Supplementary Information

Talascortenes A−G, Highly Oxygenated Diterpenoid Acids from the Sea-Anemone-Derived Endozoic Fungus *Talaromyces scorteus* AS-242

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Content

Figure S1. ^{1}H NMR (500 MHz, DMSO-d_6) spectrum of compound **1**

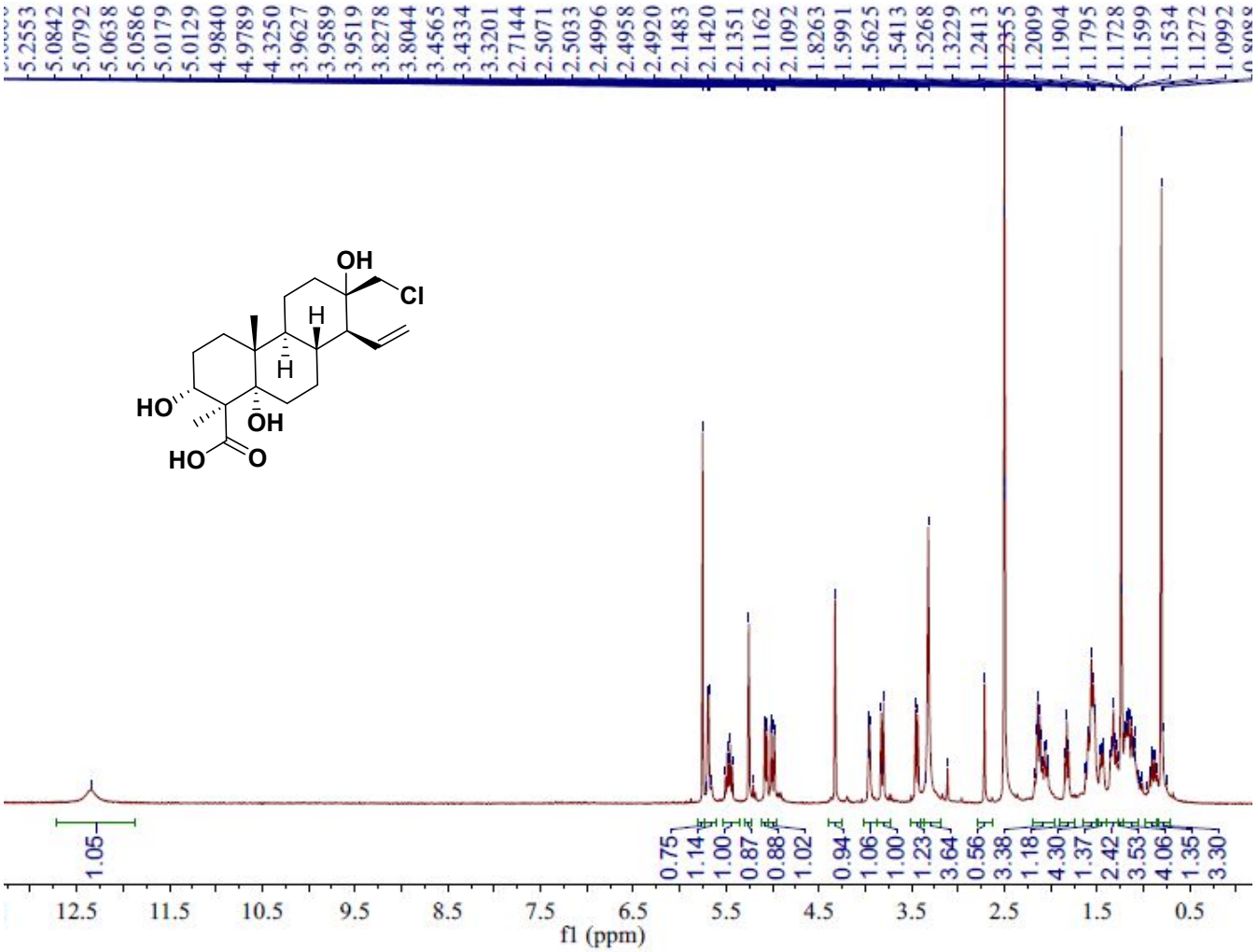

Figure S2. ^{13}C NMR (125 MHz, DMSO-d_6) and DEPT spectra of compound **1**

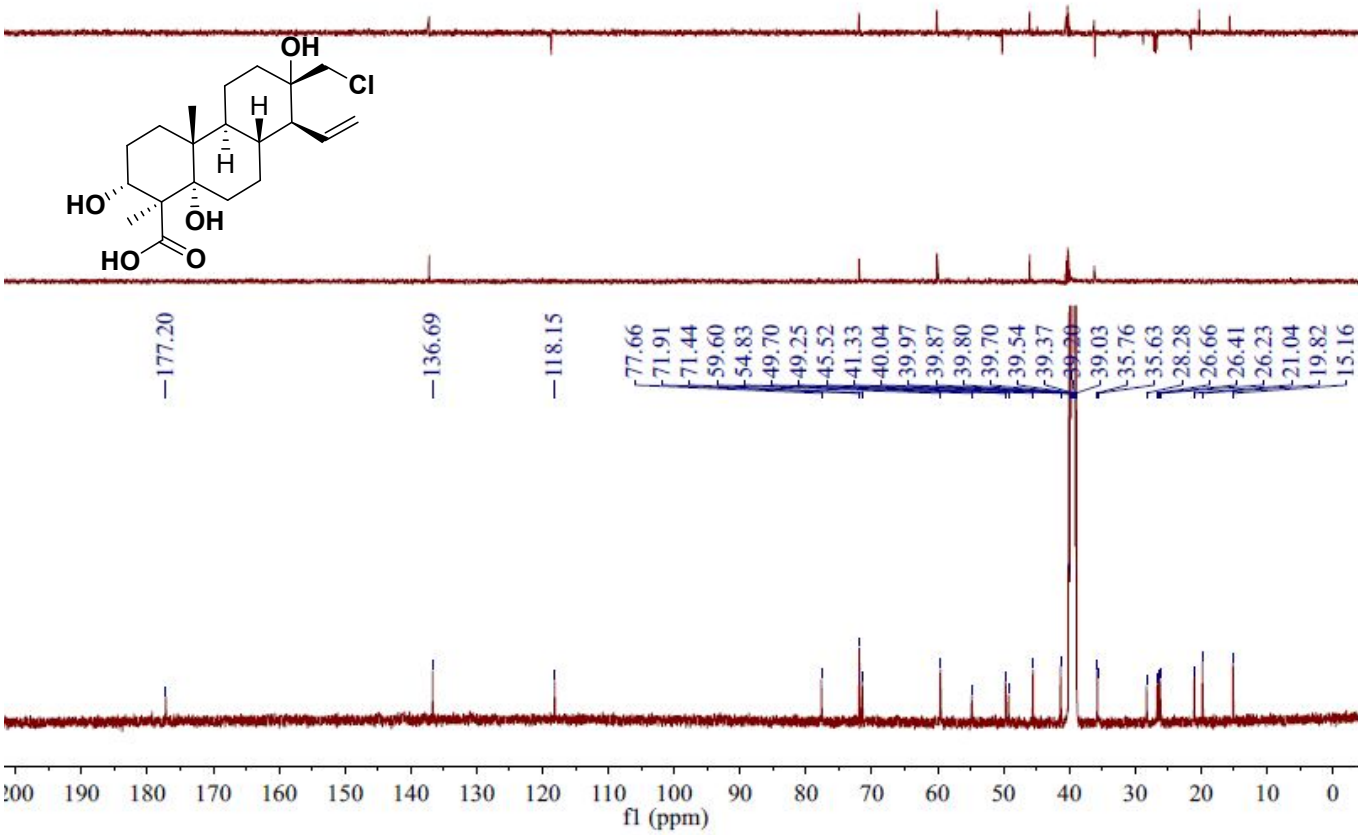

Figure S3. COSY spectrum of compound **1**

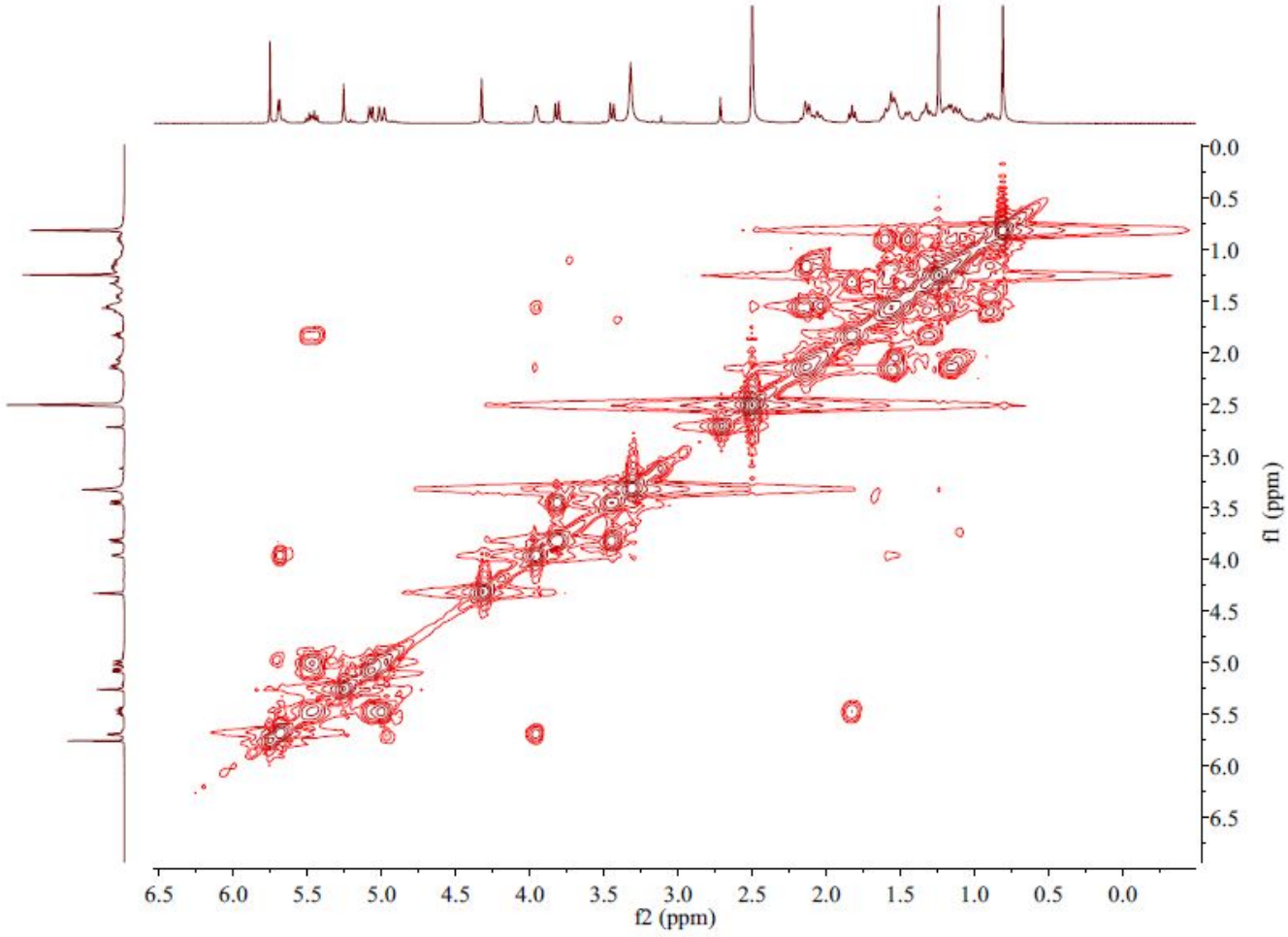

Figure S4. HSQC spectrum of compound **1**

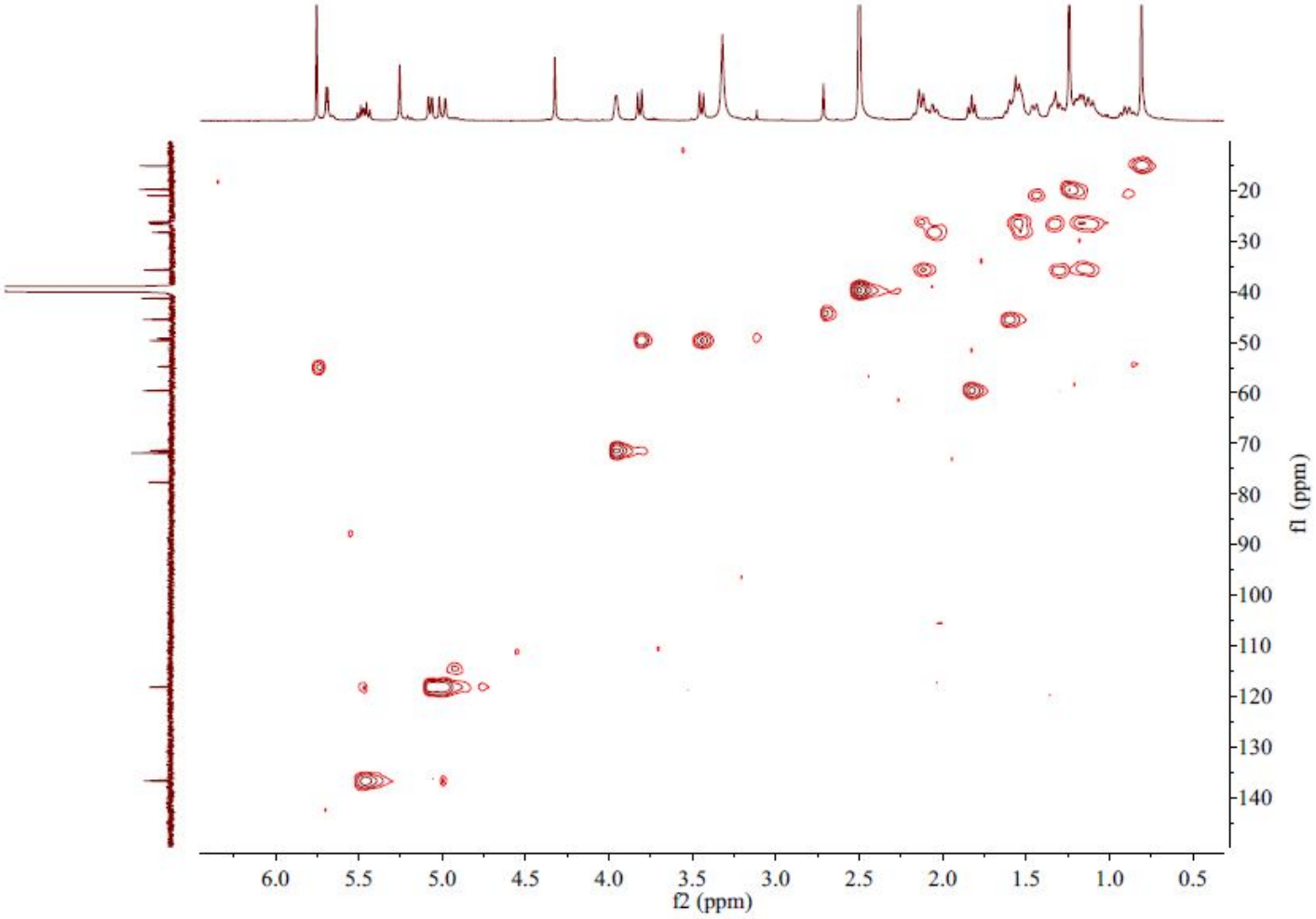

Figure S5. HMBC spectrum of compound **1**

