptides 2 and 4 containing racemic *diexo*-AOBHEC units: The peptide was analysed by HPLC-MS and

separated by RP-HPLC techniques, using a Luna 10 µ column (10 mm x 250 mm). The solvent system used was as follows: 0.1% TFA in water (A), 0.1% TFA in 80% acetonitrile (B); the gradient was 0%→20% B during 15 min, then 20%→50% during 60 min, at a flow rate of 4 mL.min^{-1}, with detection at 206 nm.

NMR experiments and signal assignments: NMR spectra were recorded at 298 K on Bruker Avance DRX 600 MHz and Avance III 500 MHz spectrometers. Samples in 4 mmol concentration were dissolved in 0.5 ml CD_3OH, DMSO-d_6, and water (H_2O/D_2O 90:10) and transferred to 5 mm NMR sample tubes. Chemical shifts are given on the δ-scale and referenced to the solvent signal. Pulse programs of all experiments (^1H, 2D-TOCSY, 2D-ROESY) were taken from Bruker software library. 2D-TOCSY experiments were taken with 80 or 120 ms mixing time, 32 scans and 2K x 256 (t_2 x t_1) data points. 2D ROESY experiments were acquired with 300 or 400 ms mixing time, 32 scans and 2K x 256 (t_2 x t_1) data points. The processing was carried out by using a cosine-bell window function, single zero filling and automatic baseline correction.

CD measurements: CD spectra were measured on a Jasco J-1500 spectropolarimeter at room temperature in a 0.1 cm cylindrical quartz cell. Three spectra were accumulated for each sample. CD curves were corrected by the spectral contribution of the blank solvent. The concentration of the sample solutions was 1 mM in CH_3OH and H_2O. Molar circular dichroism is given in M^{-1} cm^{-1}. The data were normalized for the number of chromophores.

***Ab initio* calculations:** All calculations were performed with the Gaussian16 program package[2] using the M06-2x functional[3] in combination with cc-tvz basis set[4,5]. For implicit water calculations the default PCM model was applied [6] and the original convergence criteria were kept during geometrical optimization. Considering the protonation state of the pentamers the amino group at the *N*-terminal was always protonated during the calculations.

Figure S2. NH–ND exchange plots for **1** (a), **2** (b), **6** (c) in CD_3OD. ■: NH_2; ○:NH_3; ▲: NH_4; ◊: NH_5; *: NH_4+NH_5.

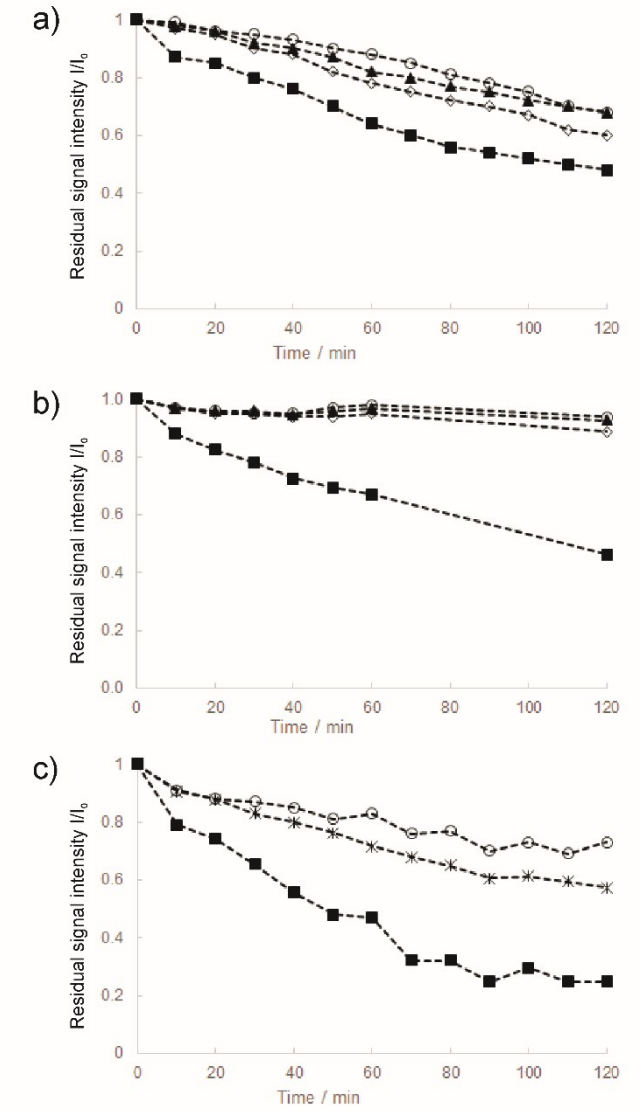


Figure S3. ECD spectra of 1 mM solutions of 1-6 in water (a,b) and methanol (c,d).

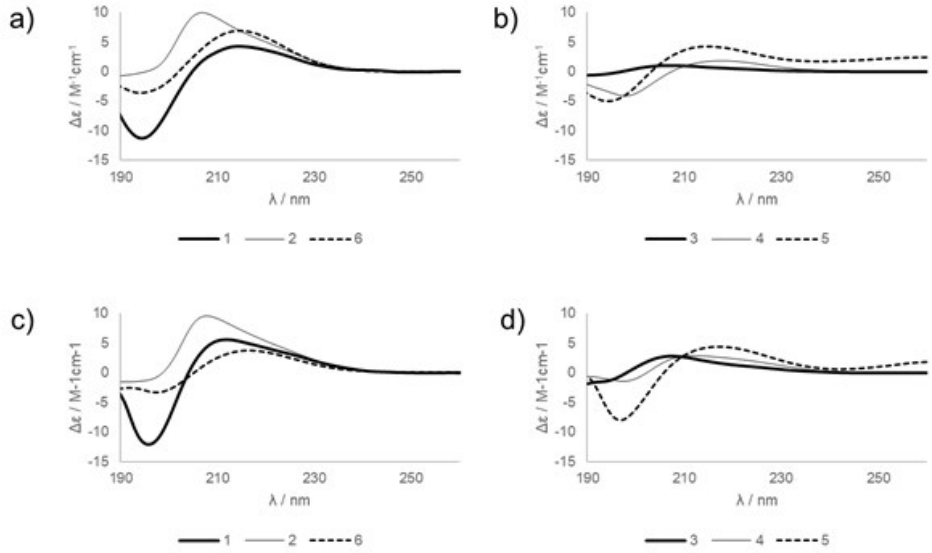


Table S1. Total energies (in Hartree) of compound **1-4** optimized at M062x/cc-tzv level of theory in implicit solvent and vacuum.

	1 [1*R*,2*R*,3*S*,4*S*]	**3** [1*S*,2*S*,3*R*,4*R*]	**2** [1*R*,2*S*,3*R*,4*S*]	**4** [1*S*,2*R*,3*S*,4*R*]
	-ABHEC		-AOBHEC	
implicit solvent	-2110.73898	-2110.72979	-2146.65102	-2146.64546
vacuum	-2110.66906	-2110.65979	-2146.58150	-2146.57485

Table S2. Optimized bond lengths (in Å) of compound **5** and **6** at M062x/cc-tzv level implicit solvent calculations. The values in parenthesis are the results of the vacuum calculations.

Compound	$(CO)_3 - (NH)_4$			
	$(CO)_2 - (NH)_3$	$(CO)_3 - (NH)_4$	$(NH)_3 - C_{\beta 3}$	$C_{\alpha 3} - (CO)_3$
5	1.38 (1.39)	1.35 (1.34)	1.37 (1.37)	1.47 (1.48)
6	1.34 (1.35)	1.34 (1.34)	1.45 (1.45)	1.51 (1.51)

