

Supplementary Data

Meroterpenoids from a Tropical *Dysidea* sp. Sponge

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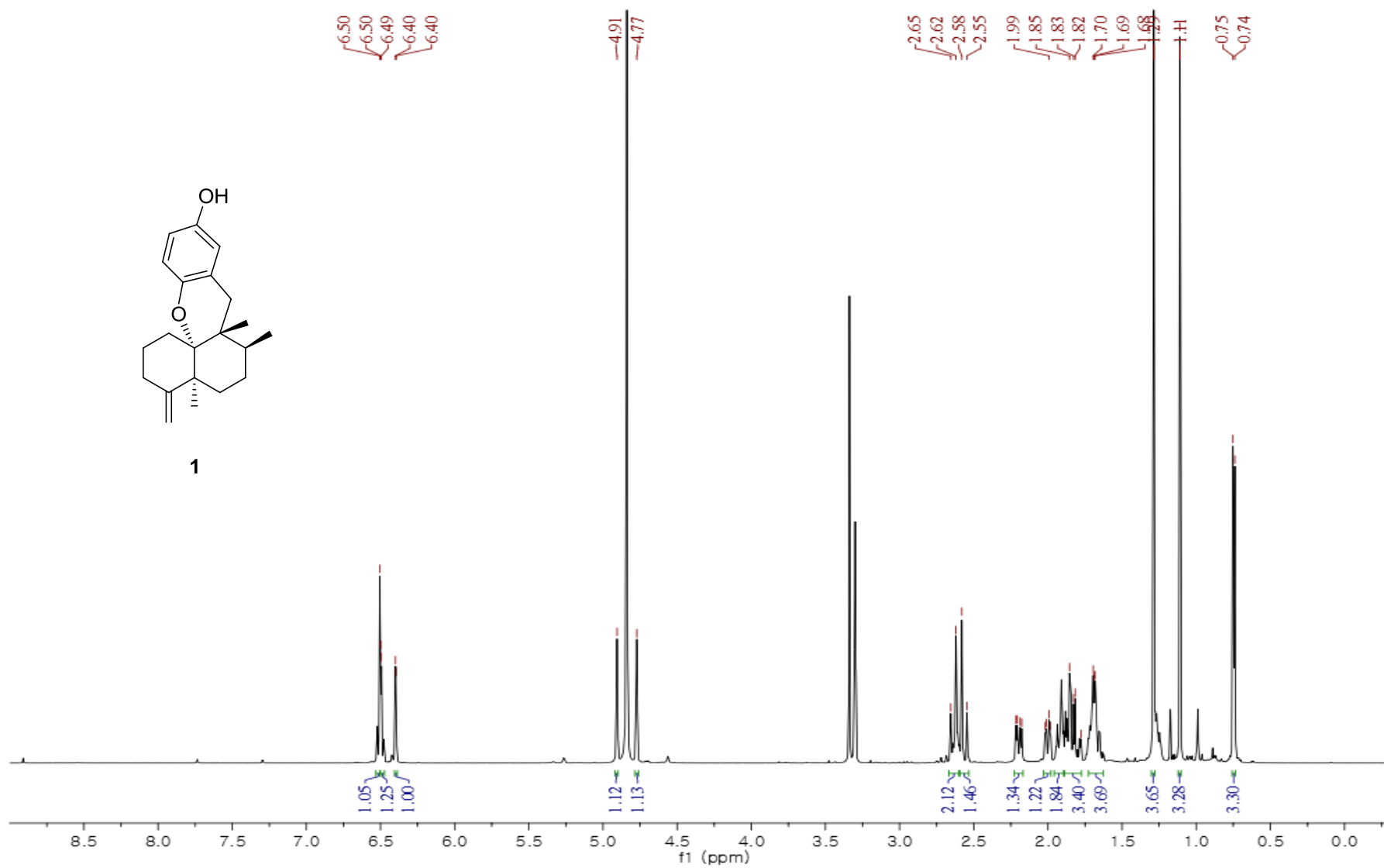