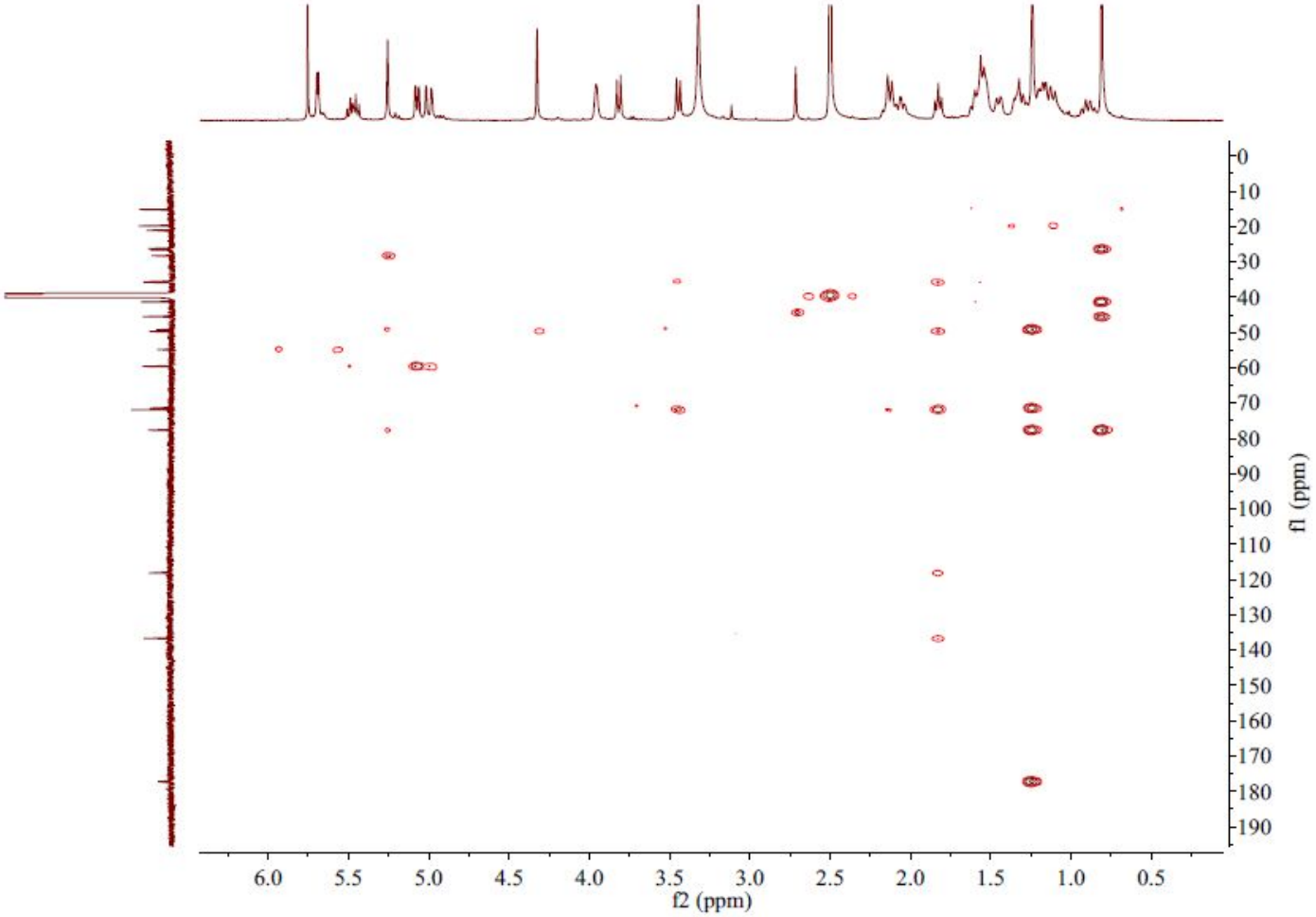

Figure S6. NOESY spectrum of compound **1**

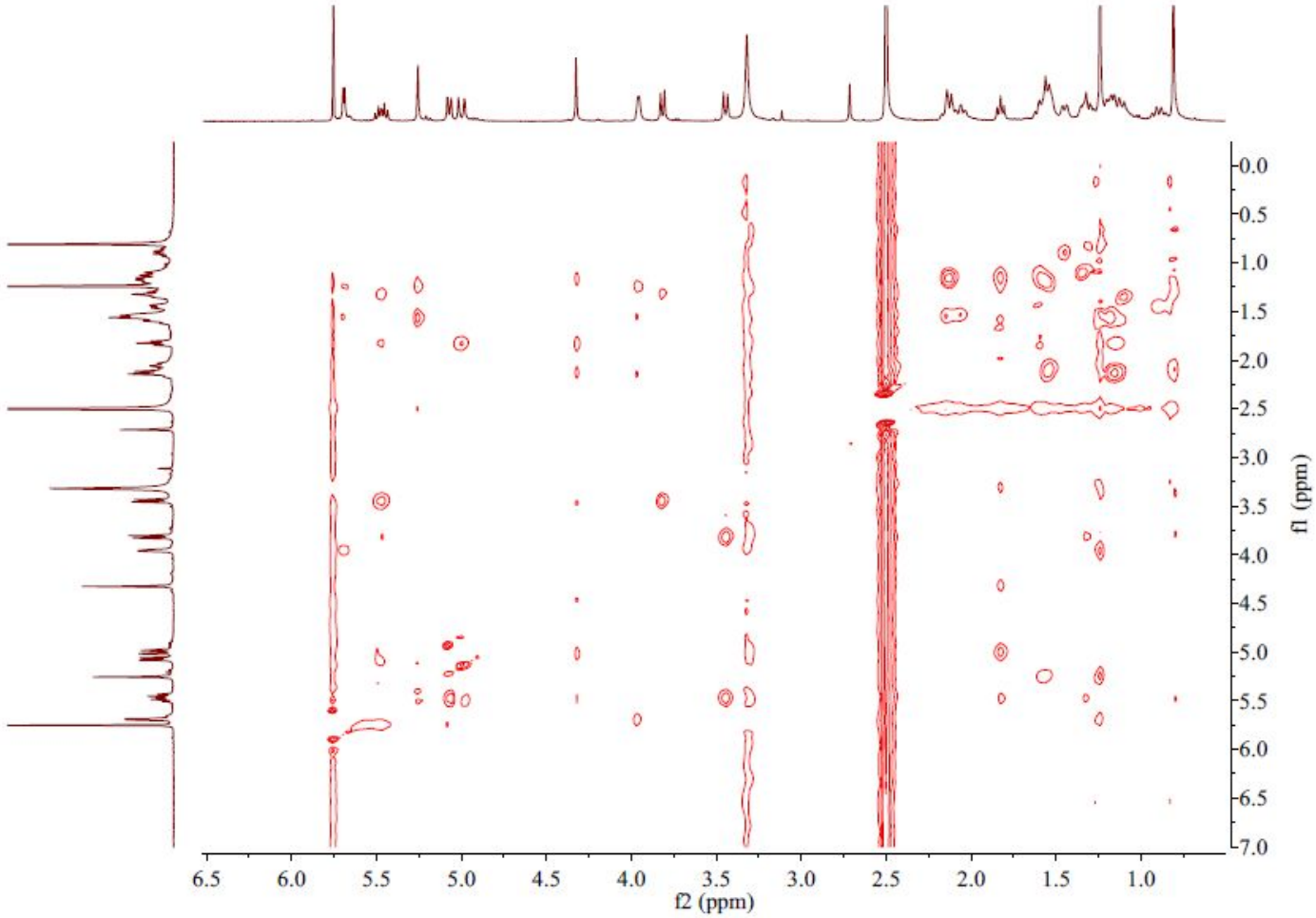

Figure S7. ECD spectrum of compound **1**

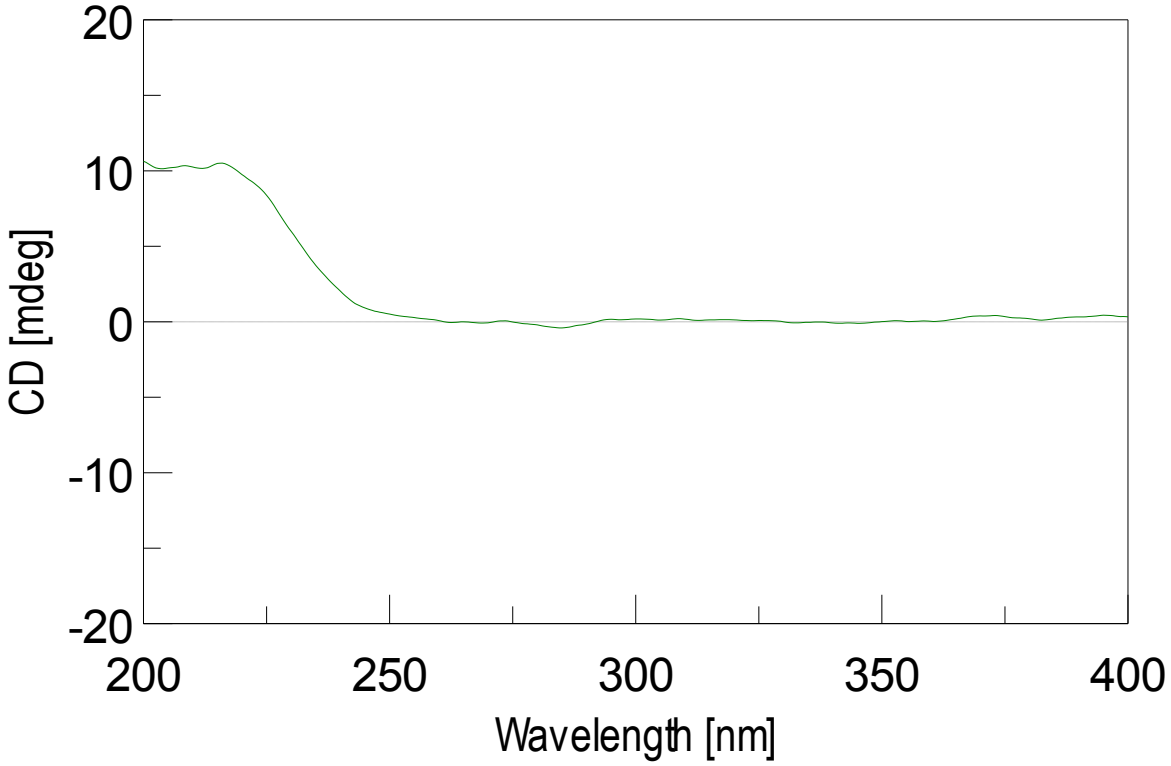

Figure S8. ^{1}H NMR (500 MHz, DMSO-d_6) spectrum of compound **2**

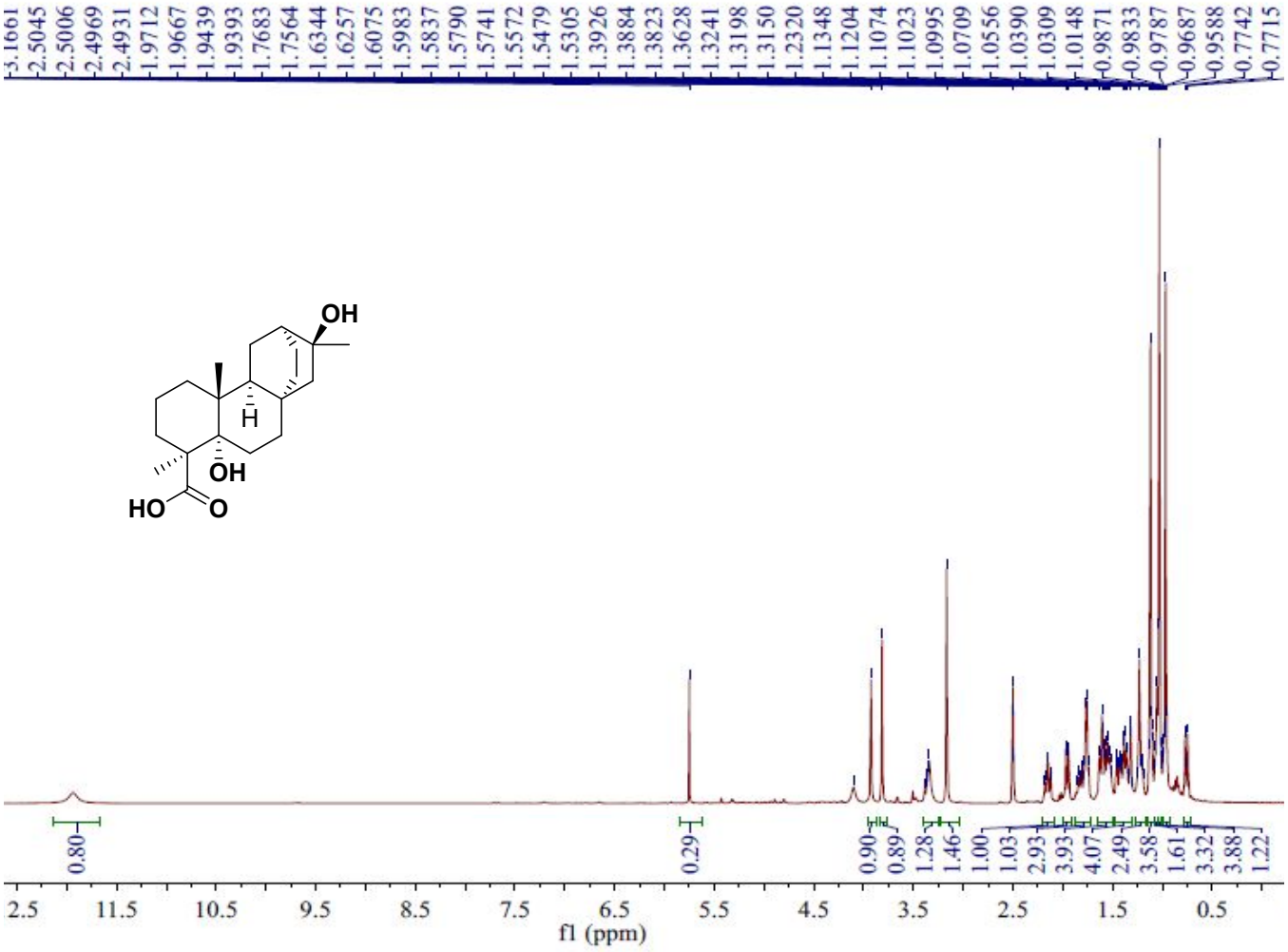

Figure S9. ^{13}C NMR (125 MHz, DMSO-d_6) and DEPT spectra of compound **2**

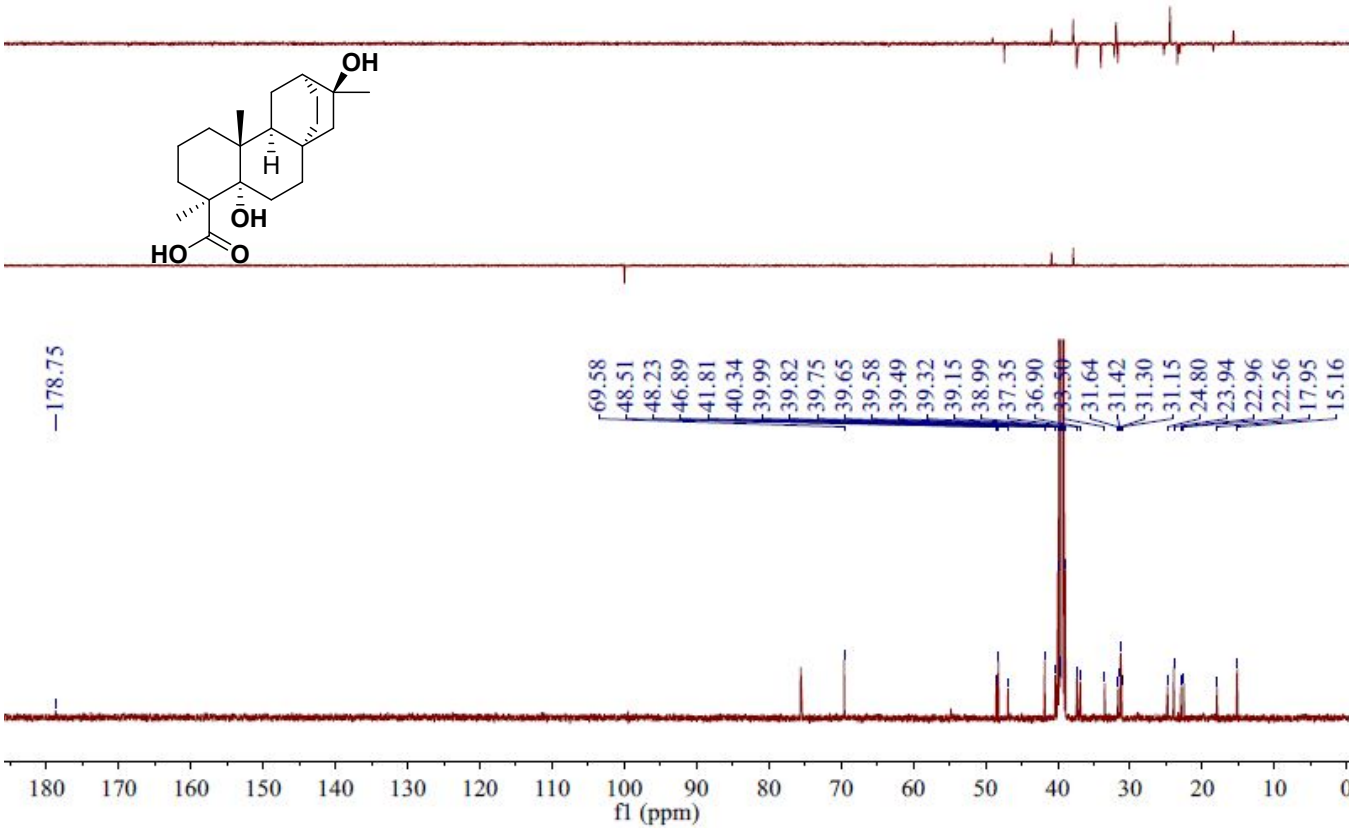

Figure S10. COSY spectrum of compound **2**

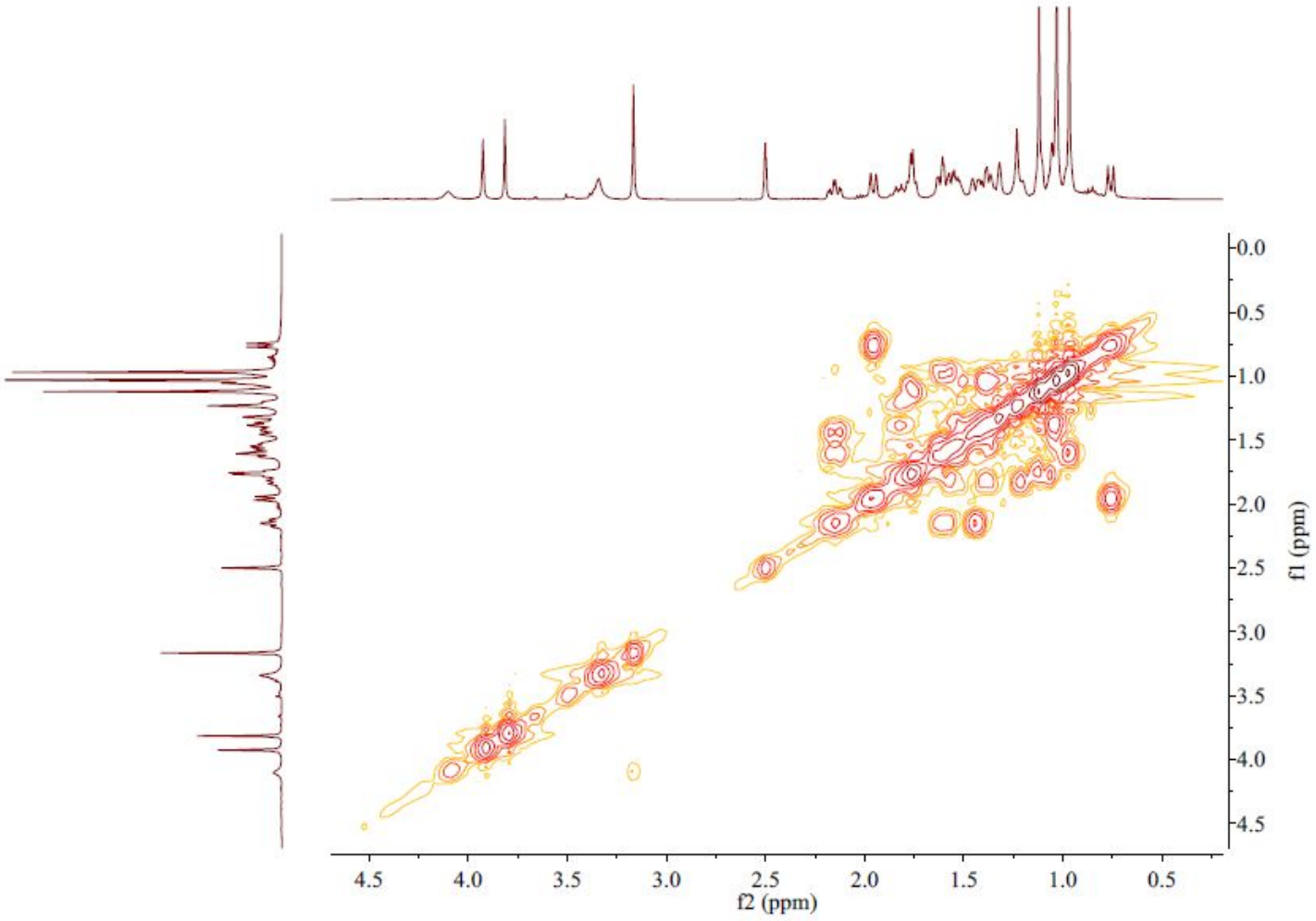

Figure S11. HSQC spectrum of compound **2**

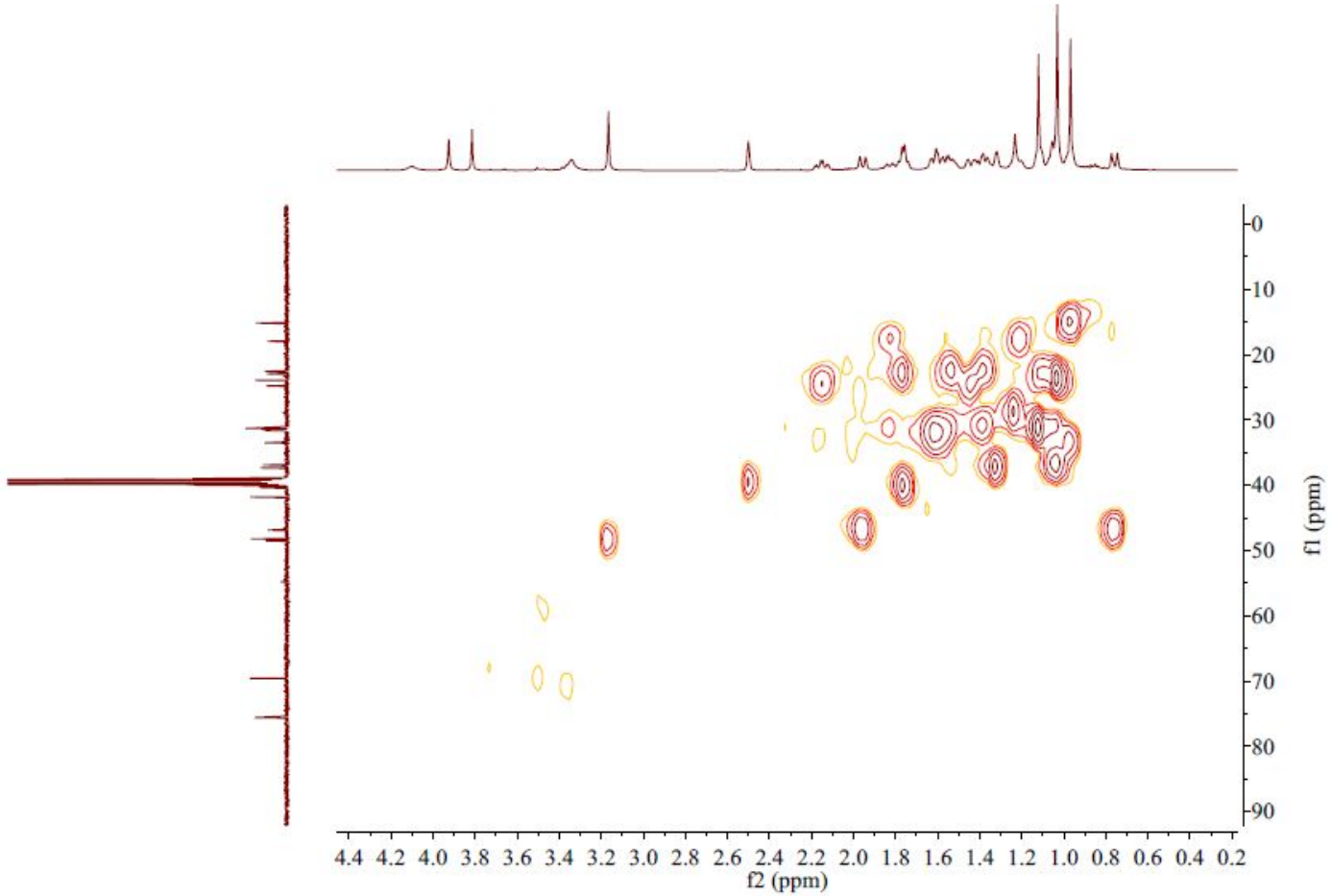