Characterization data

Figure S4. ^{1}H NMR [500 MHz, H_2O/D_2O 90:10) spectrum of compound **1**

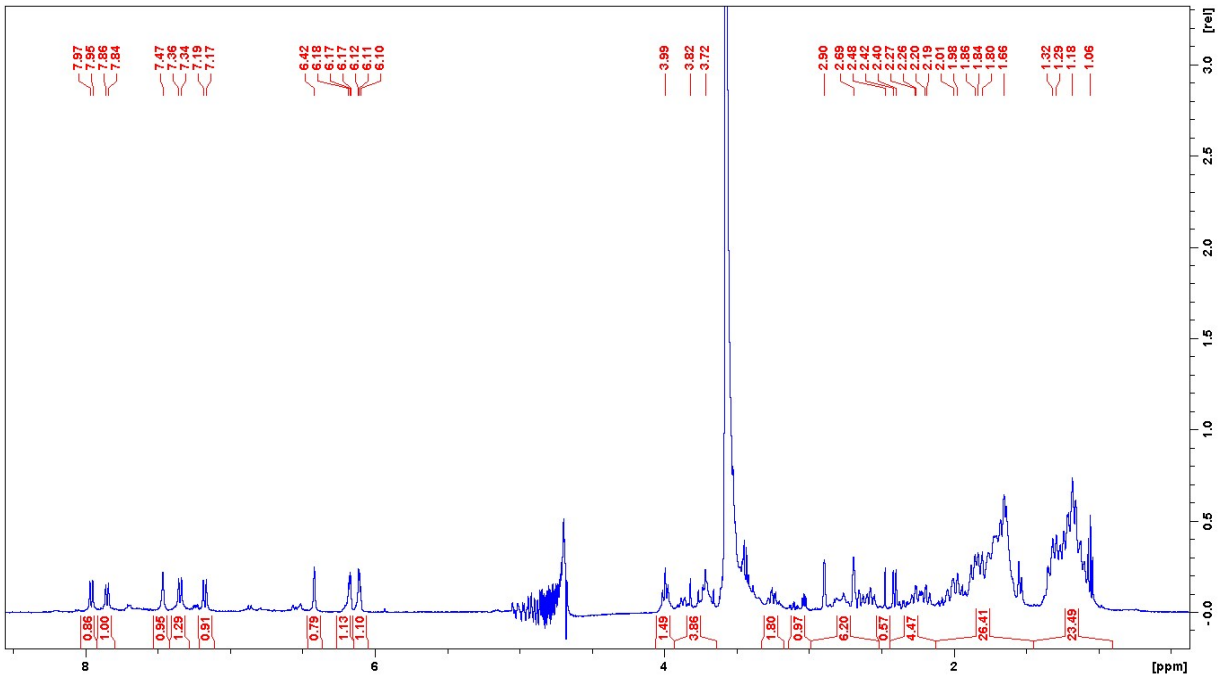


Figure S5. TOCSY NMR [500 MHz, H_2O/D_2O 90:10) spectrum of compound **1**

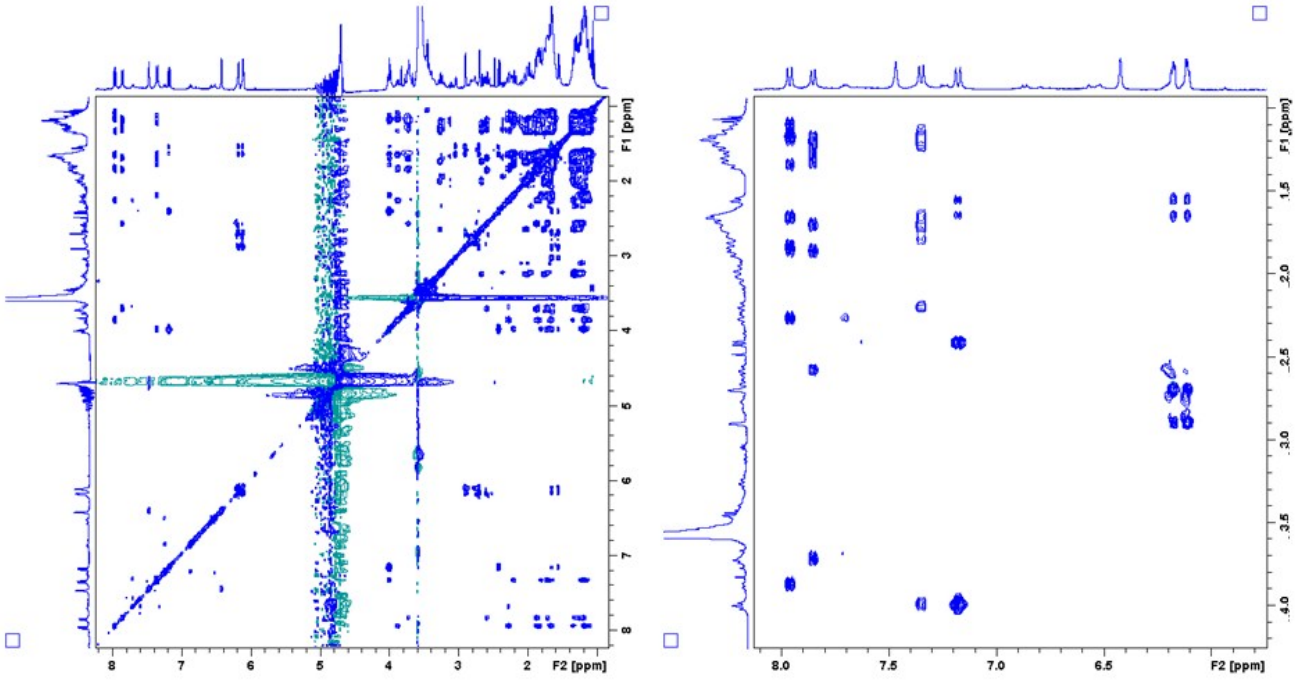


Figure S6. ROESY NMR [500 MHz, H_2O/D_2O 90:10) spectrum of compound 1

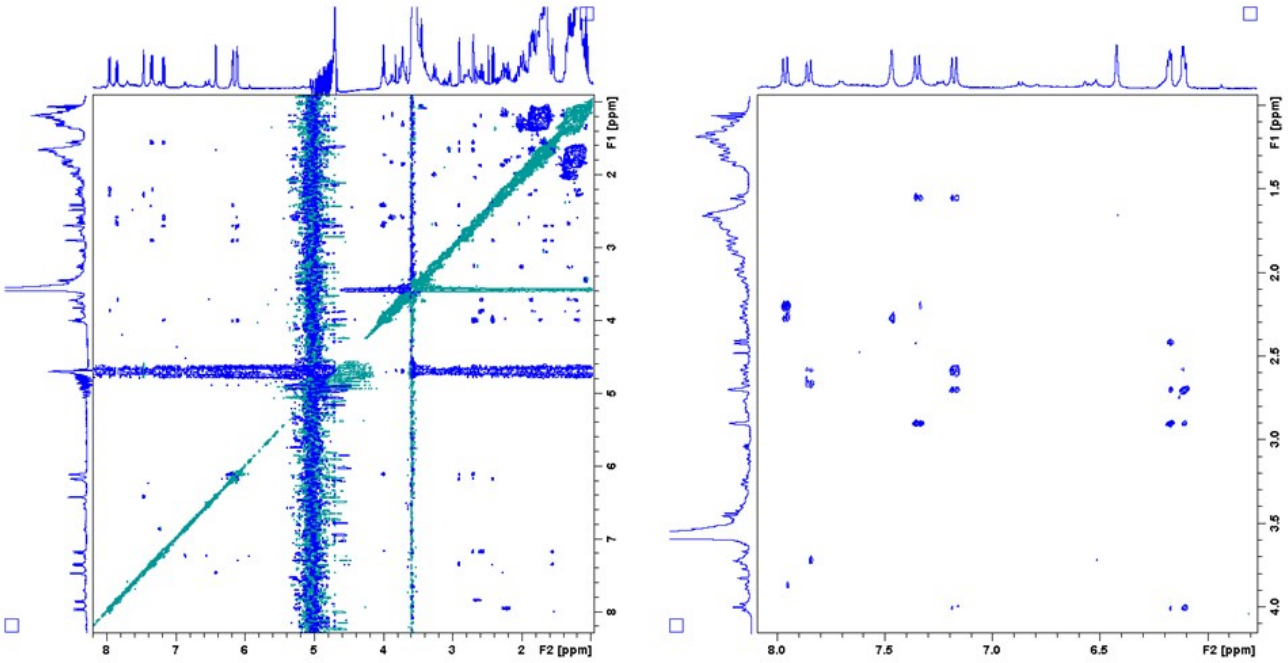


Figure S7. ^1H NMR [500 MHz, CD_3OH) spectrum of compound 1

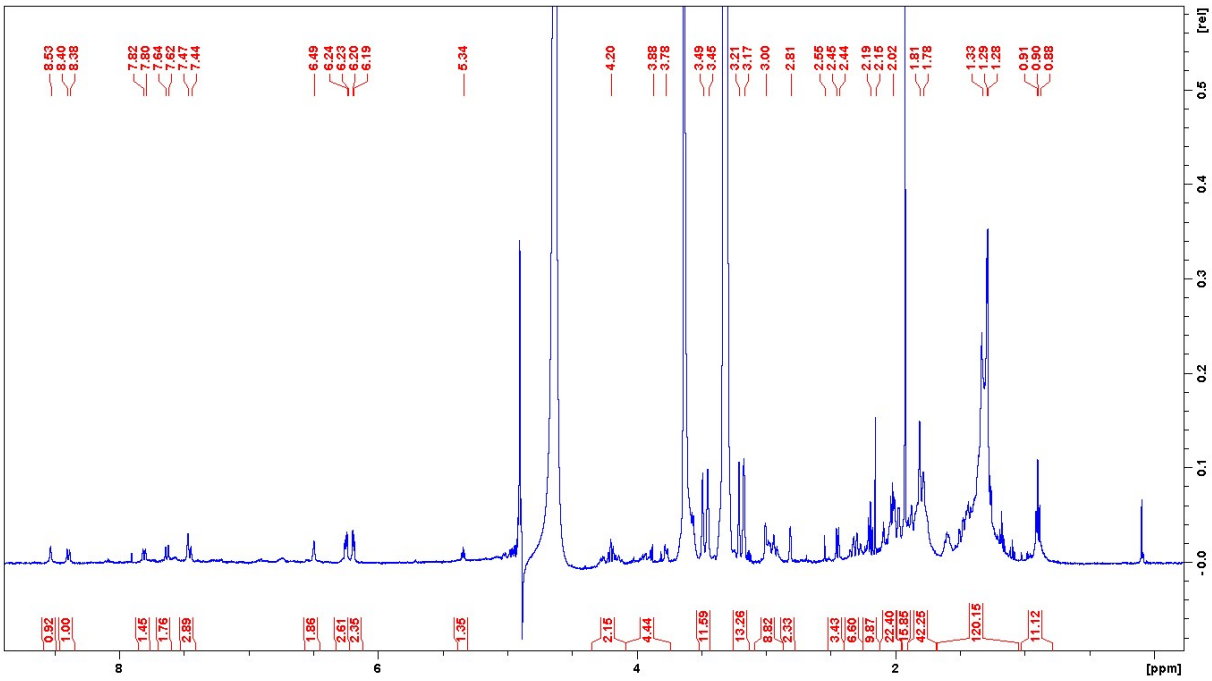


Figure S8. TOCSY NMR [500 MHz, CD_3OH) spectrum of compound **1**

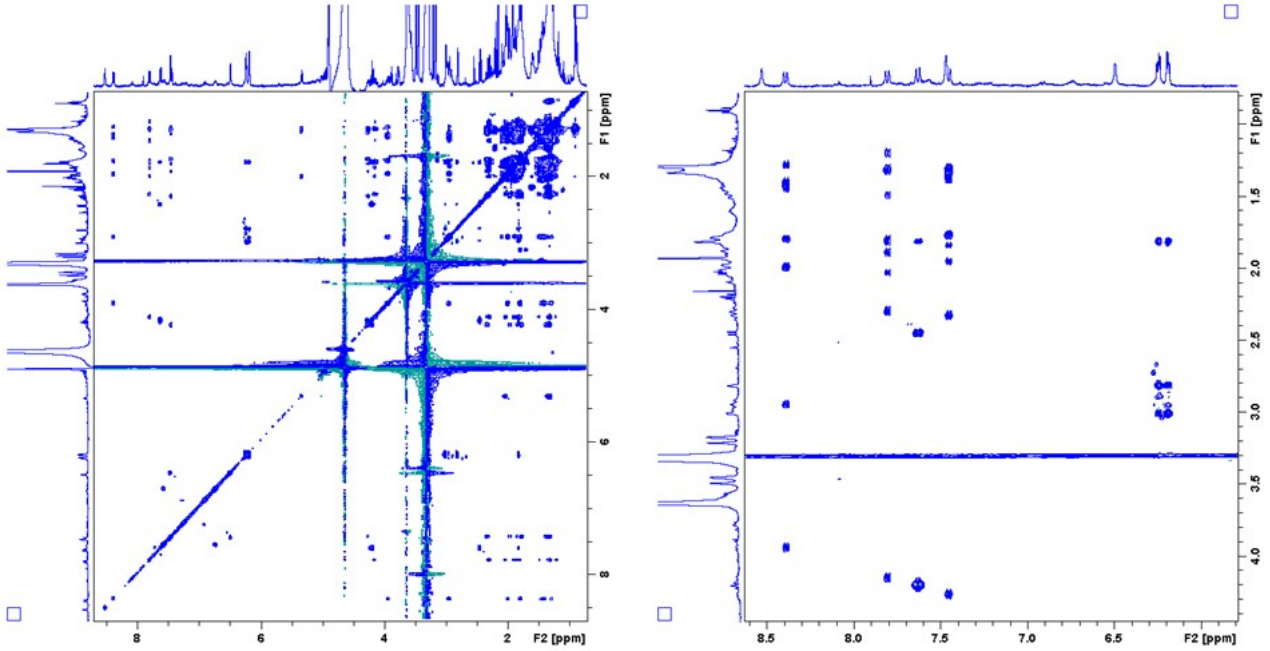


Figure S9. ROESY NMR [500 MHz, CD_3OH) spectrum of compound **1**

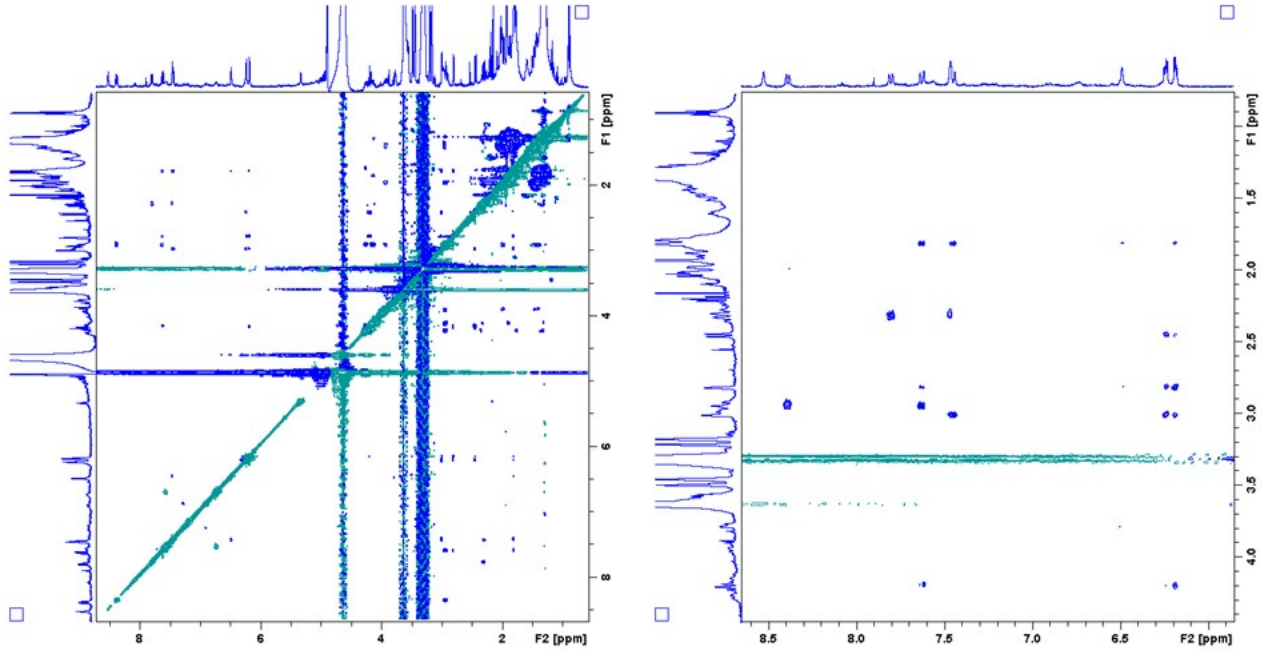


Figure S10. ^{1}H NMR [500 MHz, DMSO-d_6) spectrum of compound **1**

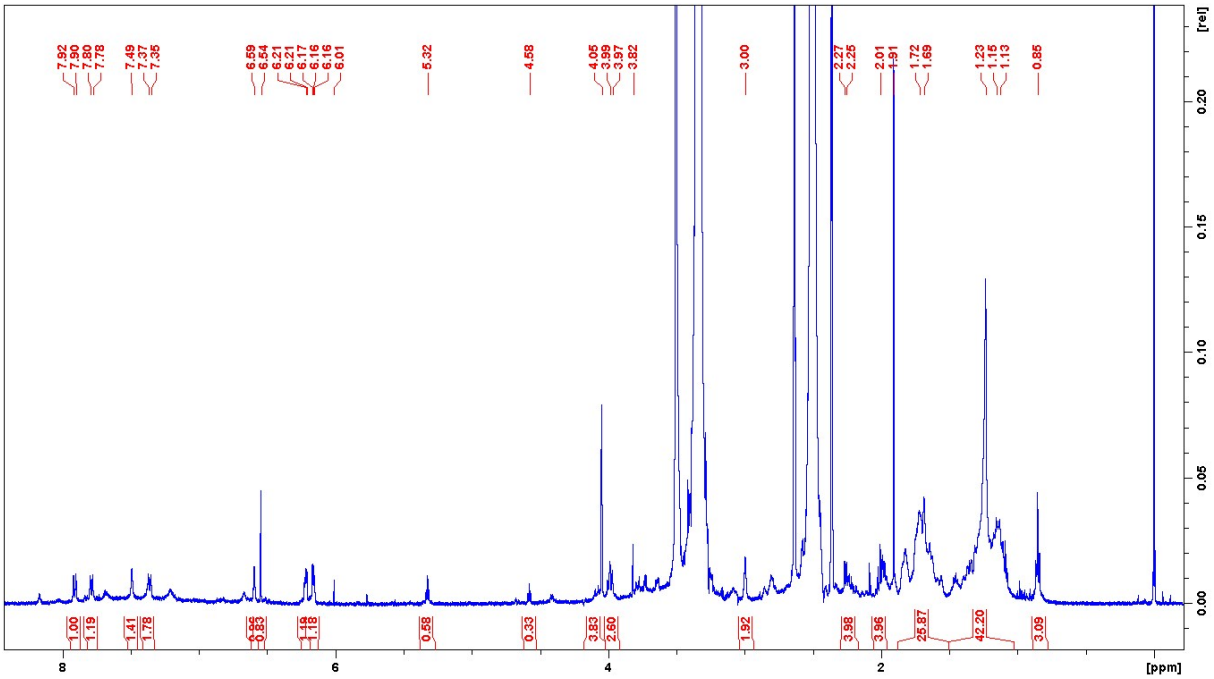


Fig. S11 TOCSY NMR [500 MHz, DMSO-d_6) spectrum of compound **1**

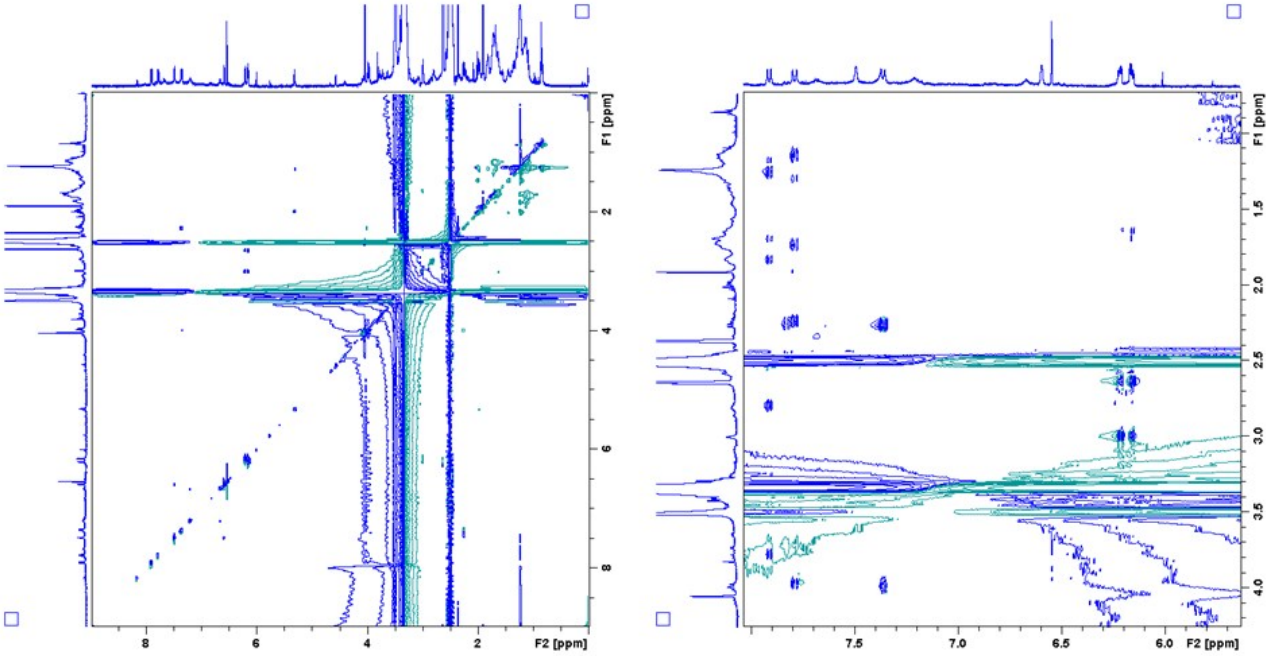


Figure S12. ROESY NMR [500 MHz, DMSO-d_6) spectrum of compound **1**

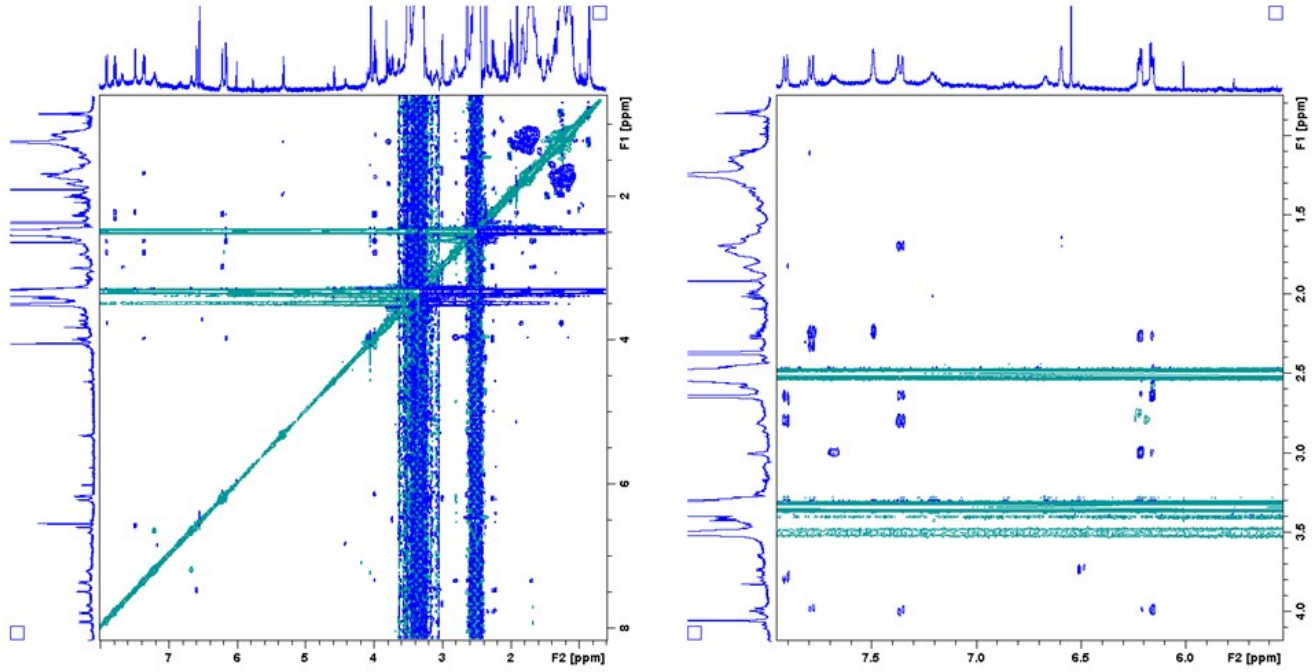


Figure S13. ^{1}H NMR [600 MHz, H_2O/D_2O 90:10) spectrum of compound **2**

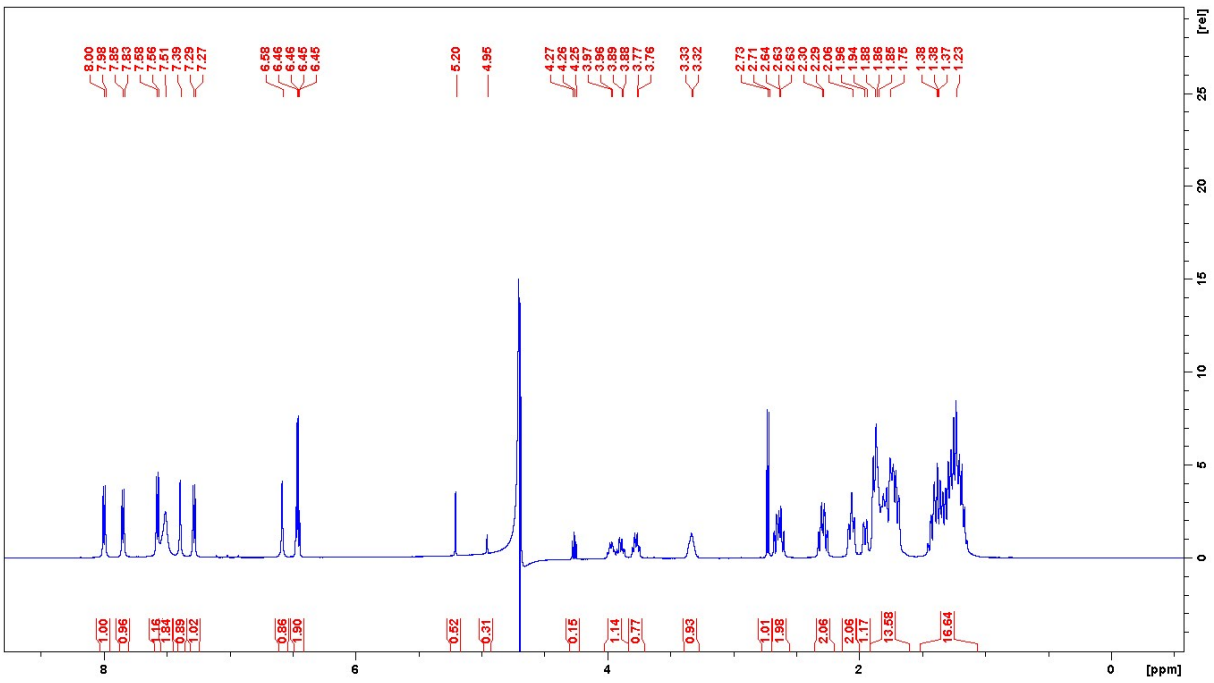


Figure S14. TOCSY NMR [600 MHz, H_2O/D_2O 90:10) spectrum of compound **2**

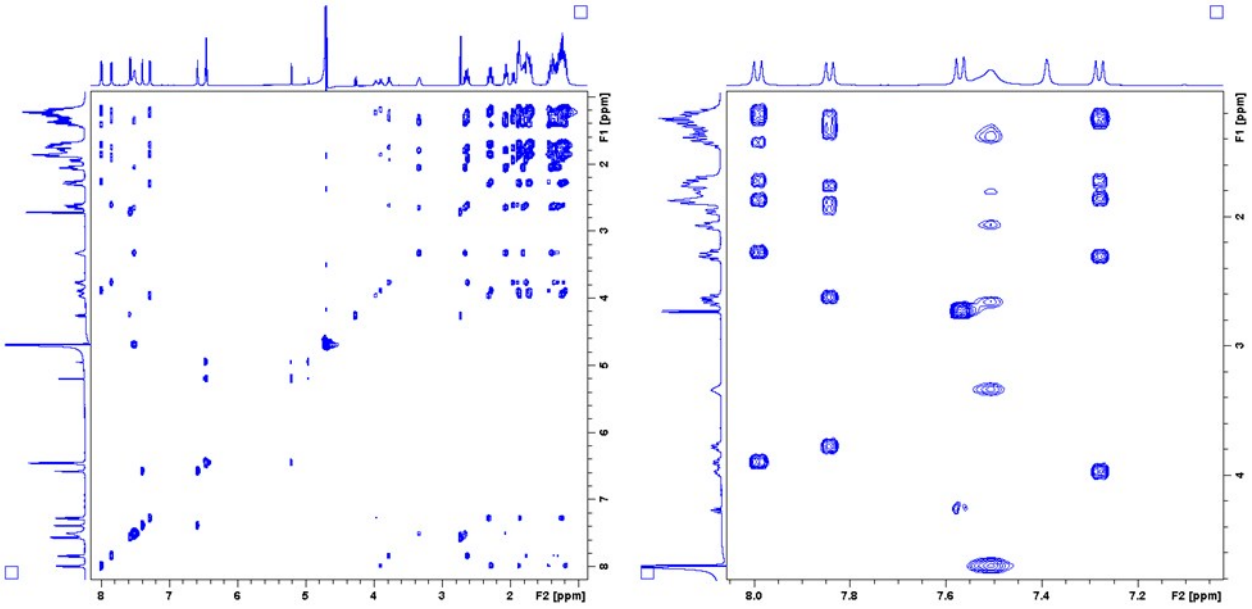


Figure S15. ROESY NMR [600 MHz, H_2O/D_2O 90:10) spectrum of compound **2**

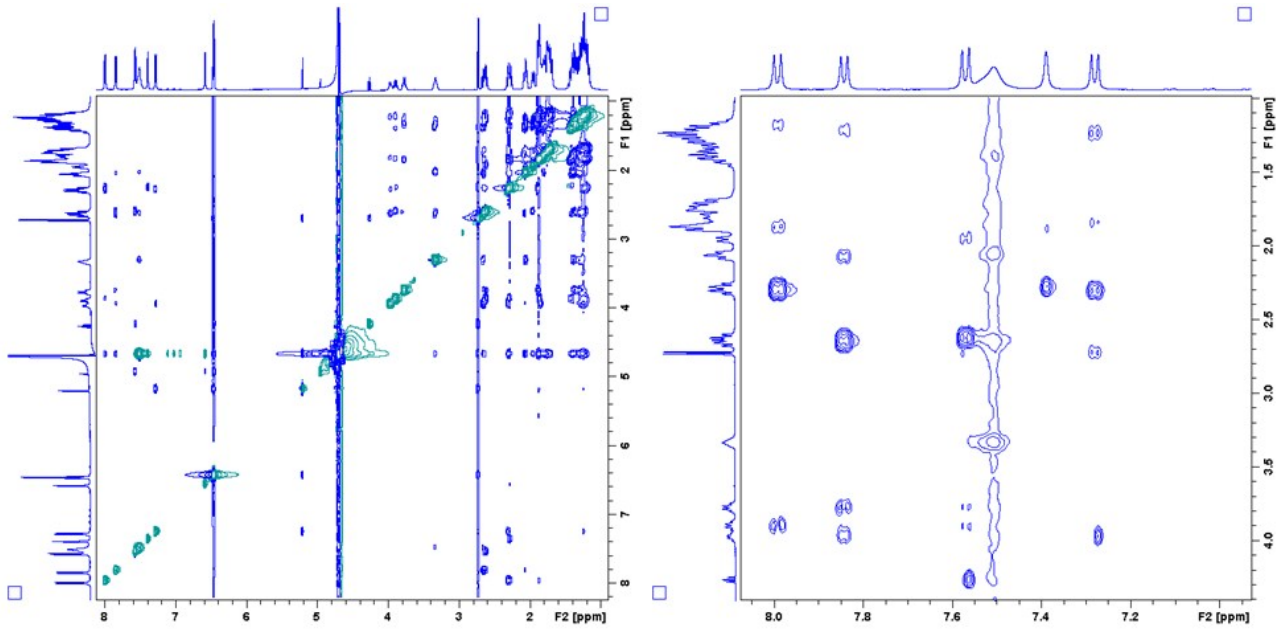


Figure S16. ^{1}H NMR [600 MHz, CD_3OH) spectrum of compound **2**

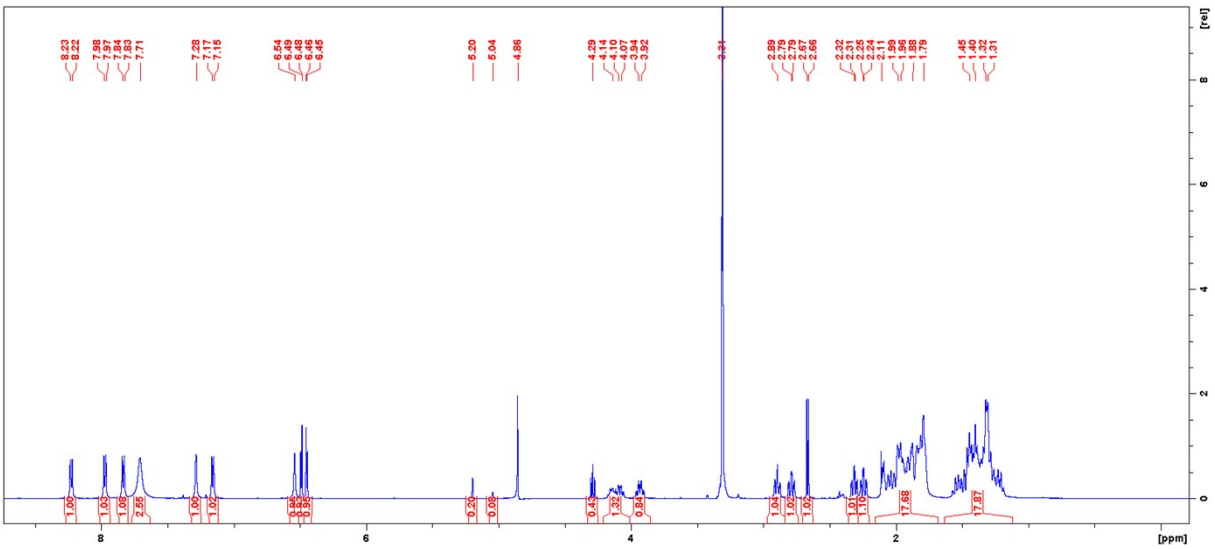


Figure S17. TOCSY NMR [600 MHz, CD_3OH) spectrum of compound **2**

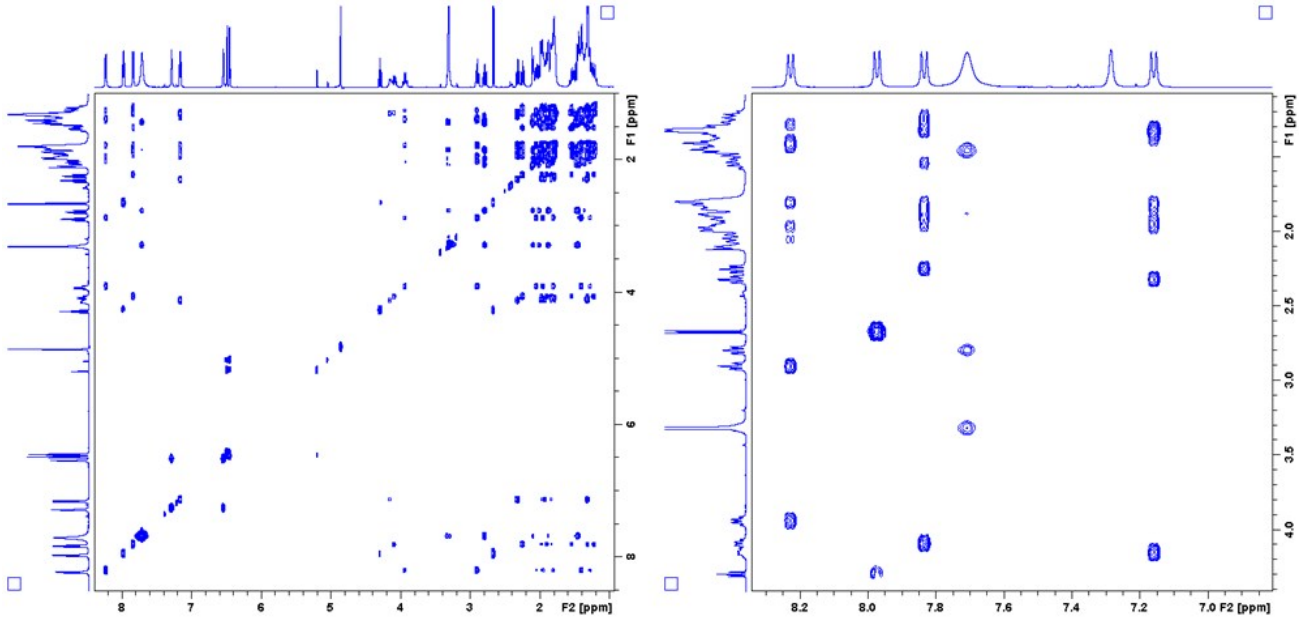


