Supporting Information

Peroxide Natural Products from *Plakortis zyggompha* and the Sponge Association *Plakortis halichondrioides-Xestospongia deweerdtae*. Antifungal Activity Against *Cryptococcus gattii*

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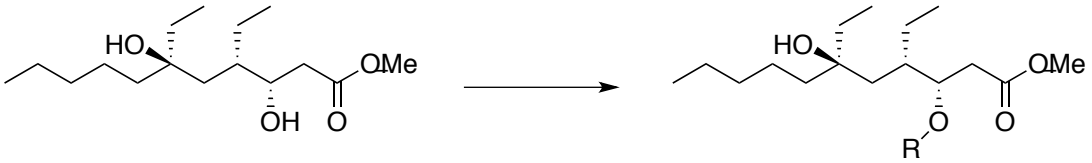
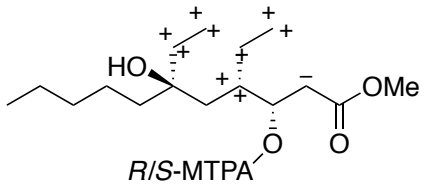


S1

S1a R = (*S*)-MTPA
S1b R = (*R*)-MTPA

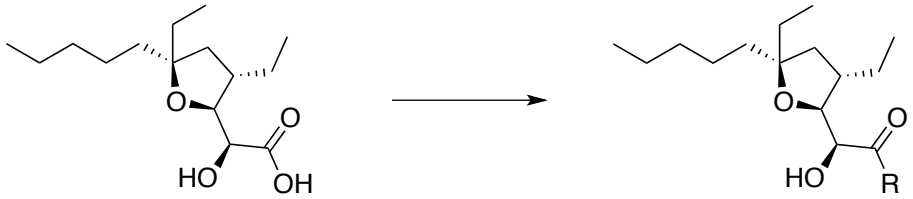
Mosher's analysis of 6-*epi*-dehydroplakortide K (1). 6-*epi*-dehydroplakortide K (**1**, 25 mg) and Pd/C (10%, 5 mg) were suspended in MeOH (0.6 mL) and stirred under an atmosphere of H_2 at 23 °C for 16 hr. The mixture was filtered through Celite® and the volatiles removed under reduced pressure to give a residue (22.8 mg) which was purified by reversed phase HPLC (Phenomenex Kinetix C_{18} column, 21.2 x 150 mm, 15 mL/min; mobile phase H_2O (0.1% TFA): CH_3CN, gradient 60–100% CH_3CN over 20 min) to provide diol **S1**. Compound **S1** (2 mg) was dissolved in $CDCl_3$ (200 μL) to which was added pyridine (5 μL) and (*R*)-MTPA-Cl (4 μL) and the mixture was stirred at 23 °C for 1hr. After removal of the volatiles, and the residue was purified by silica gel chromatography (isocratic, 4:1 *n*-hexane/EtOAc) to provide the corresponding (*S*)-MTPA ester, **S1a,** HRESITOFMS *m/z* 527.254 $[M+Na]^+$ (calcd for $C_{26}H_{39}F_3O_6Na$, 527.2591). The same procedure was repeated with S**1** and (*S*)-MTPA-Cl to yield the (*R)*-MTPA ester **S1b** HRESITOFMS *m/z* 527.2593 $[M+Na]^+$ (calcd for $C_{26}H_{39}F_3O_6Na$, 527.2591). ^{1}H NMR and gCOSY spectra of S**1a** and S**1b** were measured to determine the anisotropic shifts (δΔ(*S*-*R*, see Table S1*)* and the absolute configuration was solved after fitting of the data to the standard model.[1]

Table S1. ^{1}H NMR Data for **S1a** and **S1b** ($CDCl_3$)



#	**S1b**[a]	**S1a**[a]	δΔ(**S1a**-**S1b**)
1			
2	2.786	2.729	–0.057
	2.619	2.579	–0.040
3	5.827	5.85	+0.023
4	1.802	1.872	+0.070
5	1.289	1.319	+0.030
11	0.882	0.888	+0.006
12	1.473	1.470	+0.003
13	0.904	0.938	+0.034
14	1.385	1.484	+0.099
15	0.762	0.823	+0.061
OMe	3.660	3.618	–0.042

(1). Ohtani, I.; Kusumi, T.; Kashman, Y.; Kakisawa, H. *J. Am. Chem. Soc.* **1991**, *113*, 4092-4096.

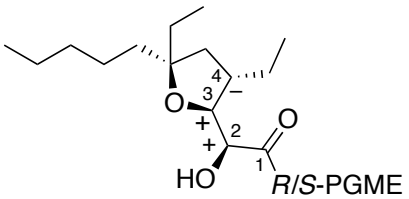


10

S2a R = (*R*)-PGME
S2b R = (*S*)-PGME

Phenylglycine methyl ester analysis of 10. 2-((3S,5R)-3,5-Diethyl-5-pentyltetrahydrofuran-2-yl)-2-hydroxyacetic acid (**10)** was dissolved in dimethylformamide (DMF, 0.4 mL). To this 1-[bis(dimethylamino)methylene]-1*H*-1,2,3-triazolo[4,5-*b*]pyridinium 3-oxid hexafluorophosphate (HATU, 4.2 mg in 100 µL DMF) and *N*.*N*-diisopropylethylamine (5 µL) were added and stirred at 23°C for 45 min before adding (R)-(−)-2-phenylglycine methyl ester (1.8 mg in 50 µL DMF). After 16 hr the mixture was diluted with EtOAc (5 mL) and successively washed with 5% HCl, sat. $NaHCO_3$, and sat. NaCl. The organic layer was dried with Na_2SO_4, evaporated, and purified on silica gel (isocratic, 15% EtOAc in Hexanes) to yield **S2a** (1.8 mg). $[a]_D$ −51 (*c* 1, MeOH); HRESITOFMS *m/z* 442.2567 $[M+Na]^+$ (calcd for $C_{24}H_{37}O_5Na$, 442.2564). The same procedure was repeated with **10** and (S)-(+)-2-Phenylglycine methyl ester to yield **S2b** (0.85 mg). $[a]_D$ +40 (*c* 0.56, MeOH); HRESITOFMS *m/z* 442.2568 $[M+Na]^+$ (calcd for $C_{24}H_{37}O_5Na$, 442.2564). ^1H NMR and gCOSY spectra of **S2a** and **S2b** were measured to determine the anisotropic shifts (δΔ(*S*-*R*, see Table S2*)* and the absolute configuration of C-2 was solved after fitting of the data to the standard model [2]

Table S2 ^1H NMR Data for **S2a** and **S2b** ($CDCl_3$)



#	**S2a**[a]	**S2b**[a]	δΔ(**S2b**-**S2a**)
1			
2	4.029	4.060	+0.03
3	3.529	3.690	+.16
4	2.224	2.143	–0.08

(2). Yabuuchi, T.; Kusumi, T. *J. Org. Chem.* **2000**, *65*, 397-404.

Figure S1. ^{1}H NMR overlay of **S1a** and **S1b** (500 MHz, $CDCl_3$)

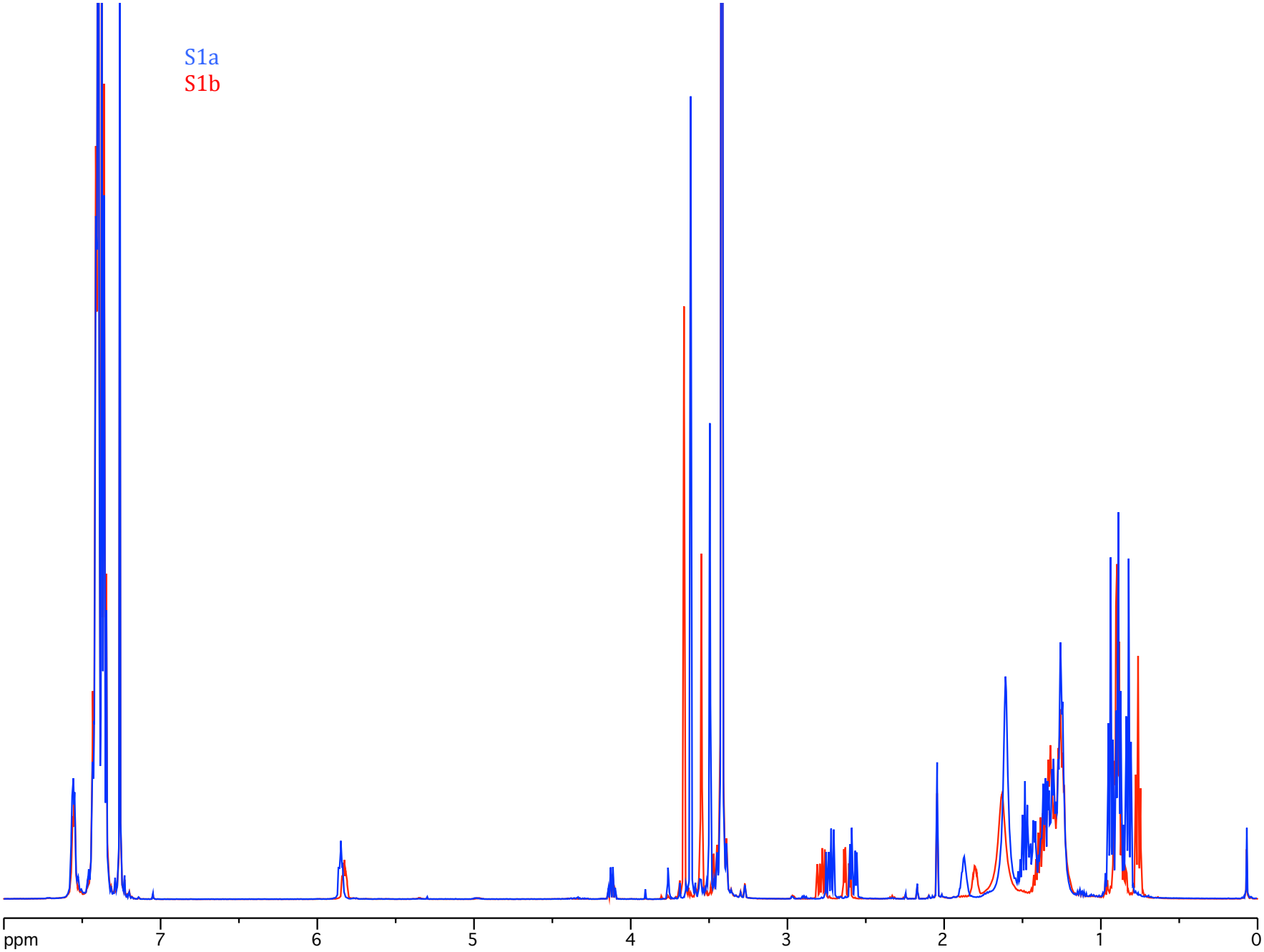


Figure S2. ^{1}H NMR of **S2a** (500 MHz, $CDCl_3$)

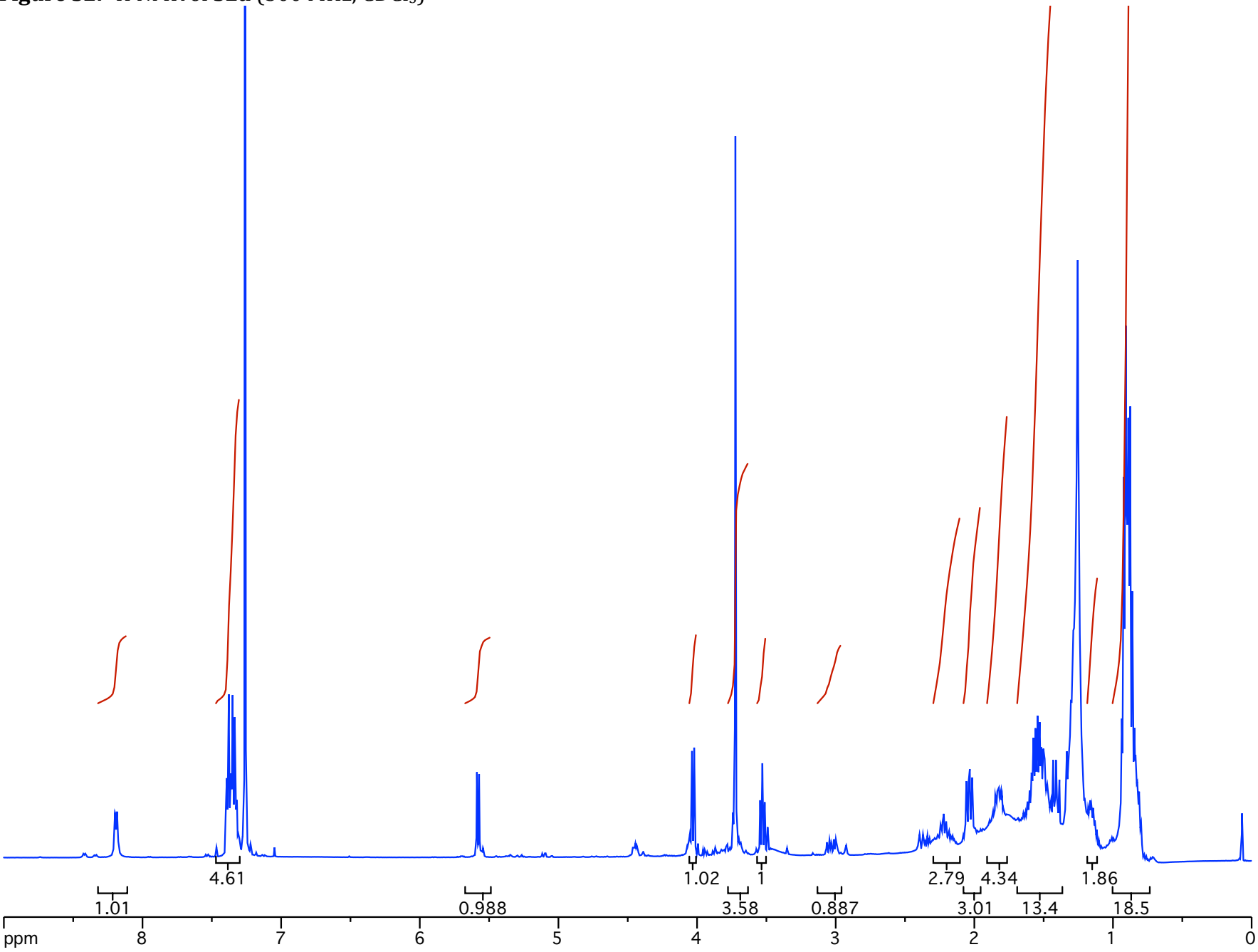


Figure S3. ^{1}H NMR of **S2b** (500 MHz, $CDCl_3$)

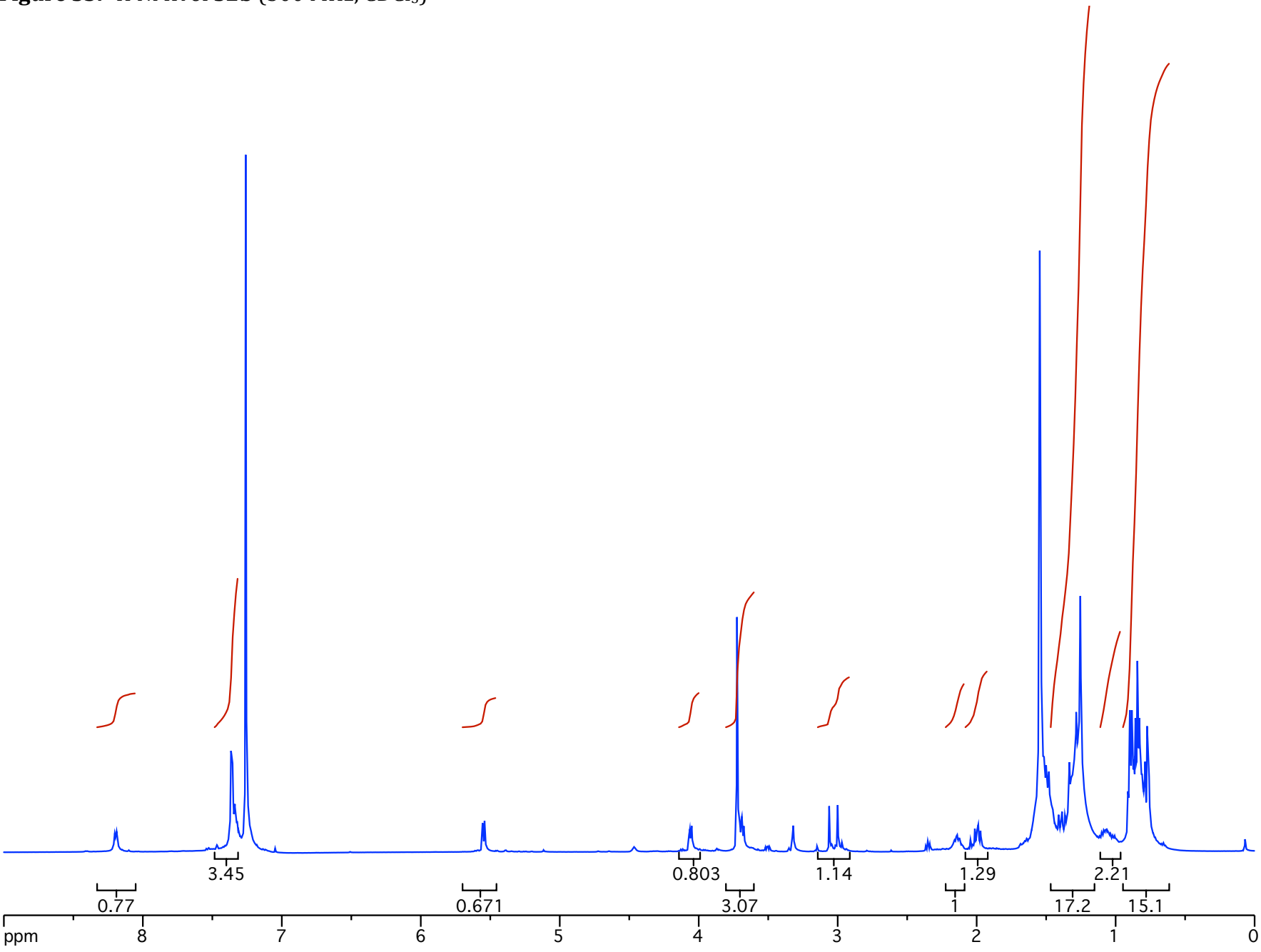


Figure S4. DQF-COSY spectrum of **S2a** (600 MHz, $CDCl_3$)

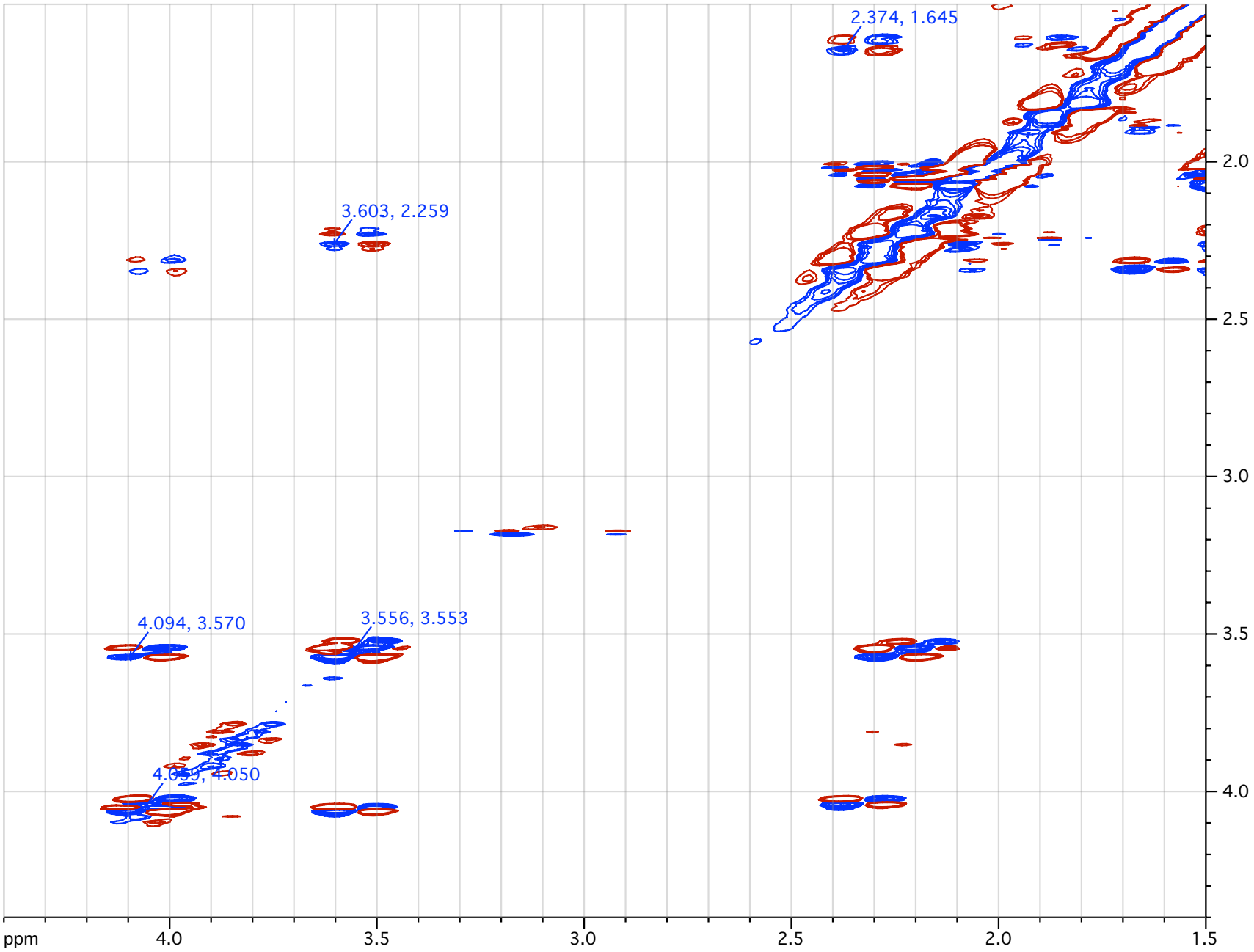


Figure S5. DQF-COSY spectrum of **S2b** (600 MHz, $CDCl_3$)

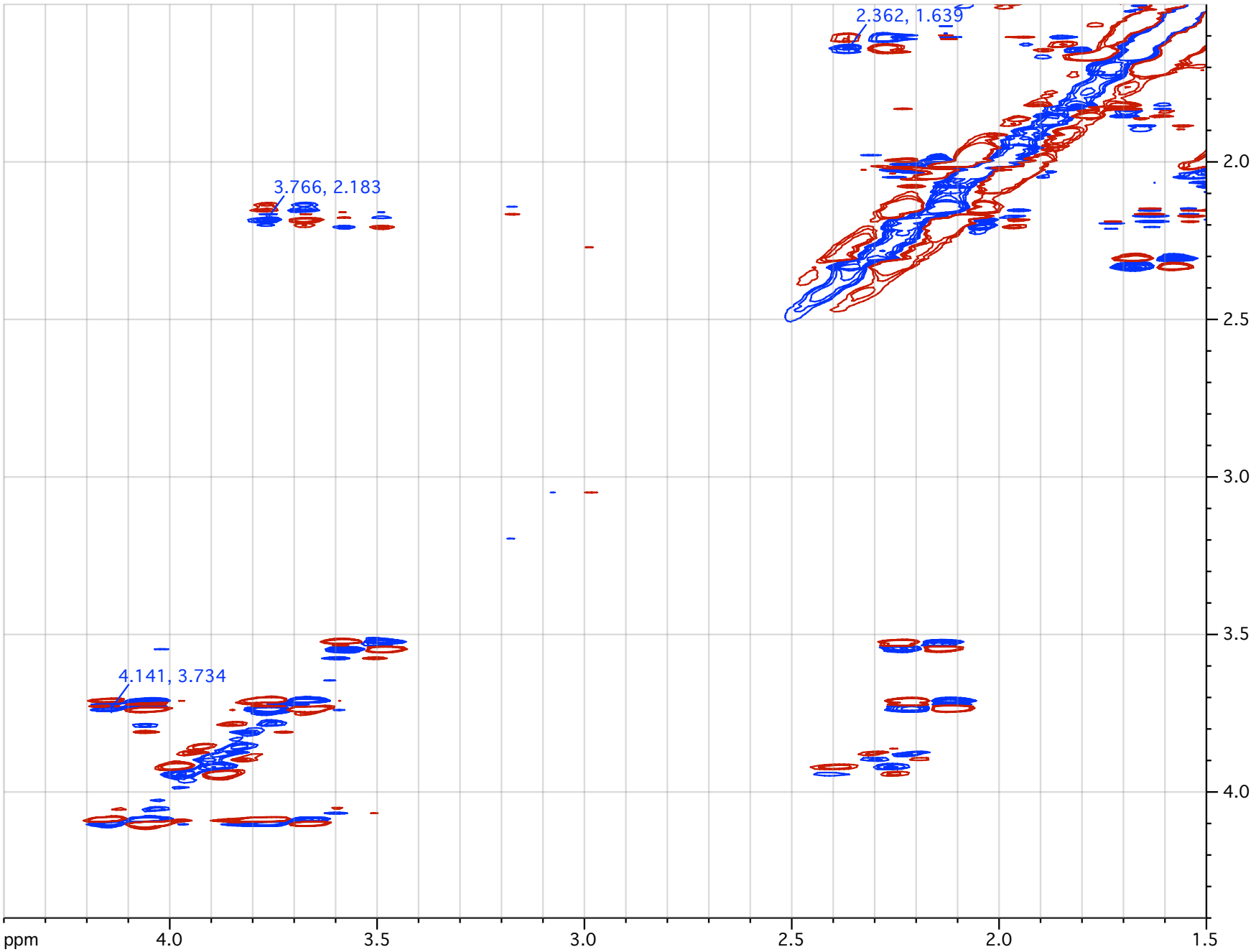


Figure S6. ^{1}H NMR spectrum of **1** (600 MHz, $CDCl_3$)

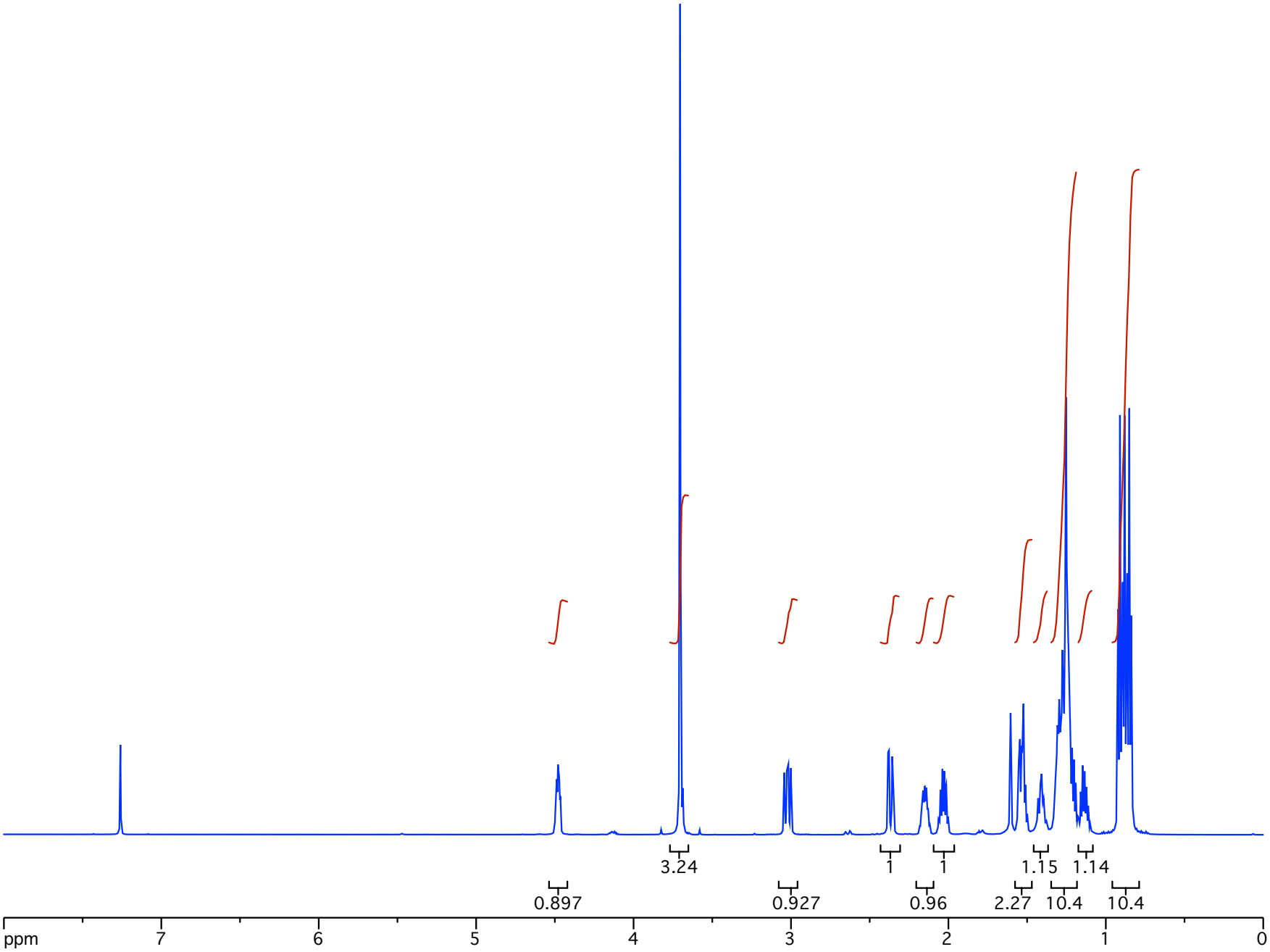


Figure S7. ^{13}C NMR spectrum of **1** (125 MHz, $CDCl_3$)

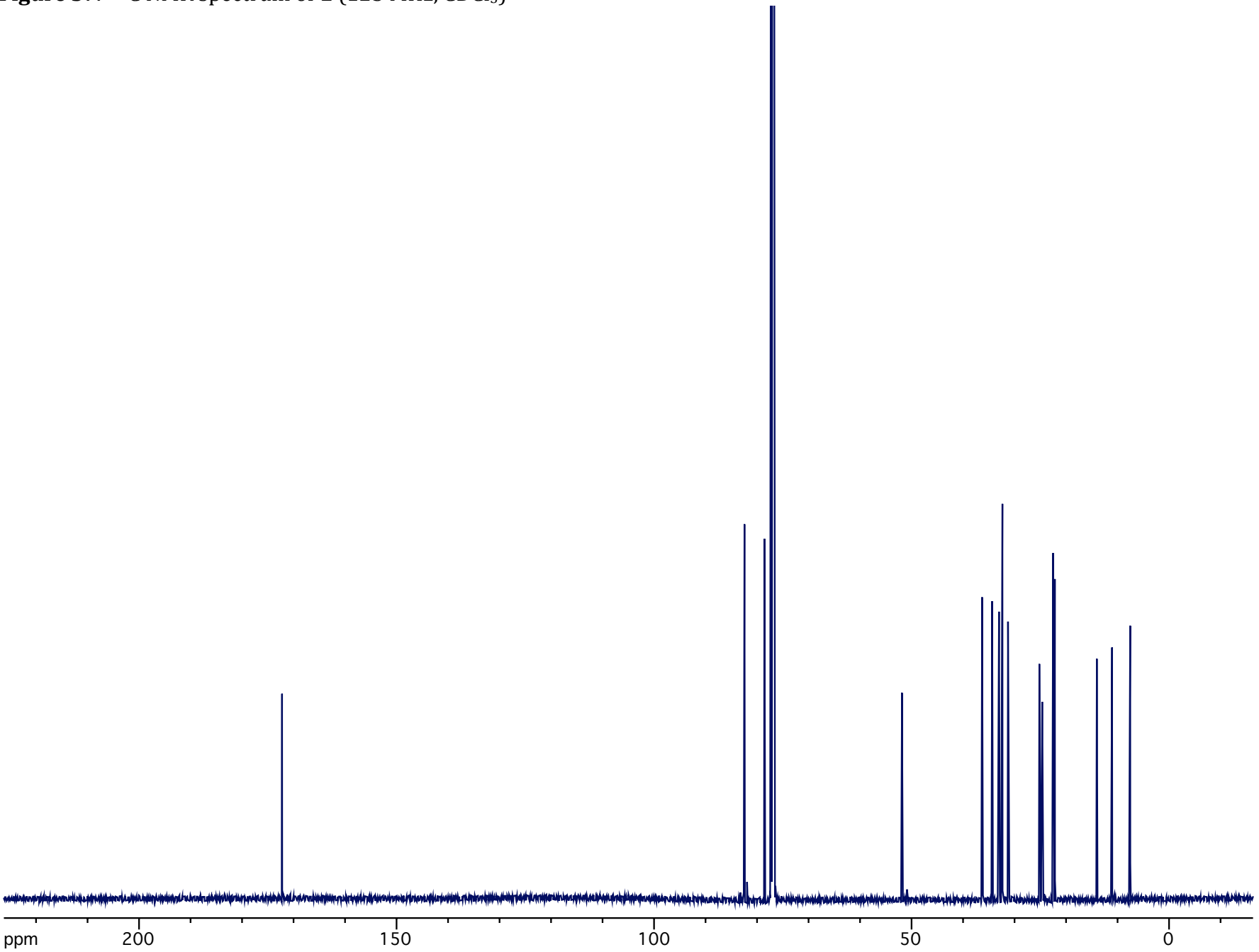


Figure S8. DQF-COSY spectrum of **1** (600 MHz, $CDCl_3$)