Figure S1. The ¹H NMR (500 MHz, CD₃OD) spectrum of compound **1**

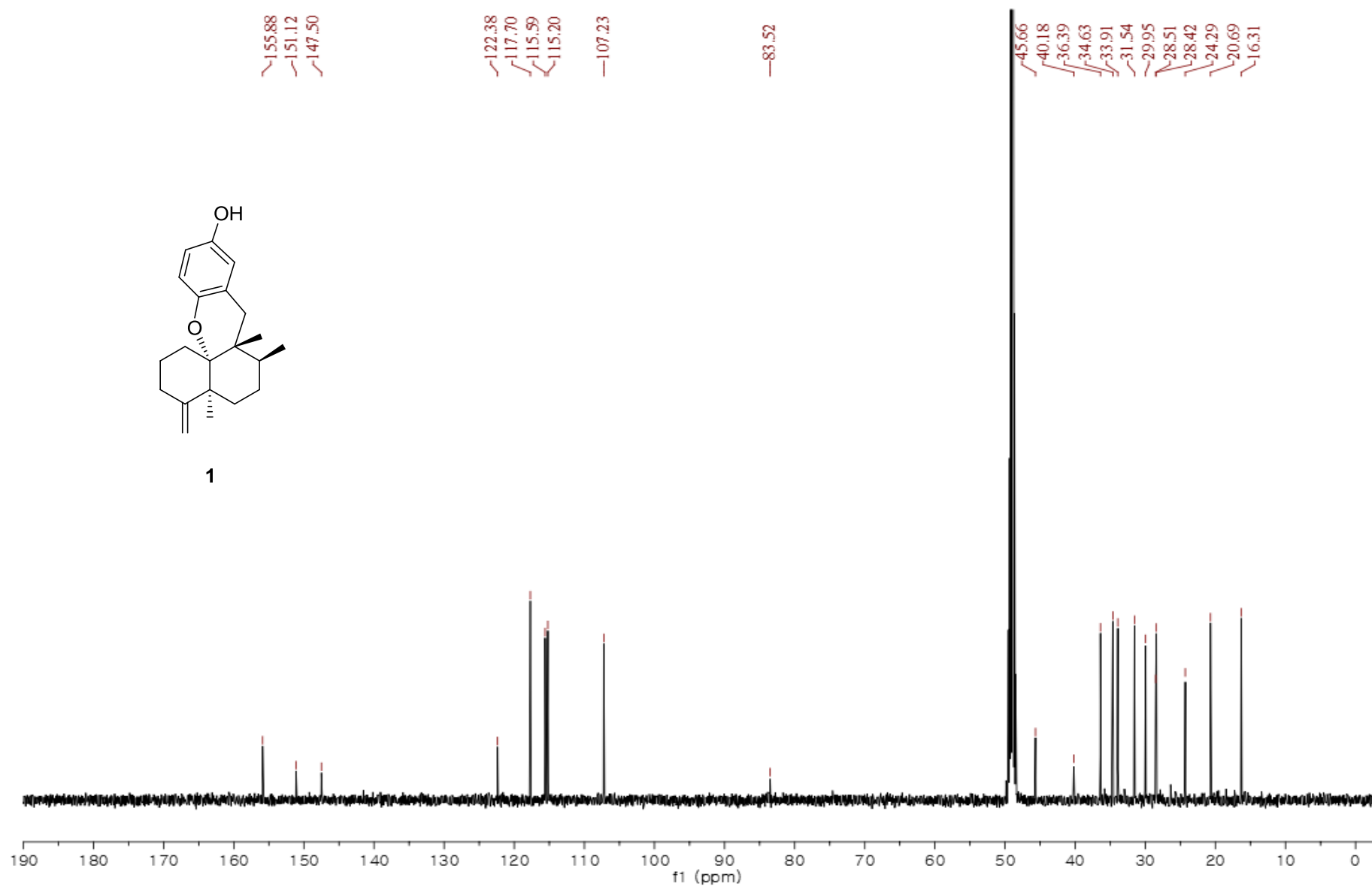


Figure S2. The ^{13}C NMR (125 MHz, CD_3OD) spectrum of compound **1**

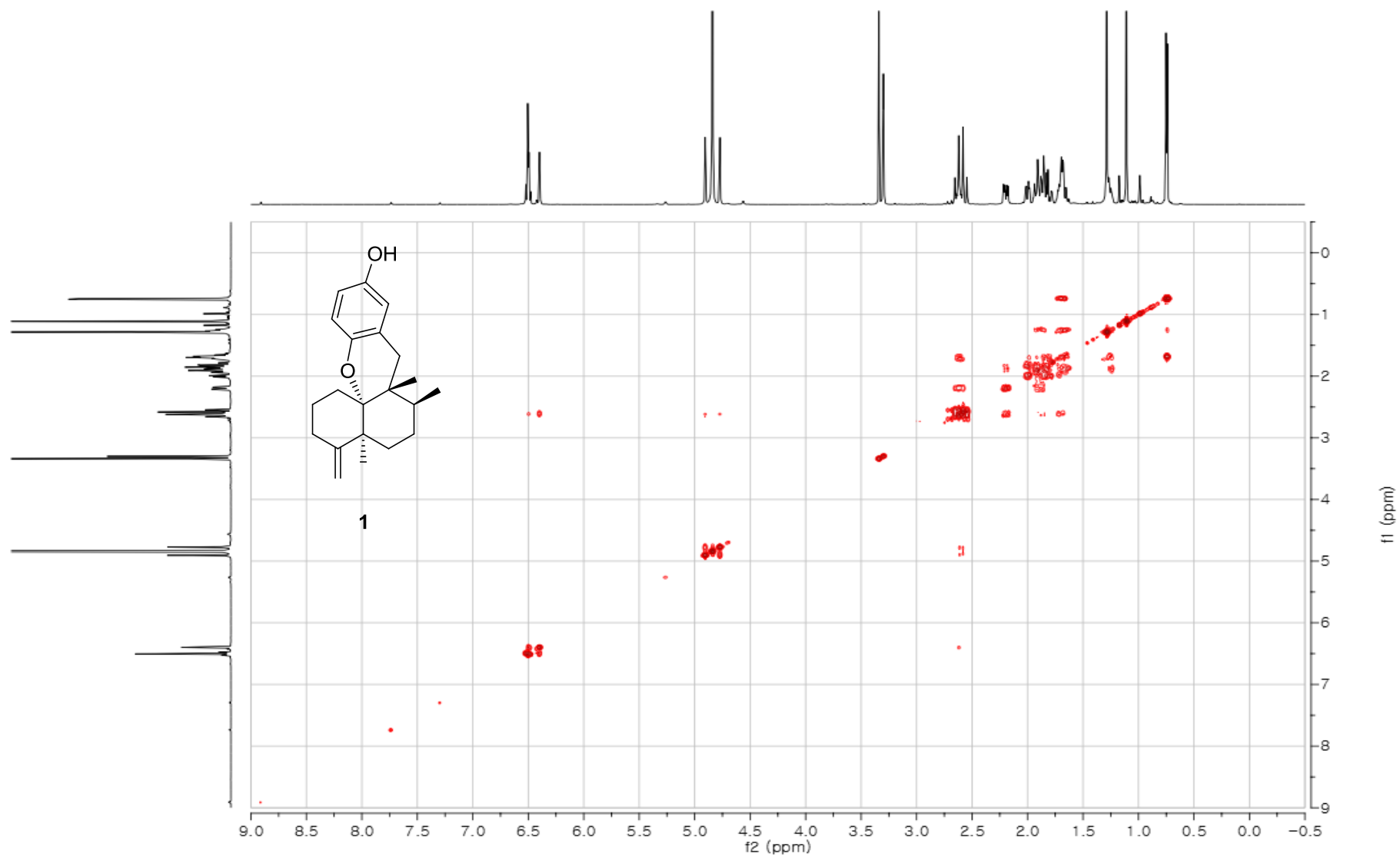


Figure S3. The COSY NMR (500 MHz, CD₃OD) spectrum of compound **1**

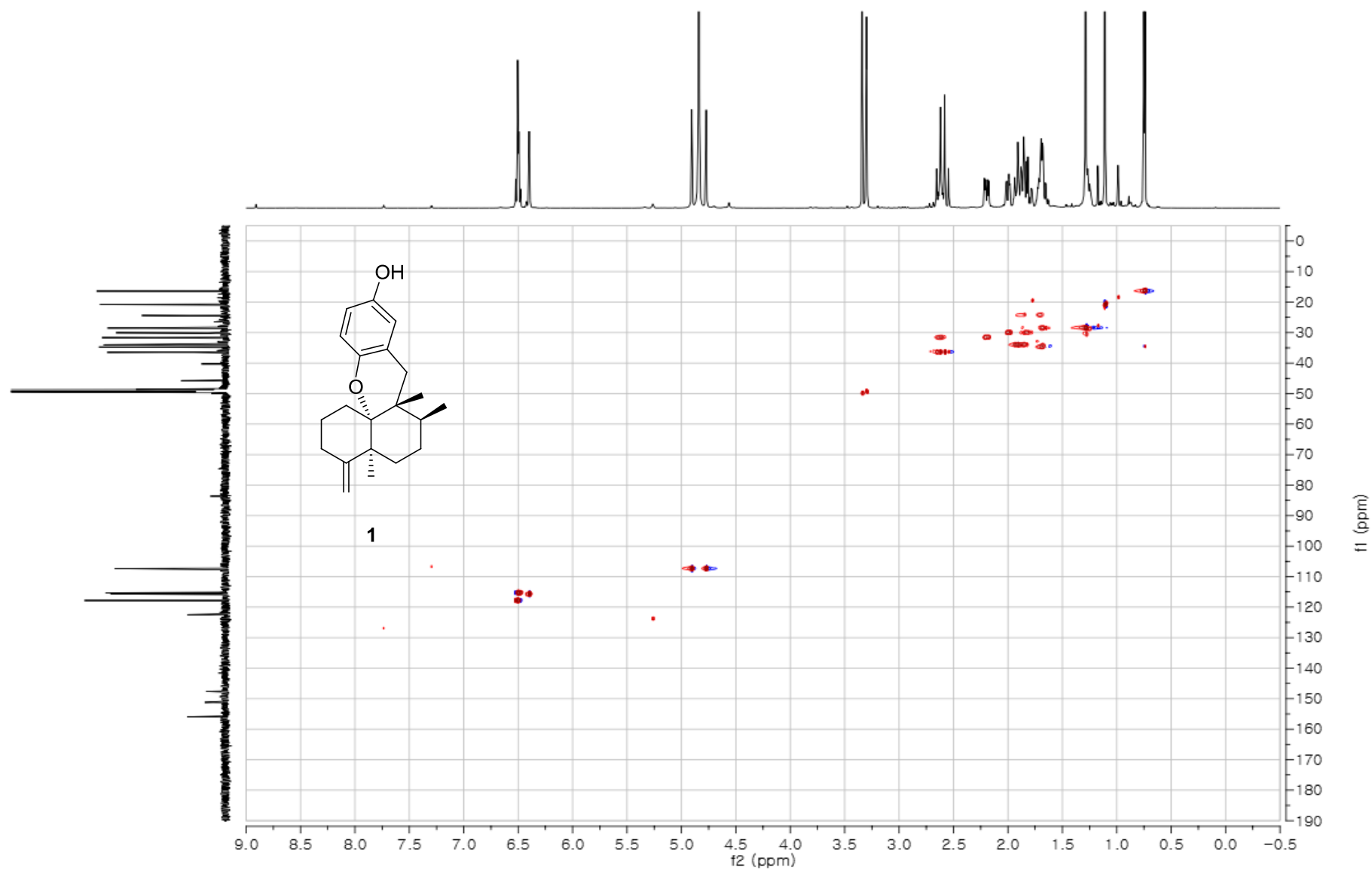


Figure S4. The HSQC NMR (500 MHz, CD₃OD) spectrum of compound **1**

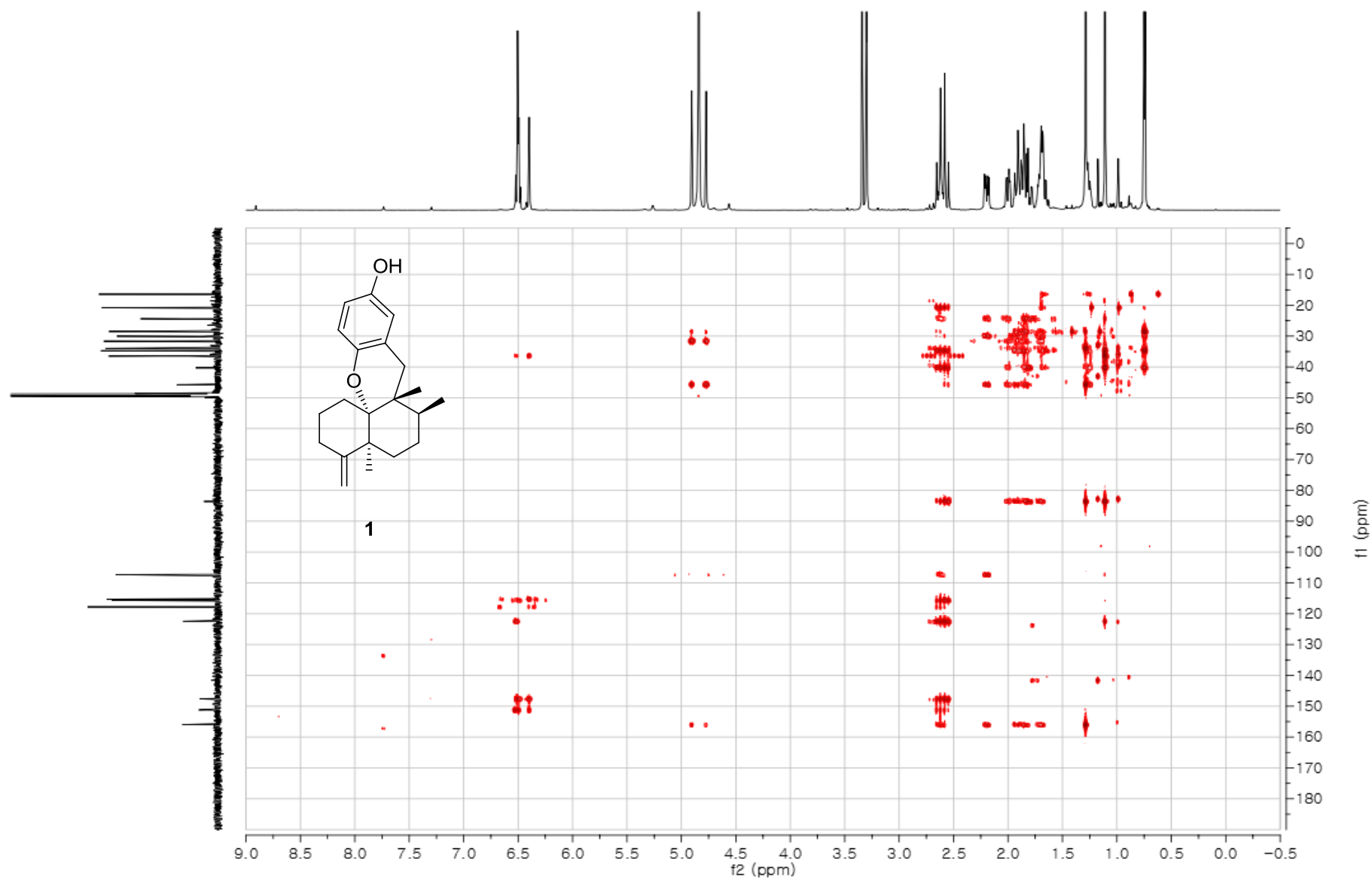


Figure S5. The HMBC NMR (500 MHz, CD_3OD) spectrum of compound **1**

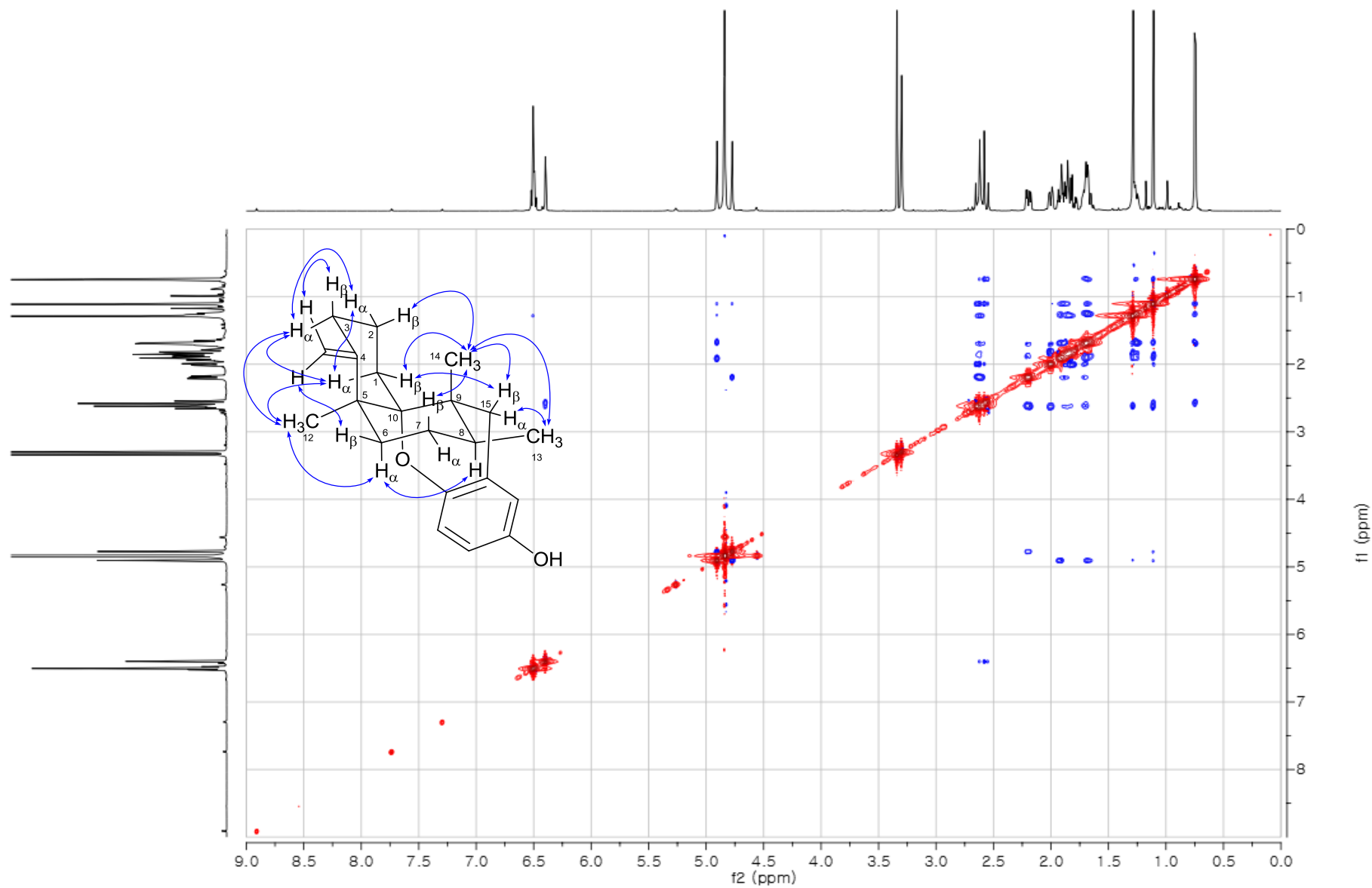


Figure S6. The NOESY NMR (500 MHz, CD₃OD) spectrum of compound **1**

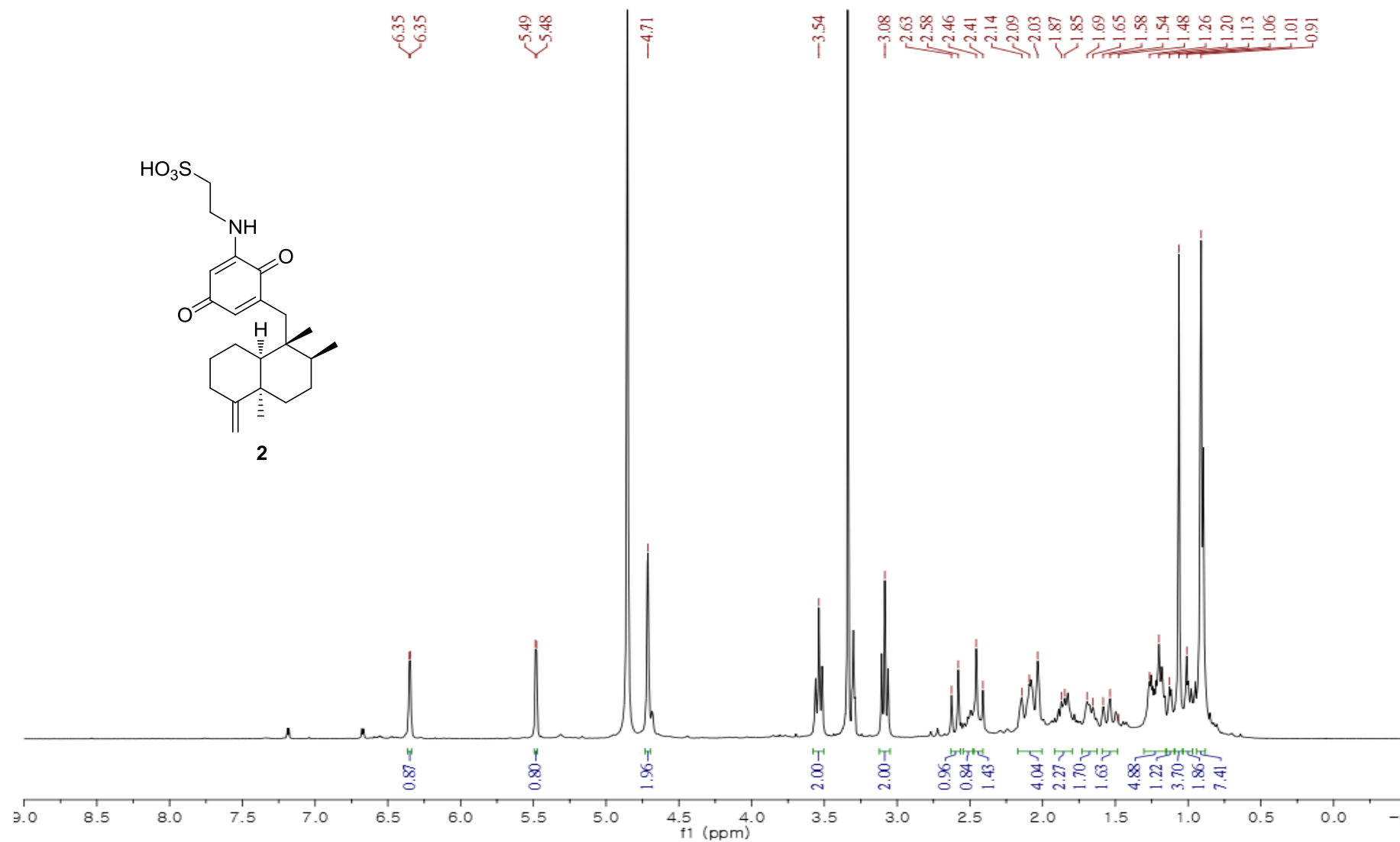


Figure S7. The ^1H NMR (500 MHz, CD_3OD) spectrum of compound **2**

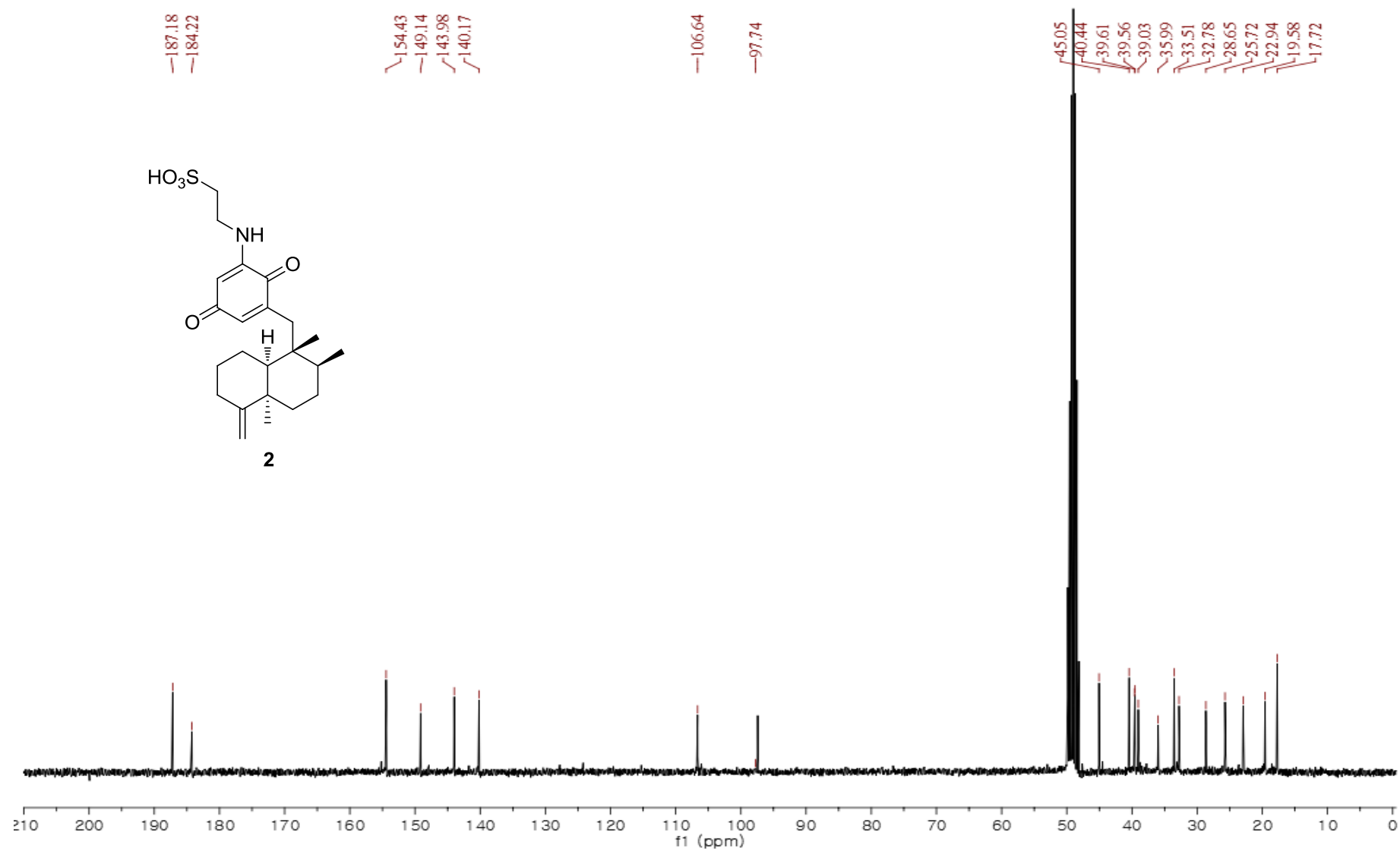