Figure S18. ROESY NMR [600 MHz, CD_3OH) spectrum of compound **2**

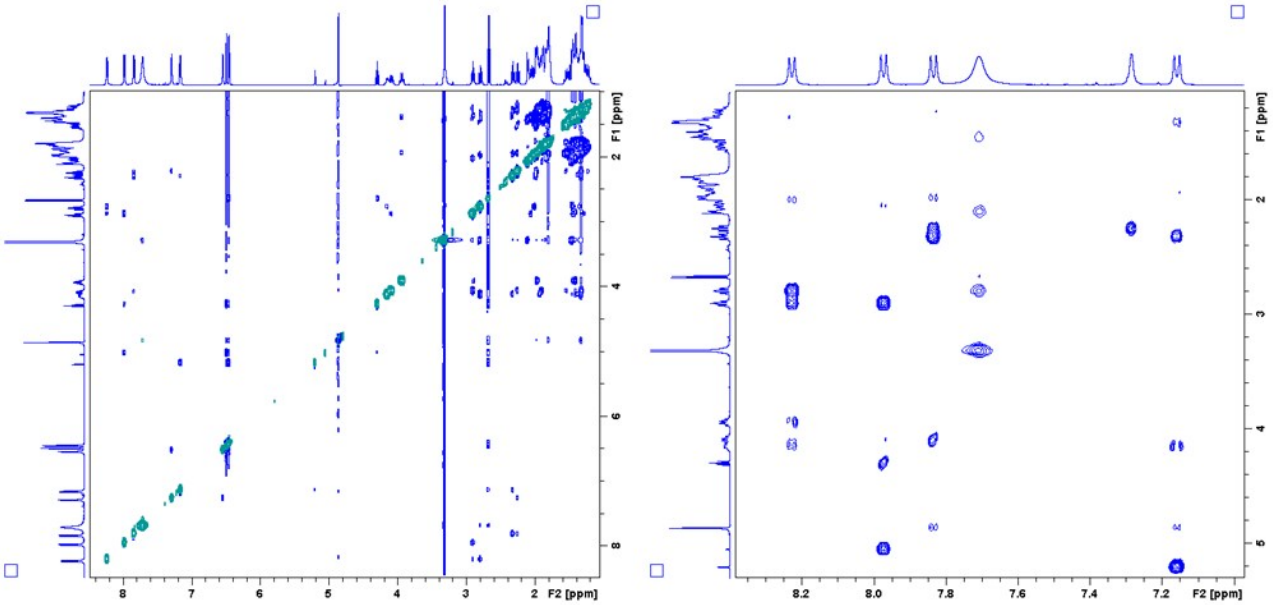


Figure S19. ^1H NMR [600 MHz, DMSO-d_6) spectrum of compound **2**

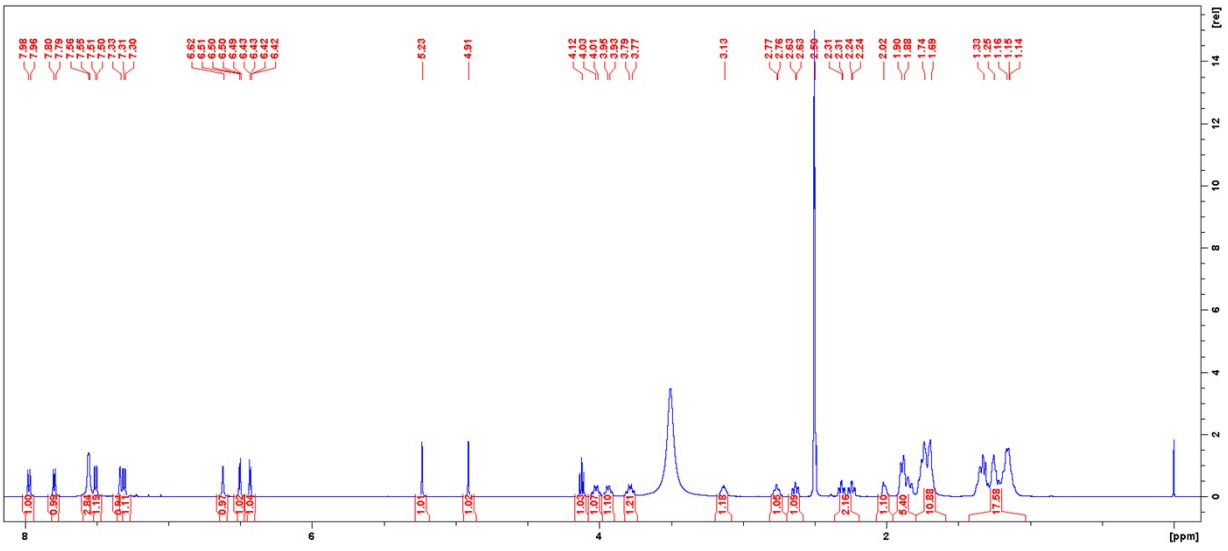


Figure S20. TOCSY NMR [600 MHz, DMSO-d_6) spectrum of compound **2**

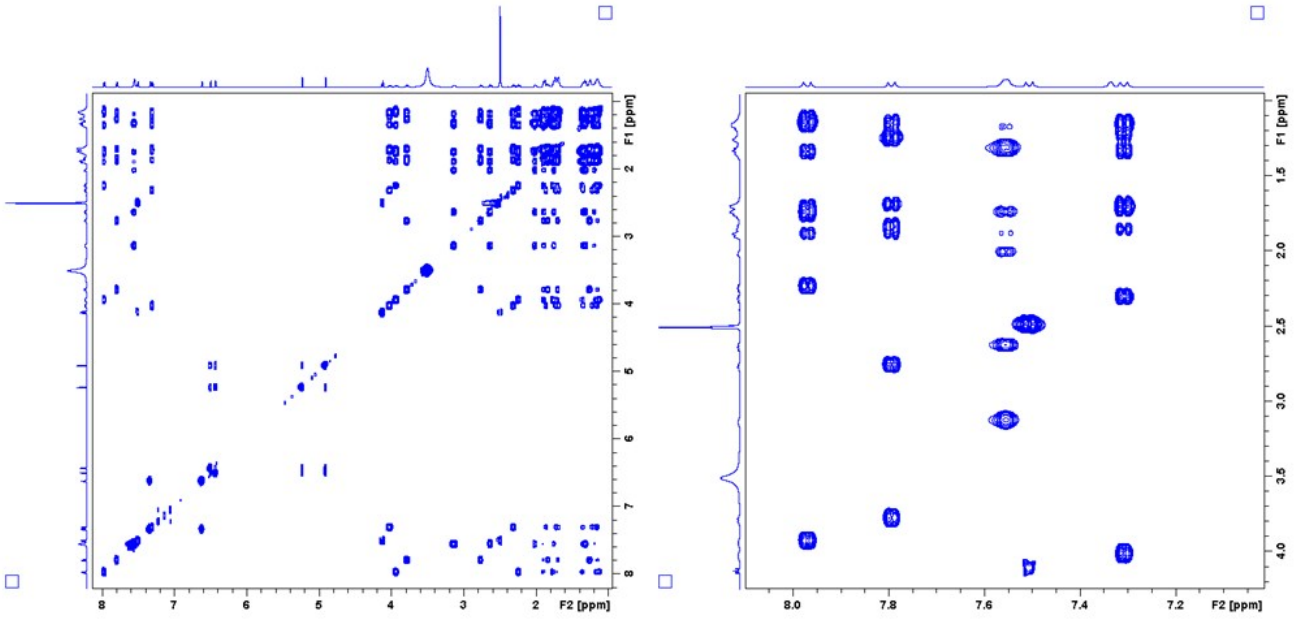


Figure S21. ROESY NMR [600 MHz, DMSO-d_6) spectrum of compound **2**

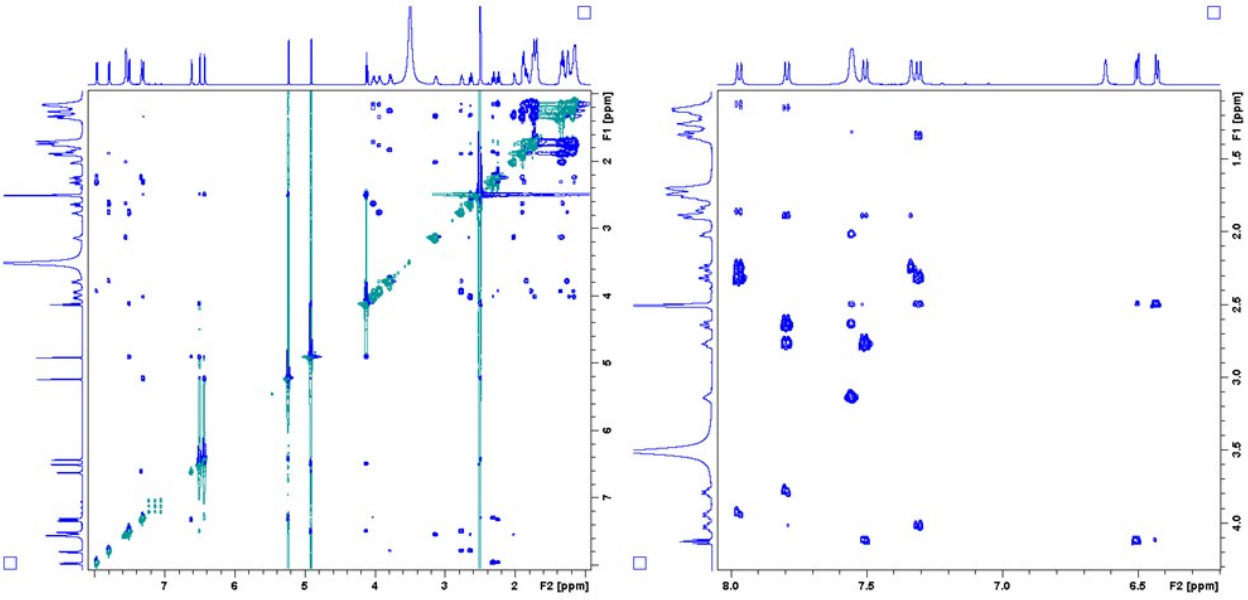


Figure S22. ^{1}H NMR [500 MHz, H_2O/D_2O 90:10) spectrum of compound **3**

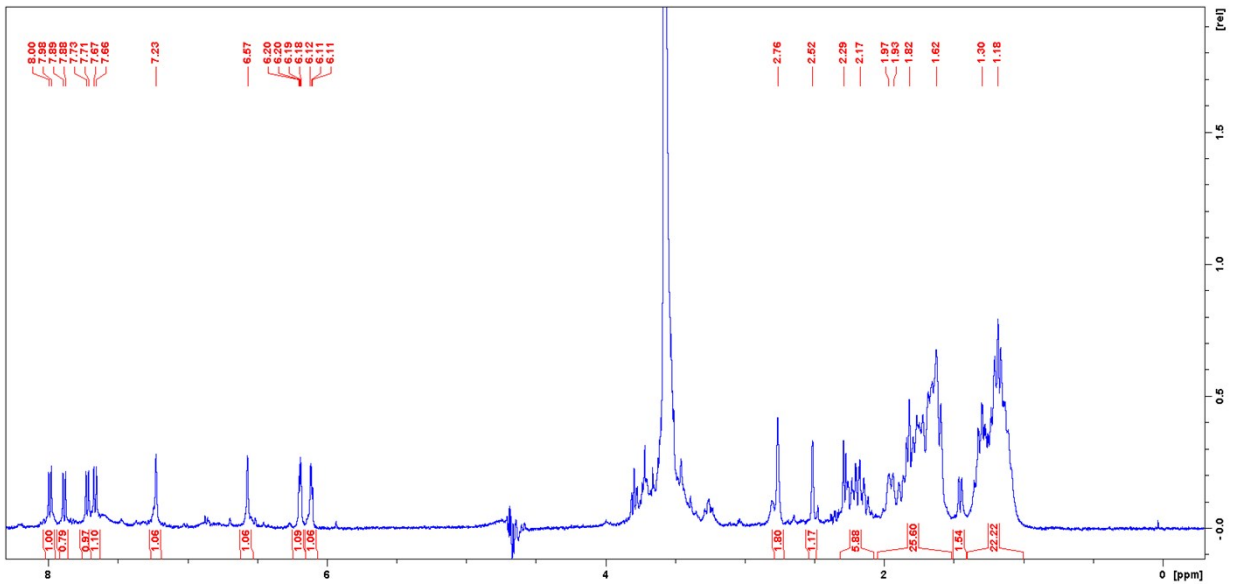


Figure S23. TOCSY NMR [500 MHz, H_2O/D_2O 90:10) spectrum of compound **3**

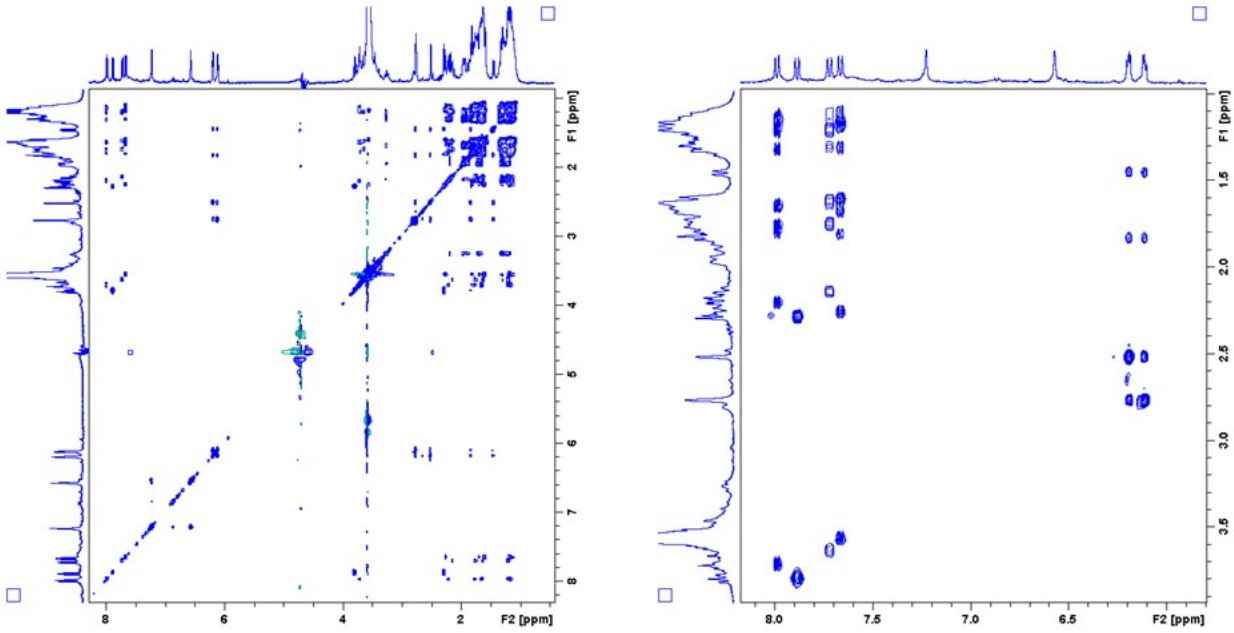


Figure S24. ROESY NMR [500 MHz, H_2O/D_2O 90:10) spectrum of compound **3**

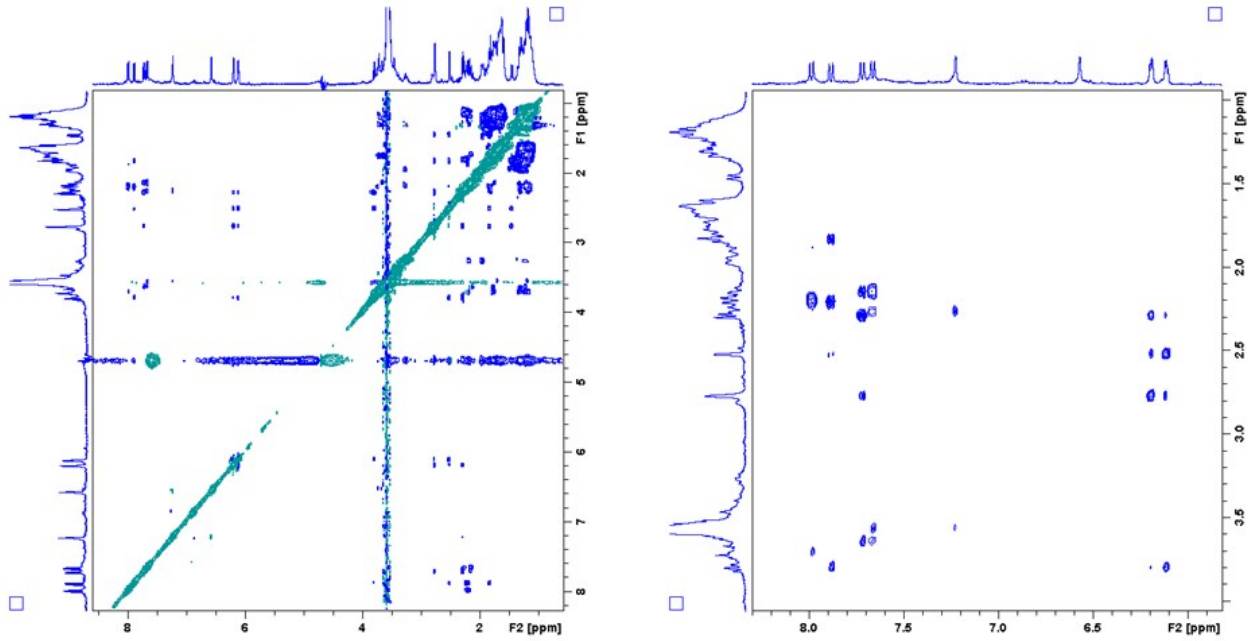


Figure S25. ^1H NMR [500 MHz, CD_3OH) spectrum of compound **3**

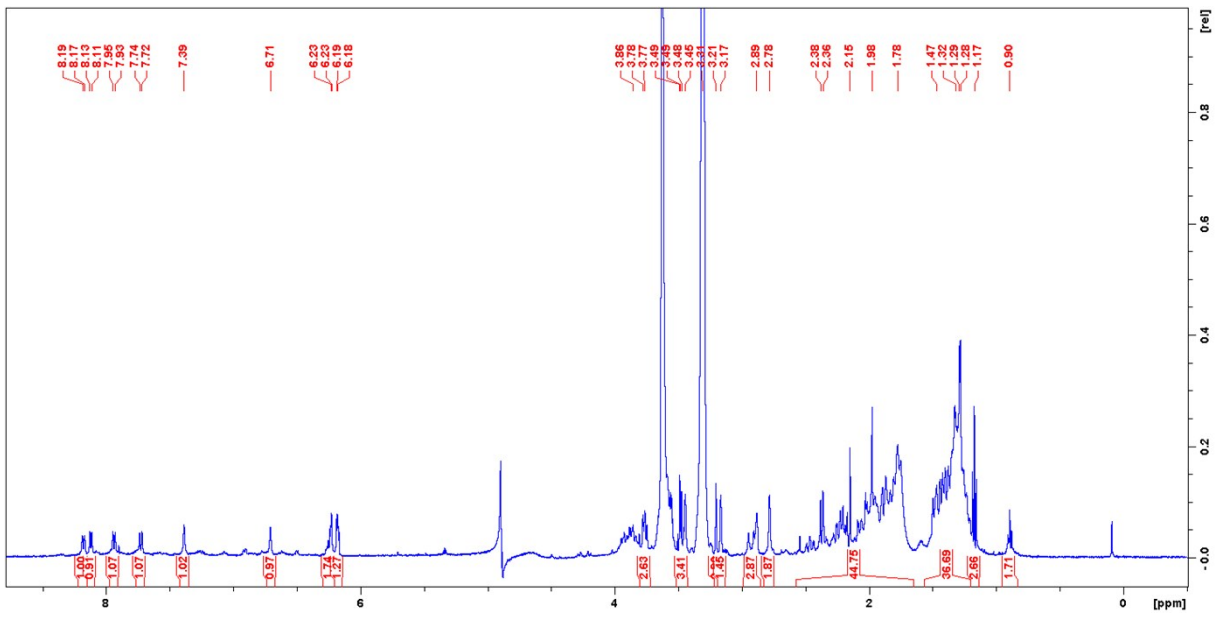


Figure S26. TOCSY NMR [500 MHz, CD_3OH) spectrum of compound **3**

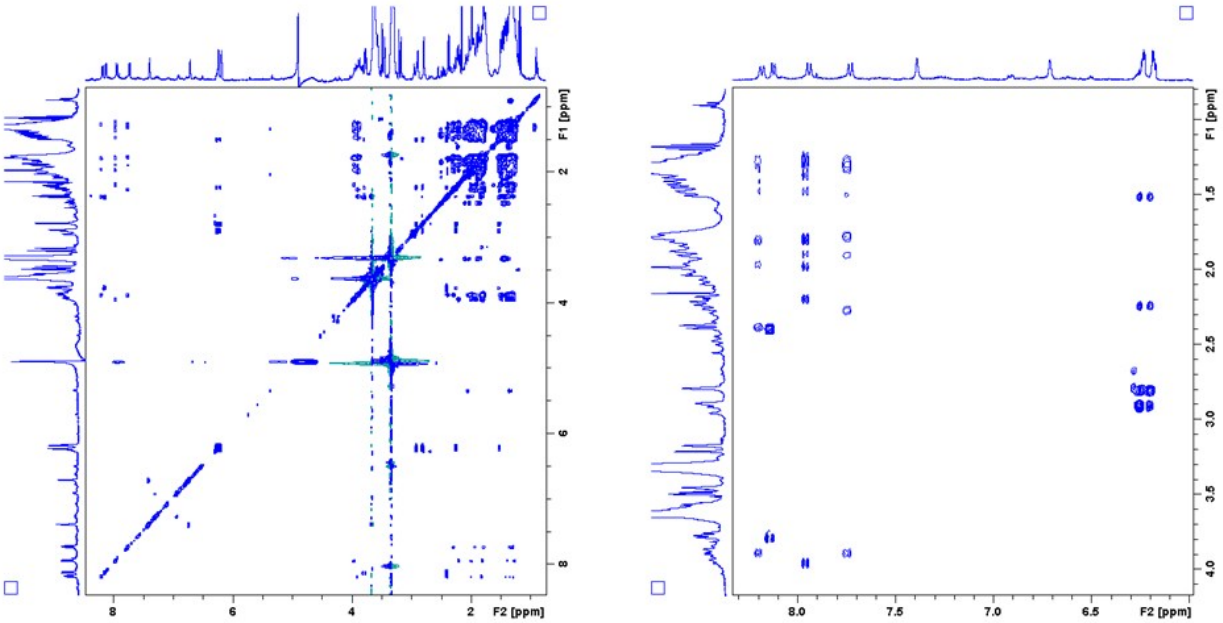


Figure S27. ROESY NMR [500 MHz, CD_3OH) spectrum of compound **3**

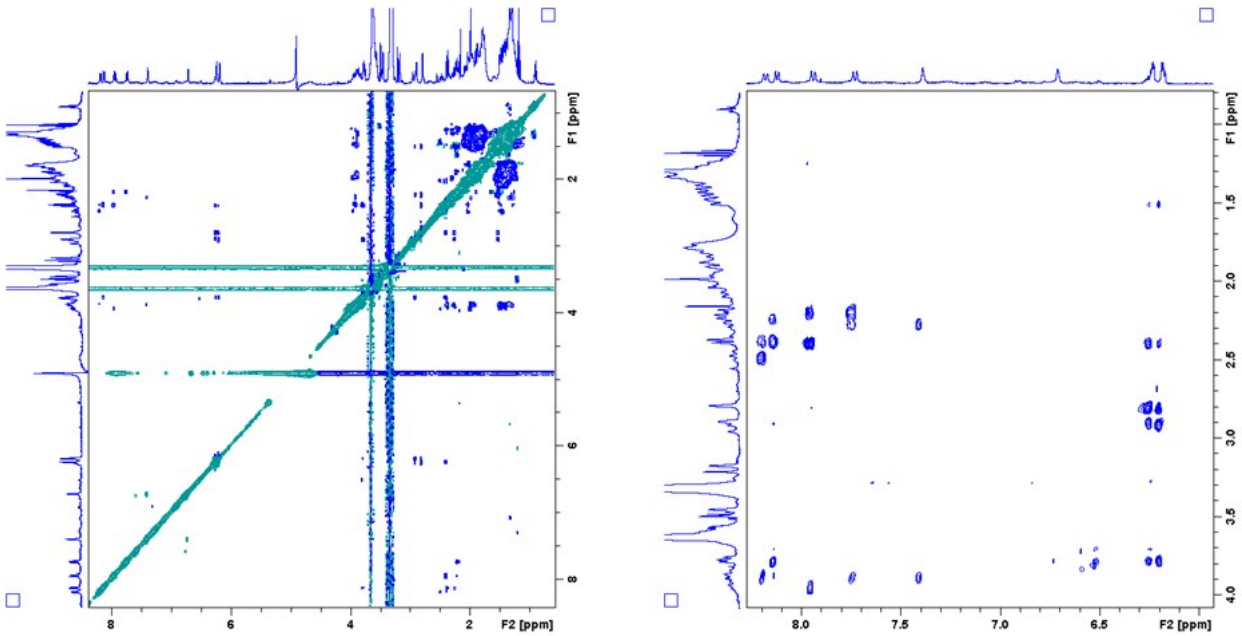


Figure S28. ^{1}H NMR [500 MHz, DMSO-d_6) spectrum of compound **3**

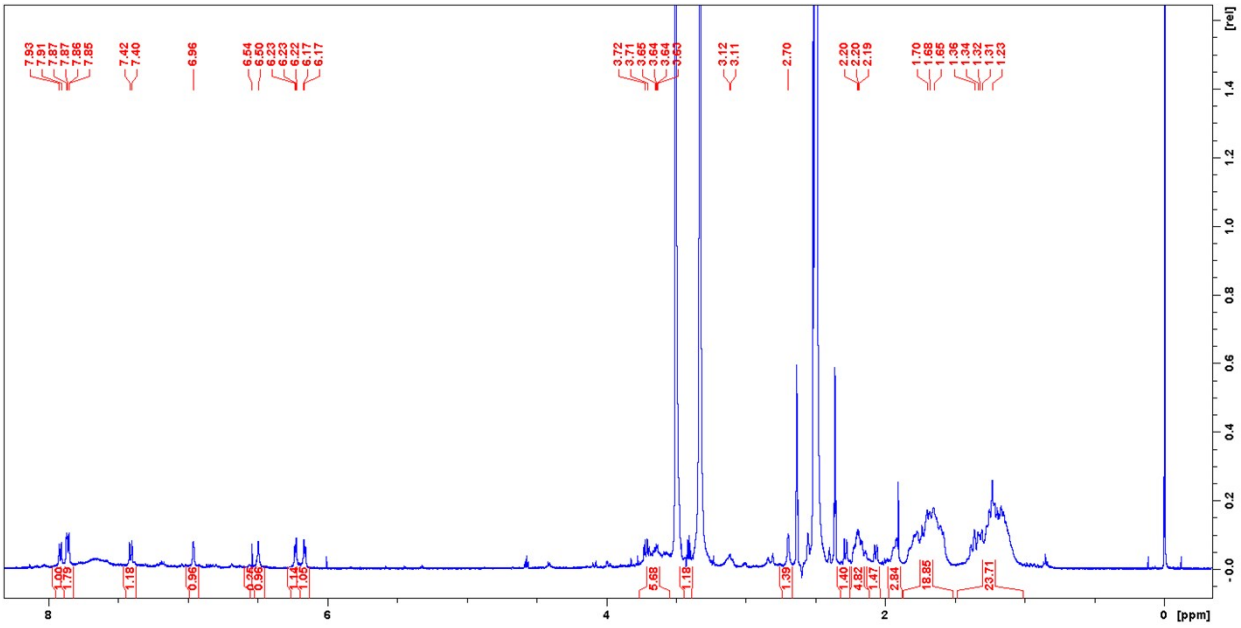


Figure S29. TOCSY NMR [500 MHz, DMSO-d_6) spectrum of compound **3**

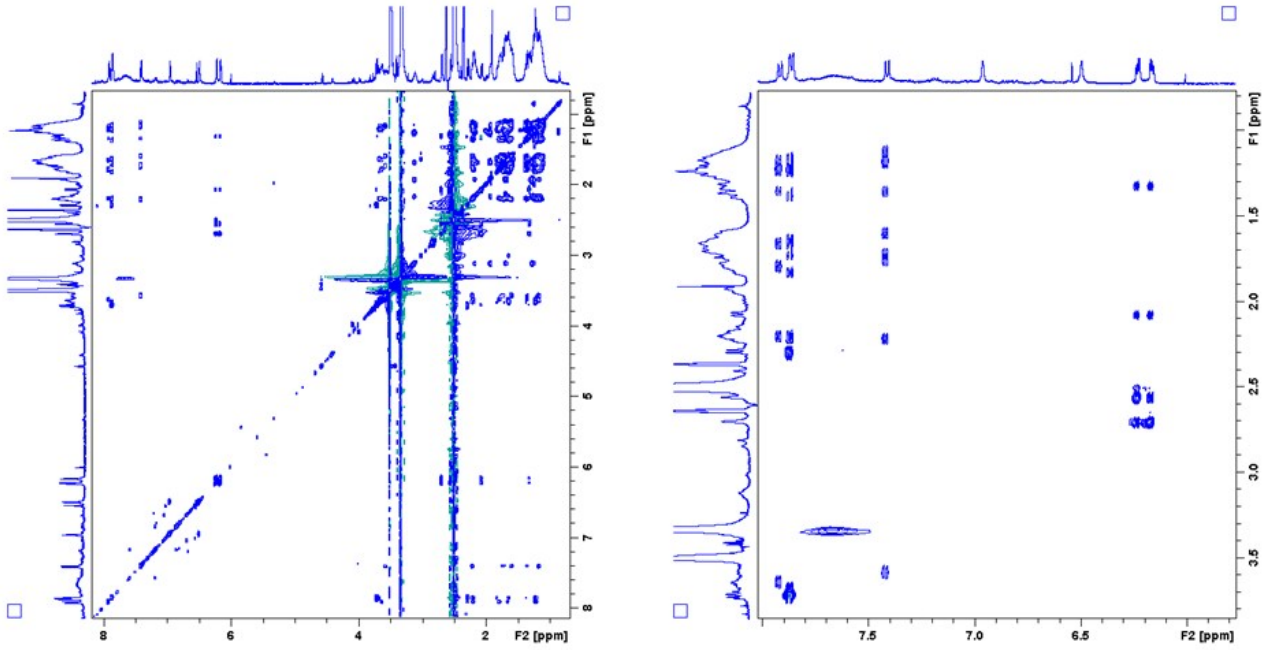


Figure S30. ROESY NMR [500 MHz, DMSO-d_6) spectrum of compound **3**

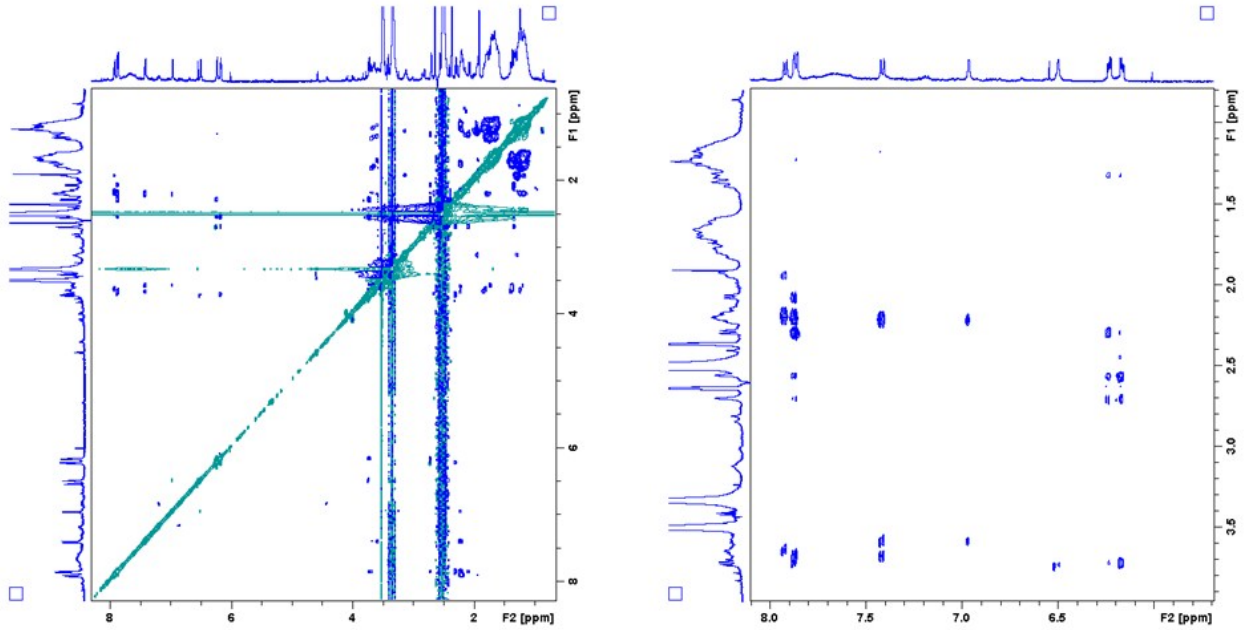


Figure S31. ^{1}H NMR [600 MHz, H_2O/D_2O 90:10) spectrum of compound **4**

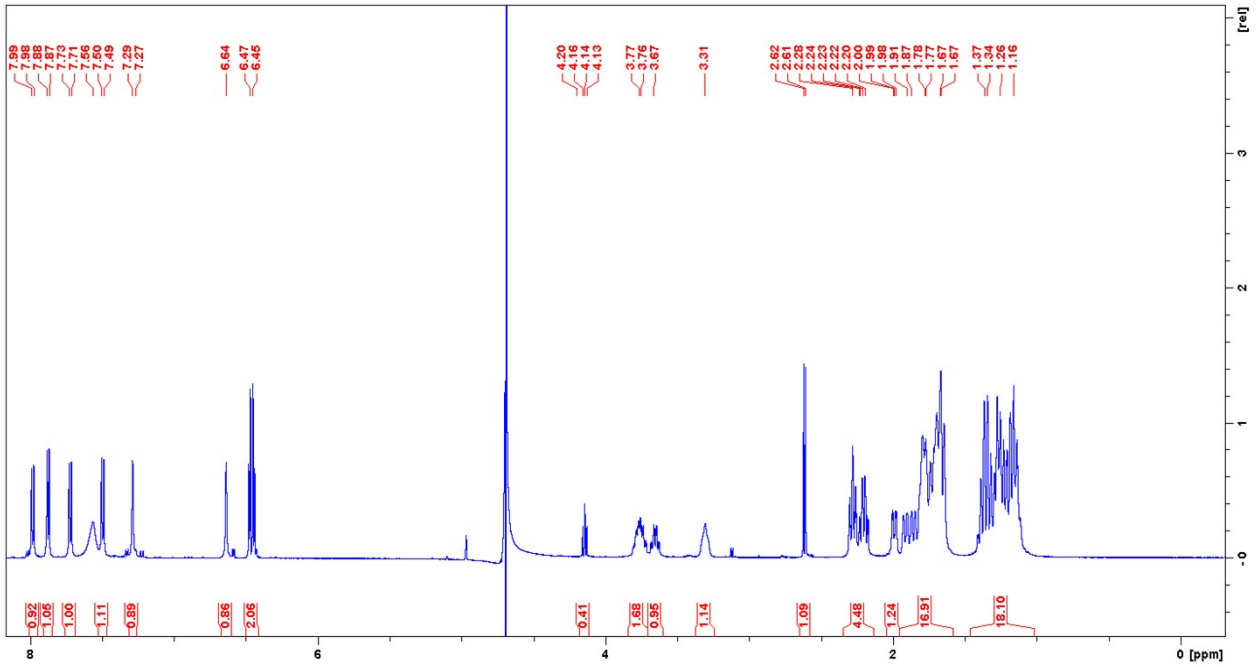