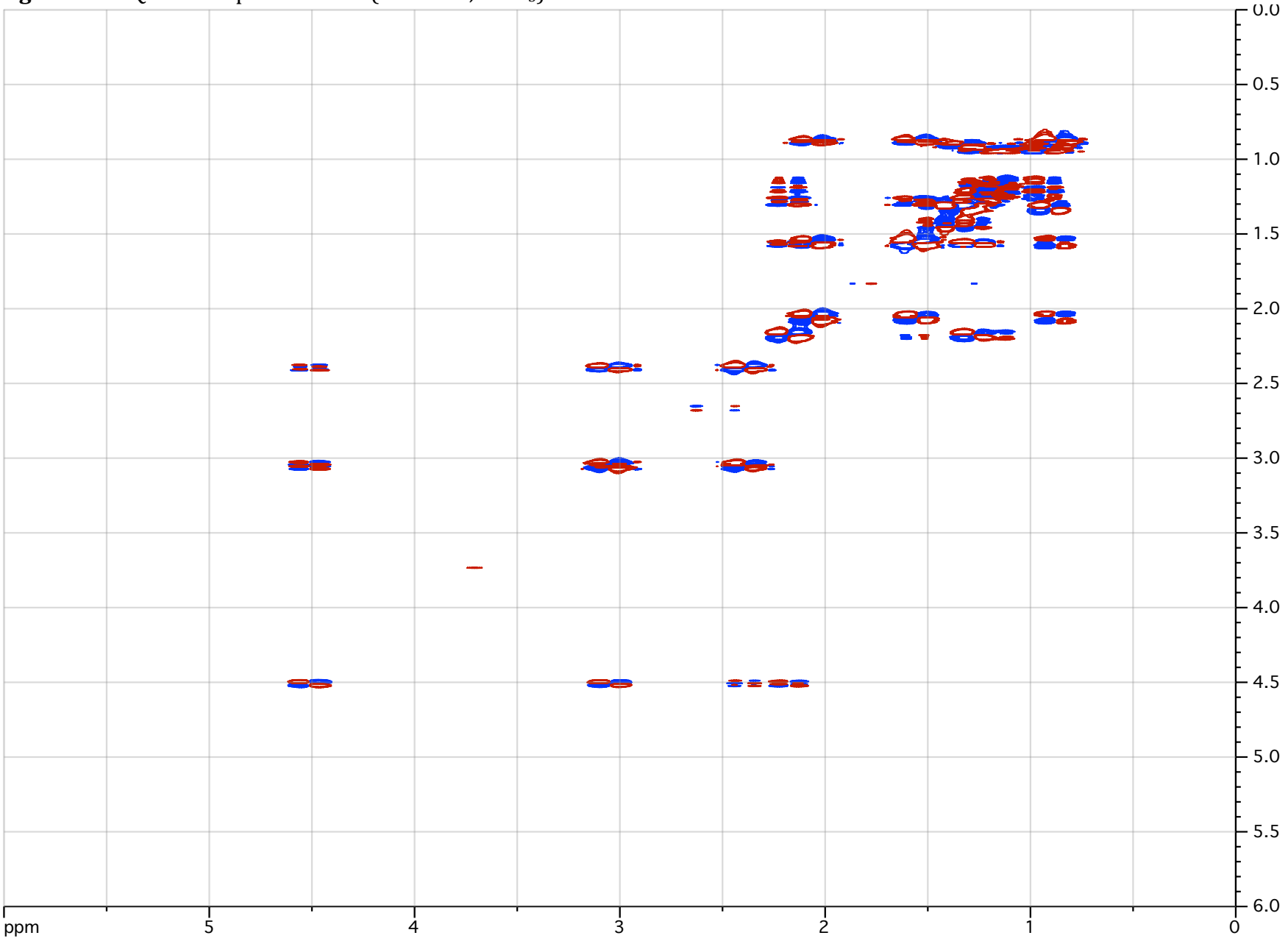


Figure S9. gHSQC spectrum of **1** (600 MHz, $CDCl_3$)

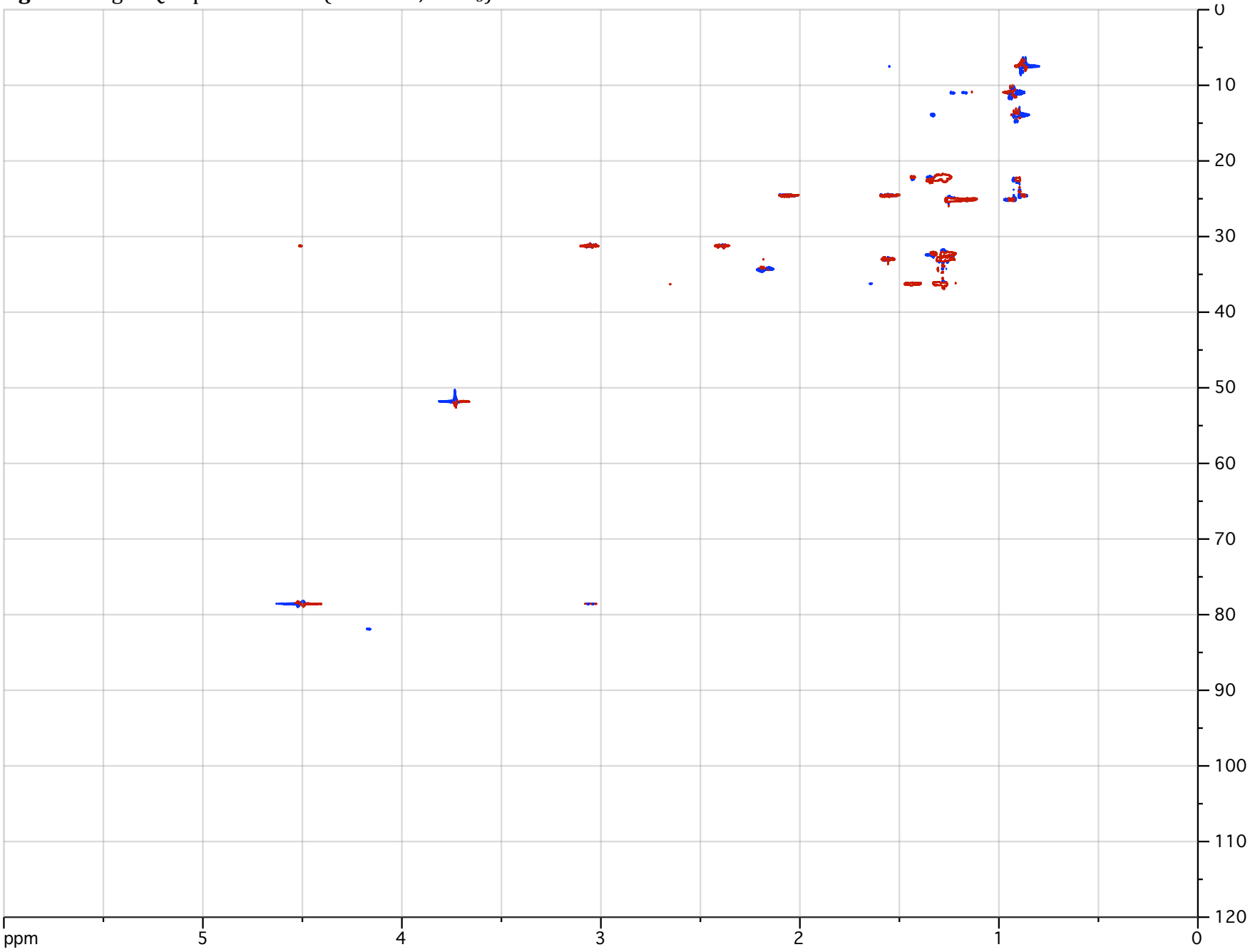


Figure S10. gHMBC spectrum of **1** (600 MHz, $CDCl_3$)

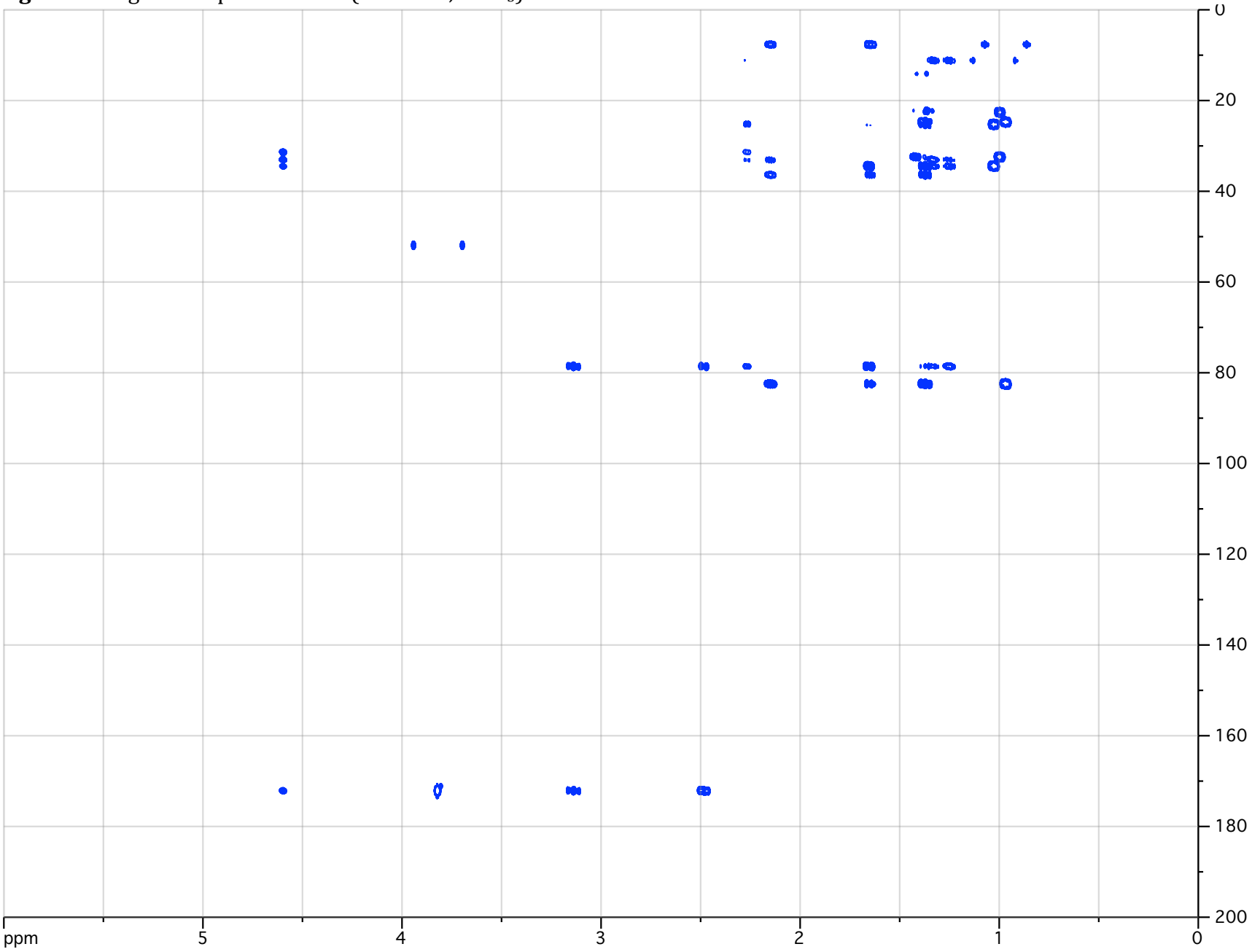


Figure S11. gNOESY spectrum of **1** (600 MHz, τ_m = 300 ms, $CDCl_3$)

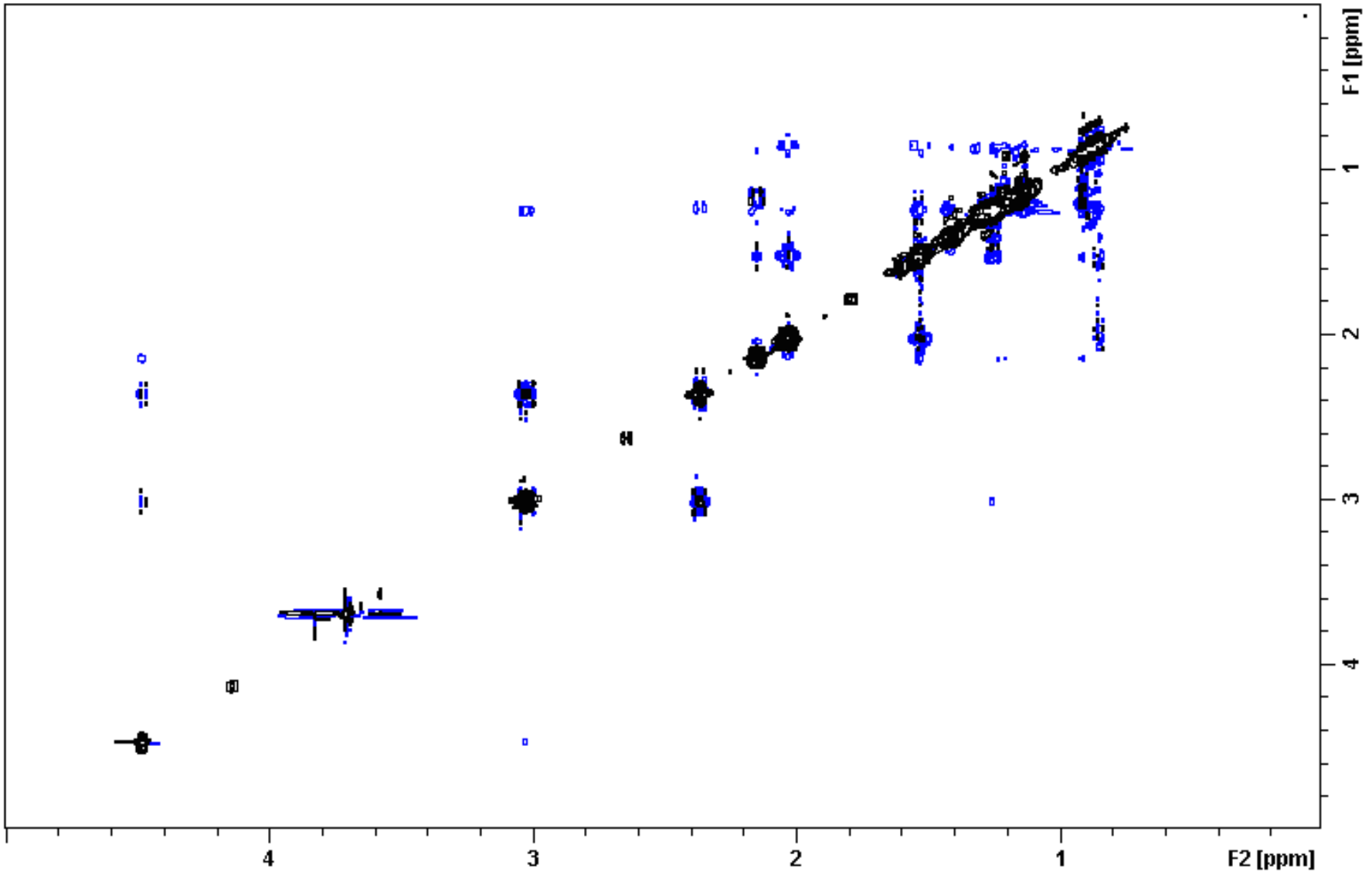


Figure S12. ^{1}H NMR spectrum of **2** (600 MHz, $CDCl_3$)

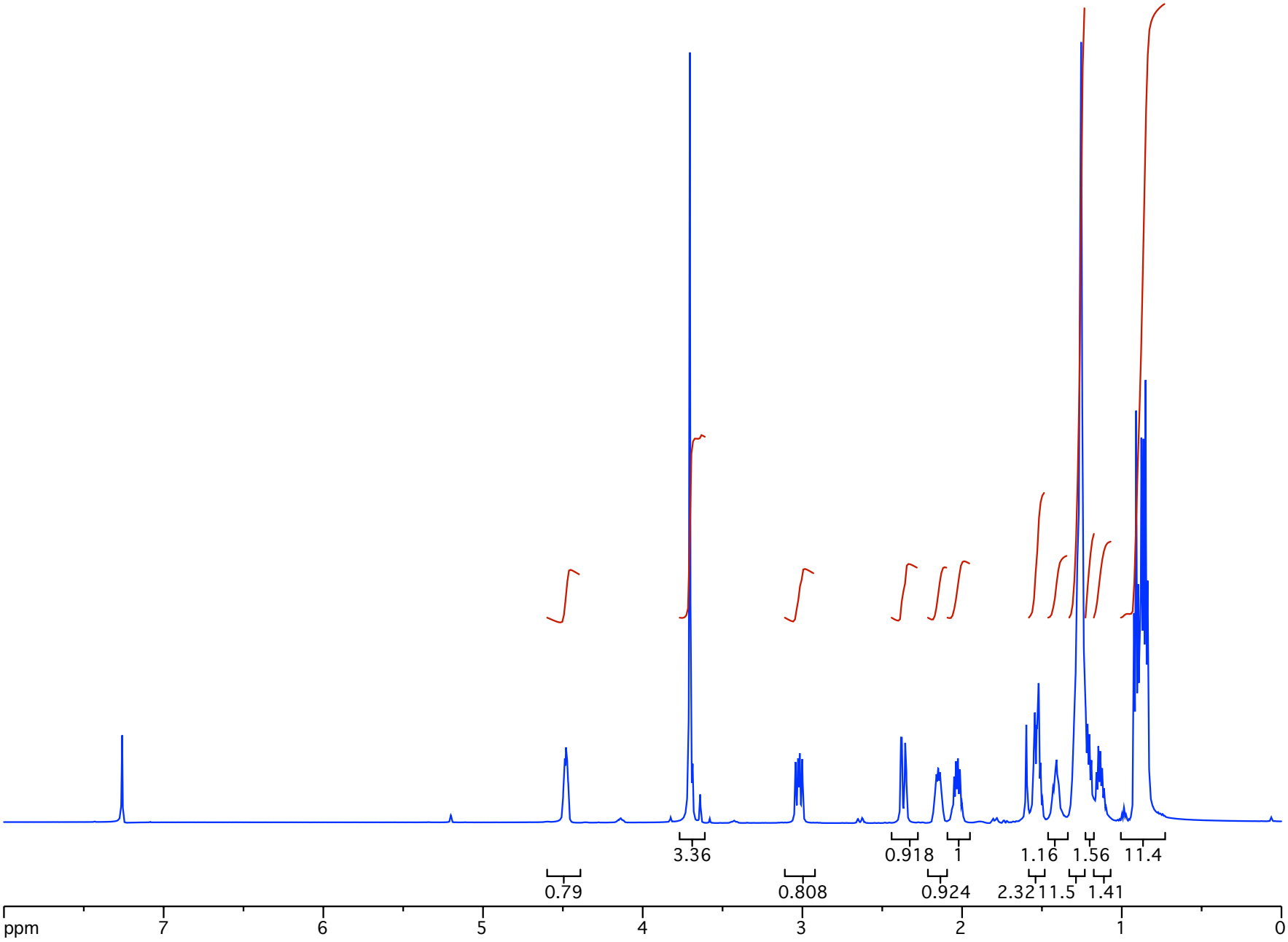


Figure S13. ^{13}C NMR spectrum of **2** (125 MHz, $CDCl_3$)

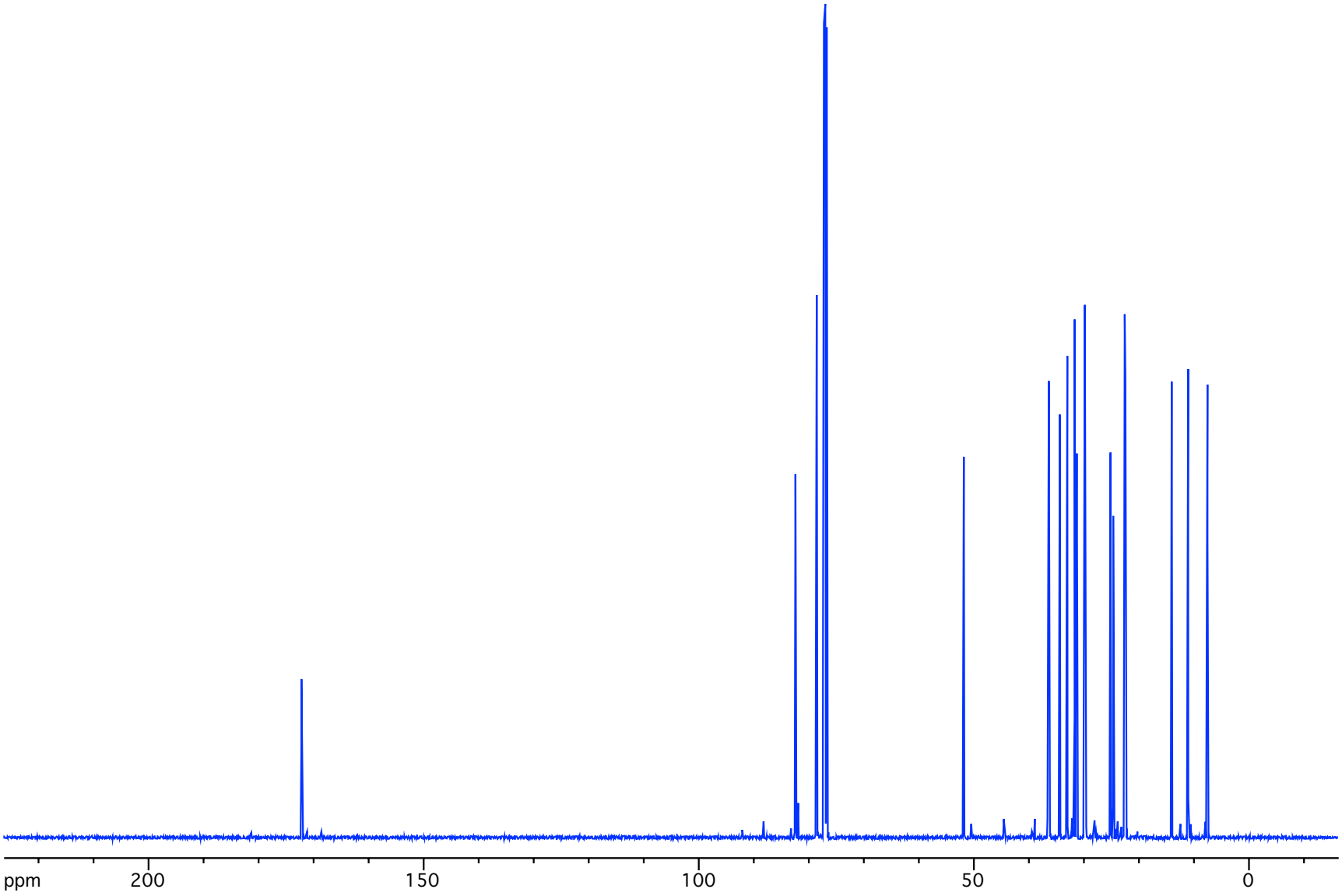


Figure S14. DQF-COSY spectrum of **2** (600 MHz, $CDCl_3$)

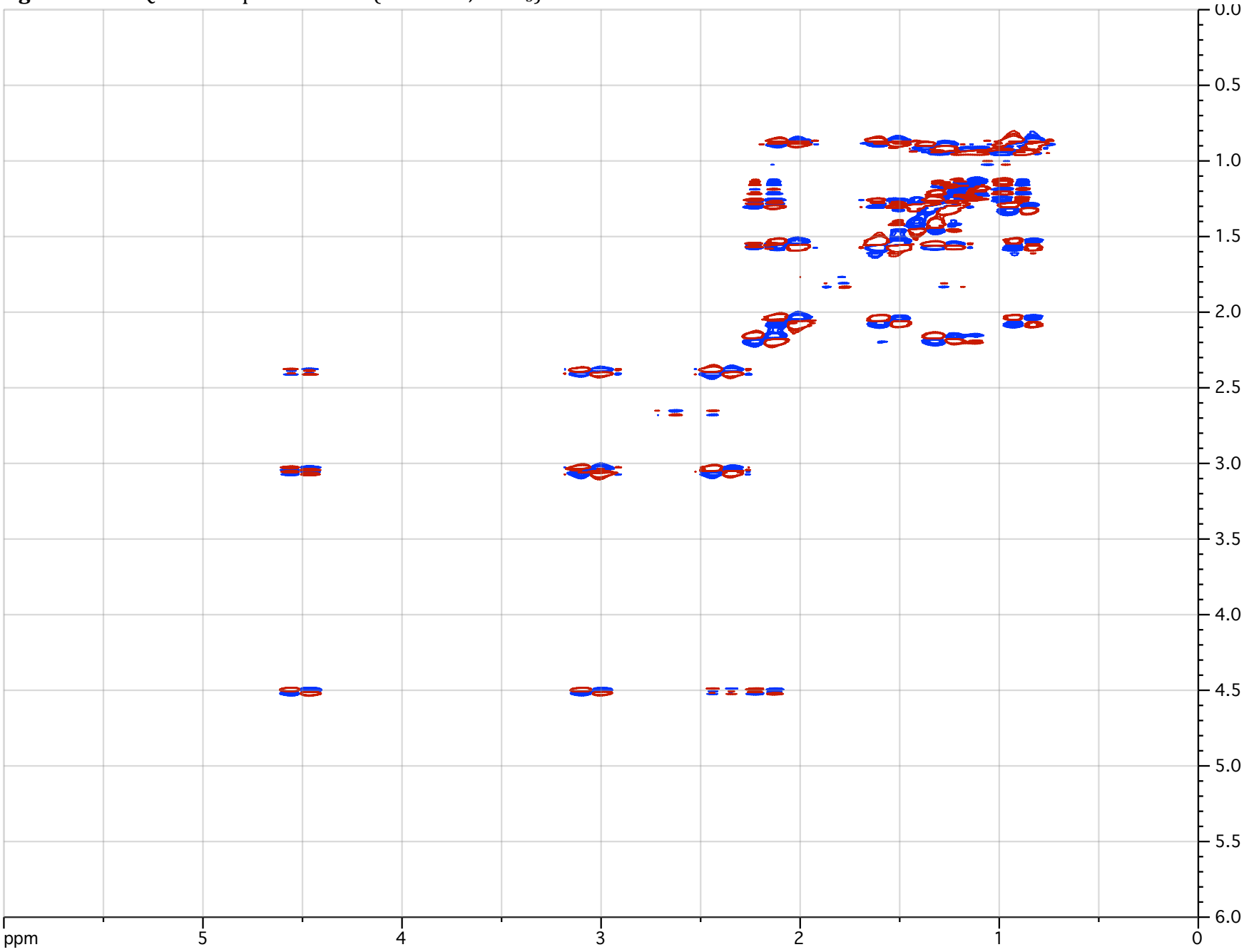


Figure S15. gHSQC spectrum of **2** (600 MHz, $CDCl_3$)

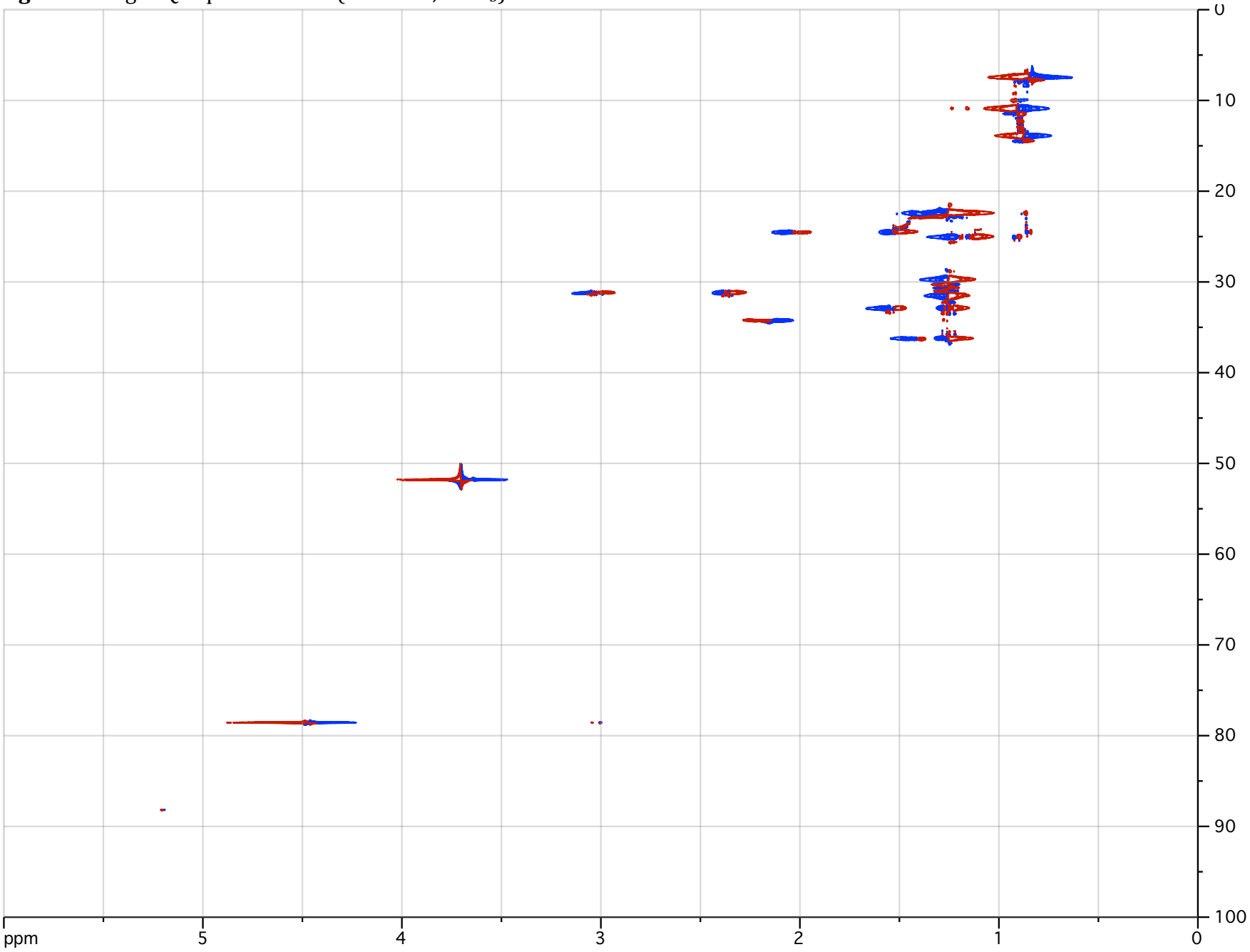


Figure S16. gHMBC spectrum of **2** (600 MHz, $CDCl_3$)