Figure S8. The ^{13}C NMR (125 MHz, CD_3OD) spectrum of compound 2

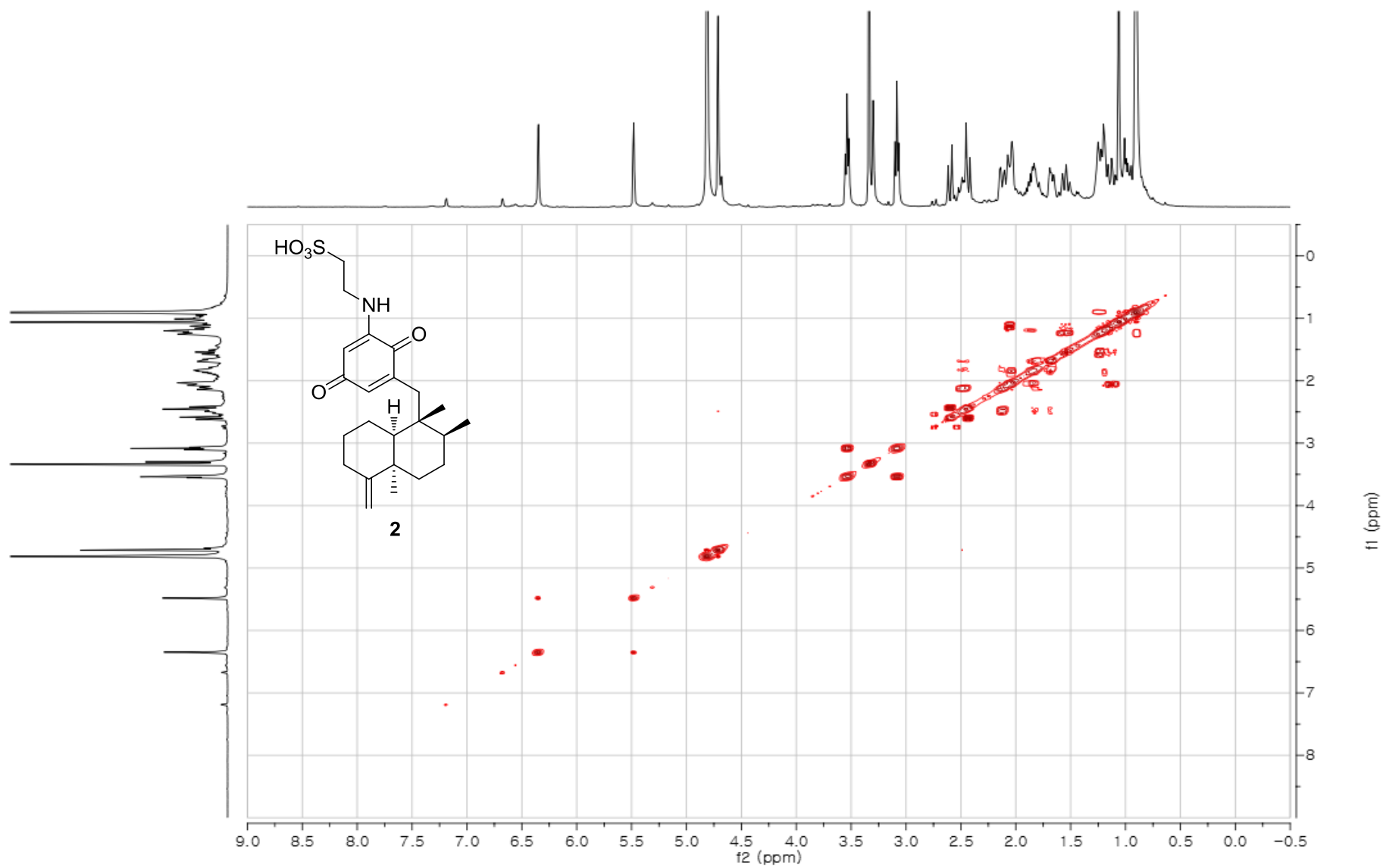


Figure S9. The COSY NMR (500 MHz, CD₃OD) spectrum of compound **2**

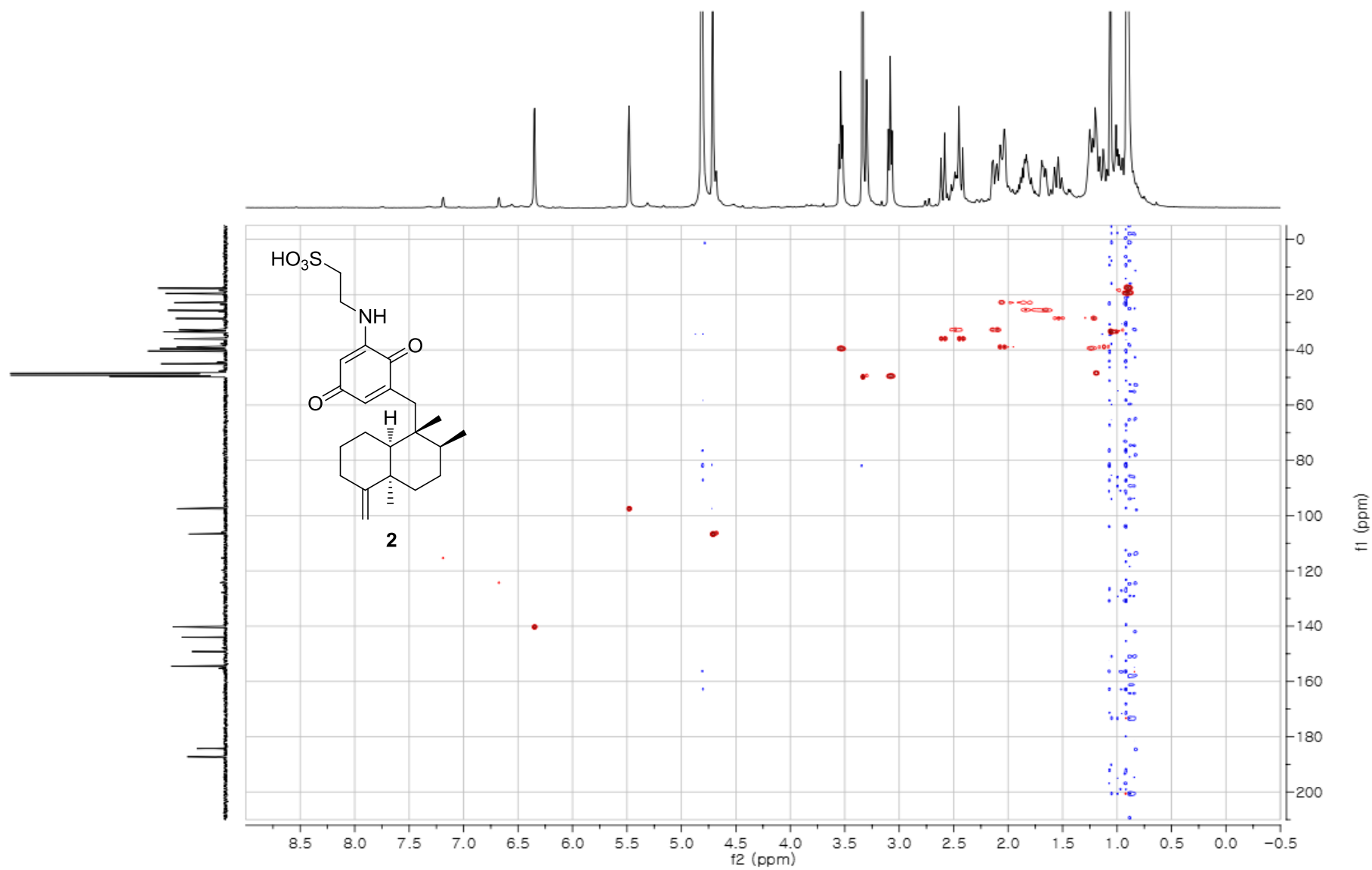


Figure S10. The HSQC NMR (500 MHz, CD_3OD) spectrum of compound **2**

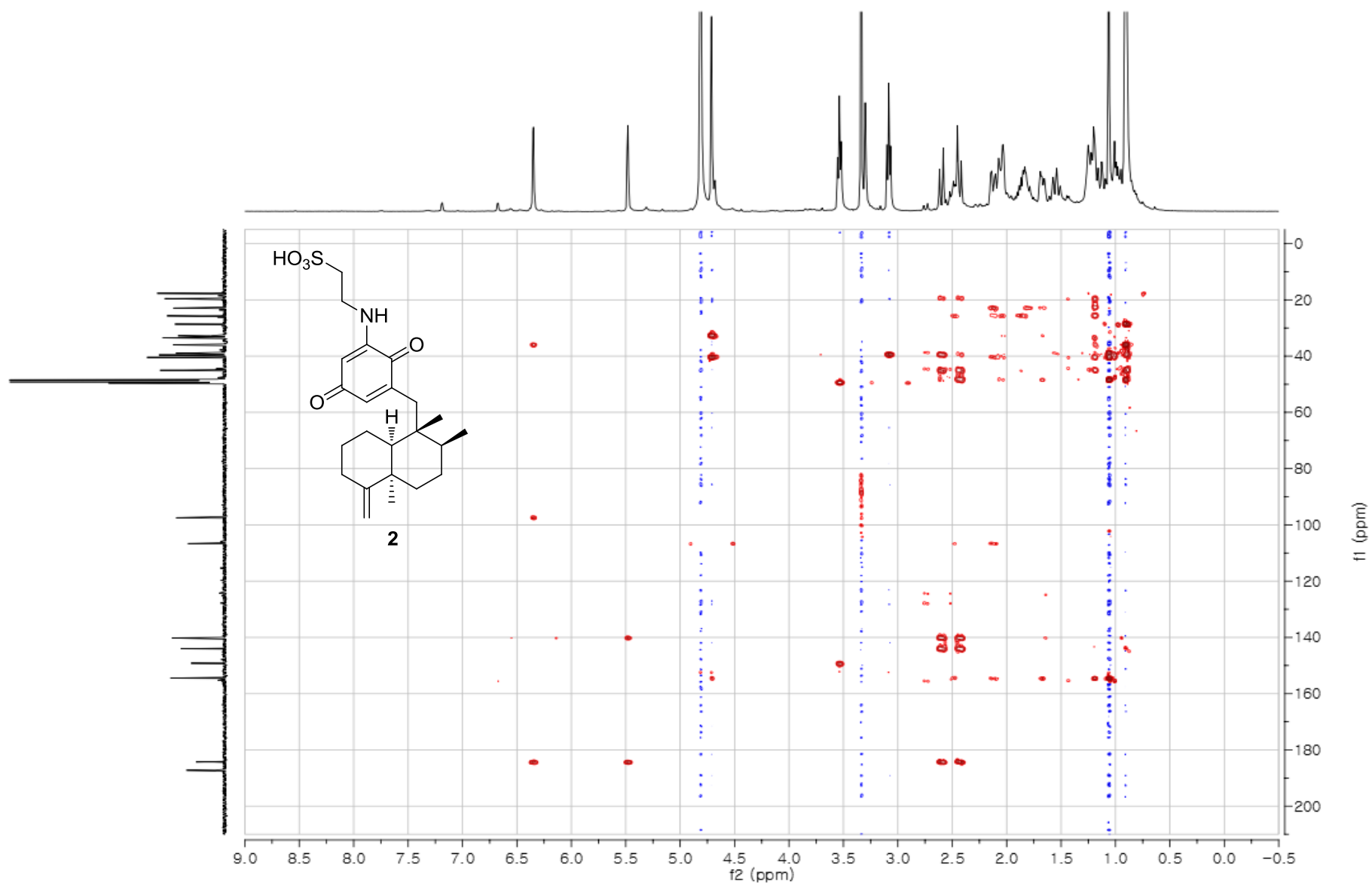


Figure S11. The HMBC NMR (500 MHz, CD₃OD) spectrum of compound **2**

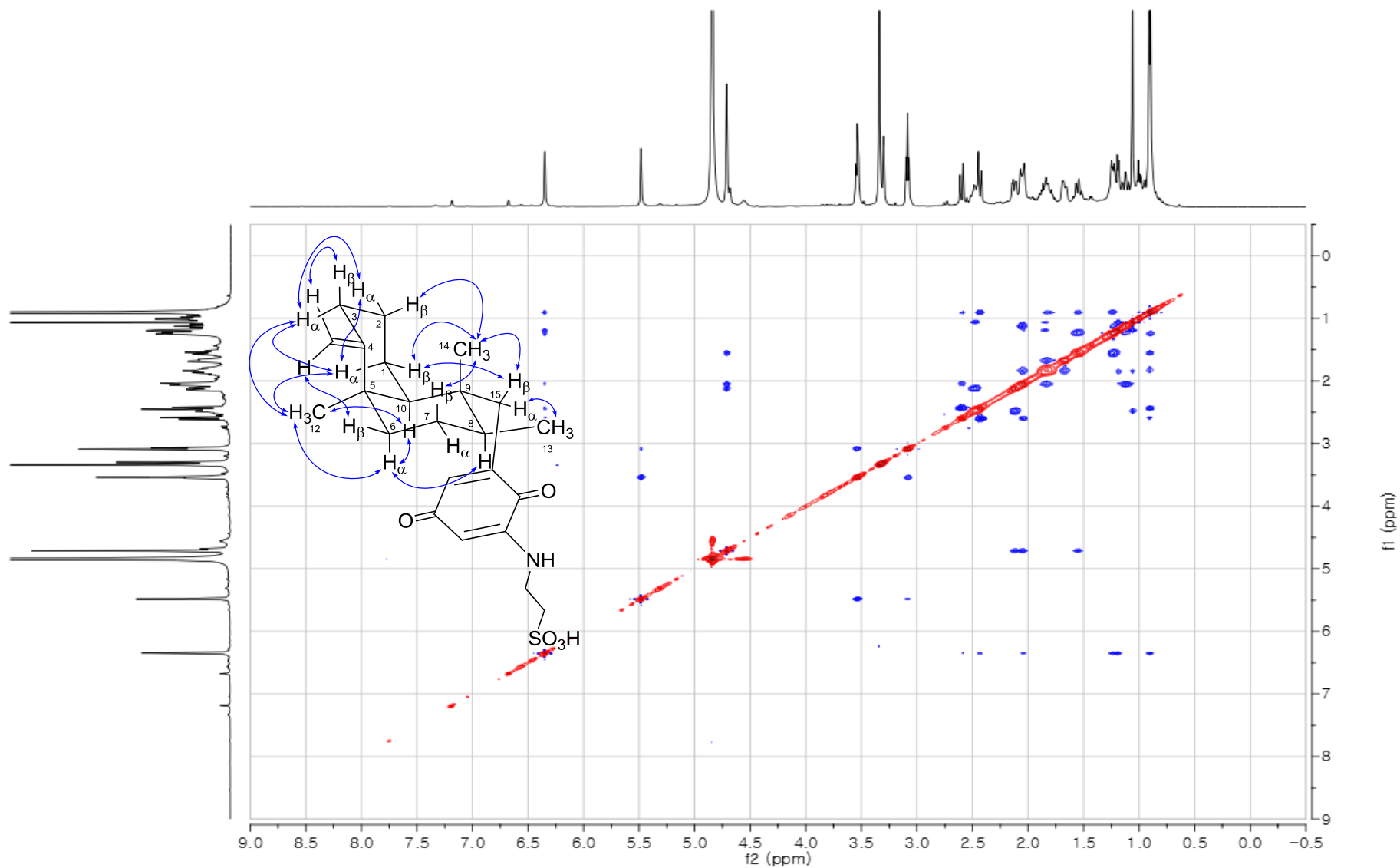


Figure S12. The NOESY NMR (500 MHz, CD₃OD) spectrum of compound **2**

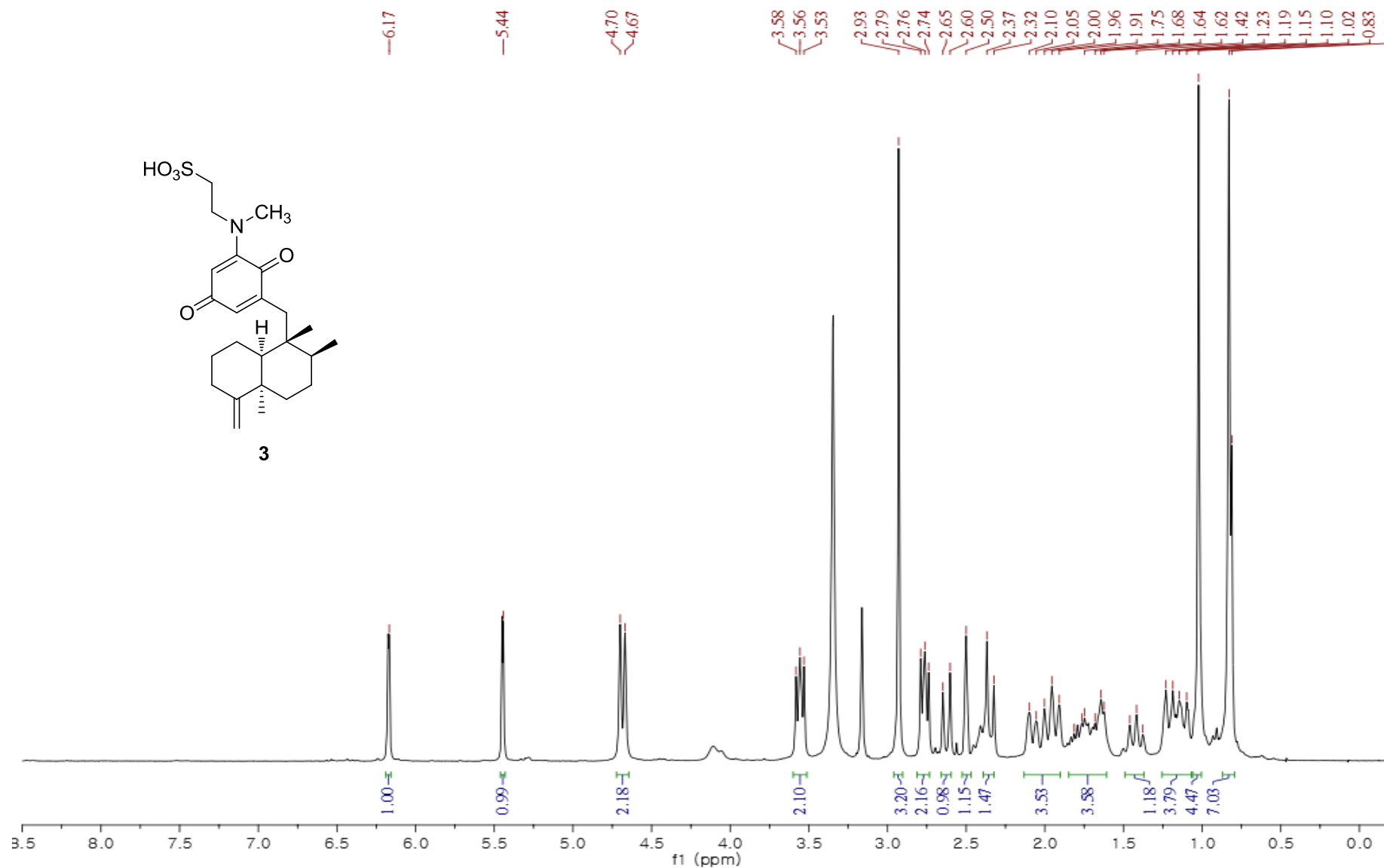


Figure S13. The ^1H NMR (400 MHz, $\text{DMSO}-d_6$) spectrum of compound **3**

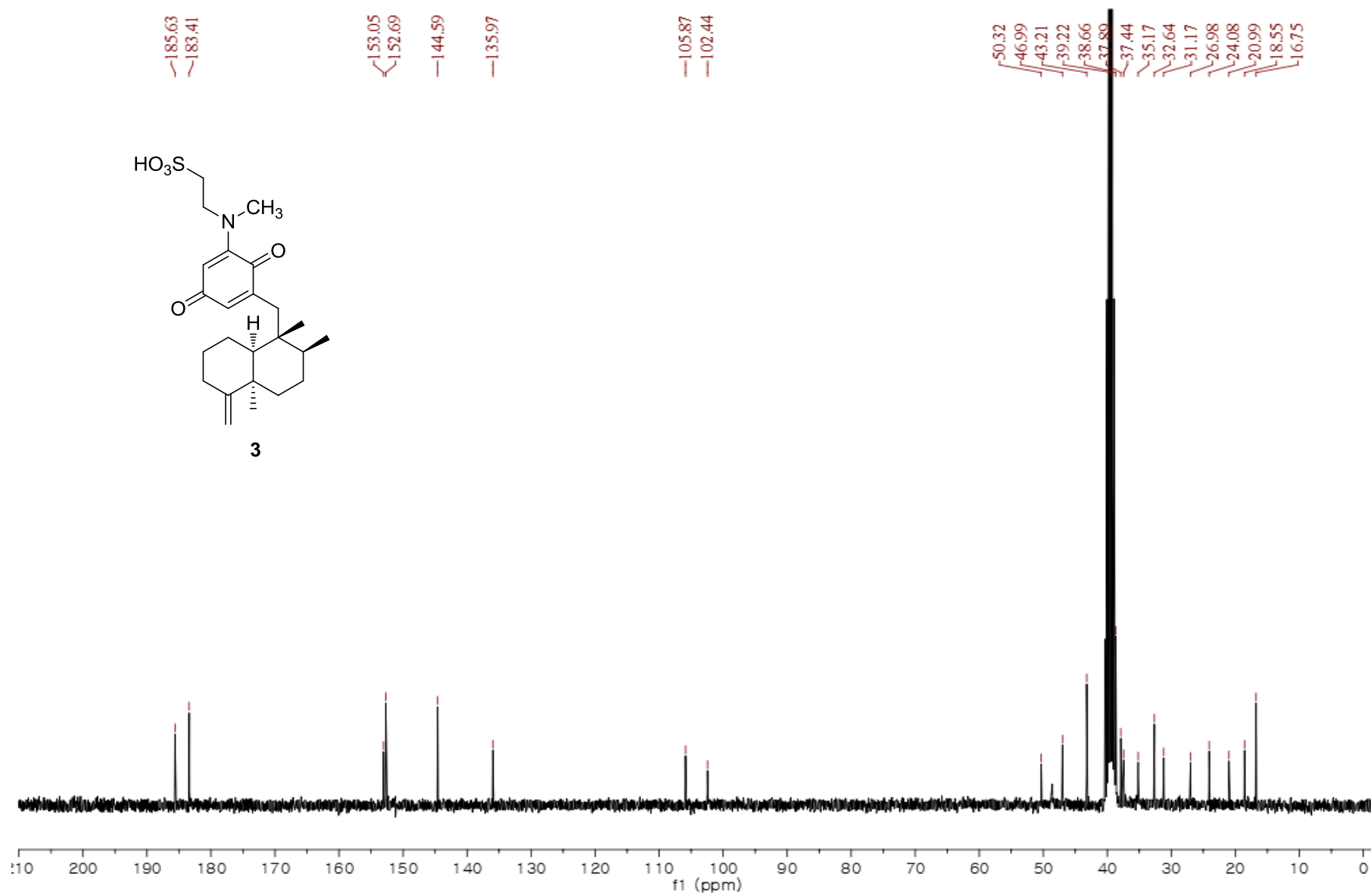


Figure S14. The ^{13}C NMR (100 MHz, $\text{DMSO}-d_6$) spectrum of compound **3**