Figure S12. HMBC spectrum of compound **2**

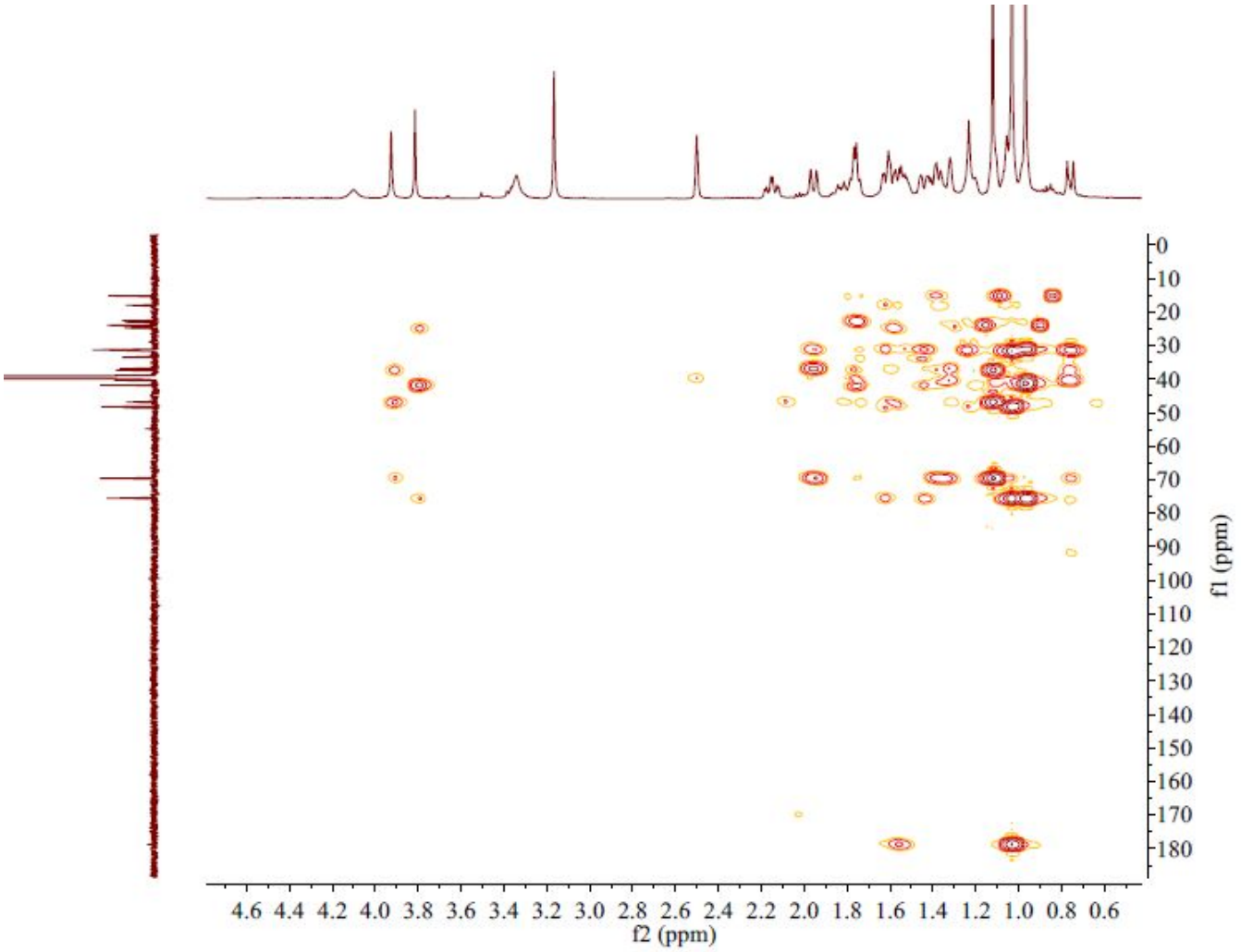

Figure S13. NOESY spectrum of compound **2**

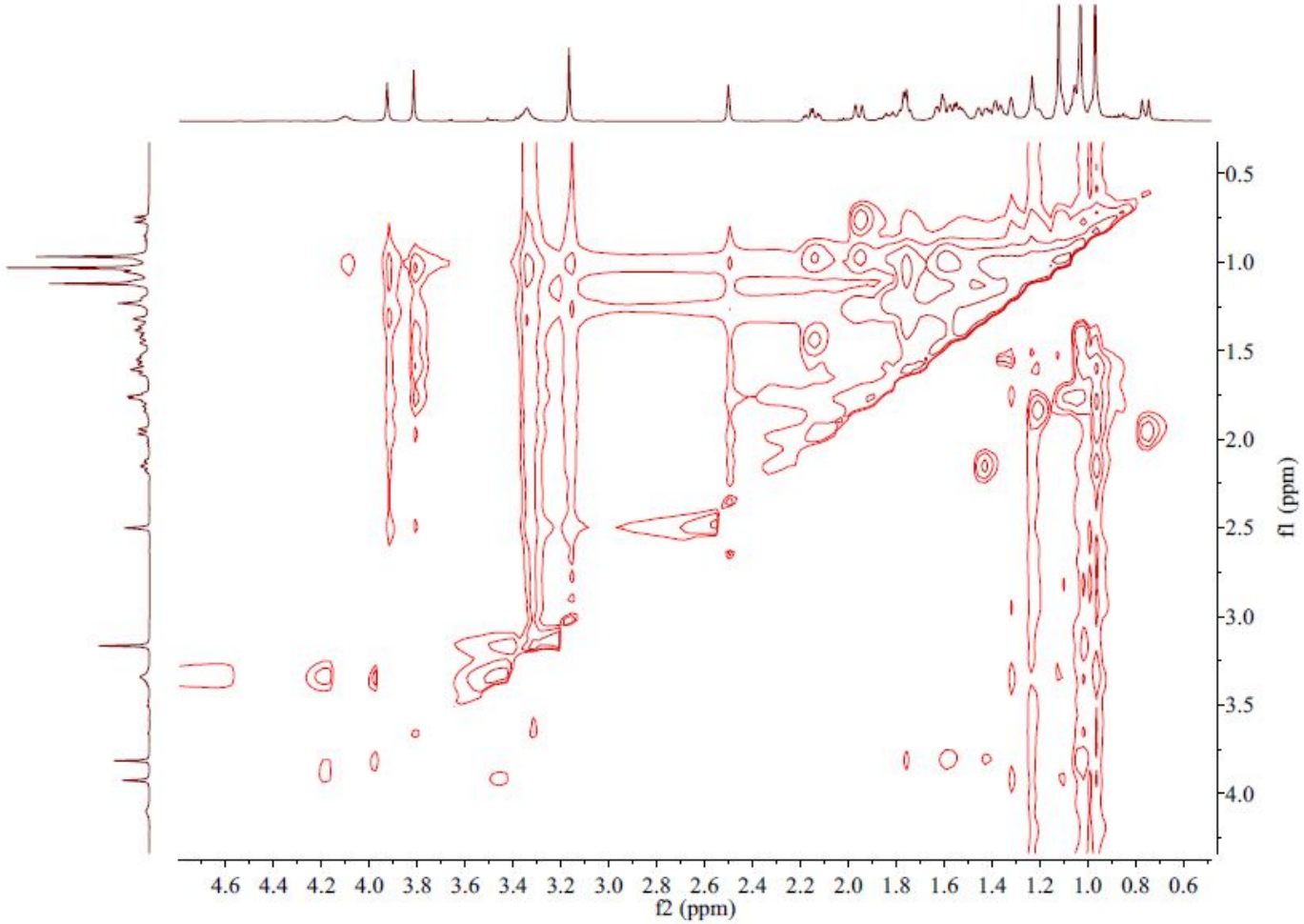

Figure S14. ECD spectrum of compound **2**

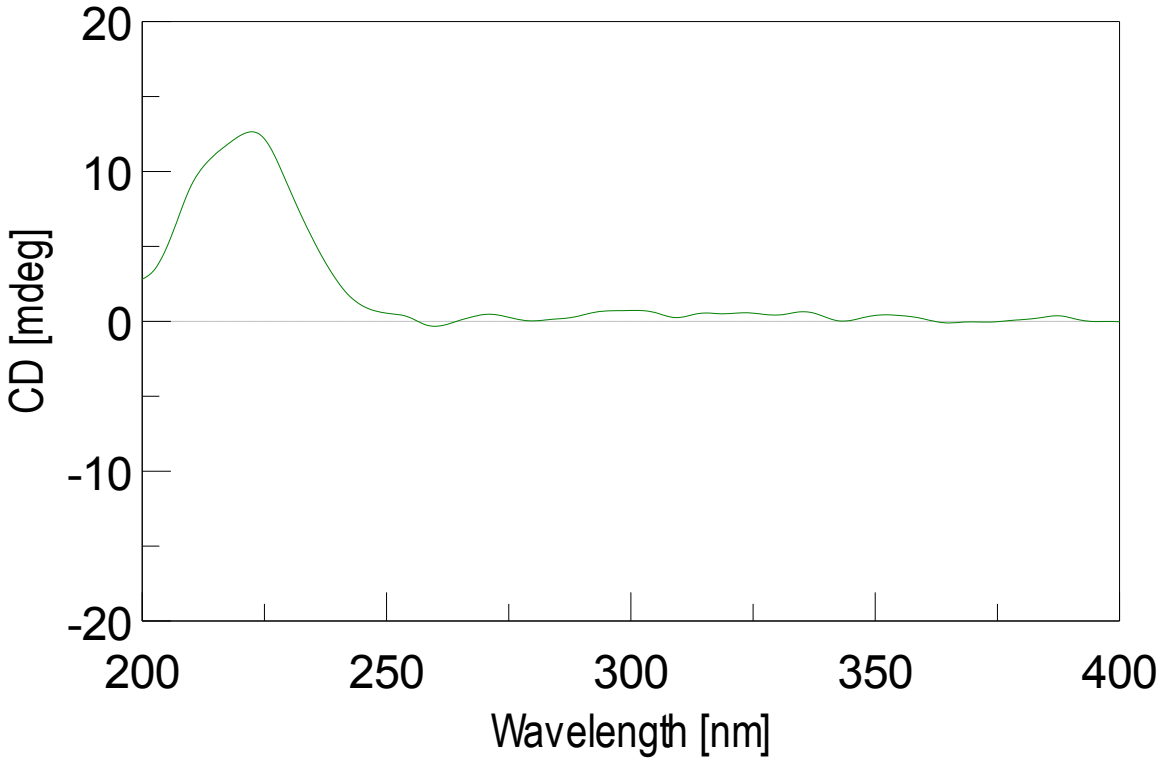

Figure S15. ^{1}H NMR (500 MHz, DMSO-d_6) spectrum of compound **3**

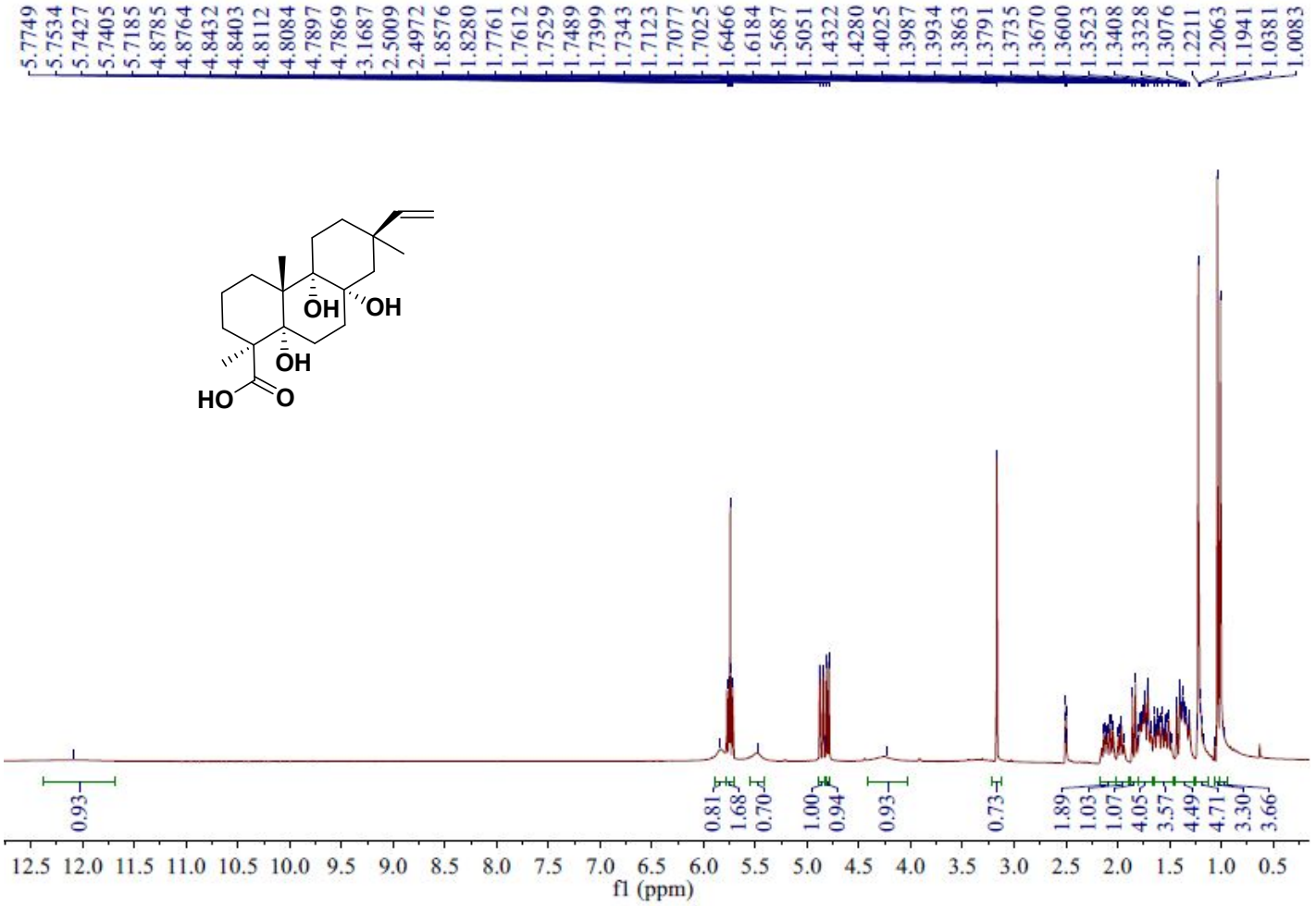

Figure S16. ^{13}C NMR (125 MHz, DMSO-d_6) and DEPT spectra of compound **3**

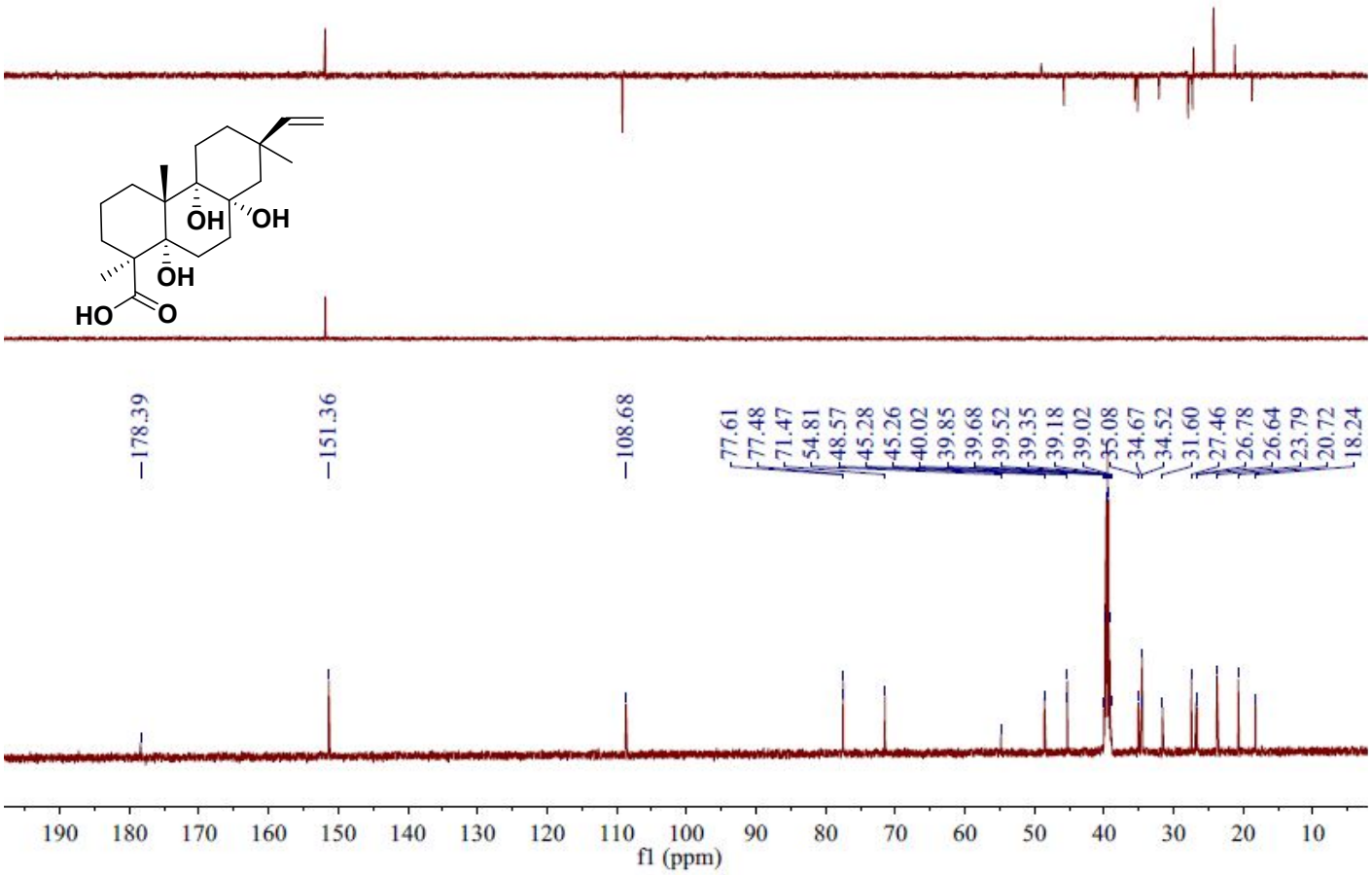

Figure S17. COSY spectrum of compound **3**

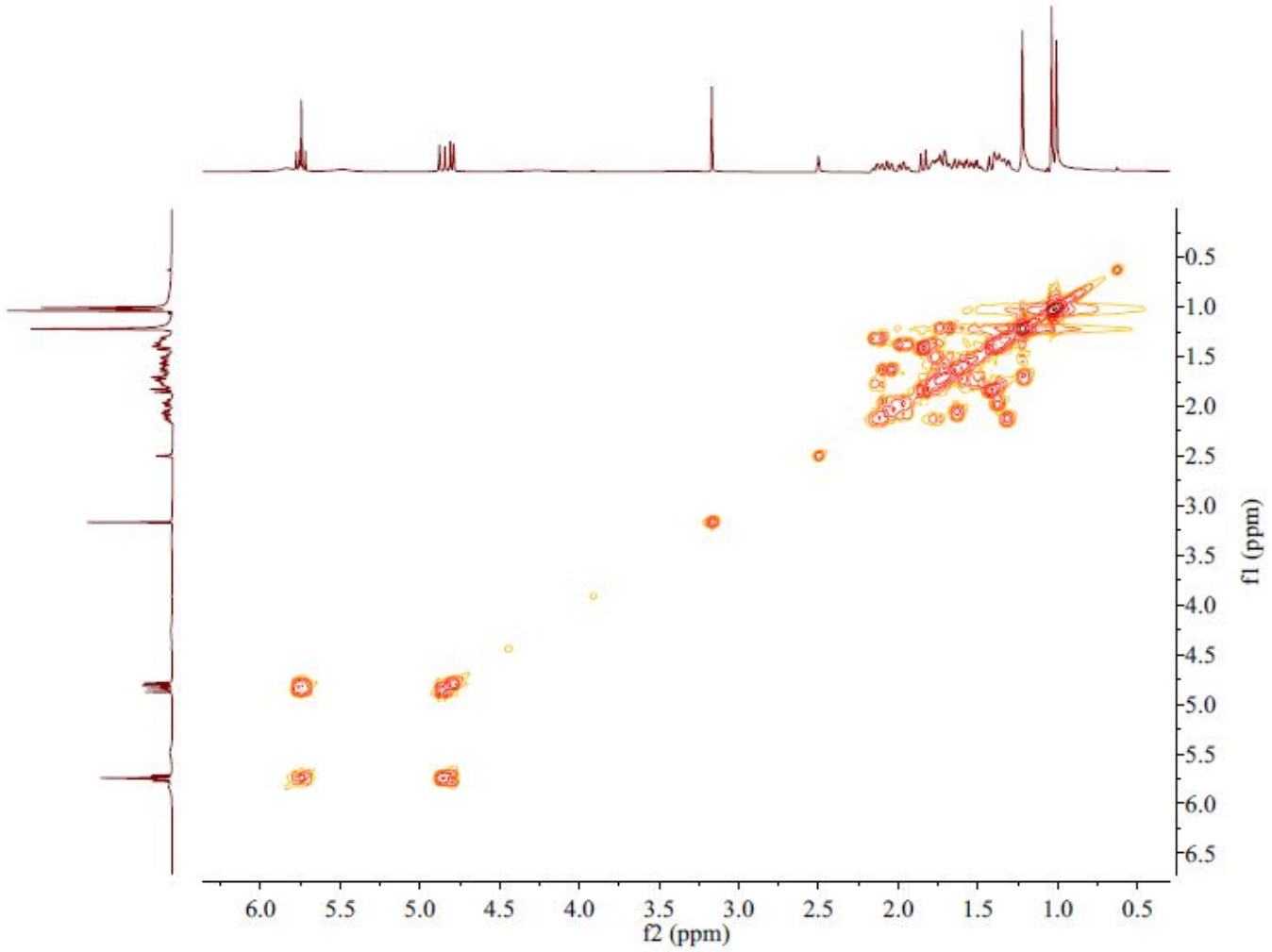

Figure S18. HSQC spectrum of compound **3**

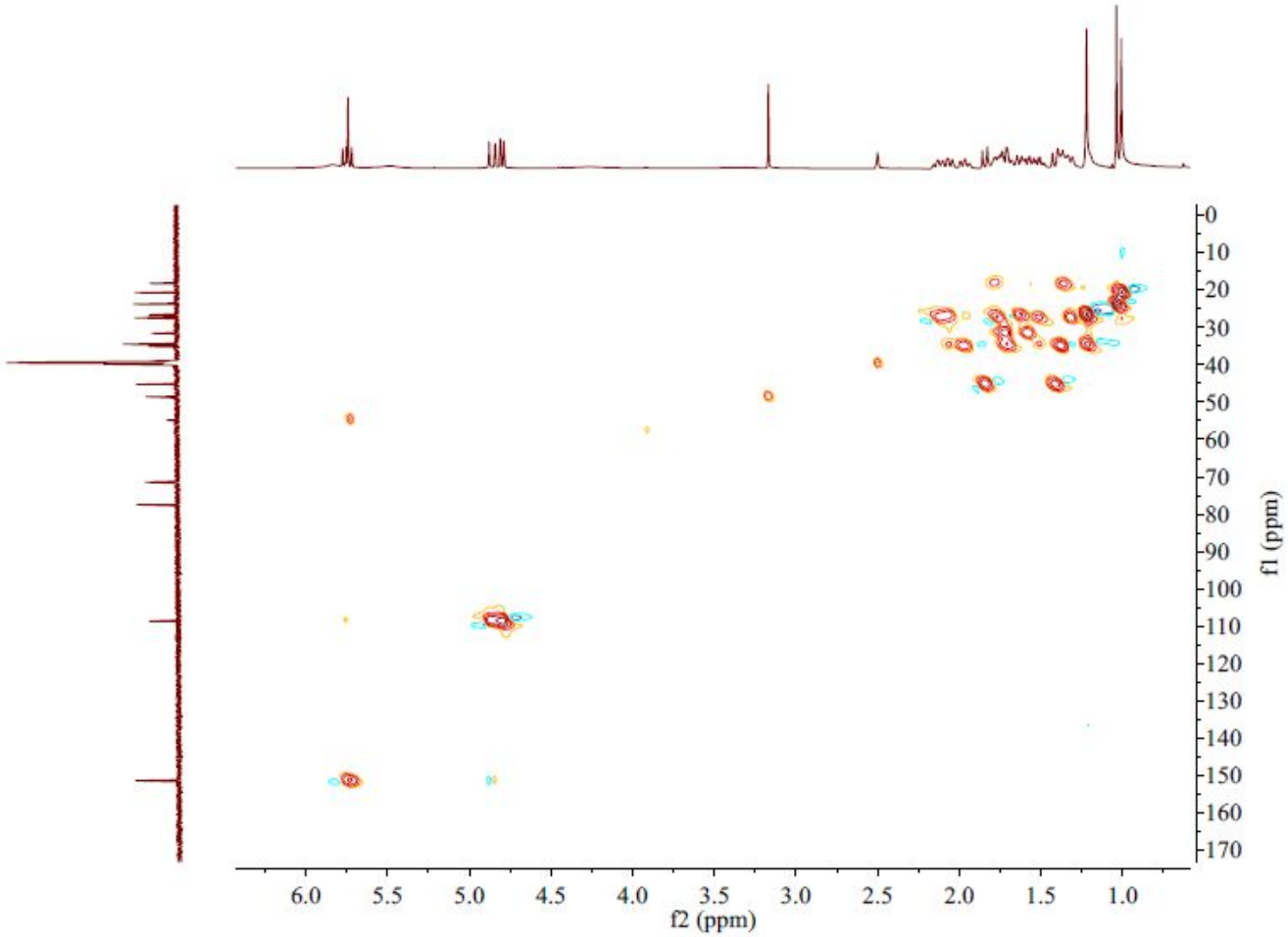