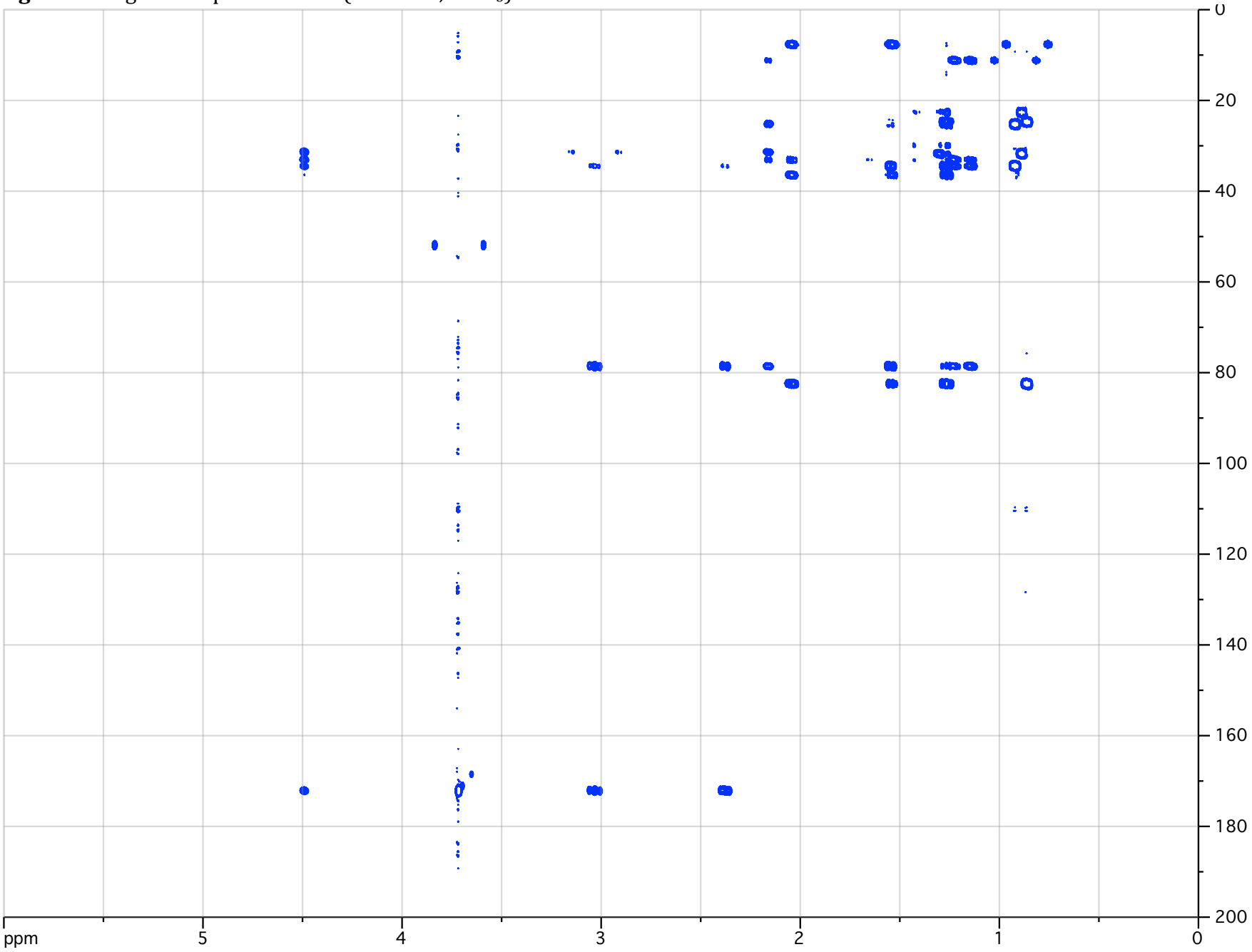


Figure S17. gNOESY spectrum of **2** (600 MHz, τ_m = 300 ms, $CDCl_3$)

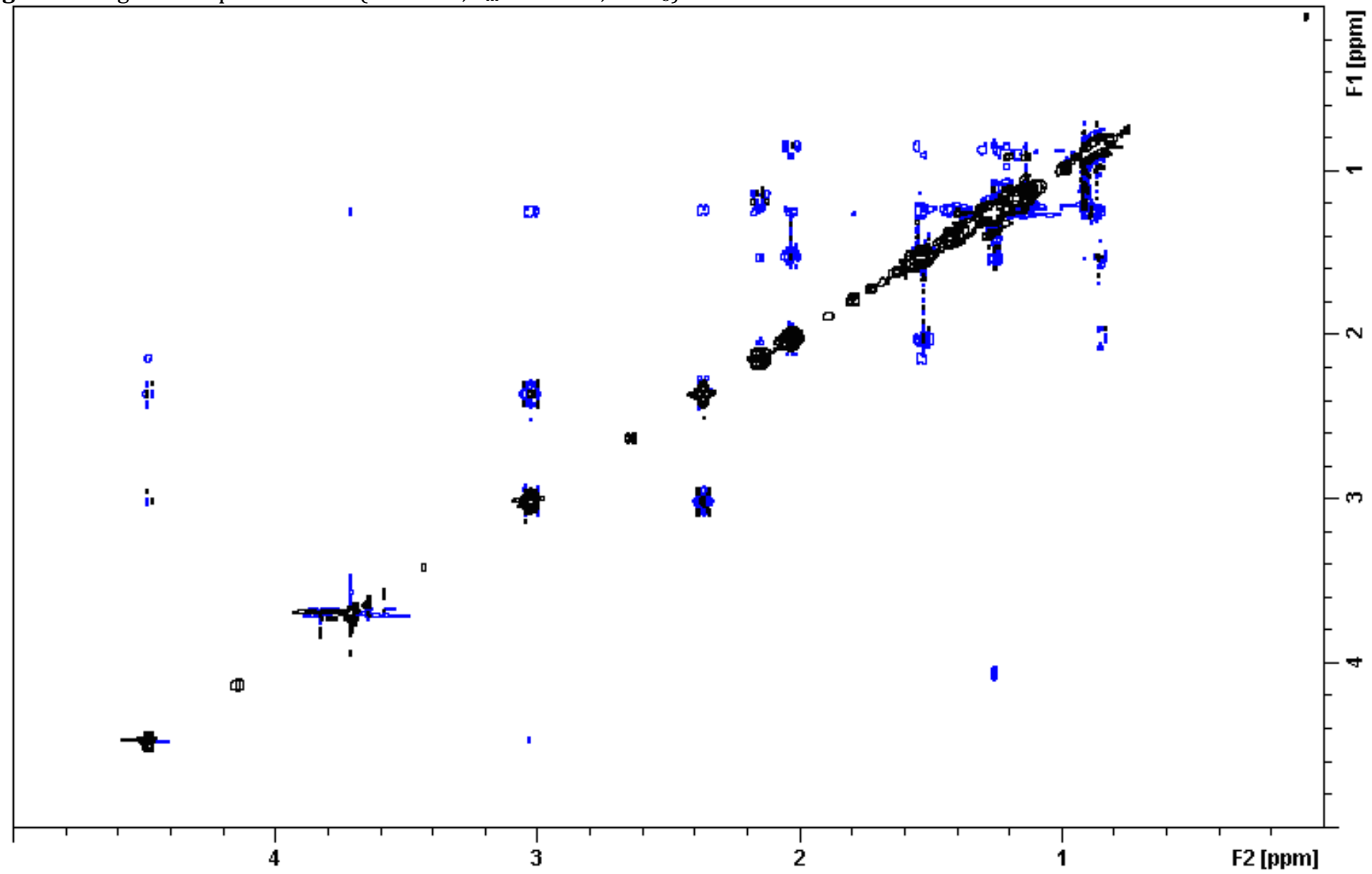


Figure S18. ^{1}H NMR spectrum of **9** (600 MHz, $CDCl_3$)

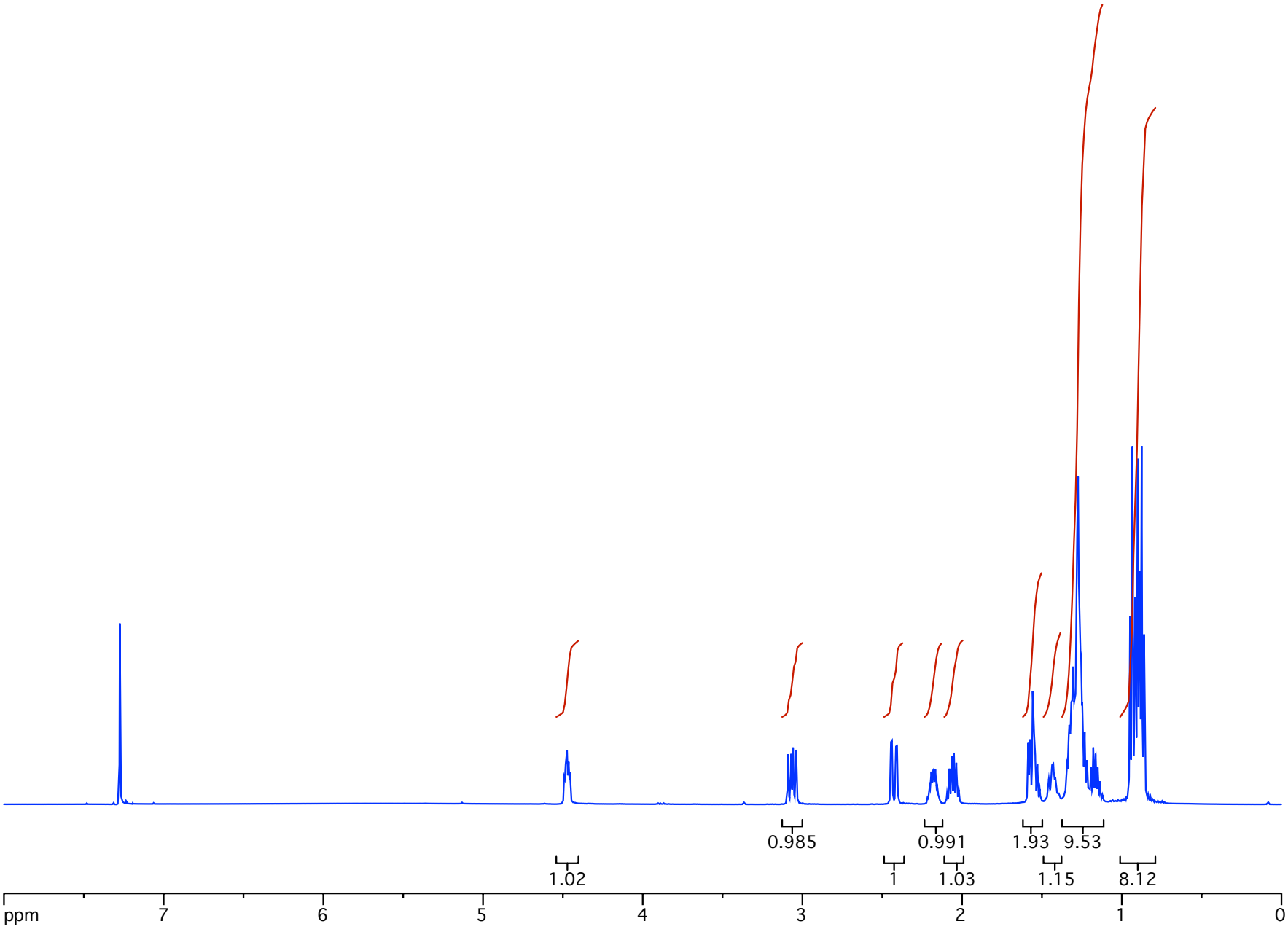


Figure S19. ^{13}C NMR spectrum of **9** (125 MHz, $CDCl_3$)

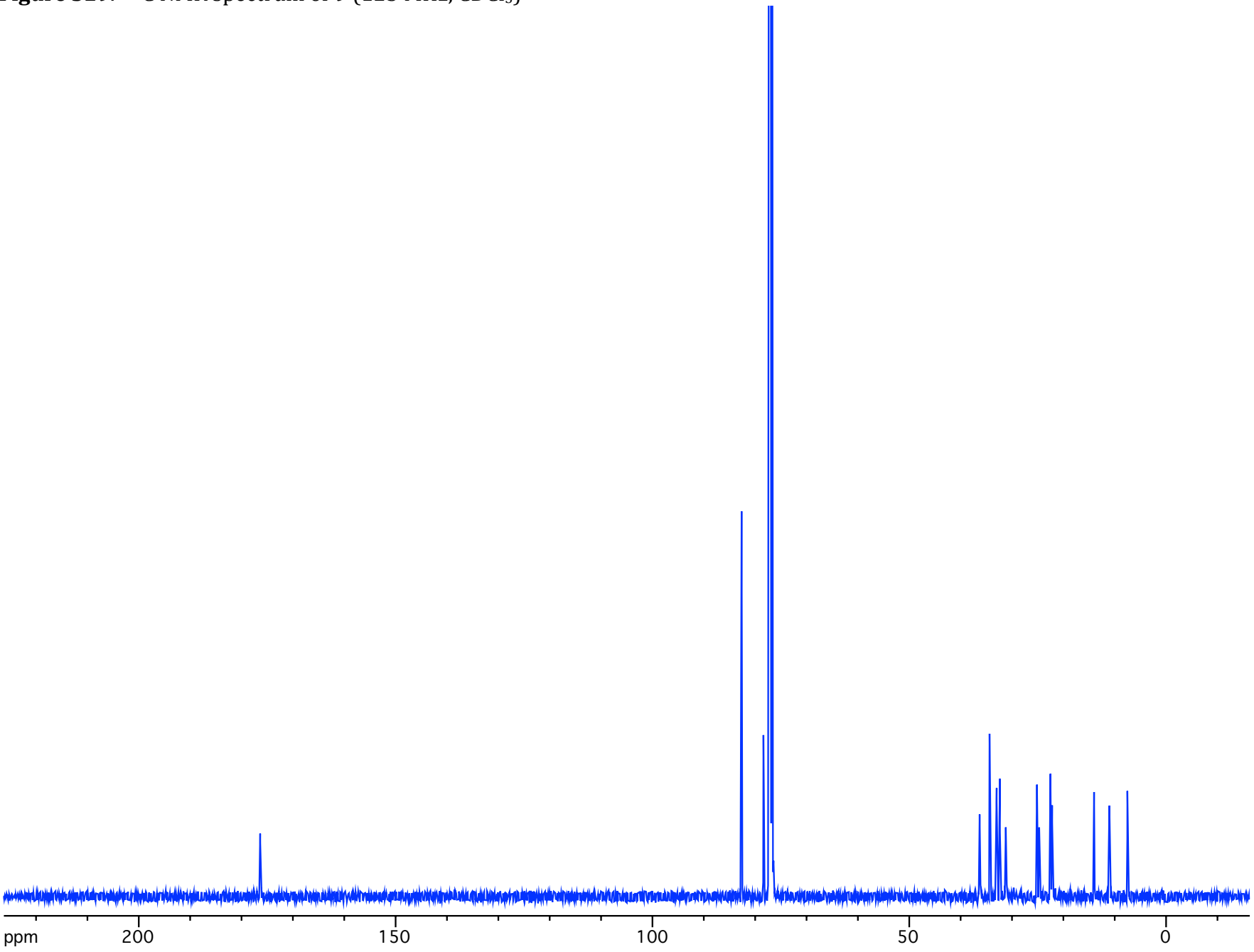


Figure S20. ^{1}H NMR spectrum of **10** (500 MHz, $CDCl_3$)

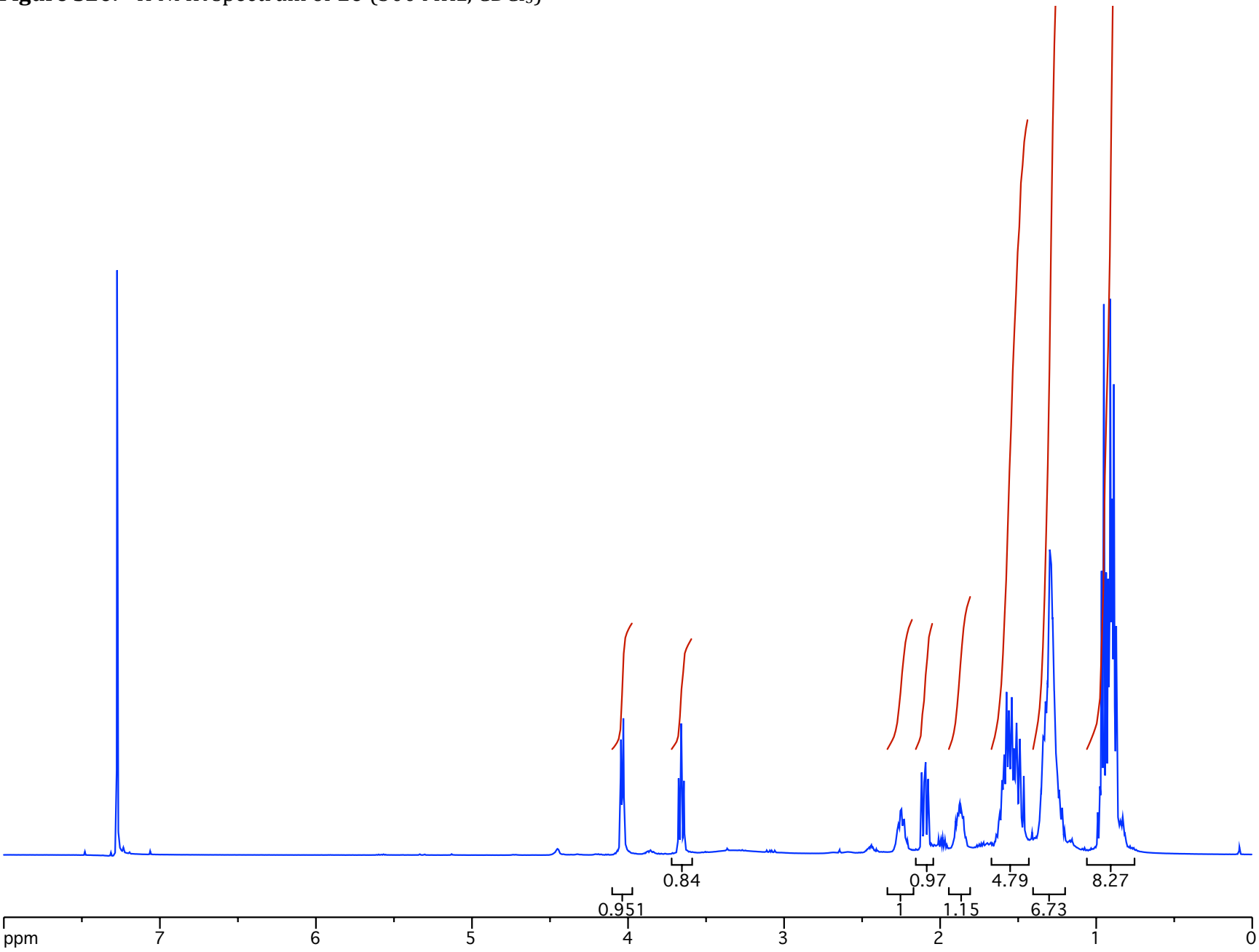


Figure S21. ^{13}C NMR spectrum of **10** (125 MHz, $CDCl_3$)

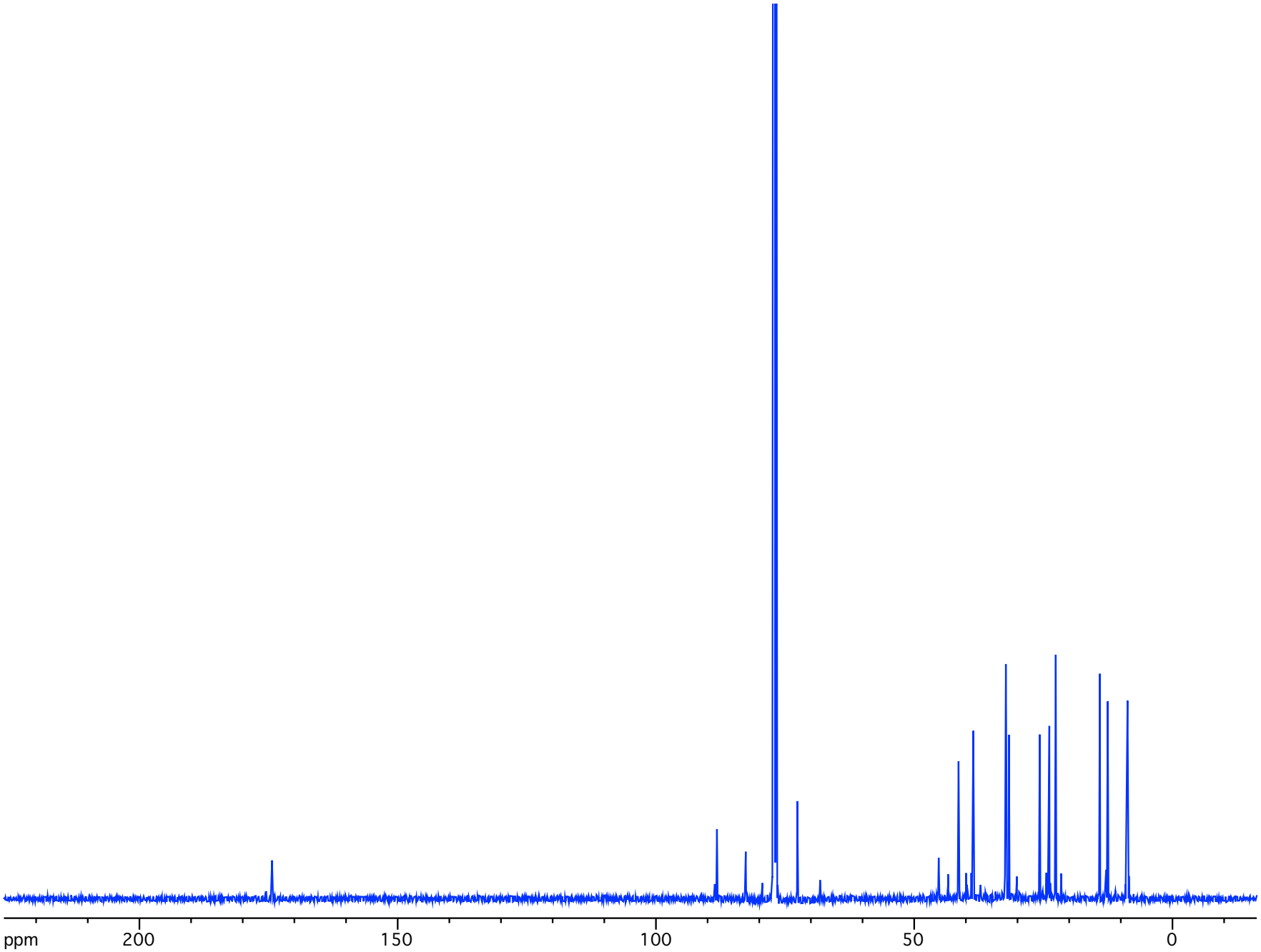


Figure S22. DQF-COSY spectrum of **10** (600 MHz, $CDCl_3$)

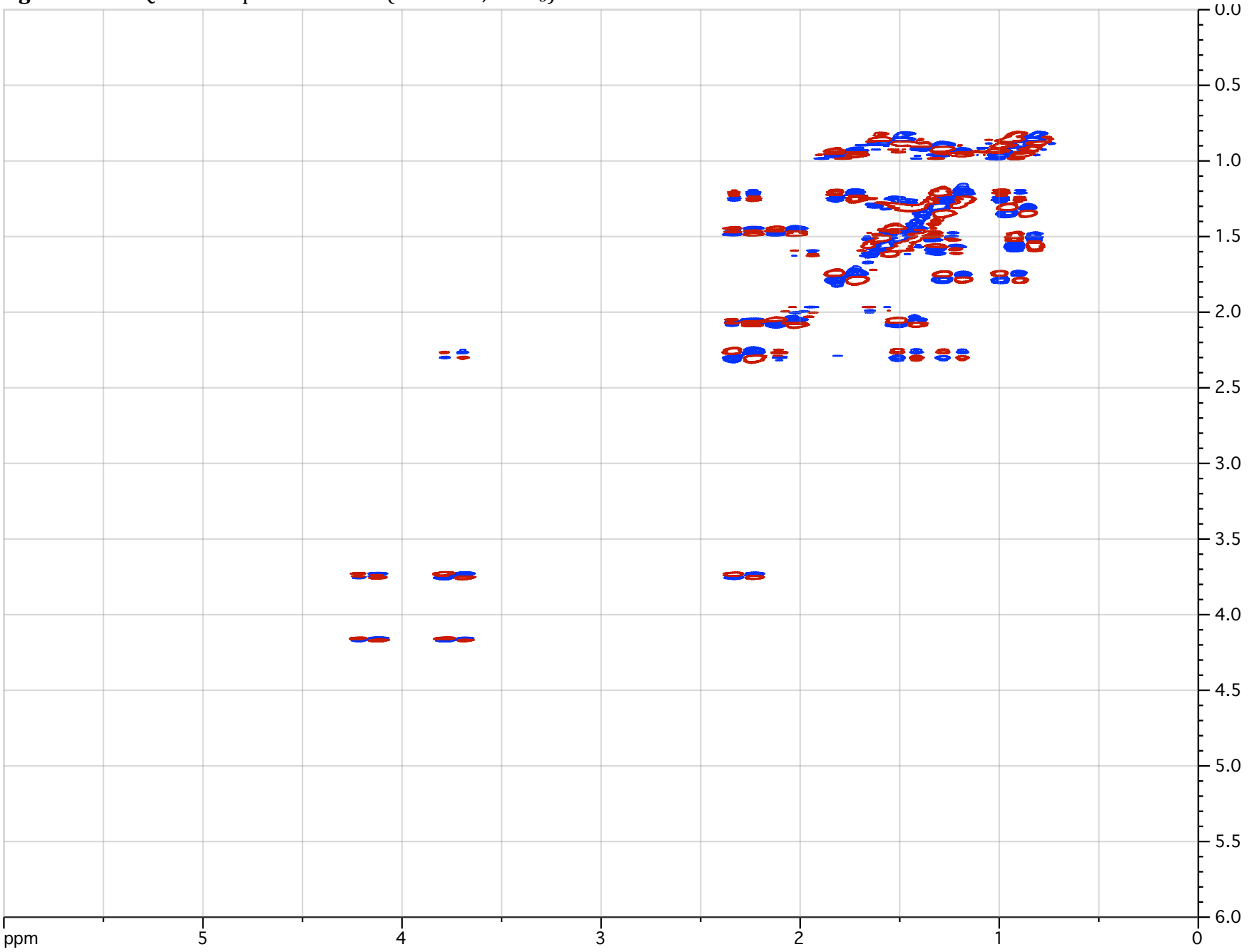


Figure S23. gHSQC spectrum of **10** (600 MHz, $CDCl_3$)

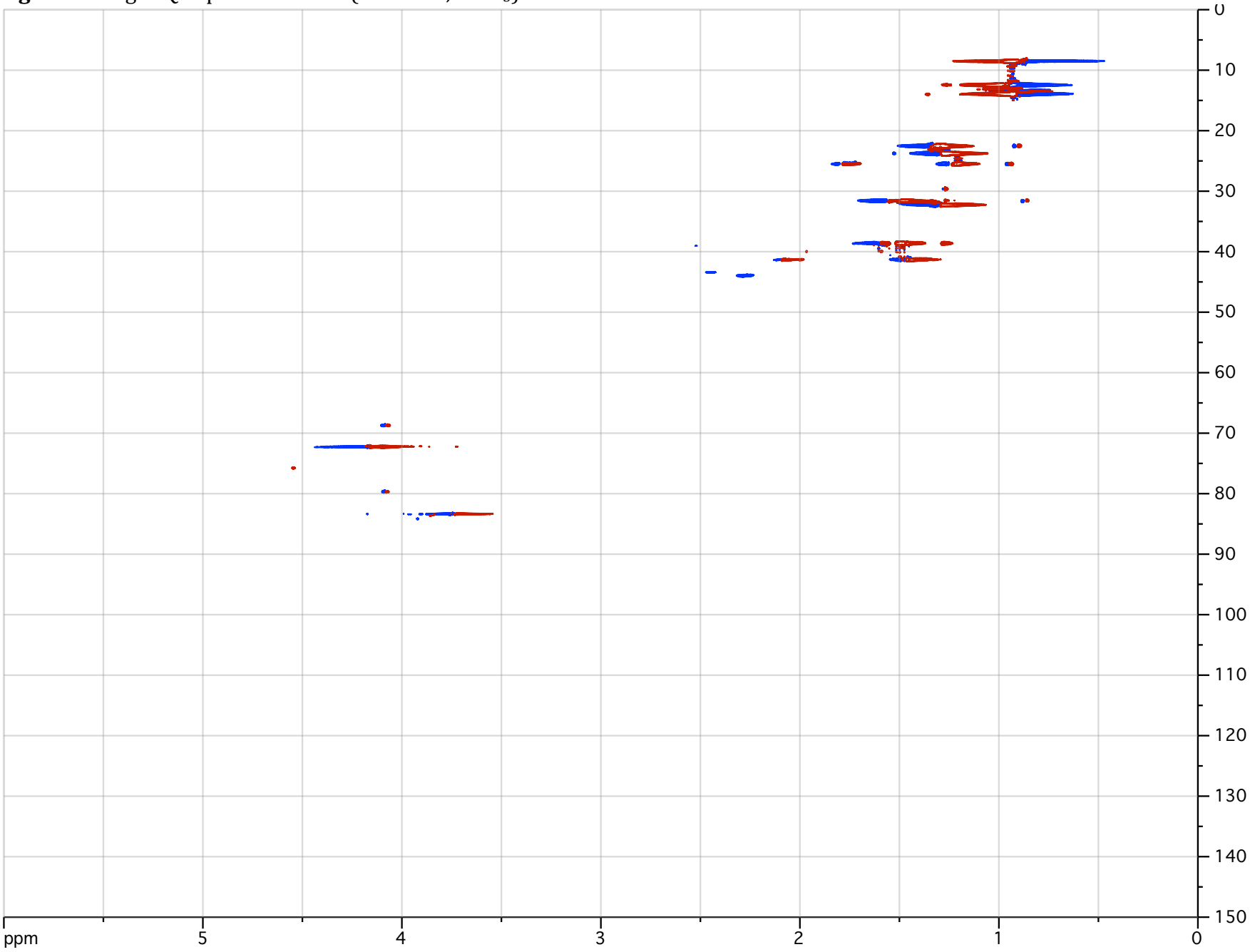


Figure S24. gHMBC spectrum of **10** (600 MHz, $CDCl_3$)

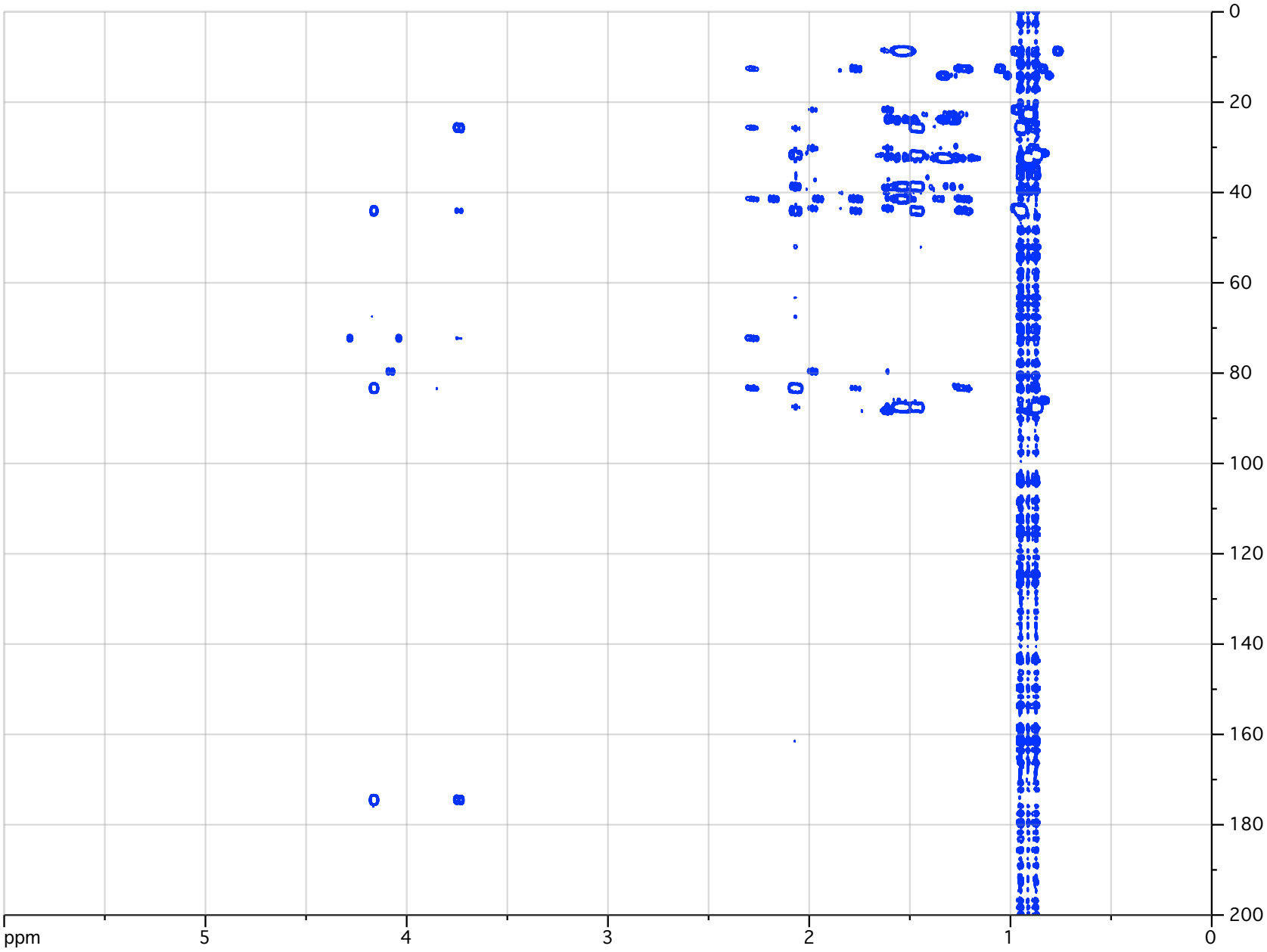


Figure S25. gNOESY spectrum of **10** (600 MHz, τ_m = 300 ms, $CDCl_3$)