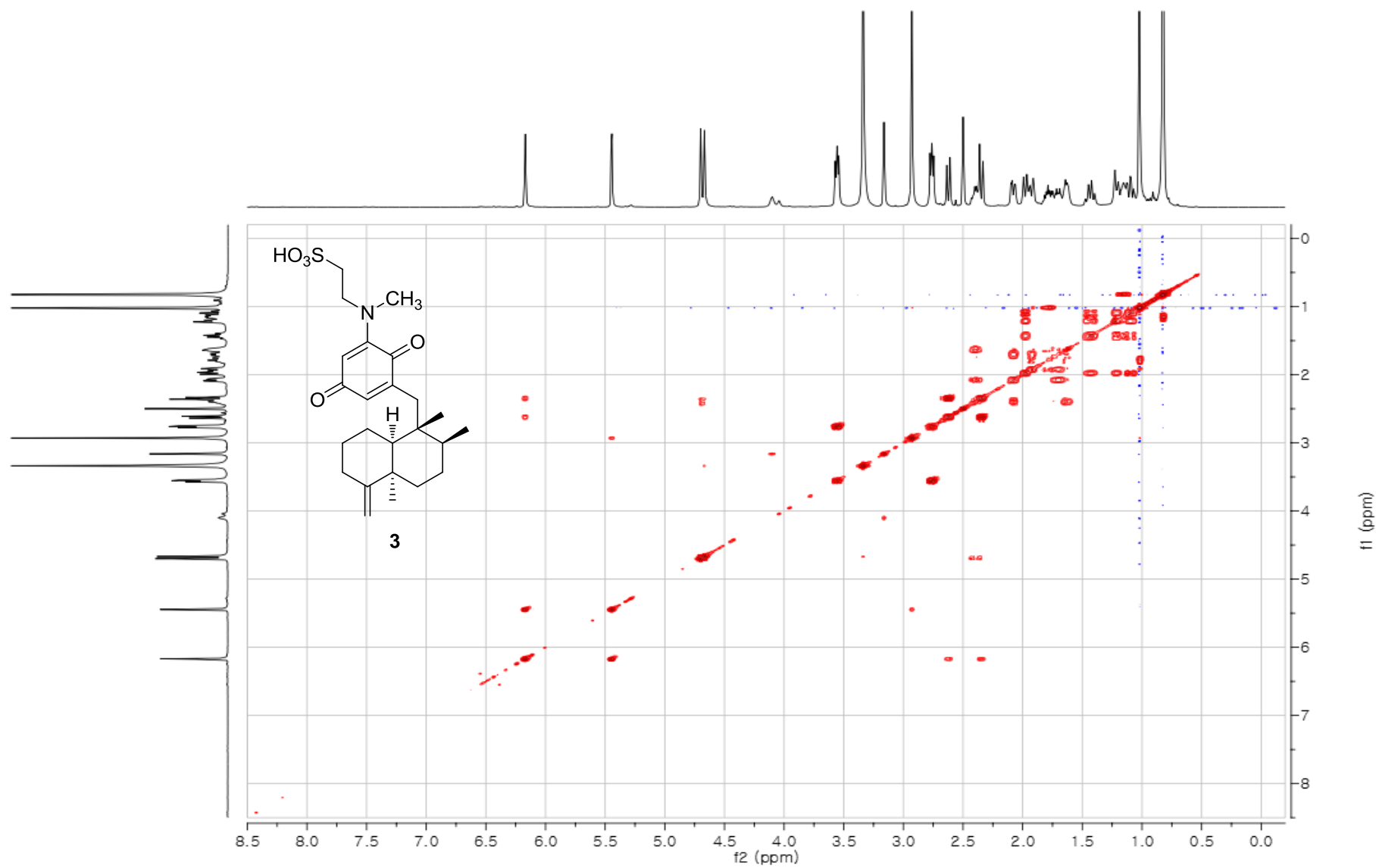


Figure S15. The COSY NMR (400 MHz, $\text{DMSO}-d_6$) spectrum of compound **3**

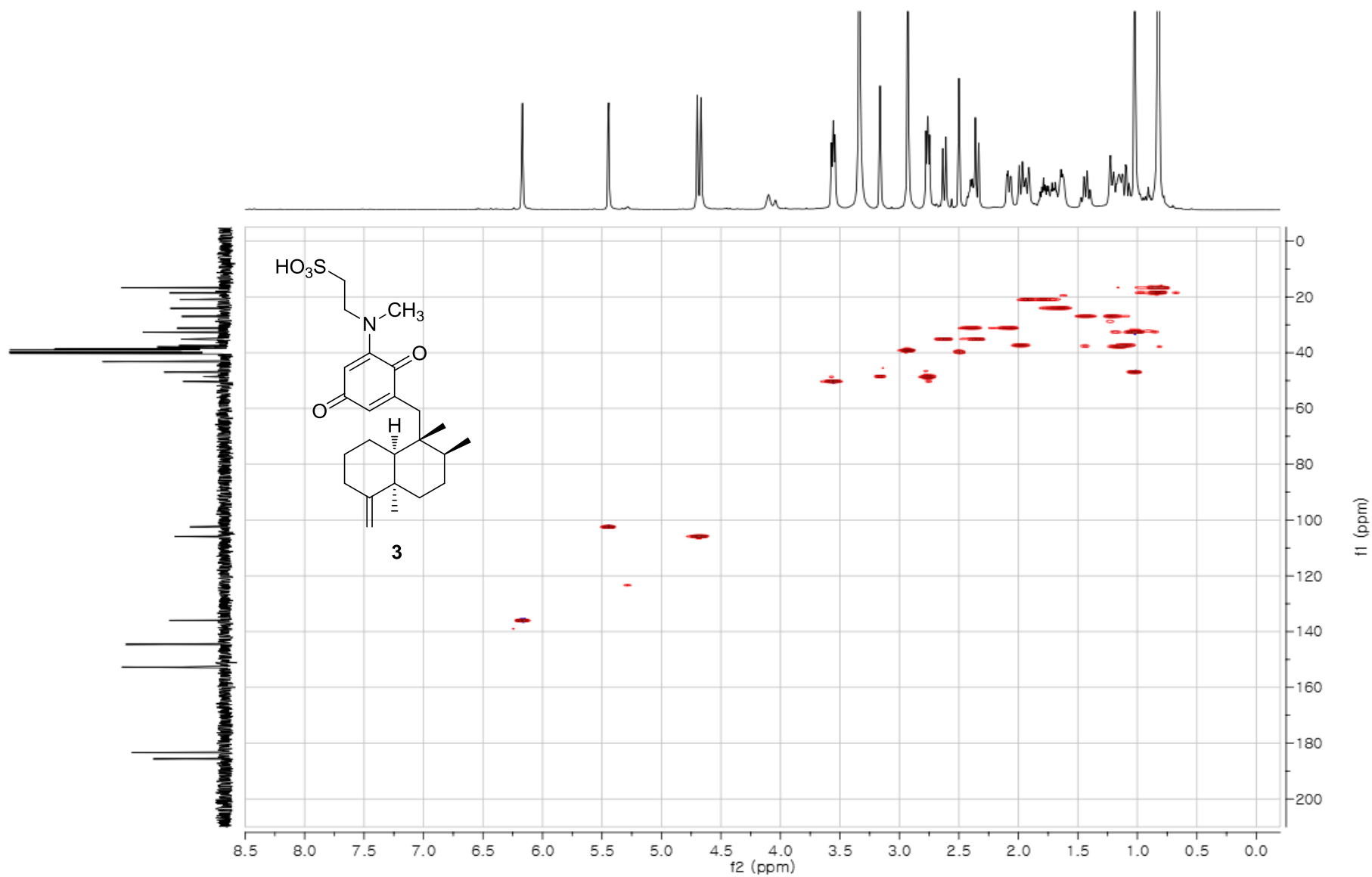


Figure S16. The HSQC NMR (400 MHz, $\text{DMSO-}d_6$) spectrum of compound **3**

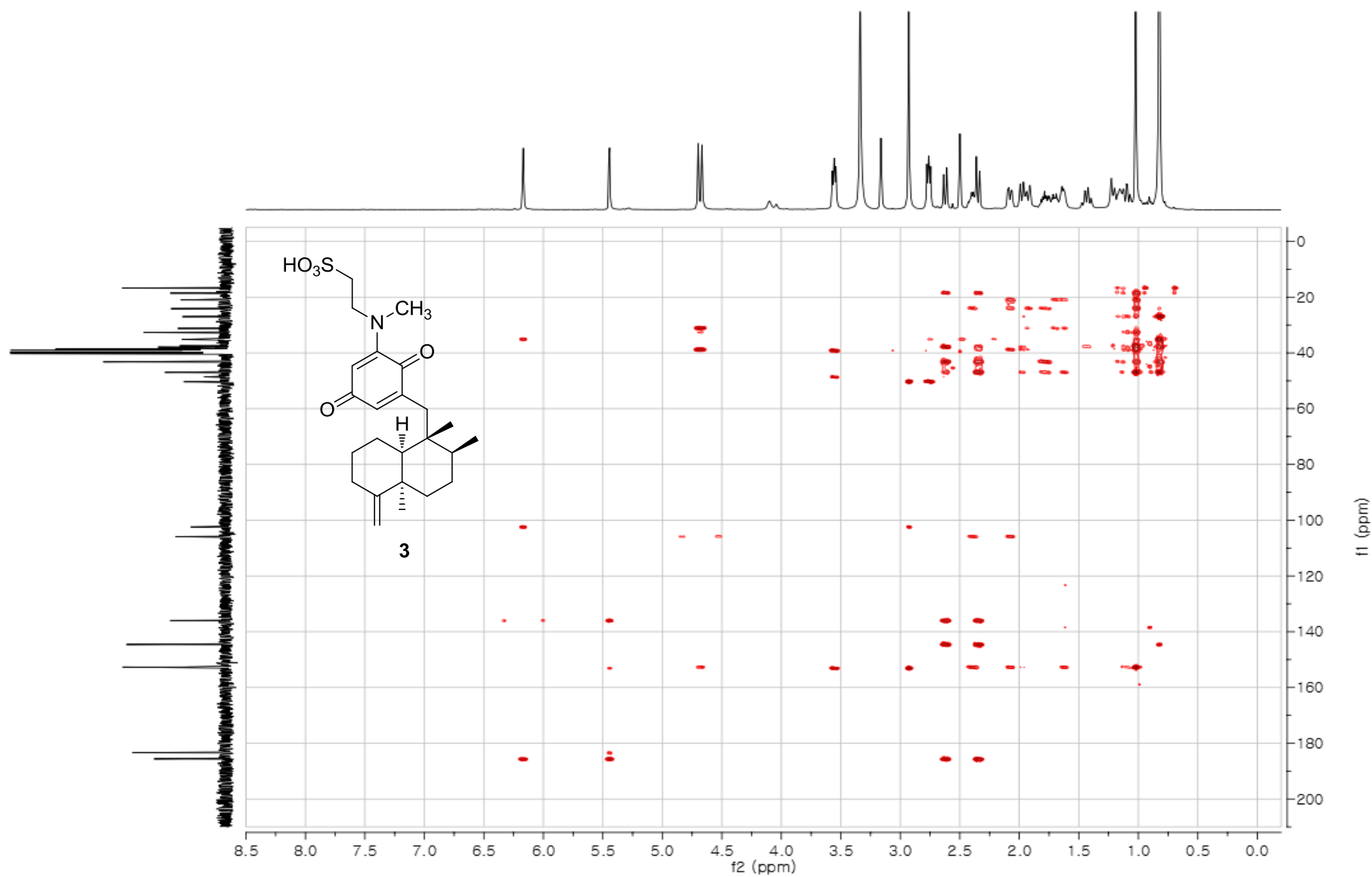


Figure S17. The HMBC NMR (400 MHz, $\text{DMSO-}d_6$) spectrum of compound **3**

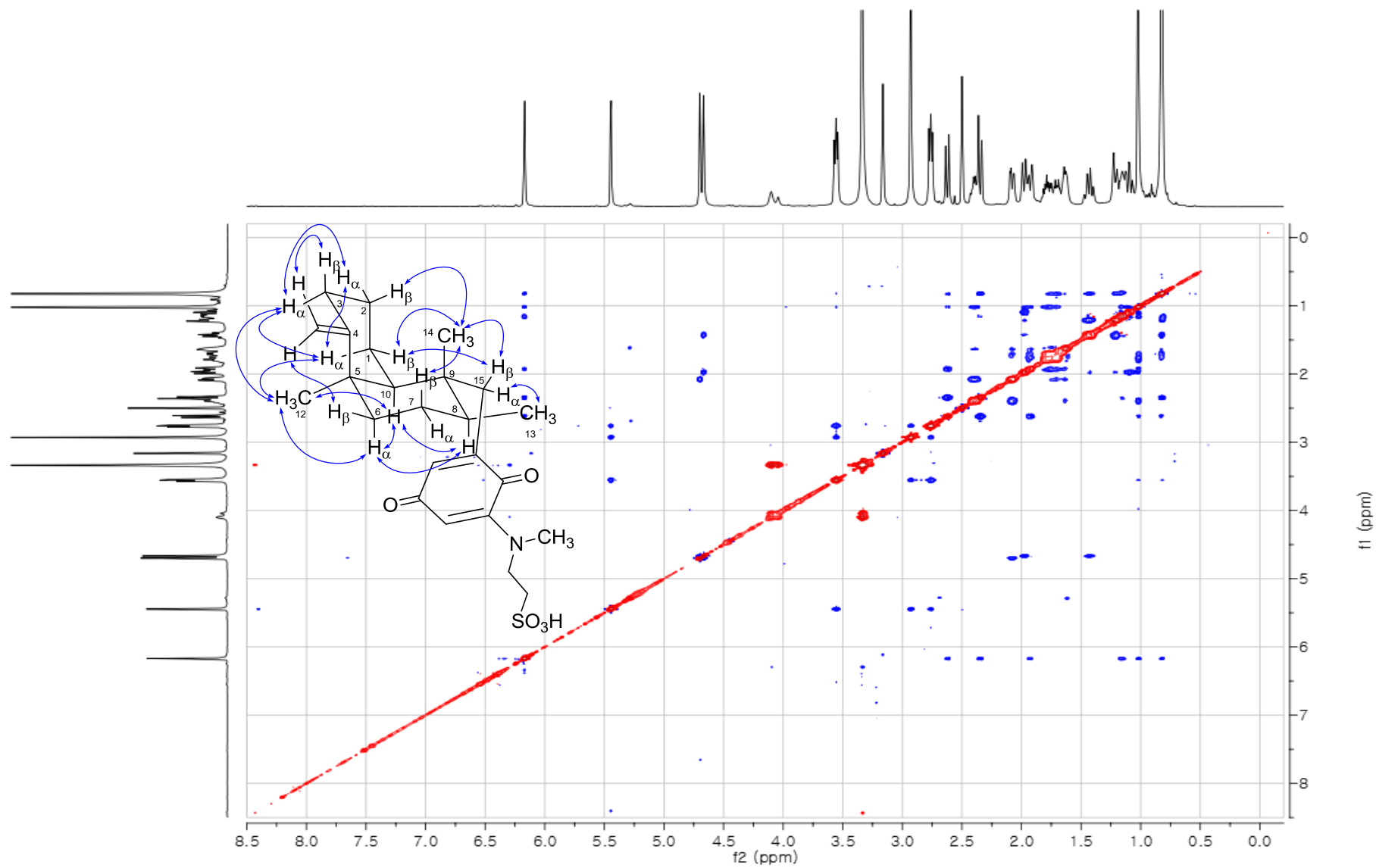


Figure S18. The NOESY NMR (400 MHz, DMSO-*d*₆) spectrum of compound **3**

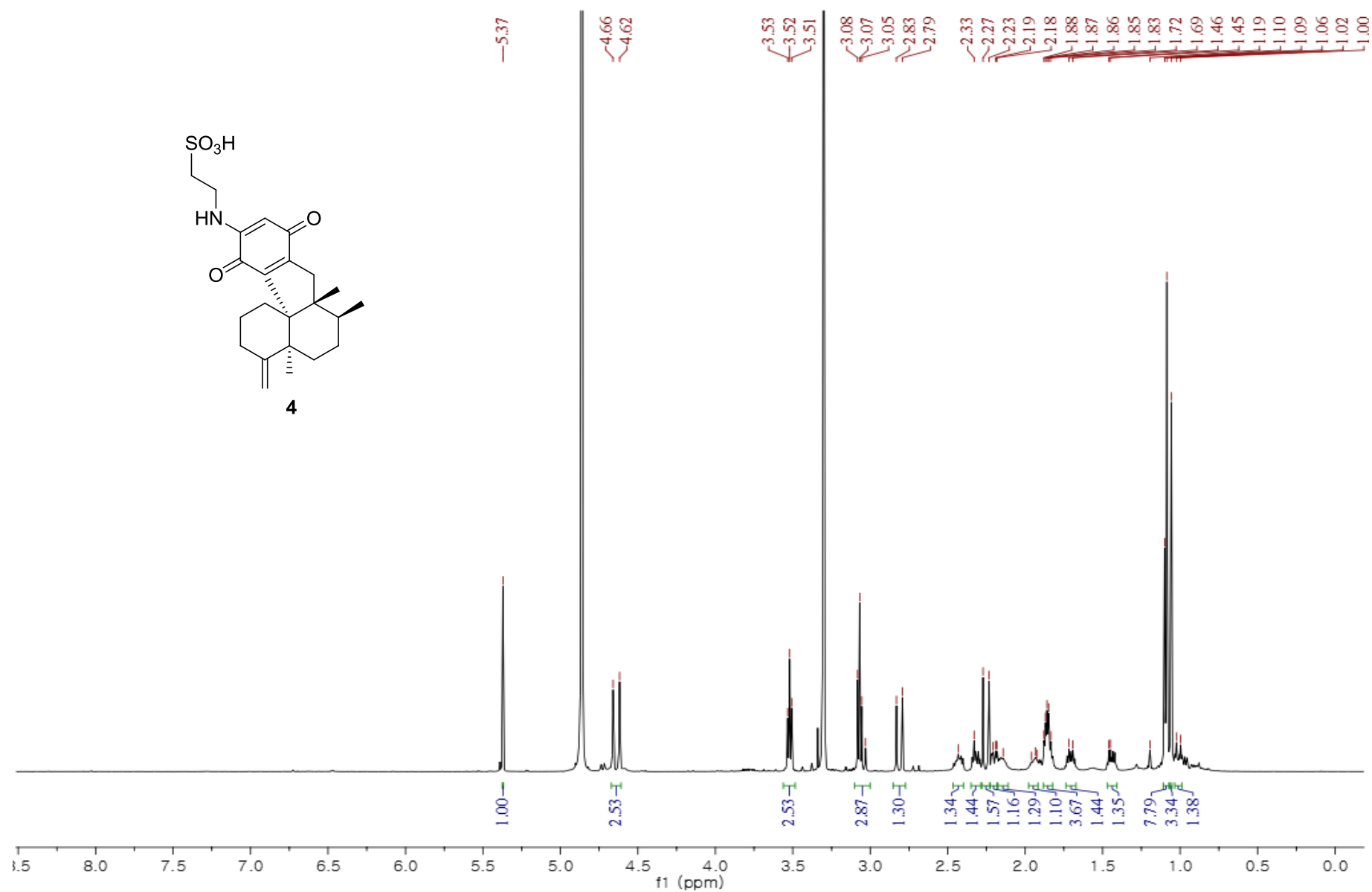


Figure S19. The ¹H NMR (500 MHz, CD₃OD) spectrum of compound **4**