Figure S19. HMBC spectrum of compound **3**

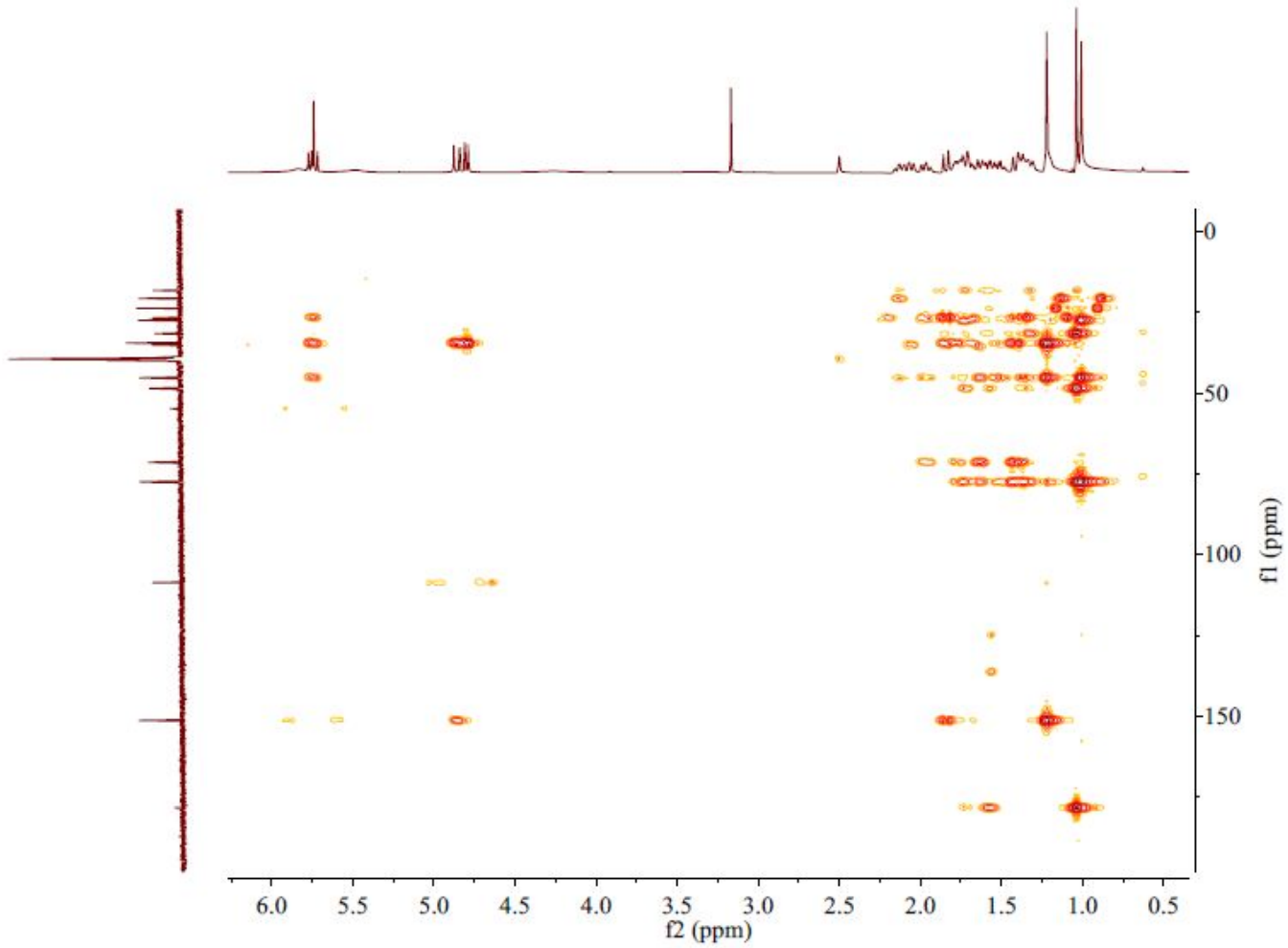

Figure S20. NOESY spectrum of compound **3**

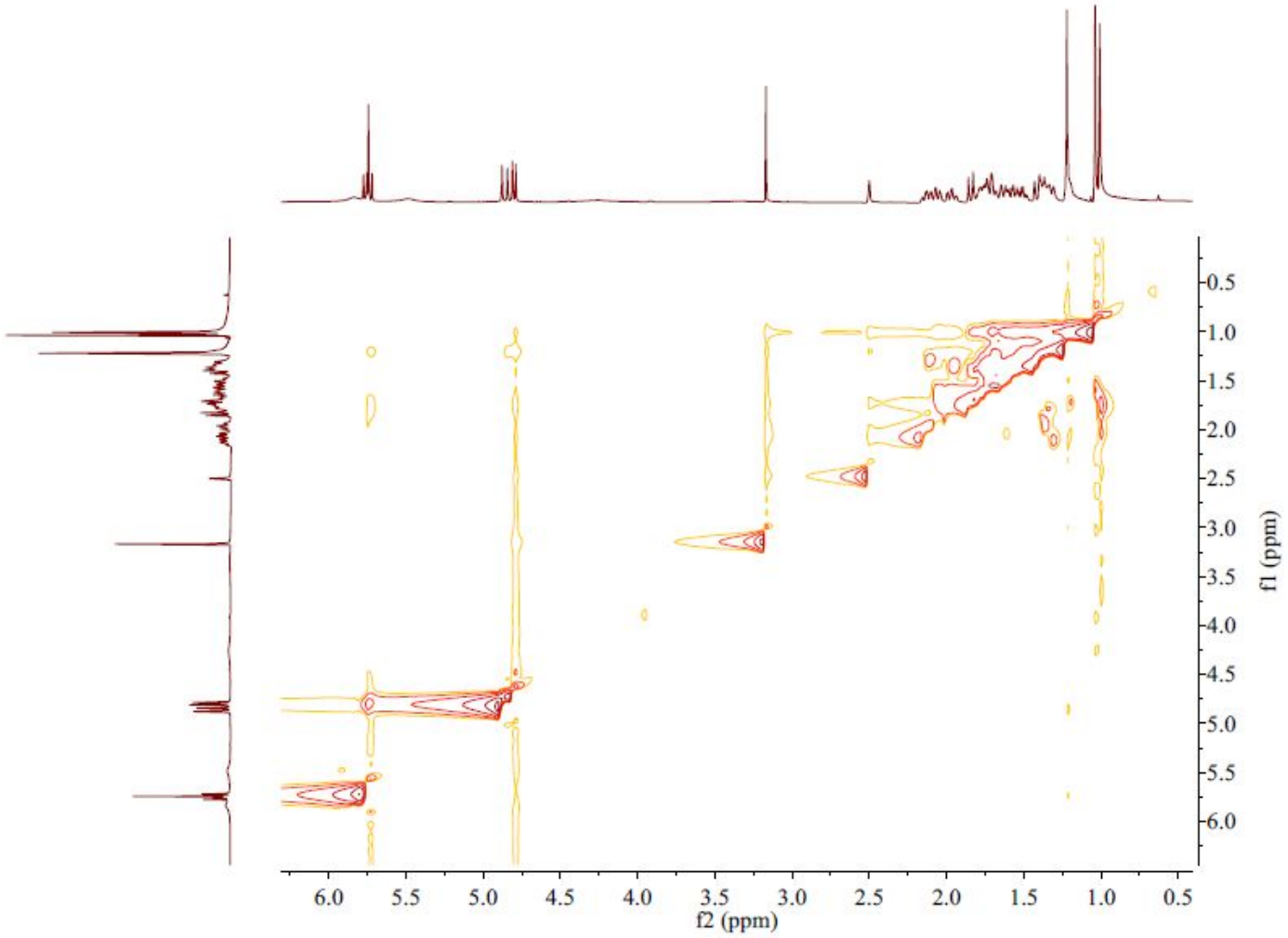

Figure S21. ECD spectrum of compound **3**

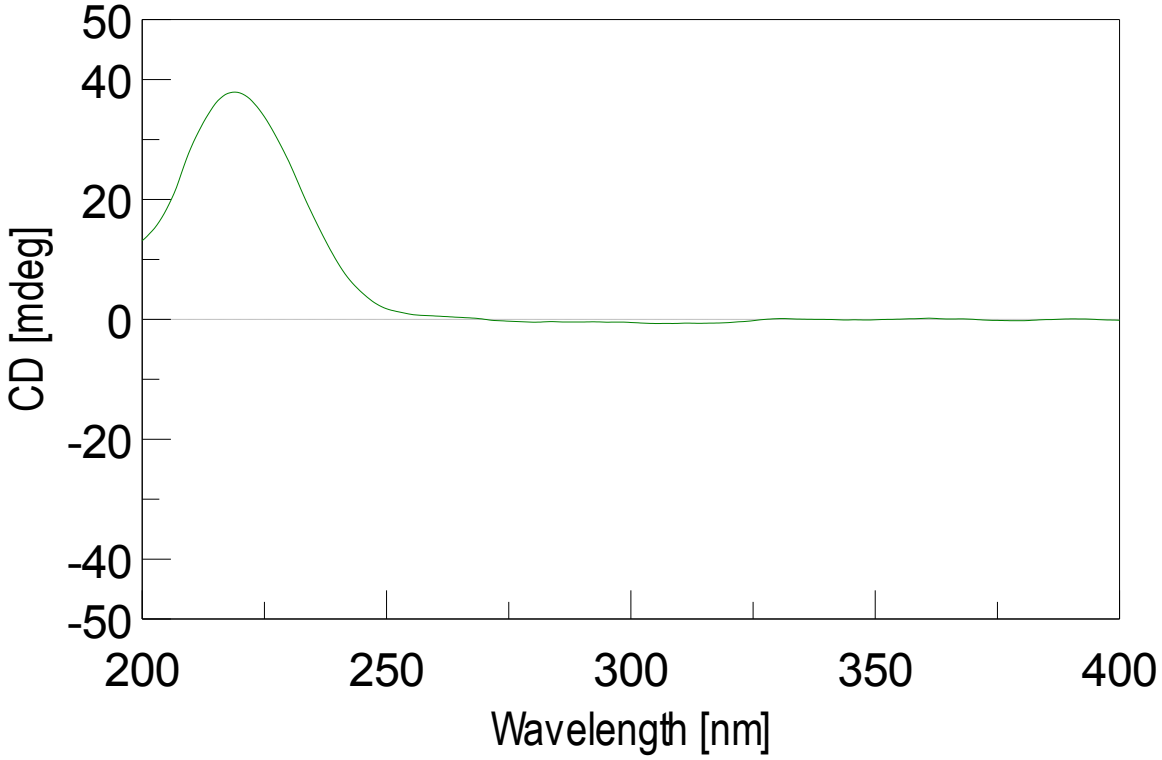

Figure S22. ^{1}H NMR (500 MHz, DMSO-d_6) spectrum of compound **4**

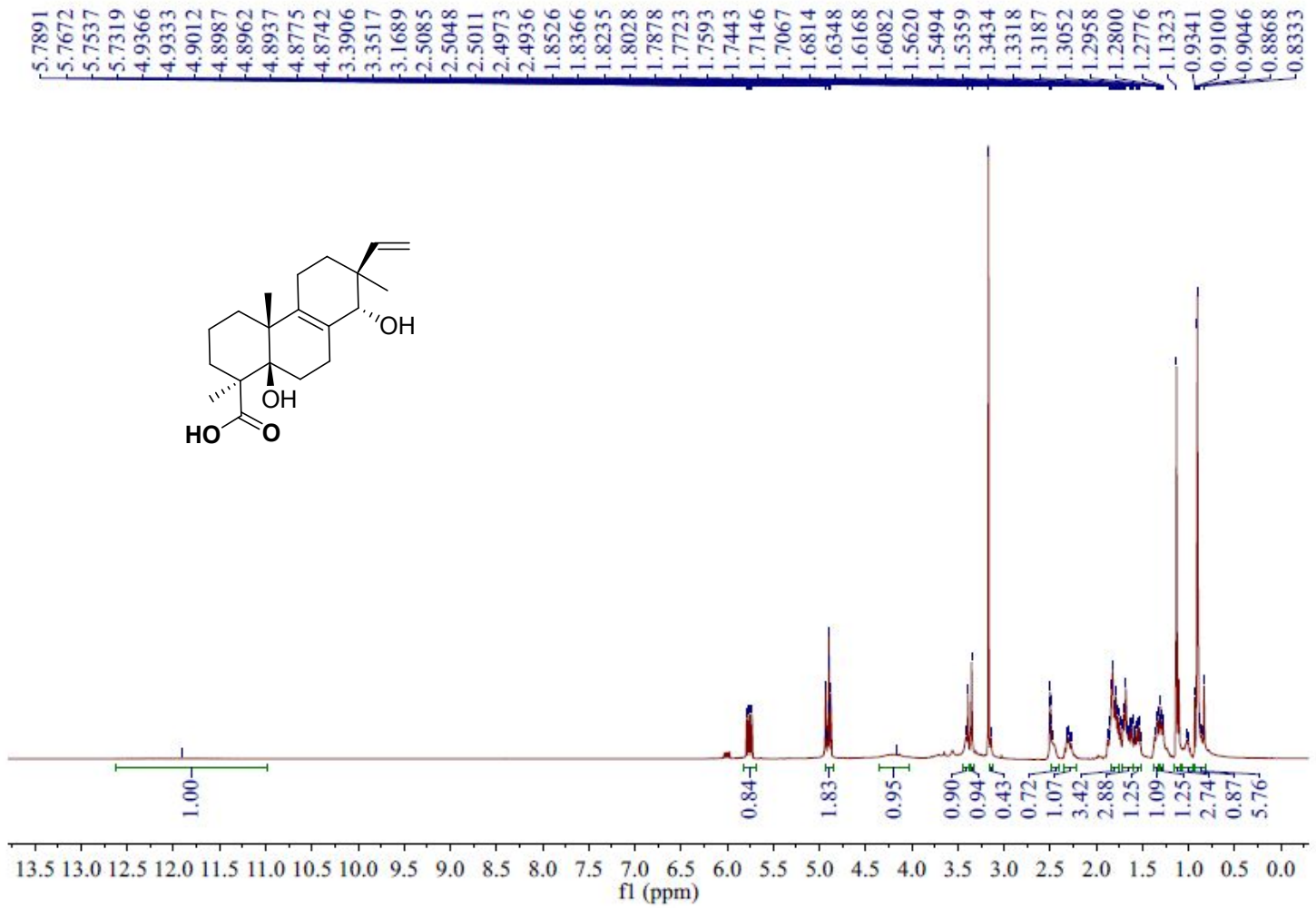

Figure S23. ^{13}C NMR (125 MHz, DMSO-d_6) and DEPT spectra of compound **4**

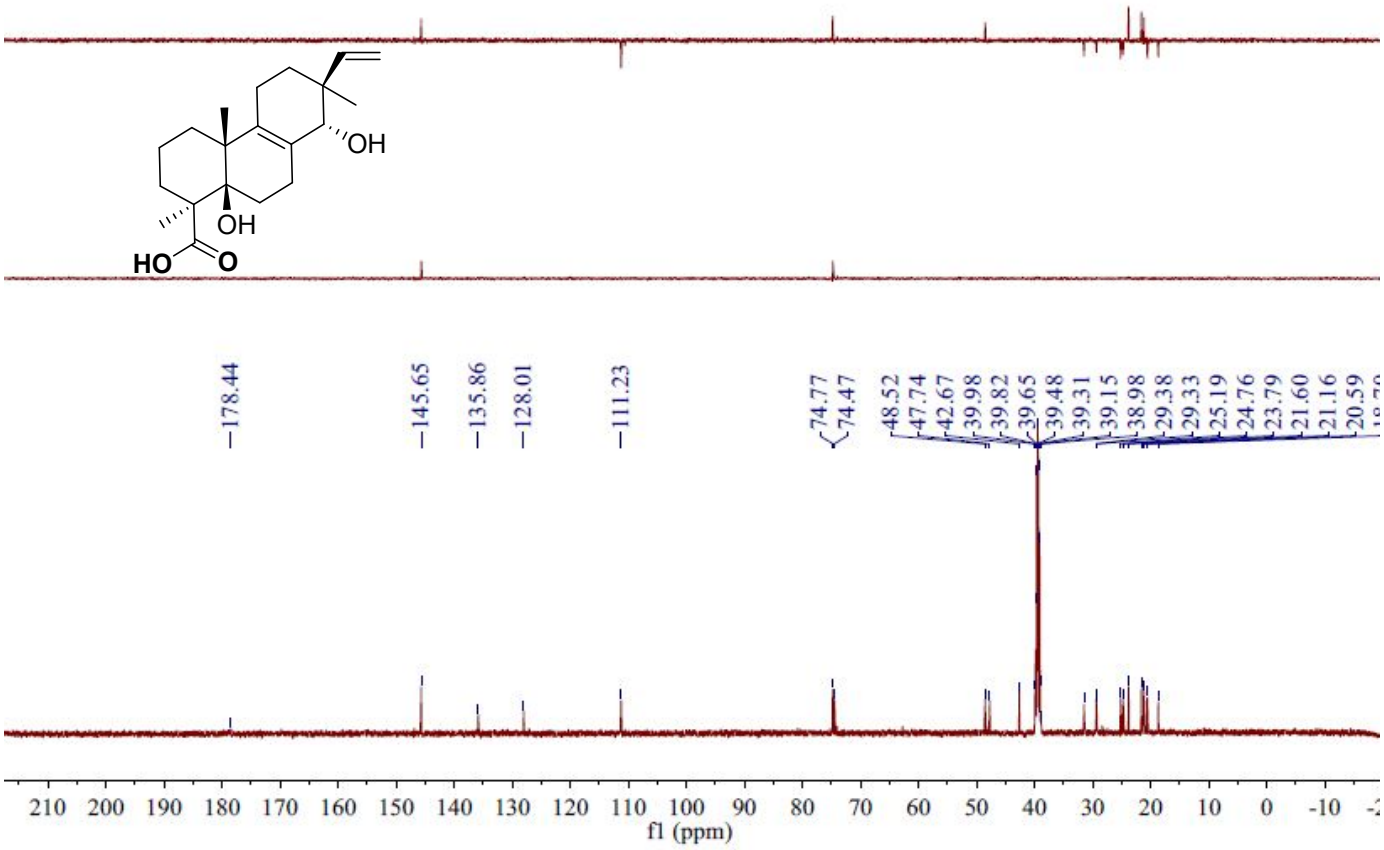

Figure S24. COSY spectrum of compound **4**

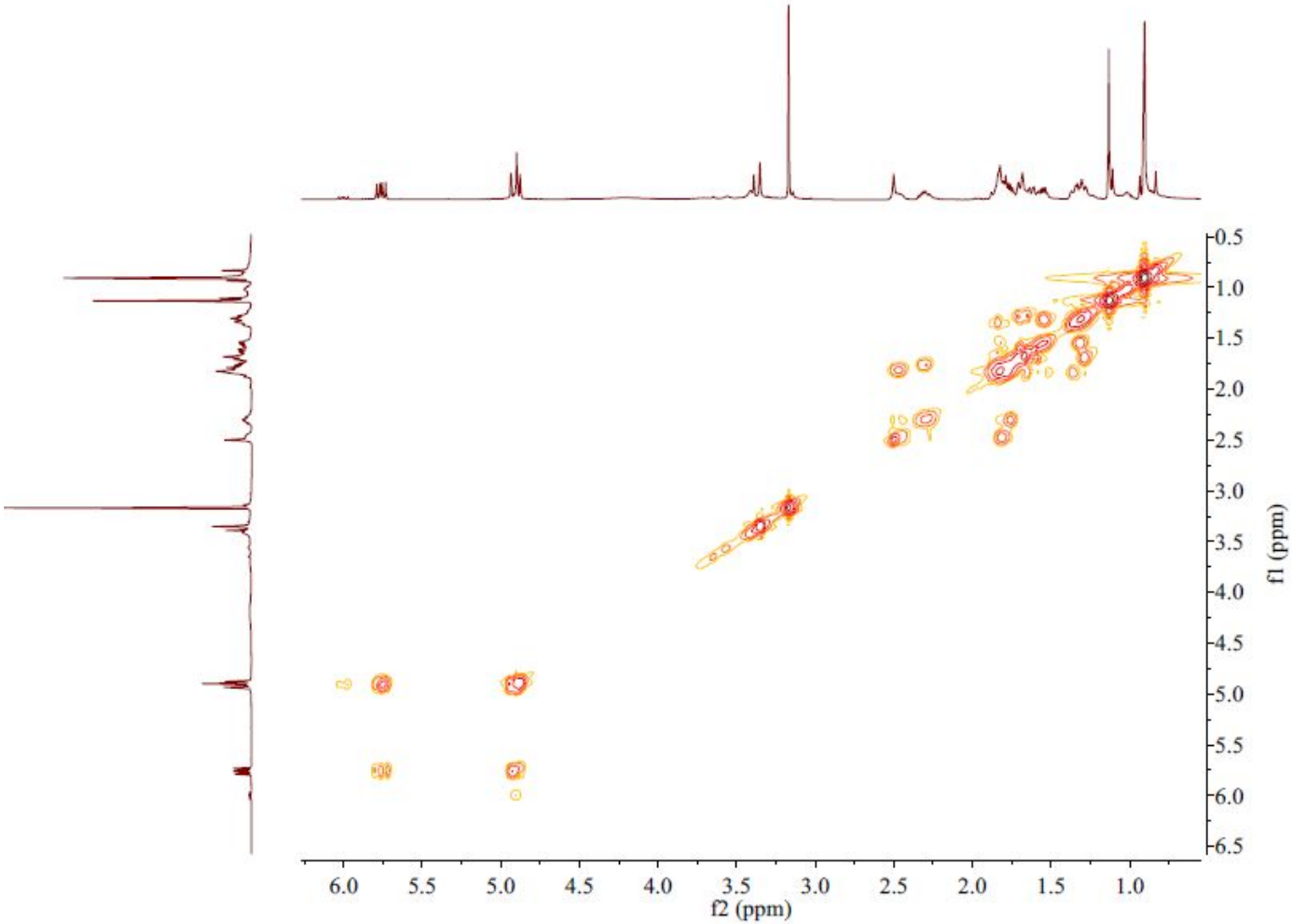

Figure S25. HSQC spectrum of compound **4**