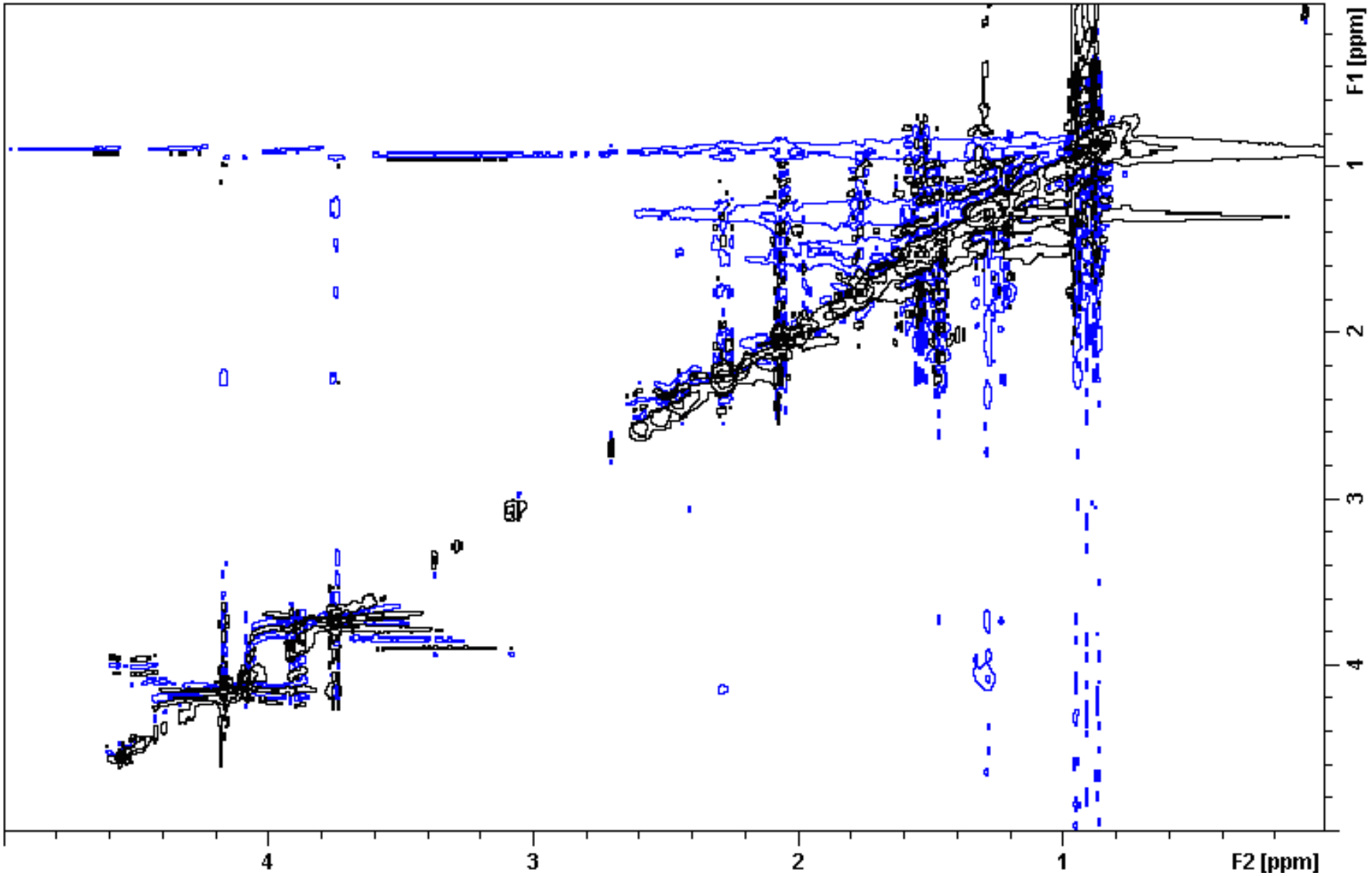


Figure S26. ^{1}H NMR spectrum of **11** (500 MHz, $CDCl_3$)

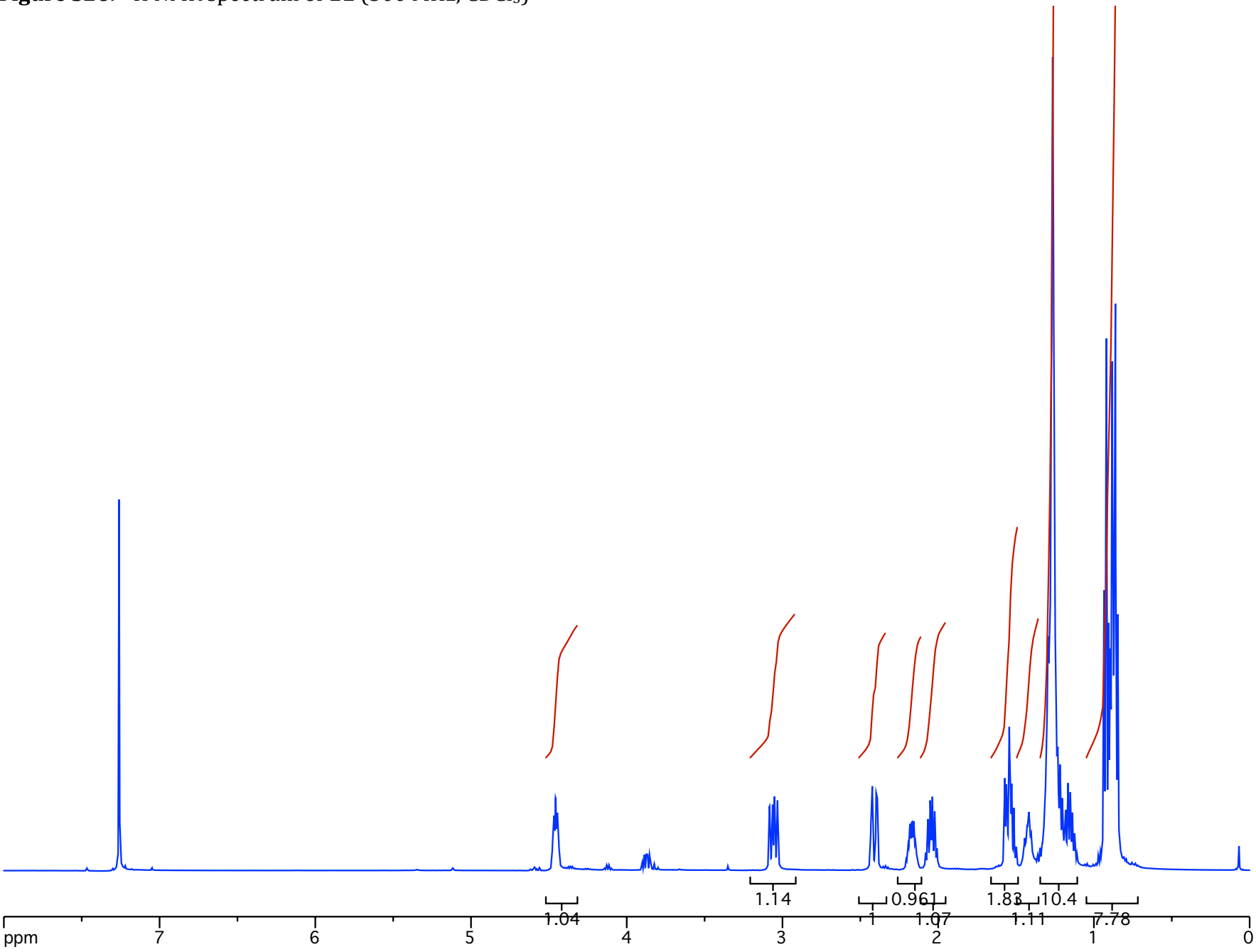


Figure S27. ^{13}C NMR spectrum of **11** (125 MHz, $CDCl_3$)

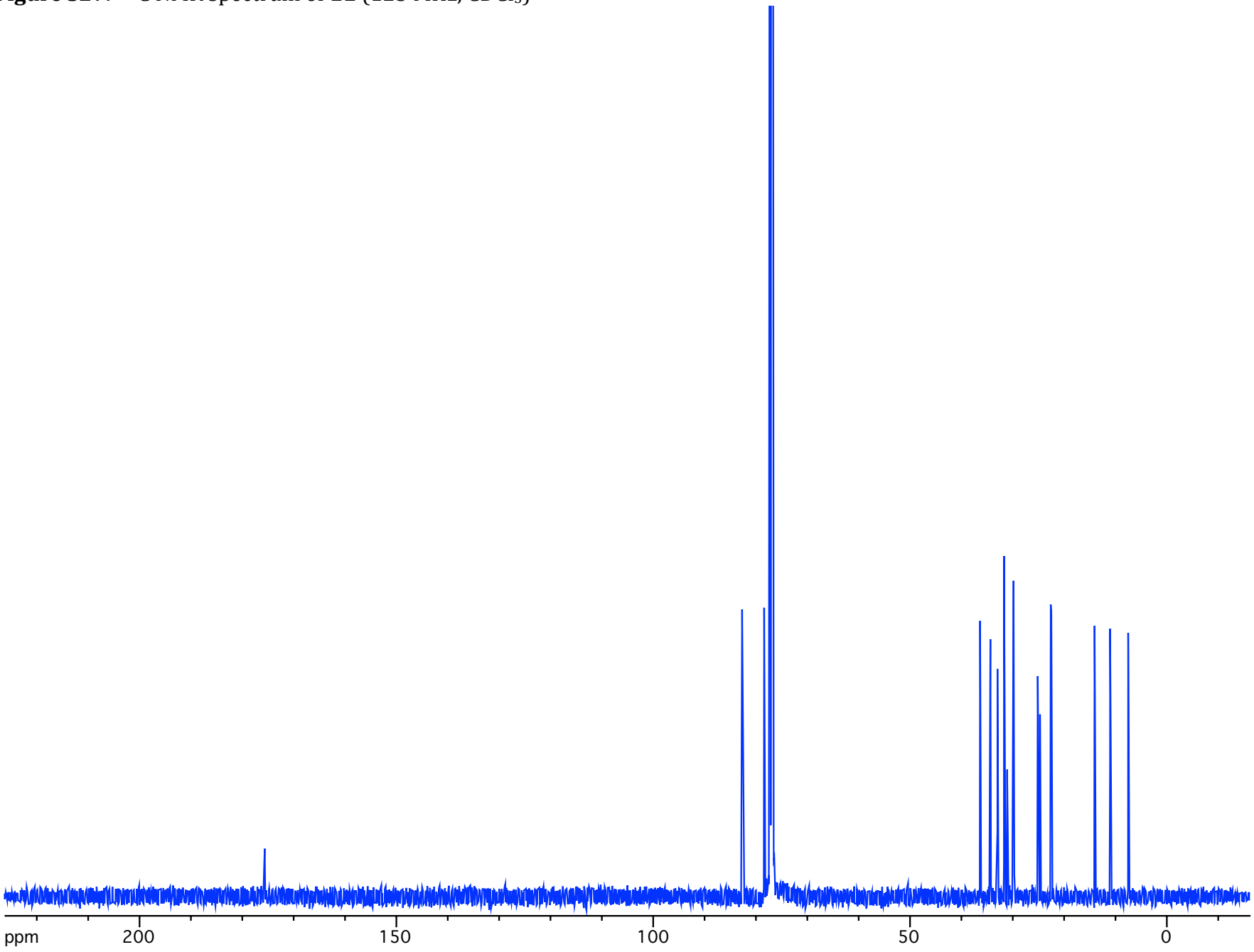


Figure S28. ^{1}H NMR spectrum of **12** (500 MHz, $CDCl_3$)

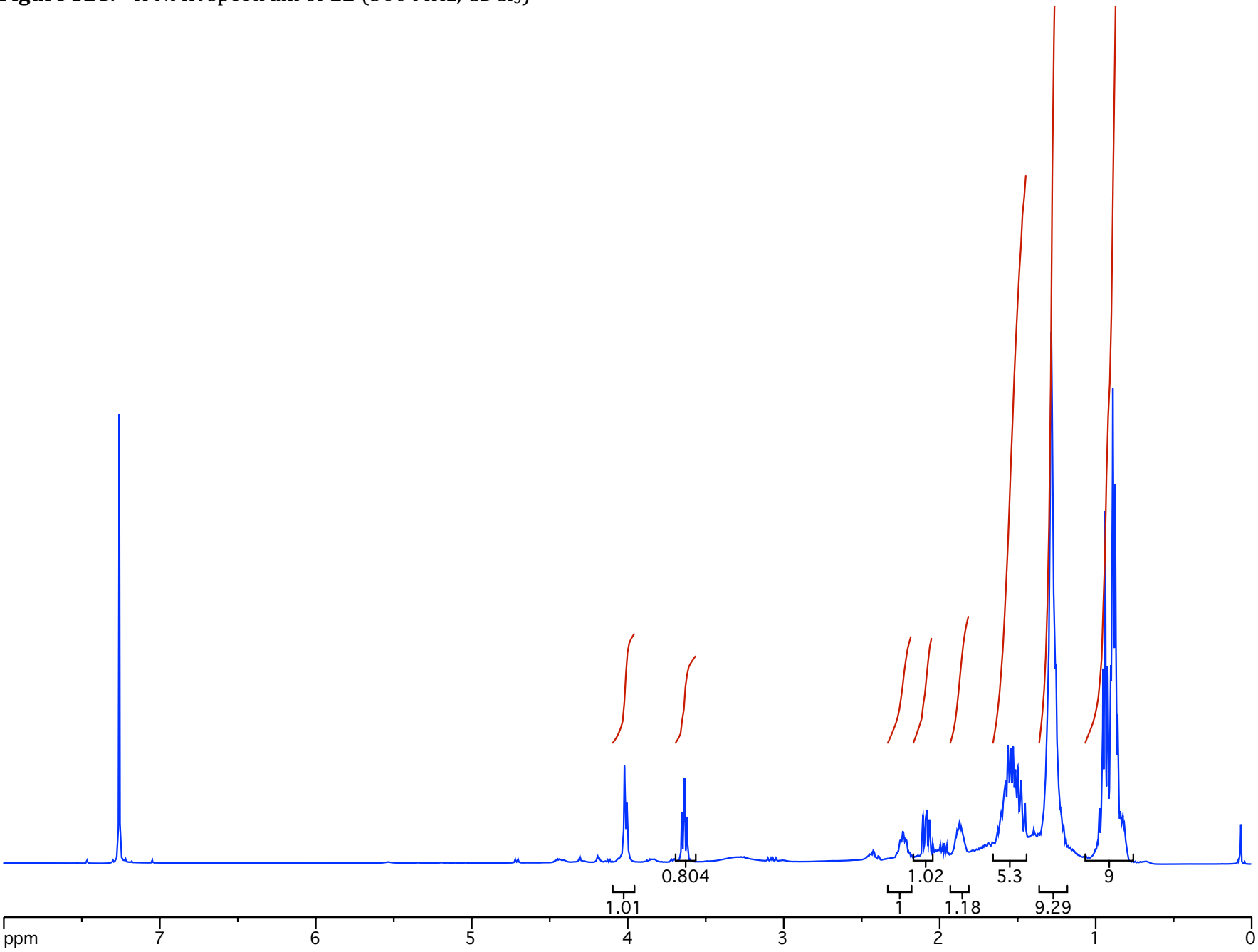


Figure S29. ^{13}C NMR spectrum of **12** (125 MHz, $CDCl_3$)

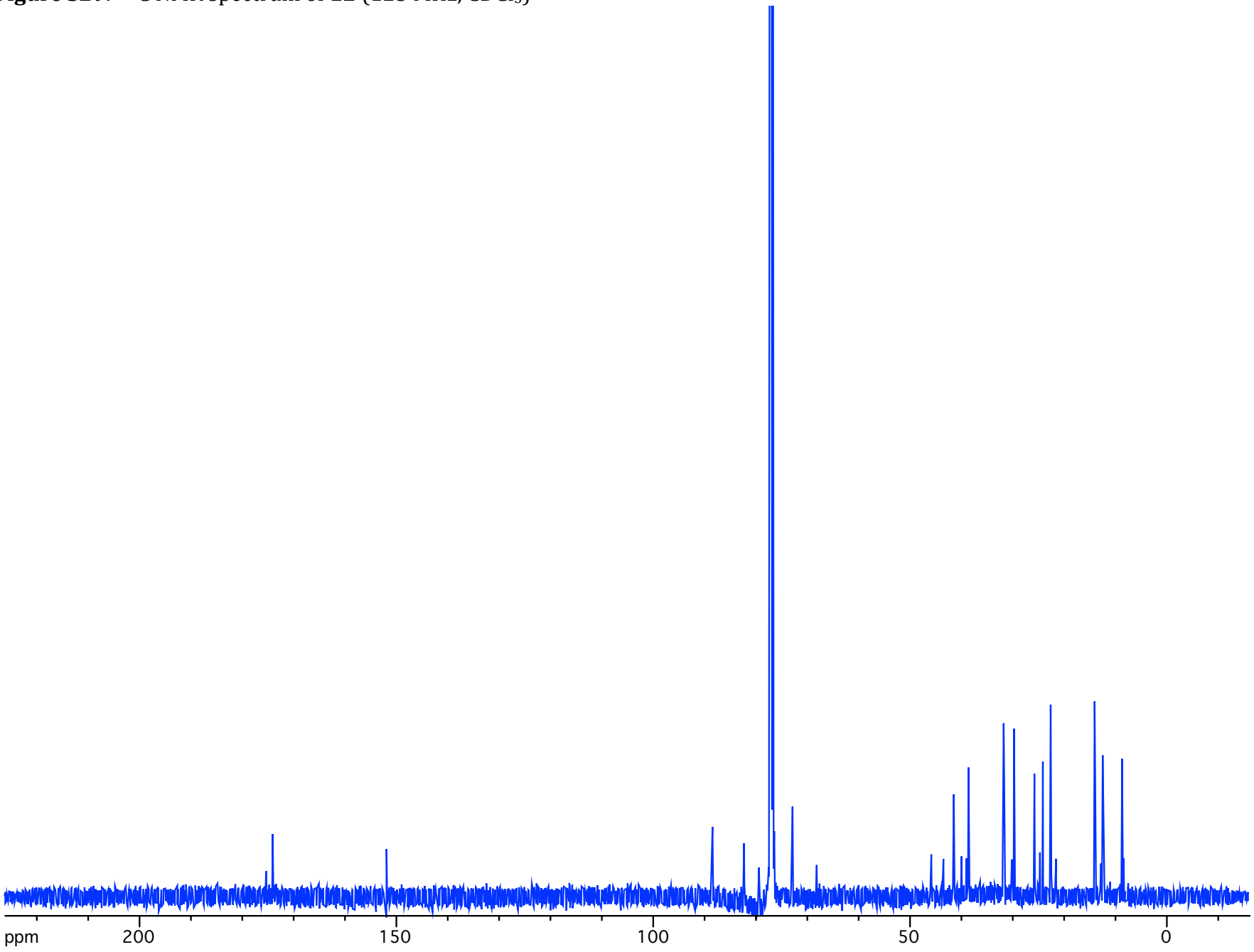


Figure S30. ^{1}H NMR spectrum of plakinic acid M (**3**) (600 MHz, $CDCl_3$)

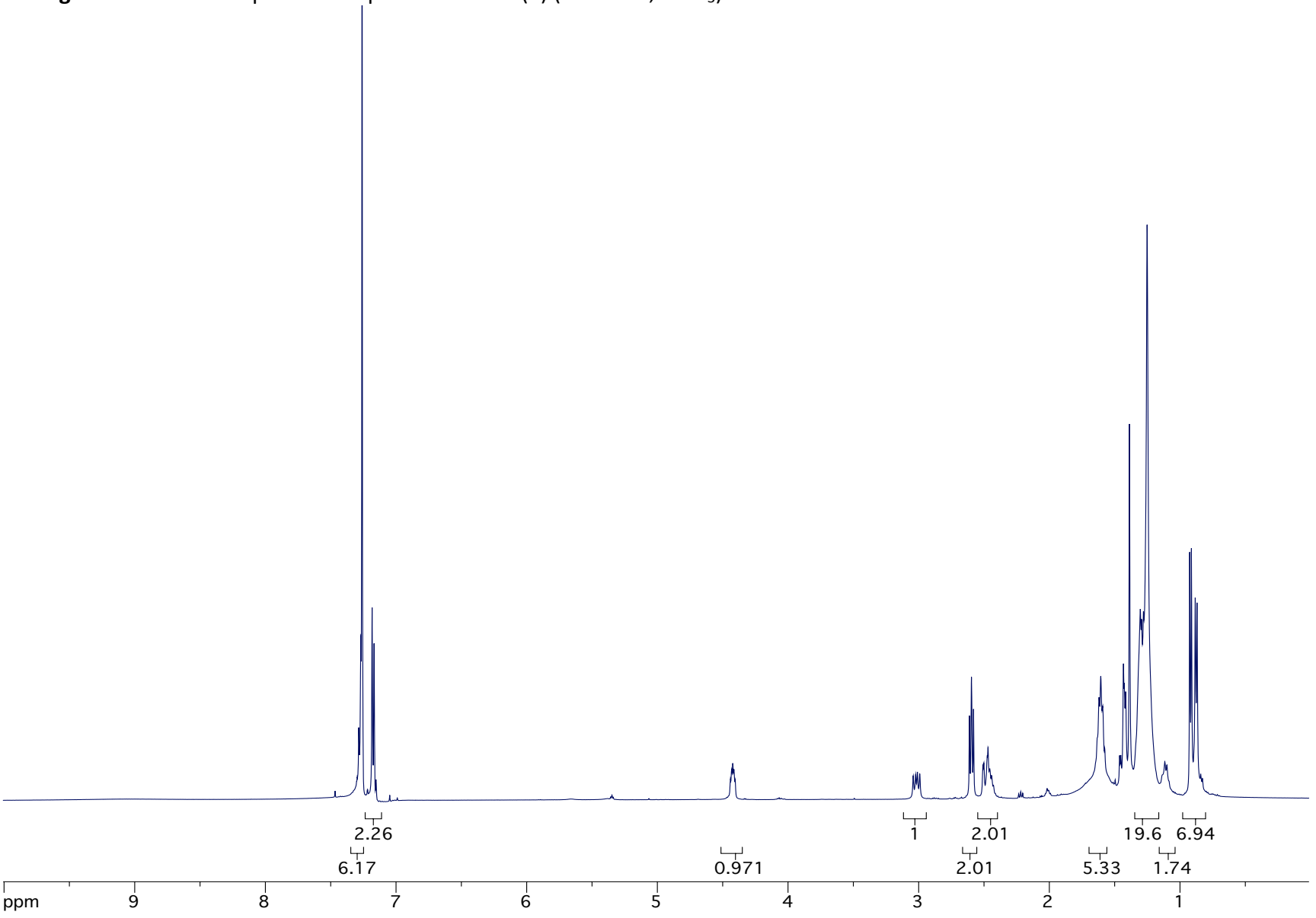


Figure S31. ^{13}C NMR spectrum of plakinic acid M (**3**) (125 MHz, $CDCl_3$)

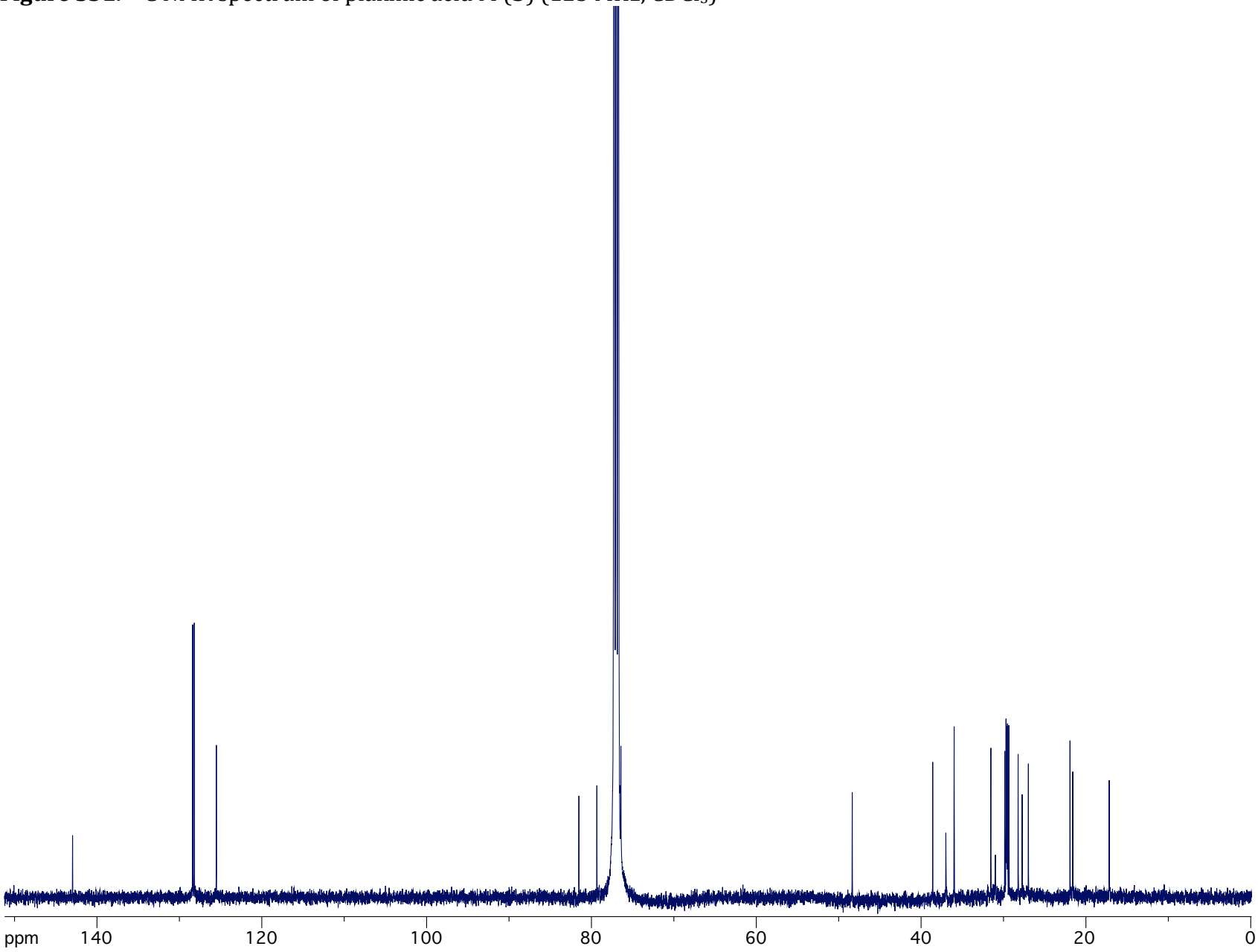


Figure S32. DQF-COSY spectrum of plakinic acid M (**3**) (600 MHz, $CDCl_3$)

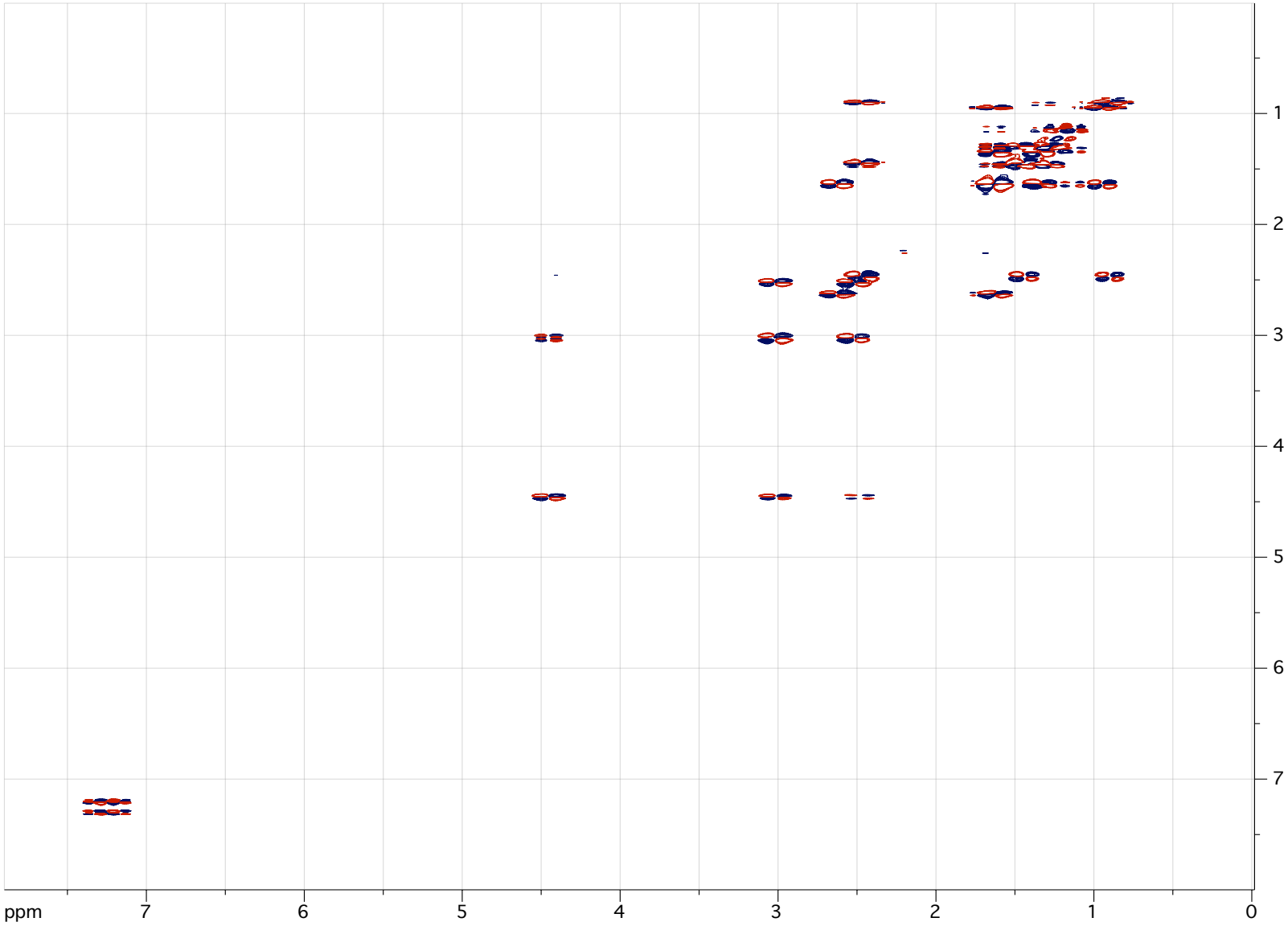


Figure S33. gHSQC spectrum of plakinic acid M (**3**) (600 MHz, $CDCl_3$)