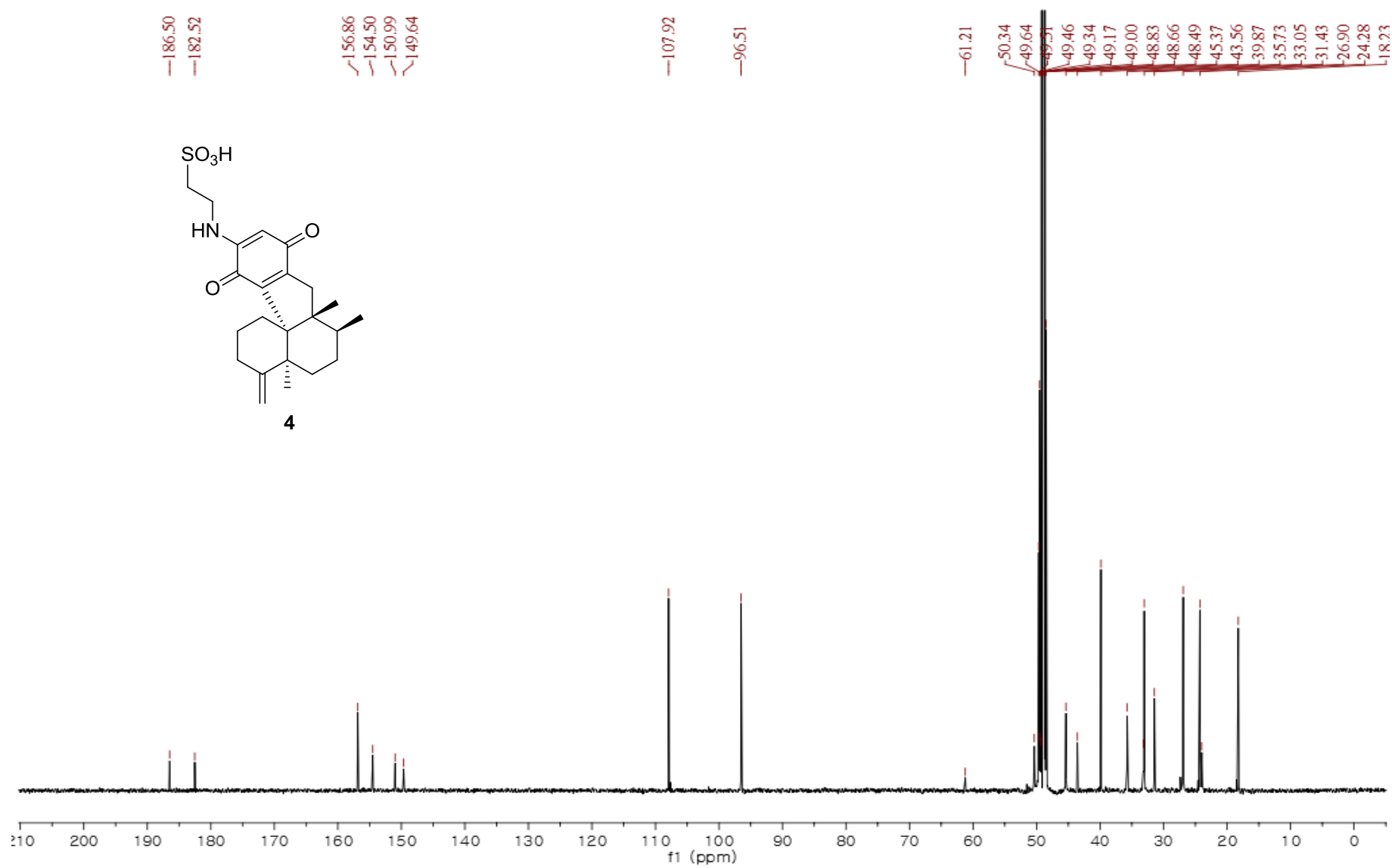


Figure S20. The ^{13}C NMR (125 MHz, CD_3OD) spectrum of compound **4**

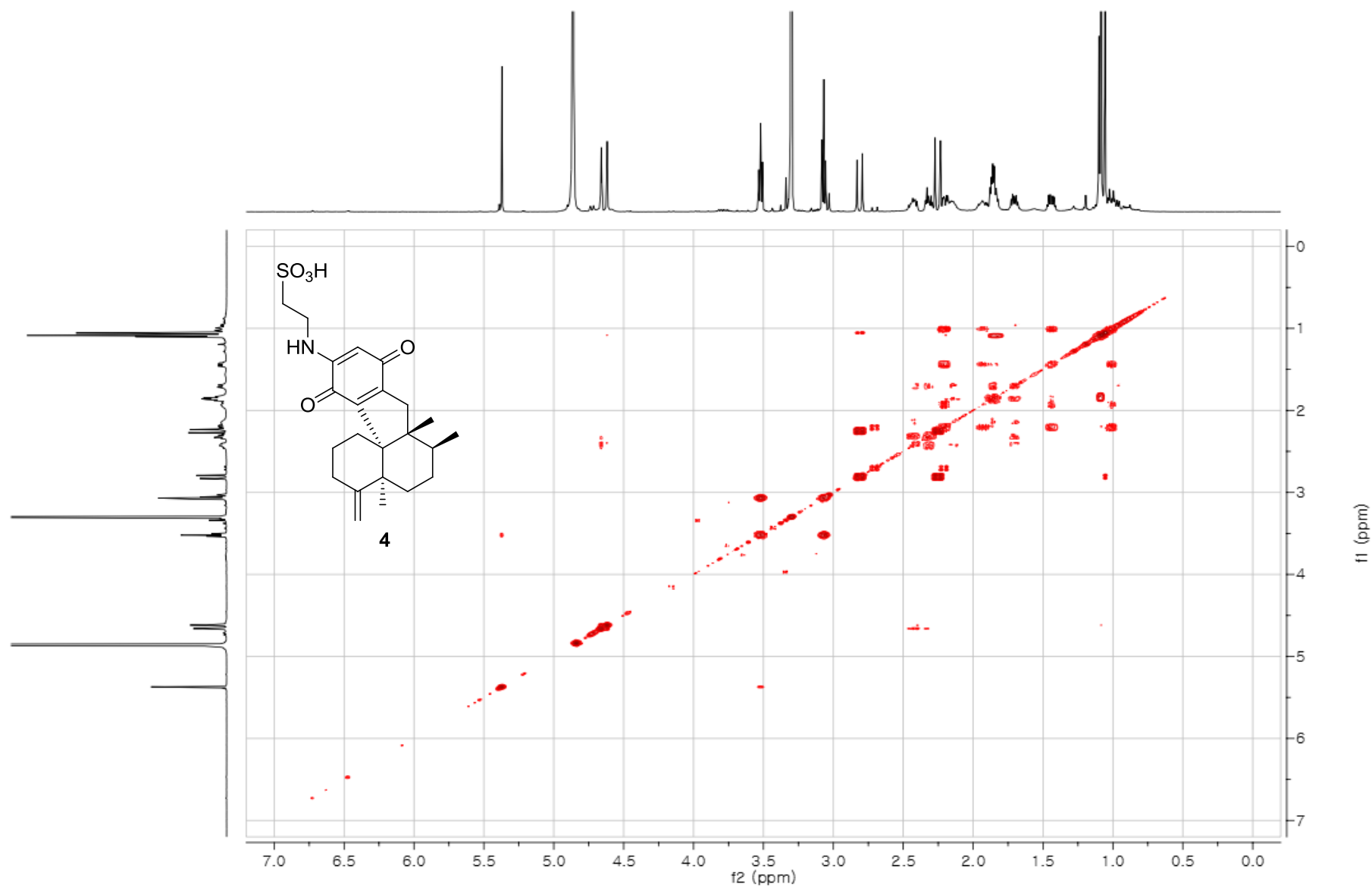


Figure S21. The COSY NMR (500 MHz, CD_3OD) spectrum of compound **4**

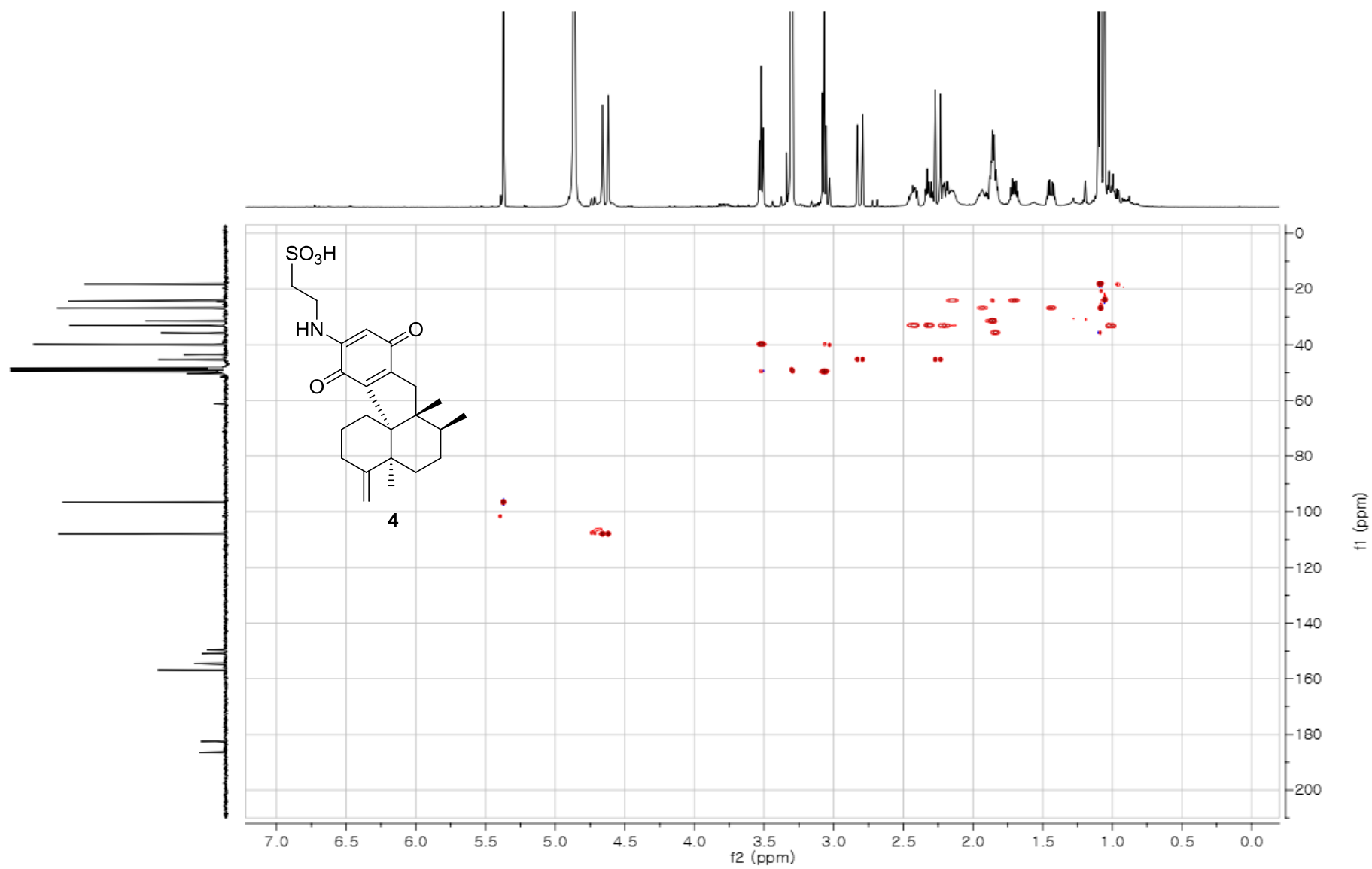


Figure S22. The HSQC NMR (500 MHz, CD_3OD) spectrum of compound **4**

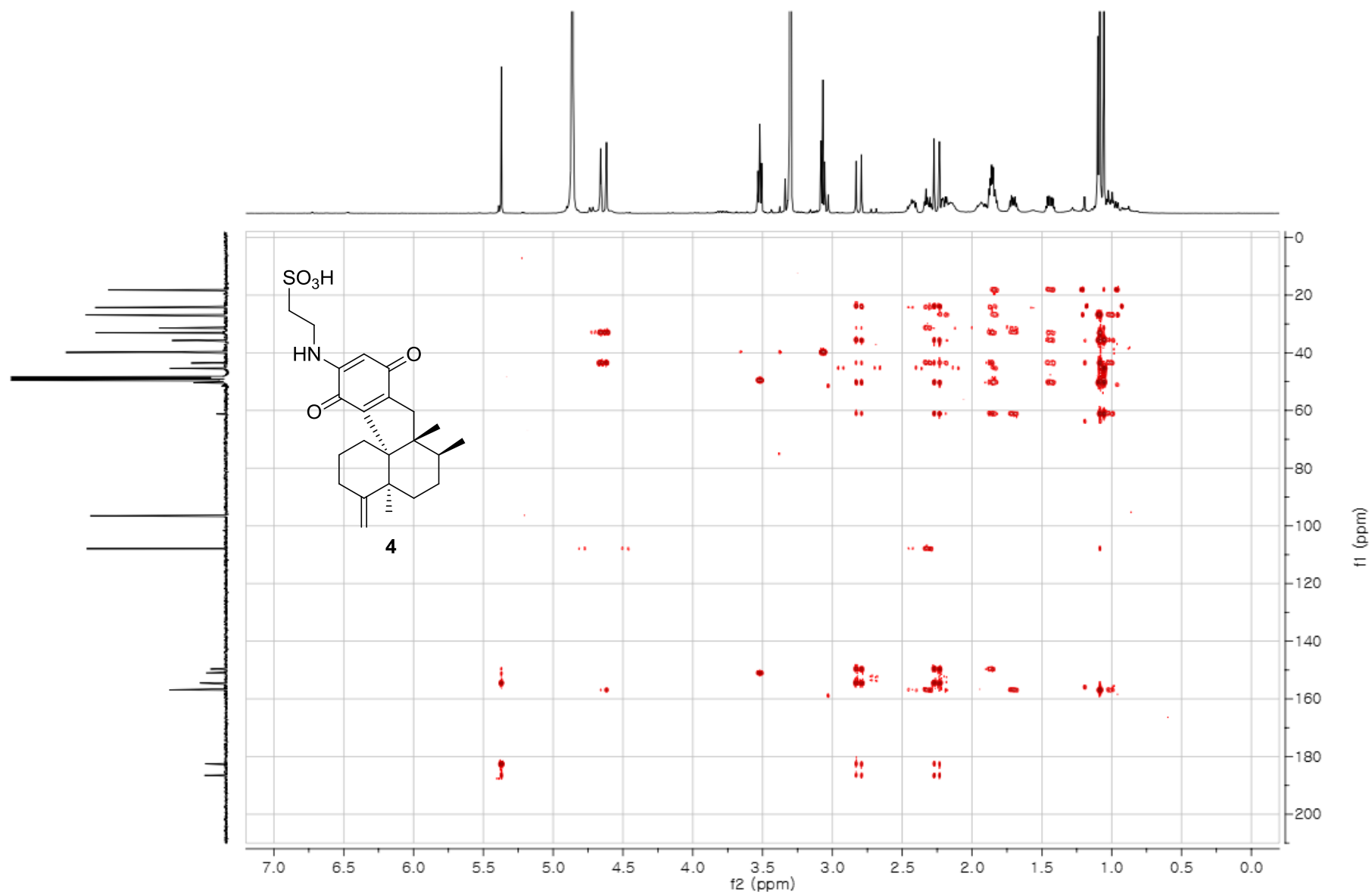


Figure S23. The HMBC NMR (500 MHz, CD_3OD) spectrum of compound **4**

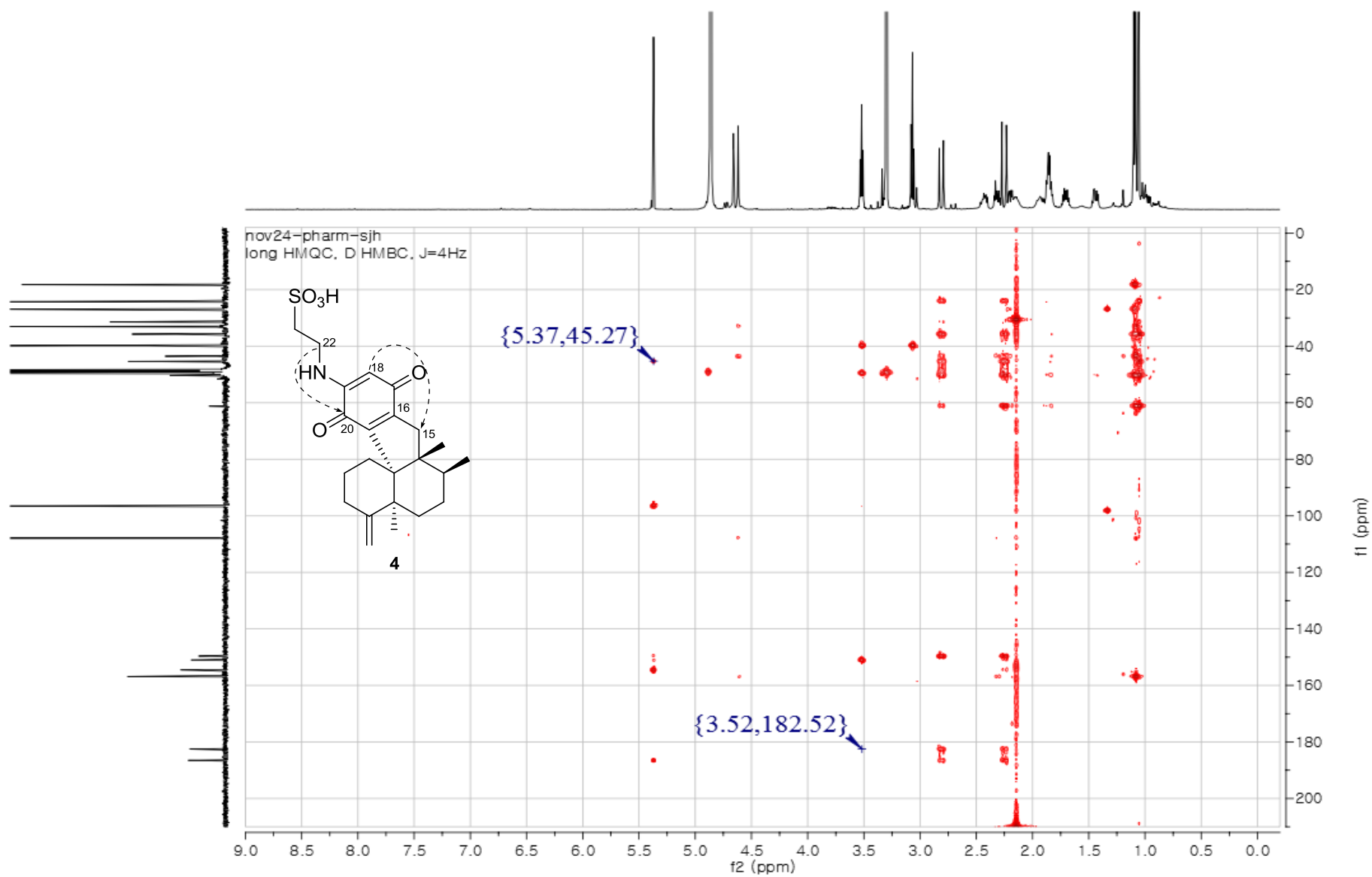


Figure S24. The D-HMBC NMR (500 MHz, CD₃OD, $J = 4$ Hz) spectrum of compound **4**