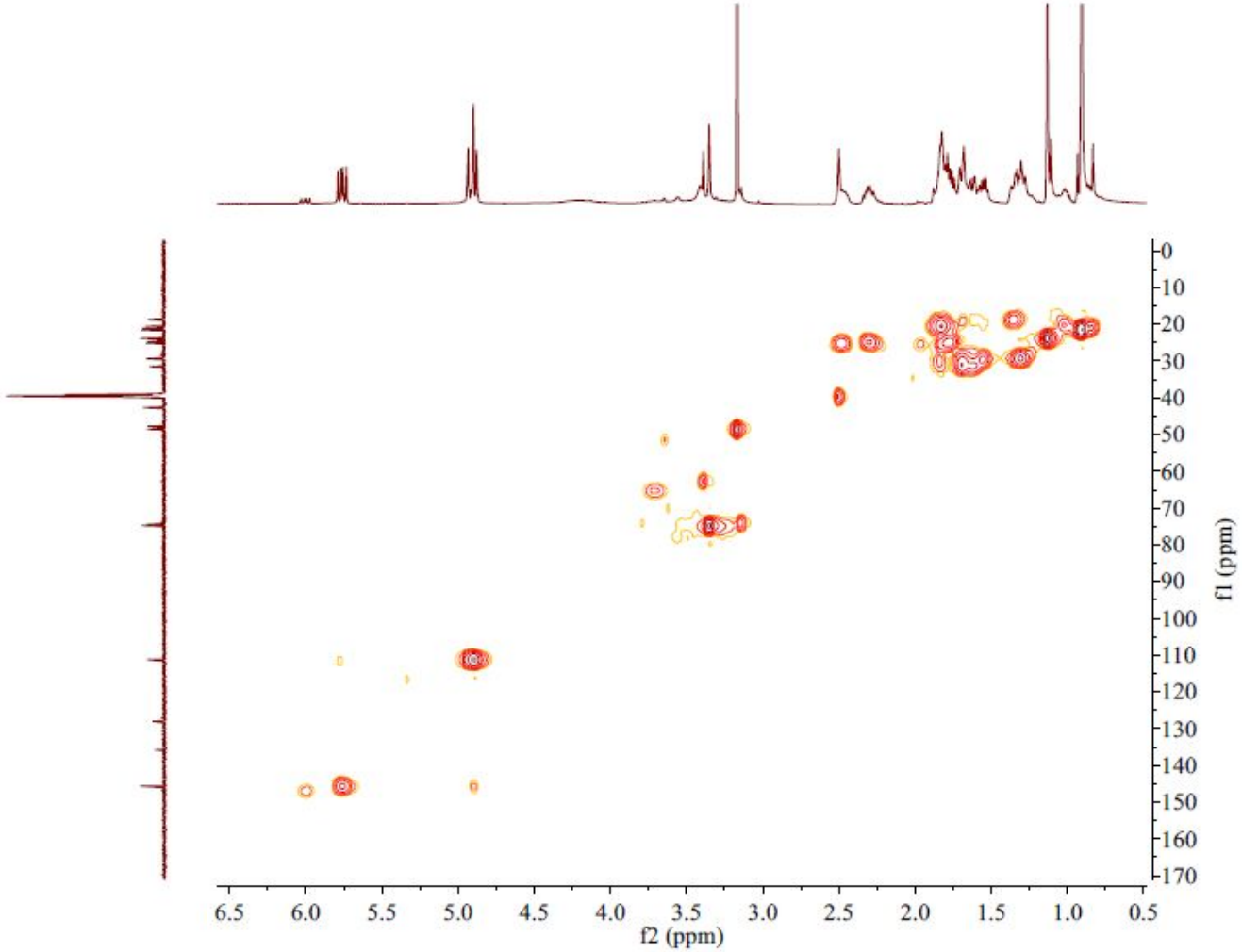

Figure S26. HMBC spectrum of compound **4**

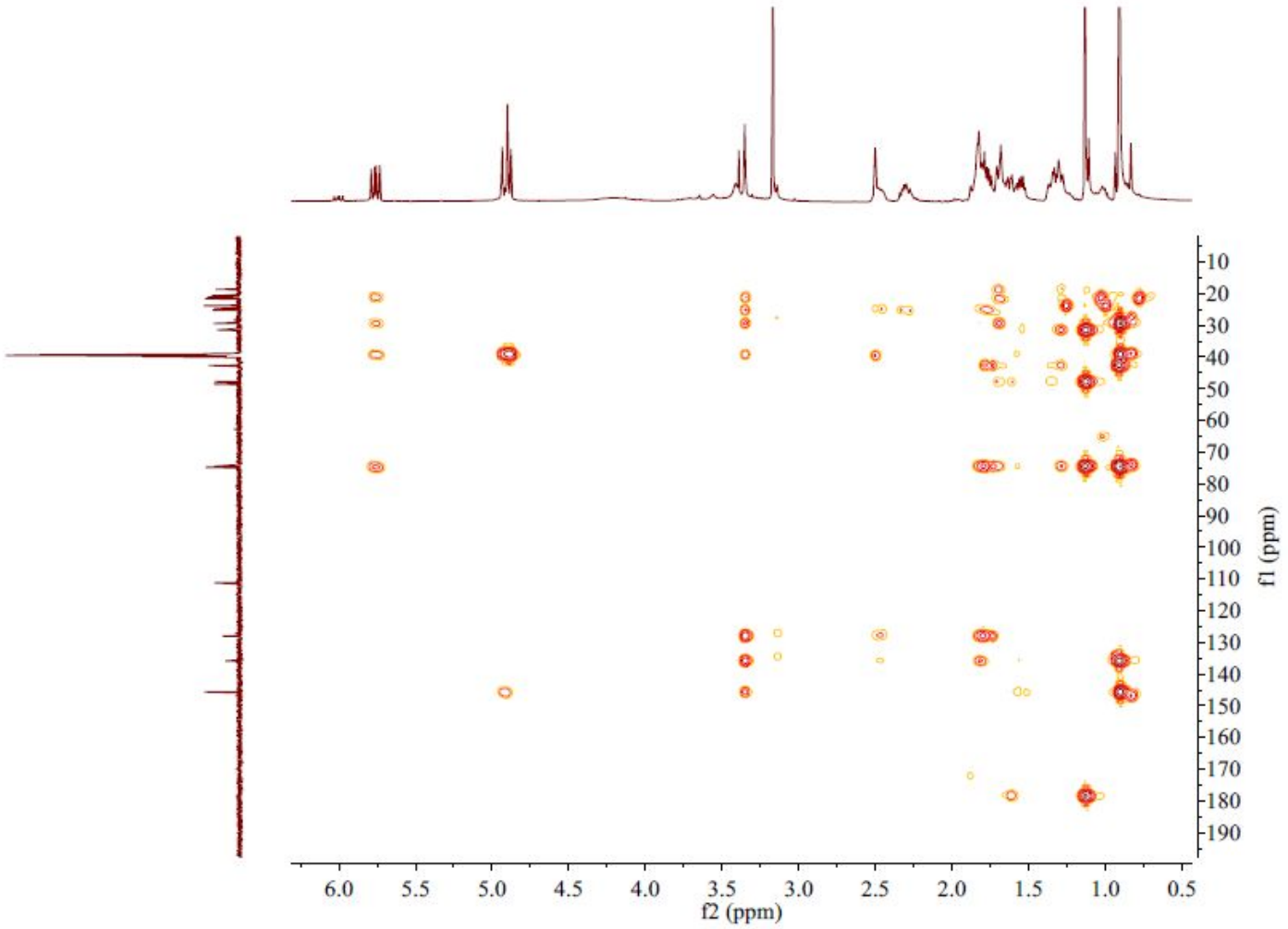

Figure S27. NOESY spectrum of compound **4**

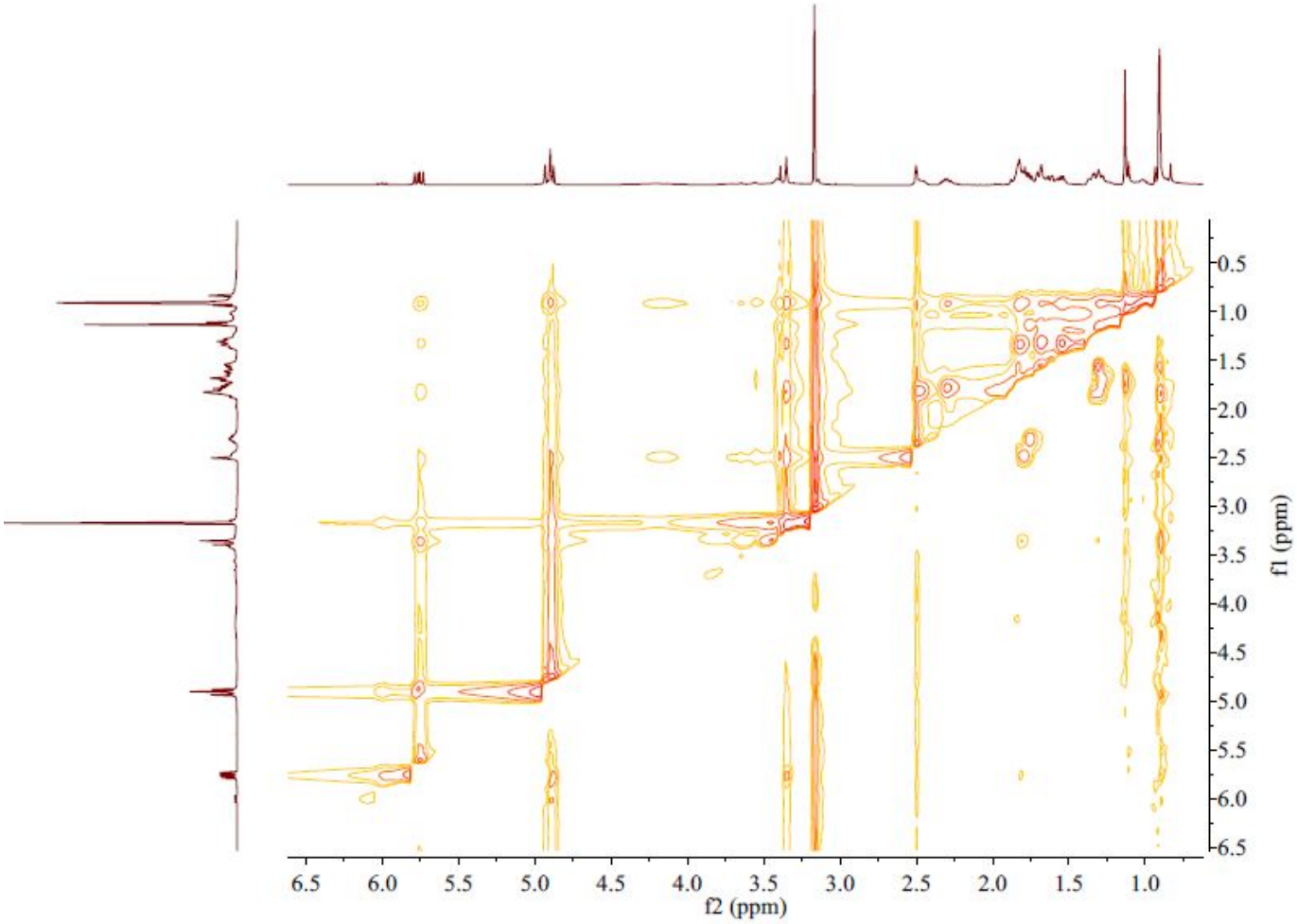

Figure S28. ECD spectrum of compound **4**

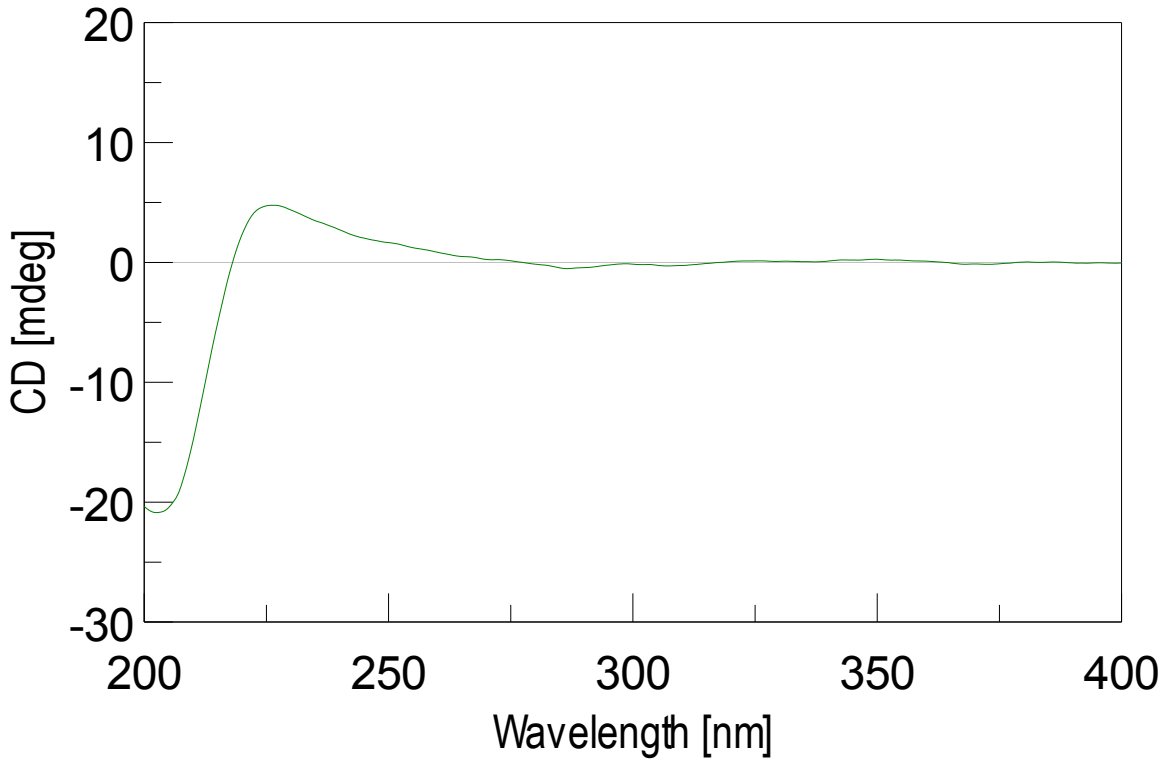

Figure S29. ^{1}H NMR (600 MHz, DMSO-d_6) spectrum of compound **5**

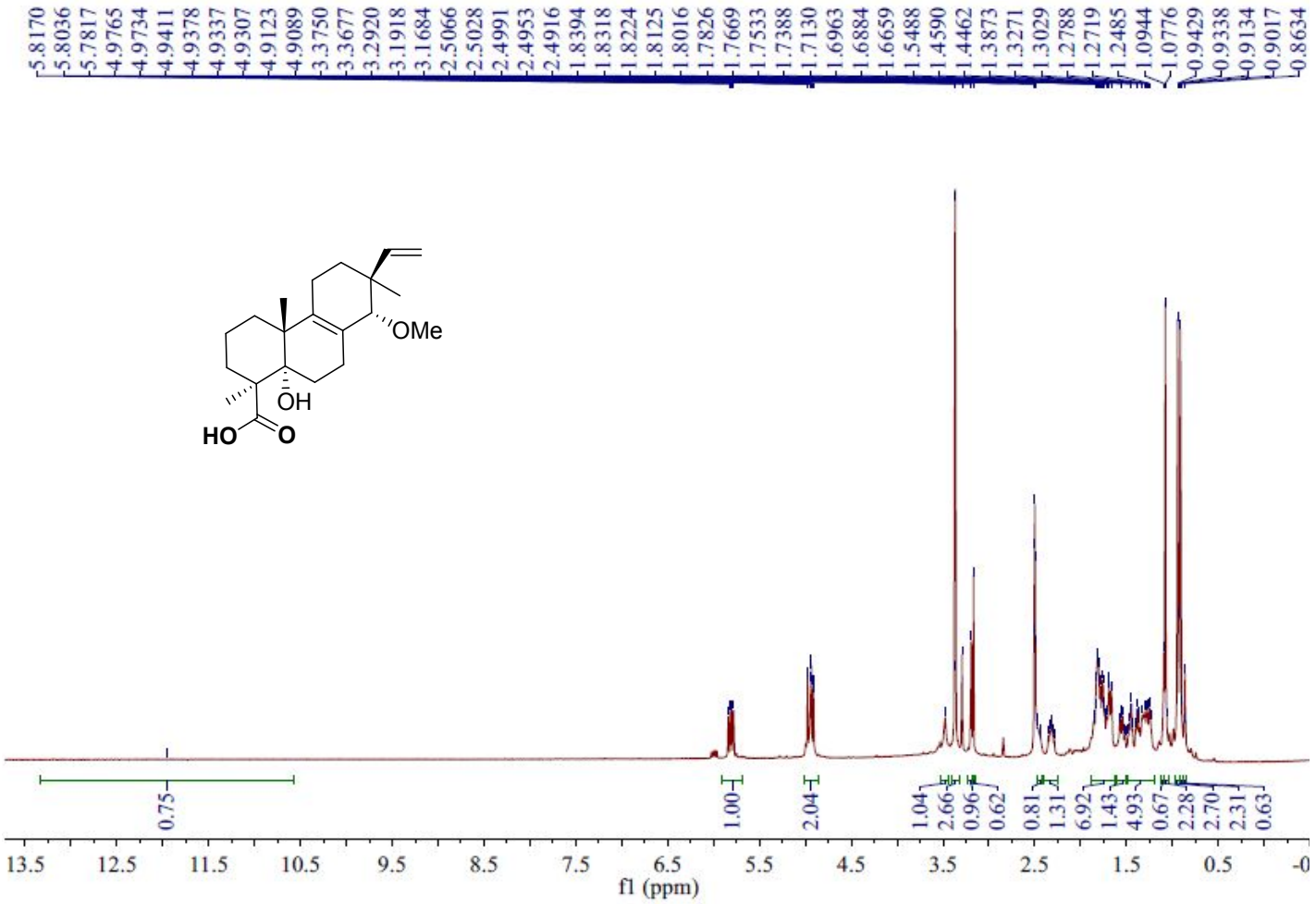

Figure S30. ^{13}C NMR (150 MHz, DMSO-d_6) and DEPT spectra of compound **5**

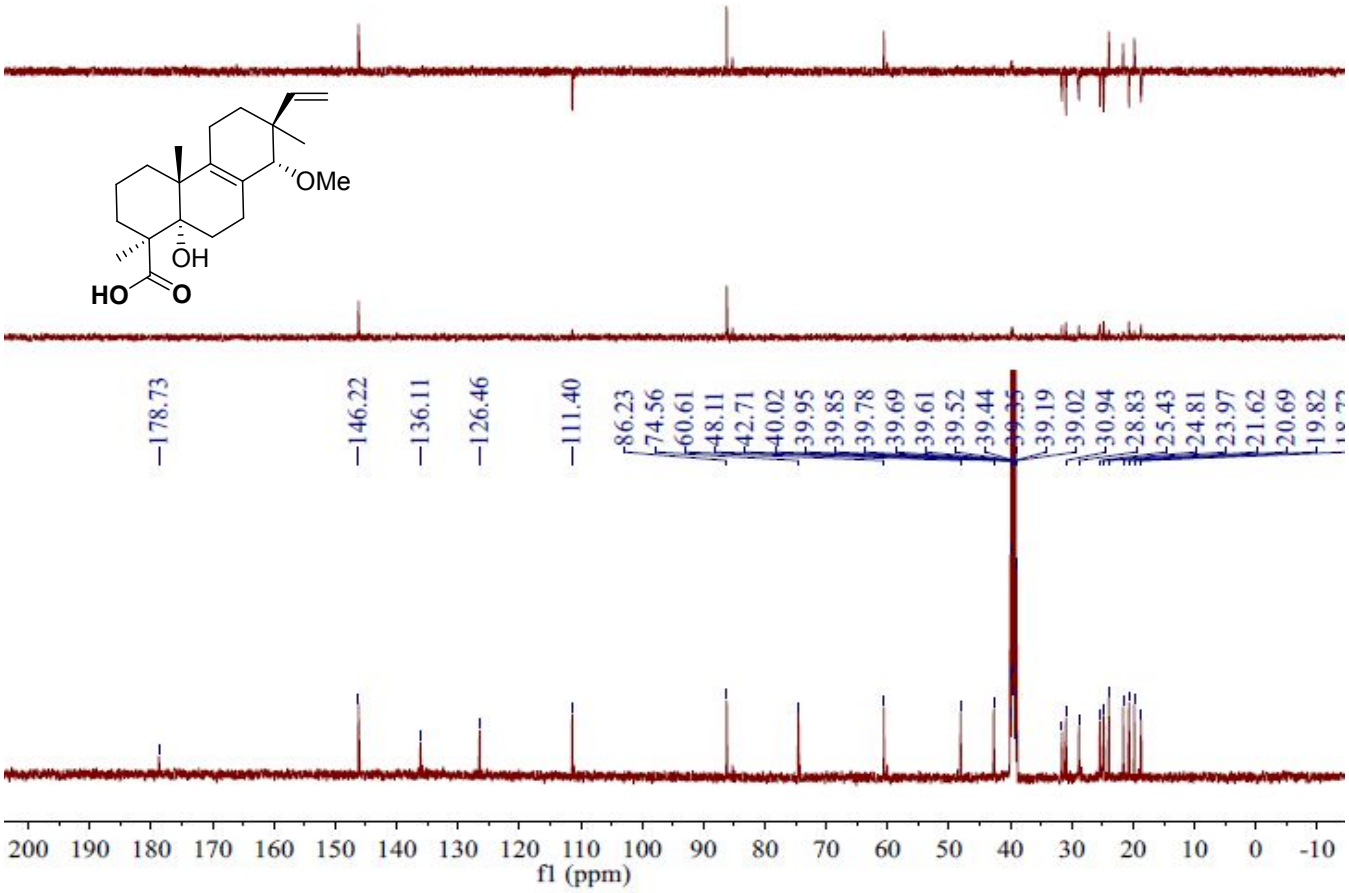

Figure S31. COSY spectrum of compound **5**

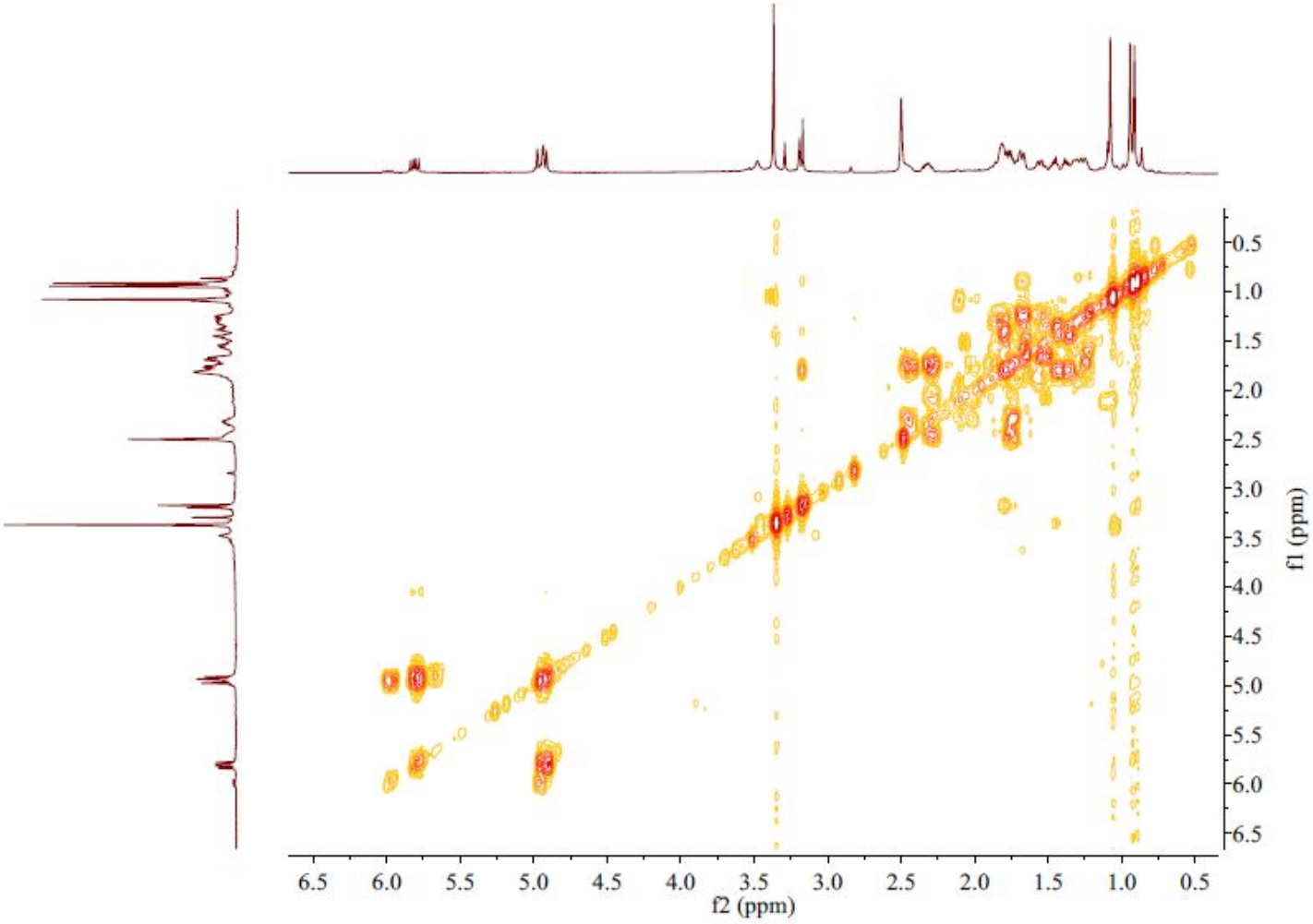

Figure S32. HSQC spectrum of compound **5**