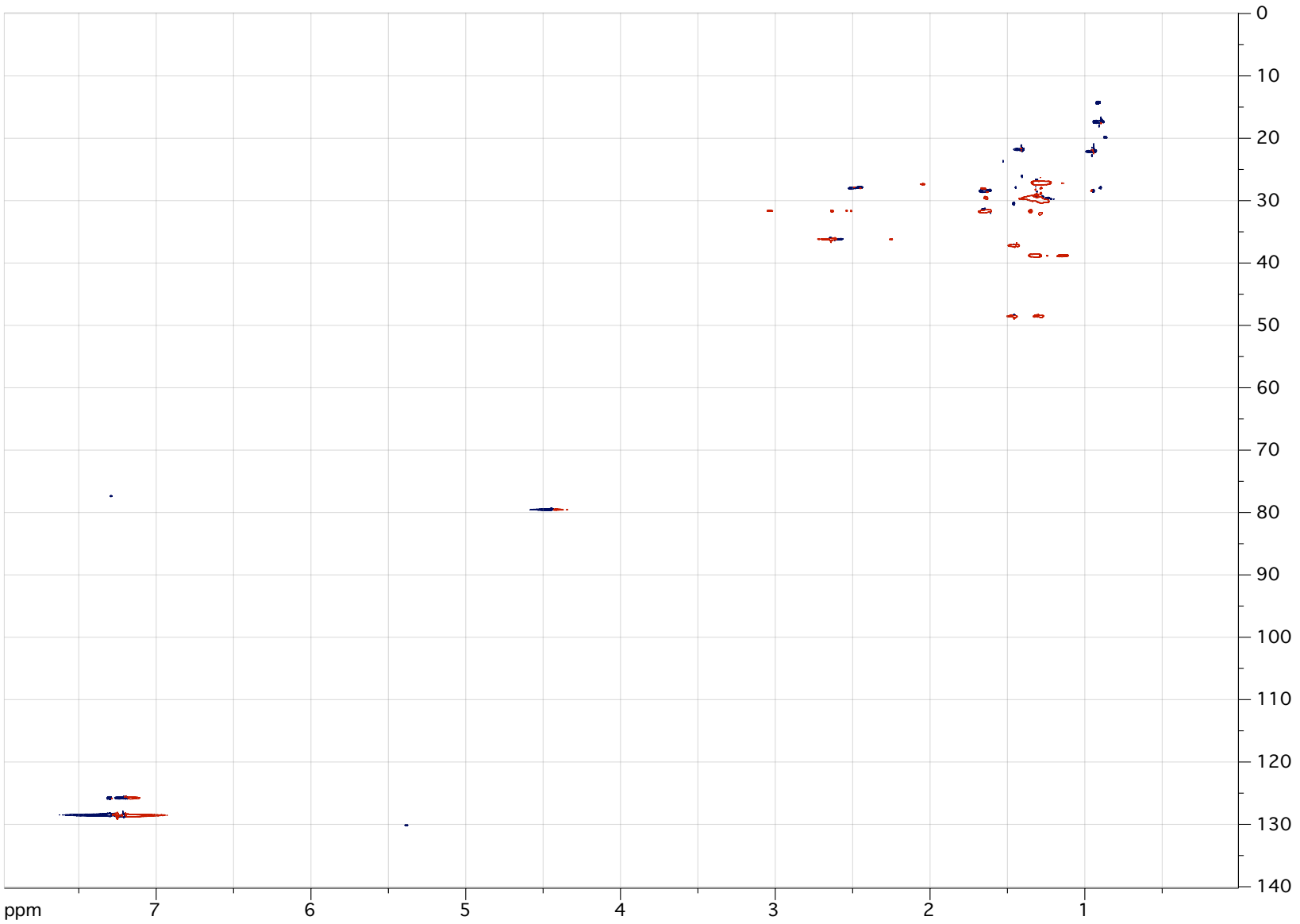


Figure S34. gHMBC spectrum of plakinic acid M (**3**) (600 MHz, $CDCl_3$)

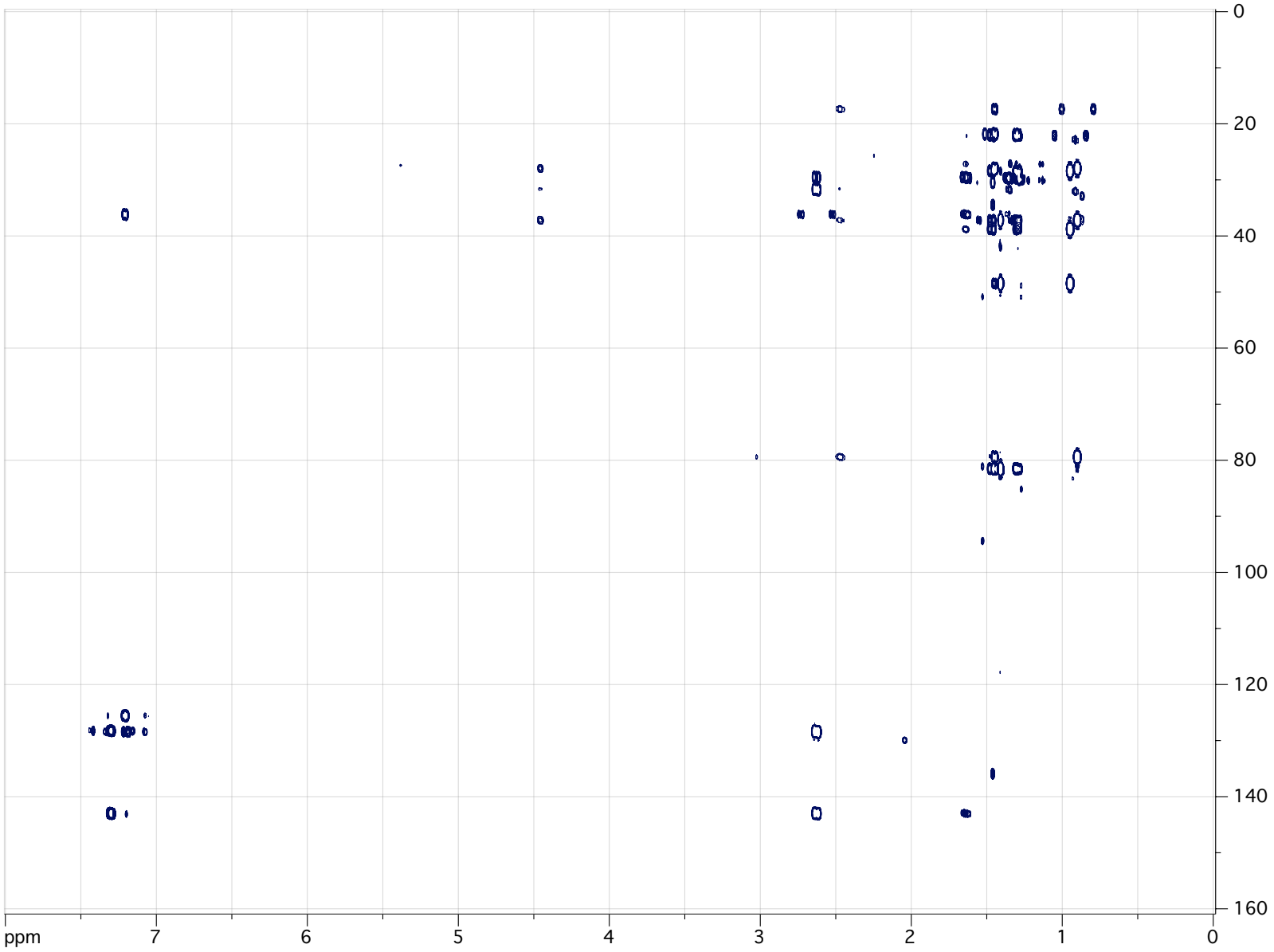


Figure S35. gNOESY spectrum of plakinic acid M (**3**) (600 MHz, τ_m = 300 ms, $CDCl_3$)

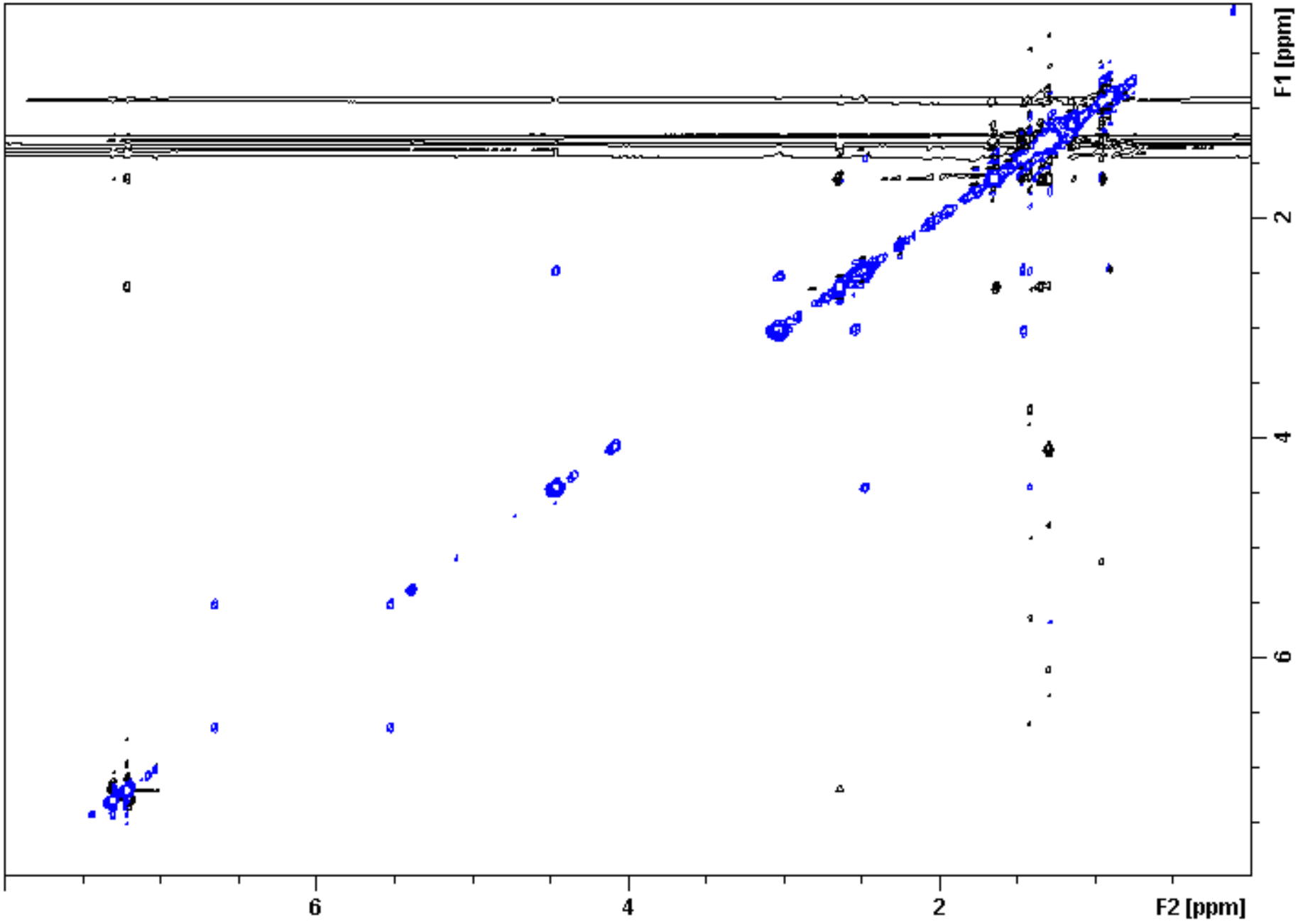


Figure S36. ^{1}H NMR spectrum of plakinic acid N (**4**) (600 MHz, $CDCl_3$)

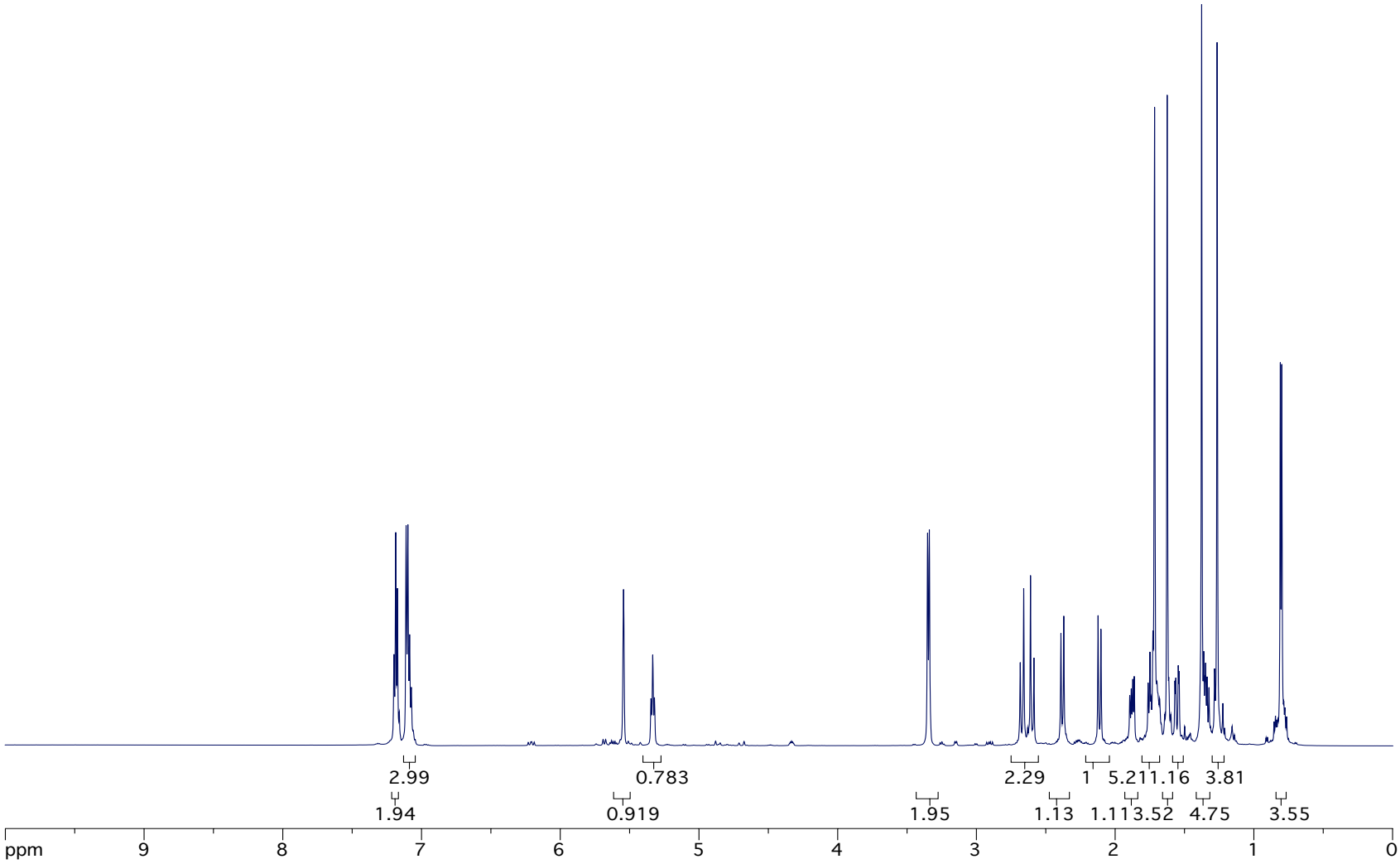


Figure S37. DQF-COSY spectrum of plakinic acid N (**4**) (600 MHz, $CDCl_3$)

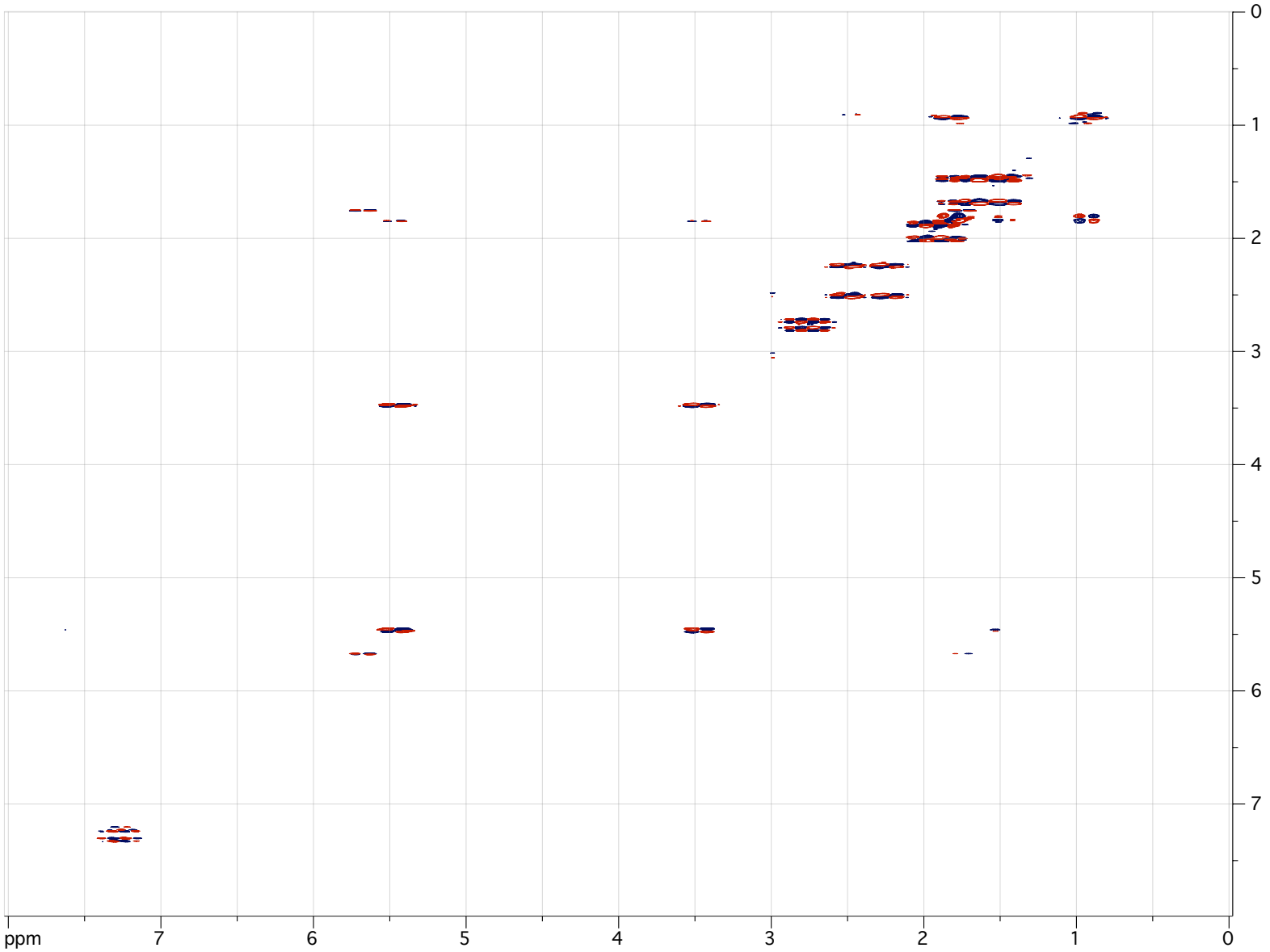


Figure S38. gHSQC spectrum of plakinic acid N (**4**) (600 MHz, $CDCl_3$)

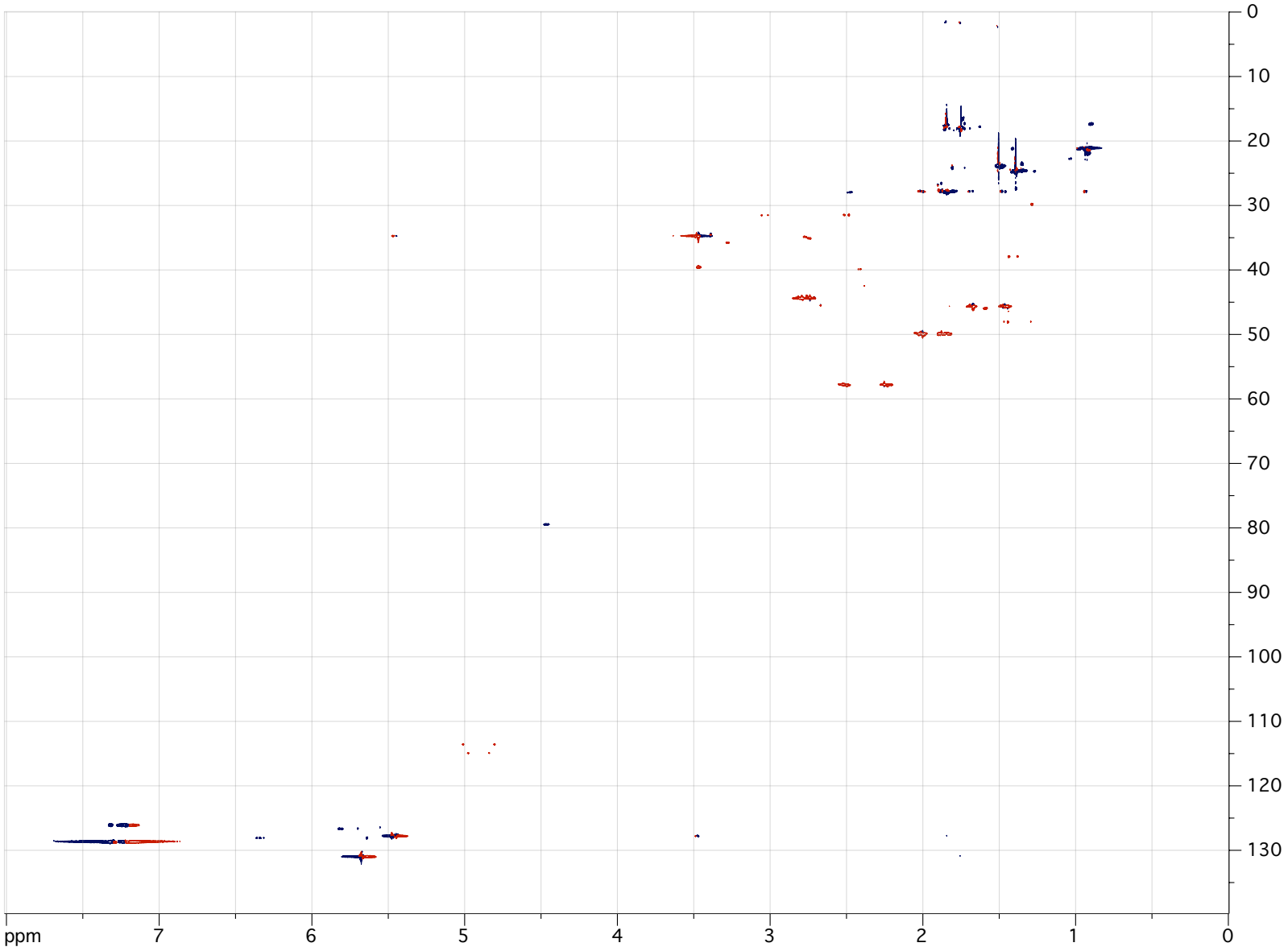


Figure S39. gHMBC spectrum of plakinic acid N (**4**) (600 MHz, $CDCl_3$)

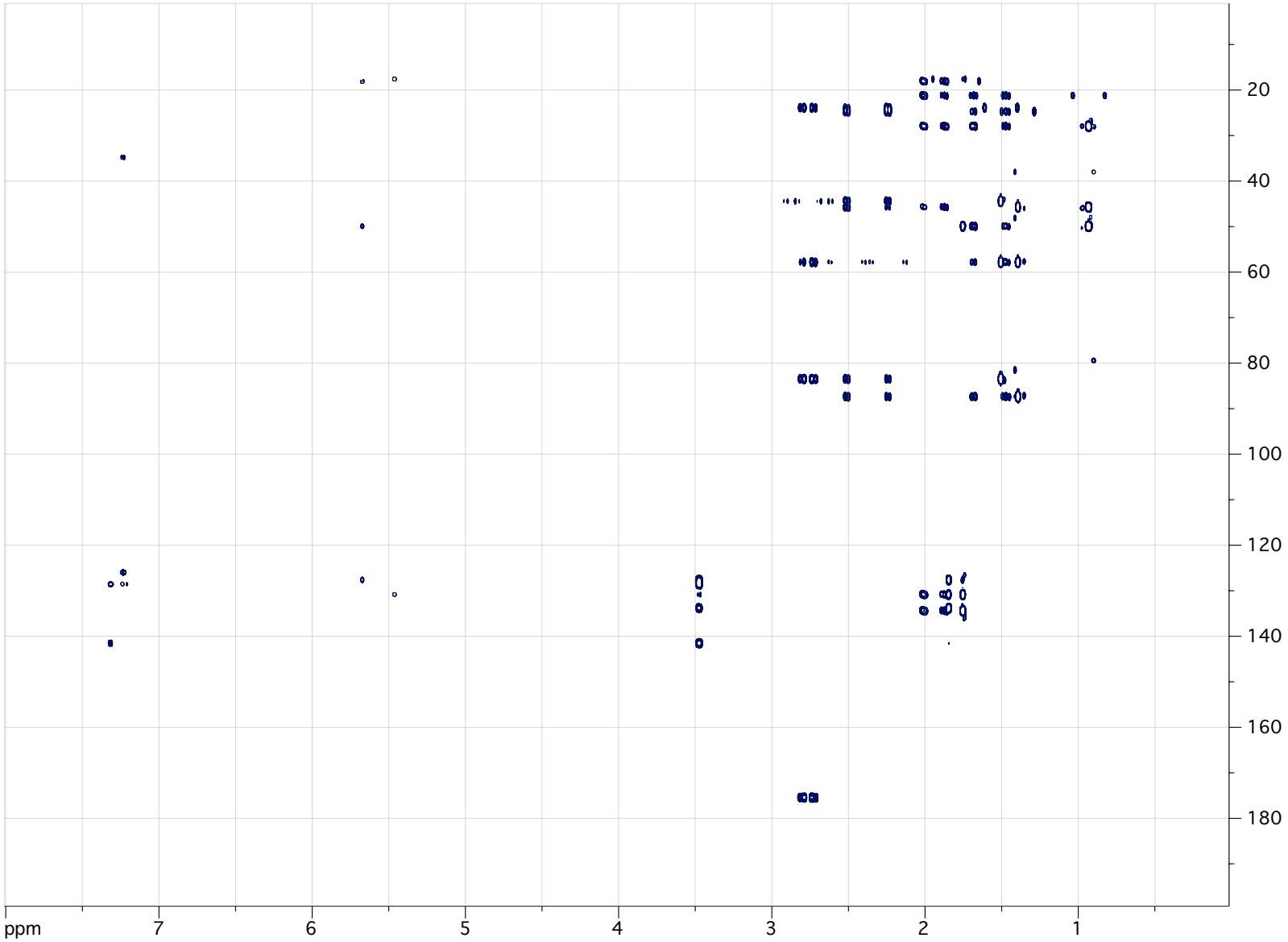


Figure S40. gNOESY spectrum of plakinic acid N (**4**) (600 MHz, τ_m = 300 ms, CD_3OD)

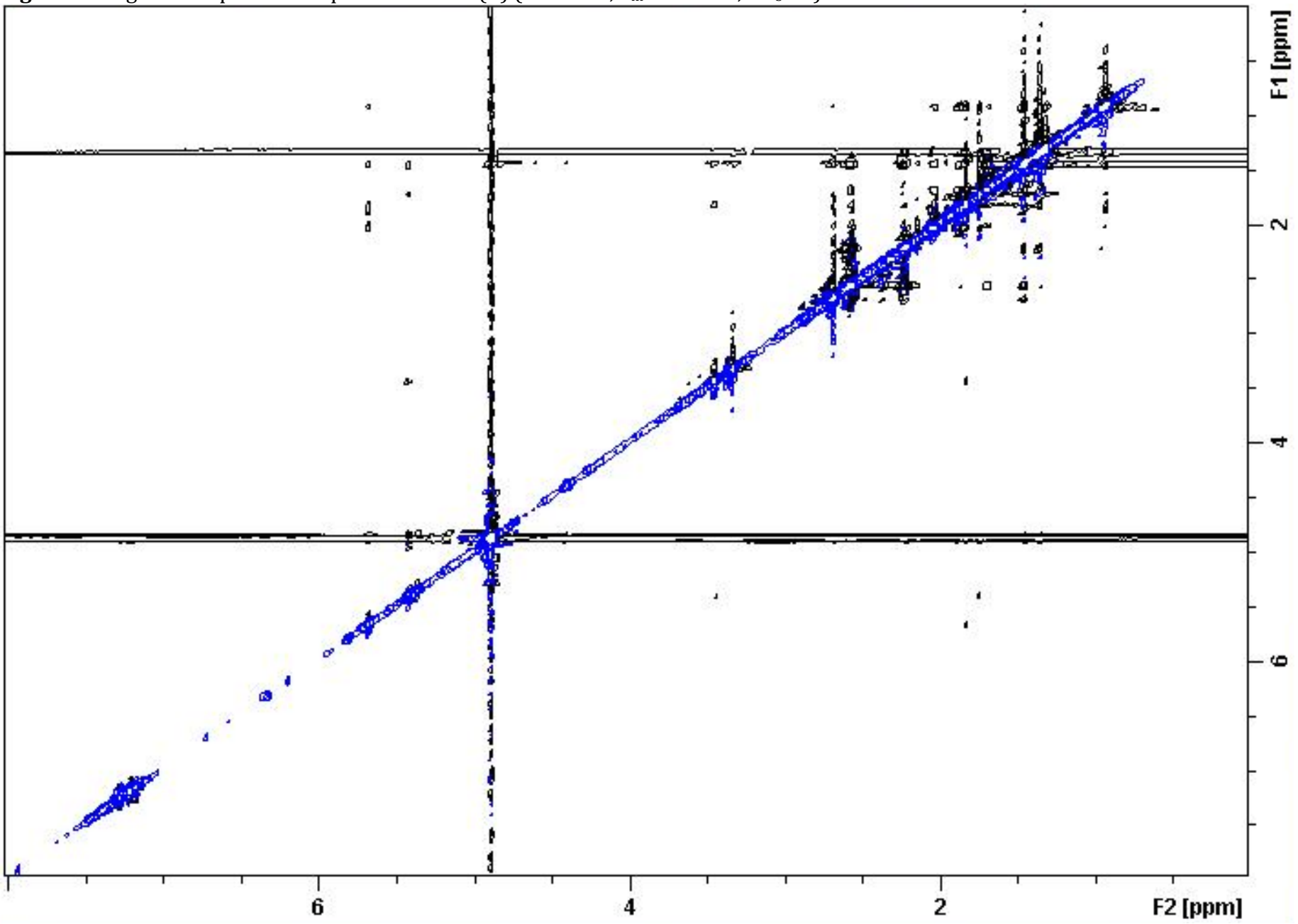


Figure S41. ^{1}H NMR spectrum of plakinic acid O (**5**) (600 MHz, $CDCl_3$)

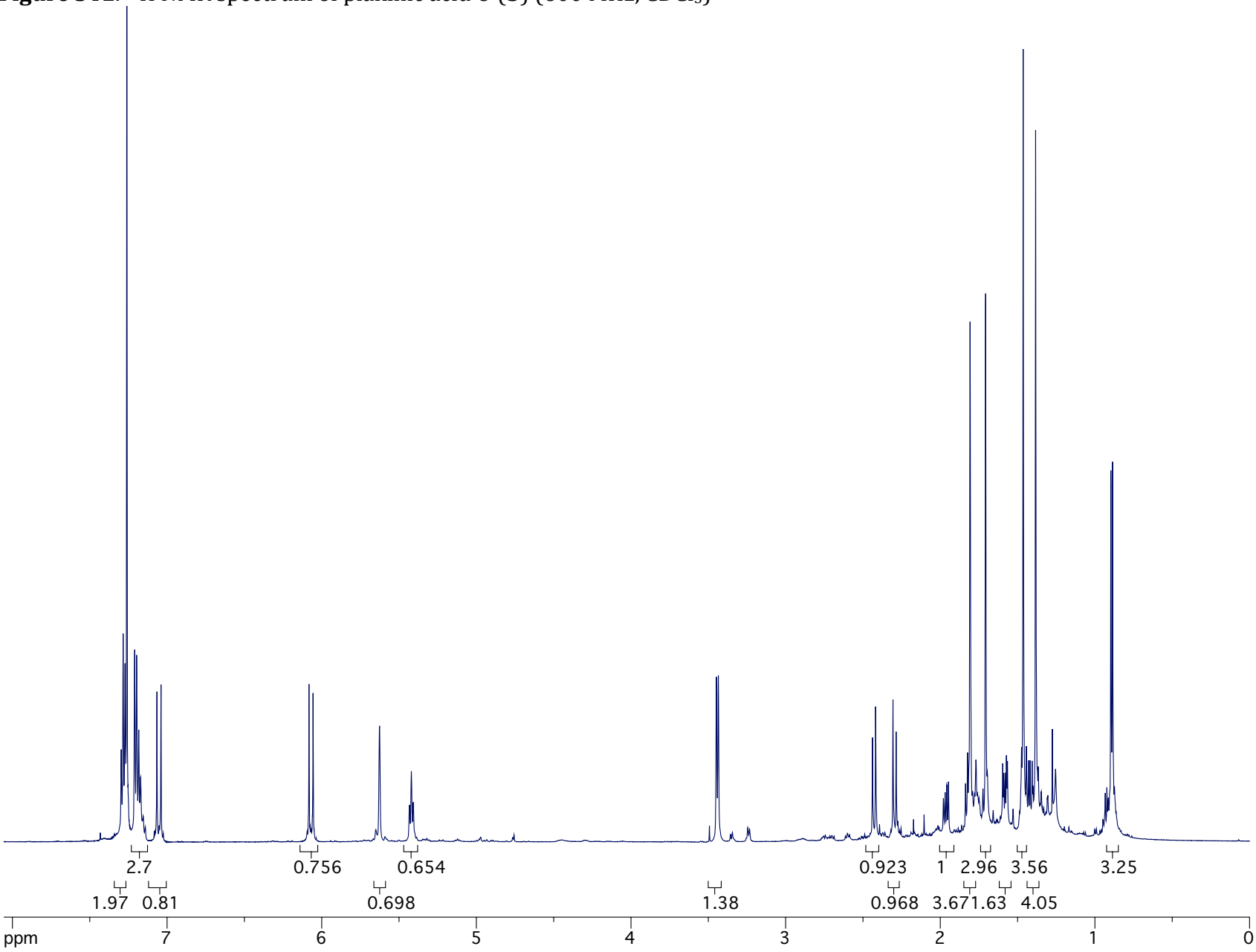


Figure S42. DQF-COSY spectrum of plakinic acid O (**5**) (600 MHz, $CDCl_3$)