Figure S32. TOCSY NMR [600 MHz, H_2O/D_2O 90:10) spectrum of compound **4**

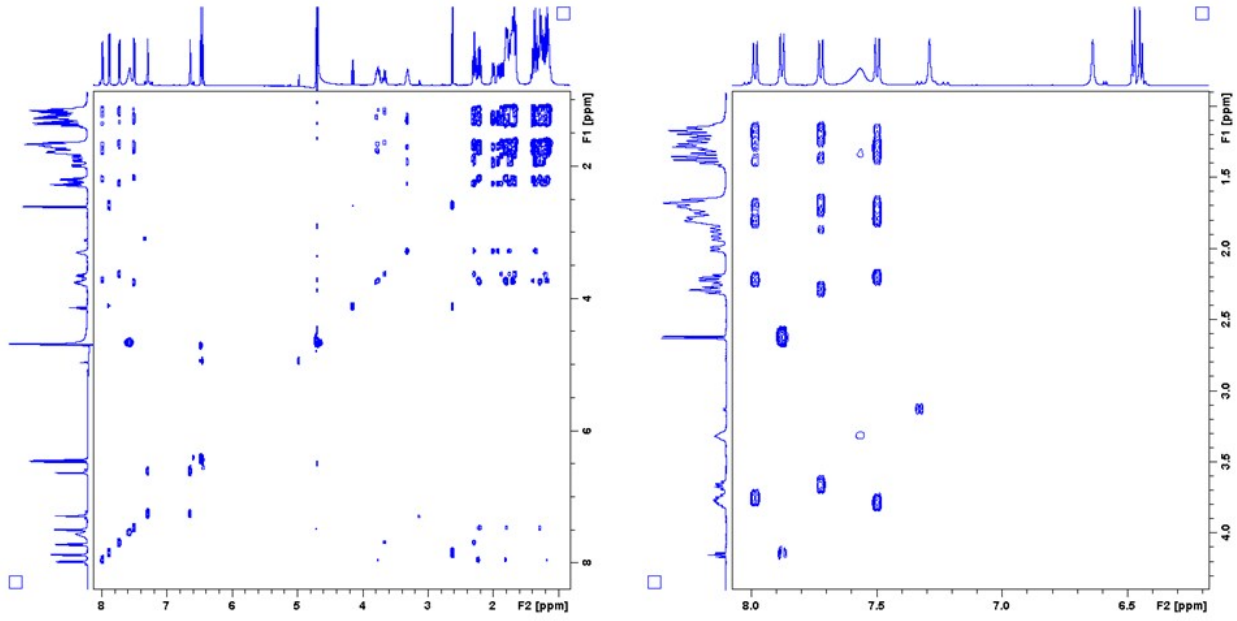


Figure S33. ROESY NMR [600 MHz, H_2O/D_2O 90:10) spectrum of compound **4**

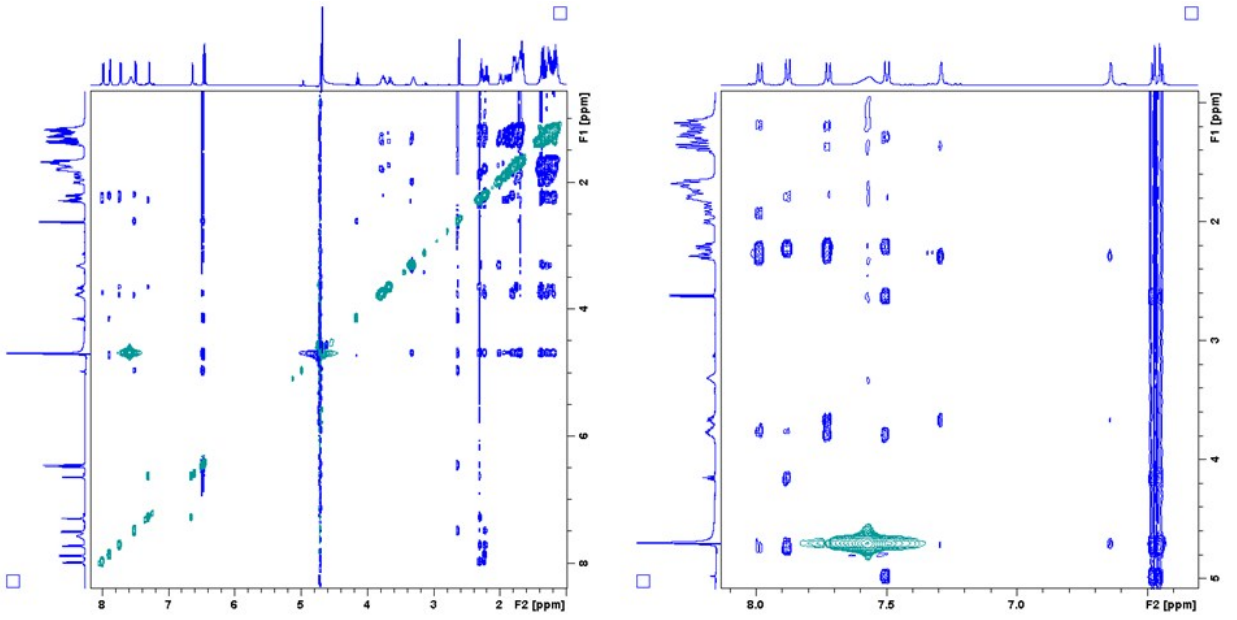


Figure S34. ^{1}H NMR [600 MHz, CD_3OH) spectrum of compound **4**

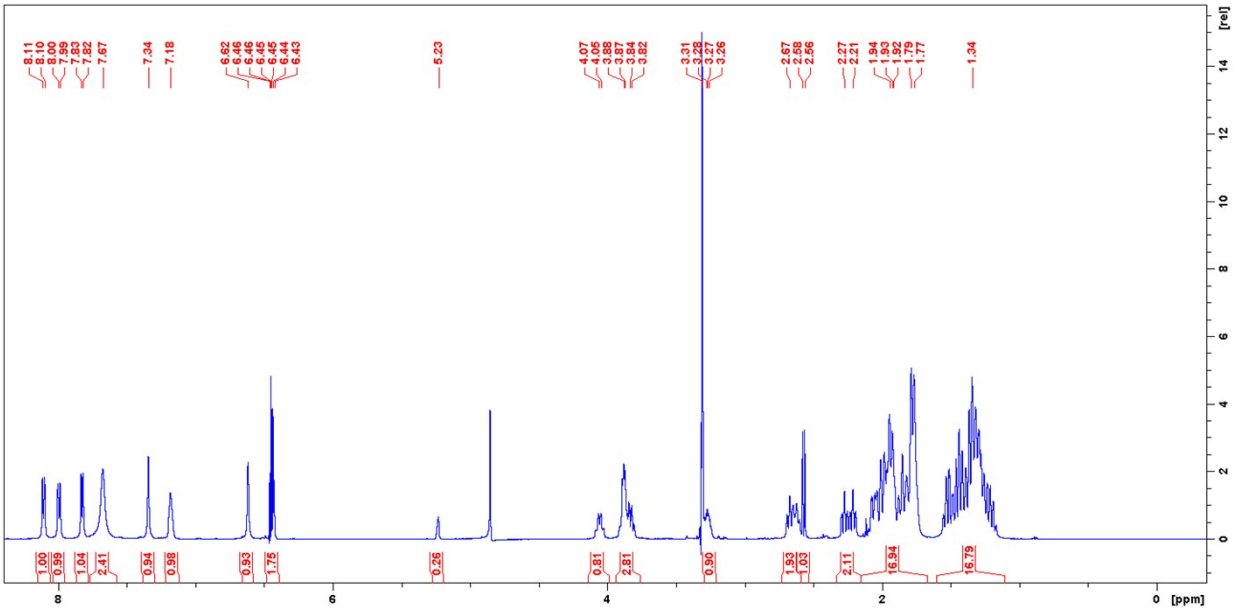


Figure S35. TOCSY NMR [600 MHz, CD_3OH) spectrum of compound **4**

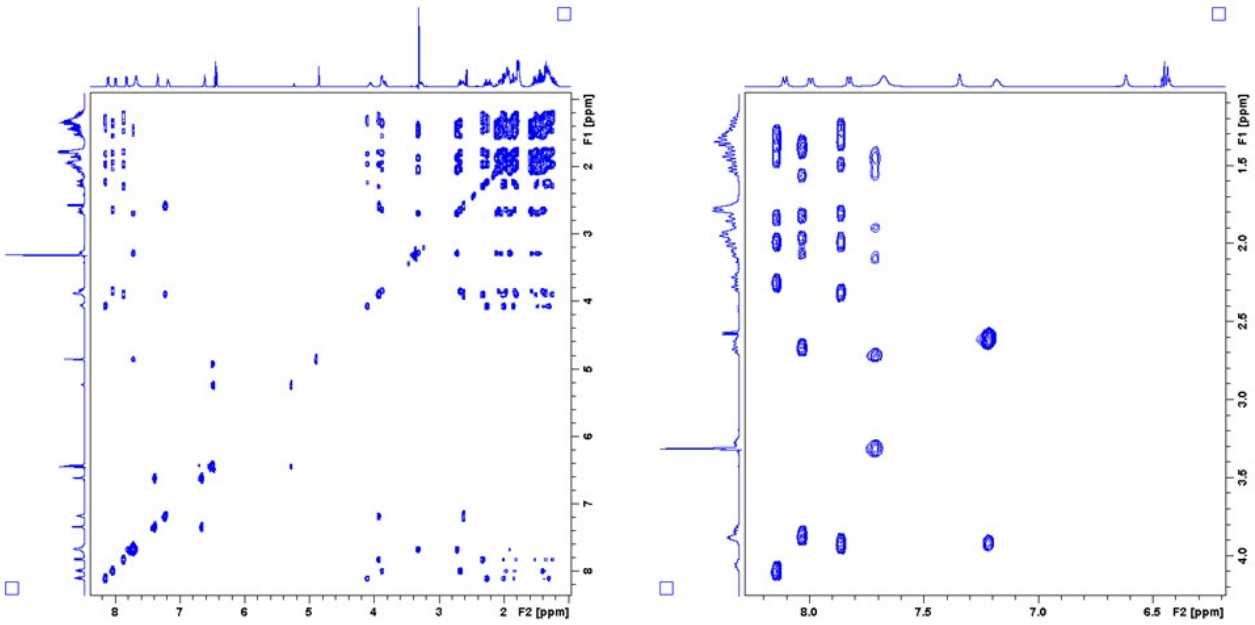


Figure S36. ROESY NMR [600 MHz, CD_3OH) spectrum of compound **4**

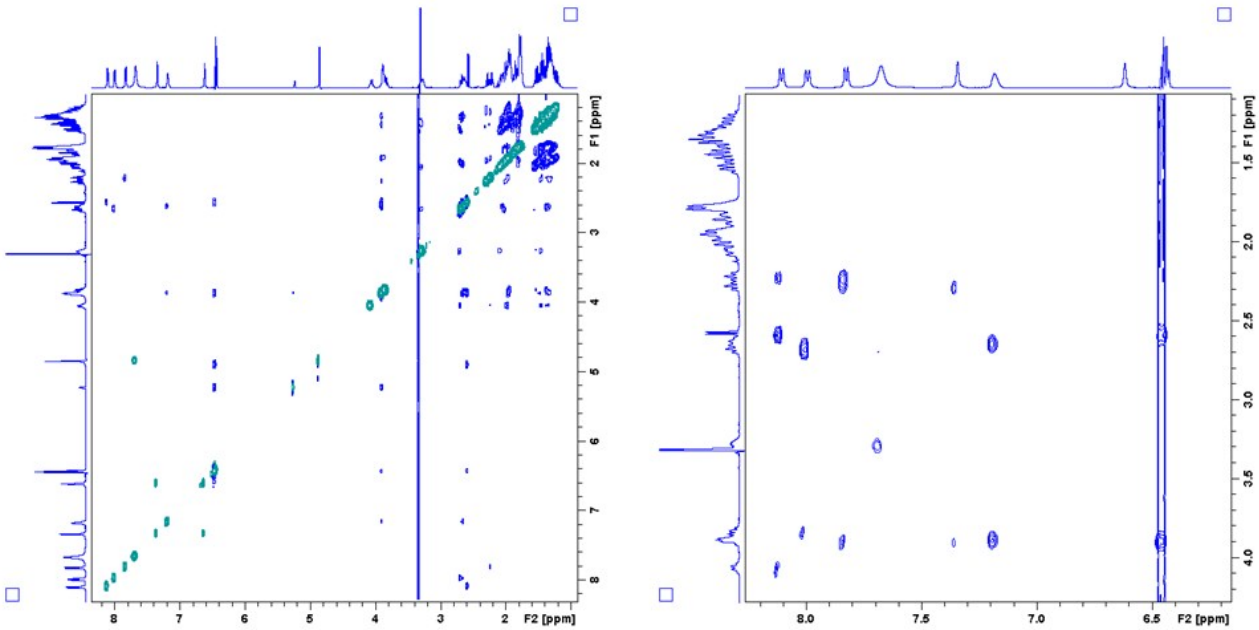


Figure S37. ^1H NMR [600 MHz, DMSO-d_6) spectrum of compound **4**

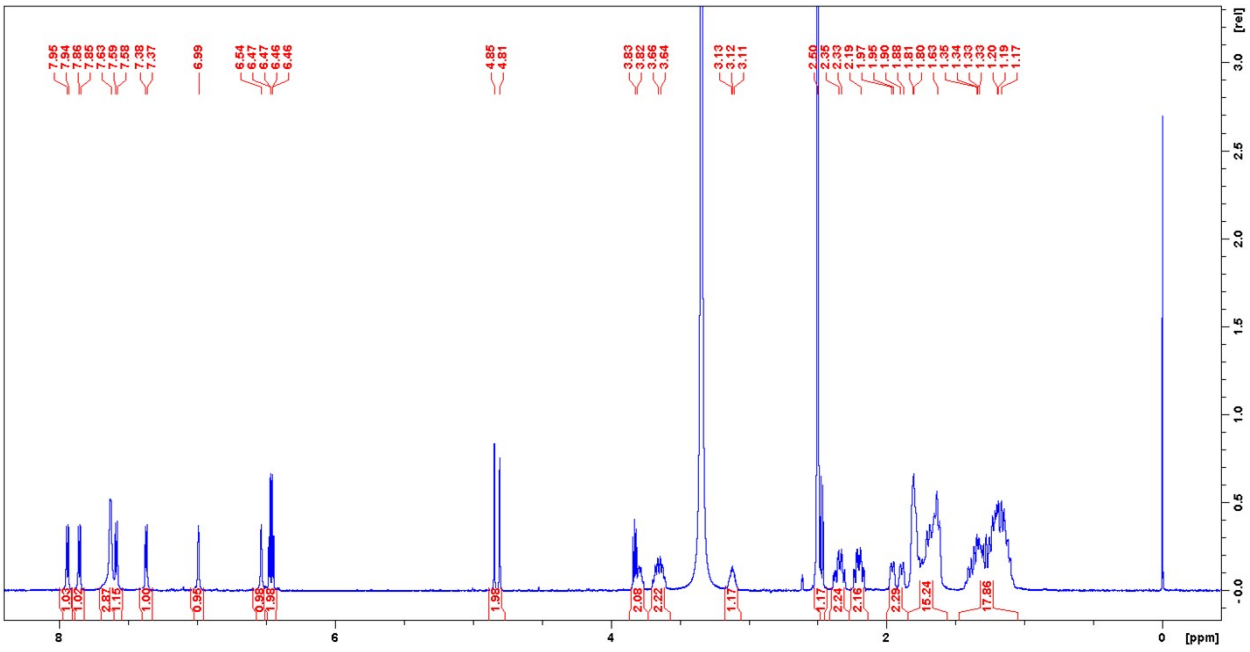


Figure S38. TOCSY NMR [600 MHz, DMSO-d_6) spectrum of compound **4**

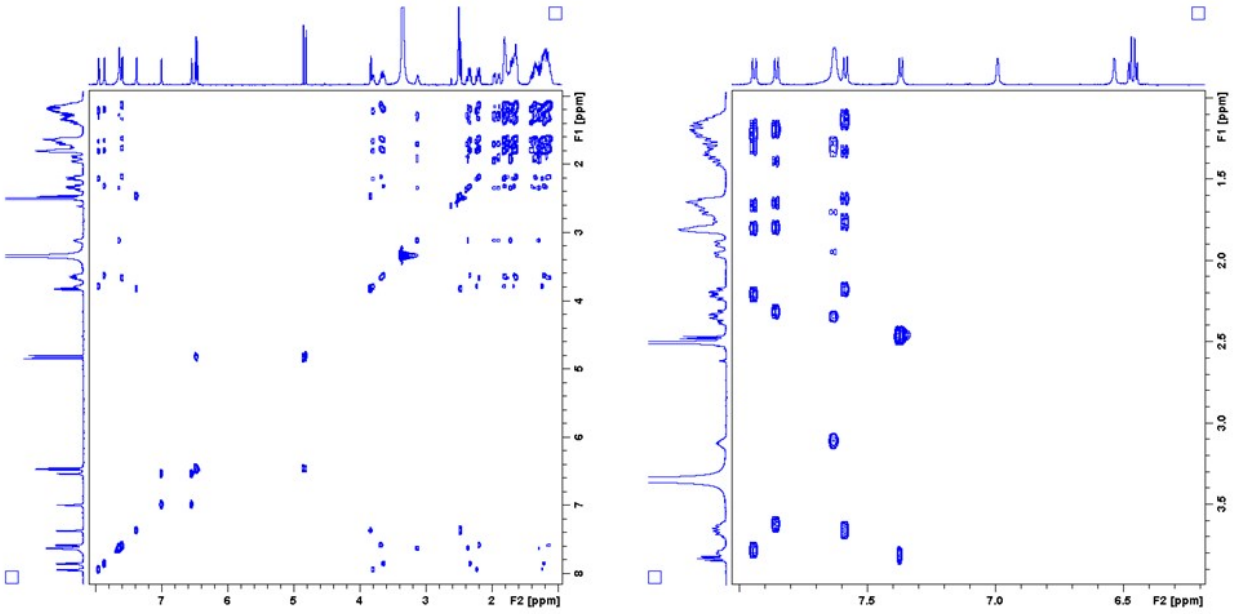


Figure S39. ROESY NMR [600 MHz, DMSO-d_6) spectrum of compound **4**

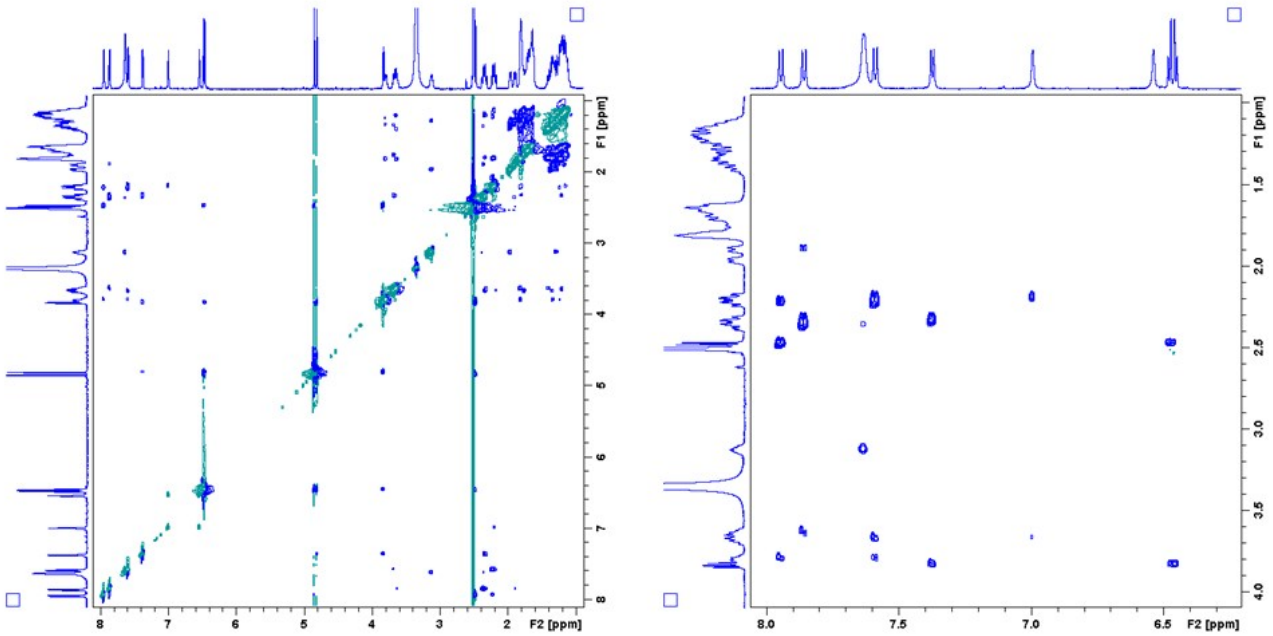


Figure S40. ^{1}H NMR [600 MHz, H_2O/D_2O 90:10) spectrum of compound **5**

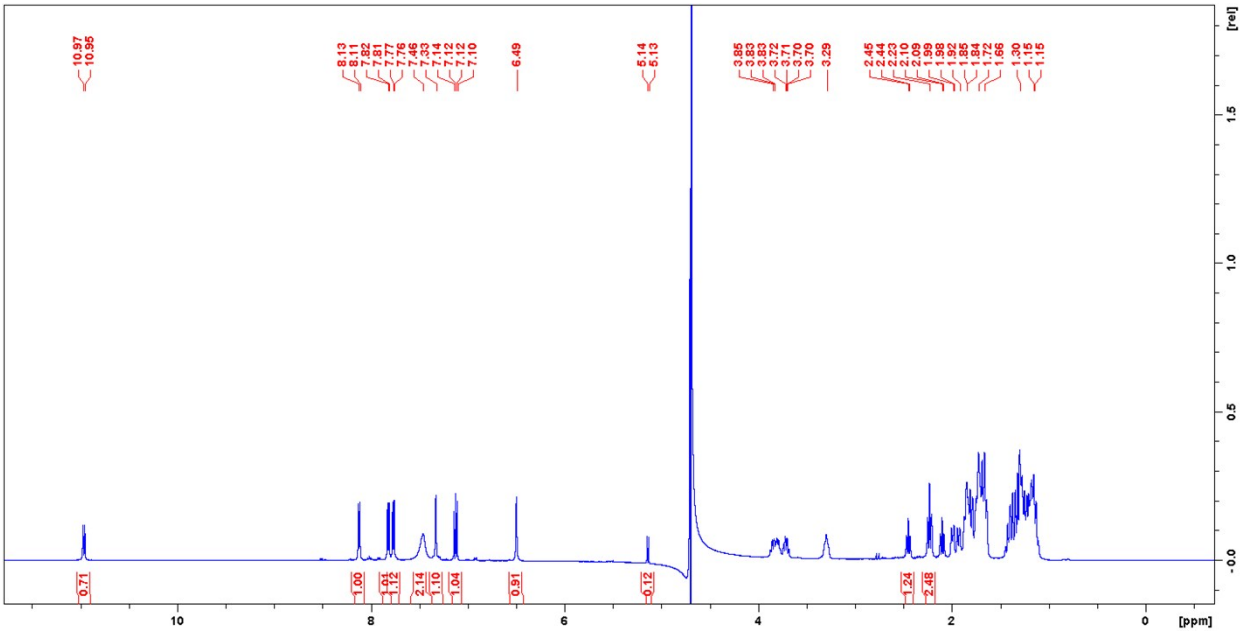


Figure S41. TOCSY NMR [600 MHz, H_2O/D_2O 90:10) spectrum of compound **5**

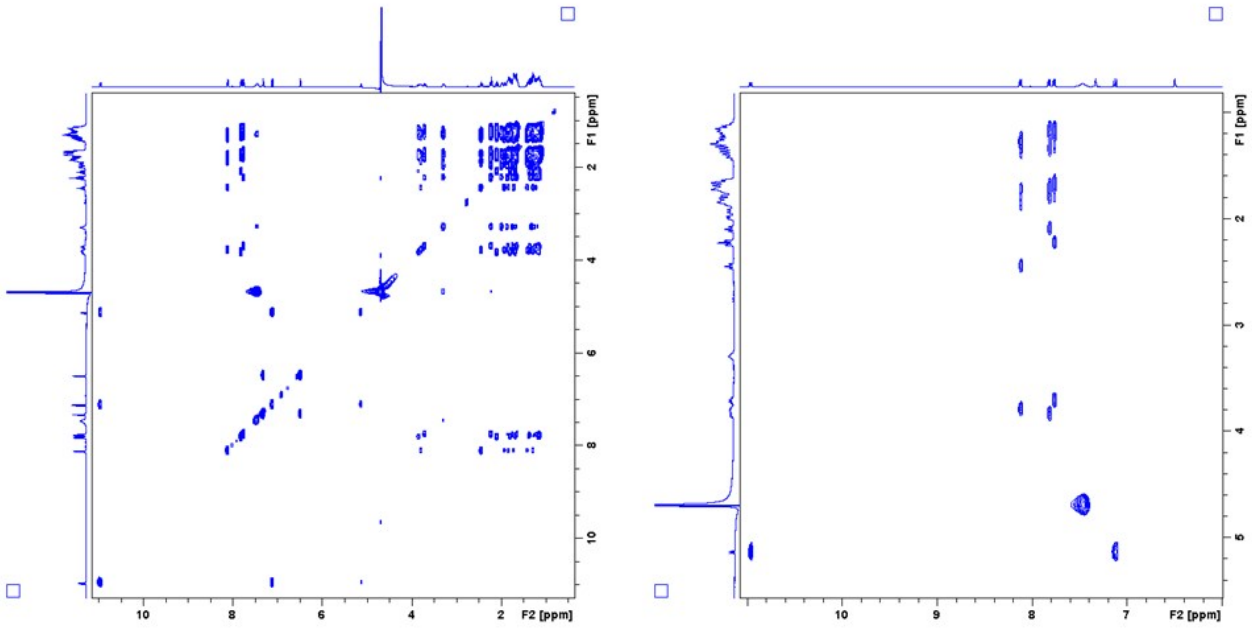


Figure S42. ROESY NMR [600 MHz, H_2O/D_2O 90:10) spectrum of compound **5**

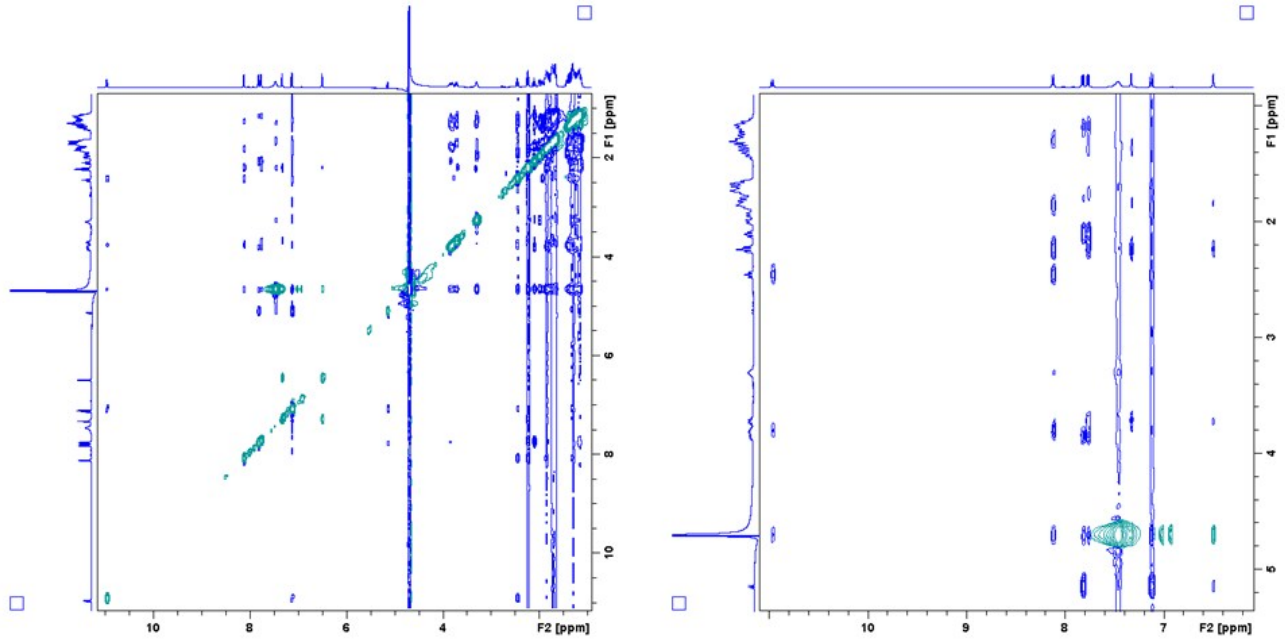


Figure S43. ^1H NMR [600 MHz, CD_3OH) spectrum of compound **5**

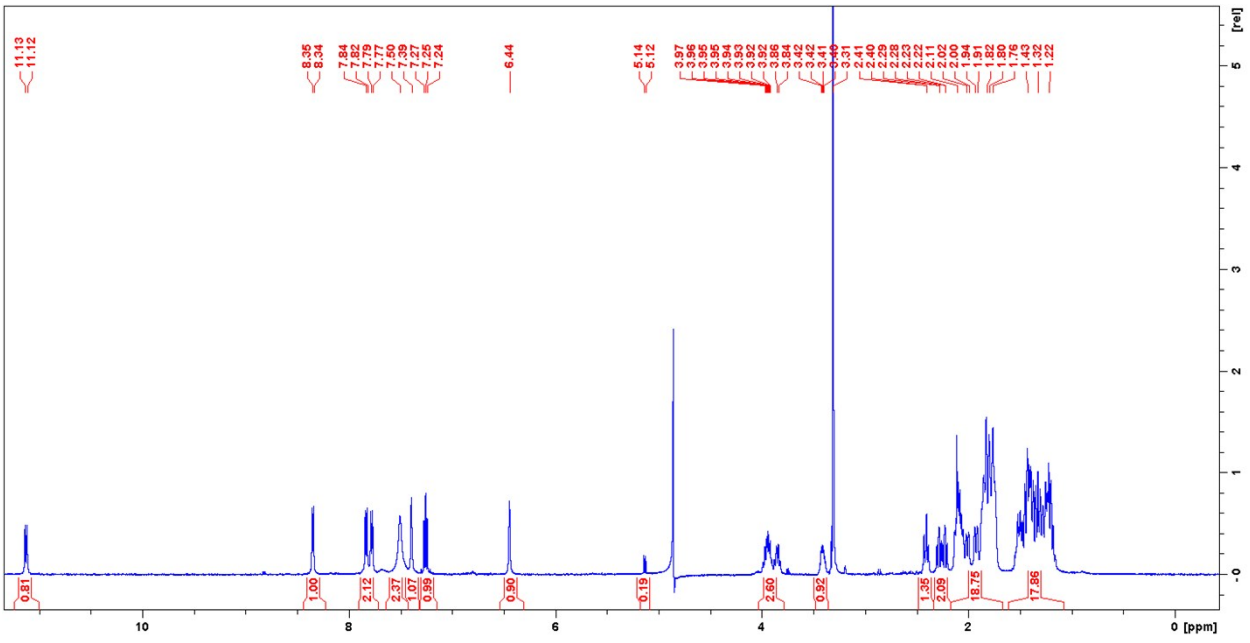


Figure S44. TOCSY NMR [600 MHz, CD_3OH) spectrum of compound **5**

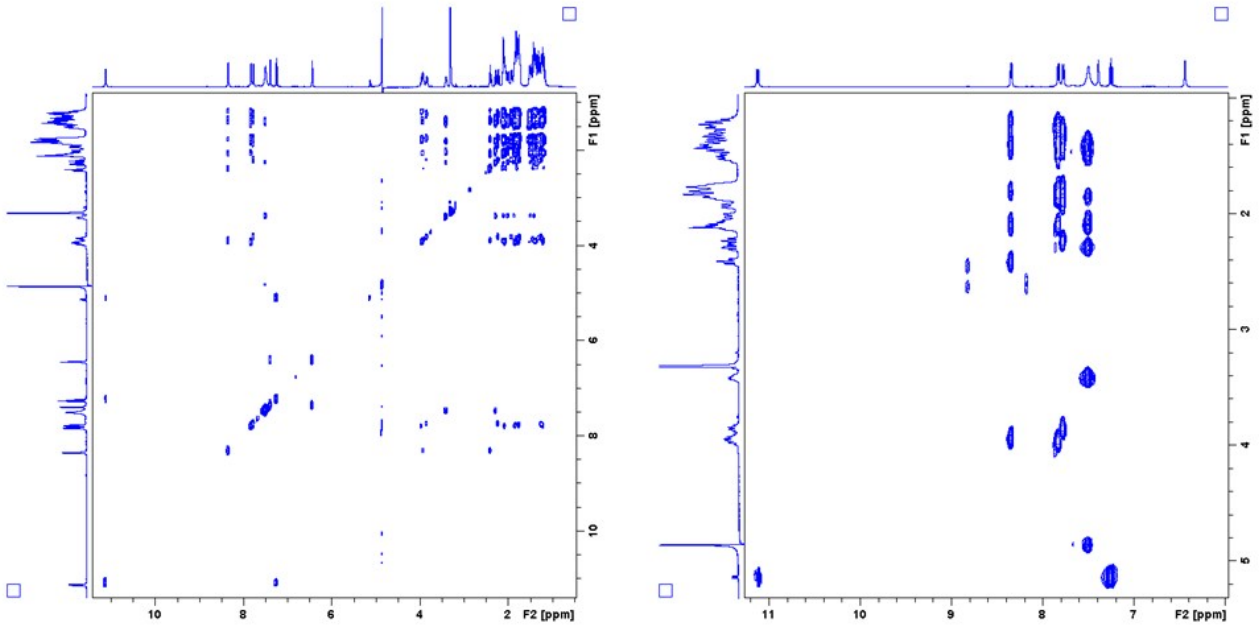


Figure S45. ROESY NMR [600 MHz, CD_3OH) spectrum of compound **5**

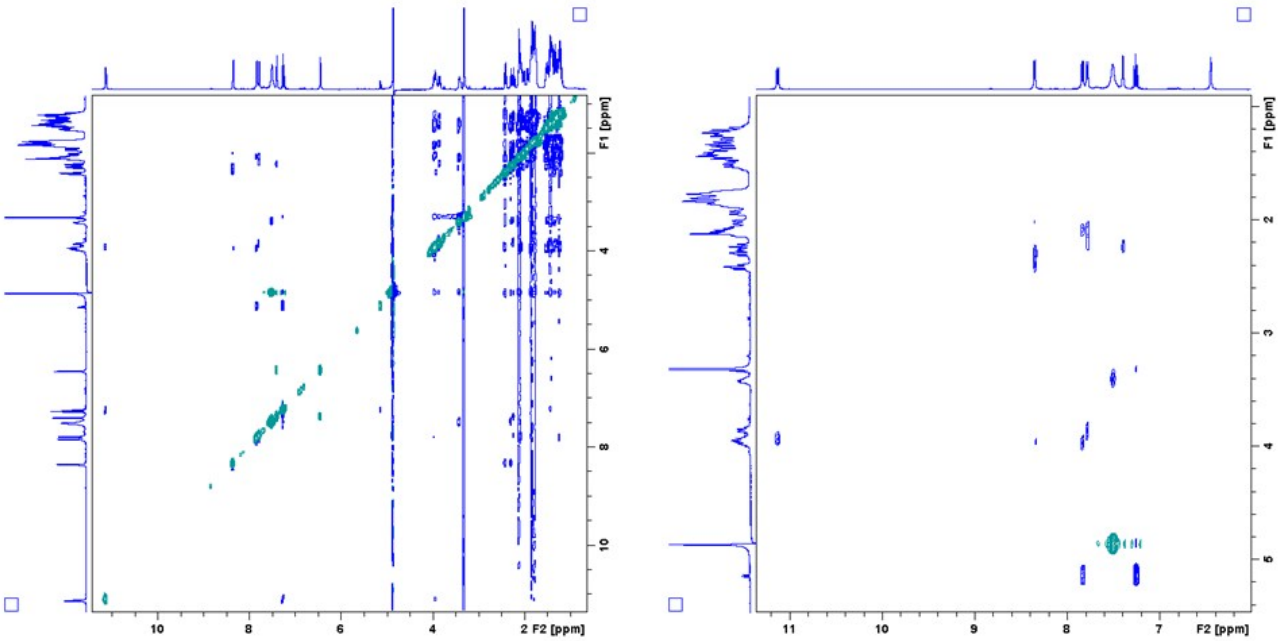