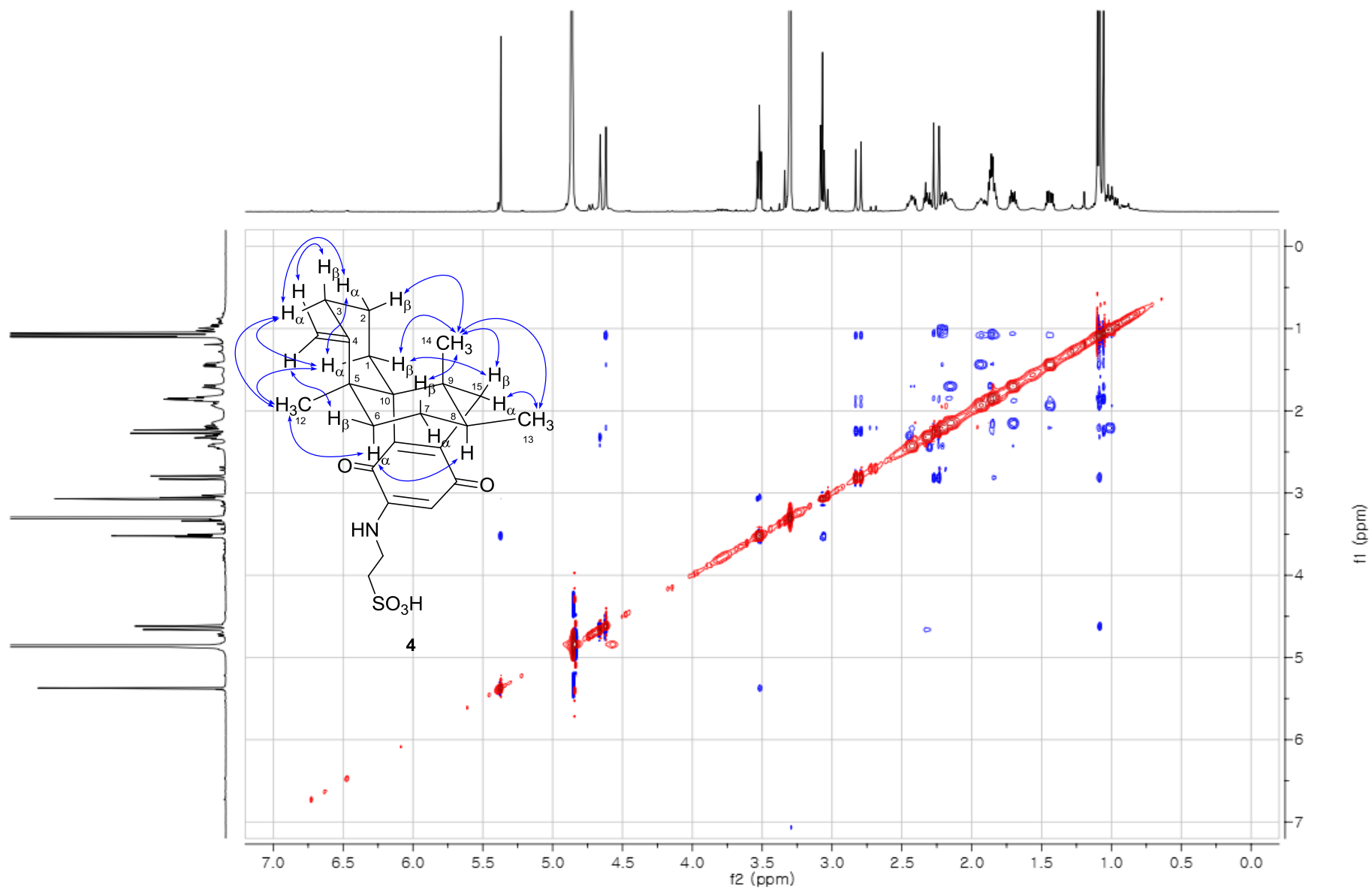


Figure S25. The NOESY NMR (500 MHz, CD₃OD) spectrum of compound **4**

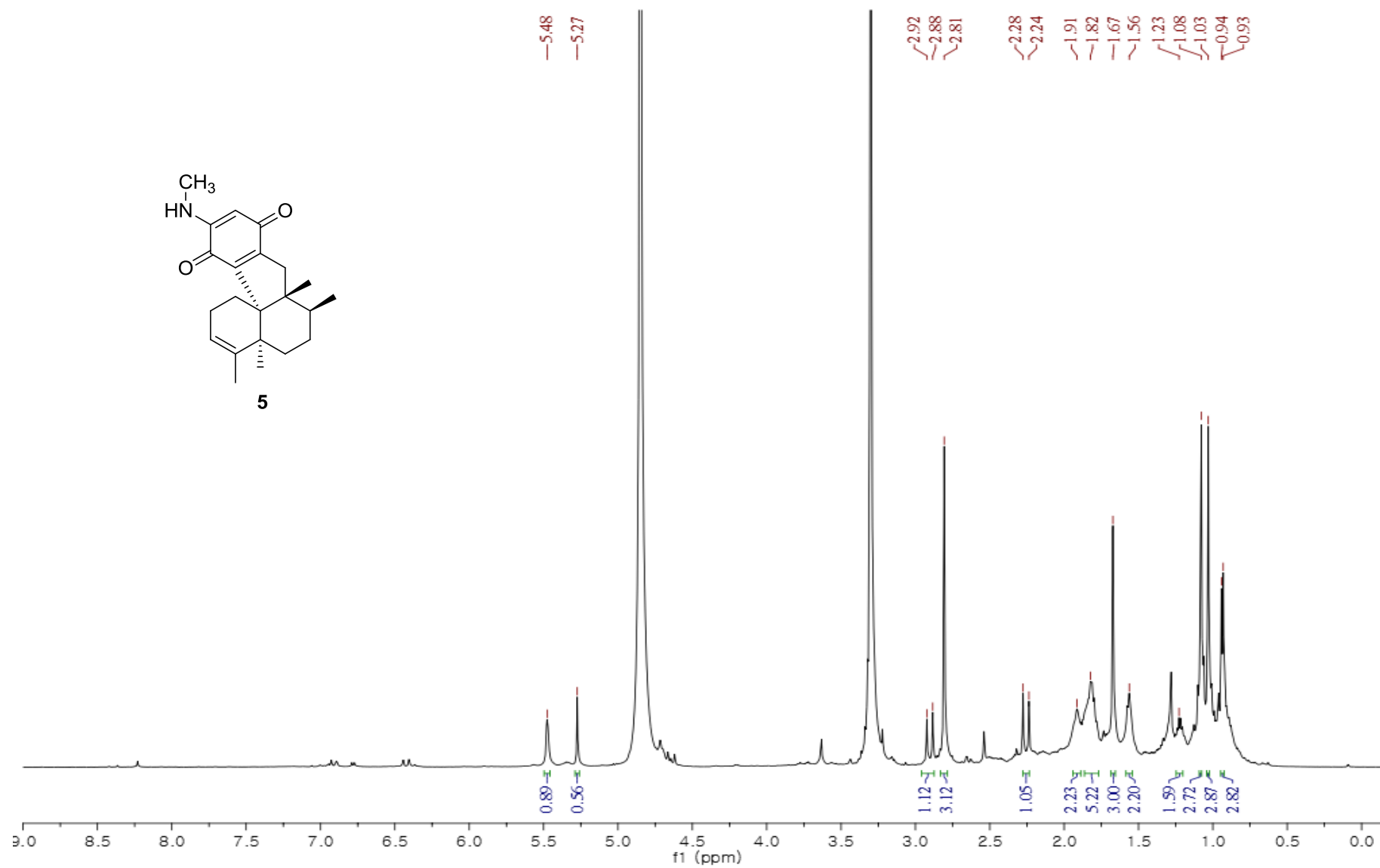


Figure S26. The ^1H NMR (600 MHz, CD_3OD) spectrum of compound **5**

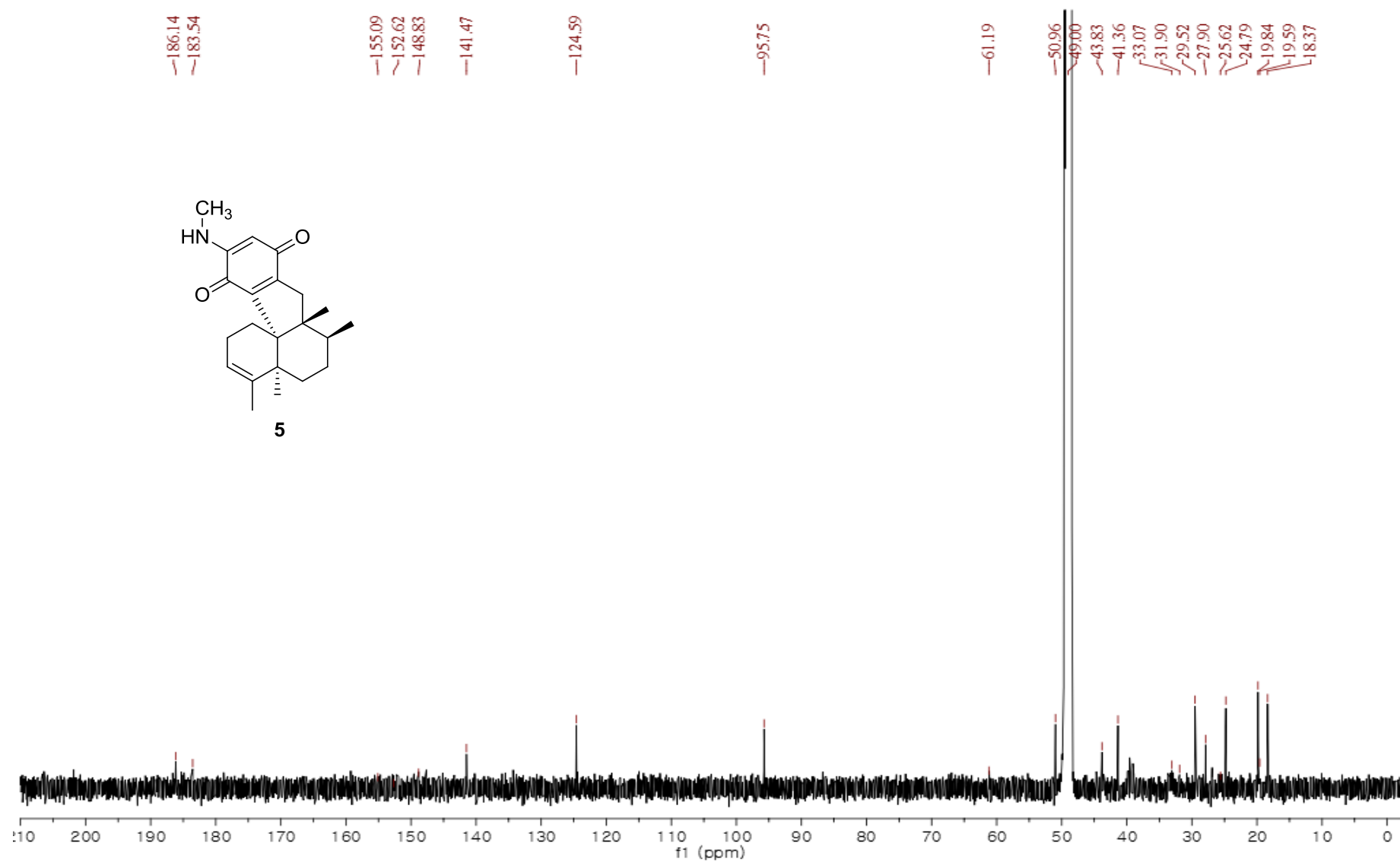


Figure S27. The ^{13}C NMR (150 MHz, CD_3OD) spectrum of compound **5**

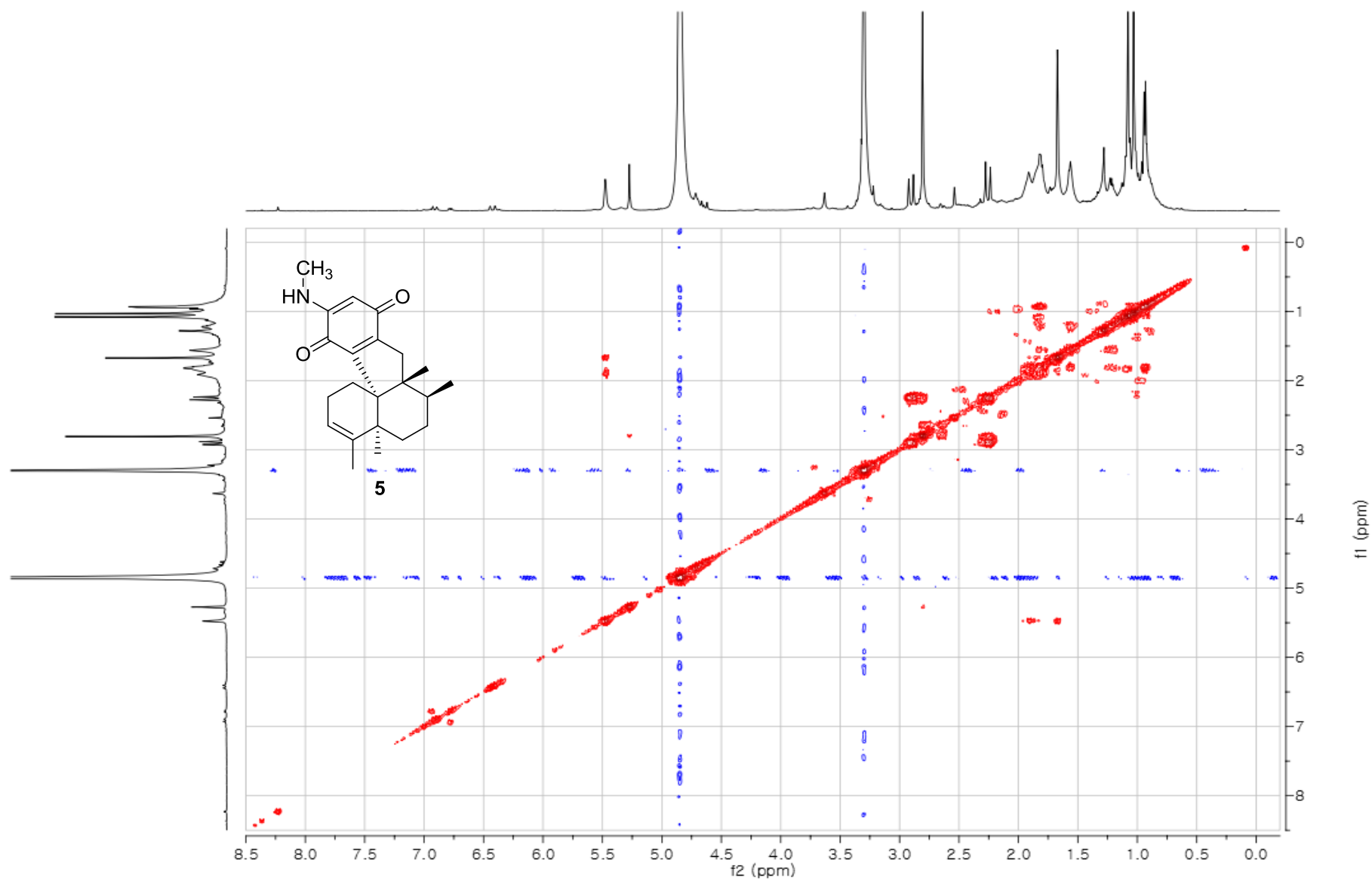


Figure S28. The COSY NMR (600 MHz, CD_3OD) spectrum of compound **5**

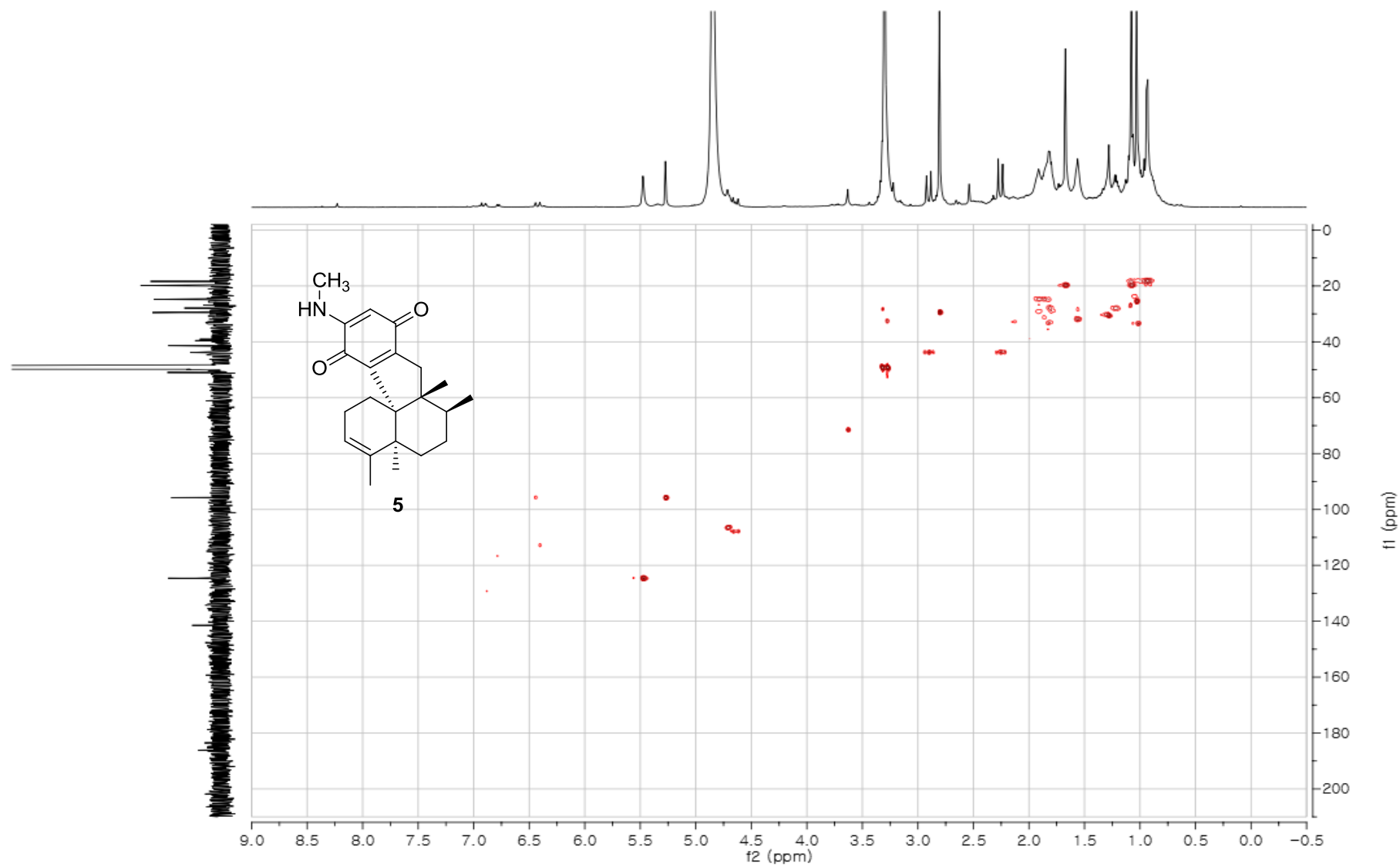


Figure S29. The HSQC NMR (600 MHz, CD_3OD) spectrum of compound **5**

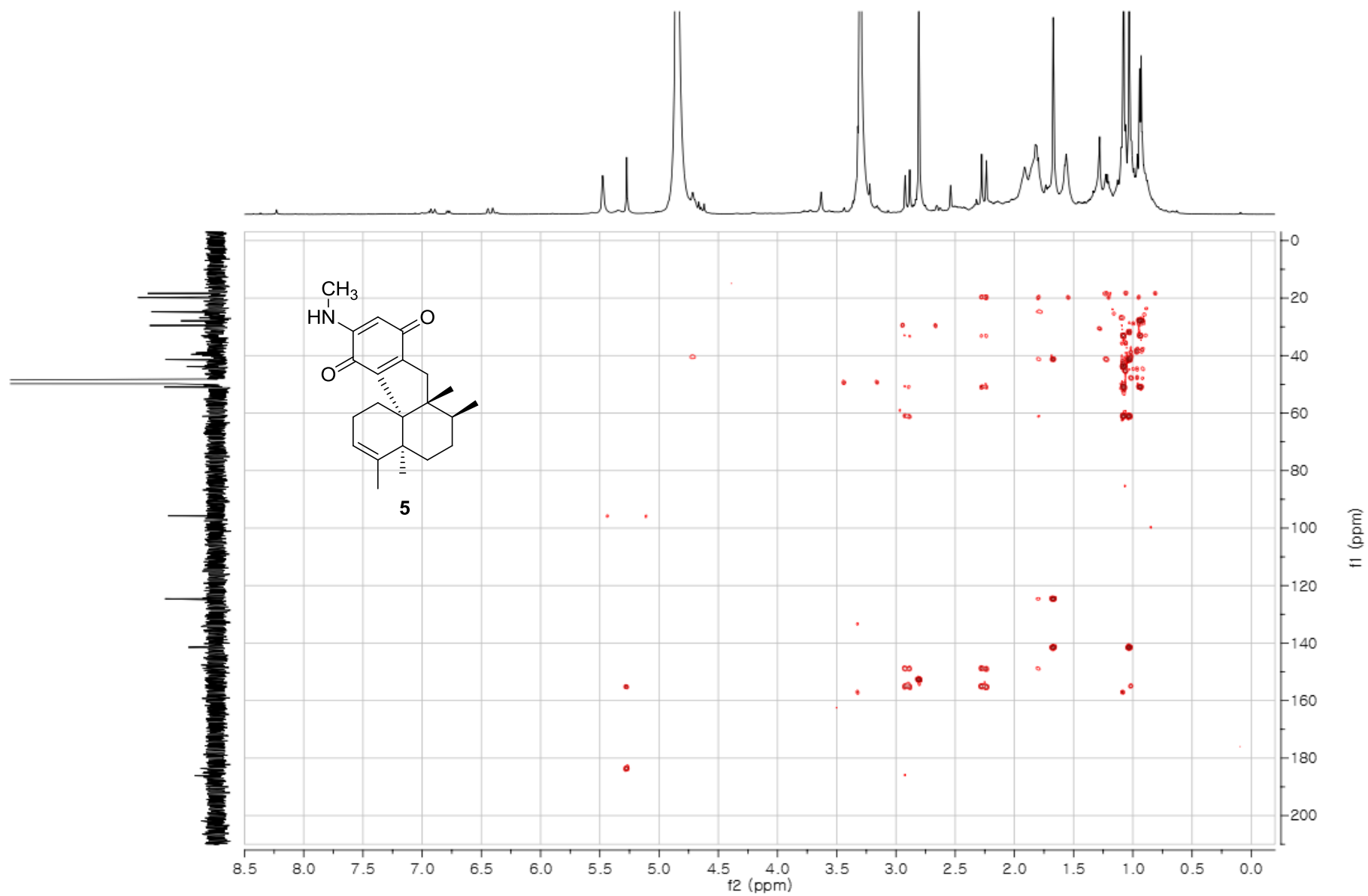


Figure S30. The HMBC NMR (600 MHz, CD_3OD) spectrum of compound **5**
S33

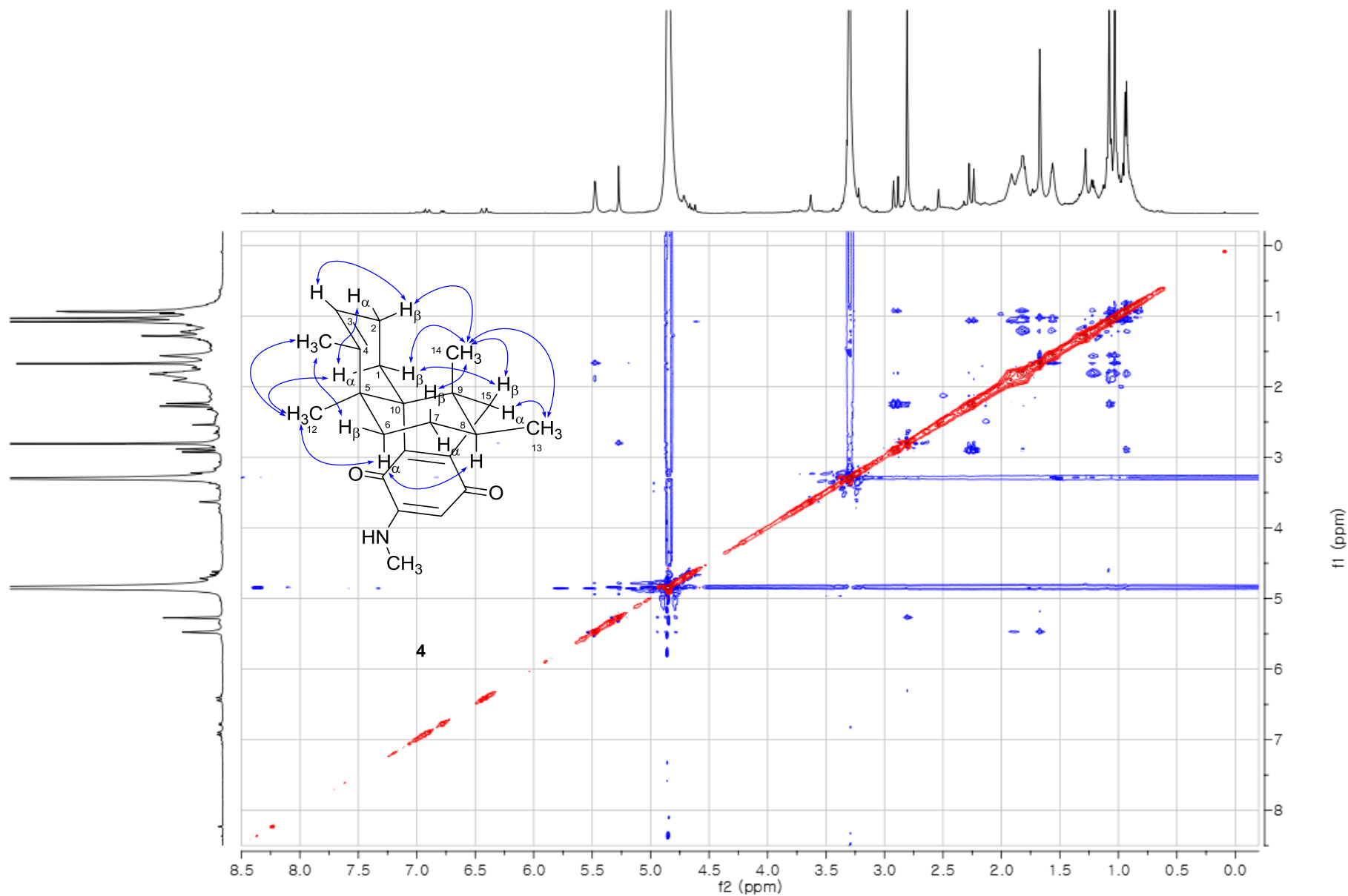


Figure S31. The NOESY NMR (600 MHz, CD₃OD) spectrum of compound **5**

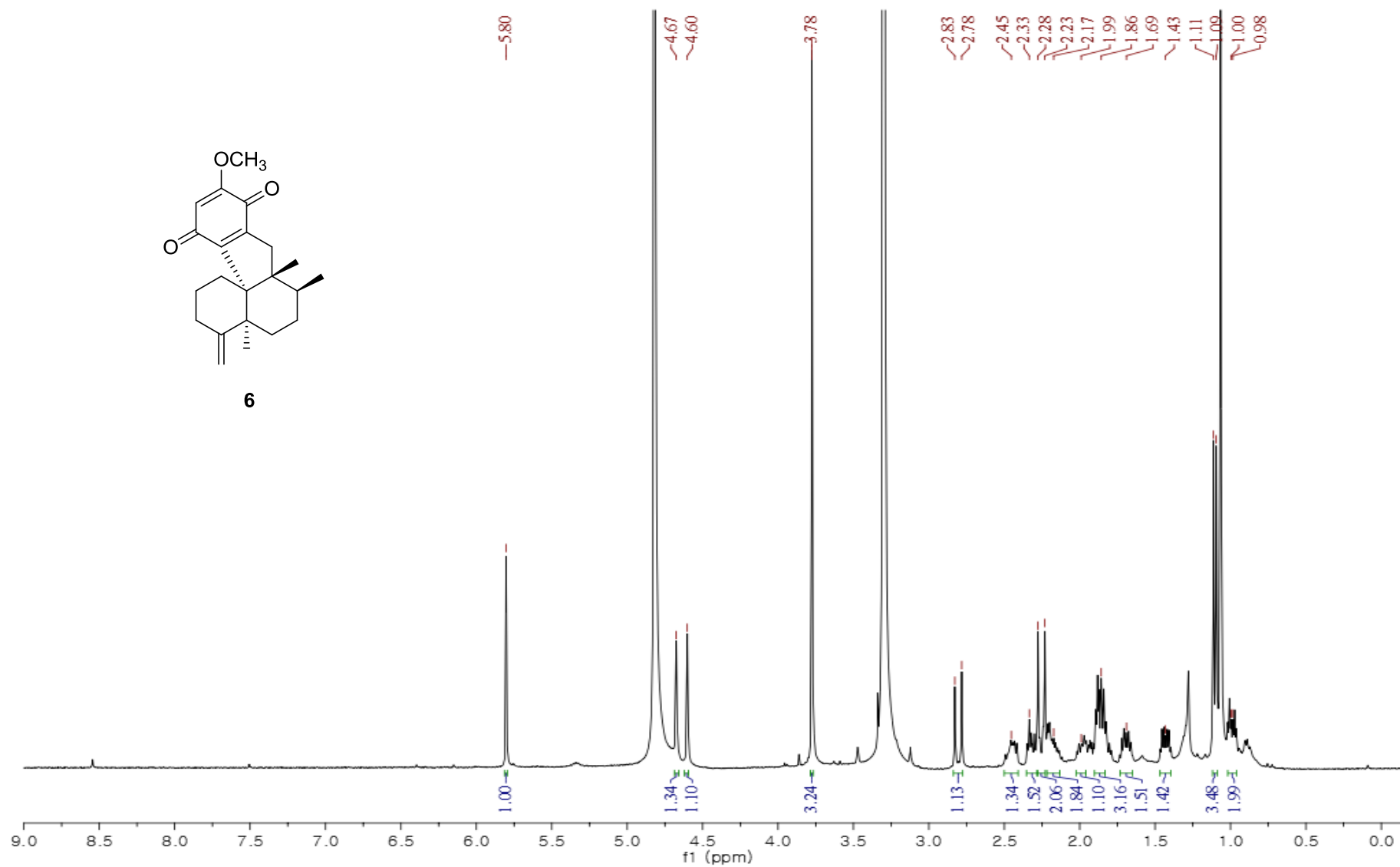


Figure S32. The ^1H NMR (500 MHz, CD_3OD) spectrum of compound **6**

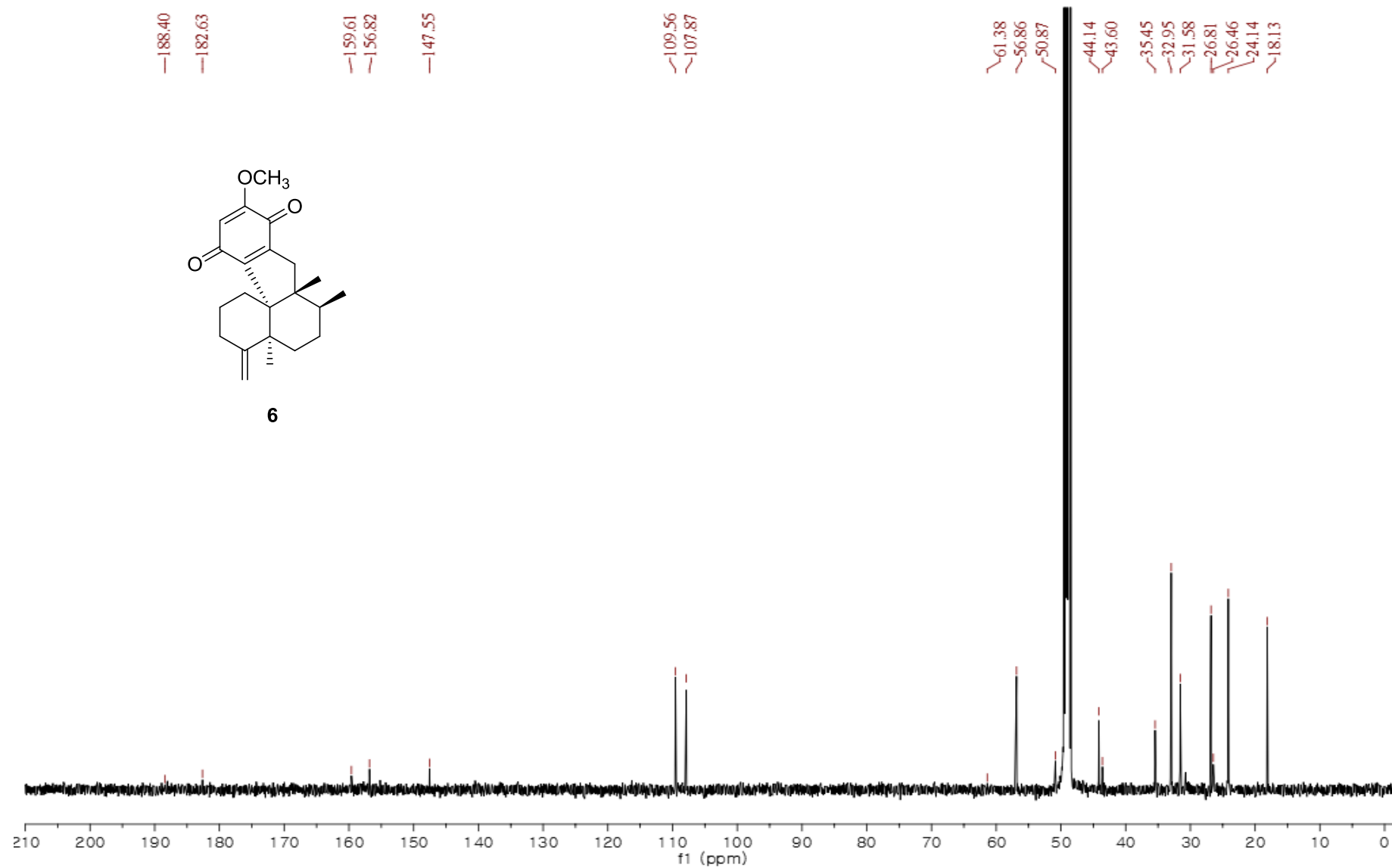


Figure S33. The ¹³C NMR (125 MHz, CD₃OD) spectrum of compound **6**

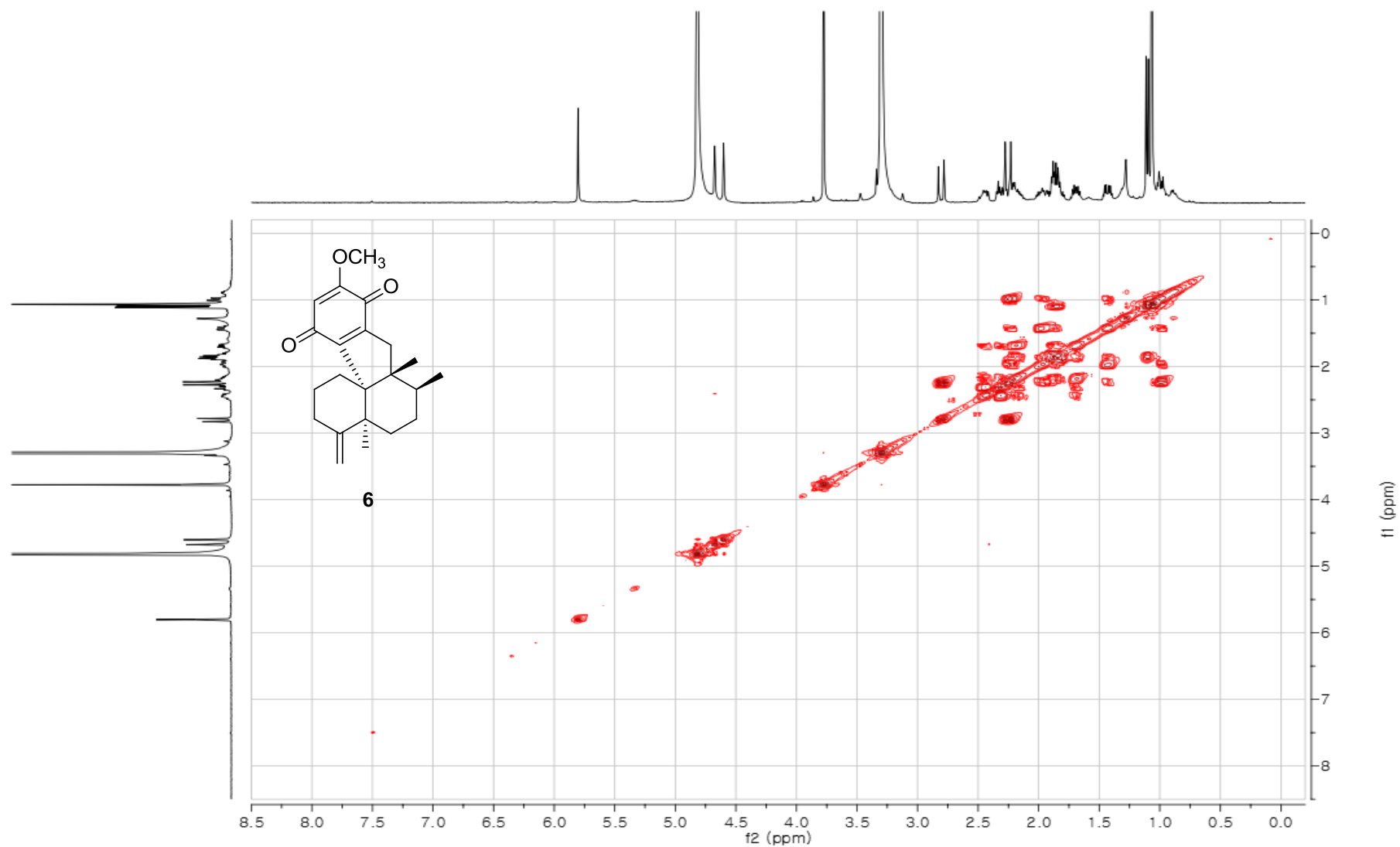


Figure S34. The COSY NMR (500 MHz, CD_3OD) spectrum of compound **6**

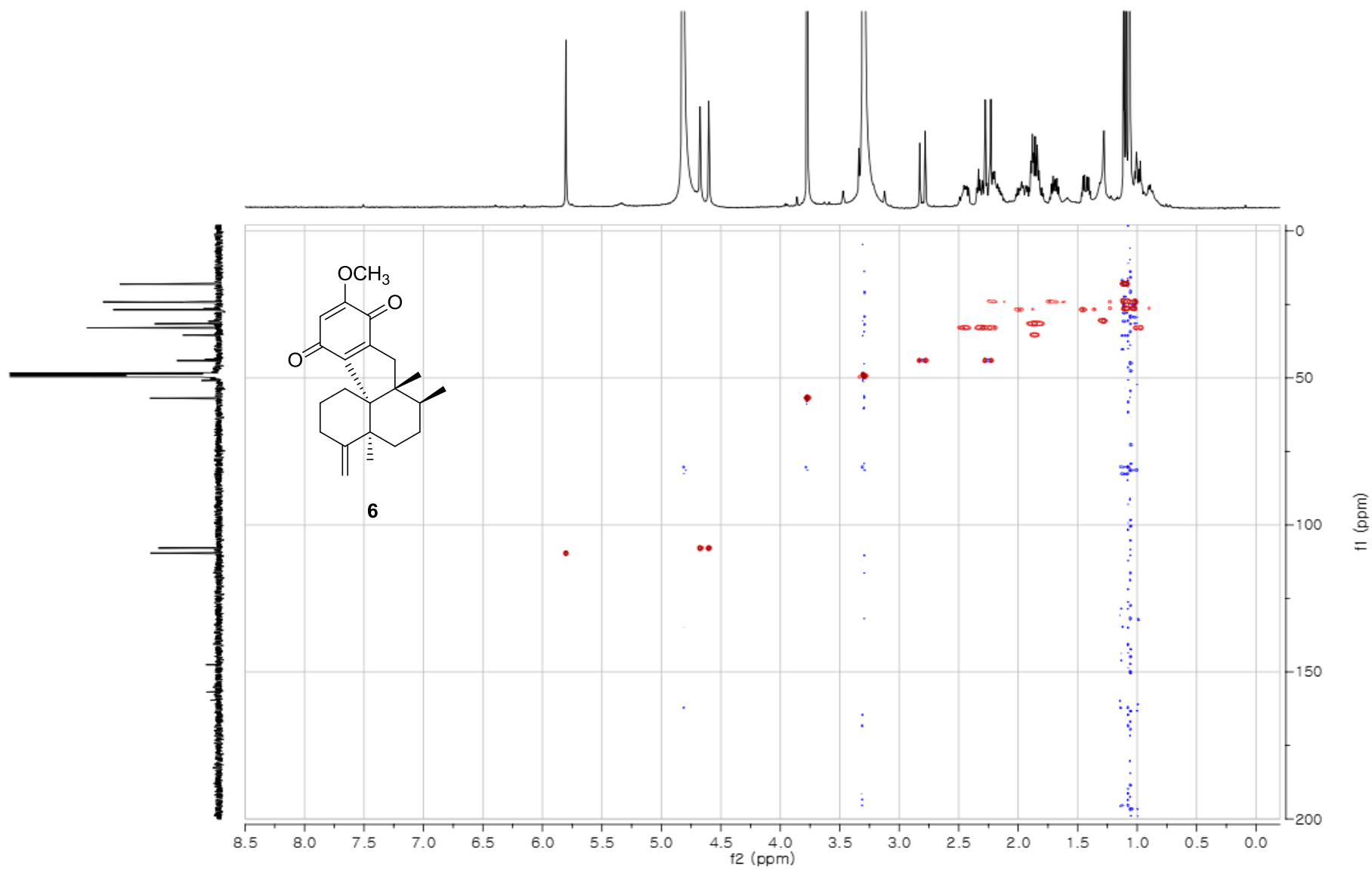


Figure S35. The HSQC NMR (500 MHz, CD₃OD) spectrum of compound **6**

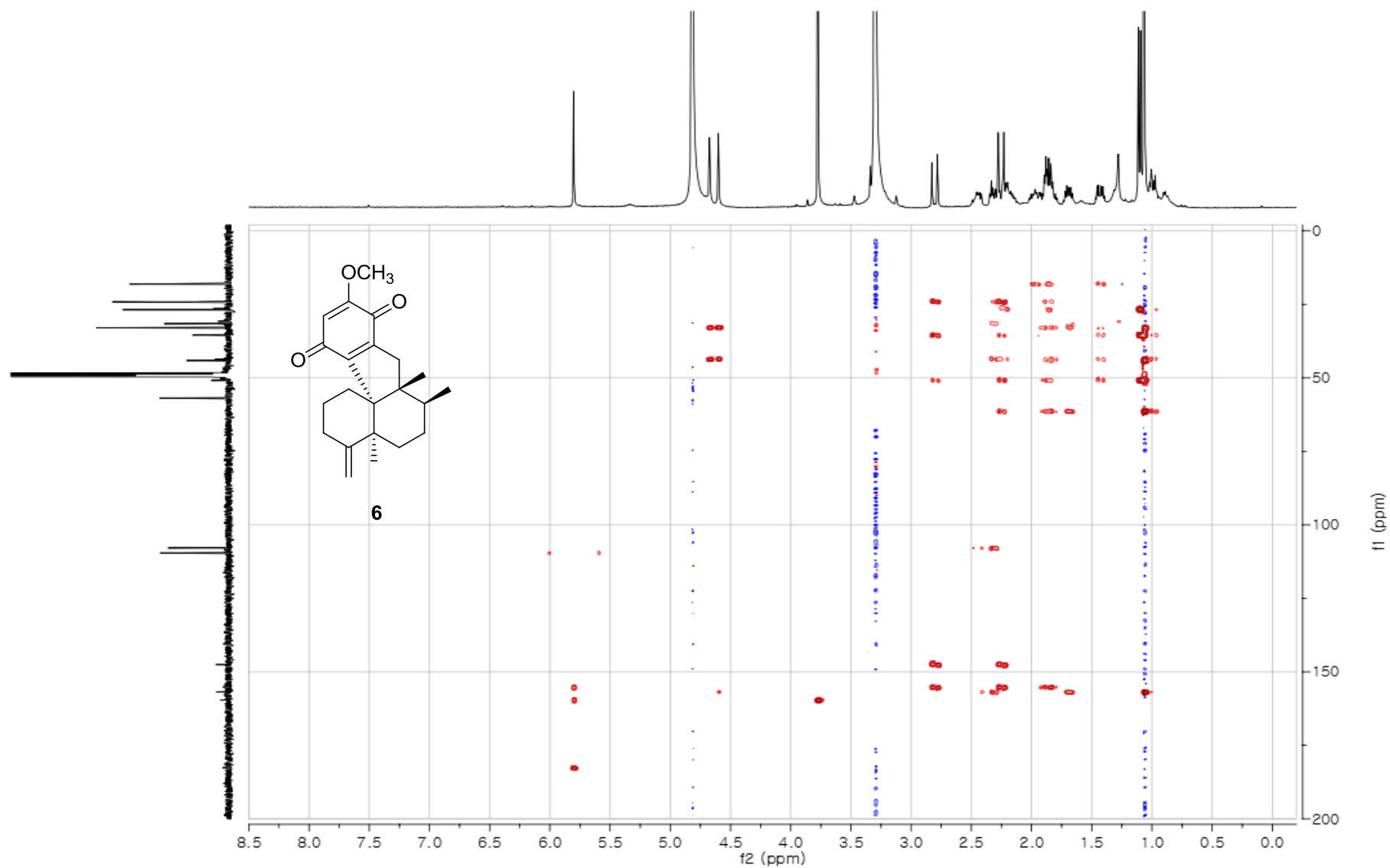


Figure S36. The HMBC NMR (500 MHz, CD_3OD) spectrum of compound **6**

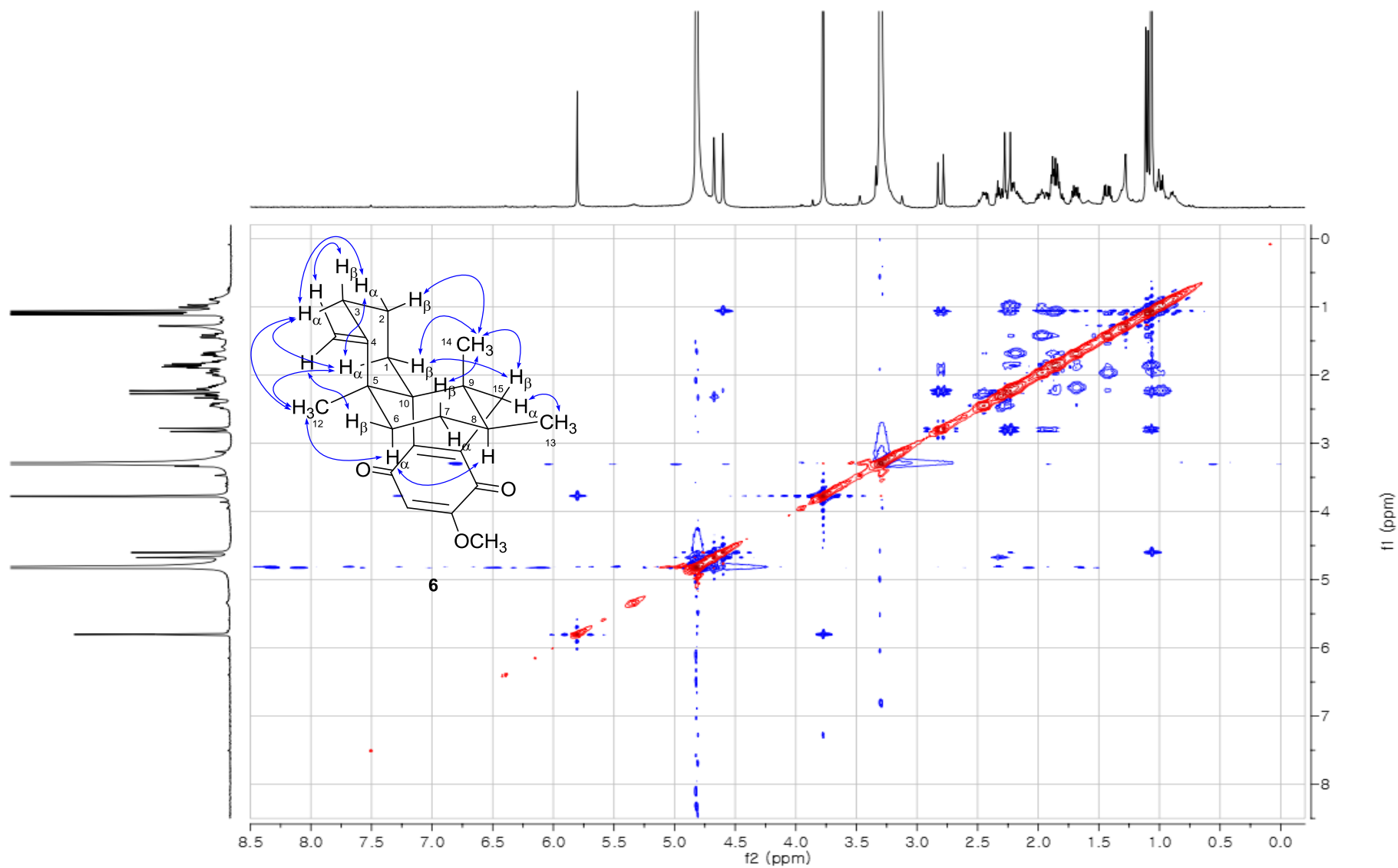
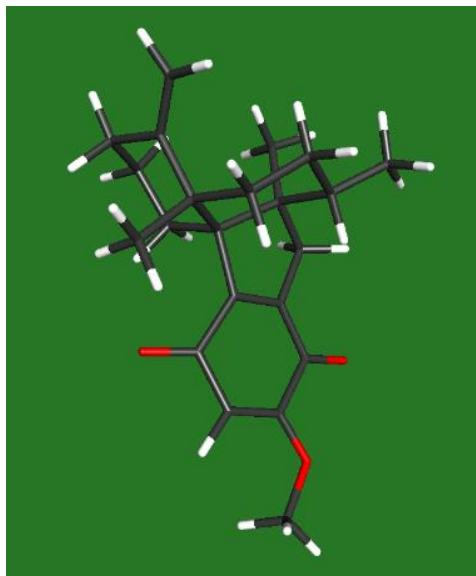


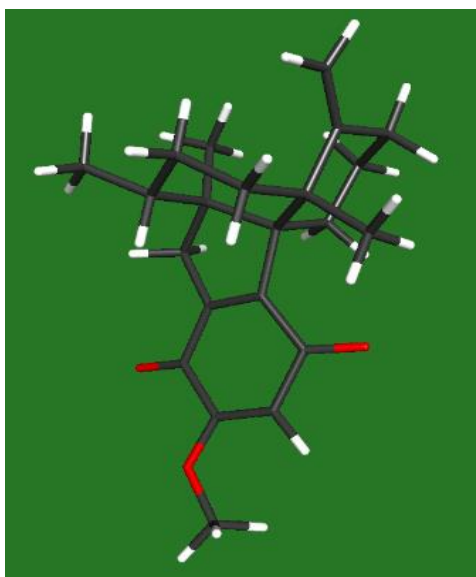