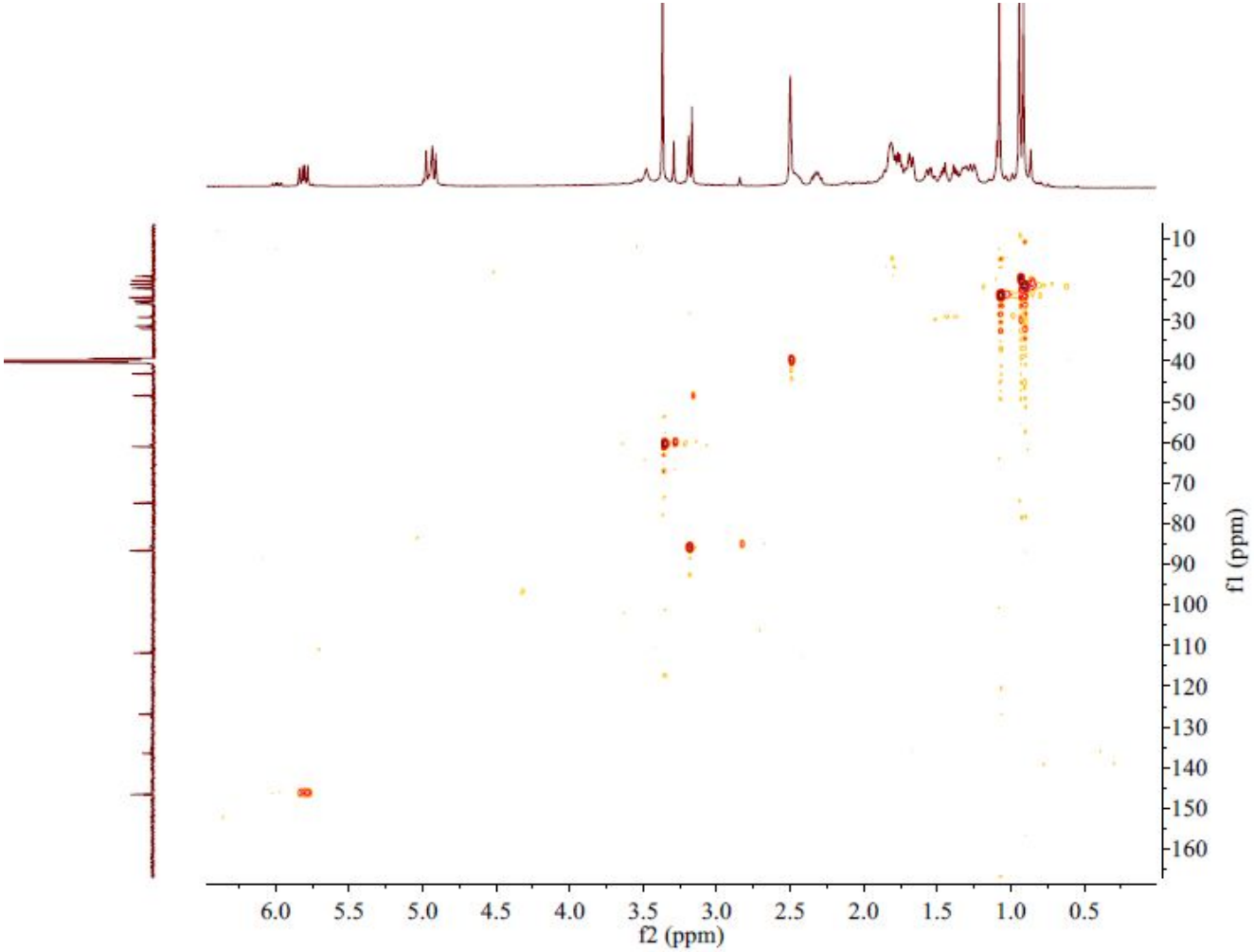

Figure S33. HMBC spectrum of compound **5**

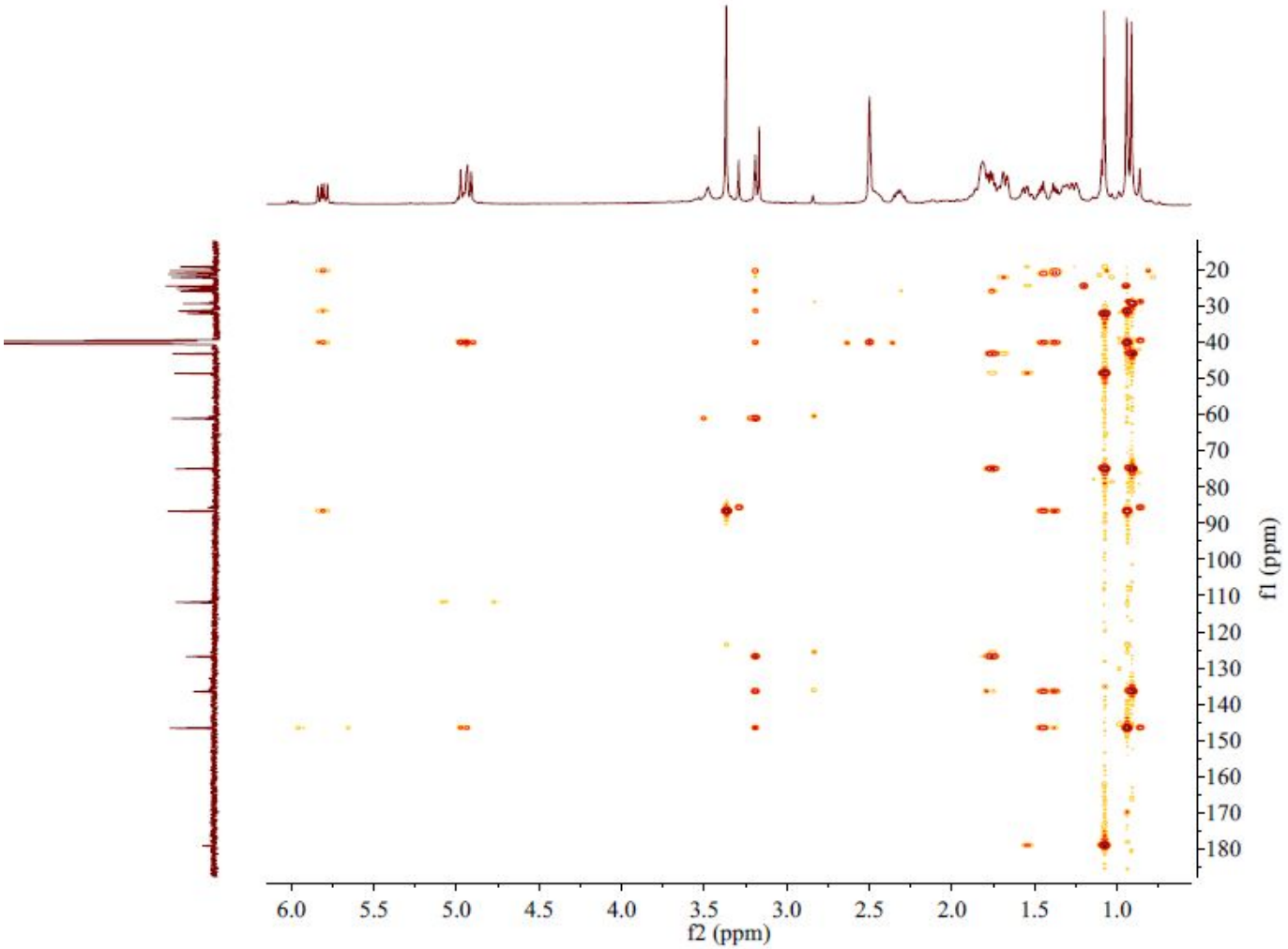

Figure S34. NOESY spectrum of compound **5**

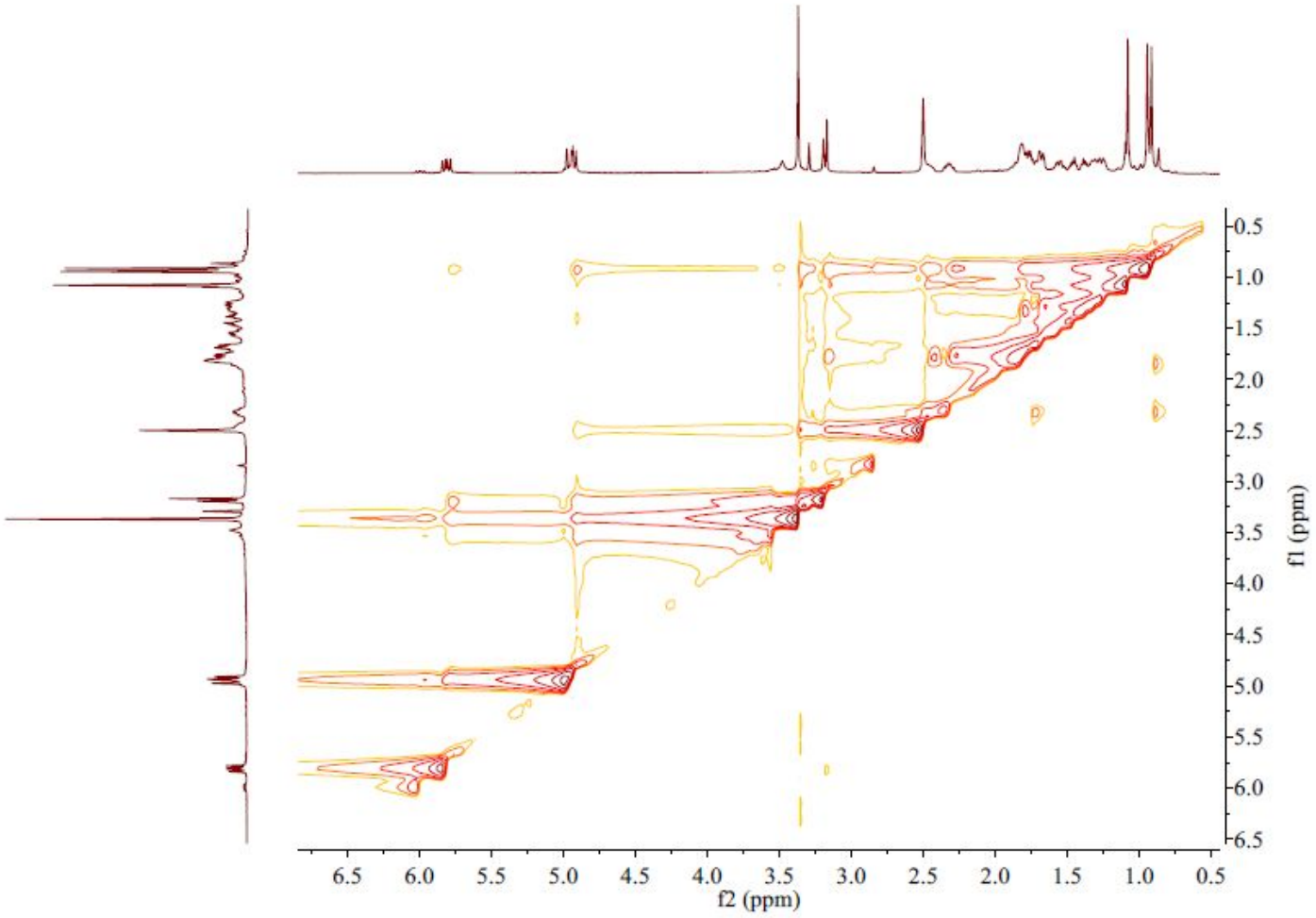

Figure S35. ECD spectrum of compound **5**

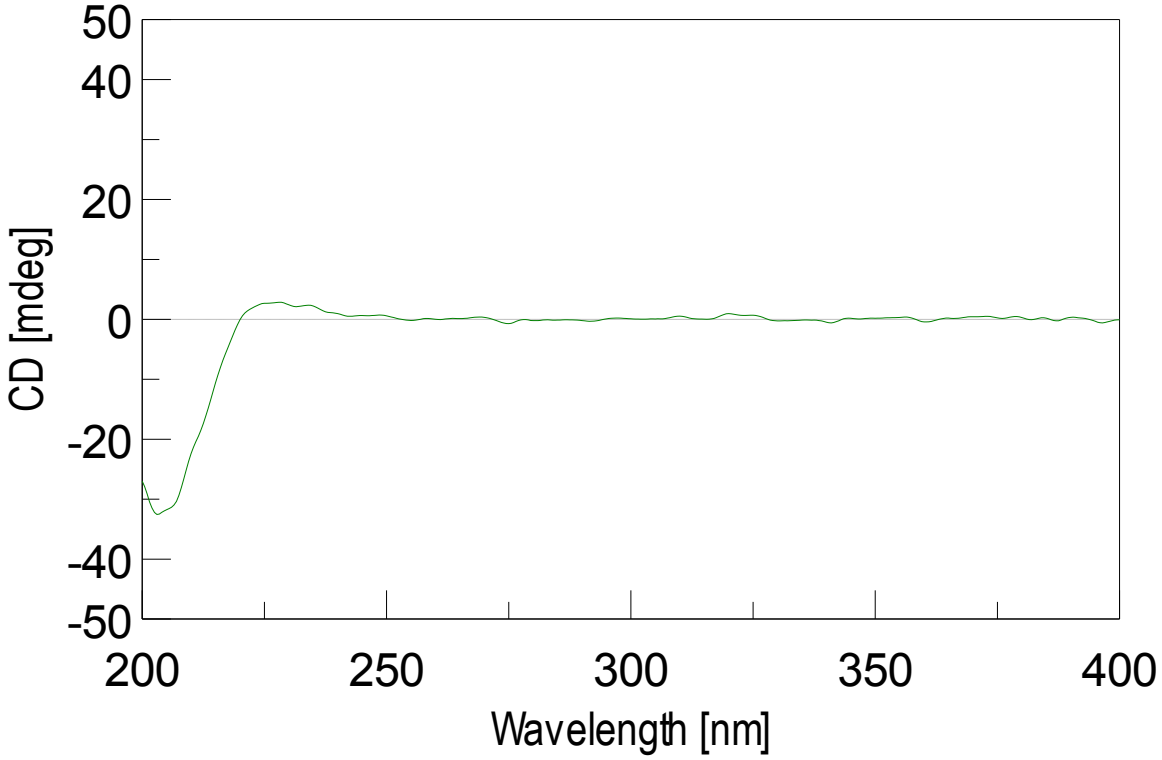

Figure S36. ^{1}H NMR (500 MHz, DMSO-d_6) spectrum of compound **6**

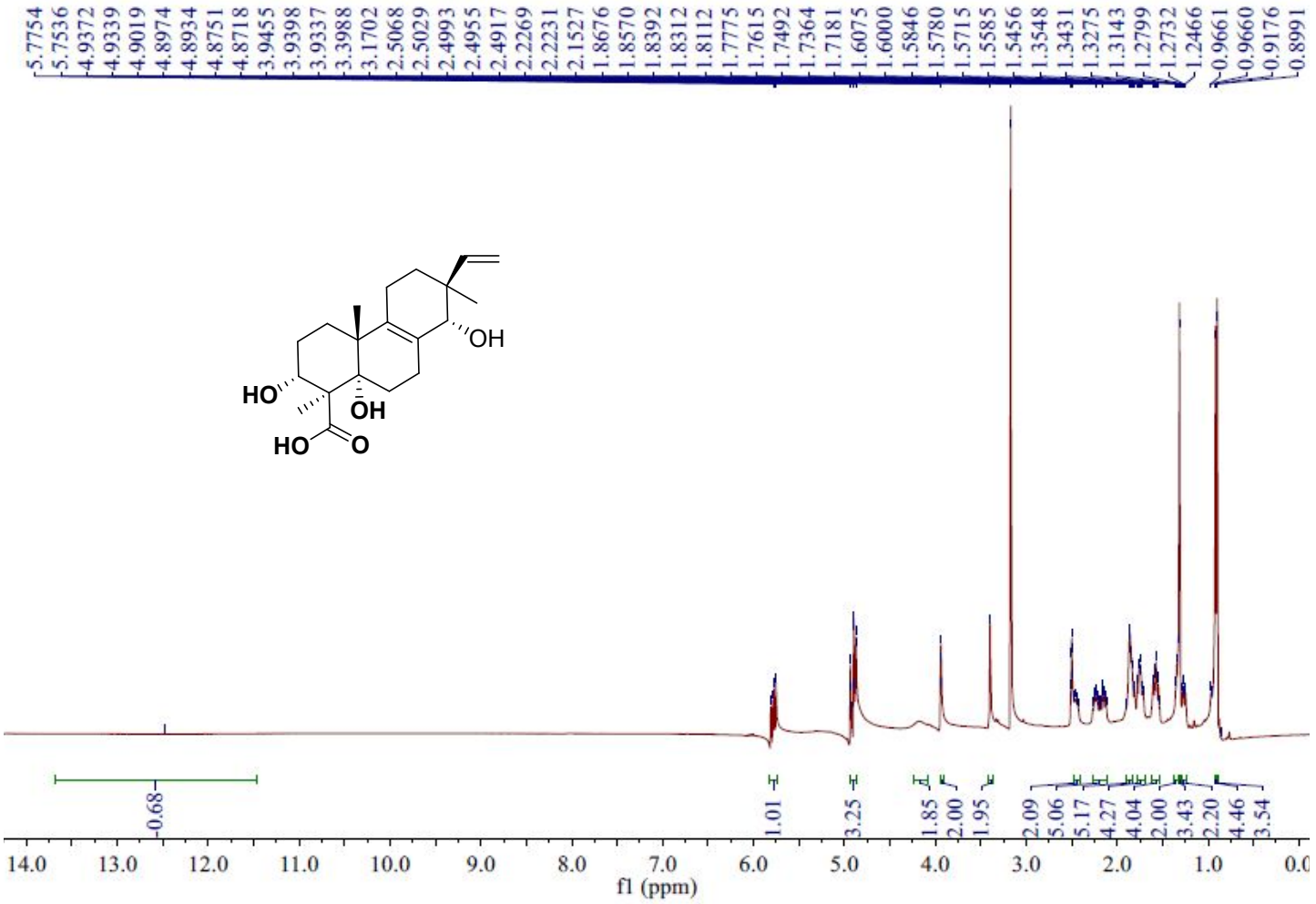

Figure S37. ^{13}C NMR (125 MHz, DMSO-d_6) and DEPT spectra of compound **6**

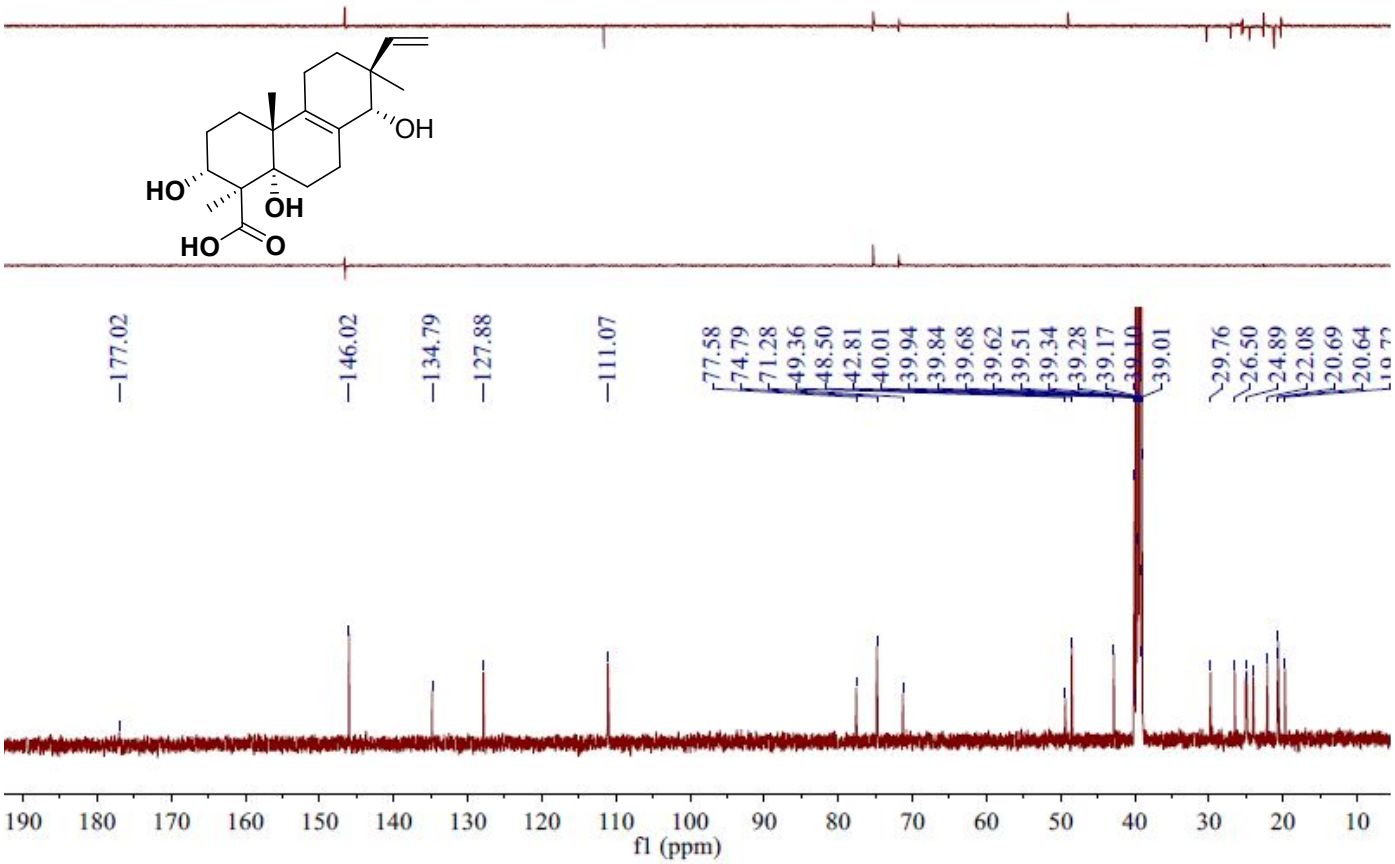

Figure S38. COSY spectrum of compound **6**

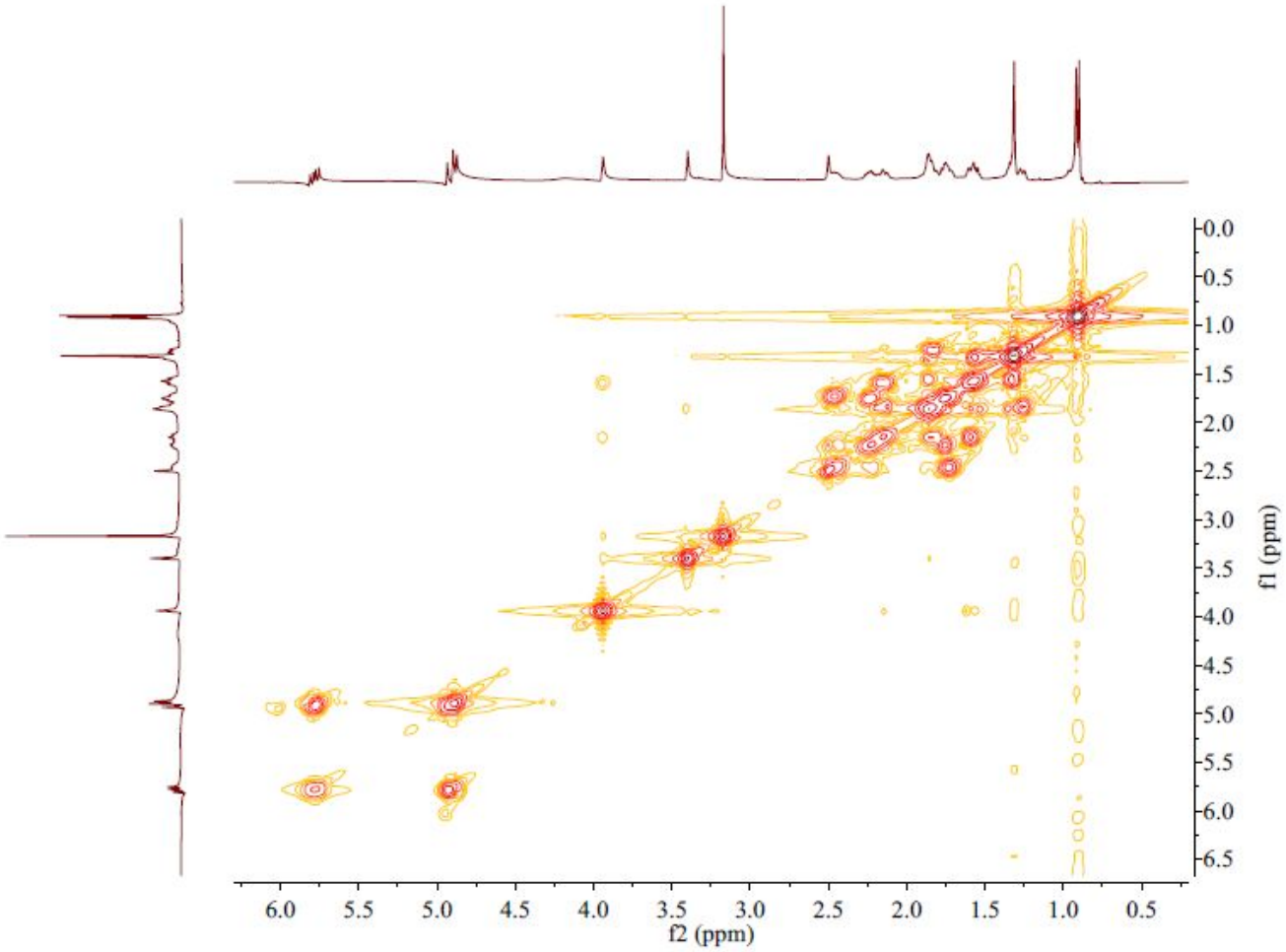