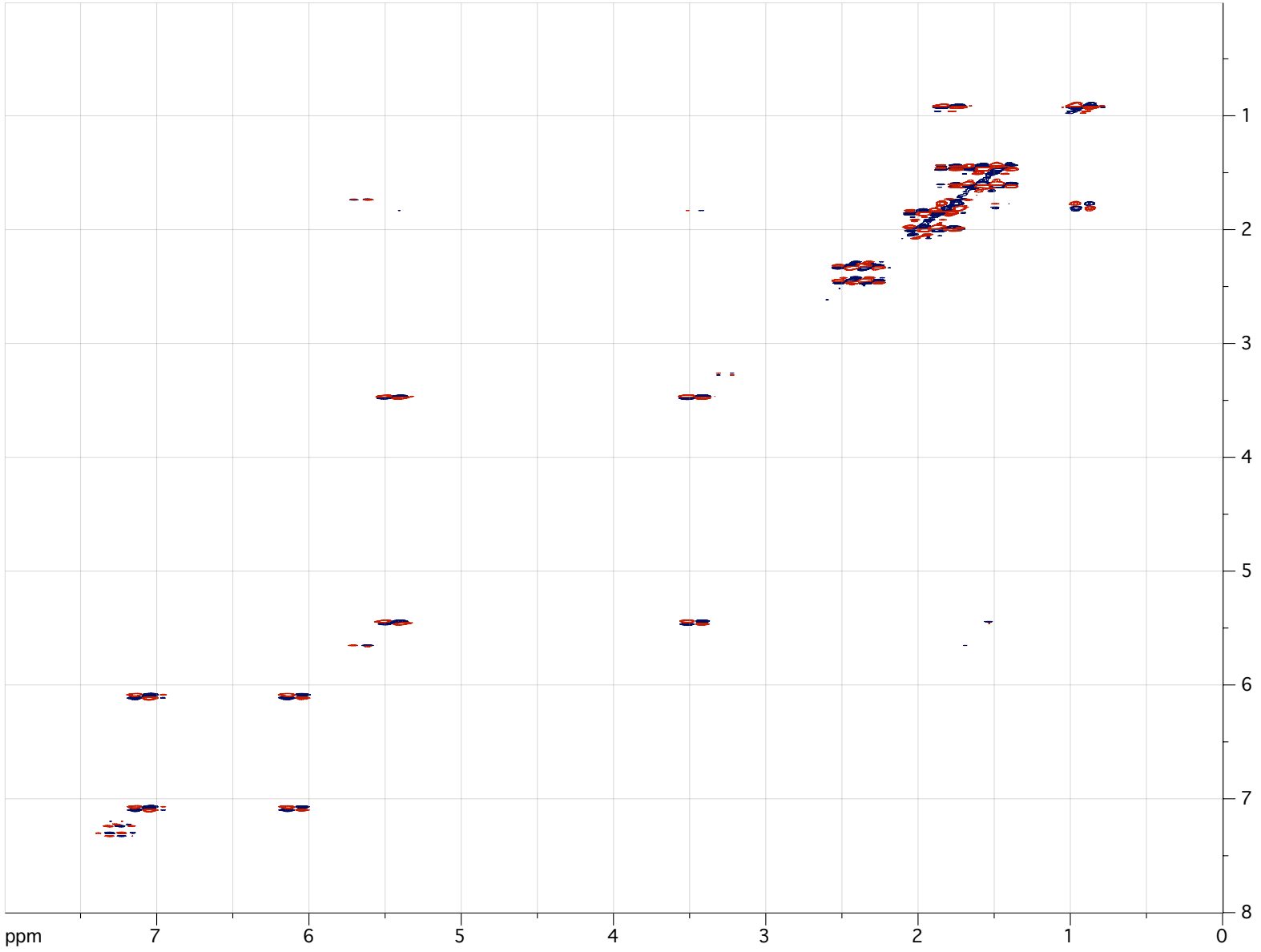


Figure S43. gHSQC spectrum of plakinic acid O (**5**) (600 MHz, $CDCl_3$)

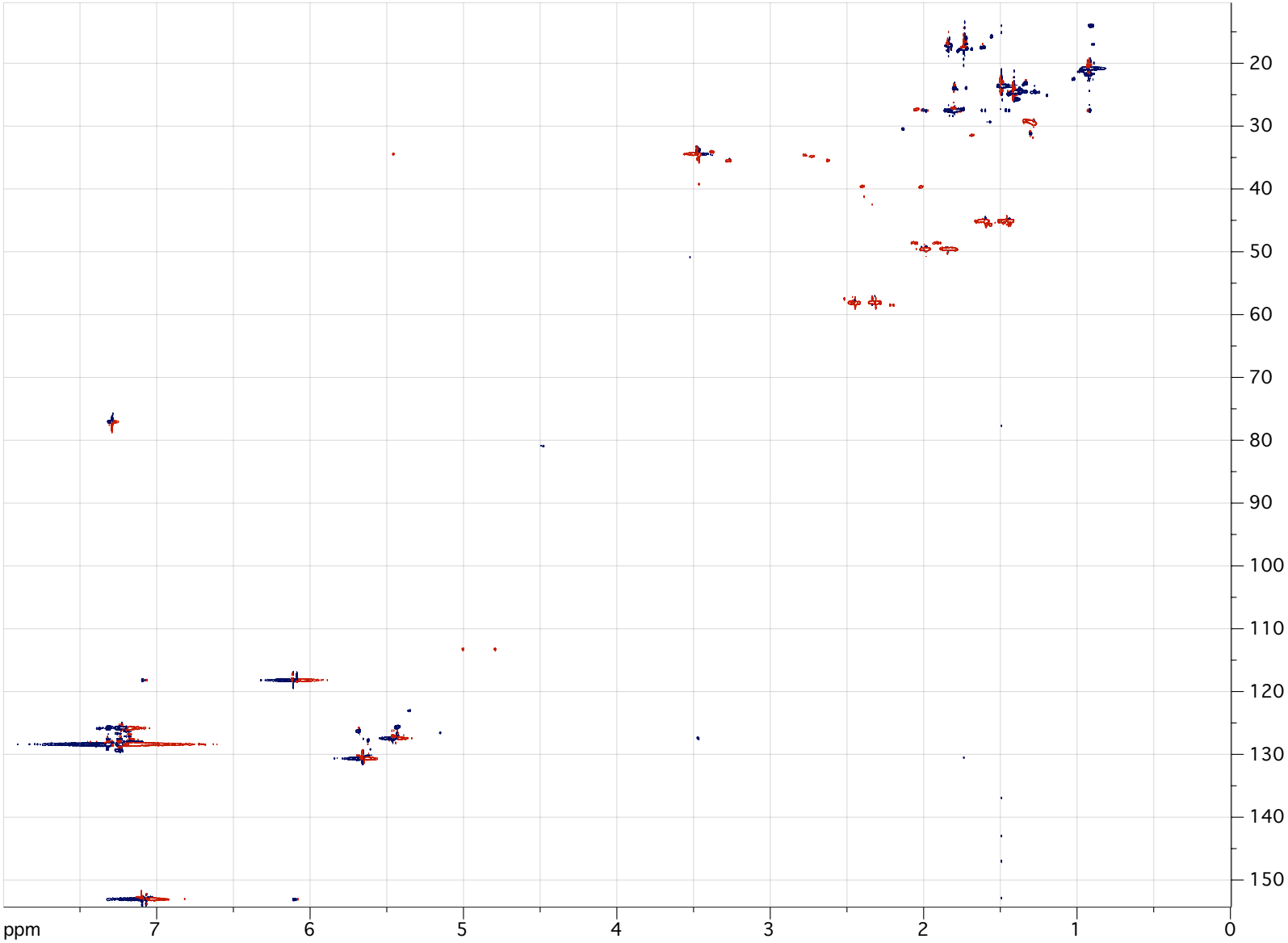


Figure S44. gHMBC spectrum of plakinic acid O (**5**) (600 MHz, $CDCl_3$)

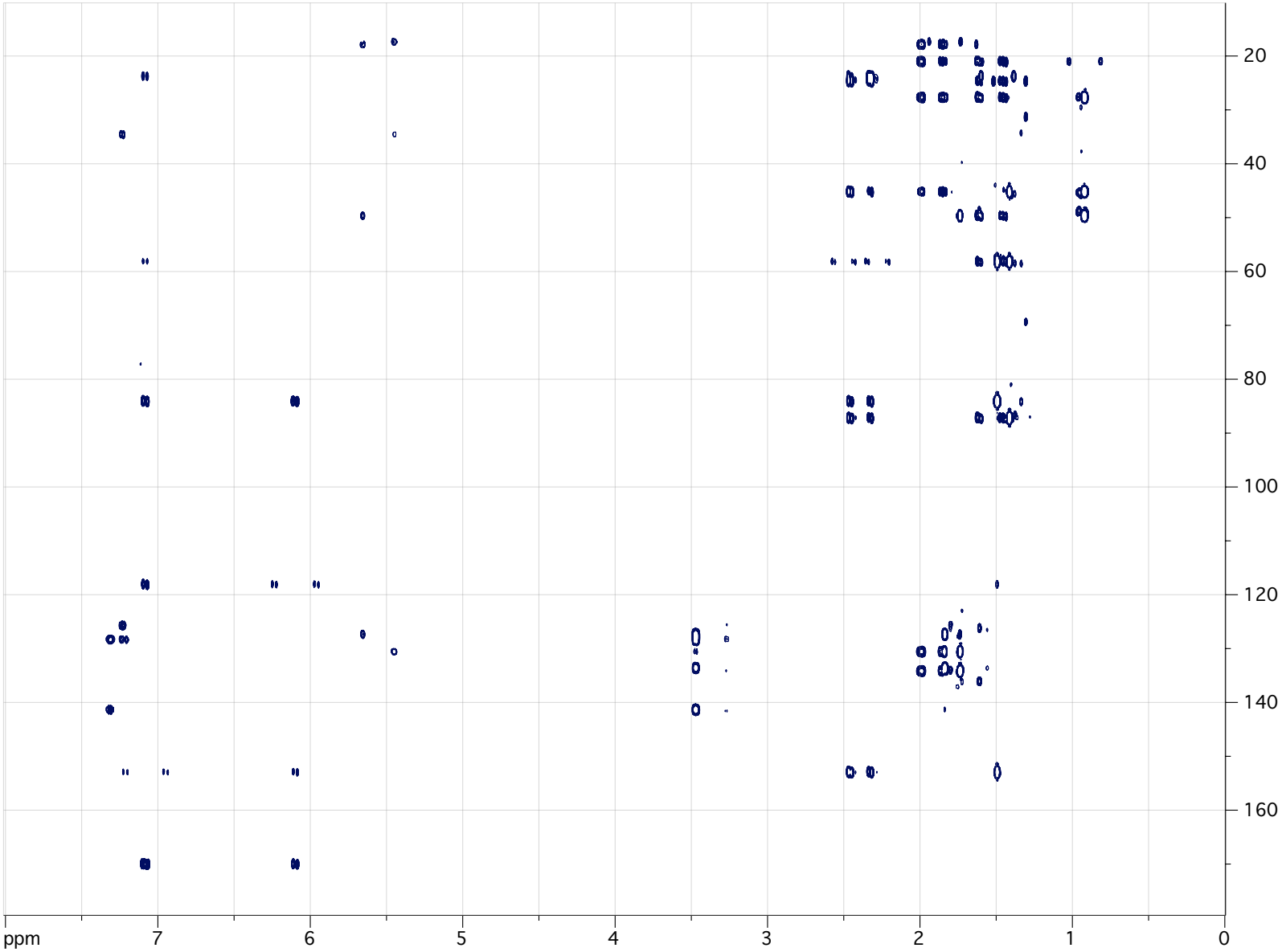


Figure S45. ^{1}H NMR spectrum of plakinic acid P (**6**) (600 MHz, $CDCl_3$)

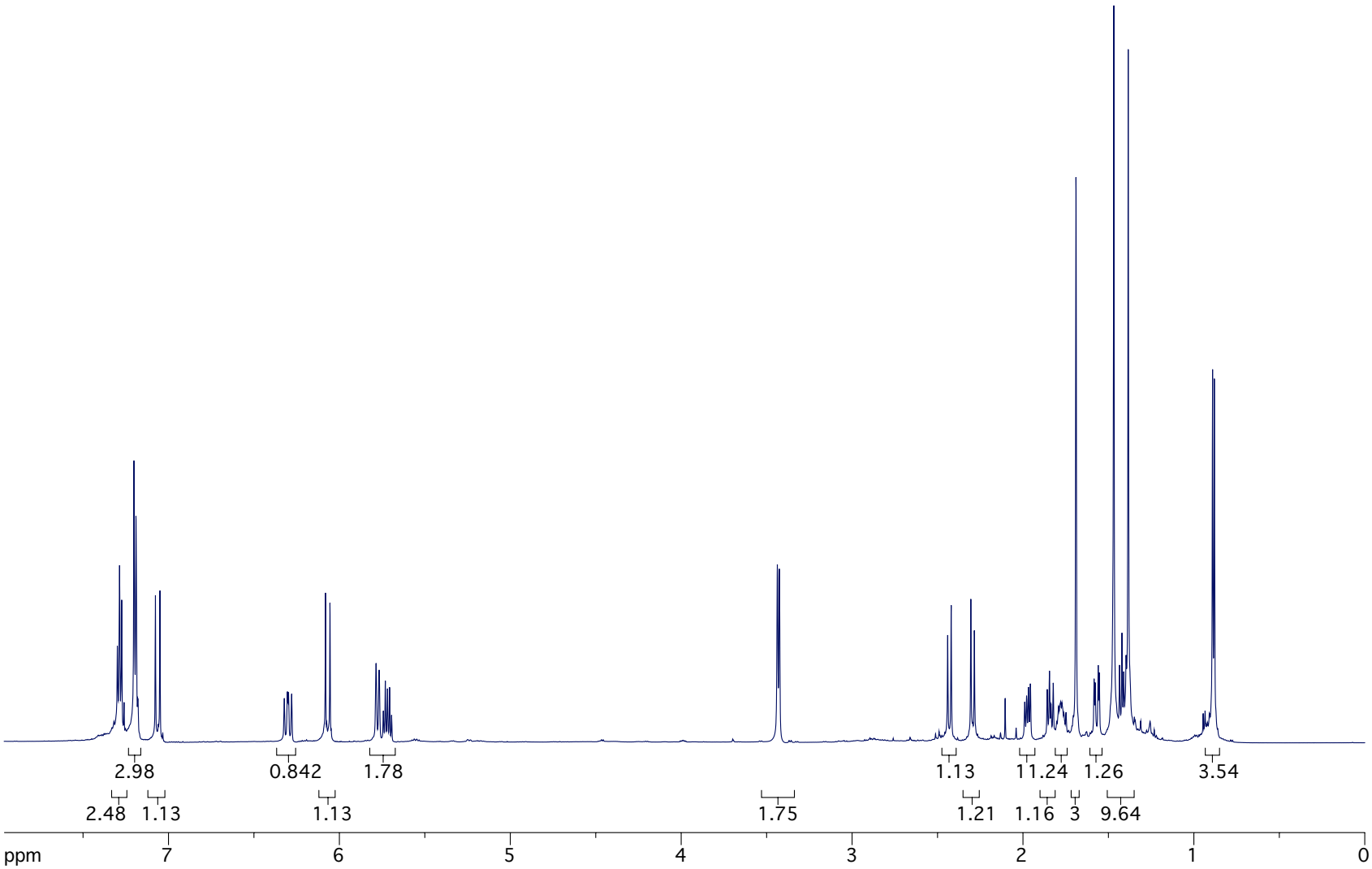


Figure S46. DQF-COSY spectrum of plakinic acid P (**6**) (600 MHz, $CDCl_3$)

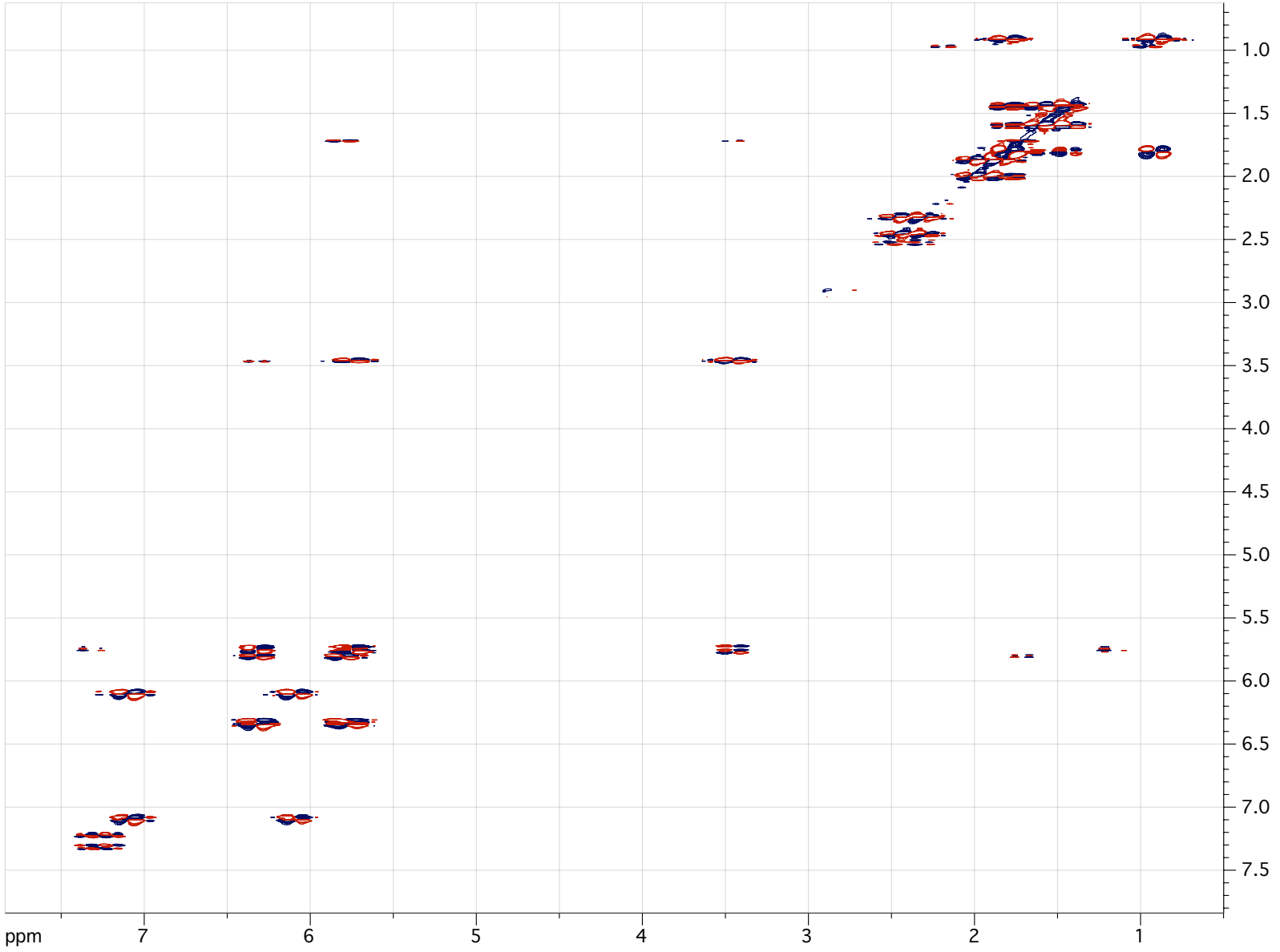


Figure S47. gHSQC spectrum of plakinic acid P (**6**) (600 MHz, $CDCl_3$)

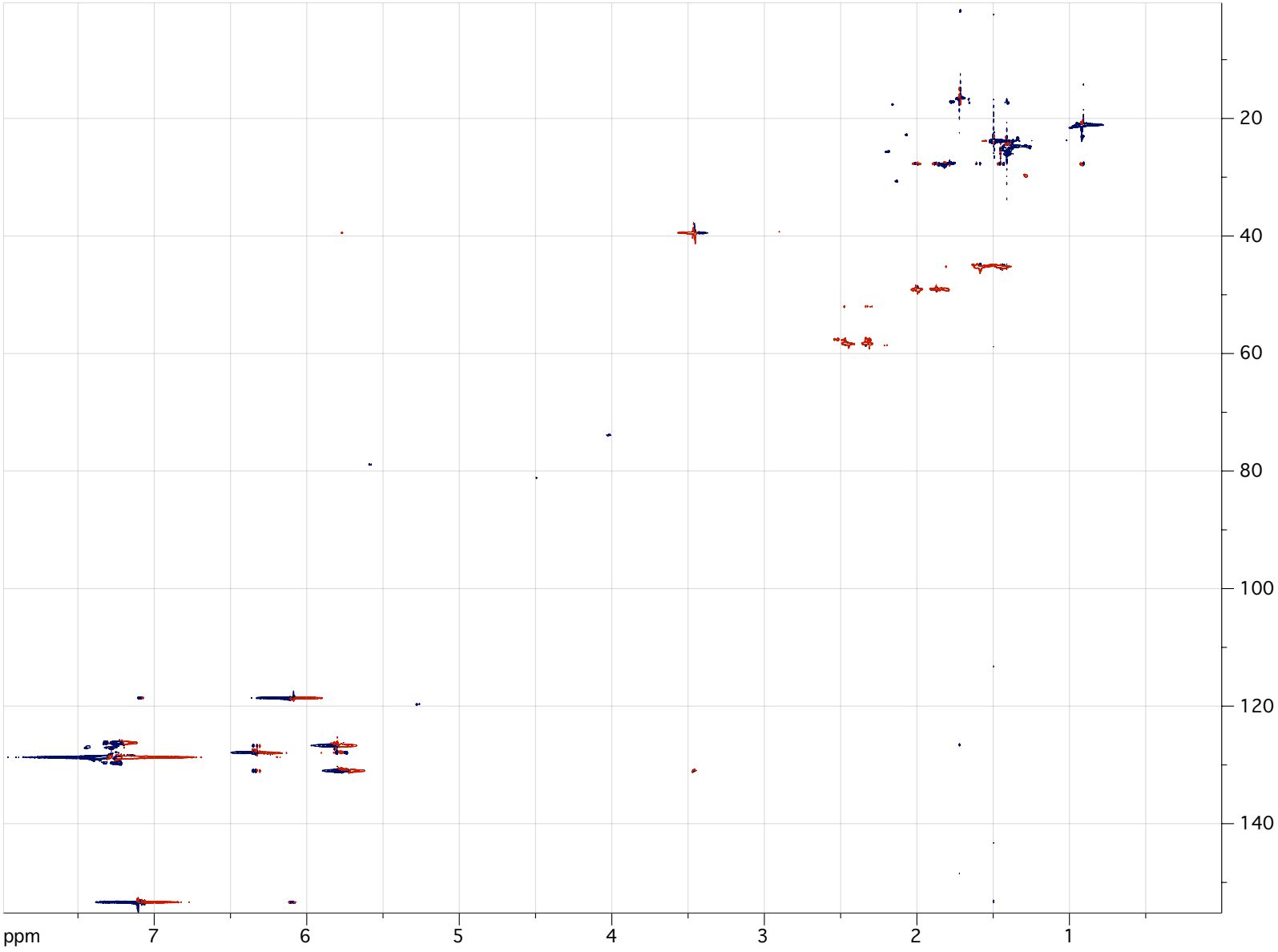


Figure S48. gHMBC spectrum of plakinic acid P (**6**) (600 MHz, $CDCl_3$)

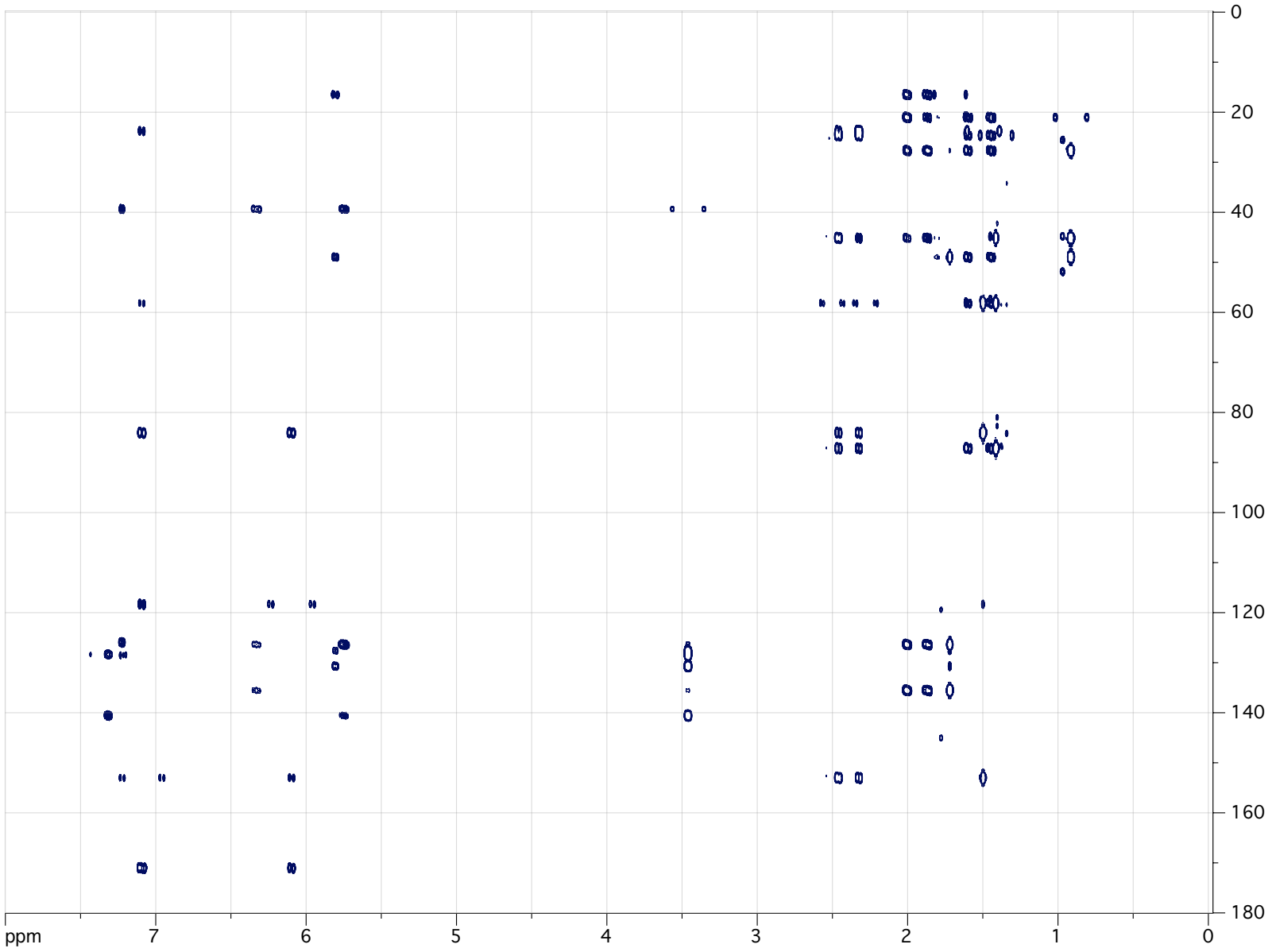


Figure S49. gNOESY spectrum of plakinic acid P (**4**) (600 MHz, τ_m = 300 ms, $CDCl_3$)

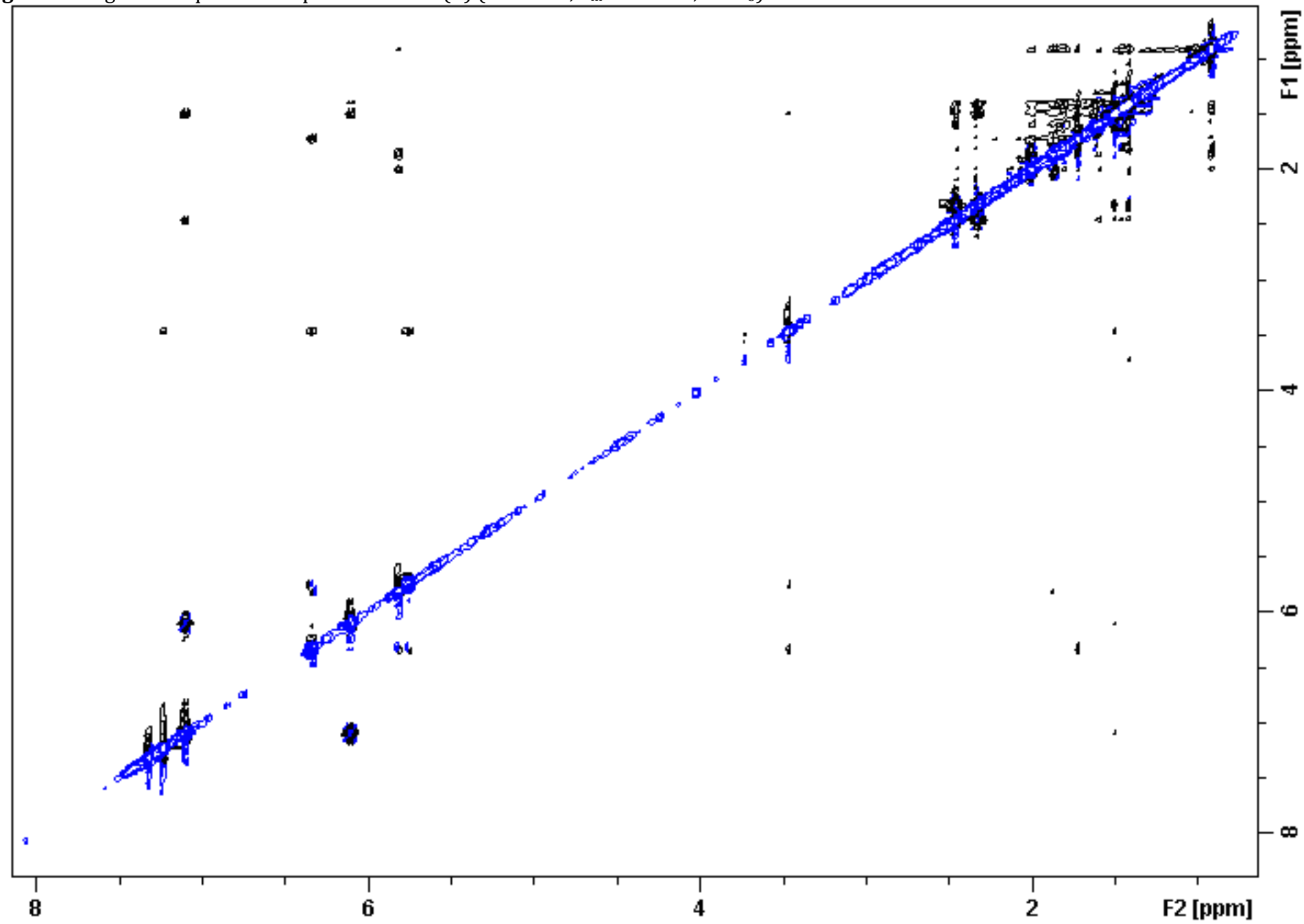
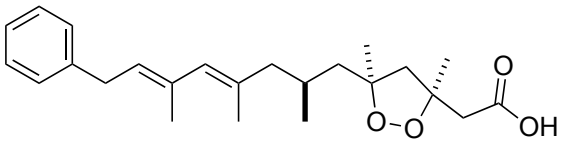


Table S3. Cartesian Coordinates and Relative Energies of Significant Conformers of 7*S*-**4**