Figure S46. ^{1}H NMR [600 MHz, DMSO-d_6) spectrum of compound **5**

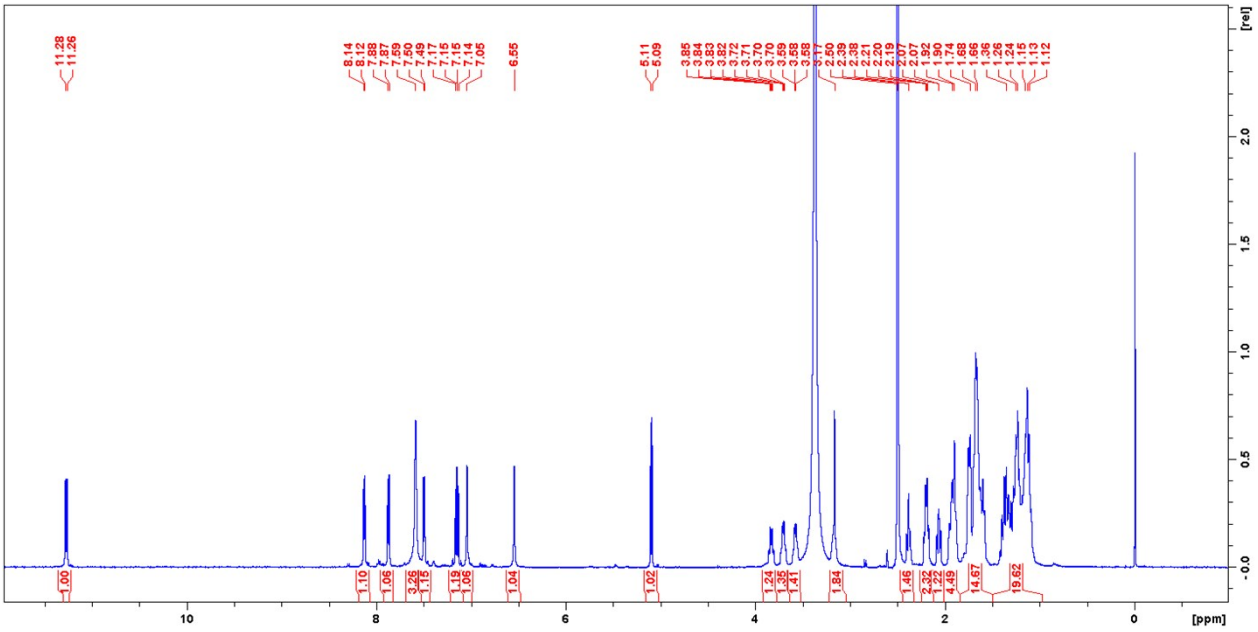


Figure S47. TOCSY NMR [600 MHz, DMSO-d_6) spectrum of compound **5**

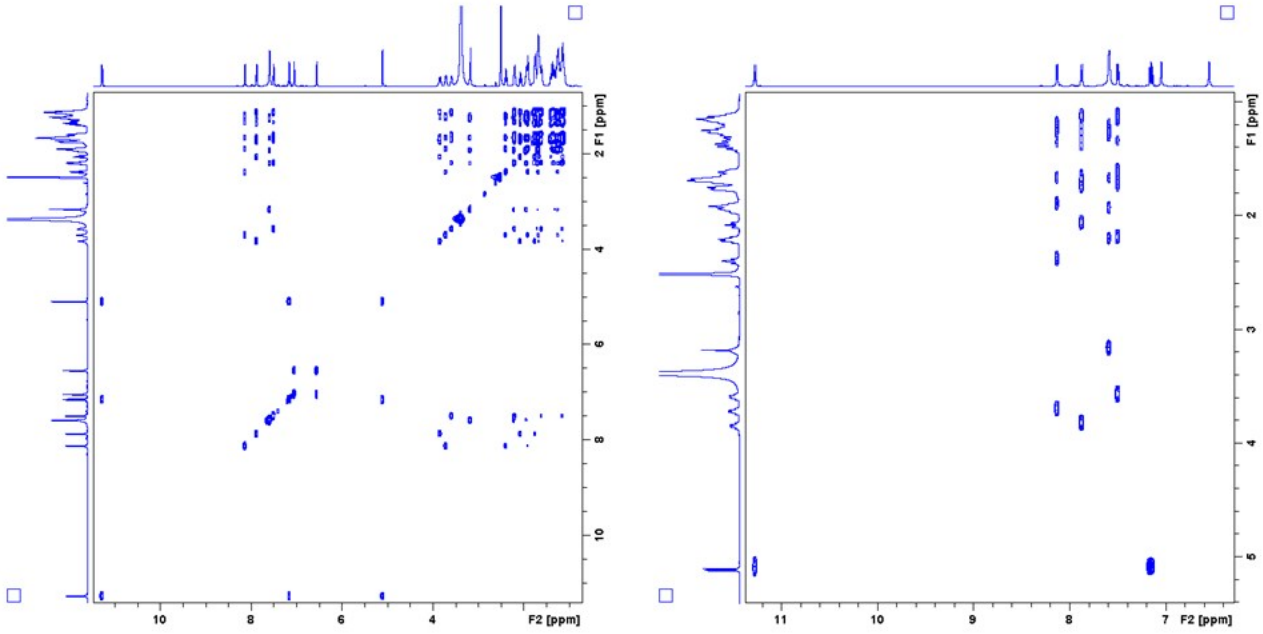


Figure S48. ROESY NMR [600 MHz, DMSO-d_6) spectrum of compound **5**

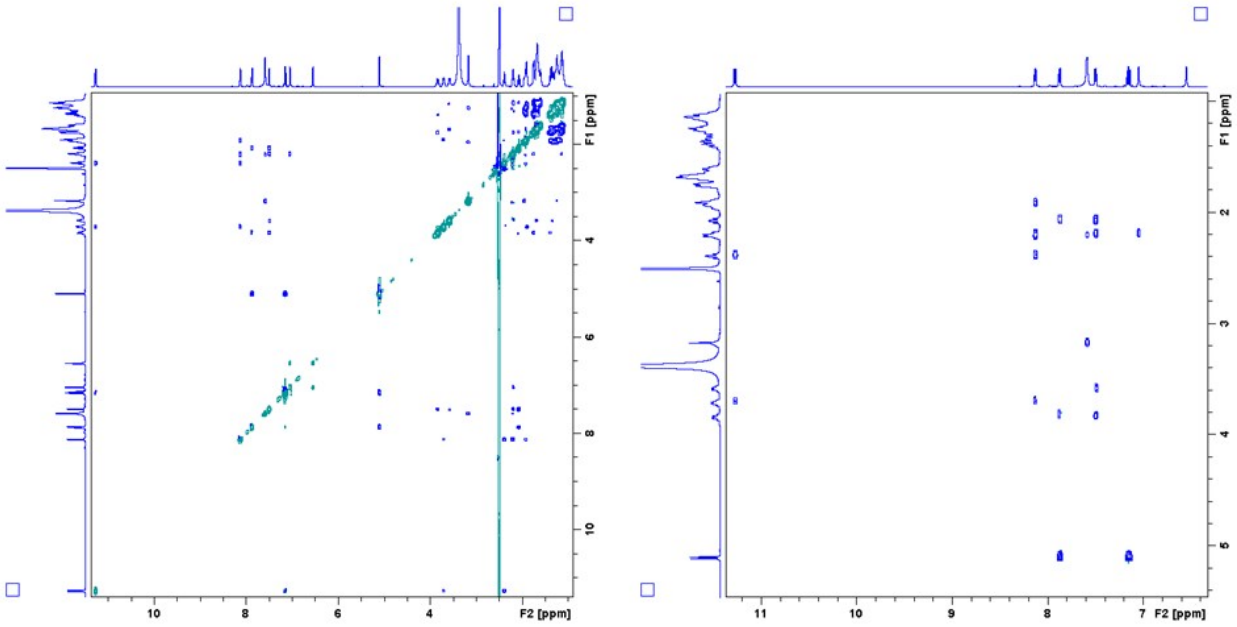


Figure S49. ^{1}H NMR [500 MHz, H_2O/D_2O 90:10) spectrum of compound **6**

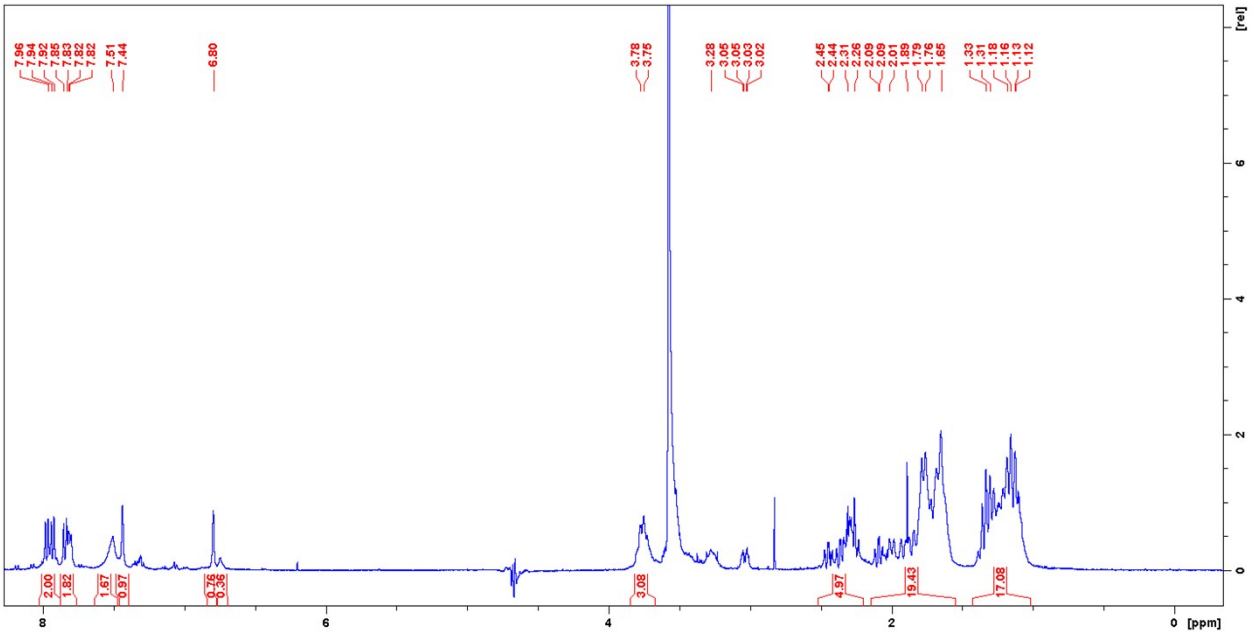


Figure S50. TOCSY NMR [500 MHz, H_2O/D_2O 90:10) spectrum of compound **6**

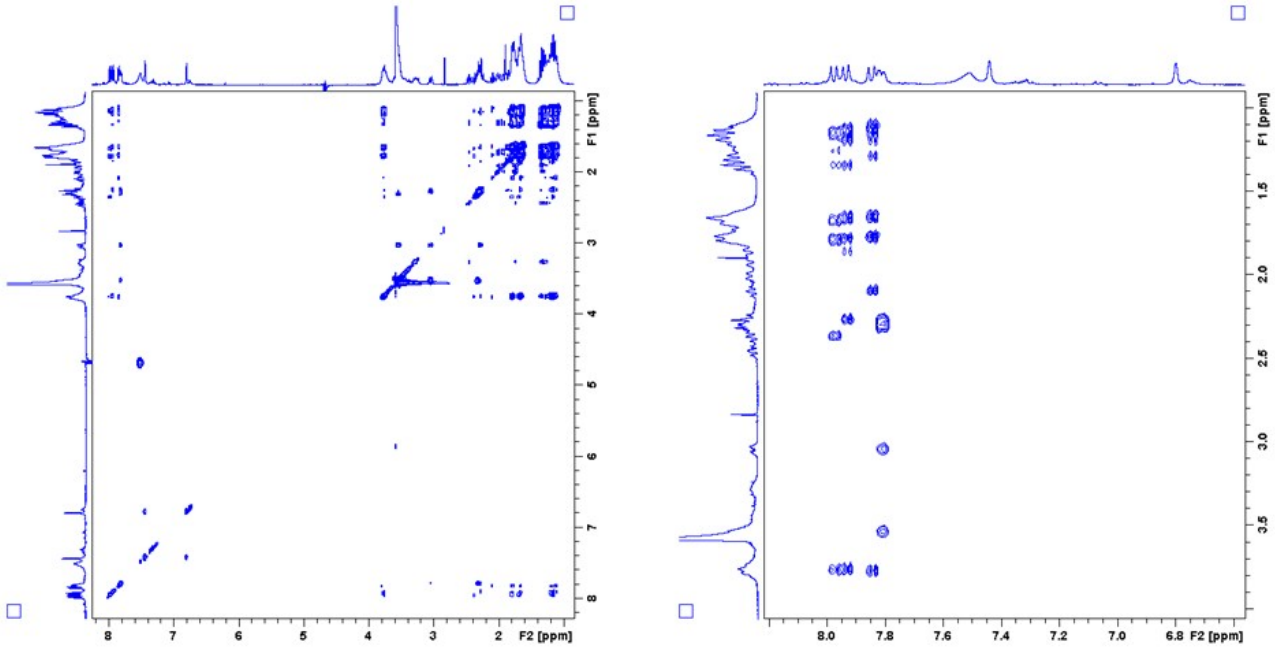


Figure S51. ROESY NMR [500 MHz, H_2O/D_2O 90:10) spectrum of compound **6**

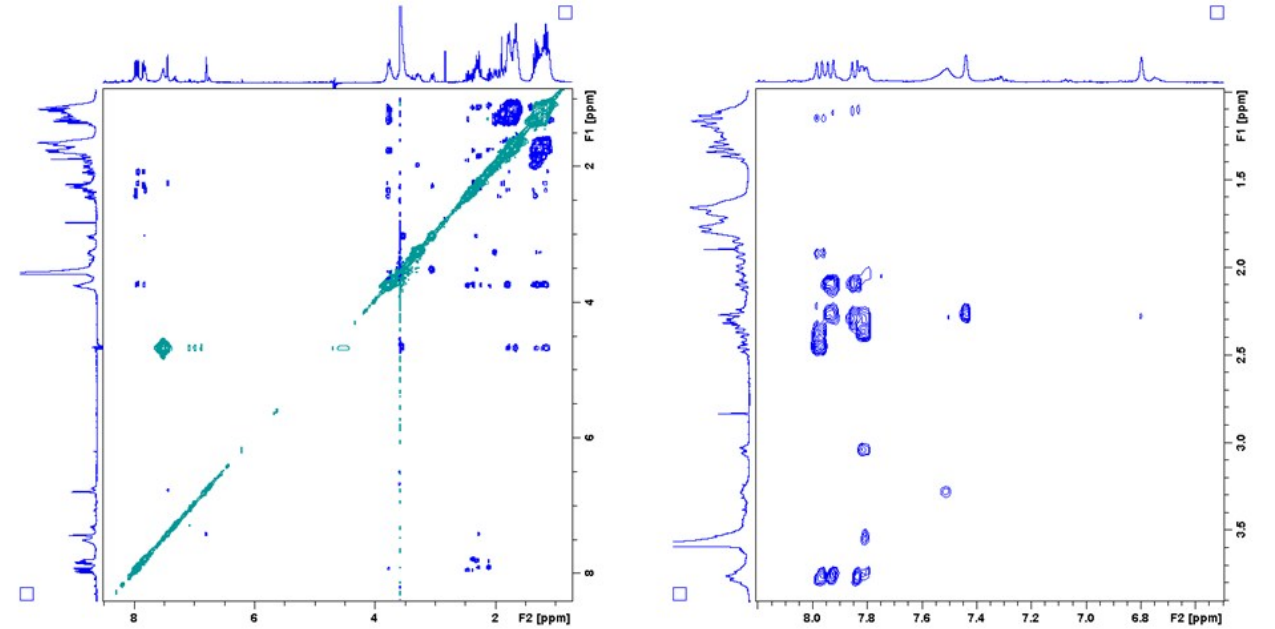


Figure S52. ^{1}H NMR [500 MHz, CD_3OH) spectrum of compound **6**

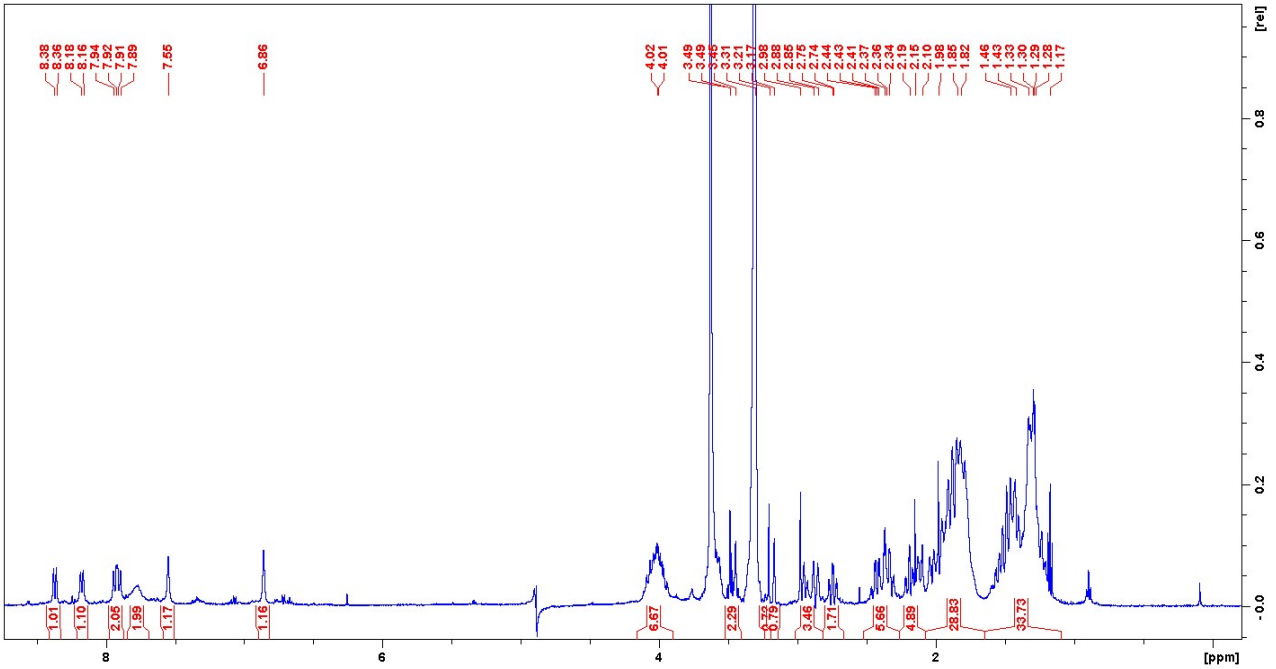


Figure S53. TOCSY NMR [500 MHz, CD_3OH) spectrum of compound **6**

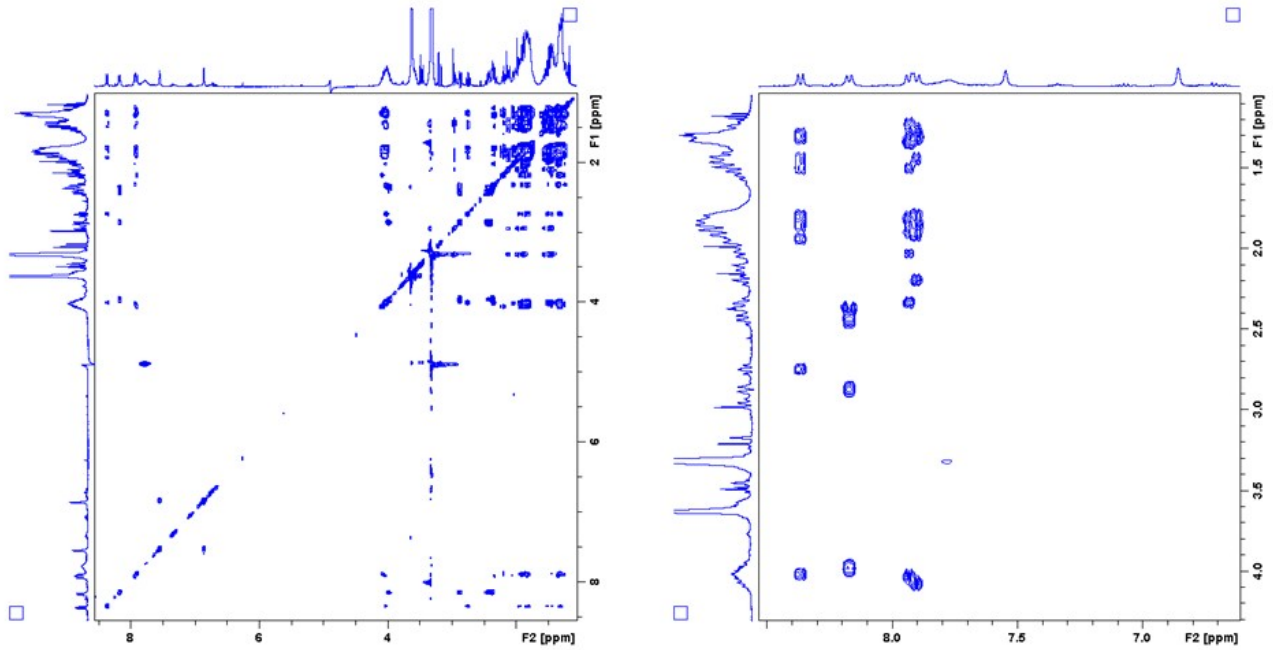


Figure S54. ROESY NMR [500 MHz, CD_3OH) spectrum of compound **6**

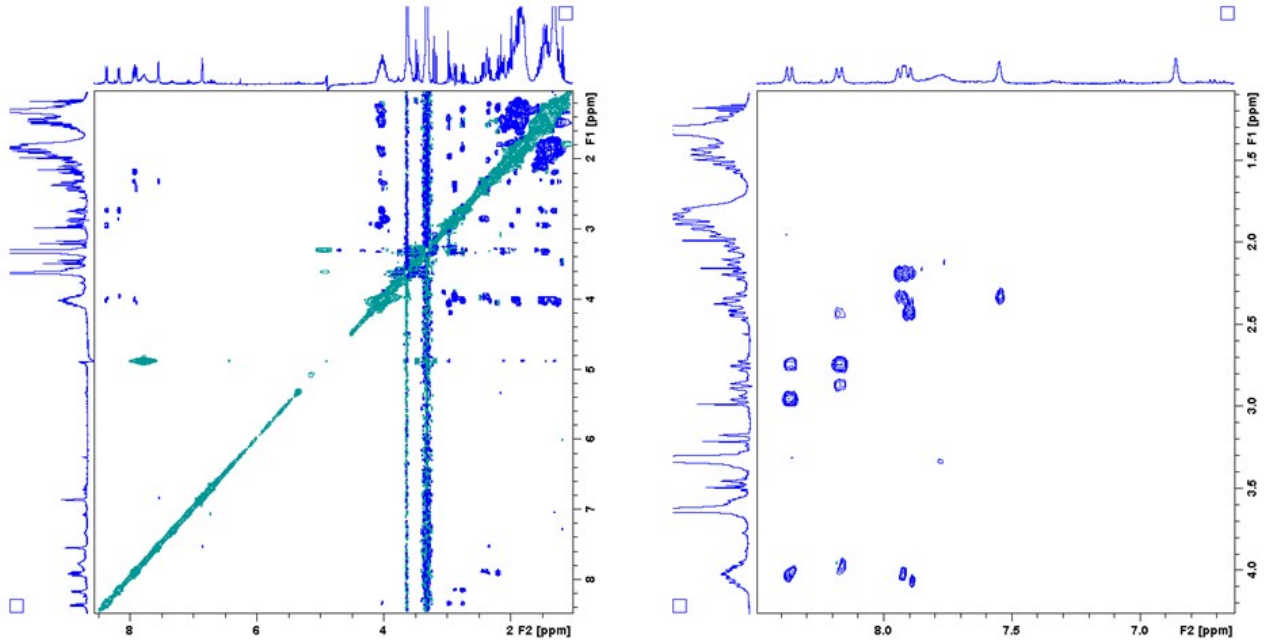


Figure S55. ^1H NMR [500 MHz, DMSO-d_6) spectrum of compound **6**

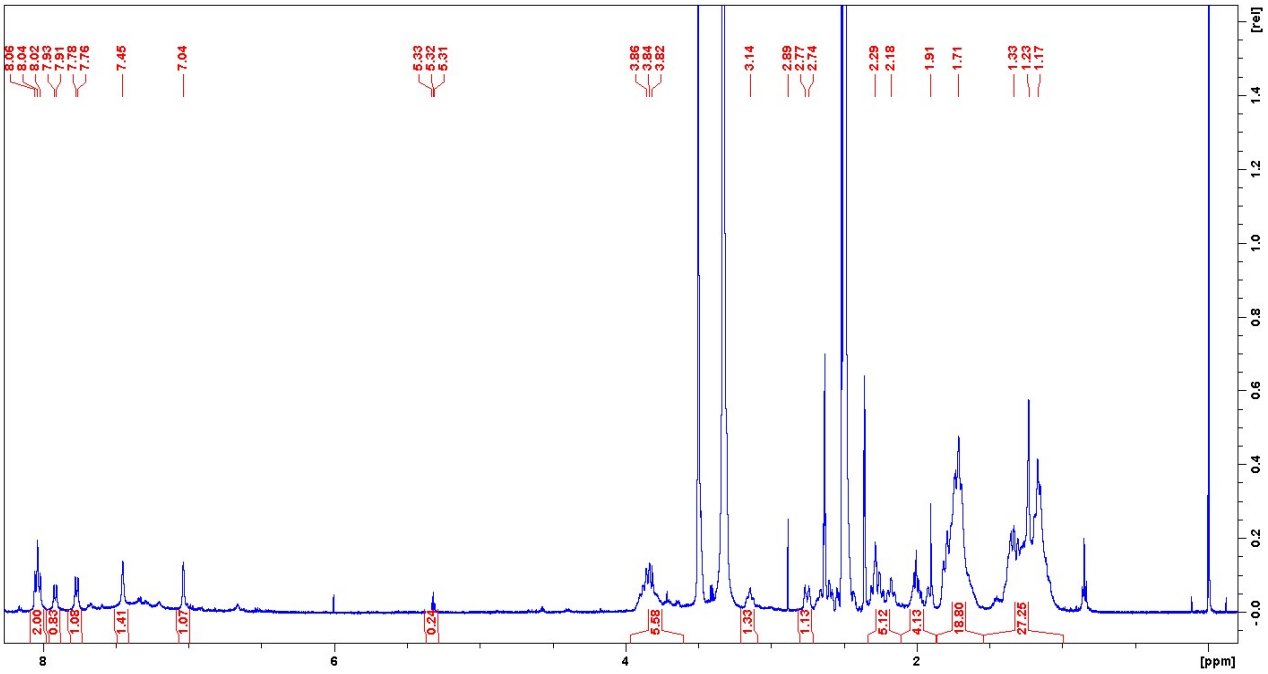


Figure S56. TOCSY NMR [500 MHz, DMSO-d_6) spectrum of compound **6**

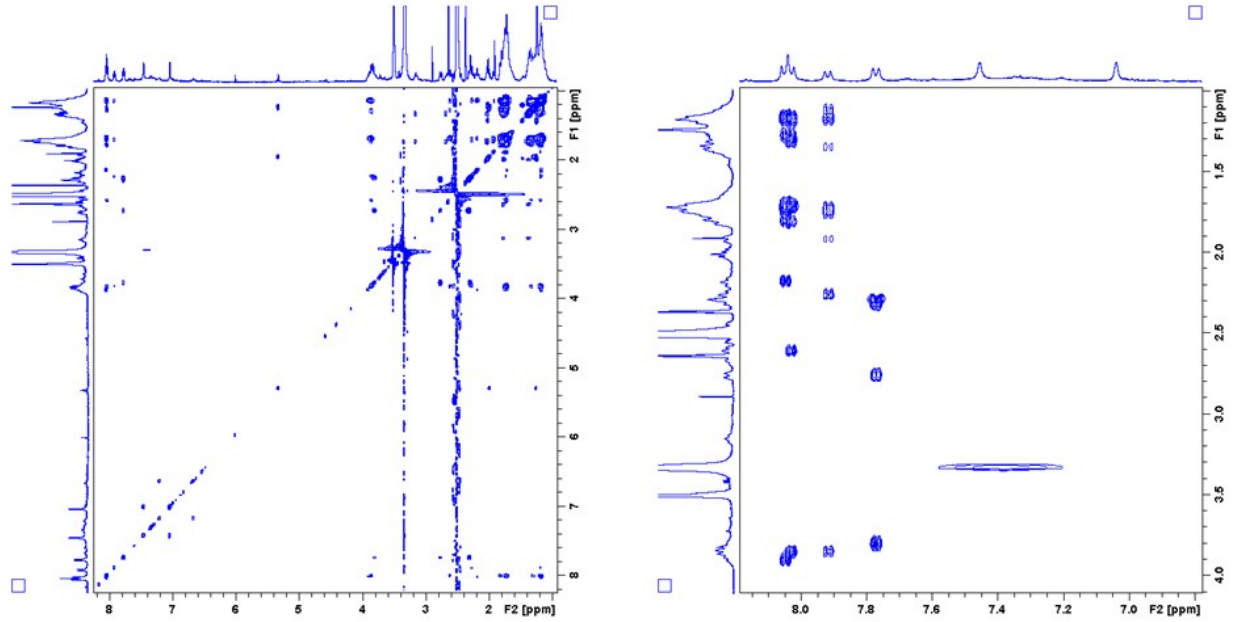


Figure S57. ROESY NMR [600 MHz, DMSO-d_6) spectrum of compound **6**

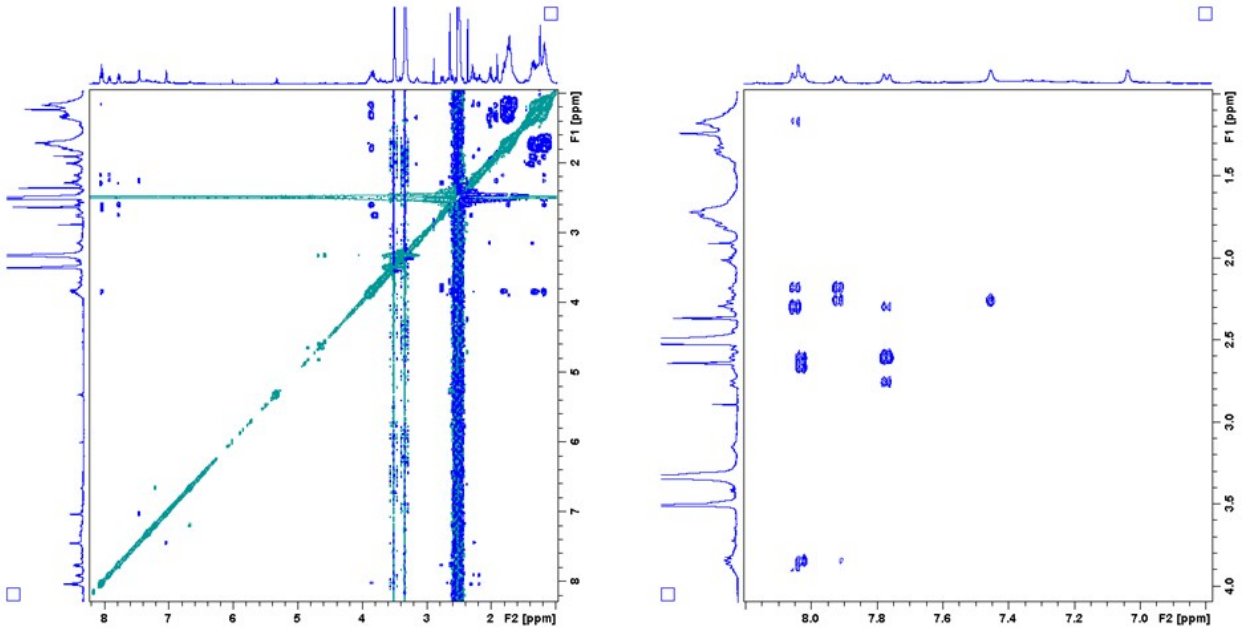
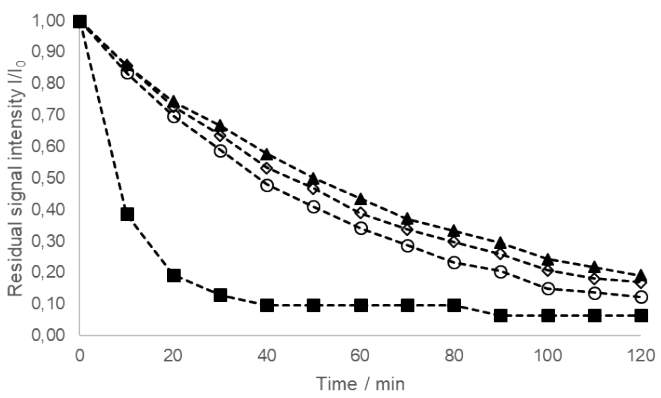


Figure S58. NH-ND exchange plots of compound **4** (a) and **5** (b)

a)



b)

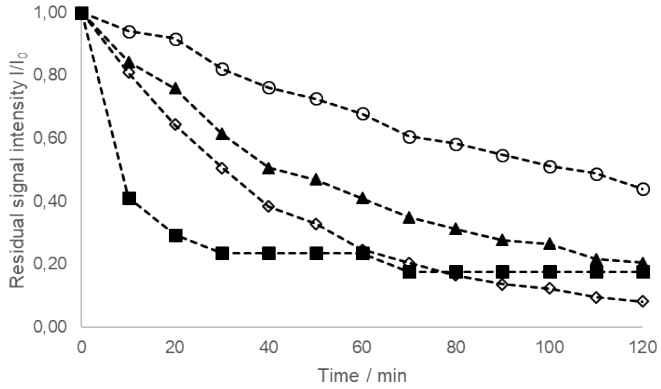


Figure S59. Assignment of backbone protons of compound **1** (a: H_2O/D_2O 90:10; b: CH_3OH; c: DMSO-d_6)