Figure S39. HSQC spectrum of compound **6**

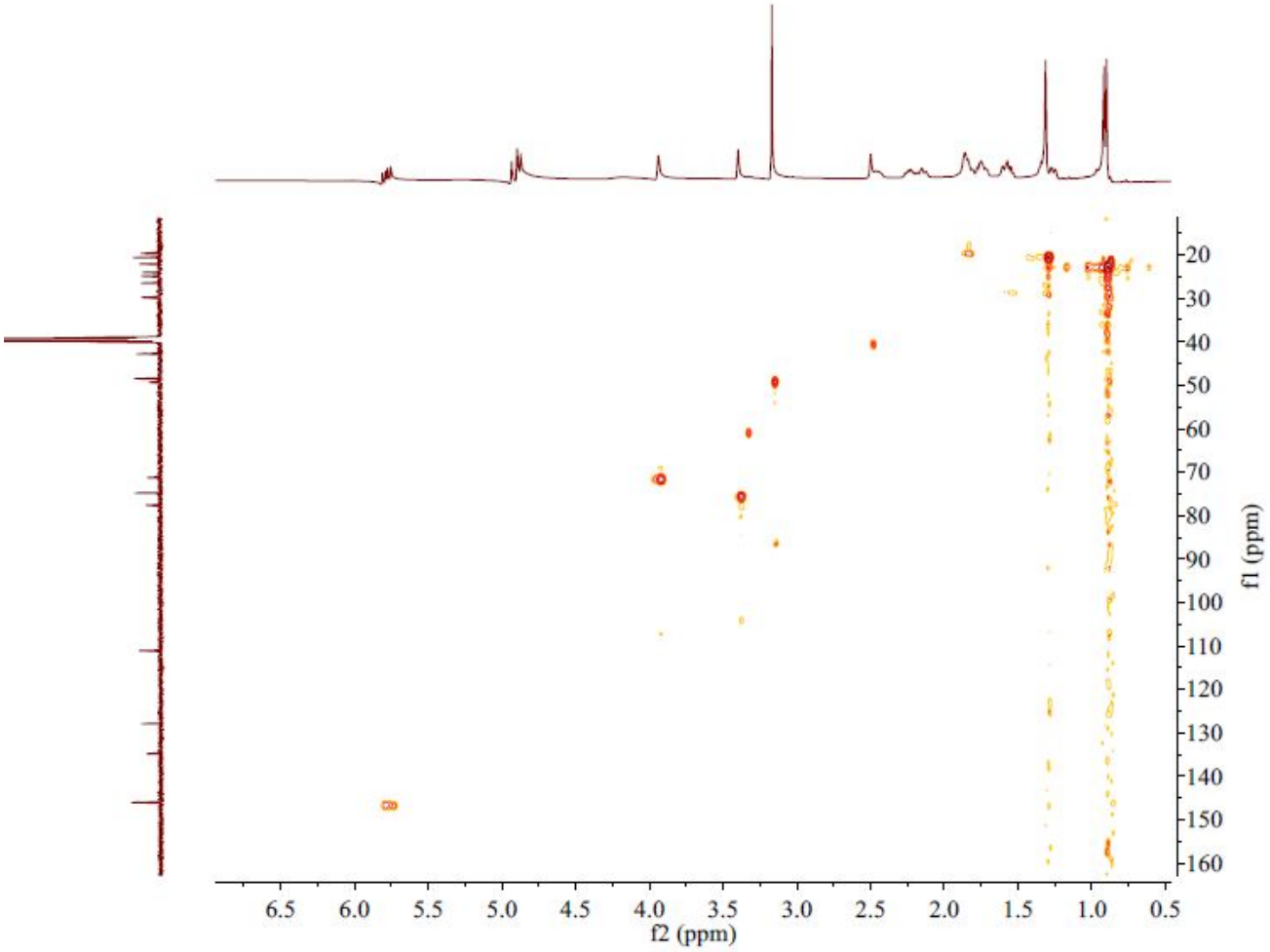

Figure S40. HMBC spectrum of compound **6**

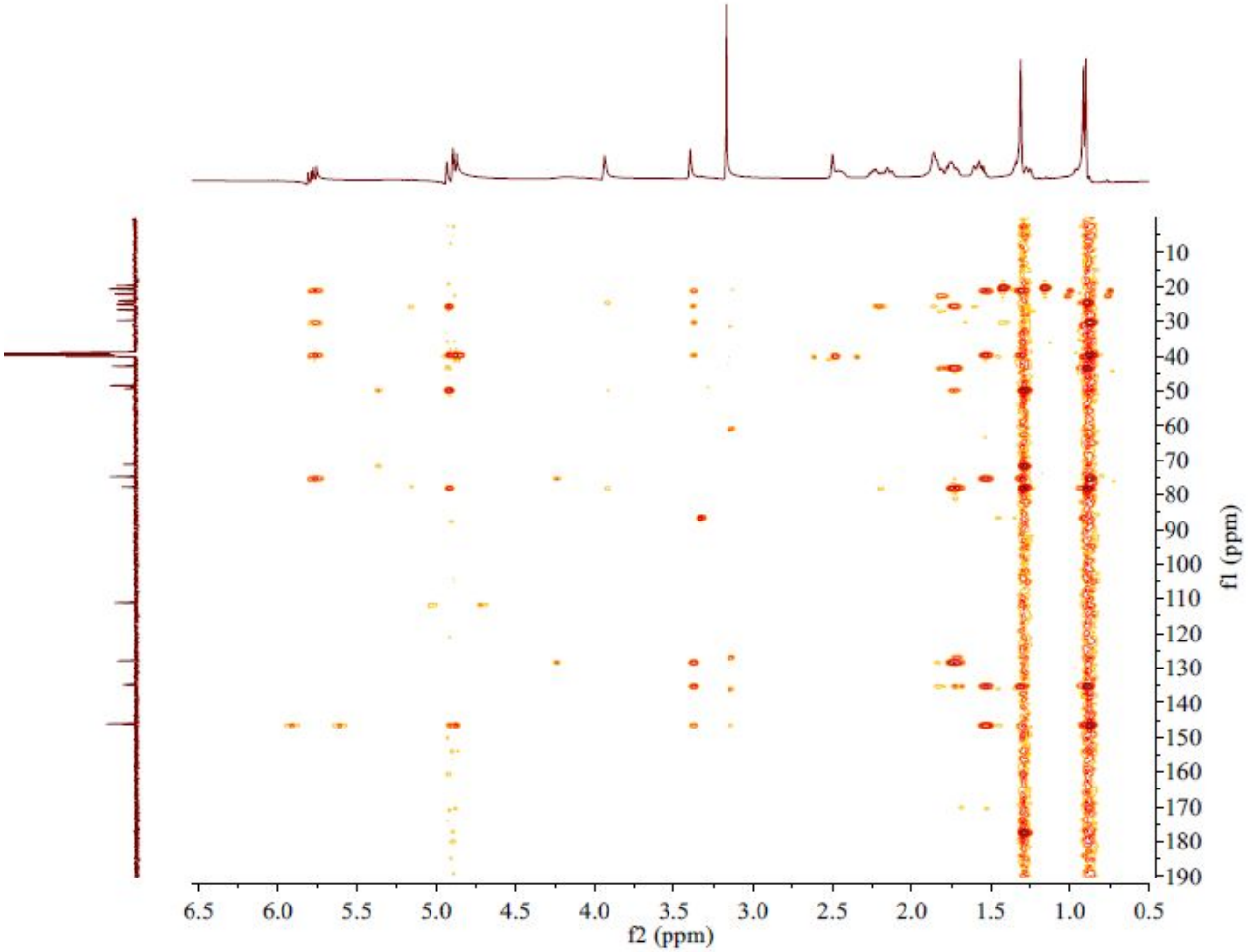

Figure S41. NOESY spectrum of compound **6**

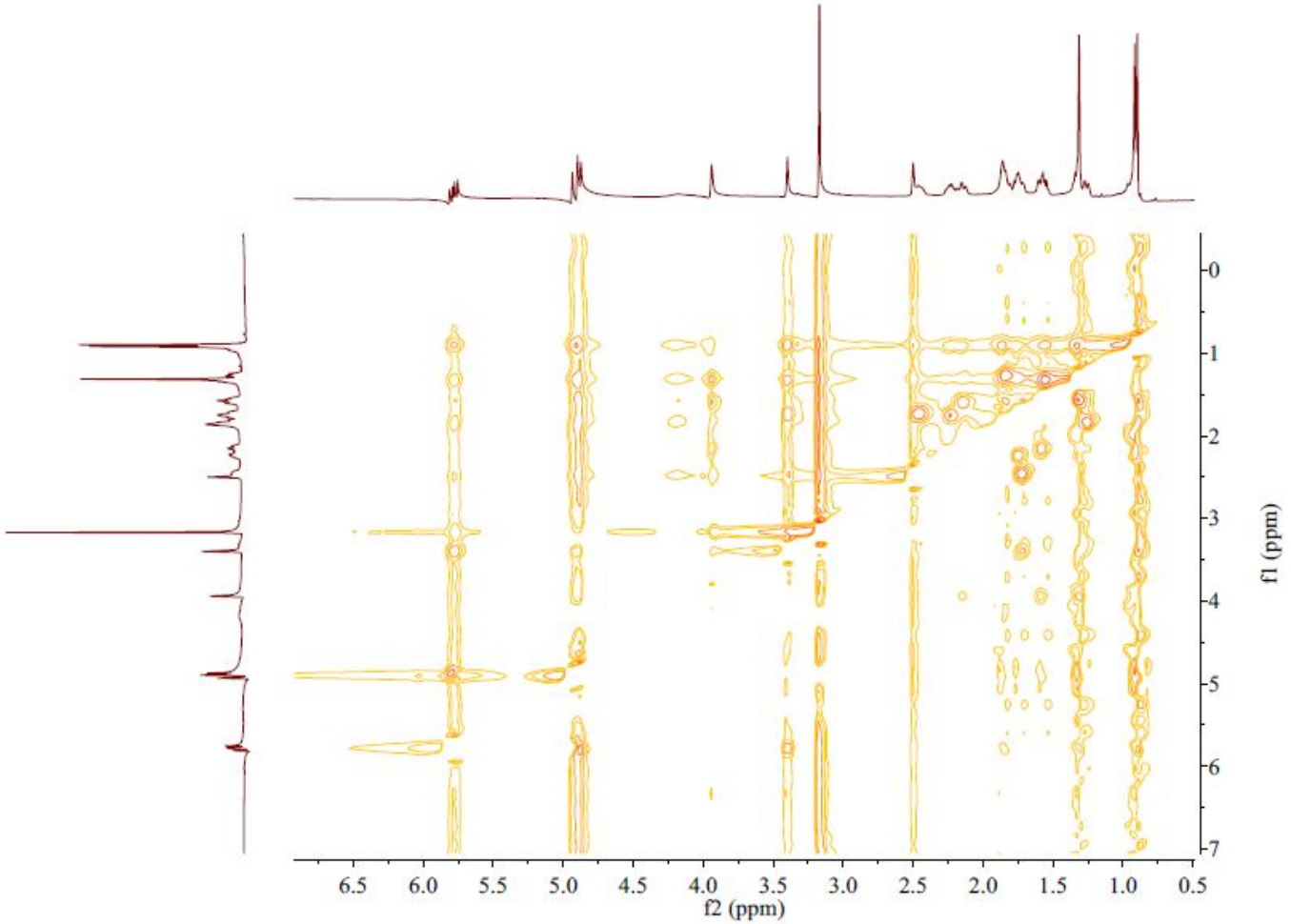

Figure S42. ECD spectrum of compound **6**

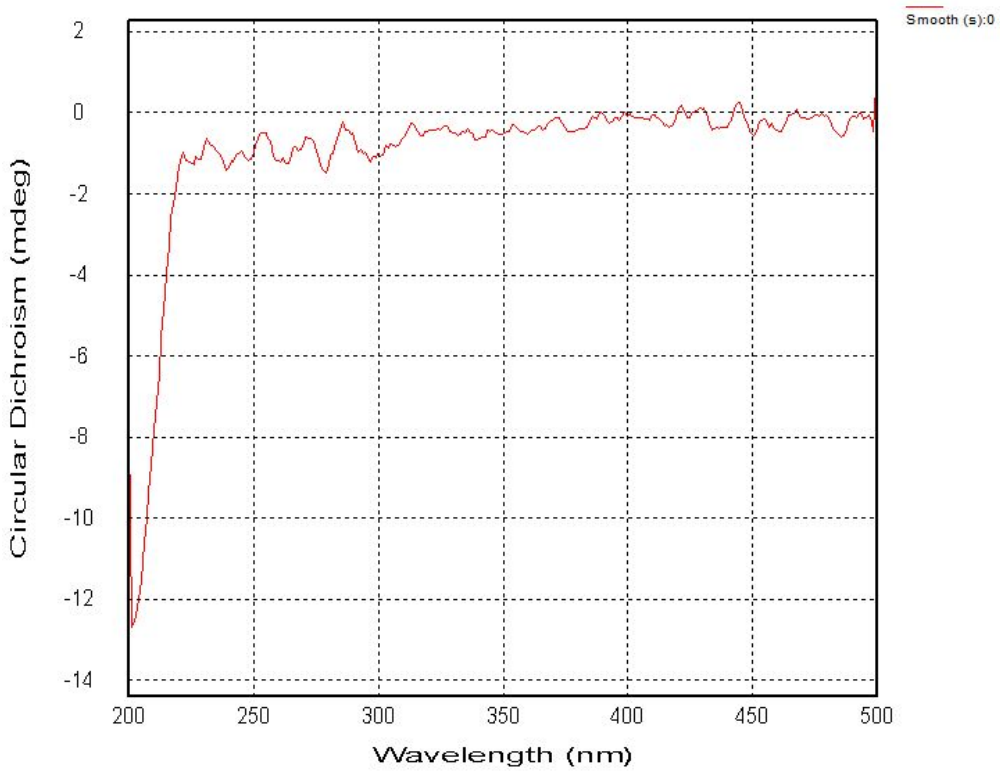

Figure S43. ^{1}H NMR (600 MHz, DMSO-d_6) spectrum of compound **7**

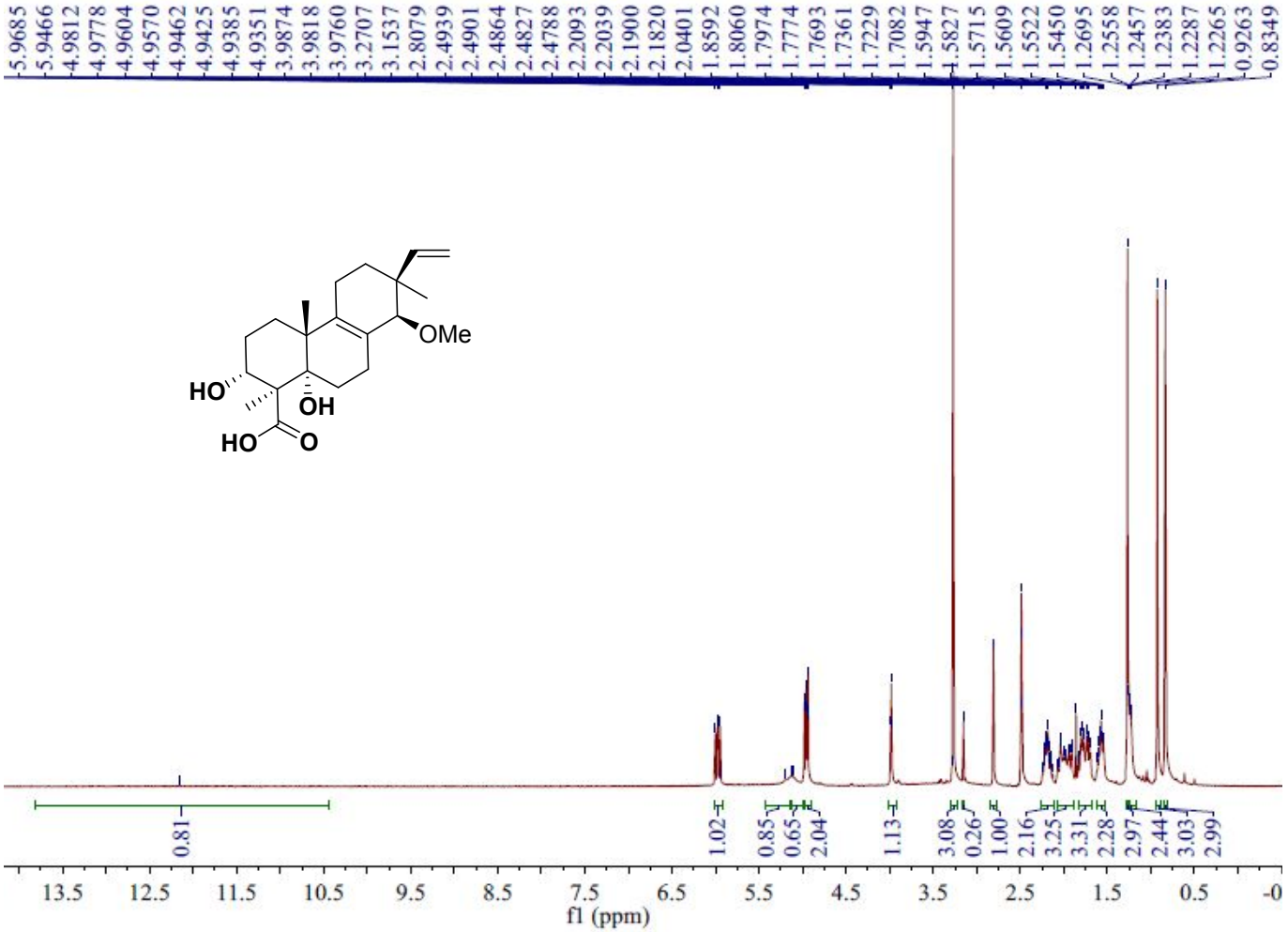

Figure S44. ^{13}C NMR (150 MHz, DMSO-d_6) and DEPT spectra of compound **7**

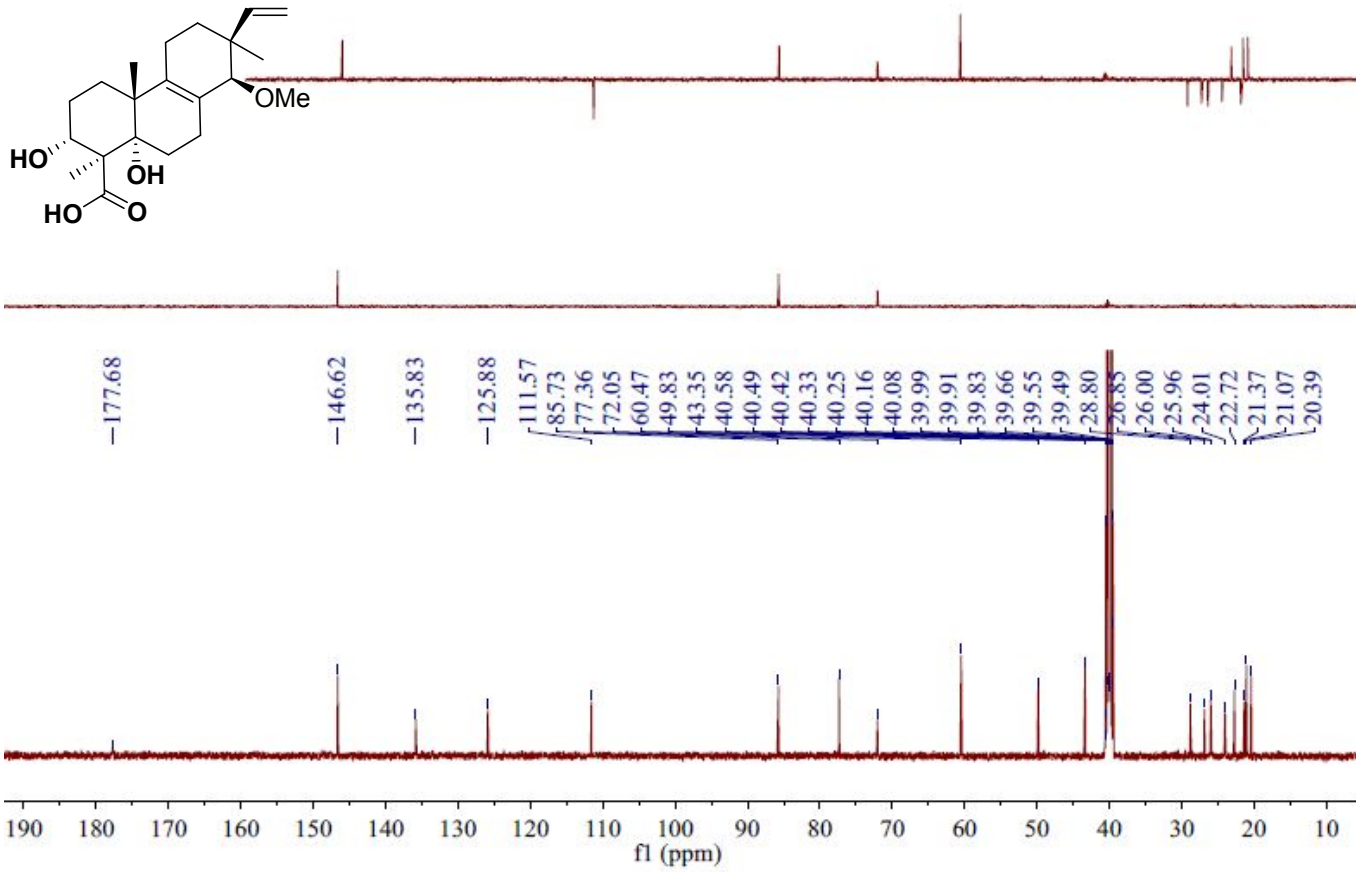

Figure S45. COSY spectrum of compound **7**

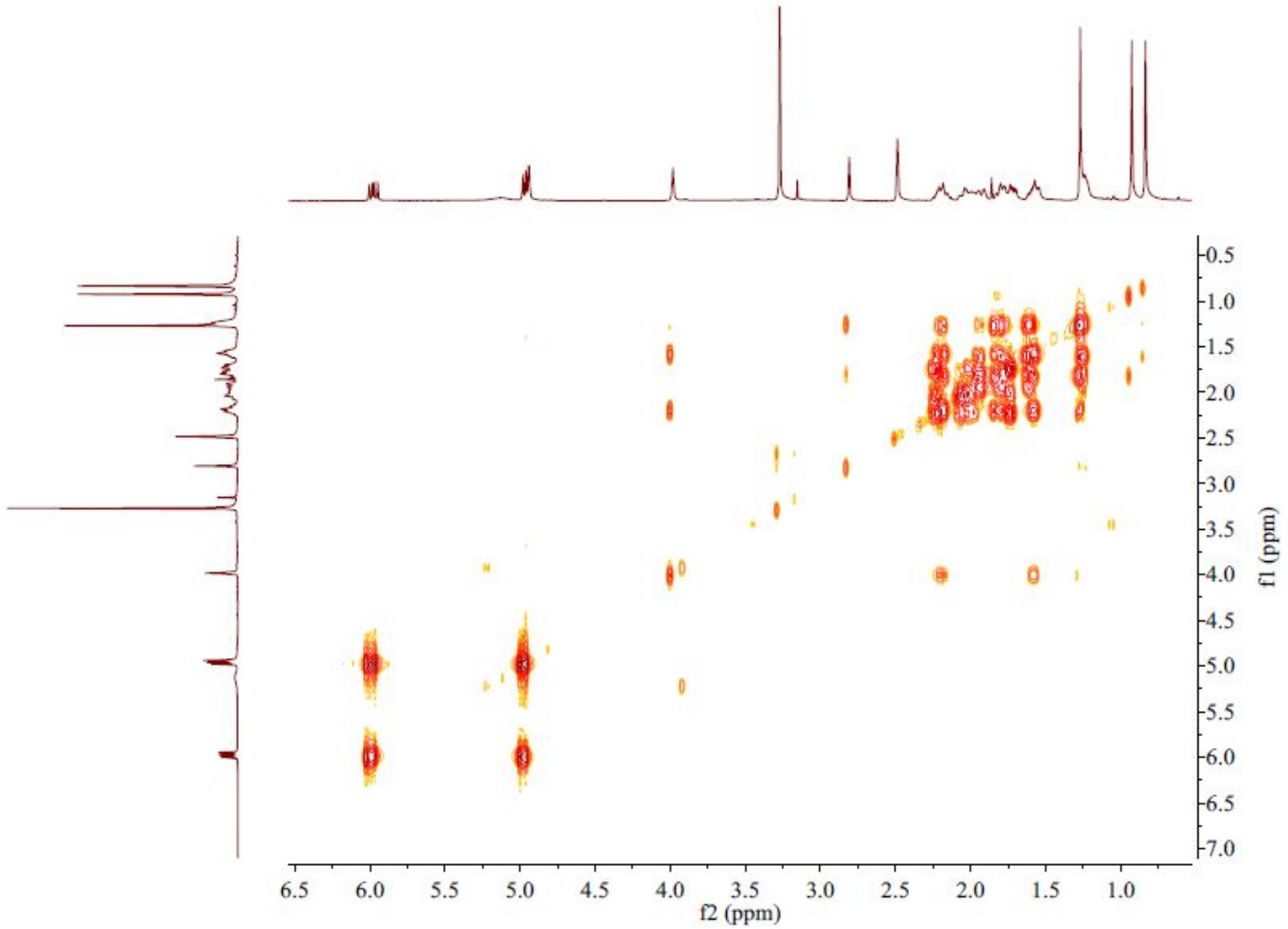