7*S*-**4**

Conformation 1

SCF Done: E(RB3LYP) = -1235.88827875 A.U. after 14 cycles

Atom	X	Y	Z
C	1.082000	3.427200	−0.086200
H	0.986200	3.156600	0.971400
C	−0.324000	3.476500	−0.729700
H	−0.221300	3.490500	−1.823300
H	−0.814500	4.427000	−0.478000
C	−1.263900	2.364800	−0.292600
C	−1.691600	1.440400	−1.177400
H	−1.327700	1.487400	−2.204300
C	−2.681700	0.394200	−0.947300
C	−2.526000	−0.523000	0.027900
H	−1.629000	−0.476500	0.645900
C	−3.494100	−1.596300	0.444300
H	−3.659000	−1.500500	1.525600
H	−4.486900	−1.462000	0.002700
C	1.993700	2.409200	−0.809600
H	1.385100	1.667400	−1.344500
H	2.552800	2.916300	−1.608600
C	−3.003600	−2.989300	0.131800
C	−2.091100	−5.578000	−0.450900
C	−3.101700	−3.503300	−1.169100
C	−2.435600	−3.787600	1.135100
C	−1.983700	−5.076200	0.844700
C	−2.648400	−4.791700	−1.457800
H	−3.534200	−2.900400	−1.964900
H	−2.335100	−3.406400	2.149800
H	−1.547300	−5.687300	1.631200
H	−2.732100	−5.182400	−2.469000
H	−1.741300	−6.582500	−0.676200
C	−3.836700	0.446800	−1.912000
H	−4.514200	−0.405400	−1.823500
H	−3.474800	0.451000	−2.946600
H	−4.425200	1.356500	−1.749900
C	−1.746300	2.470700	1.133000
H	−1.969200	3.513300	1.384800
H	−0.977700	2.107100	1.822000
H	−2.665300	1.908800	1.319200
C	1.687900	4.837700	−0.158300
H	1.065700	5.552300	0.391900
H	1.759900	5.185000	−1.195000
H	2.688200	4.878200	0.278200

C	2.987700	1.634900	0.080700
C	2.296500	0.566100	0.930500
C	3.045500	-0.729500	0.614700
O	4.261200	-0.267000	-0.003500
O	3.837300	0.881100	-0.802500
H	1.228100	0.480600	0.705900
H	2.348700	0.823600	1.995500
C	3.896000	2.535700	0.919400
H	3.336900	3.094500	1.675500
H	4.662800	1.949500	1.439400
H	4.437500	3.241600	0.280100
C	3.459000	-1.483400	1.878400
H	4.034300	-2.381000	1.624500
H	2.602300	-1.781500	2.488400
H	4.117900	-0.865200	2.499800
C	2.345500	-1.630100	-0.411600
H	3.008600	-2.462900	-0.677500
H	2.157800	-1.067900	-1.335000
C	1.037200	-2.201300	0.050400
O	0.498000	-2.040400	1.131300
O	0.471100	-2.957700	-0.910500
H	-0.388100	-3.255900	-0.538700

Conformation 2

7S-SP-3

SCF Done: E(RB3LYP) = -1235.88480463 A.U. after 14 cycles

C	2.929700	-1.108300	1.472100
H	3.980200	-0.865700	1.675800
C	2.965900	-2.152200	0.323900
H	3.464100	-3.066300	0.673000
H	3.634300	-1.757400	-0.454900
C	1.635700	-2.524700	-0.311100
C	1.295100	-1.999000	-1.506300
H	1.990300	-1.319800	-2.001000
C	0.069500	-2.227800	-2.259600
C	-1.130700	-1.929100	-1.723600
H	-1.159300	-1.537700	-0.705600
C	-2.489200	-2.065900	-2.356700
H	-2.455000	-2.515600	-3.352900
H	-3.070100	-2.761000	-1.737100
C	2.206000	0.183900	1.023200
H	2.611800	0.476900	0.045100
H	1.148800	-0.061900	0.863400
C	-3.220500	-0.745200	-2.464400
C	-4.592600	1.695400	-2.681600
C	-2.665300	0.326100	-3.181000
C	-4.480500	-0.579600	-1.871400
C	-5.161500	0.635000	-1.978900
C	-3.345300	1.541000	-3.283000
H	-1.694200	0.219900	-3.661200
H	-4.941000	-1.396100	-1.318800
H	-6.138200	0.752000	-1.515400

```
 H   -2.901200    2.366200   -3.834900
 H   -5.123600    2.640300   -2.766600
 C    0.308600   -2.738400   -3.654300
 H    0.813600   -3.710400   -3.620300
 H    0.942100   -2.041800   -4.215000
 H   -0.607700   -2.871600   -4.232600
 C    0.807000   -3.541600    0.427900
 H    0.225900   -3.063700    1.220800
 H    1.448000   -4.306600    0.878500
 H    0.111200   -4.072400   -0.229100
 C    2.354200   -1.701700    2.759000
 H    2.723600   -2.719100    2.925500
 H    1.261100   -1.730400    2.742400
 H    2.659400   -1.111200    3.628500
 C    2.277500    1.416500    1.953200
 C    1.473000    2.572100    1.344200
 C    0.281600    2.737400    2.276100
 O    0.854300    2.329400    3.531300
 O    1.629800    1.129200    3.200800
 H    1.197100    2.408700    0.298300
 H    2.083000    3.485100    1.345200
 C    3.718900    1.832600    2.249100
 H    4.245800    1.065700    2.826100
 H    4.277300    2.030000    1.328700
 H    3.743700    2.736600    2.869100
 C   -0.136100    4.201100    2.419000
 H    0.696700    4.811200    2.788200
 H   -0.938000    4.306200    3.158600
 H   -0.478500    4.628400    1.472500
 C   -0.922600    1.824500    1.998800
 H   -1.703600    2.013100    2.746200
 H   -0.639100    0.771900    2.114300
 C   -1.532000    1.987300    0.635900
 O   -1.260800    2.823700   -0.207000
 O   -2.481200    1.057300    0.413400
 H   -2.796900    1.217400   -0.504000
```

Conformation 3

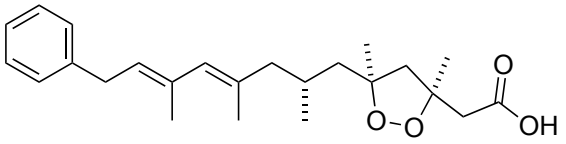
7S-SP-17

SCF Done: E(RB3LYP) = -1235.88456271   A.U. after   14 cycles

```
 C   -2.844300   -0.391900   -2.275300
 H   -3.051600   -1.241600   -1.614900
 C   -1.547600   -0.679100   -3.069000
 H   -1.150600    0.258500   -3.480000
 H   -1.768600   -1.303200   -3.945400
 C   -0.495800   -1.407100   -2.244000
 C    0.647800   -0.782100   -1.893700
 H    0.770400    0.244100   -2.248100
 C    1.778800   -1.258600   -1.096400
 C    2.970700   -0.641000   -1.244300
 H    3.059800    0.163100   -1.974600
```

C	4.268500	−0.973400	−0.555000
H	4.271300	−1.999800	−0.170700
H	5.076400	−0.952700	−1.298200
C	−2.725800	0.906100	−1.440800
H	−1.675100	1.215600	−1.360800
H	−3.203300	1.736700	−1.979500
C	4.597400	−0.000400	0.552100
C	5.137800	1.832400	2.607100
C	4.413800	−0.359700	1.895200
C	5.059500	1.289800	0.253600
C	5.327600	2.200600	1.276700
C	4.682300	0.552800	2.916500
H	4.051600	−1.352000	2.156800
H	5.208800	1.594400	−0.780200
H	5.683600	3.199100	1.035200
H	4.533800	0.264300	3.954400
H	5.346600	2.542800	3.403000
C	1.557900	−2.342500	−0.073800
H	0.562900	−2.270900	0.377300
H	2.259600	−2.273200	0.761800
H	1.680700	−3.332500	−0.522200
C	−0.826500	−2.851000	−1.966400
H	−1.495400	−3.253400	−2.735600
H	−1.330600	−2.952700	−1.000800
H	0.059800	−3.488800	−1.988600
C	−4.013600	−0.278800	−3.263600
H	−3.841600	0.521500	−3.991700
H	−4.955900	−0.070900	−2.749300
H	−4.142600	−1.215200	−3.817300
C	−3.307000	0.844400	−0.012000
C	−2.384000	0.095900	0.956700
C	−2.011300	1.131300	2.015200
O	−3.101600	2.067100	1.923900
O	−3.331900	2.196800	0.485400
H	−1.503800	−0.335400	0.471200
H	−2.917300	−0.753800	1.401300
C	−4.747200	0.331300	0.042600
H	−5.397800	0.936600	−0.598400
H	−4.828400	−0.716500	−0.259800
H	−5.155300	0.419500	1.056400
C	−2.044100	0.552700	3.429100
H	−1.344500	−0.277000	3.558700
H	−3.048500	0.188600	3.676200
H	−1.810300	1.325100	4.170700
C	−0.725400	1.918600	1.724200
H	−0.609600	2.719900	2.464800
H	−0.804200	2.410500	0.746600
C	0.535400	1.103900	1.723800
O	0.688900	−0.031000	2.138500
O	1.564700	1.808500	1.211900
H	2.344800	1.213700	1.263300

Table S4. Cartesian Coordinates and Relative Energies of Significant Conformers of 7*R*-**4**