Figure S37. The NOESY NMR (500 MHz, CD₃OD) spectrum of compound **6**

Figure S38. Energy minimized conformation of cycloaurenone C (**6**) at the basis set def-SV(P) for all atoms and functional B3LYP/DFT level.



cycloaurenone C (**6**) : total energy = -1079.28129245278
 kinetic energy = 1068.71443177919, potential energy = -2147.99572423196
 DFT settings (Functional B3-LYP / Gridsize M3), Geometry optimization options (Energy 10^{-6} Hartree, Gradient norm $|dE / dxyz| = 10^{-3}$ Hartree/Bohr)

Figure S39. Energy minimized conformation of cycloaurenone C (*ent*-**6**) at the basis set def-SV(P) for all atoms and functional B3LYP/DFT level.



cycloaurenone C (*ent*-**6**) : total energy = -1079.28122946455
 kinetic energy = 1068.71203078936, potential energy = -2147.99326025390
 DFT settings (Functional B3-LYP / Gridsize M3), Geometry optimization options (Energy 10^{-6} Hartree, Gradient norm $|dE / dxyz| = 10^{-3}$ Hartree/Bohr)

Table S1. Energy minimized coordinates of cycloaurenone C (**6**) at the basis set def-SV(P) for all atoms (Å)

atom	x	y	z
C	-3.2476	-0.3831	-2.273
C	-4.108	-1.4169	-2.8944
C	-2.922	-0.4078	-0.9566
H	-5.6607	-3.5529	0.3521
H	-4.0533	-4.1394	0.7783
C	-3.1398	-6.3265	-2.5715
H	-2.5401	-4.5734	-3.6432
H	-3.0426	-5.8888	-4.7011
H	-3.8269	-7.1858	-2.6513
C	-5.8909	-5.9091	-0.8443
H	-6.8603	-5.4163	-0.6735
H	-5.639	-6.43	0.0948
H	-3.6491	-7.4682	-0.1374
C	-4.3213	-2.6922	-2.1275
C	-4.1081	-2.6388	-0.7898
C	-3.4098	-1.54	-0.0877
C	-5.0878	-3.9841	-2.5199