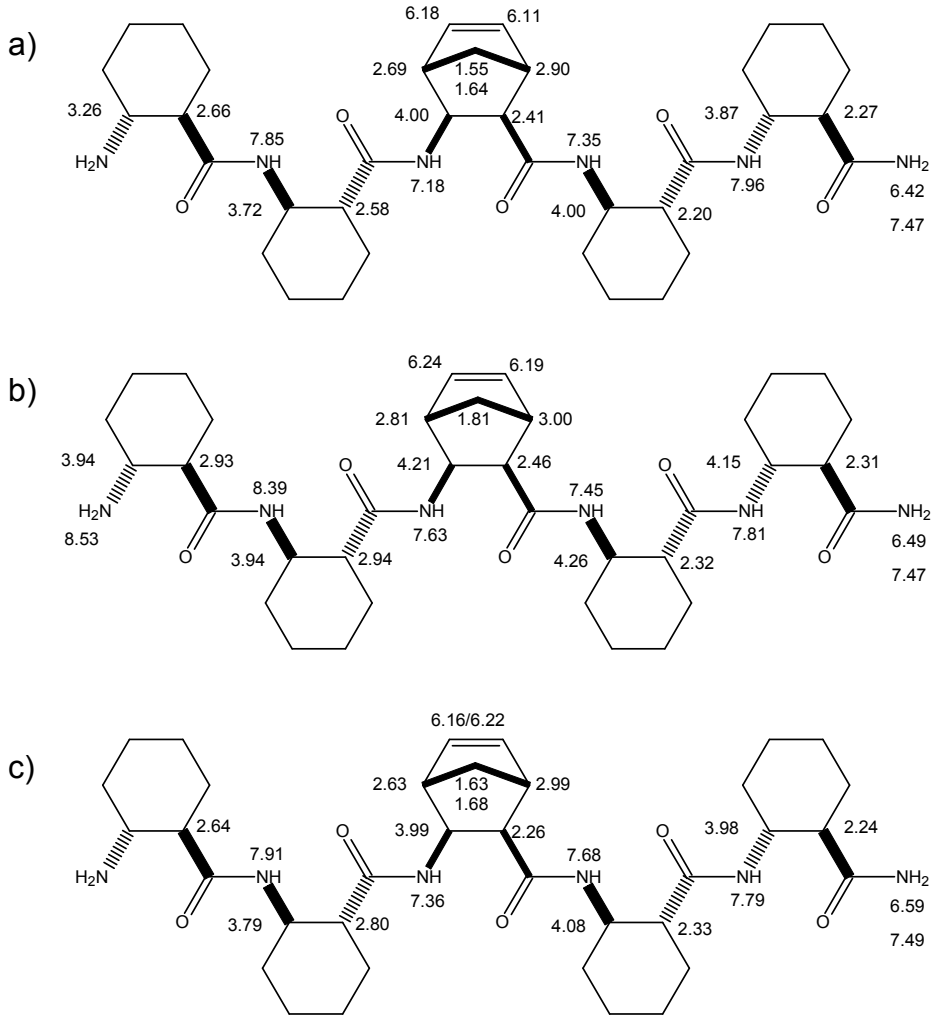


Figure S60. Assignment of backbone protons of compound **2** (a: H_2O/D_2O 90:10; b: CH_3OH; c: DMSO- d_6)

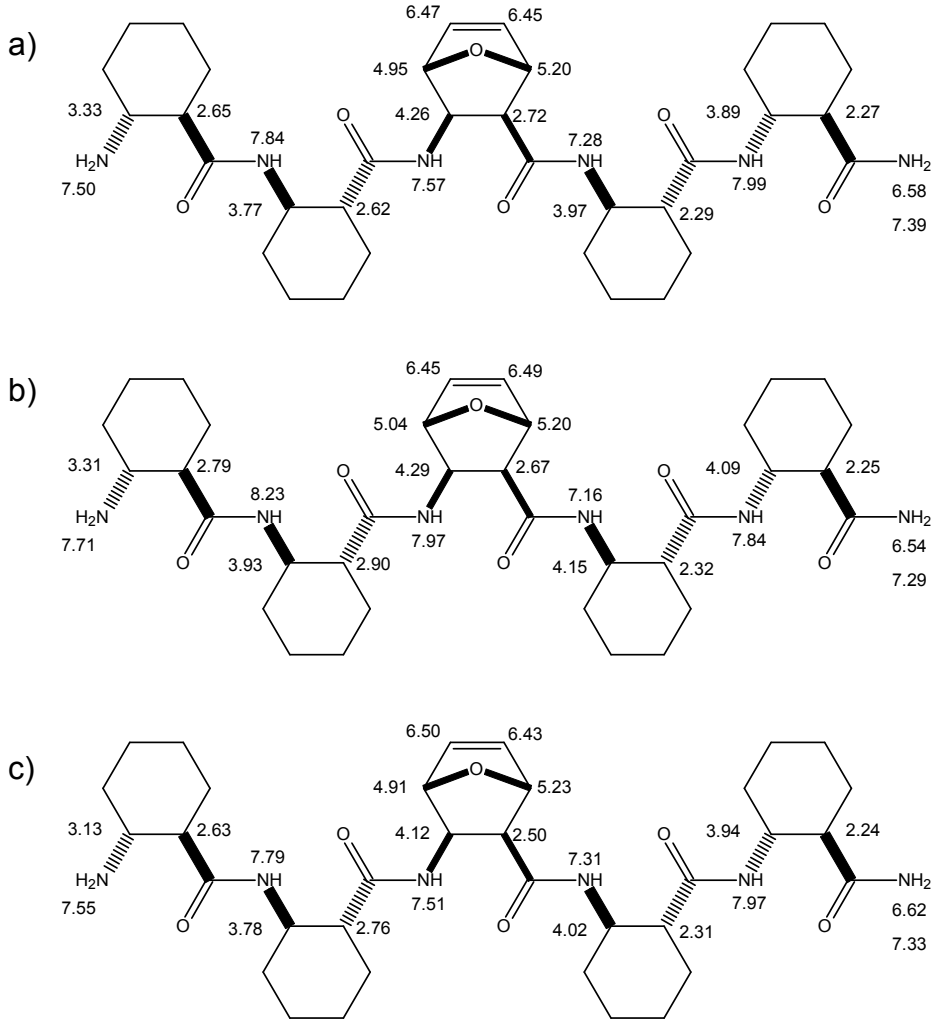


Figure S61. Assignment of backbone protons of compound **3** (a: H_2O/D_2O 90:10; b: CH_3OH; c: DMSO-d_6)

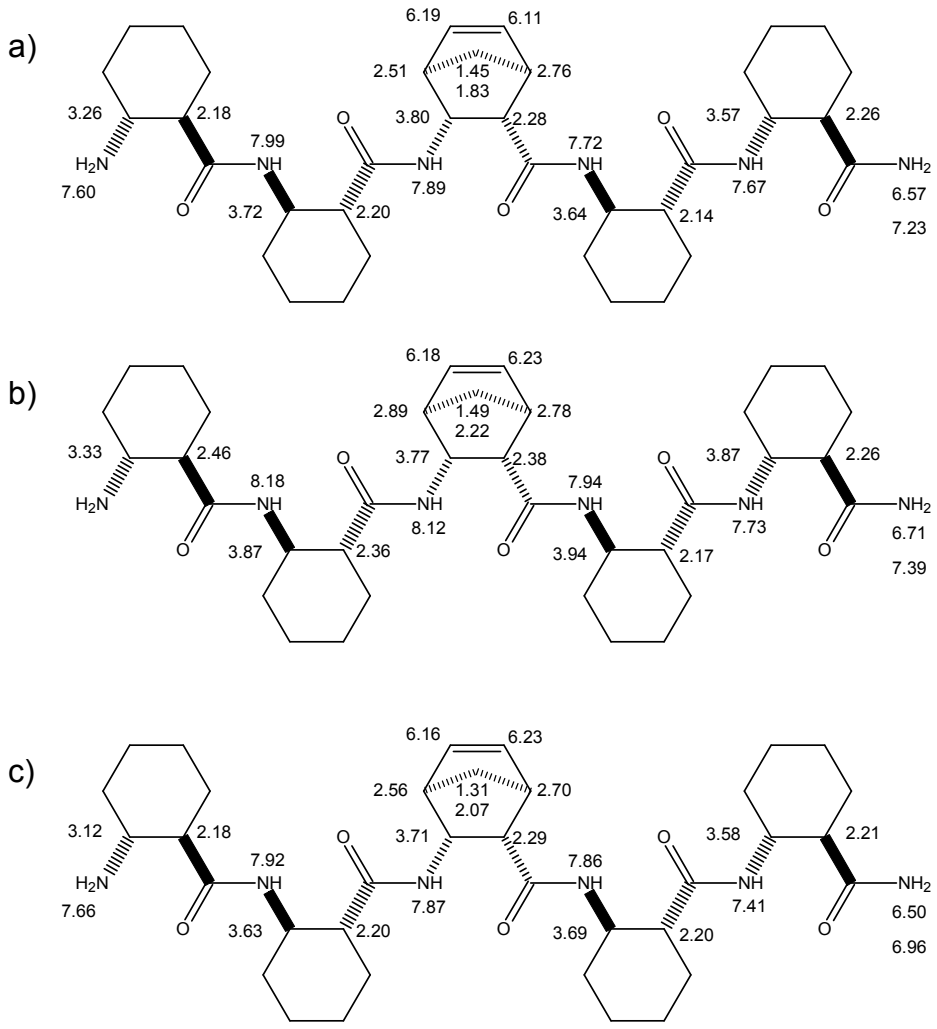


Figure S62. Assignment of backbone protons of compound **4** (a: H_2O/D_2O 90:10; b: CH_3OH; c: DMSO-d_6)

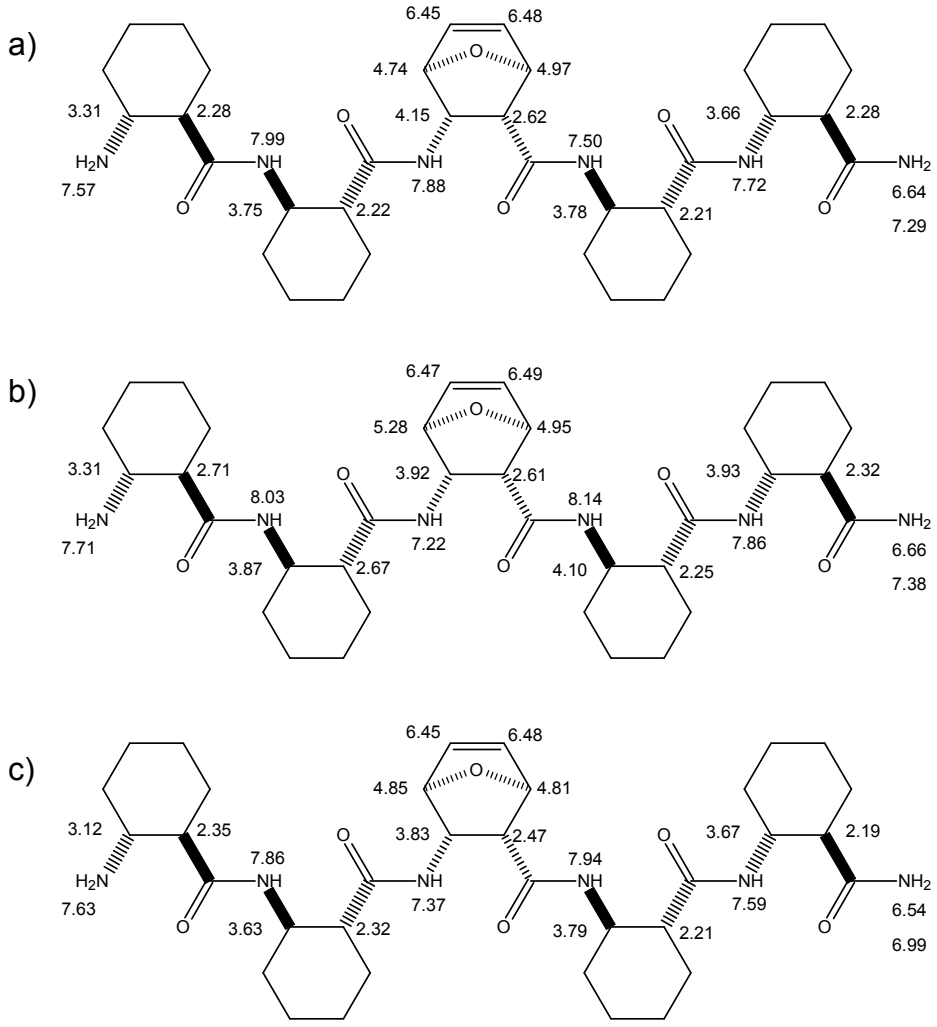
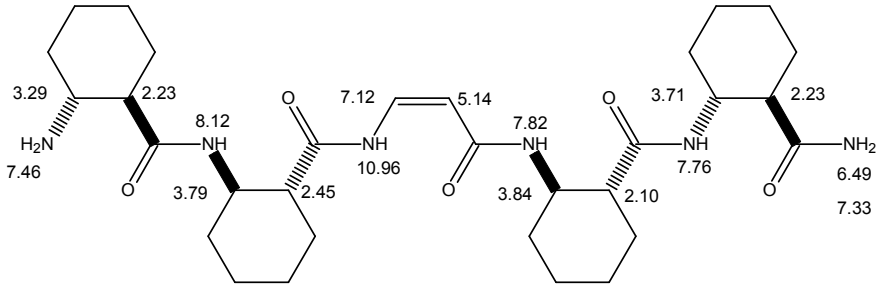
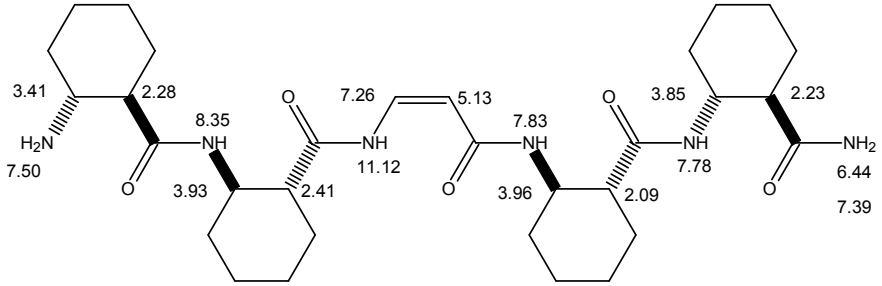


Figure S63. Assignment of backbone protons of compound **5** (a: H_2O/D_2O 90:10; b: CH_3OH; c: DMSO-d_6)

a)



b)



c)

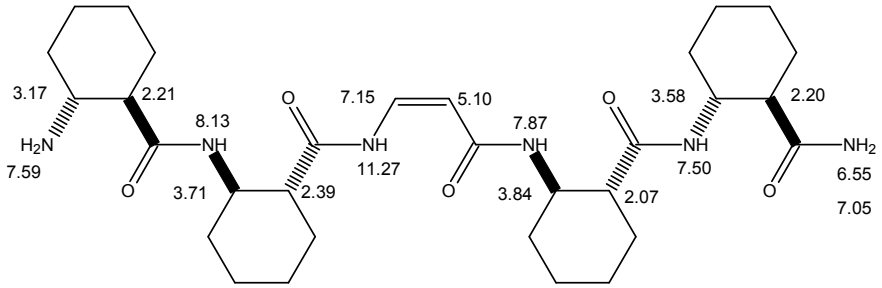


Figure S64. Assignment of backbone protons of compound **6** (a: H_2O/D_2O 90:10; b: CH_3OH; c: DMSO-d_6)

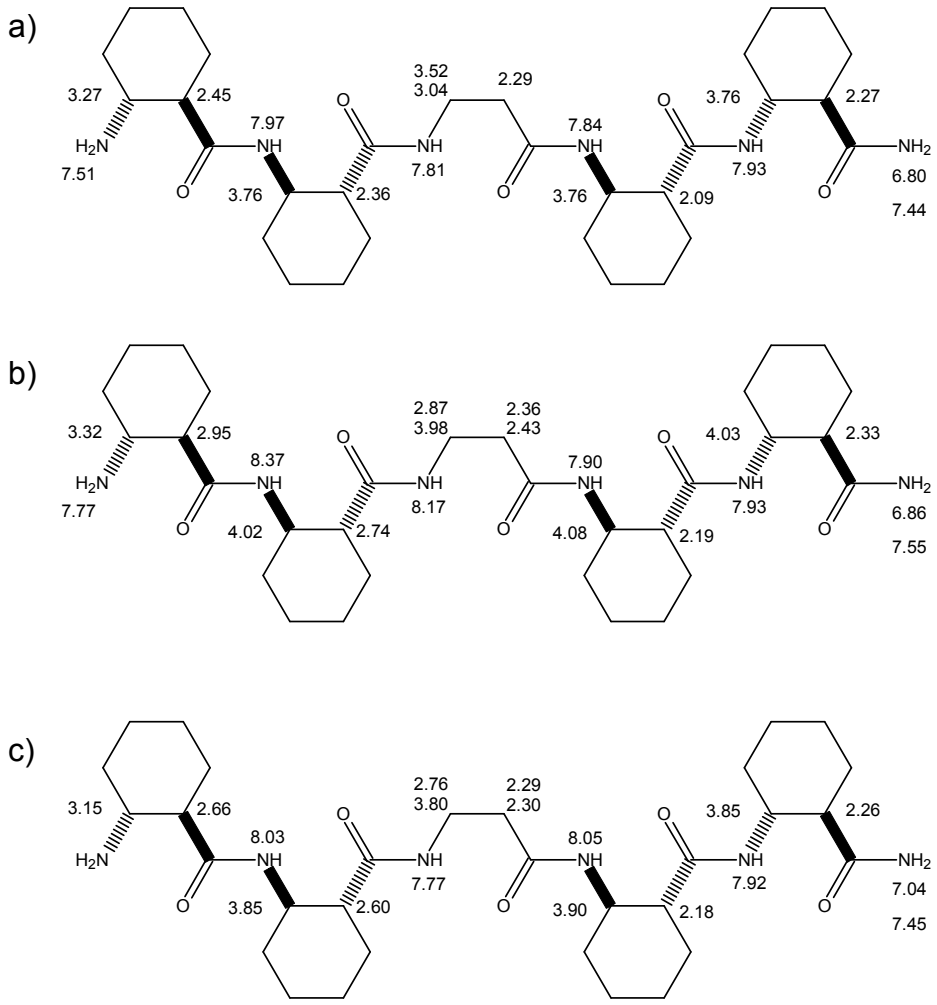


Figure S65. NOE correlations in compound **3**, **4** and **5**

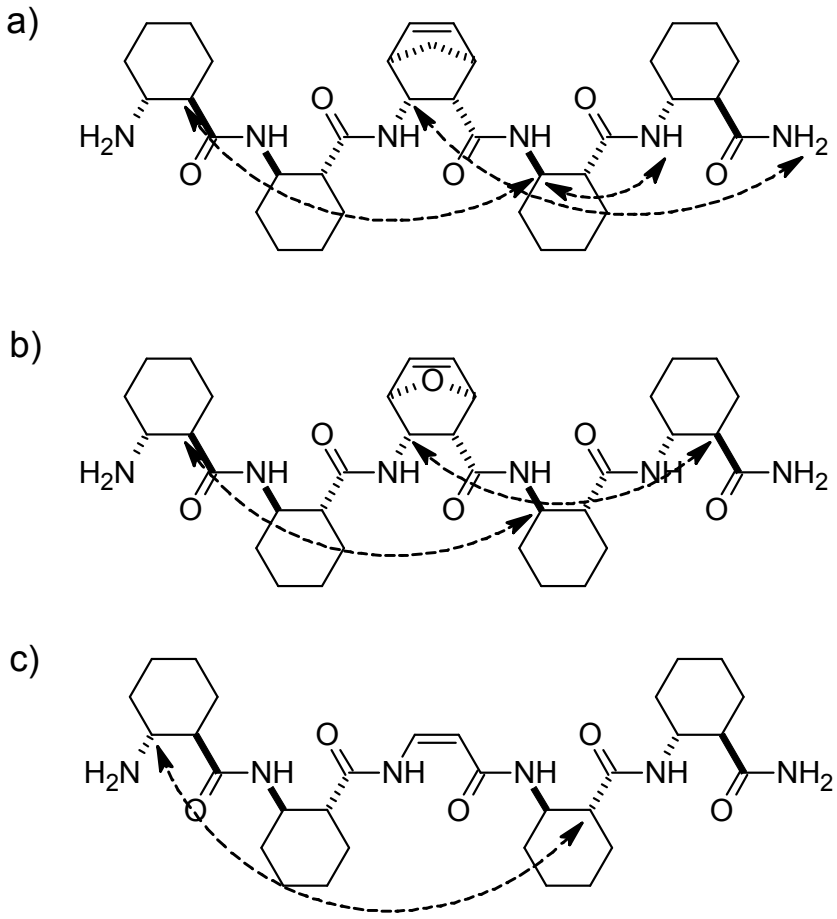


Figure S66. HPLC-MS chromatogram and mass spectrum of **1**: The following retention time and molecular weight were determined: **1**: {RT= 17.58, m/z = 653 $[M + H]^+$}.

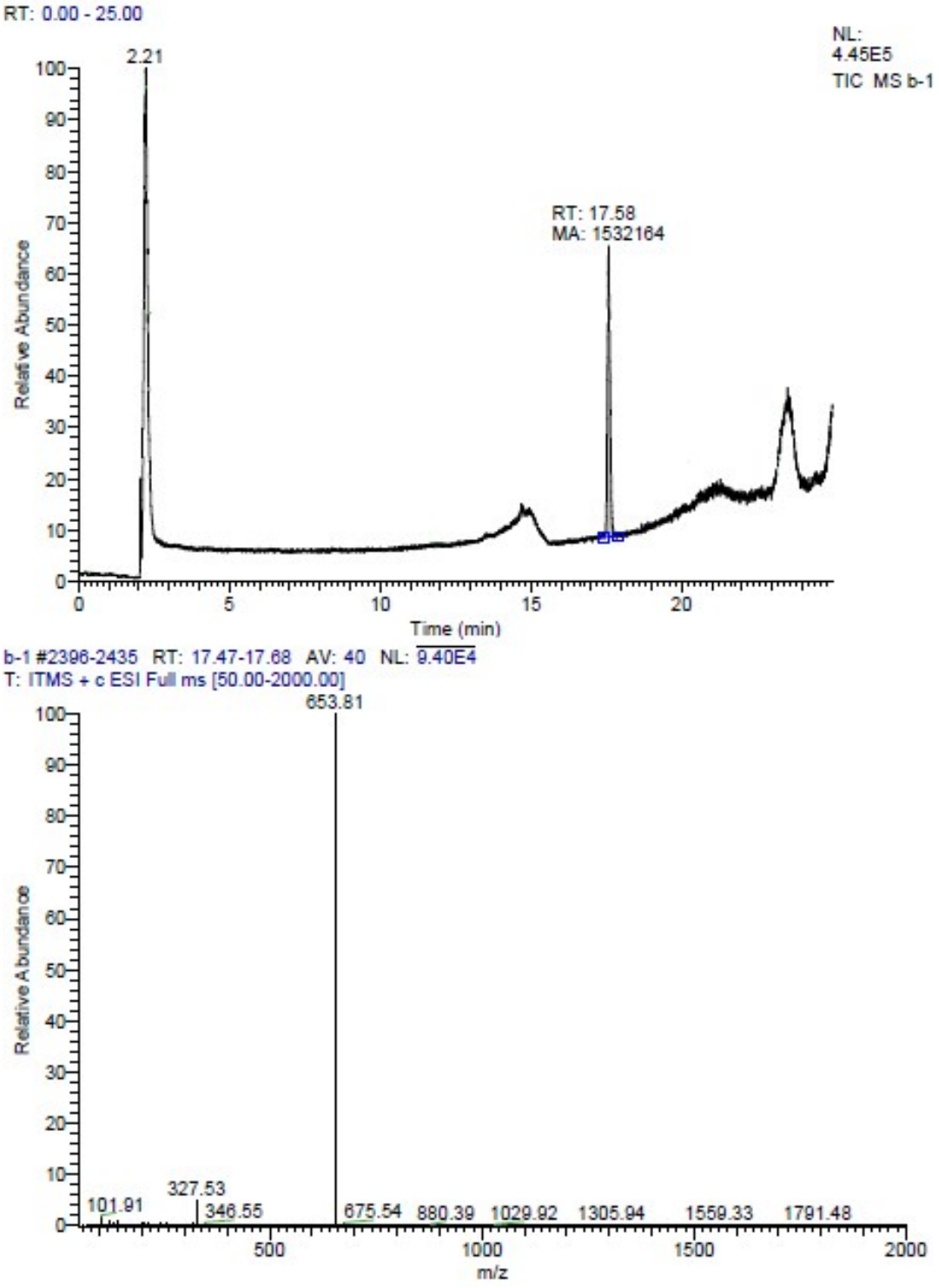


Figure S67. HPLC-MS chromatogram and mass spectrum of **2**: The following retention time and molecular weight were determined: **2**: {RT= 16.82, m/z = 655 $[M + H]^+$}.

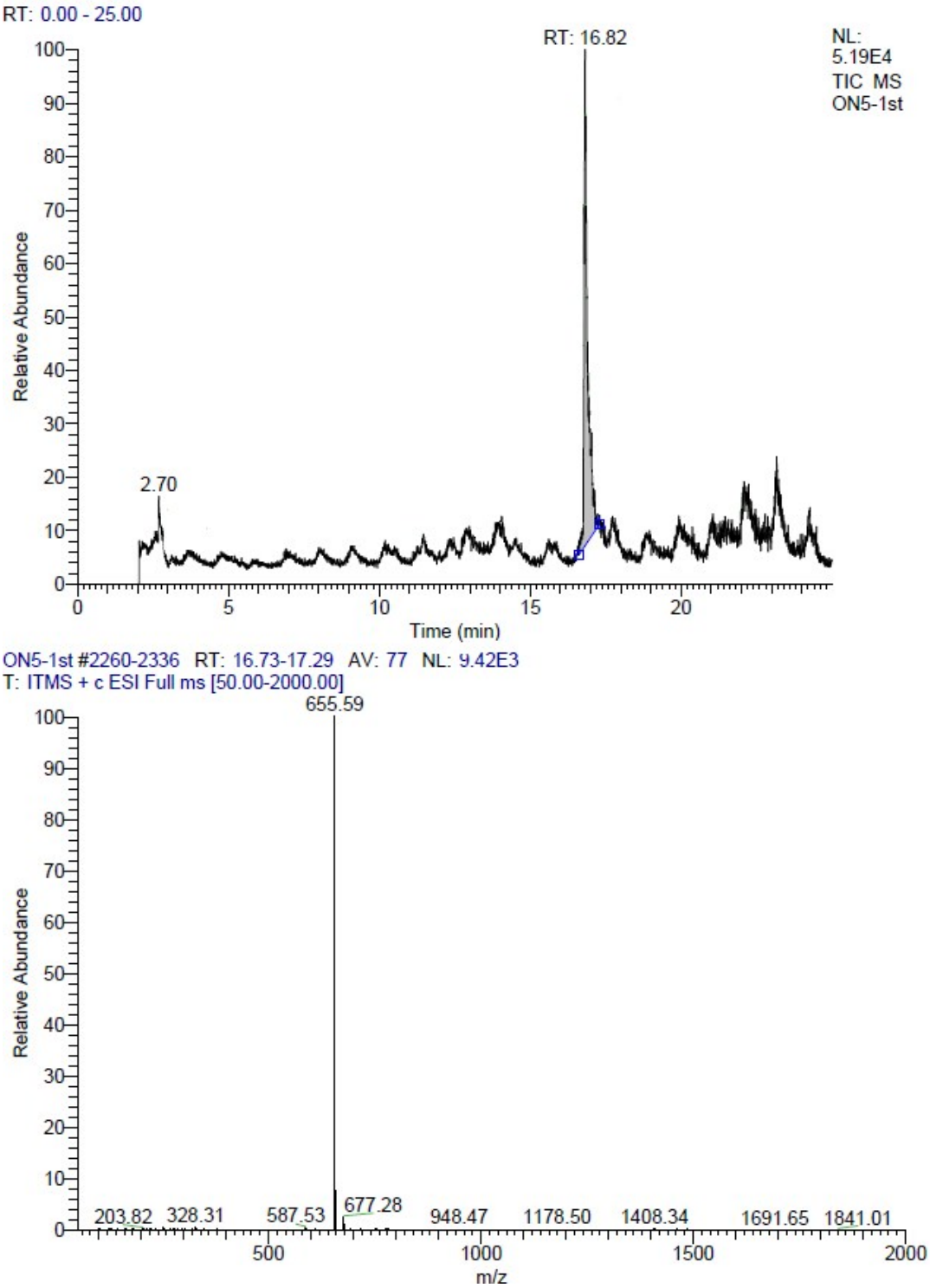


Figure S68. HPLC-MS chromatogram and mass spectrum of **3**: The following retention time and molecular weight were determined: **3**: {RT= 14.97, m/z = 653 $[M + H]^+$}.

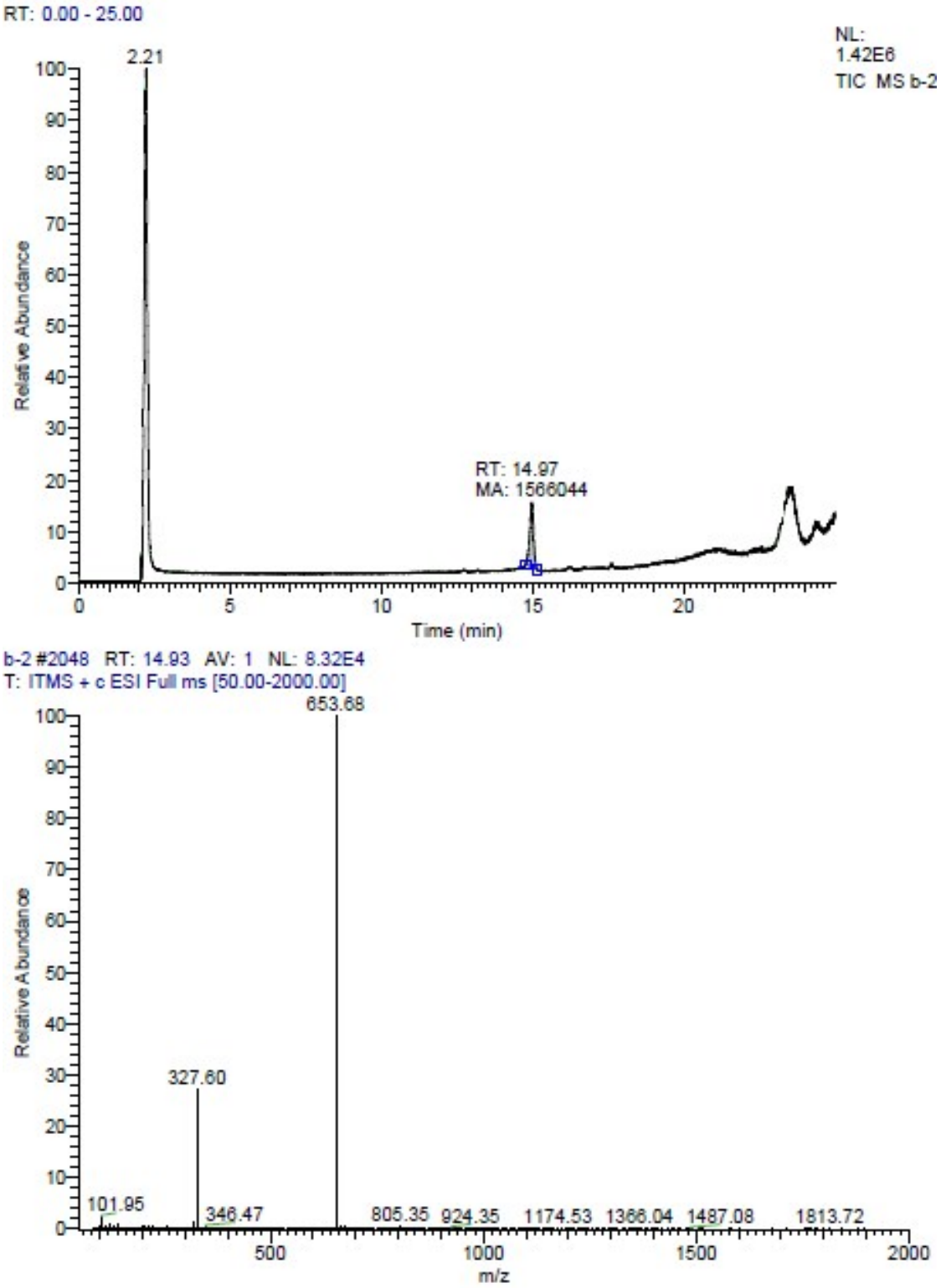


Figure S69. HPLC-MS chromatogram and mass spectrum of **4**: The following retention time and molecular weight were determined: **4**: {RT= 13.61, m/z = 655 $[M + H]^+$}.