7*R*-**4**

Conformation 1

7R-SP-39

SCF Done: E(RB3LYP) = -1235.88464332 A.U. after 14 cycles

Atom	X	Y	Z
C	-0.884100	-0.746100	-0.820300
C	-0.450500	-0.161300	0.542800
H	-0.950200	-0.721600	1.344200
H	-0.799400	0.872700	0.637500
C	1.051700	-0.140600	0.771300
C	1.599500	-0.890200	1.749500
H	0.949800	-1.490500	2.386500
C	3.013000	-0.991600	2.083500
C	3.892400	-1.462500	1.177600
H	3.513700	-1.755400	0.197600
C	5.374600	-1.654600	1.333400
H	5.717900	-1.503400	2.361200
H	5.610500	-2.702200	1.106200
C	-2.424400	-0.782100	-0.995100
H	-2.833600	-1.449200	-0.223400
H	-2.640500	-1.252200	-1.964500
C	6.162800	-0.746500	0.418600
C	7.597400	0.956400	-1.287900
C	6.708200	-1.232700	-0.777800
C	6.338000	0.606600	0.743900
C	7.053300	1.452600	-0.104800
C	7.424000	-0.384900	-1.625000
H	6.576700	-2.275200	-1.058100
H	5.909800	1.007700	1.659900
H	7.182400	2.499500	0.156300
H	7.844500	-0.770900	-2.549800
H	8.153200	1.615800	-1.948900
C	3.336800	-0.562300	3.487200
H	4.407300	-0.561500	3.703200
H	2.977800	0.457700	3.666000
H	2.854800	-1.228000	4.211600
C	1.824700	0.795200	-0.122800
H	1.898800	0.382900	-1.133800
H	2.837600	0.994100	0.237900
H	1.319700	1.765400	-0.181700
C	-3.185100	0.559800	-0.939000
C	-4.665300	0.347500	-1.252700
C	-5.408500	1.278000	-0.291200
O	-4.363300	1.957500	0.433900
O	-3.226600	1.036900	0.408100

```
 H    -4.896300     0.538400    -2.307100
 H    -4.953600    -0.694700    -1.069200
 C    -2.558600     1.625300    -1.843900
 H    -2.467400     1.267800    -2.874600
 H    -3.153700     2.544500    -1.856100
 H    -1.568000     1.921800    -1.483900
 C    -6.198800     2.360600    -1.029100
 H    -6.670700     3.048600    -0.318300
 H    -5.536800     2.973400    -1.651300
 H    -6.976500     1.942100    -1.674000
 C    -6.265000     0.543500     0.748200
 H    -6.651600     1.271300     1.473100
 H    -5.648800    -0.167200     1.312400
 C    -7.426300    -0.206800     0.161600
 O    -7.610500    -0.495900    -1.007800
 O    -8.305400    -0.593600     1.106800
 H    -8.999000    -1.080600     0.613900
 H    -0.461200    -0.132300    -1.624800
 C    -0.341700    -2.172000    -1.012500
 H    -0.679300    -2.835300    -0.208900
 H    -0.683300    -2.593100    -1.964300
 H     0.752500    -2.186600    -1.031200

Conformation 2

7R-SP-1

SCF Done:  E(RB3LYP) =  -1235.88424322     A.U. after   14 cycles

 C    -1.532300     0.277900     2.835800
 C    -0.182100    -0.252100     3.375200
 H    -0.342700    -1.172700     3.951700
 H     0.234000     0.471000     4.089400
 C     0.822900    -0.558100     2.275400
 C     1.877100     0.254200     2.059400
 H     2.023200     1.121100     2.703900
 C     2.887300     0.109000     1.020500
 C     2.538700     0.203500    -0.278400
 H     1.491800     0.390100    -0.517900
 C     3.422600     0.092700    -1.489600
 H     3.447400     1.073400    -1.981200
 H     4.461700    -0.139600    -1.239400
 C    -1.418900     1.752600     2.365600
 H    -0.370800     2.022800     2.191800
 H    -1.756800     2.400000     3.186300
 C     2.933100    -0.953000    -2.467500
 C     2.060600    -2.898700    -4.293200
 C     2.380300    -0.577200    -3.699900
 C     3.033900    -2.317400    -2.158500
 C     2.599300    -3.284300    -3.066900
 C     1.949400    -1.545800    -4.608900
 H     2.280900     0.474600    -3.961900
 H     3.457100    -2.631600    -1.206100
 H     2.687700    -4.339300    -2.819000
 H     1.527900    -1.241500    -5.564200
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H	1.730100	-3.652500	-5.003600
C	4.279000	-0.093800	1.551100
H	4.335500	-1.029200	2.118900
H	5.038500	-0.143300	0.768300
H	4.559700	0.729800	2.217300
C	0.568400	-1.836800	1.516600
H	1.407100	-2.136300	0.882400
H	-0.314000	-1.737000	0.880400
H	0.396700	-2.662100	2.215900
C	-2.212700	2.113600	1.088100
C	-1.686100	1.407000	-0.155800
C	-2.886700	0.663500	-0.719500
O	-3.732300	0.494000	0.431200
O	-3.585600	1.727800	1.211000
H	-1.237300	2.090400	-0.886100
H	-0.887700	0.710500	0.119100
C	-2.187600	3.634300	0.895900
H	-2.766800	3.933100	0.015500
H	-2.648800	4.142200	1.750700
H	-1.165000	4.008400	0.779900
C	-3.659800	1.473100	-1.764600
H	-3.053700	1.685900	-2.649800
H	-4.012200	2.426000	-1.356500
H	-4.558700	0.932600	-2.082900
C	-2.543800	-0.739400	-1.235600
H	-3.393400	-1.184600	-1.766100
H	-2.344300	-1.392900	-0.376600
C	-1.343500	-0.768000	-2.139600
O	-0.961200	0.122300	-2.879000
O	-0.684300	-1.939600	-2.058800
H	0.108500	-1.836300	-2.631100
H	-1.845400	-0.362600	2.005800
C	-2.600900	0.150300	3.928800
H	-2.325800	0.720600	4.822700
H	-2.727700	-0.896800	4.224400
H	-3.571800	0.513900	3.579300

Conformation 3

7R-SP-11

SCF Done: E(RB3LYP) = -1235.88416963 A.U. after 14 cycles

C	2.103500	2.139200	-1.216500
C	1.830300	1.650900	-2.666600
H	2.783200	1.335800	-3.112700
H	1.512400	2.509800	-3.274100
C	0.815000	0.530500	-2.827700
C	-0.503800	0.810000	-2.860000
H	-0.821600	1.851400	-2.799400
C	-1.612500	-0.129300	-2.953400
C	-1.759600	-1.106200	-2.036300
H	-1.002700	-1.199000	-1.256200
C	-2.881400	-2.103100	-1.923100
H	-3.728400	-1.861800	-2.572400

H	-2.497700	-3.075500	-2.255300
C	2.588700	0.985500	-0.310300
H	3.431300	0.495000	-0.819000
H	1.810700	0.214500	-0.250600
C	-3.411900	-2.221100	-0.509000
C	-4.409500	-2.447400	2.105900
C	-3.411300	-3.458900	0.150000
C	-3.932900	-1.101000	0.157100
C	-4.422900	-1.213300	1.459200
C	-3.907000	-3.570200	1.450900
H	-3.022700	-4.346700	-0.344900
H	-3.954900	-0.130900	-0.336600
H	-4.817500	-0.336600	1.967400
H	-3.902200	-4.535100	1.952300
H	-4.796700	-2.534800	3.118100
C	-2.557300	0.154200	-4.088300
H	-3.103100	1.086700	-3.908100
H	-2.004300	0.255900	-5.029300
H	-3.291500	-0.639700	-4.244200
C	1.398400	-0.847600	-3.016700
H	0.660500	-1.584600	-3.345000
H	1.847900	-1.212000	-2.089200
H	2.174800	-0.825100	-3.789200
C	3.037300	1.318600	1.130700
C	1.869900	1.438200	2.114100
C	2.006200	0.233000	3.034200
O	3.425600	0.009000	3.004100
O	3.785000	0.170500	1.593300
H	1.965200	2.371000	2.684800
H	0.891000	1.486000	1.634400
C	3.985900	2.515800	1.196200
H	3.485000	3.455900	0.948900
H	4.418600	2.616100	2.198500
H	4.830200	2.378400	0.511100
C	1.632100	0.565600	4.478600
H	2.262900	1.373000	4.868900
H	1.805200	-0.296400	5.133000
H	0.587500	0.872600	4.578100
C	1.319300	-1.050900	2.541500
H	1.514400	-1.866400	3.249000
H	1.749400	-1.365800	1.583300
C	-0.168100	-0.935400	2.359000
O	-0.890900	-0.015300	2.697900
O	-0.672600	-2.025100	1.747700
H	-1.637700	-1.855600	1.662800
H	2.921600	2.866400	-1.302800
C	0.899800	2.896200	-0.651700
H	0.070000	2.223700	-0.414900
H	0.538200	3.642300	-1.367600
H	1.165900	3.439000	0.259900

Conformation 4

7R-SP-9

SCF Done: E(RB3LYP) = -1235.88336631   A.U. after   15 cycles

C	-2.312000	-2.443100	-0.136900
C	-3.128300	-1.144300	0.069800
H	-3.766400	-1.236900	0.958800
H	-3.819100	-1.005200	-0.772200
C	-2.252000	0.082900	0.259700
C	-2.093700	0.974600	-0.740800
H	-2.594900	0.789600	-1.691300
C	-1.242500	2.158000	-0.744200
C	-1.340200	3.098100	0.215800
H	-2.093500	2.970700	0.992600
C	-0.502800	4.335500	0.377900
H	-0.142600	4.711900	-0.585700
H	-1.135000	5.142100	0.771500
C	-1.766700	-2.577700	-1.585200
H	-1.938900	-1.660800	-2.162000
H	-2.352600	-3.351600	-2.099500
C	0.658200	4.113400	1.321700
C	2.809700	3.667800	3.070400
C	0.455500	4.081300	2.709000
C	1.952500	3.906800	0.823800
C	3.023000	3.690700	1.693800
C	1.526000	3.859600	3.577600
H	-0.540700	4.230400	3.120200
H	2.136700	3.909500	-0.248600
H	4.022500	3.537400	1.293400
H	1.357800	3.841800	4.651600
H	3.643600	3.502100	3.748000
C	-0.284900	2.206100	-1.905200
H	0.384200	3.068700	-1.879300
H	0.347400	1.312500	-1.918500
H	-0.835100	2.250500	-2.851700
C	-1.611100	0.185600	1.623200
H	-2.372900	0.418500	2.374400
H	-0.834400	0.949900	1.682200
H	-1.133100	-0.755600	1.907900
C	-0.267300	-2.947500	-1.688400
C	0.636100	-1.756700	-1.416900
C	1.819600	-2.325600	-0.640000
O	1.544200	-3.737500	-0.516700
O	0.092900	-3.881300	-0.669200
H	0.929800	-1.236500	-2.335900
H	0.117000	-1.010400	-0.811600
C	0.018400	-3.573500	-3.058700
H	-0.229800	-2.884300	-3.872400
H	1.069000	-3.863900	-3.161200
H	-0.563200	-4.493000	-3.191500
C	3.129900	-2.219700	-1.425200
H	3.955000	-2.674400	-0.865000
H	3.065500	-2.770600	-2.370300
H	3.399100	-1.186200	-1.657900
C	1.948800	-1.749600	0.778000
H	2.812700	-2.187900	1.291200
H	1.061500	-2.031800	1.358900

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 C     2.080800    -0.249800     0.814900
 O     2.395300     0.486500    -0.104200
 O     1.811700     0.248500     2.037800
 H     1.860800     1.225700     1.932400
 H    -1.480200    -2.452300     0.574900
 C    -3.190900    -3.654800     0.200800
 H    -3.524500    -3.613300     1.243200
 H    -2.635500    -4.589200     0.067700
 H    -4.080500    -3.691500    -0.437300

Conformation 5

7R-SP-13

SCF Done:  E(RB3LYP) =  -1235.88325774     A.U. after   14 cycles

 C     1.488600     1.138500    -2.642600
 C     0.451400     0.382300    -3.506500
 H     0.904000    -0.535900    -3.906100
 H     0.198400     0.988200    -4.385900
 C    -0.809900    -0.011100    -2.749100
 C    -0.732800    -0.964100    -1.796300
 H     0.241300    -1.440300    -1.657500
 C    -1.749800    -1.460000    -0.874100
 C    -1.630200    -2.722300    -0.411800
 H    -0.817500    -3.343300    -0.789000
 C    -2.532700    -3.434700     0.559600
 H    -3.486900    -2.913700     0.695500
 H    -2.803700    -4.410300     0.135600
 C     1.011300     2.567800    -2.276900
 H    -0.076600     2.656500    -2.369800
 H     1.426300     3.264800    -3.017600
 C    -1.865800    -3.646200     1.898600
 C    -0.567600    -3.991600     4.362200
 C    -2.100900    -2.759700     2.959000
 C    -0.968600    -4.707200     2.089000
 C    -0.324100    -4.878400     3.315300
 C    -1.455700    -2.933000     4.184500
 H    -2.779200    -1.917800     2.833700
 H    -0.765100    -5.405900     1.280100
 H     0.368300    -5.705100     3.454000
 H    -1.644200    -2.236900     4.998400
 H    -0.066200    -4.126300     5.317300
 C    -2.798600    -0.503200    -0.371500
 H    -3.098800    -0.726300     0.656500
 H    -2.425500     0.526600    -0.350200
 H    -3.695200    -0.544000    -0.996600
 C    -2.070400     0.670500    -3.206300
 H    -2.061100     0.808600    -4.293100
 H    -2.171800     1.653100    -2.737300
 H    -2.965200     0.081300    -2.994300
 C     1.405500     3.044300    -0.861100
 C     0.628400     2.326700     0.237000
 C     1.662000     2.046700     1.327900
 O     2.857200     2.717700     0.875900
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 O     2.767900     2.717700    -0.584800
 H    -0.216300     2.927400     0.594900
 H     0.182600     1.396300    -0.125700
 C     1.236500     4.565700    -0.763100
 H     1.513300     4.938500     0.229100
 H     1.896000     5.074600    -1.475300
 H     0.204000     4.867500    -0.967600
 C     1.285800     2.702500     2.658300
 H     0.336800     2.333000     3.055500
 H     1.204100     3.789900     2.545500
 H     2.065800     2.532400     3.409200
 C     2.011400     0.561100     1.487300
 H     2.800100     0.445500     2.240800
 H     2.418600     0.177100     0.544000
 C     0.849900    -0.308000     1.883100
 O    -0.272800     0.051600     2.192400
 O     1.187400    -1.613200     1.874900
 H     0.370800    -2.093100     2.139200
 H     1.665600     0.559500    -1.729700
 C     2.821500     1.197000    -3.402100
 H     2.710100     1.716400    -4.360200
 H     3.192400     0.187300    -3.609000
 H     3.590000     1.717200    -2.823100

Conformation 6

7R-SP-43

SCF Done:  E(RB3LYP) =  -1235.88317581     A.U. after   14 cycles

 C     0.054000    -0.707500     1.162200
 C     0.679700     0.064400    -0.021100
 H     1.687300    -0.329500    -0.208900
 H     0.813200     1.118200     0.245800
 C    -0.143700     0.038800    -1.298500
 C     0.335900    -0.570500    -2.402000
 H     1.327900    -1.021500    -2.371200
 C    -0.330800    -0.694500    -3.690300
 C    -1.501800    -1.354200    -3.788000
 H    -1.928800    -1.780600    -2.879500
 C    -2.330200    -1.600700    -5.017200
 H    -1.821600    -1.305100    -5.939800
 H    -2.487400    -2.682700    -5.113500
 C     0.950100    -0.703000     2.428000
 H     1.884200    -1.226800     2.181600
 H     0.444000    -1.308900     3.192400
 C    -3.665700    -0.897300    -4.950900
 C    -6.134900     0.425600    -4.799900
 C    -3.754500     0.478400    -5.209400
 C    -4.829200    -1.599400    -4.606600
 C    -6.057800    -0.940400    -4.534200
 C    -4.983600     1.135300    -5.135700
 H    -2.861300     1.044900    -5.463100
 H    -4.784900    -2.664300    -4.390600
 H    -6.954800    -1.493100    -4.267900
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 H    -5.041200     2.201600    -5.337100
 H    -7.091400     0.937800    -4.741500
 C     0.423100    -0.062200    -4.826600
 H     1.378800    -0.574300    -4.983500
 H    -0.121400    -0.085300    -5.773000
 H     0.629900     0.991600    -4.607000
 C    -1.459200     0.771700    -1.229900
 H    -1.892500     0.968400    -2.214400
 H    -1.324300     1.746700    -0.749400
 H    -2.186200     0.197600    -0.647200
 C     1.300900     0.663800     3.061600
 C     2.086800     0.476400     4.366500
 C     3.484300     1.005500     4.063300
 O     3.536000     0.960700     2.627700
 O     2.200100     1.380100     2.206800
 H     1.632800     0.996600     5.218200
 H     2.111900    -0.583300     4.649300
 C     0.068700     1.537200     3.293100
 H     0.345500     2.479100     3.781200
 H    -0.404900     1.823600     2.348400
 H    -0.671000     1.028700     3.919500
 C     3.676800     2.463800     4.496300
 H     3.608300     2.584300     5.581300
 H     2.928700     3.120000     4.037500
 H     4.652900     2.837700     4.166700
 C     4.608700     0.103600     4.579400
 H     5.573500     0.500800     4.239200
 H     4.513600    -0.901600     4.150300
 C     4.643800    -0.027600     6.074800
 O     3.763900     0.260200     6.866900
 O     5.803100    -0.561900     6.506300
 H     5.703800    -0.612600     7.480400
 H    -0.907500    -0.247500     1.420900
 C    -0.236500    -2.169300     0.782500
 H     0.675000    -2.681600     0.456000
 H    -0.974200    -2.236600    -0.023100
 H    -0.645800    -2.719400     1.636900

Conformation 7

7R-SP-5

SCF Done:  E(RB3LYP) =  -1235.88299047     A.U. after   14 cycles

 C    -3.154000    -0.500000     0.992200
 C    -3.139500     0.920900     1.623200
 H    -2.981200     0.830300     2.706700
 H    -4.146300     1.349800     1.527800
 C    -2.133600     1.908200     1.051400
 C    -0.864900     1.942800     1.509000
 H    -0.573700     1.275200     2.320200
 C     0.215100     2.792400     1.024400
 C     0.603600     2.725000    -0.264800
 H     0.084200     2.025300    -0.921200
 C     1.659800     3.535700    -0.961400
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H	1.203600	4.020300	-1.834700
H	2.028800	4.362300	-0.346200
C	-1.960200	-1.341400	1.502500
H	-2.000200	-1.341300	2.601400
H	-1.021500	-0.829800	1.262000
C	2.823800	2.690100	-1.420500
C	4.975700	1.097400	-2.259200
C	3.955000	2.536600	-0.606900
C	2.779800	2.024900	-2.654700
C	3.851800	1.234000	-3.071700
C	5.027000	1.747200	-1.027100
H	4.006100	3.032100	0.360500
H	1.907400	2.118600	-3.298800
H	3.808400	0.724400	-4.031400
H	5.902000	1.637800	-0.390900
H	5.811800	0.484000	-2.585900
C	0.841300	3.652300	2.086400
H	0.124300	4.401800	2.438900
H	1.150700	3.042900	2.943200
H	1.731700	4.183000	1.741600
C	-2.683500	2.861000	0.017600
H	-2.856100	2.348700	-0.932500
H	-2.024300	3.712300	-0.174200
H	-3.634700	3.283400	0.359500
C	-1.838900	-2.809700	1.035100
C	-1.130100	-2.937000	-0.316400
C	0.224900	-3.549000	0.012700
O	-0.109400	-4.350100	1.158700
O	-0.952100	-3.467100	1.971400
H	-1.705600	-3.610200	-0.965100
H	-1.048600	-1.997000	-0.864900
C	-3.161600	-3.574200	1.093400
H	-3.886100	-3.219800	0.356200
H	-3.000100	-4.644600	0.918900
H	-3.610600	-3.492500	2.090000
C	0.709500	-4.493300	-1.086800
H	-0.018000	-5.294300	-1.263600
H	0.880700	-3.972100	-2.032800
H	1.639900	-4.990700	-0.790000
C	1.324000	-2.566800	0.447700
H	2.229600	-3.131300	0.704600
H	1.027100	-2.036400	1.360000
C	1.695500	-1.531900	-0.575000
O	1.252900	-1.403600	-1.702600
O	2.632200	-0.692600	-0.091000
H	2.792300	-0.030000	-0.798900
H	-4.068300	-0.980500	1.365700
C	-3.270000	-0.440100	-0.531400
H	-4.105200	0.203300	-0.828800
H	-3.465500	-1.425900	-0.961100
H	-2.356900	-0.051000	-0.992500

Conformation 8

7R-SP-25

SCF Done: E(RB3LYP) = -1235.88292829   A.U. after   14 cycles

C	-3.554400	0.150500	0.876700
C	-3.456000	-0.953200	-0.203400
H	-4.407400	-1.014400	-0.749300
H	-3.338300	-1.927200	0.290600
C	-2.360900	-0.741300	-1.234800
C	-1.371300	-1.646500	-1.381200
H	-1.361300	-2.532700	-0.747500
C	-0.290300	-1.601300	-2.357000
C	0.603600	-0.592800	-2.348500
H	0.499600	0.180900	-1.585800
C	1.731500	-0.354200	-3.312400
H	1.637800	-0.956300	-4.222300
H	1.668500	0.684500	-3.662800
C	-2.372200	0.088800	1.877300
H	-1.564800	-0.506100	1.434500
H	-2.681100	-0.454200	2.780100
C	3.088800	-0.594000	-2.696100
C	5.599000	-1.048000	-1.527100
C	3.627700	-1.887700	-2.643500
C	3.820600	0.467900	-2.147000
C	5.070400	0.240800	-1.567700
C	4.877700	-2.112400	-2.064000
H	3.072900	-2.728000	-3.055100
H	3.417600	1.478900	-2.158300
H	5.624900	1.071200	-1.136400
H	5.288700	-3.118400	-2.033200
H	6.572200	-1.220800	-1.074800
C	-0.277100	-2.774500	-3.297500
H	0.594100	-2.790400	-3.956200
H	-0.265400	-3.716500	-2.737400
H	-1.170300	-2.762900	-3.931800
C	-2.524200	0.481600	-2.102200
H	-1.943300	0.431600	-3.027300
H	-2.219200	1.380200	-1.557700
H	-3.571500	0.597400	-2.401900
C	-1.787400	1.463900	2.287200
C	-0.601500	1.308400	3.236400
C	0.631700	1.358600	2.325400
O	0.098200	1.430700	0.995500
O	-1.200100	2.093200	1.143700
H	-0.561400	2.118700	3.975300
H	-0.671200	0.387000	3.826800
C	-2.828800	2.411300	2.877900
H	-3.599300	2.671300	2.145200
H	-3.307500	1.979600	3.762300
H	-2.369600	3.364600	3.166000
C	1.452400	2.624700	2.586500
H	0.812500	3.515100	2.564700
H	1.951300	2.586200	3.559900
H	2.202900	2.787400	1.806900
C	1.443800	0.070100	2.479100
H	0.788600	-0.797100	2.322300

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 H     1.857400    -0.026300     3.489700
 C     2.580900    -0.041400     1.503800
 O     3.541400     0.705900     1.425400
 O     2.465000    -1.120400     0.707900
 H     3.203200    -1.050200     0.063100
 H    -3.573100     1.126000     0.377800
 C    -4.889300    -0.014700     1.618300
 H    -5.731100     0.085900     0.924600
 H    -5.015300     0.741400     2.397700
 H    -4.960500    -1.000300     2.091500

Conformation 9

7R-SP-35

SCF Done:  E(RB3LYP) =  -1235.88266658     A.U. after   14 cycles

 C     1.322900    -1.201500    -3.167100
 C     1.572200     0.290500    -2.860200
 H     1.776700     0.795200    -3.815600
 H     2.496500     0.381500    -2.278800
 C     0.499100     1.125700    -2.174300
 C    -0.759100     0.701800    -1.934300
 H    -1.069400    -0.289500    -2.257700
 C    -1.837100     1.456000    -1.302100
 C    -1.697000     1.956200    -0.058400
 H    -0.754000     1.786700     0.463000
 C    -2.672300     2.794400     0.719900
 H    -2.172500     3.733400     0.991400
 H    -3.537800     3.101500     0.124800
 C     1.261800    -2.160300    -1.952300
 H     1.224700    -3.187200    -2.345800
 H     0.279200    -2.046600    -1.473800
 C    -3.159200     2.105500     1.972500
 C    -4.059600     0.817200     4.296000
 C    -2.578700     2.392400     3.216600
 C    -4.189200     1.156600     1.906400
 C    -4.637700     0.517500     3.063500
 C    -3.029700     1.753000     4.372700
 H    -1.767900     3.114800     3.291200
 H    -4.647500     0.912100     0.950300
 H    -5.439600    -0.214200     3.003000
 H    -2.576300     1.986400     5.333100
 H    -4.412100     0.321000     5.196900
 C    -3.076700     1.558300    -2.149200
 H    -2.876200     2.159300    -3.043000
 H    -3.407000     0.563900    -2.470900
 H    -3.921200     2.013800    -1.627800
 C     0.988600     2.518000    -1.840000
 H     1.689400     2.476200    -0.999800
 H     0.186800     3.215000    -1.584600
 H     1.509200     2.952200    -2.700800
 C     2.328400    -2.123600    -0.834200
 C     2.089600    -1.021300     0.200000
 C     2.096600    -1.729600     1.556100
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 O     2.666900   -3.016000    1.255500
 O     2.139300   -3.334800   -0.069900
 H     2.862900   -0.246700    0.132800
 H     1.141100   -0.502700    0.042000
 C     3.772700   -2.149700   -1.334700
 H     3.927100   -2.983400   -2.028600
 H     4.059300   -1.217100   -1.825900
 H     4.476100   -2.311800   -0.509400
 C     3.036600   -1.056600    2.555300
 H     3.059900   -1.610200    3.500900
 H     4.066100   -1.055600    2.177800
 H     2.753800   -0.021900    2.765700
 C     0.700600   -1.992000    2.138400
 H     0.785300   -2.565300    3.069700
 H     0.126100   -2.613900    1.439700
 C    -0.103300   -0.755500    2.419500
 O     0.298900    0.393100    2.480800
 O    -1.400800   -1.054000    2.627600
 H    -1.850900   -0.192200    2.770900
 H     0.348500   -1.284200   -3.668300
 C     2.333500   -1.688000   -4.218800
 H     3.368100   -1.498600   -3.925200
 H     2.169800   -1.166000   -5.168700
 H     2.218900   -2.759300   -4.413800

Conformation 10

7R-SP-31

SCF Done:  E(RB3LYP) =  -1235.88266024     A.U. after   15 cycles

 C     2.472300    1.019400   -1.590900
 C     3.269700    0.042100   -0.688500
 H     4.147500    0.562900   -0.282600
 H     3.667000   -0.768000   -1.315000
 C     2.499000   -0.531600    0.485600
 C     2.384700   -1.867100    0.635400
 H     2.874400   -2.535800   -0.071500
 C     1.644000   -2.544600    1.687500
 C     0.299400   -2.473100    1.695800
 H    -0.186000   -1.929800    0.883600
 C    -0.660600   -3.043600    2.700100
 H    -1.281200   -3.795500    2.197300
 H    -0.159800   -3.569000    3.518600
 C     1.207100    0.342200   -2.182200
 H     0.608400    0.005800   -1.326400
 H     1.486700   -0.572600   -2.720800
 C    -1.540600   -1.967000    3.296400
 C    -3.150900    0.065700    4.364100
 C    -1.013300   -1.049900    4.217500
 C    -2.884600   -1.850500    2.916000
 C    -3.685800   -0.840000    3.449900
 C    -1.815100   -0.038400    4.747400
 H     0.029600   -1.119000    4.520900
 H    -3.312300   -2.540200    2.190800
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H	-4.726900	-0.757600	3.148400
H	-1.397500	0.668200	5.460200
H	-3.775200	0.853500	4.777800
C	2.502900	-3.285200	2.671500
H	1.926100	-3.845200	3.410700
H	3.144200	-4.007200	2.153400
H	3.145100	-2.585600	3.217900
C	1.937600	0.481500	1.451300
H	2.696600	1.234100	1.691000
H	1.625300	0.040100	2.401800
H	1.071900	0.989400	1.015900
C	0.284200	1.208800	-3.076800
C	-1.188700	0.774100	-2.975000
C	-1.856900	1.896200	-2.183200
O	-0.760800	2.588300	-1.577800
O	0.282000	2.561600	-2.605900
H	-1.665100	0.653700	-3.956000
H	-1.274700	-0.209400	-2.505000
C	0.713300	1.195400	-4.546000
H	1.709800	1.613900	-4.696300
H	0.700400	0.180100	-4.955700
H	0.042500	1.818000	-5.150100
C	-2.568400	2.884700	-3.123400
H	-2.924700	3.759800	-2.567700
H	-1.891100	3.267700	-3.894900
H	-3.423900	2.416900	-3.621900
C	-2.851200	1.447400	-1.113300
H	-3.721600	0.957200	-1.566600
H	-3.240300	2.315800	-0.565300
C	-2.282300	0.495900	-0.100800
O	-2.180400	-0.711800	-0.246100
O	-1.912800	1.098600	1.042400
H	-1.625600	0.376300	1.644300
H	2.153300	1.865800	-0.969500
C	3.421000	1.576000	-2.654400
H	3.667900	0.817700	-3.404500
H	2.986000	2.444100	-3.156900
H	4.358600	1.918700	-2.202600

Conformation 11

7R-SP-21

SCF Done: E(RB3LYP) = -1235.88246974 A.U. after 14 cycles

C	2.535400	-1.693600	-1.699800
C	1.472700	-1.265600	-2.741000
H	0.646000	-1.986200	-2.711800
H	1.896900	-1.393100	-3.746500
C	0.923000	0.148300	-2.634900
C	-0.294300	0.356000	-2.093800
H	-0.875800	-0.503300	-1.756400
C	-0.970600	1.626700	-1.876400
C	-0.380700	2.596700	-1.150600
H	0.629800	2.423400	-0.779300

C	−0.954600	3.924100	−0.742800
H	−0.223300	4.708000	−0.977000
H	−1.850300	4.193500	−1.310900
C	2.055800	−1.679000	−0.226200
H	1.651600	−0.682900	−0.005200
H	2.937900	−1.800100	0.418200
C	−1.273700	3.944900	0.734000
C	−1.836500	3.896400	3.481300
C	−0.364400	4.481800	1.655500
C	−2.465500	3.376900	1.208000
C	−2.744600	3.353600	2.574800
C	−0.647200	4.460000	3.022300
H	0.572000	4.917500	1.314400
H	−3.178900	2.934900	0.514400
H	−3.669800	2.906800	2.930000
H	0.062400	4.880600	3.730100
H	−2.054700	3.878200	4.545700
C	−2.372500	1.665800	−2.421700
H	−2.355300	1.572500	−3.513200
H	−2.969000	0.841100	−2.015900
H	−2.904000	2.589600	−2.183800
C	1.752700	1.242300	−3.255600
H	2.499600	1.615400	−2.550700
H	1.142800	2.090300	−3.583000
H	2.270000	0.876600	−4.148800
C	1.027200	−2.751200	0.200700
C	0.702500	−2.614600	1.687800
C	−0.797700	−2.891600	1.778200
O	−1.211300	−3.194300	0.440000
O	−0.236400	−2.519200	−0.420800
H	1.307100	−3.297000	2.297600
H	0.937200	−1.615200	2.068000
C	1.495700	−4.169100	−0.147700
H	0.818000	−4.928500	0.256200
H	1.499800	−4.330900	−1.230700
H	2.497600	−4.366900	0.246300
C	−1.056000	−4.148200	2.619800
H	−0.750800	−4.003000	3.661300
H	−0.517300	−5.013600	2.218700
H	−2.118200	−4.418400	2.602700
C	−1.640400	−1.743700	2.343400
H	−1.300600	−1.452800	3.344800
H	−2.682500	−2.071300	2.459400
C	−1.702100	−0.516000	1.479000
O	−2.643800	−0.179900	0.779300
O	−0.610800	0.262100	1.594700
H	−0.808100	1.037100	1.022000
H	2.827400	−2.718300	−1.959500
C	3.821900	−0.865500	−1.818300
H	3.701200	0.136800	−1.398000
H	4.141400	−0.775500	−2.861500
H	4.635900	−1.349600	−1.266800

Conformation 12

7R-SP-15

SCF Done: E(RB3LYP) = -1235.88231487   A.U. after   15 cycles

C	-1.228500	-0.213200	3.119500
C	-1.322000	1.300500	2.795300
H	-0.779600	1.883000	3.551800
H	-2.367600	1.628200	2.867200
C	-0.741200	1.650200	1.433500
C	-1.551700	1.846600	0.372700
H	-2.628800	1.753300	0.516600
C	-1.166100	2.087900	-1.012200
C	-0.326400	3.084500	-1.353100
H	0.060400	3.731300	-0.566400
C	0.164100	3.435300	-2.730200
H	-0.603100	3.238900	-3.487800
H	0.329600	4.519600	-2.781000
C	-2.294200	-1.043200	2.352800
H	-3.074400	-1.341800	3.066400
H	-2.805700	-0.424000	1.607000
C	1.452300	2.728600	-3.088000
C	3.845800	1.421700	-3.760700
C	1.454400	1.668600	-4.006300
C	2.666400	3.116100	-2.502600
C	3.855900	2.466300	-2.838200
C	2.645000	1.021200	-4.342900
H	0.527000	1.342700	-4.472600
H	2.691400	3.931700	-1.782900
H	4.791700	2.779200	-2.381500
H	2.633500	0.205600	-5.062300
H	4.773800	0.921500	-4.026500
C	-1.810100	1.135200	-1.985300
H	-1.519200	0.104000	-1.757800
H	-2.902000	1.205800	-1.926400
H	-1.532700	1.324400	-3.024300
C	0.764700	1.728500	1.396800
H	1.174400	1.662600	0.386900
H	1.216100	0.911600	1.966200
H	1.097900	2.671000	1.843500
C	-1.774300	-2.316800	1.642400
C	-0.820800	-2.018400	0.493300
C	0.434100	-2.814800	0.804400
O	0.371900	-2.975600	2.232500
O	-1.049500	-3.149500	2.554700
H	-1.238700	-2.260400	-0.490700
H	-0.597500	-0.950000	0.459700
C	-2.974500	-3.132900	1.146500
H	-3.579000	-2.565000	0.431600
H	-3.615600	-3.430800	1.984300
H	-2.652900	-4.062400	0.664900
C	0.439000	-4.205500	0.164300
H	1.323200	-4.771700	0.478900
H	-0.424300	-4.798900	0.482100
H	0.433900	-4.152400	-0.928300
C	1.730200	-2.053300	0.496300

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 H     2.602400    -2.711500     0.583700
 H     1.863400    -1.267100     1.250000
 C     1.752500    -1.405500    -0.861100
 O     1.128100    -1.745800    -1.851000
 O     2.586400    -0.347600    -0.890500
 H     2.471300     0.061300    -1.777100
 H    -0.224400    -0.561800     2.861400
 C    -1.391300    -0.421700     4.630200
 H    -0.605100     0.105500     5.181000
 H    -1.321200    -1.483600     4.887600
 H    -2.358800    -0.047300     4.981900
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Conformation 13

7R-SP-23

SCF Done: E(RB3LYP) = -1235.88218107   A.U. after   15 cycles

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 C    -1.760100     2.125900    -1.542000
 C    -2.180000     1.134200    -2.663800
 H    -1.885800     1.558000    -3.633300
 H    -3.277500     1.091600    -2.702300
 C    -1.634900    -0.279900    -2.554500
 C    -2.254000    -1.185500    -1.769900
 H    -3.169600    -0.895800    -1.253700
 C    -1.821800    -2.542500    -1.466600
 C    -0.602700    -2.755500    -0.933300
 H     0.051800    -1.893000    -0.796100
 C    -0.010500    -4.048400    -0.445600
 H    -0.742800    -4.860300    -0.401900
 H     0.761600    -4.367700    -1.156100
 C    -0.224700     2.286000    -1.462900
 H     0.138900     2.518100    -2.474300
 H     0.235500     1.321600    -1.214000
 C     0.598000    -3.889100     0.931900
 C     1.713900    -3.502800     3.475700
 C    -0.226300    -3.760800     2.060100
 C     1.988900    -3.824500     1.096000
 C     2.542900    -3.633100     2.362800
 C     0.330100    -3.568500     3.325300
 H    -1.308600    -3.803100     1.953300
 H     2.649700    -3.913600     0.236200
 H     3.622400    -3.580300     2.482300
 H    -0.315700    -3.469900     4.194400
 H     2.148200    -3.348700     4.460700
 C    -2.864600    -3.594600    -1.717400
 H    -3.705500    -3.473700    -1.026000
 H    -3.247200    -3.515600    -2.741500
 H    -2.482000    -4.611800    -1.604500
 C    -0.431100    -0.579000    -3.412400
 H     0.459600    -0.075000    -3.028600
 H    -0.605100    -0.235500    -4.438000
 H    -0.210000    -1.647900    -3.481000
 C     0.351700     3.346700    -0.498800
 C     0.444700     2.862000     0.951900
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C	1.935200	2.850100	1.269400
O	2.445500	3.828100	0.350600
O	1.726400	3.551000	-0.894200
H	-0.091600	3.558400	1.609300
H	-0.016200	1.886600	1.123400
C	-0.345700	4.702900	-0.620700
H	0.191000	5.471400	-0.052200
H	-0.352000	5.042000	-1.662800
H	-1.376500	4.673400	-0.256700
C	2.217600	3.355700	2.683200
H	1.738100	2.733600	3.444800
H	1.860700	4.384800	2.808500
H	3.295500	3.381500	2.879400
C	2.643900	1.522800	0.977700
H	3.726700	1.621500	1.128100
H	2.545300	1.240500	-0.078200
C	2.162900	0.387100	1.830900
O	2.454700	0.189100	2.997900
O	1.331200	-0.436800	1.168800
H	1.138100	-1.174500	1.791000
H	-2.184500	3.094300	-1.837900
C	-2.400900	1.754400	-0.202900
H	-1.943000	0.862000	0.234100
H	-3.472500	1.562600	-0.323800
H	-2.307400	2.569800	0.520200

Conformation 14

7R-SP-3

SCF Done: E(RB3LYP) = -1235.88205835 A.U. after 14 cycles

C	0.690700	2.169600	-2.366100
C	1.503500	1.063200	-3.078800
H	2.571500	1.321900	-3.057700
H	1.233100	1.036000	-4.142500
C	1.355300	-0.320800	-2.464900
C	1.896600	-0.581500	-1.256600
H	2.444200	0.207900	-0.740300
C	1.883100	-1.852200	-0.548000
C	0.727600	-2.370400	-0.087400
H	-0.194500	-1.814700	-0.258400
C	0.527700	-3.684100	0.616000
H	-0.331500	-4.193000	0.159200
H	1.366600	-4.370000	0.455600
C	-0.828800	2.034700	-2.638600
H	-1.079900	1.002700	-2.906100
H	-1.071300	2.637900	-3.524100
C	0.281000	-3.525900	2.097300
C	-0.175000	-3.223300	4.850900
C	-1.018800	-3.341700	2.588800
C	1.350600	-3.544000	3.003900
C	1.122700	-3.396700	4.373700
C	-1.244900	-3.193300	3.958700
H	-1.865300	-3.305200	1.905600

H	2.369600	-3.677600	2.647100
H	1.959000	-3.420400	5.068200
H	-2.258300	-3.050700	4.326500
H	-0.353200	-3.112500	5.917700
C	3.248800	-2.454800	-0.364800
H	3.919100	-1.743900	0.131700
H	3.242600	-3.361200	0.244600
H	3.682600	-2.715200	-1.336600
C	0.670300	-1.344500	-3.331900
H	-0.388400	-1.099300	-3.454000
H	0.732000	-2.360200	-2.932200
H	1.135400	-1.368500	-4.323300
C	-1.761400	2.451500	-1.476500
C	-1.637600	1.539200	-0.259900
C	-1.224300	2.461600	0.877500
O	-0.635500	3.581500	0.193800
O	-1.448600	3.767900	-1.011500
H	-2.562500	0.995400	-0.034300
H	-0.883800	0.764900	-0.440200
C	-3.208800	2.484600	-1.978900
H	-3.894100	2.809700	-1.188100
H	-3.321000	3.206800	-2.795700
H	-3.533600	1.502000	-2.336500
C	-2.413000	2.981100	1.692700
H	-2.078100	3.707900	2.441600
H	-2.944300	2.175500	2.207300
H	-3.132800	3.510400	1.059300
C	-0.135500	1.864200	1.775900
H	0.100500	2.555300	2.593800
H	0.785700	1.737800	1.192600
C	-0.496500	0.529500	2.362600
O	-1.573400	-0.037700	2.299700
O	0.550200	-0.027200	3.002300
H	0.240500	-0.921300	3.269800
H	0.890300	2.097300	-1.292700
C	1.200900	3.540000	-2.832900
H	1.086200	3.658200	-3.915900
H	2.263300	3.658000	-2.593600
H	0.663300	4.357800	-2.345300

Conformation 15

7R-SP-17

SCF Done: E(RB3LYP) = -1235.88195071 A.U. after 14 cycles

C	-1.173300	1.246700	-2.751000
C	-2.511300	1.614300	-2.060200
H	-3.290600	0.898500	-2.354900
H	-2.841000	2.587900	-2.446900
C	-2.469500	1.654800	-0.536200
C	-2.072200	0.570000	0.162500
H	-1.862000	-0.334400	-0.412700
C	-1.855000	0.397700	1.597000
C	-1.984100	-0.839300	2.122300

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H   -2.291800   -1.657900    1.471100
C   -1.813500   -1.245700    3.561900
H   -1.712100   -0.384600    4.231400
H   -2.734400   -1.746100    3.888900
C   -0.072700    2.302800   -2.468300
H   -0.267400    2.809700   -1.515600
H   -0.143700    3.081000   -3.240400
C   -0.641500   -2.177000    3.765000
C    1.541600   -3.905200    4.121600
C   -0.819700   -3.567600    3.729200
C    0.647500   -1.664900    3.970700
C    1.732300   -2.525300    4.150300
C    0.266500   -4.426400    3.909500
H   -1.808600   -3.990400    3.563900
H    0.816400   -0.590200    3.987700
H    2.727400   -2.115300    4.307600
H    0.116300   -5.503100    3.887400
H    2.386700   -4.573900    4.265400
C   -1.373900    1.574500    2.404500
H   -2.214300    2.099500    2.867800
H   -0.689100    1.270200    3.202000
H   -0.806300    2.280700    1.788700
C   -2.960900    2.949000    0.055000
H   -2.182700    3.715800   -0.003500
H   -3.285900    2.847600    1.091900
H   -3.838900    3.308600   -0.493500
C    1.382800    1.776200   -2.418400
C    1.630400    0.789200   -1.280200
C    2.059700   -0.499400   -1.967200
O    1.554700   -0.346400   -3.305300
O    1.717600    1.074900   -3.619100
H    2.383600    1.139600   -0.564400
H    0.719800    0.648500   -0.689700
C    2.343700    2.965700   -2.314300
H    2.170000    3.545300   -1.401800
H    3.387200    2.631000   -2.319700
H    2.232600    3.632800   -3.176900
C    3.581500   -0.650700   -2.055100
H    4.038200    0.200300   -2.572200
H    3.847900   -1.538700   -2.639600
H    4.045500   -0.734700   -1.068300
C    1.394000   -1.752300   -1.388900
H    1.768300   -2.648500   -1.898200
H    0.314600   -1.708800   -1.583500
C    1.587200   -1.927700    0.090200
O    2.340300   -1.305900    0.818500
O    0.797000   -2.907600    0.572000
H    0.950800   -2.910400    1.543100
H   -0.857900    0.266900   -2.382600
C   -1.424400    1.104800   -4.258700
H   -1.784900    2.044500   -4.691400
H   -2.180000    0.335700   -4.452400
H   -0.518200    0.813900   -4.795900
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Conformation 16

7R-SP-7

SCF Done: E(RB3LYP) = -1235.88123366   A.U. after   14 cycles

C	2.651400	-1.938900	-0.510200
C	3.100600	-1.617800	0.941200
H	4.170900	-1.370800	0.944800
H	3.004700	-2.546600	1.521500
C	2.386600	-0.507700	1.701200
C	1.878500	0.586800	1.097700
H	2.012100	0.724800	0.026200
C	1.164700	1.682300	1.739500
C	-0.017800	1.462200	2.347200
H	-0.418700	0.448200	2.342400
C	-0.865800	2.450800	3.097800
H	-1.213300	1.978900	4.026300
H	-0.281900	3.315700	3.431400
C	1.169900	-2.394200	-0.534500
H	0.584100	-1.576100	-0.099200
H	1.027600	-3.237000	0.155400
C	-2.066000	2.910700	2.305500
C	-4.282300	3.751800	0.803000
C	-2.067100	4.164300	1.677300
C	-3.189300	2.082500	2.166400
C	-4.290900	2.501700	1.418600
C	-3.171200	4.582900	0.932200
H	-1.205800	4.823300	1.764300
H	-3.209100	1.100000	2.634100
H	-5.154500	1.848900	1.314900
H	-3.163700	5.558800	0.452800
H	-5.142500	4.078400	0.223800
C	1.839800	3.018100	1.598400
H	2.035100	3.241100	0.543300
H	1.242600	3.844700	1.990300
H	2.796000	3.018700	2.133000
C	2.357000	-0.731200	3.194100
H	3.361100	-0.979700	3.555400
H	1.687200	-1.562900	3.435800
H	2.029300	0.144300	3.760500
C	0.540100	-2.745100	-1.906500
C	-0.940300	-2.340800	-1.944700
C	-0.976500	-1.158000	-2.899700
O	0.078200	-1.512700	-3.812300
O	1.166900	-1.979900	-2.947100
H	-1.535400	-3.166600	-2.357300
H	-1.370800	-2.140400	-0.960000
C	0.690200	-4.234000	-2.236200
H	0.189600	-4.860900	-1.491100
H	0.260900	-4.458400	-3.220000
H	1.737100	-4.540100	-2.294800
C	-2.277800	-1.107500	-3.701000
H	-2.247500	-0.299100	-4.440500
H	-2.423600	-2.032900	-4.270600

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 H   -3.151400    -0.959400    -3.059700
 C   -0.624500     0.209600    -2.298200
 H   -0.548500     0.940800    -3.113800
 H    0.358000     0.190300    -1.815400
 C   -1.617800     0.722300    -1.296600
 O   -2.465100     0.081600    -0.699600
 O   -1.455500     2.041500    -1.077200
 H   -2.088800     2.264300    -0.359200
 H    2.757200    -1.033400    -1.119300
 C    3.606100    -2.986800    -1.089900
 H    4.649400    -2.678500    -0.959100
 H    3.451900    -3.116000    -2.164500
 H    3.478700    -3.956800    -0.598100

Conformation 17

7R-SP-27

SCF Done:  E(RB3LYP) =  -1235.88107580     A.U. after   15 cycles

 C    1.489000    -2.485100     2.187000
 C    2.164000    -2.857200     0.845200
 H    2.406100    -3.928400     0.836200
 H    3.130000    -2.339400     0.773000
 C    1.308800    -2.566100    -0.377300
 C    1.665000    -1.597300    -1.245700
 H    2.583400    -1.038800    -1.061100
 C    0.959300    -1.188300    -2.453400
 C   -0.330000    -0.799400    -2.400100
 H   -0.836900    -0.824300    -1.434500
 C   -1.213100    -0.361200    -3.533800
 H   -0.797400    -0.617300    -4.513600
 H   -2.155800    -0.921100    -3.477000
 C    1.399700    -0.948900     2.378300
 H    1.556700    -0.459200     1.410200
 H    2.220100    -0.605800     3.022300
 C   -1.505800     1.119400    -3.480100
 C   -2.025600     3.872000    -3.351400
 C   -0.661400     2.033800    -4.125500
 C   -2.610100     1.602500    -2.763800
 C   -2.868500     2.972600    -2.701300
 C   -0.923400     3.403300    -4.064200
 H    0.204100     1.682900    -4.684300
 H   -3.278500     0.911600    -2.252800
 H   -3.731500     3.338600    -2.150100
 H   -0.266400     4.106200    -4.571400
 H   -2.228300     4.939400    -3.305100
 C    1.821300    -1.187400    -3.686600
 H    2.139900    -2.207700    -3.926900
 H    2.716800    -0.575100    -3.530300
 H    1.315400    -0.785800    -4.567300
 C    0.113200    -3.469300    -0.546200
 H   -0.287800    -3.461100    -1.563400
 H   -0.687500    -3.176800     0.139700
 H    0.388200    -4.507900    -0.332800
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C	0.058500	-0.430900	2.942700
C	0.057500	1.100900	3.001400
C	-1.059400	1.523200	2.056300
O	-1.913200	0.363500	2.055500
O	-0.985800	-0.768800	2.015400
H	1.027000	1.538100	2.743900
H	-0.147800	1.438500	4.025400
C	-0.293800	-1.037400	4.301500
H	-1.234200	-0.621000	4.681800
H	0.489800	-0.845600	5.041200
H	-0.458500	-2.117200	4.229100
C	-1.885600	2.681900	2.615500
H	-2.718300	2.923800	1.945100
H	-2.338800	2.408800	3.575800
H	-1.288100	3.585000	2.766700
C	-0.624900	1.769000	0.603800
H	-1.524200	1.911200	-0.006100
H	-0.105100	0.891900	0.205000
C	0.276500	2.959200	0.407700
O	0.824900	3.587200	1.299200
O	0.455000	3.266500	-0.896800
H	-0.051800	2.698600	-1.515200
H	0.485800	-2.926100	2.205600
C	2.290900	-3.118100	3.332500
H	3.326900	-2.761700	3.335800
H	2.311400	-4.208700	3.232900
H	1.851900	-2.885300	4.306600

Conformation 18

7R-SP-19

SCF Done: E(RB3LYP) = -1235.88097696 A.U. after 14 cycles

C	0.929700	-2.394400	1.843400
C	1.763600	-2.856400	0.614500
H	1.350800	-3.793500	0.219100
H	2.766300	-3.125900	0.976000
C	1.903200	-1.850500	-0.516500
C	3.003400	-1.074000	-0.601100
H	3.808600	-1.194700	0.123100
C	3.218500	-0.006200	-1.565700
C	2.443300	1.095100	-1.512600
H	1.683300	1.147400	-0.731100
C	2.485900	2.299100	-2.410000
H	2.976200	3.119300	-1.871100
H	3.081600	2.128300	-3.312400
C	-0.579500	-2.343500	1.514500
H	-0.873200	-3.339600	1.152600
H	-0.745800	-1.682800	0.660500
C	1.100900	2.736000	-2.835400
C	-1.470300	3.536200	-3.621500
C	0.456100	3.798700	-2.186200
C	0.433700	2.068500	-3.872400
C	-0.844400	2.469500	-4.264700

C	−0.821900	4.198600	−2.580700
H	0.947600	4.324600	−1.369800
H	0.910800	1.232700	−4.380800
H	−1.351600	1.949300	−5.073700
H	−1.310400	5.028500	−2.075400
H	−2.464300	3.849700	−3.930800
C	4.359300	−0.241800	−2.513200
H	4.124200	−1.068600	−3.192200
H	4.595800	0.632800	−3.124000
H	5.271400	−0.498200	−1.962300
C	0.799400	−1.817600	−1.542600
H	0.328700	−2.801300	−1.641100
H	1.173300	−1.554500	−2.537700
H	0.031800	−1.090600	−1.266800
C	−1.572500	−1.928000	2.623700
C	−1.689100	−0.409500	2.776300
C	−3.041800	−0.061800	2.172600
O	−3.793000	−1.243600	2.496300
O	−2.883000	−2.348900	2.173700
H	−1.674900	−0.153200	3.843900
H	−0.868900	0.151800	2.327400
C	−1.319400	−2.644800	3.949500
H	−2.138000	−2.458300	4.654600
H	−1.286100	−3.730300	3.801300
H	−0.386700	−2.330600	4.424700
C	−3.700200	1.116000	2.891000
H	−4.711100	1.291000	2.505500
H	−3.123400	2.038900	2.785000
H	−3.817800	0.906200	3.960700
C	−3.080900	0.112200	0.644900
H	−4.092800	0.394100	0.328200
H	−2.868900	−0.843100	0.150200
C	−2.122000	1.134100	0.101700
O	−1.555700	2.021500	0.714700
O	−1.946800	0.983200	−1.226100
H	−1.316600	1.686400	−1.500300
H	1.066400	−3.173200	2.605700
C	1.493900	−1.096900	2.427900
H	1.322200	−0.243500	1.764700
H	2.573600	−1.185200	2.591900
H	1.047600	−0.864900	3.398400

Table S5. Calculated (GIAO)[3] ^{1}H and ^{13}C NMR δ Values of (7*S*)- and (7*R*)-**4** and Comparison to δ_{exp}.

locant	δ **4**$_{exp}$	δ (7*S*)-**4**$_{calc}$	δ (7*R*)-**4**$_{calc}$	Δδ[(7*S*)-**4**$_{calc}$–[**4**$_{exp}$]	Δδ[(7*R*)-**4**$_{calc}$]–[**4**$_{exp}$]	Δδ (7*S*)-**4**$_{calc}$– Δδ(7*R*)-**4**$_{calc}$
C-1	175.2	166.1	165.1	–9.1	–10.1	1.0
C-2	43.8	41.5	41.5	–2.3	–2.3	0.0
C-3	83.3	82.3	80.9	–1.0	–2.4	1.4
C-4	57.6	55.8	57.7	–1.8	0.1	**–1.9**
C-5	87.2	83.3	81.7	–3.9	–5.5	**1.6**
C-6	45.4	44.9	46.4	–0.5	1.0	**–1.5**
C-7	27.7	31.1	31.3	3.4	3.6	–0.2
C-8	49.6	52.7	47.7	3.1	–1.9	**5.0**
C-9	134.1	133	133.2	–1.1	–0.9	–0.2
C-10	130.7	127.6	127.5	–3.1	–3.2	0.1
C–11	133.6	128.9	129.7	–4.7	–3.9	–0.8
C-12	127.4	125.4	125.4	–2.0	–2.0	0.0
C-13	34.5	36.9	36.7	2.4	2.2	0.2
C-4	141.4	135.9	136.5	–5.5	–4.9	–0.6
C-15	128.3	123.4	123.9	–4.9	–4.4	–0.5
C-16	128.4	122.6	123.3	–5.8	–5.1	–0.7
C-17	125.8	119.7	119.4	–6.1	–6.4	0.3
C-18	128.4	122.9	122.9	–5.5	–5.5	0.0
C-19	128.3	125.9	123.5	–2.4	–4.8	2.4
C-20	23.5	23.9	25.4	0.4	1.9	–1.5
C-21	24.3	26.7	26	2.4	1.7	0.7
C-22	20.9	26.1	22.9	5.2	2.0	3.2
C-23	17.7	18.4	19.5	0.7	1.8	–1.1
C-24	17.3	17.6	17.1	0.3	–0.2	0.5
H-2	2.735	2.52	2.48	–0.22	–0.26	0.0
H-4	2.345	2.34	2.43	–0.01	0.09	–0.1
H-6	1.545	1.335	1.46	–0.21	–0.09	–0.1
H-7	1.85	1.53	1.99	–0.32	0.14	–0.5
H-8	1.905	1.84	1.92	–0.06	0.01	–0.1
H-10	5.64	5.81	5.88	0.17	0.24	–0.1
H-12	5.43	5.63	5.45	0.20	0.02	0.2
H-13	3.44	3.33	3.27	–0.11	–0.17	0.1
H-15	7.2	7.42	7.37	0.22	0.17	0.0
H-16	7.29	7.38	7.44	0.09	0.15	–0.1
H-17	7.19	7.23	7.21	0.04	0.02	0.0
H-18	7.29	7.42	7.37	0.13	0.08	0.0
H-19	7.2	7.57	7.42	0.37	0.22	0.2
H-20	1.47	1.30	1.35	–0.17	–0.12	–0.1
H-21	1.37	1.27	1.22	–0.10	–0.15	0.1
H-22	0.9	0.96	0.89	0.06	–0.01	0.1
H-23	1.73	1.68	1.55	–0.05	–0.18	0.1
H-24	1.82	1.71	1.70	–0.11	–0.12	0.0

(3). Smith, S. G.; Goodman, J. M. *J. Am. Chem. Soc.* **2010**, *132,* 12946-1295