C	-4.6731	-3.8212	-0.074
C	-4.7949	-4.8897	-1.1932
C	-4.6761	-4.7106	-3.8925
H	-6.0265	-6.6721	-1.6284
C	-3.078	-6.525	-0.0734
H	-2.0062	-6.7944	-0.0863
C	-4.535	-3.7529	-5.111
H	-5.3944	-3.0881	-5.2636
H	-4.405	-4.3705	-6.0178
H	-3.6466	-3.1116	-5.0138
C	-7.1697	-5.1286	-4.4454
C	-7.6321	-4.4673	-3.1451
C	-3.3841	-5.5885	-1.2571
H	-2.1162	-6.7467	-2.5663
C	-3.2908	-5.3794	-3.753
H	-2.6376	-4.7724	-1.217
H	-3.2865	-6.0695	0.9104
C	-5.7768	-5.7114	-4.3177

Table S2. Energy minimized coordinates of cycloaurenone C (*ent*-6) at the basis set def-SV(P) for all atoms (Å)

atom	x	y	z
C	-6.7165	-8.1566	-7.0617
C	-8.0185	-7.6081	-6.6138
C	-6.0113	-7.6069	-8.0816
C	-10.1473	-5.1613	-8.827
H	-8.3949	-4.7333	-10.1493
C	-11.7152	-7.7035	-8.4589
C	-11.8773	-6.8676	-9.7196
H	-10.8878	-8.419	-8.6271
H	-12.7278	-6.1702	-9.6342
H	-12.1048	-7.5323	-10.5744
C	-10.9613	-3.8575	-8.8174
H	-12.0314	-4.0256	-8.6112
H	-11.6352	-4.7369	-11.4146
C	-8.7205	-6.6514	-7.5361
C	-7.952	-6.0247	-8.4605
C	-6.5734	-6.4199	-8.8231
H	-6.3279	-8.9614	-6.4346
C	-10.109	-5.9674	-7.4081
C	-8.6468	-4.8595	-9.085
H	-8.3195	-3.9267	-8.5835
H	-10.8808	-3.3534	-9.7952
H	-10.5749	-3.146	-8.0713
H	-10.8333	-6.1258	-12.1778
H	-9.8632	-4.7424	-11.6262
C	-11.2034	-7.9913	-6.0737
H	-10.5029	-8.775	-6.3978
H	-10.8293	-7.6025	-5.1187
C	-12.5894	-6.0635	-6.6824
C	-12.3331	-5.2327	-5.4409
H	-12.611	-8.3235	-8.278
C	-10.5972	-6.0897	-10.018
C	-11.3903	-6.9084	-7.1748
C	-10.7333	-5.3735	-11.3743
H	-9.7964	-6.8436	-10.1361
H	-12.1833	-8.47	-5.896