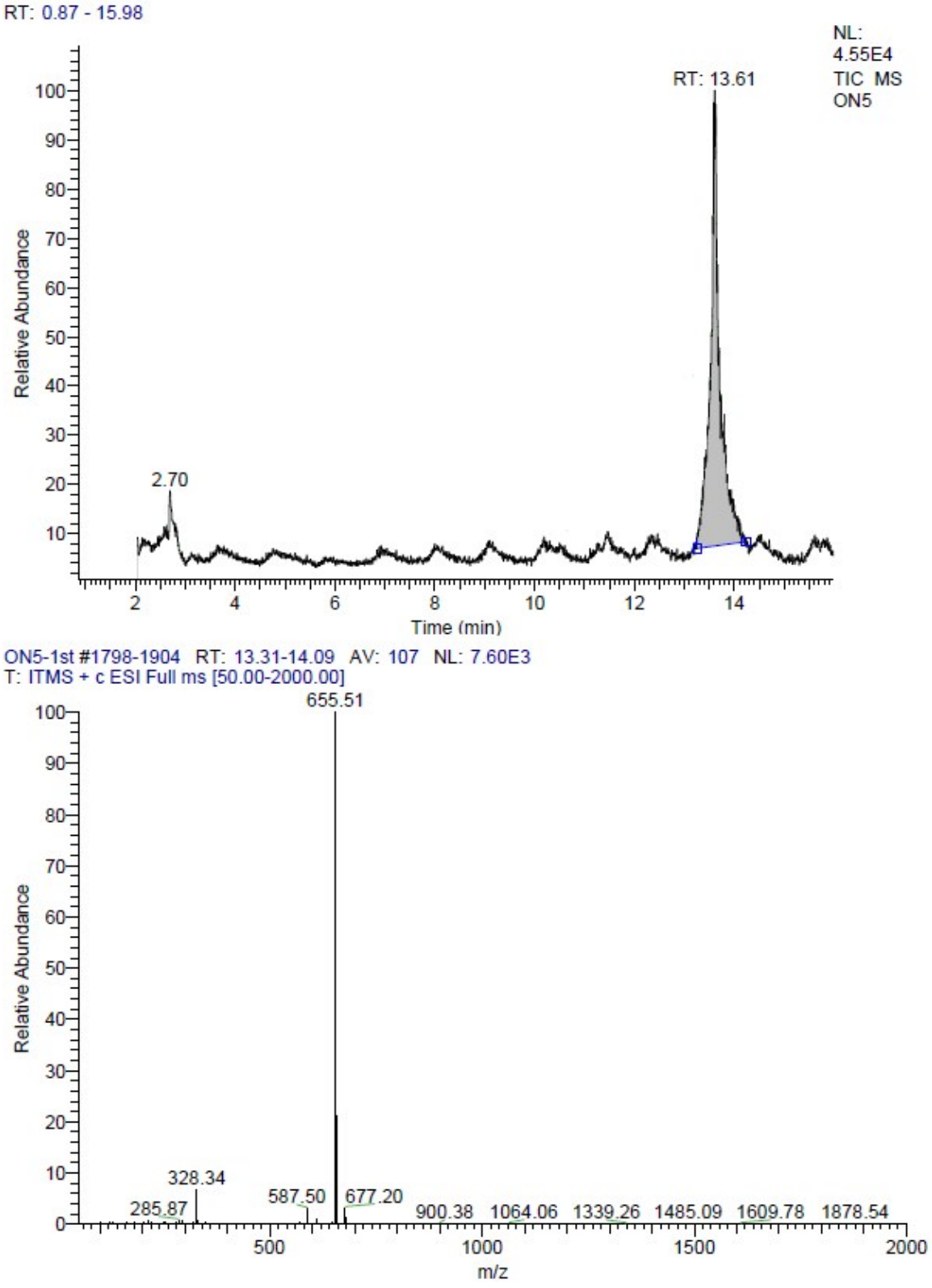


Figure S70. HPLC-MS chromatogram and mass spectrum of **5**: The following retention time and molecular weight were determined: **5**: {RT= 13.74, m/z = 587 $[M + H]^+$}.

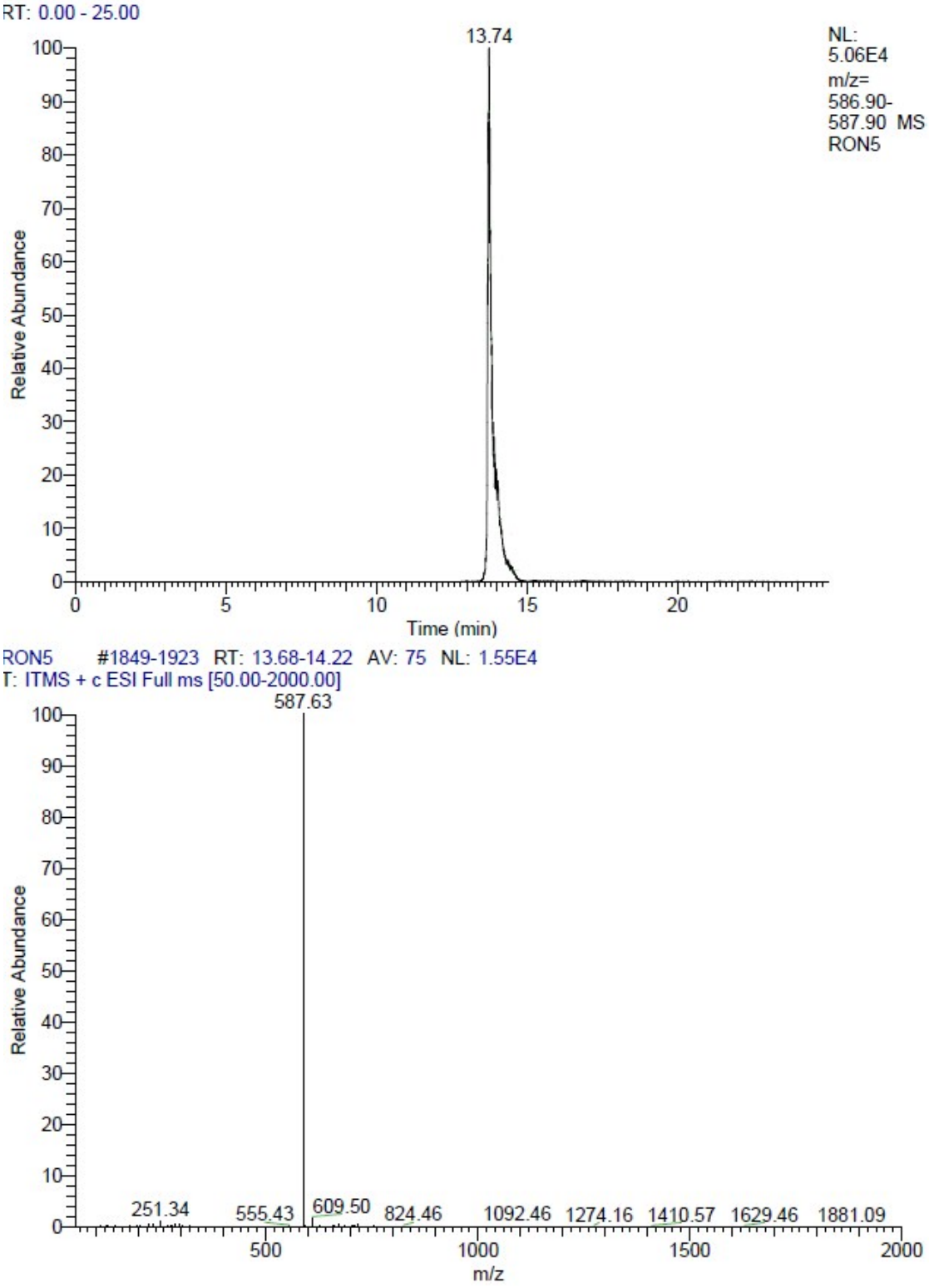


Figure S71. HPLC-MS chromatogram and mass spectrum of **6**: The following retention time and molecular weight were determined: **6**: {RT= 14.60, m/z = 589 $[M + H]^+$}.

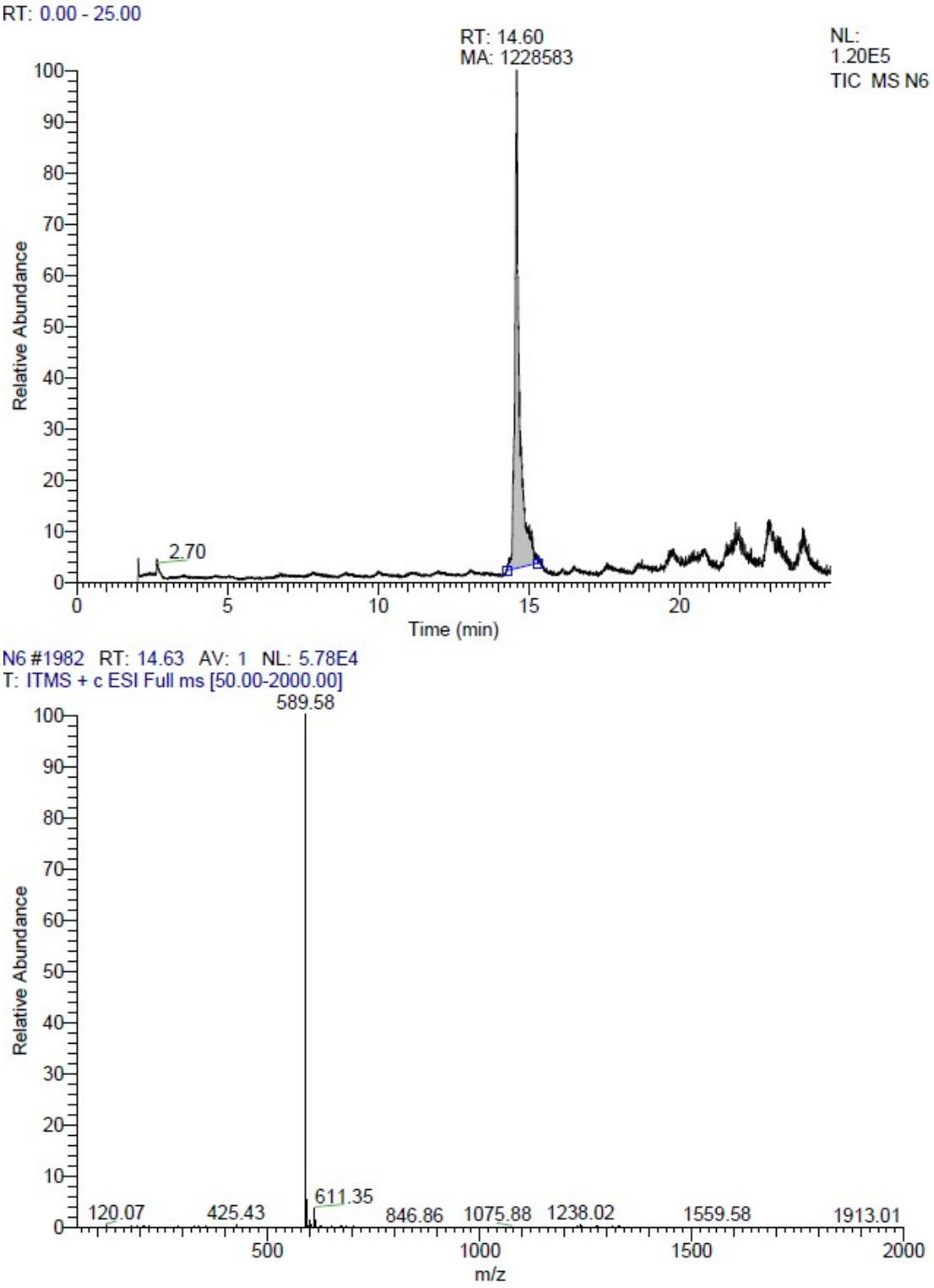


Figure S72. ^{1}H NMR spectrum of compound **(+)-9** 1.41 (d, *J* = 8.6 Hz, 1H), 2.14 (d, *J* = 8.3 Hz, 1H), 2.42 (d, *J* = 6.8 Hz, 1H) 2.59-2.64 (m, 1H) 2.85-2.90 (m, 1H), 3.77-3.85 (t, *J* = 7.1 Hz, 1H), 4.15-4.27 (m, 3H), 6.15-6.25 (m, 2H), 7.29-7.48 (m, 5H), 7.89 (d, *J* = 7.6 Hz, 2H)

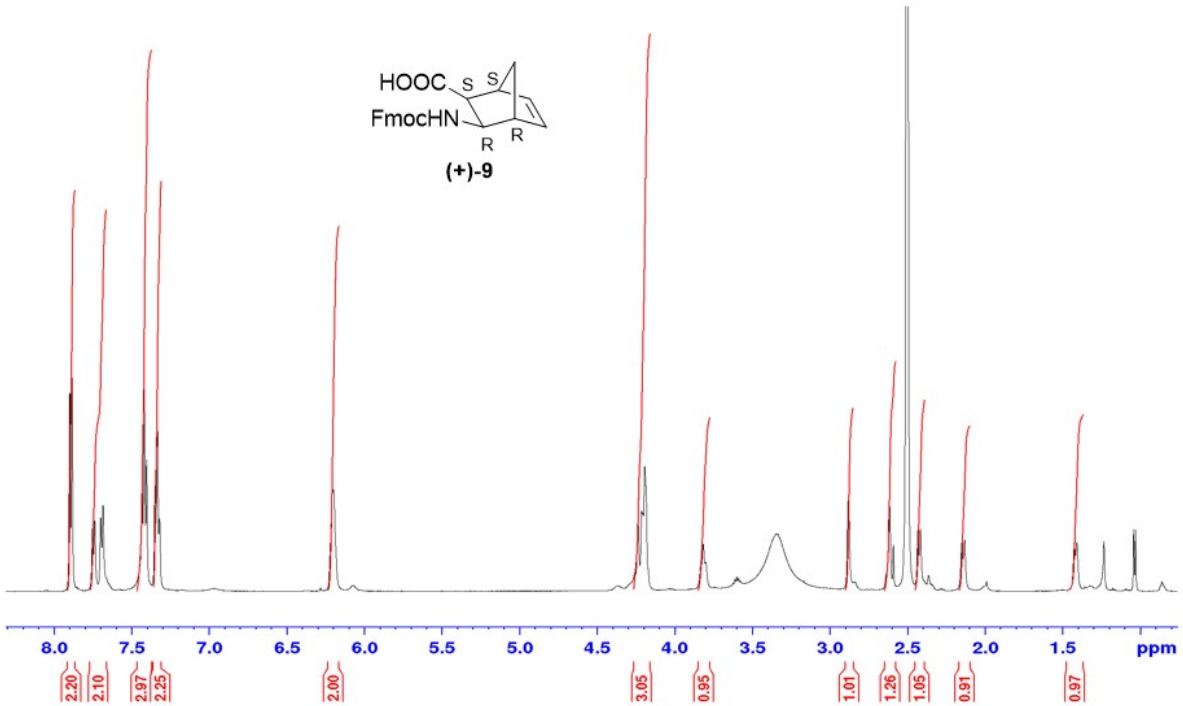


Figure S73. ^{13}C NMR spectrum of compound **(+)-9** 23.3, 25.7, 45.1, 45.4, 47.2, 47.4, 48.0, 57.3, 66.2, 120.6, 125.8, 126.0, 127.6, 127.6, 128.1, 137.2, 139.5, 141.1, 141.2, 144.2, 144.5, 156.2, 174.8.

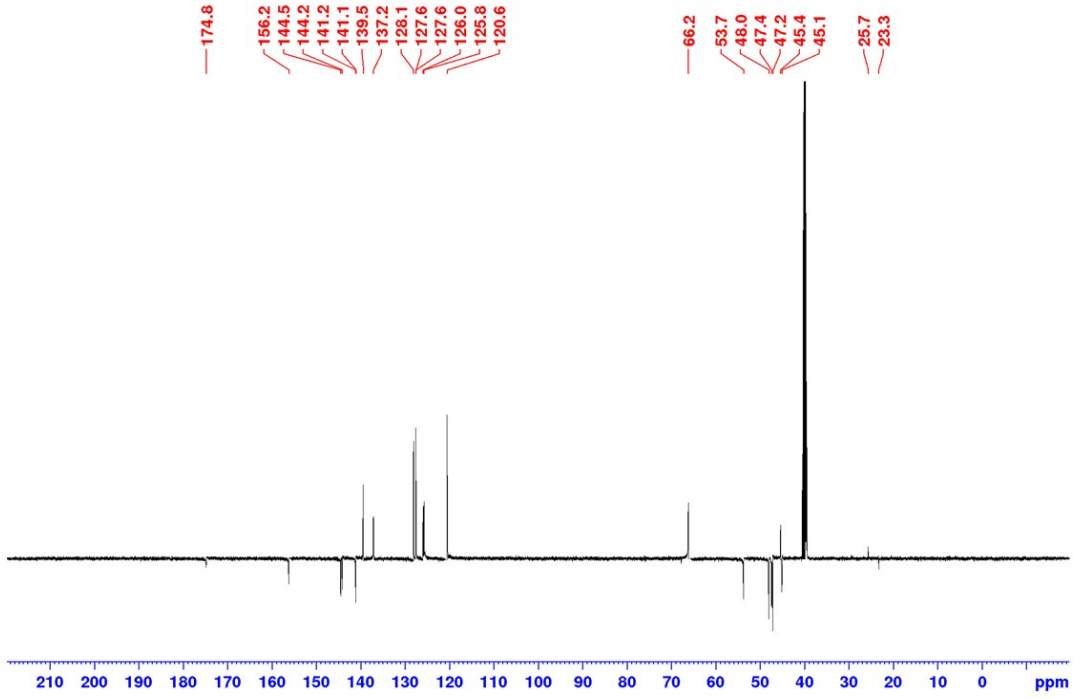


Figure S74. HPLC chromatogram of **(+)-9**

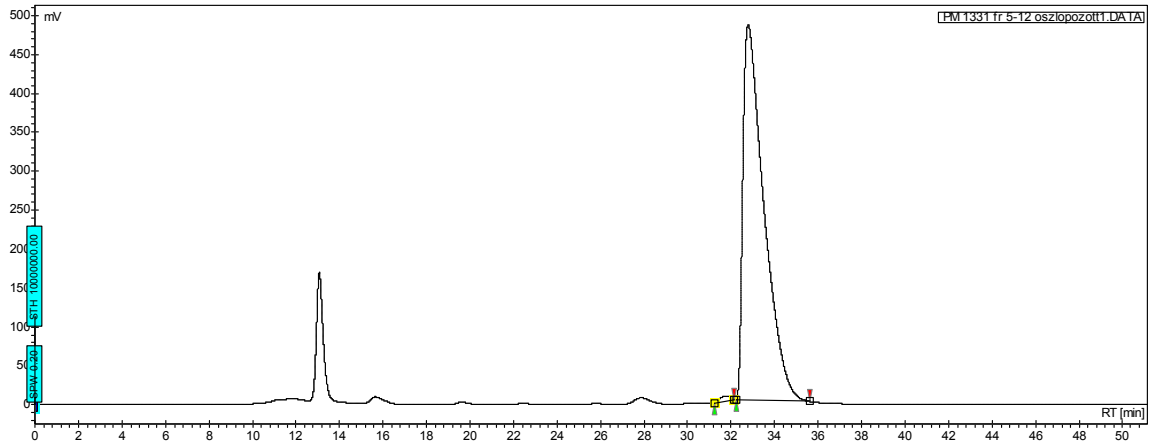


Figure S75. HPLC chromatogram of **(–)-9**

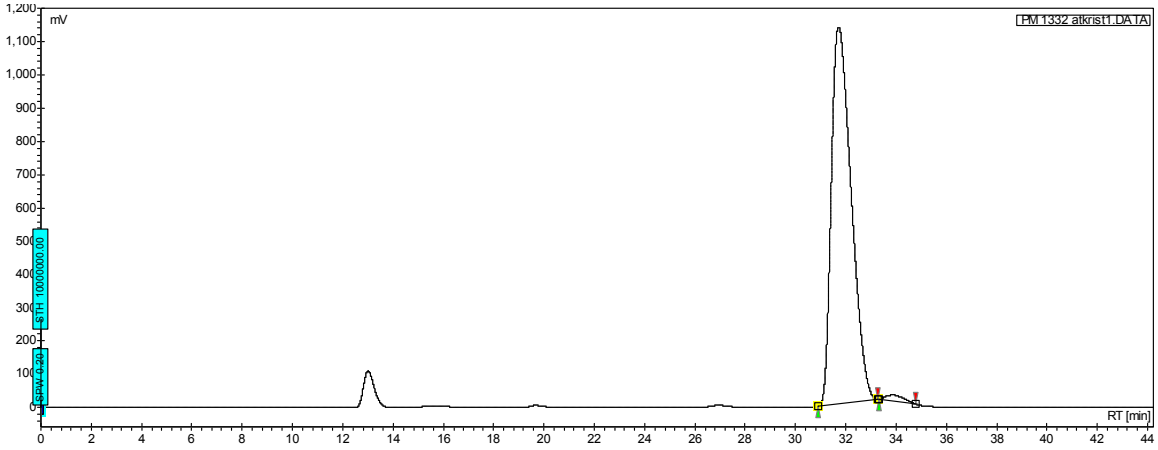


Figure S76. ^{1}H NMR spectrum of racemic *N*-Fmoc-protected *diexo*-AOBHEC (DMSO-d6) 2.67 (d, *J* = 7.8 Hz, 1H), 4.05 (t, *J* = 8.3 Hz, 1H), 4.10-4.25 (m, 3H), 4.71 (s, 1H), 5.06 (s, 1H), 6.43-6.54 (m, 2H), 7.23 (d, *J* = 9.3 Hz, 1H) 7.30-7.44 (m, 5H), 7.73 (d, *J* = 7.8 Hz, 1H), 7.78 (d, *J* = 7.5 Hz, 1H), 7.89 (d, *J* = 7.3 Hz, 2H), 12.3 (s, 1H).

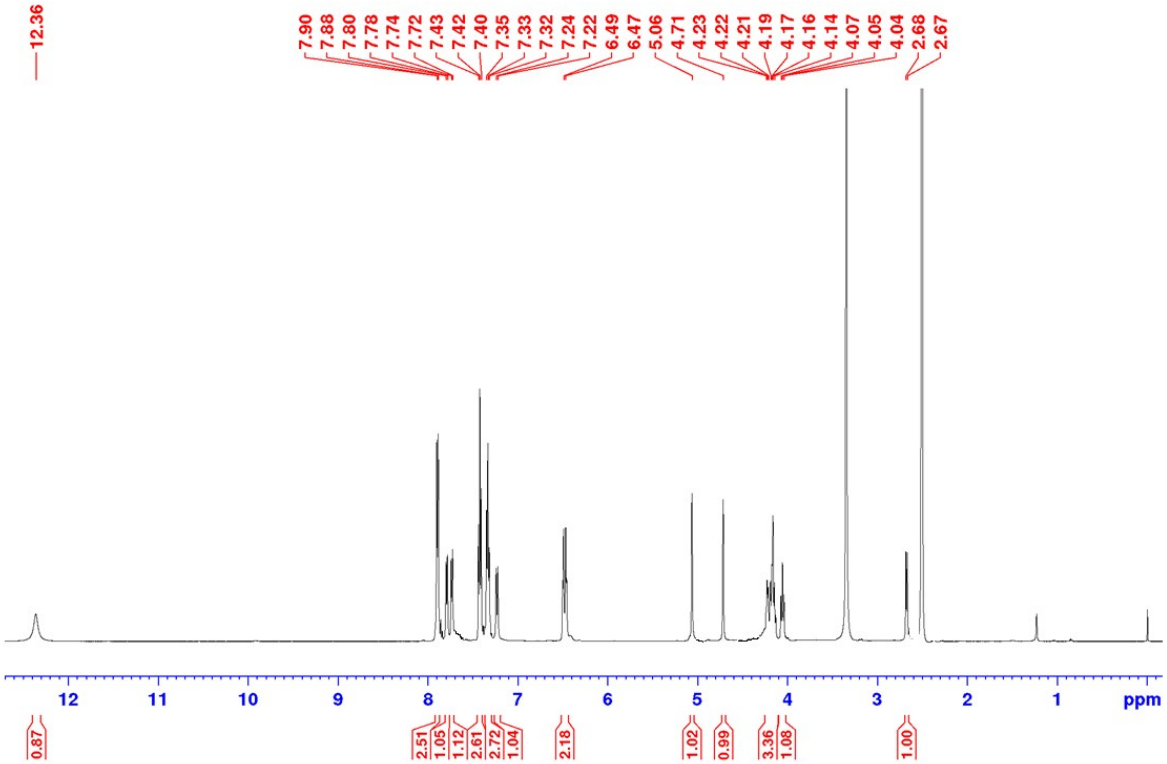
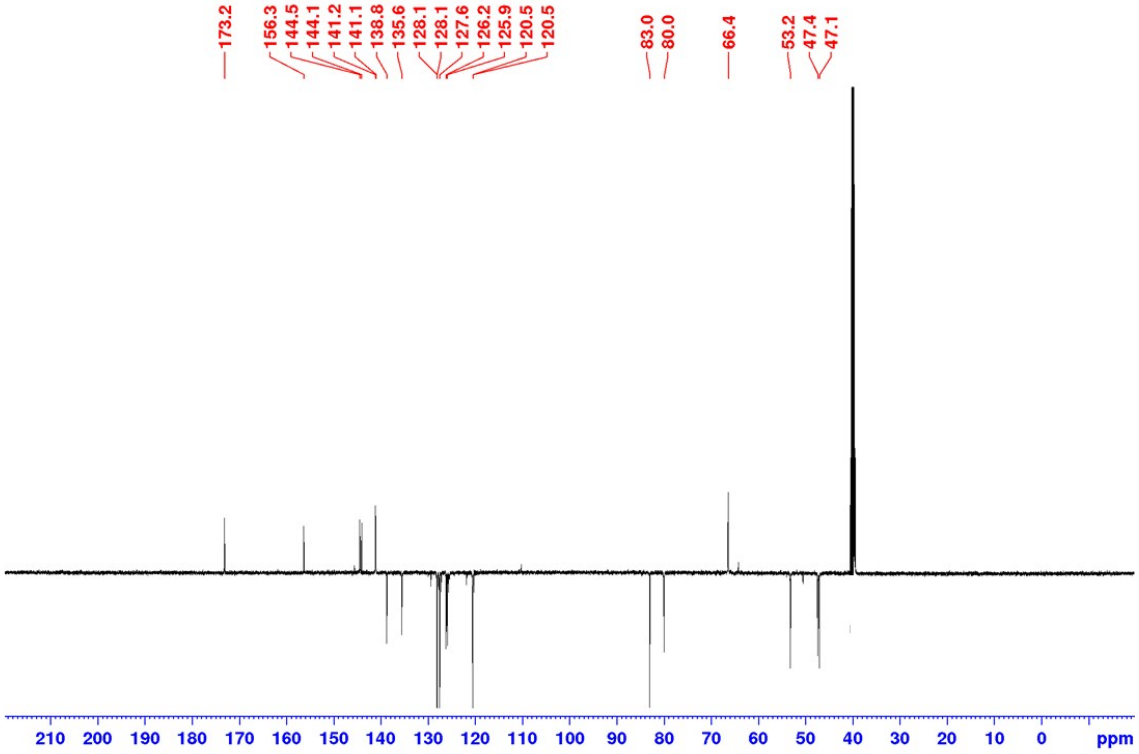


Figure S77. ^{13}C NMR spectrum of racemic *N*-Fmoc-protected *diexo*-AOBHEC (DMSO-d6) 47.1, 47.4, 53.2, 66.4, 80.0, 83.0, 120.5, 120.5, 125.9, 126.2, 127.6, 128.1, 128.1, 135.6, 138.8, 141.1, 141.2, 144.1, 144.5, 156.3, 173.2.



Coordinates of the optimized geometries for 1 in implicit water

N	-2.43084600	-1.72872600	-1.38484200
C	-3.47989900	-1.35541900	-0.44617000
C	-4.47808100	-0.42636600	-1.13859500
C	-3.75044100	0.80681700	-1.63304200
O	-3.05753200	1.47703400	-0.86960900
C	-4.17680500	-2.57652300	0.14541100
C	-5.59139500	-0.01480100	-0.16718900
C	-6.28449800	-1.23534100	0.42940200
C	-5.27897200	-2.15652100	1.11377100
N	-3.91216000	1.12815100	-2.92179900
N	0.82132400	-0.13481500	-2.40847500
C	1.08841600	-1.54789400	-2.16598800
C	-0.21216300	-2.34560800	-2.14029700
C	-1.13450000	-1.83409700	-1.05158700
O	-0.71449300	-1.57221300	0.07440800
C	2.06082100	-2.10570700	-3.20355700
C	0.08870300	-3.83026500	-1.88114600
C	1.05059000	-4.38860300	-2.92431300
C	2.34566100	-3.58304500	-2.95374700
N	-0.35056100	2.22162300	-0.24678100
C	0.24458700	3.01900700	-1.30738100
C	1.21475400	2.24972300	-2.28636400
C	1.53260600	0.84355000	-1.83114300
O	2.39770200	0.58533200	-0.98853800
C	1.10110200	4.25558300	-0.89225500
C	1.16898300	5.08783100	-2.16131600
C	2.45907100	3.18773200	-2.32855300
C	1.96831900	4.45166600	-3.01487500
C	2.52299300	3.67975000	-0.87521800
N	0.54597600	-0.44454400	2.40913000
C	-0.43374900	0.46967800	2.97227500
C	-1.03799300	1.30466800	1.84690800
C	0.03059600	2.02318300	1.02958700
O	1.09225800	2.40196400	1.52055000
C	-1.52989300	-0.26152300	3.74125400
C	-2.04862400	2.31251000	2.40883400
C	-3.13941000	1.59225100	3.19696900
C	-2.54639500	0.72669400	4.30477900
N	3.75376500	1.02867300	1.30319500
C	4.07857900	-0.36644900	1.74575300
C	2.78632700	-1.16506800	1.85971600
C	1.83052700	-0.42670700	2.77963800
O	2.25592900	0.17457700	3.76503500
C	5.04538500	-1.01801100	0.77291800
C	3.10876400	-2.57487600	2.36572700
C	4.09135100	-3.26294700	1.42166900

C	5.36286500	-2.43753000	1.24232000
H	-2.70605800	-2.02175900	-2.31048400
H	-3.43152500	-3.19746400	0.64484400
H	-4.60321700	-3.16903200	-0.67008800
H	-2.99208400	-0.79628100	0.35327500
H	-4.92565800	-0.95671800	-1.98494500
H	-5.14489700	0.58552300	0.62955800
H	-5.77912200	-3.03905300	1.51237900
H	-4.82940600	-1.63370600	1.96417000
H	-6.79698300	-1.78467500	-0.36555300
H	-7.04762900	-0.91201100	1.13760200
H	-6.30889200	0.62079600	-0.68769200
H	-3.47765700	1.96240900	-3.28301200
H	-4.49246100	0.58238200	-3.53436600
H	0.18704100	0.10897400	-3.15440900
H	1.54343000	-1.61097900	-1.17812100
H	2.97998000	-1.51889000	-3.17073800
H	1.62488300	-1.97487800	-4.19885900
H	-0.70526700	-2.25180800	-3.11300300
H	0.57677900	-4.34983600	-3.90938900
H	1.25820500	-5.43684000	-2.70891300
H	2.85875400	-3.69290000	-1.99382800
H	3.01884200	-3.96661900	-3.72024800
H	-0.84552000	-4.39332100	-1.87478800
H	0.53138900	-3.92037100	-0.88468600
H	-1.27825200	1.87722500	-0.47463200
H	0.74098100	4.74903300	0.00454100
H	0.57249000	5.96796300	-2.35383300
H	-0.60964900	3.36070900	-1.88751500
H	2.16275300	4.70622700	-4.04683500
H	3.34794000	2.72134400	-2.74255100
H	3.27986100	4.44902500	-0.73506900
H	2.63467400	2.88865600	-0.14702500
H	0.75791000	2.18393700	-3.27196000
H	0.28754300	-0.92017600	1.54984200
H	-1.07419500	-0.85061900	4.53825800
H	-2.02699700	-0.96179100	3.06036600
H	0.11215700	1.12488000	3.65123700
H	-1.57397400	0.62922600	1.17405900
H	-3.33650700	0.19197400	4.83261700
H	-2.05094400	1.37020600	5.03805400
H	-3.84077100	2.31695900	3.61148000
H	-3.70546900	0.95398800	2.51072000
H	-2.48645800	2.88105400	1.58728800
H	-1.52330900	3.01819200	3.05966000
H	3.10354000	1.48378100	1.95446500
H	3.28071400	1.00746900	0.37374700
H	5.95897800	-0.42598500	0.70063500
H	4.58449000	-1.04342900	-0.21987700
H	4.52716300	-0.27357500	2.73382600

H	2.33798400	-1.24222800	0.86509300
H	6.03045200	-2.91644500	0.52702000
H	5.89800200	-2.38608100	2.19453400
H	4.33752600	-4.25492200	1.79998600
H	3.60956700	-3.40057300	0.44896300
H	2.18447800	-3.14784100	2.44513100
H	3.53669900	-2.50070400	3.36929200
H	4.59520100	1.59943600	1.23686100

Coordinates of the optimized geometries for 2 in implicit water

N	-2.74576800	-1.87079600	-0.71635300
C	-3.68949000	-1.06499700	0.04355100
C	-4.62561600	-0.34142700	-0.92171600
C	-3.81926300	0.55186500	-1.84516400
O	-2.88282300	1.22753900	-1.42429100
C	-4.46310500	-1.89987700	1.05822400
C	-5.65329100	0.50725200	-0.15853100
C	-6.41617900	-0.33181600	0.86195000
C	-5.46193900	-1.03624000	1.82212000
N	-4.20763200	0.58646500	-3.12628000
N	0.66320500	-1.08215200	-2.22742600
C	0.74330600	-2.37292300	-1.54936600
C	-0.64776600	-2.93565200	-1.28321600
C	-1.44472300	-1.98764300	-0.40778200
O	-0.92981900	-1.40103800	0.54272200
C	1.59949400	-3.35222300	-2.34948600
C	-0.53846100	-4.29575100	-0.57505500
C	0.31092900	-5.27440500	-1.37937900
C	1.69885800	-4.70004600	-1.64307200
N	-0.10231900	1.95810800	-0.98592300
C	0.62531100	2.31047100	-2.18967200
C	1.44987900	1.13543800	-2.84012900
C	1.52690600	-0.09434200	-1.96450600
O	2.35851300	-0.19569900	-1.05857000
C	1.74517800	3.38379600	-2.03861400
C	2.02709900	3.86368500	-3.45259200
C	2.84737700	1.80966100	-2.96717300
C	2.70819000	2.88435300	-4.03196300
O	2.89365800	2.58119500	-1.76787600
N	0.63110500	0.28460500	2.34959600
C	-0.36331000	1.31837400	2.59258100
C	-0.91644900	1.81289500	1.25686400
C	0.19520700	2.21270100	0.30255600
O	1.23278000	2.74566900	0.69264700
C	-1.50694900	0.84872400	3.48601300
C	-1.88348200	2.98047300	1.48245900
C	-3.02327700	2.54327200	2.39832300
C	-2.50005400	1.98487800	3.71922100

N	3.73067100	1.34173100	0.68189400
C	4.13795200	0.26286600	1.63417300
C	2.90612700	-0.51914200	2.08685000
C	1.91340000	0.44298100	2.71352200
O	2.30323000	1.32011000	3.48008500
C	5.15970600	-0.64987900	0.97615800
C	3.33457200	-1.60400400	3.08167100
C	4.36561300	-2.53436900	2.45040500
C	5.57594700	-1.75282800	1.94714800
H	-3.10534000	-2.42952600	-1.47578800
H	-3.75131600	-2.37047900	1.73837500
H	-4.99069600	-2.70079100	0.53131400
H	-3.09817800	-0.31625500	0.57107500
H	-5.16435100	-1.08722200	-1.51532100
H	-5.12653000	1.31950100	0.34851500
H	-6.01924400	-1.64893900	2.53053300
H	-4.91814900	-0.28763100	2.40808800
H	-7.01541600	-1.08082300	0.33612300
H	-7.10954700	0.30430900	1.41237200
H	-6.34095600	0.96566900	-0.87031700
H	-3.74562200	1.21040800	-3.76807700
H	-4.98083000	0.03784600	-3.45984300
H	0.06496900	-0.99837000	-3.03593100
H	1.21773700	-2.18248100	-0.58719500
H	2.58737200	-2.91284400	-2.49526100
H	1.15108400	-3.48372000	-3.33914100
H	-1.16558200	-3.07738000	-2.23712800
H	-0.18327200	-5.48093300	-2.33321600
H	0.38416100	-6.22172700	-0.84494300
H	2.22177000	-4.56992400	-0.69092700
H	2.29245200	-5.39038900	-2.24220500
H	-1.53877800	-4.69820700	-0.41024100
H	-0.08569600	-4.13515000	0.40756800
H	-1.02626800	1.56952200	-1.15058100
H	1.58140900	4.12176800	-1.26589900
H	1.64192800	4.77298200	-3.88660400
H	-0.12307200	2.65475000	-2.89903600
H	3.02368100	2.78848700	-5.05880600
H	3.68782700	1.12759900	-3.02873500
H	1.04067800	0.86585000	-3.81079900
H	0.38730800	-0.43344400	1.67481700
H	-1.10063100	0.48753300	4.43162900
H	-2.00748800	0.00335200	3.00027300
H	0.16568800	2.13442300	3.08431800
H	-1.47229800	0.99380500	0.79672200
H	-3.32896100	1.63719800	4.33669400
H	-2.00153400	2.78496900	4.27457300
H	-3.70328500	3.37648600	2.57841900
H	-3.59829500	1.76488400	1.88759600
H	-2.27581400	3.31989900	0.52271100

H	-1.33873800	3.81496900	1.93416700
H	3.02172400	1.97845800	1.07050900
H	3.28298800	0.93399100	-0.16715200
H	6.02882800	-0.06875100	0.66344400
H	4.71317400	-1.08865500	0.07876600
H	4.57159200	0.76138100	2.50058400
H	2.45524800	-0.99344000	1.21169800
H	6.28530400	-2.42027600	1.45898000
H	6.09422300	-1.30223500	2.79825500
H	4.67860100	-3.28775200	3.17331400
H	3.90291700	-3.06437600	1.61260900
H	2.45468300	-2.16335900	3.40127400
H	3.75625700	-1.12239300	3.96812400
H	4.52695600	1.90276700	0.38519100

Coordinates of the optimized geometries for 3 in implicit water

N	2.25338600	0.28602800	2.10014100
C	3.18713800	-0.65932700	1.50349200
C	4.39739100	0.09430000	0.95708500
C	3.95114300	1.08437700	-0.10017500
O	3.14487000	0.76279100	-0.97113300
C	3.60114900	-1.74525500	2.49232200
C	5.40860800	-0.87940100	0.33444800
C	5.81187700	-1.96873600	1.32327200
C	4.58895300	-2.71379500	1.85000800
N	4.50501700	2.30250200	-0.05439700
N	-0.73928900	2.27898300	0.91271000
C	-1.12052400	1.59095400	2.14238200
C	0.11684300	1.11086900	2.89499000
C	0.91807700	0.13938400	2.05047100
O	0.37251100	-0.75186900	1.40252800
C	-1.99331100	2.48845500	3.01664800
C	-0.29722200	0.40219100	4.19466500
C	-1.16065400	1.30506800	5.06854200
C	-2.39372100	1.78004200	4.30665500
N	0.42235500	0.86800900	-1.96755400
C	-0.09469500	2.12068700	-2.47343500
C	-0.99071300	2.91974900	-1.44642200
C	-1.36682100	2.07827300	-0.24991600
O	-2.24953600	1.21869200	-0.35910500
C	1.08138200	3.11080200	-2.71637400
C	0.48813700	4.32392100	-3.40121700
C	-0.14902800	4.20617500	-1.19330200
C	-0.23719000	4.97772200	-2.49850700
C	1.28870700	3.66232200	-1.29484100
N	-1.16923200	-2.28821300	-0.54908900
C	-0.09216000	-2.70432900	-1.43459800
C	0.76947300	-1.49364500	-1.78230900

C	-0.06237000	-0.33911200	-2.30630500
O	-1.06945200	-0.49553100	-2.99765400
C	0.77324700	-3.80815400	-0.83456900
C	1.86096500	-1.88298800	-2.78636700
C	2.72297100	-3.00342400	-2.21150900
C	1.87956000	-4.20933500	-1.80716100
N	-3.73420400	-0.25507600	-2.02359200
C	-4.46840800	-1.08366900	-1.01459700
C	-3.47167700	-1.71820900	-0.04656400
C	-2.45588500	-2.50588800	-0.85320200
O	-2.82700000	-3.24614900	-1.76207500
C	-5.48619600	-0.22863600	-0.27984100
C	-4.23456800	-2.59955100	0.94772400
C	-5.27238600	-1.77317300	1.70221900
C	-6.23594700	-1.08279500	0.74079900
H	2.62862900	0.99126900	2.71718400
H	2.70495600	-2.26599600	2.83365900
H	4.05879700	-1.27260400	3.36683900
H	2.66719200	-1.12131200	0.66419900
H	4.88598200	0.62626500	1.77943700
H	4.95197000	-1.33216400	-0.54940700
H	4.88773700	-3.47485900	2.57073000
H	4.09627900	-3.23428400	1.02212200
H	6.34611100	-1.51440200	2.16279400
H	6.50257400	-2.66139700	0.84206900
H	6.28339700	-0.32261900	-0.00368600
H	4.29544400	2.96902300	-0.78050500
H	5.17374500	2.55432800	0.65246500
H	-0.08153900	3.04064800	0.98345900
H	-1.69167700	0.71561700	1.83592700
H	-2.87301100	2.78462500	2.44342300
H	-1.43666000	3.40059000	3.25415300
H	0.73697900	1.97602700	3.14948500
H	-0.57283700	2.17175500	5.38470000
H	-1.45296800	0.76943800	5.97187100
H	-3.02183300	0.91782700	4.06389800
H	-2.99335300	2.44719500	4.92570200
H	0.59677600	0.08334100	4.73253600
H	-0.85681400	-0.49907700	3.92885800
H	1.31128100	0.88404700	-1.47518700
H	1.93046800	2.63790000	-3.20102600
H	0.57167000	4.53501700	-4.45697100
H	-0.65208700	1.90447700	-3.38000400
H	-0.87735700	5.83273400	-2.65907100
H	1.53451700	2.89075700	-0.56187500
H	2.03392600	4.45405800	-1.25795900
H	-0.42516800	4.76316400	-0.30206500
H	-1.94134900	3.17072900	-1.91321100
H	-0.93252100	-1.63067000	0.18739800
H	0.14422100	-4.66373200	-0.58519400

H	1.21022100	-3.43827000	0.10004700
H	-0.57096900	-3.07334700	-2.34206300
H	1.25857100	-1.15264500	-0.86780400
H	2.51005900	-4.97849300	-1.35994000
H	1.42691900	-4.64759100	-2.70164300
H	3.48703400	-3.29692400	-2.93212400
H	3.24524400	-2.62253400	-1.32803000
H	2.47371700	-1.00876800	-3.01083200
H	1.39144400	-2.21204800	-3.71830000
H	-3.05343900	-0.80268600	-2.56377800
H	-3.17226900	0.48327900	-1.53832600
H	-6.18390400	0.21370900	-0.99308000
H	-4.96322300	0.58912800	0.22510000
H	-4.96576700	-1.87606900	-1.57283400
H	-2.96334100	-0.92055400	0.49999900
H	-6.94150300	-0.46025400	1.28977000
H	-6.82081400	-1.83954900	0.21061200
H	-5.82422700	-2.41048000	2.39302400
H	-4.75778400	-1.01712200	2.30259600
H	-3.52594900	-3.05322700	1.64135700
H	-4.72269800	-3.41057900	0.40096500
H	-4.38102900	0.18296100	-2.67655100

Coordinates of the optimized geometries for 4 in implicit water

N	2.40450400	0.09953200	2.26632000
C	3.39068600	-0.69055100	1.54505700
C	4.39235600	0.25928600	0.86921200
C	3.60886900	1.17409500	-0.04870700
O	3.01667500	0.70951300	-1.02400500
C	4.10091100	-1.70047100	2.43951400
C	5.44105100	-0.53246000	0.08600800
C	6.14548200	-1.54737800	0.98112700
C	5.14037300	-2.48494500	1.64365600
N	3.56332200	2.47447800	0.25825800
N	-0.57009500	2.11927700	0.77530300
C	-0.96152900	1.49502700	2.03862600
C	0.25495900	1.04722500	2.83898400
C	1.07820200	0.04086400	2.05620500
O	0.55289400	-0.78924400	1.31808700
C	-1.84429000	2.44027700	2.85161200
C	-0.19970400	0.39784400	4.15739900
C	-1.08094000	1.33907600	4.97119800
C	-2.28860000	1.79223500	4.15805100
N	0.35709300	0.76439600	-1.99463600
C	-0.12192900	2.01455800	-2.52803900
C	-1.00454600	2.85453800	-1.53149000
C	-1.37491200	2.07831000	-0.28888000
O	-2.42636200	1.42585800	-0.26985900

C	1.08794000	2.97844100	-2.70149100
C	0.59968100	4.18989100	-3.46552000
C	-0.08969200	4.09294800	-1.30935300
C	-0.13108900	4.88323900	-2.60356200
O	1.21058500	3.49053000	-1.36641100
N	-1.22092800	-2.30109700	-0.43872900
C	-0.18020300	-2.77292700	-1.34059300
C	0.68321800	-1.59323500	-1.77982100
C	-0.15101900	-0.43964200	-2.30010300
O	-1.17943400	-0.59032200	-2.96370000
C	0.69937900	-3.85661100	-0.72473000
C	1.70712900	-2.04661200	-2.82694400
C	2.58808400	-3.14832000	-2.24367700
C	1.75501300	-4.31891800	-1.72687100
N	-3.80934300	-0.20441000	-1.90900600
C	-4.51833000	-1.02288500	-0.87289400
C	-3.49992500	-1.63517800	0.08621600
C	-2.52139000	-2.47191900	-0.71920200
O	-2.93456500	-3.21946300	-1.60256300
C	-5.52887600	-0.15723200	-0.13958300
C	-4.23841000	-2.48044100	1.13047100
C	-5.26489400	-1.63657500	1.88028400
C	-6.25410000	-0.98841300	0.91623600
H	2.74788100	0.80691200	2.89903400
H	3.35688600	-2.36776400	2.87670400
H	4.58732700	-1.16880100	3.26318400
H	2.84270000	-1.22071400	0.76375700
H	4.89036500	0.84669100	1.64671900
H	4.93851300	-1.04748900	-0.73607400
H	5.65094700	-3.19235500	2.29691600
H	4.63183200	-3.07233800	0.87221600
H	6.71026600	-1.01928800	1.75506400
H	6.86544800	-2.11760600	0.39383600
H	6.16136100	0.15674100	-0.35659000
H	2.97734500	3.08626500	-0.29561000
H	4.04132100	2.84279000	1.06185800
H	0.28512000	2.65546800	0.72622000
H	-1.53492400	0.60577300	1.77722500
H	-2.70378500	2.72226900	2.24231300
H	-1.27771800	3.35250600	3.06226200
H	0.87193100	1.92098300	3.07216700
H	-0.49547600	2.21366800	5.26923200
H	-1.40054200	0.84053300	5.88643800
H	-2.91932900	0.92660300	3.93477200
H	-2.89689700	2.49094100	4.73220400
H	0.67764000	0.09826600	4.73149100
H	-0.75658500	-0.51222000	3.91510200
H	1.24195500	0.78932500	-1.49075200
H	2.00409500	2.49247400	-3.01929000
H	0.75687800	4.36272800	-4.51804100

H	-0.65027300	1.81954300	-3.45626900
H	-0.72737900	5.76590900	-2.77084100
H	-0.23500000	4.63412200	-0.38050800
H	-1.94701800	3.13585800	-1.99293100
H	-0.93896500	-1.64385700	0.28165500
H	0.07411200	-4.69245500	-0.40796800
H	1.18068200	-3.44673200	0.16985400
H	-0.69777000	-3.17962800	-2.20957200
H	1.23372600	-1.23377000	-0.90768600
H	2.40118100	-5.06875800	-1.26947100
H	1.25502100	-4.80243000	-2.57147900
H	3.30219700	-3.49356500	-2.99200700
H	3.16954300	-2.72788500	-1.41661500
H	2.31584500	-1.19440100	-3.13225100
H	1.17965100	-2.41453300	-3.71214000
H	-3.08751100	-0.73474800	-2.41621000
H	-3.30574400	0.58570900	-1.44713300
H	-6.24055800	0.26392700	-0.85181600
H	-5.00238300	0.67554900	0.33628000
H	-5.01924900	-1.82807000	-1.40865100
H	-2.96795500	-0.82497600	0.59055400
H	-6.95778300	-0.35722800	1.45764700
H	-6.83804300	-1.76774600	0.41877900
H	-5.79484700	-2.25501500	2.60447100
H	-4.74493800	-0.85569300	2.44299300
H	-3.51199200	-2.90871200	1.82177800
H	-4.73537000	-3.31096300	0.62208700
H	-4.46770200	0.16914000	-2.59024100

Coordinates of the optimized geometries for 5 in implicit water

N	-4.76435600	0.32183000	-0.52548200
C	-5.32614400	-1.01245400	-0.38141500
C	-5.49636900	-1.33211000	1.10049400
C	-4.18505800	-1.18458300	1.85480600
O	-3.09251500	-1.31084000	1.30798900
C	-6.64382800	-1.18286100	-1.13188800
C	-6.03388400	-2.76178700	1.27341500
C	-7.34618200	-2.94520000	0.51672700
C	-7.18385900	-2.59953500	-0.96058100
N	-4.30162000	-0.93839900	3.16838100
N	-1.27394200	0.58727600	-0.29957400
C	-1.59746500	1.62918400	-1.27009200
C	-3.09893200	1.91944900	-1.26957400
C	-3.85382000	0.61952000	-1.47261900
O	-3.61177900	-0.12285700	-2.41606300
C	-0.81503800	2.91505400	-1.01820800
C	-3.42451200	2.93844500	-2.36569300
C	-2.63360200	4.22838200	-2.16170400

C	-1.13361000	3.95400700	-2.09013600
N	2.22330000	-1.84067300	-0.21746100
C	1.14836300	-1.96726600	0.62287700
C	0.04597200	-1.19796600	0.58395100
C	-0.12353900	-0.10658200	-0.39130400
O	0.74628100	0.17858500	-1.22832500
N	4.52114000	0.15200600	-0.15121700
C	5.33612000	-1.02679300	-0.41942400
C	4.49685100	-2.18242500	-1.01523200
C	3.38397700	-2.56793800	-0.06247900
O	3.49757000	-3.43011500	0.78322000
C	6.47604800	-0.65474000	-1.36089300
C	5.39338800	-3.38223300	-1.31582900
C	6.52566900	-3.00037500	-2.26137800
C	7.35433500	-1.86032600	-1.67794700
N	1.72983100	0.51844700	2.93811500
C	2.39736300	1.77953100	2.47492700
C	2.98988100	1.58623500	1.08053600
C	3.91191400	0.37263900	1.02106100
O	4.05652700	-0.37972900	1.98666200
C	1.41140000	2.93502500	2.51213500
C	3.70144100	2.88815100	0.67132100
C	2.74745300	4.07799000	0.71522600
C	2.10427900	4.22700100	2.08937000
H	-4.90374700	0.98262000	0.22251300
H	-6.47817900	-0.95063800	-2.18422700
H	-7.36625900	-0.45801900	-0.74465900
H	-4.58827500	-1.70017400	-0.79991600
H	-6.22616700	-0.63789900	1.53146300
H	-5.28543500	-3.46207200	0.89113400
H	-8.13566000	-2.70281900	-1.48154900
H	-6.48840000	-3.30746000	-1.42109800
H	-8.10657400	-2.29476300	0.95880400
H	-7.69566400	-3.97129800	0.63256200
H	-6.16904700	-2.97766400	2.33345300
H	-3.47326200	-0.89014200	3.73897500
H	-5.19800100	-0.83329200	3.61103700
H	-1.98983300	0.22410300	0.32165100
H	-1.32934700	1.24512000	-2.25798400
H	0.24899800	2.68066700	-1.00979100
H	-1.08320100	3.30123000	-0.02956200
H	-3.36666700	2.35021000	-0.29962500
H	-2.95797600	4.70152600	-1.23018500
H	-2.85364800	4.92845600	-2.96802300
H	-0.78722300	3.58398100	-3.05949000
H	-0.58770400	4.87599900	-1.88817500
H	-4.49606700	3.14243100	-2.36520900
H	-3.17779900	2.49451700	-3.33363700
H	1.25459200	-2.75580100	1.35614400
H	-0.76191200	-1.40349000	1.27141900

H	2.14838100	-1.12293200	-0.93153600
H	4.33487100	0.77696100	-0.92120600
H	7.05978400	0.14462800	-0.90355700
H	6.05034300	-0.25914600	-2.28896500
H	5.73918200	-1.35671800	0.53921200
H	4.05065300	-1.81630400	-1.94516200
H	8.14431100	-1.56604200	-2.36857900
H	7.84089000	-2.20110500	-0.75957200
H	7.15631800	-3.86848000	-2.45322200
H	6.10791600	-2.68872300	-3.22320500
H	4.78860600	-4.18563800	-1.73742200
H	5.80427900	-3.75324300	-0.37458100
H	2.45188000	-0.21794200	2.94392800
H	0.98289000	0.21896900	2.30270100
H	0.99723600	3.03390400	3.51619800
H	0.58111300	2.71721700	1.83234900
H	3.20564900	1.94754900	3.18758500
H	2.17608500	1.39844000	0.36625300
H	1.38254200	5.04265100	2.08666500
H	2.87113600	4.47862800	2.82668700
H	3.28870700	4.98598300	0.45152300
H	1.96766400	3.93956200	-0.03817600
H	4.12034600	2.78920700	-0.32850700
H	4.53932100	3.05640000	1.35366100
H	1.33152700	0.62447900	3.87100200

Coordinates of the optimized geometries for 6 in implicit water

N	-2.32340400	1.93340200	-0.46991300
C	-3.27700800	0.89007400	-0.82160200
C	-4.45016700	0.92034100	0.15513200
C	-3.95017600	0.67978200	1.56556800
O	-3.13859100	-0.21161600	1.80805500
C	-3.74671800	1.01787600	-2.26779300
C	-5.48163700	-0.16044200	-0.20026900
C	-5.94072900	-0.03477100	-1.64957600
C	-4.75423700	-0.07552300	-2.60805500
N	-4.46313900	1.45914500	2.52586100
N	0.75764900	2.18533500	1.71677500
C	1.09143200	2.74198200	0.40927800
C	-0.17585700	3.05459100	-0.38080600
C	-0.99313600	1.79781600	-0.60783800
O	-0.46572200	0.73881700	-0.94274200
C	1.97712100	3.97705700	0.55676400
C	0.18867500	3.65411900	-1.74847200
C	1.06520600	4.89220100	-1.59612200
C	2.32820400	4.56914000	-0.80429200
N	-0.39530400	-0.95345900	2.39120200
C	0.17368600	-0.59690900	3.67244400

C	1.07628900	0.69955600	3.64815500
C	1.40037900	1.13665900	2.23922900
O	2.25533600	0.52303500	1.58922900
N	1.06042000	-1.75281800	-1.03645300
C	-0.01283000	-2.70327500	-0.78719700
C	-0.82595600	-2.23934200	0.41806700
C	0.05460400	-1.95846800	1.62023400
O	1.06898000	-2.60792100	1.87694000
C	-0.92667600	-2.89277400	-1.99399800
C	-1.91041100	-3.26761500	0.76111900
C	-2.82093700	-3.48721700	-0.44371000
C	-2.02695300	-3.90317000	-1.67887500
N	3.72101600	-1.70222500	1.37301900
C	4.40699400	-1.40811500	0.07431700
C	3.37074300	-1.01951300	-0.97847700
C	2.34458000	-2.13339600	-1.07434400
O	2.70785300	-3.30698400	-1.12421500
C	5.43882900	-0.31041300	0.26720700
C	4.08387800	-0.76928300	-2.31121700
C	5.13437300	0.32658100	-2.15382900
C	6.13924800	-0.02266800	-1.05945700
H	-2.68634500	2.85394700	-0.27045000
H	-2.87550200	0.96787900	-2.92302200
H	-4.20488300	2.00204400	-2.40606700
H	-2.75691200	-0.05996500	-0.69866700
H	-4.93622700	1.89927600	0.09680300
H	-5.02362500	-1.13993800	-0.04050200
H	-5.09258700	0.03609900	-3.63809900
H	-4.26360000	-1.05190300	-2.53741700
H	-6.47536600	0.91087700	-1.77816800
H	-6.64511400	-0.83416000	-1.88026100
H	-6.33030400	-0.08611700	0.48078700
H	-4.21703900	1.28627500	3.48760700
H	-5.13647800	2.17710000	2.32234000
H	0.12490300	2.70775300	2.30370500
H	1.63834700	1.96374700	-0.12136400
H	2.87729900	3.69707100	1.10582100
H	1.44728100	4.72280800	1.15791600
H	-0.77105800	3.78562900	0.17520900
H	0.50115900	5.67297400	-1.07759100
H	1.32162600	5.28270800	-2.58106000
H	2.93124800	3.84917000	-1.36540900
H	2.93806100	5.46299500	-0.67403100
H	-0.72587600	3.89232100	-2.29350400
H	0.72237000	2.89247600	-2.32392800
H	-1.29253300	-0.54796200	2.13935800
H	0.74084800	-1.45125700	4.02981800
H	2.04375400	0.47627800	4.09396800
H	0.83197400	-0.76711300	-0.95274200
H	-0.33201600	-3.21783700	-2.84874300

H	-1.36883600	-1.92341800	-2.25112000
H	0.47063700	-3.65076100	-0.54749600
H	-1.32079100	-1.30323300	0.15225600
H	-2.69174700	-4.01194600	-2.53640300
H	-1.57223700	-4.88227100	-1.50098800
H	-3.58044200	-4.23386000	-0.20941100
H	-3.34696700	-2.55134000	-0.65774000
H	-2.48865900	-2.91152700	1.61489900
H	-1.43439500	-4.21020900	1.04774700
H	3.03262300	-2.46038800	1.29287200
H	3.17520000	-0.86524200	1.68601400
H	6.16482800	-0.61183600	1.02433700
H	4.93426200	0.59023700	0.62976000
H	4.88785900	-2.33555100	-0.23475200
H	2.87931300	-0.09809900	-0.65772400
H	6.85478800	0.78786600	-0.92614400
H	6.70822300	-0.90663000	-1.36066100
H	5.65078100	0.48514600	-3.10044500
H	4.63422800	1.26549400	-1.89852800
H	3.34697100	-0.49025900	-3.06501000
H	4.55466700	-1.69887100	-2.64168100
H	4.39485800	-1.95812000	2.09209400
H	0.59683400	1.50023200	4.20598900
H	-0.64379300	-0.42616900	4.36872600

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