Figure S46. HSQC spectrum of compound **7**

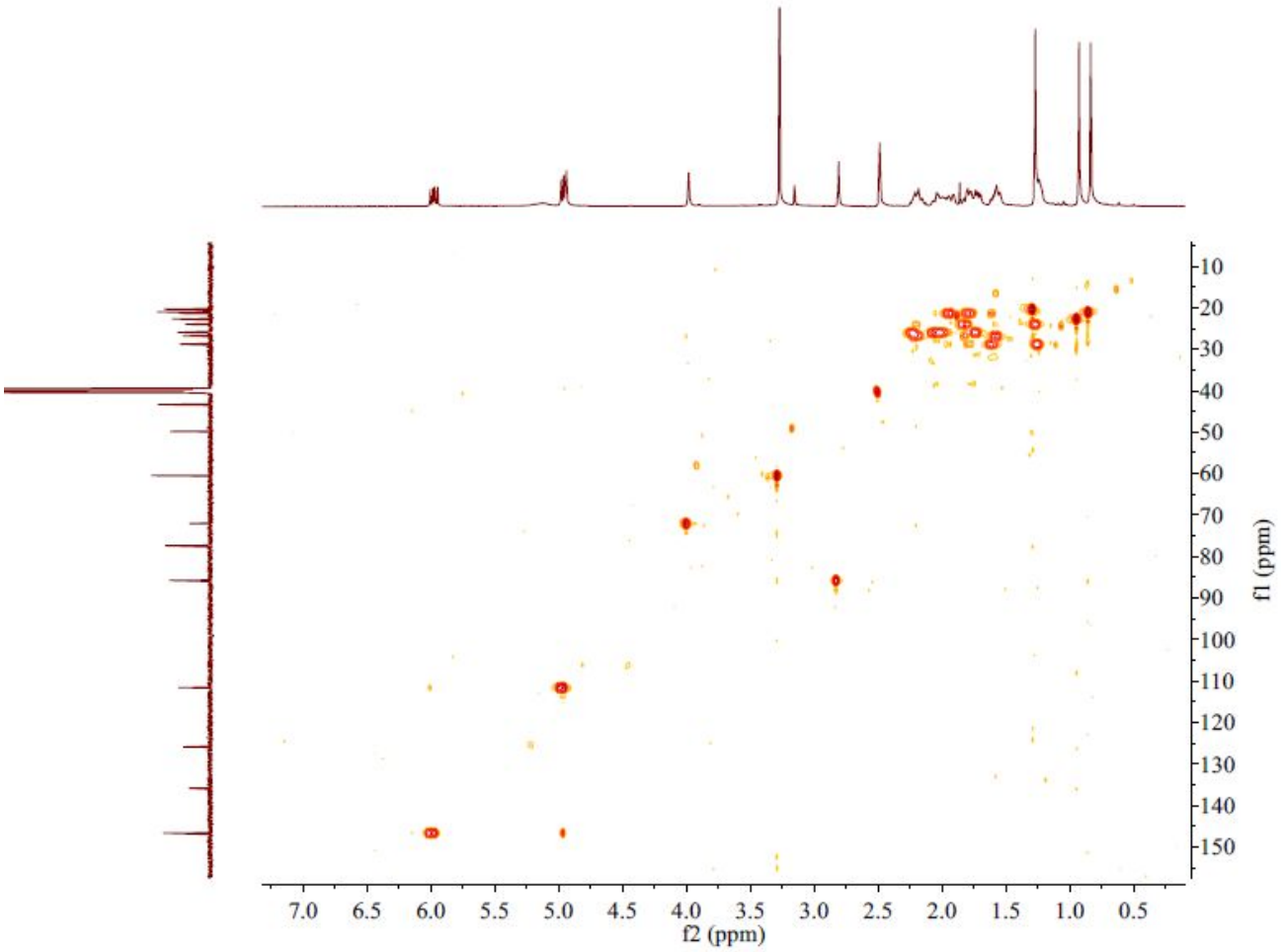

Figure S47. HMBC spectrum of compound **7**

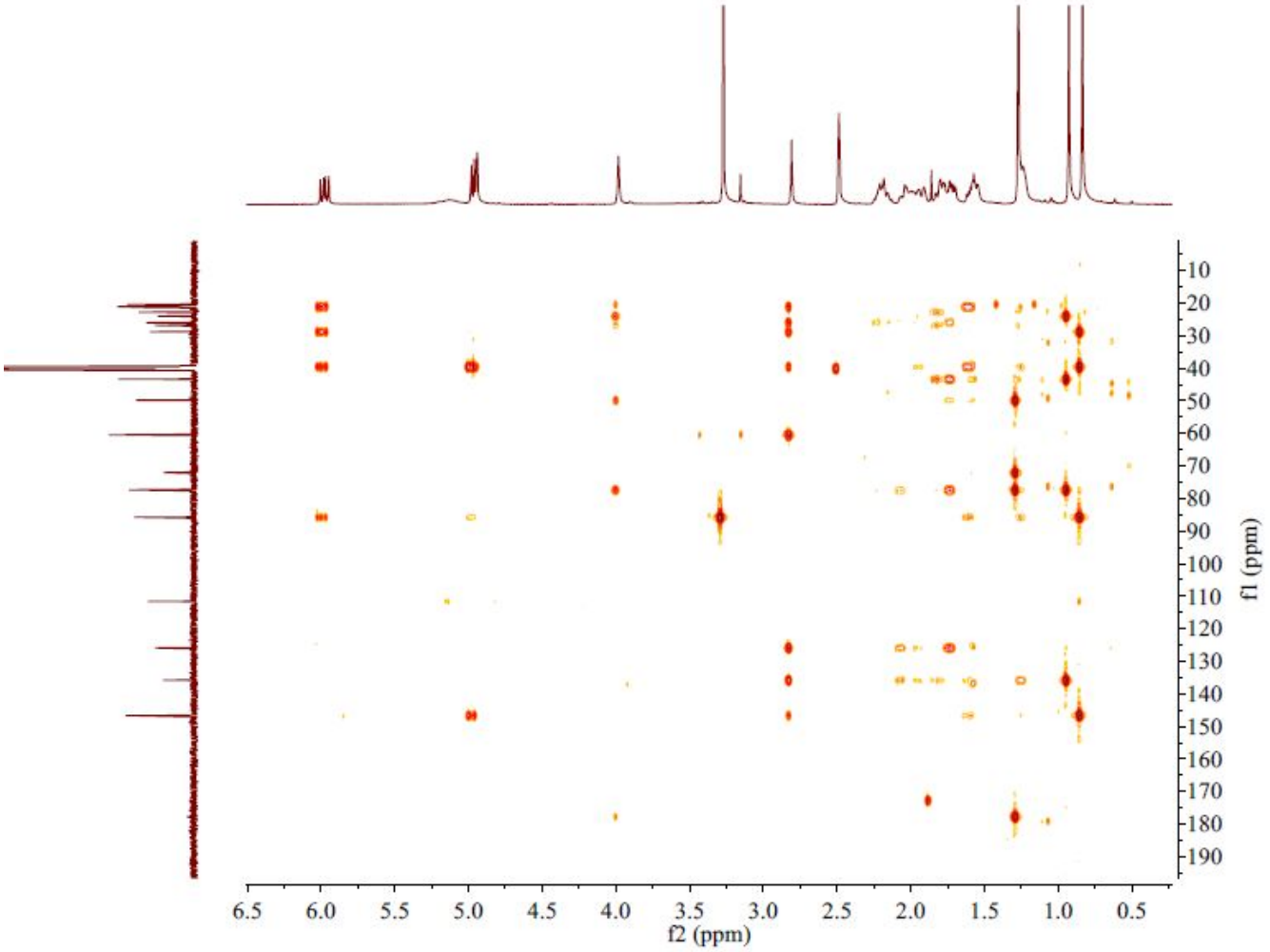

Figure S48. NOESY spectrum of compound **7**

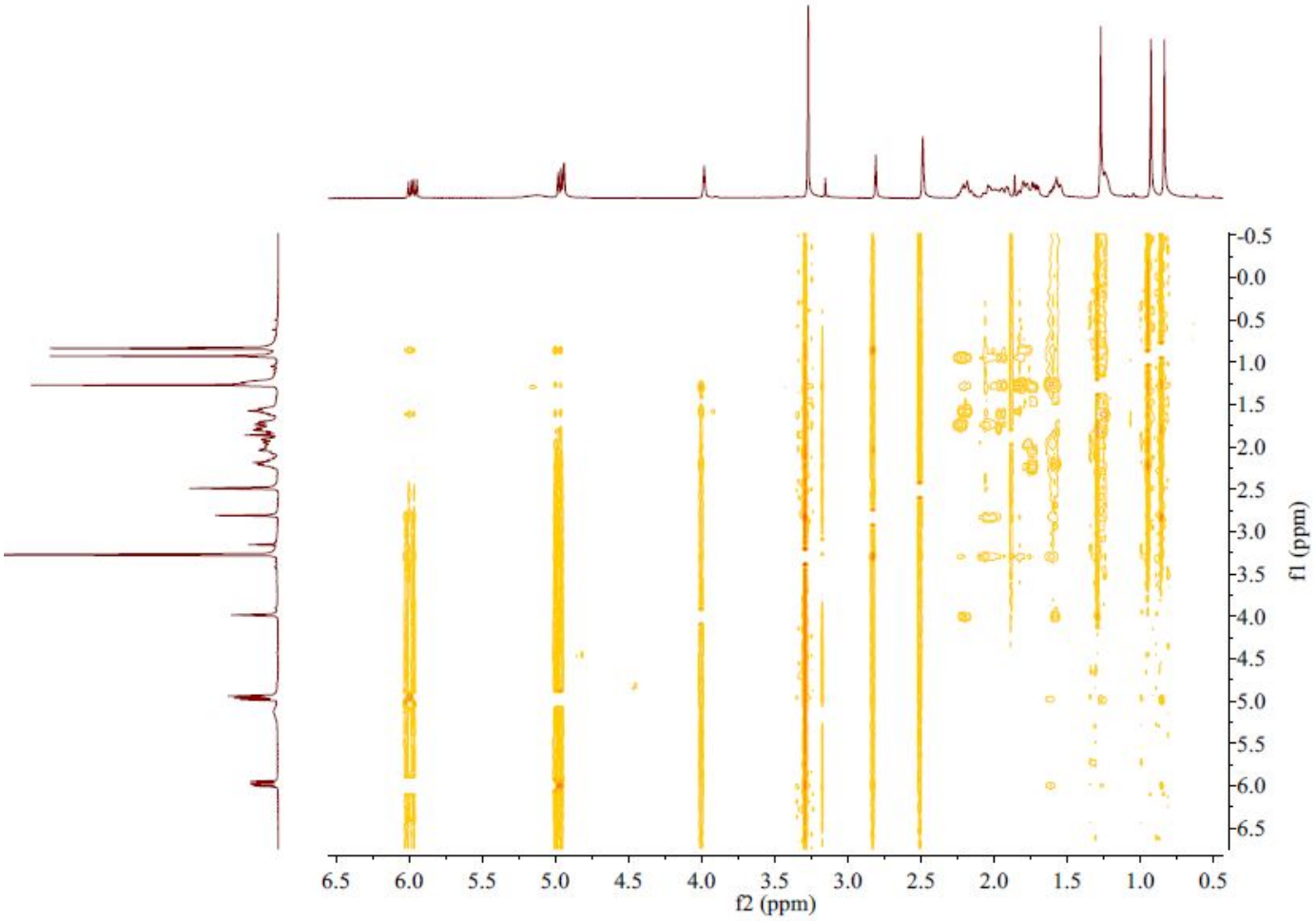

Figure S49. ECD spectrum of compound **7**

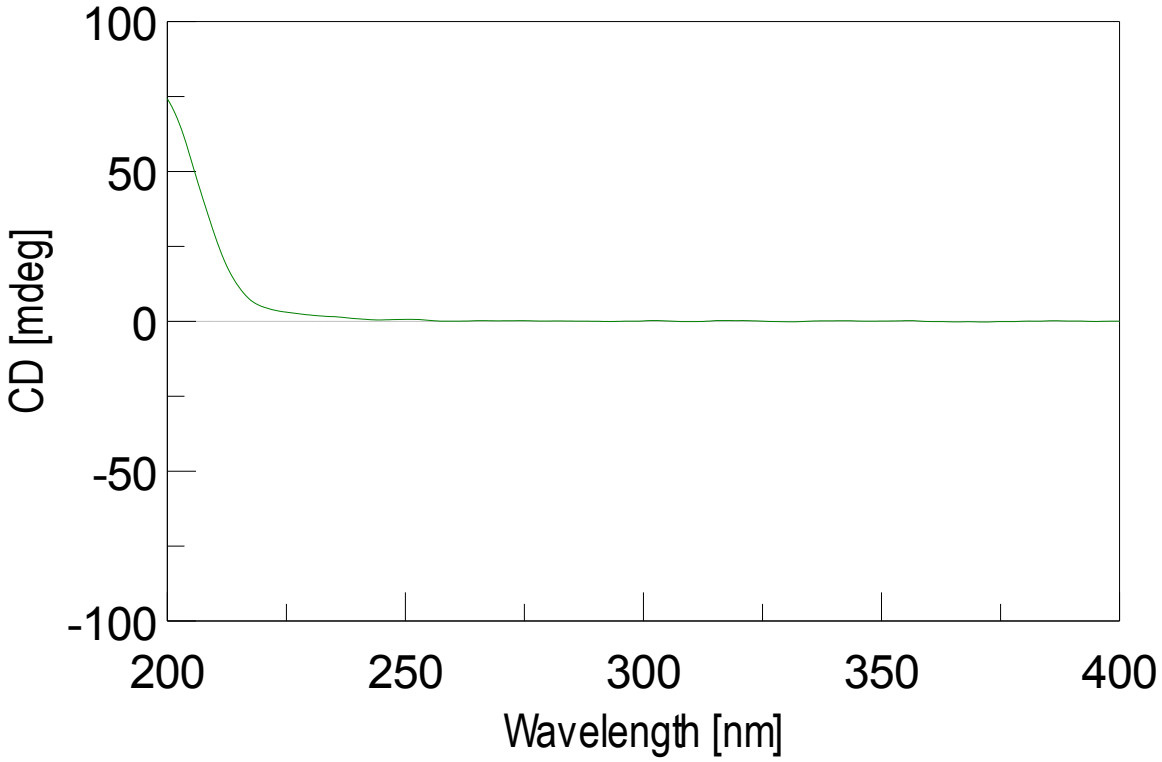

Figure S50. ^{1}H NMR (600 MHz, DMSO-d_6) spectrum of compound **8**

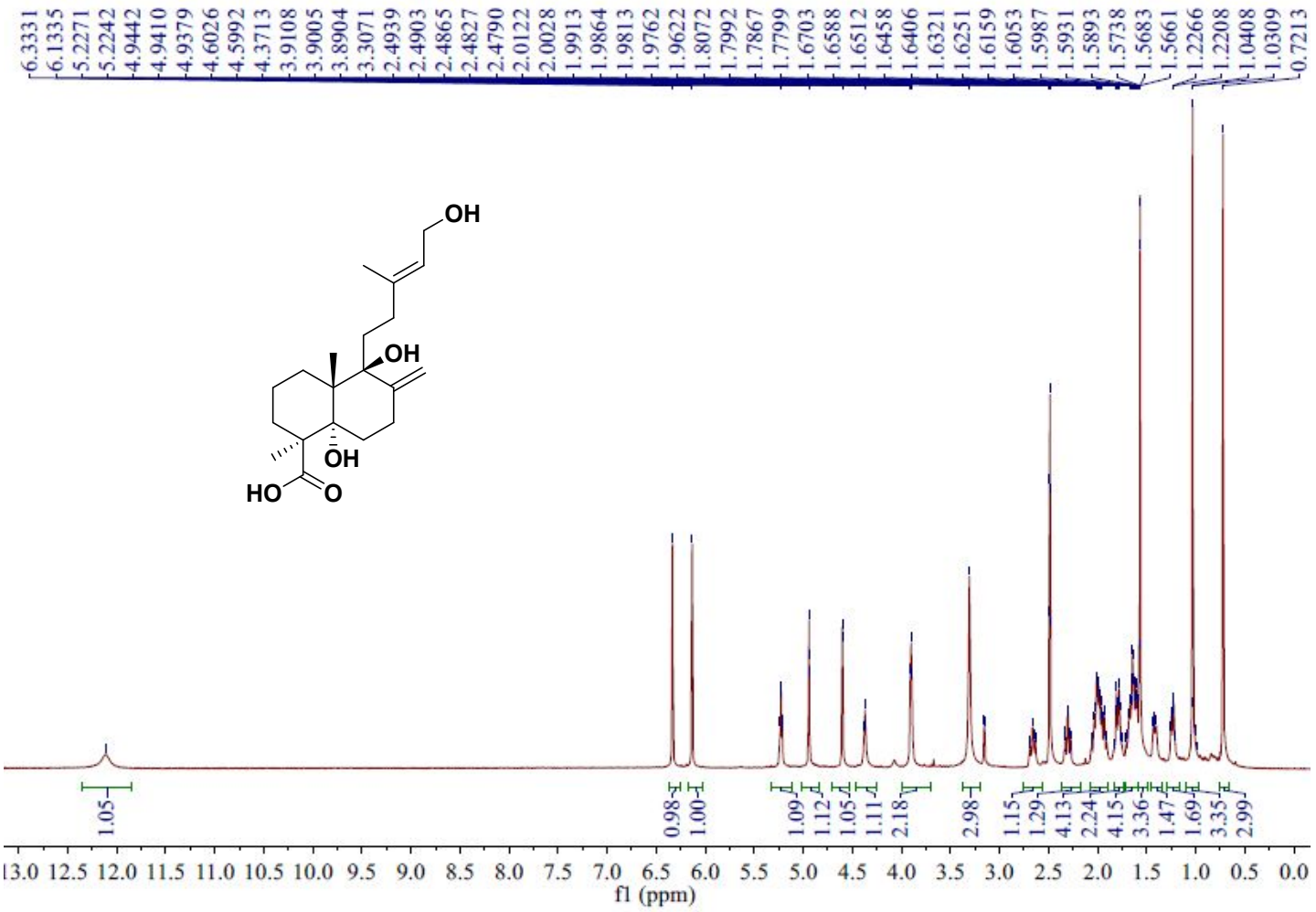

Figure S51. ^{13}C NMR (150 MHz, DMSO-d_6) and DEPT spectra of compound **8**

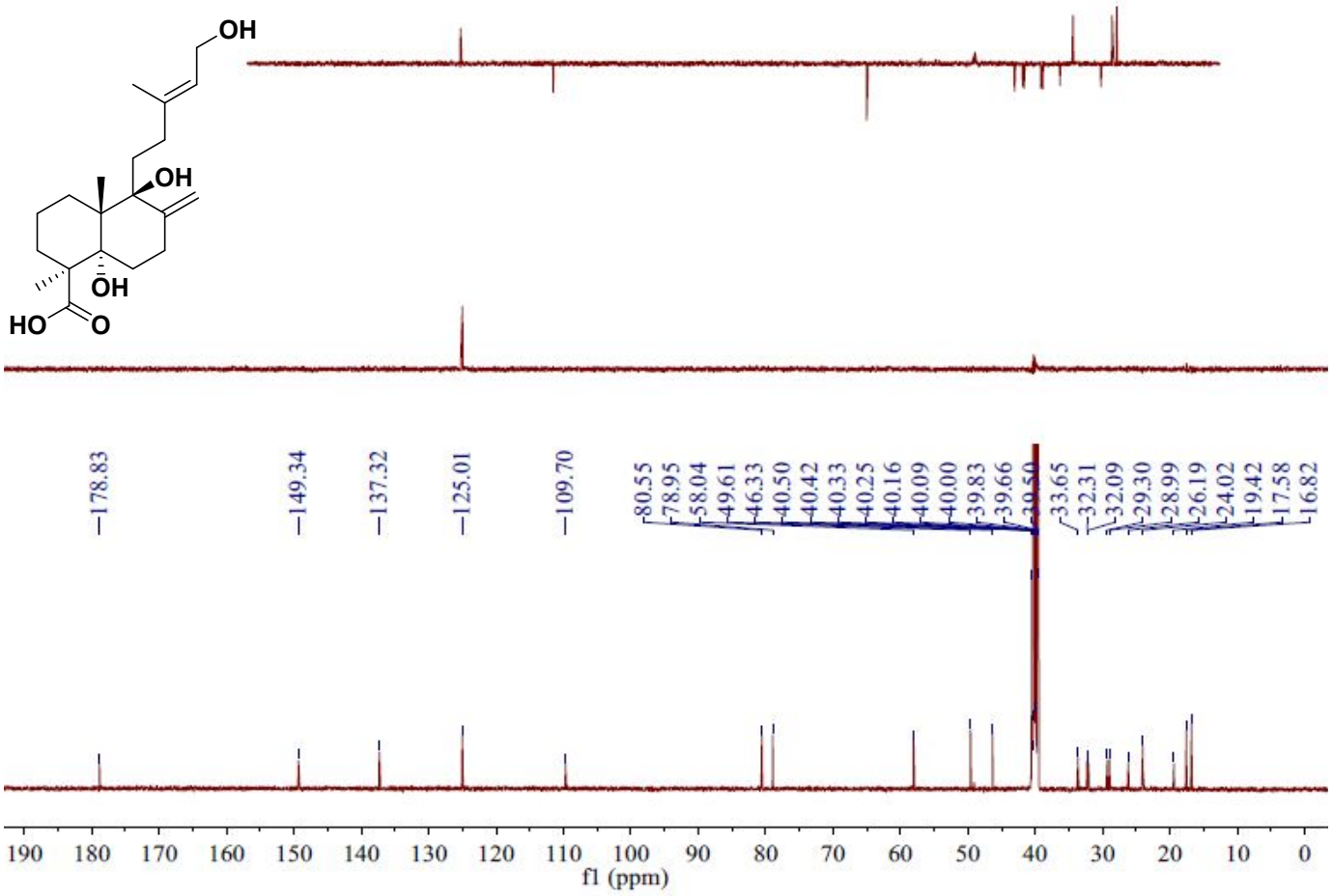

Figure S52. COSY spectrum of compound **8**

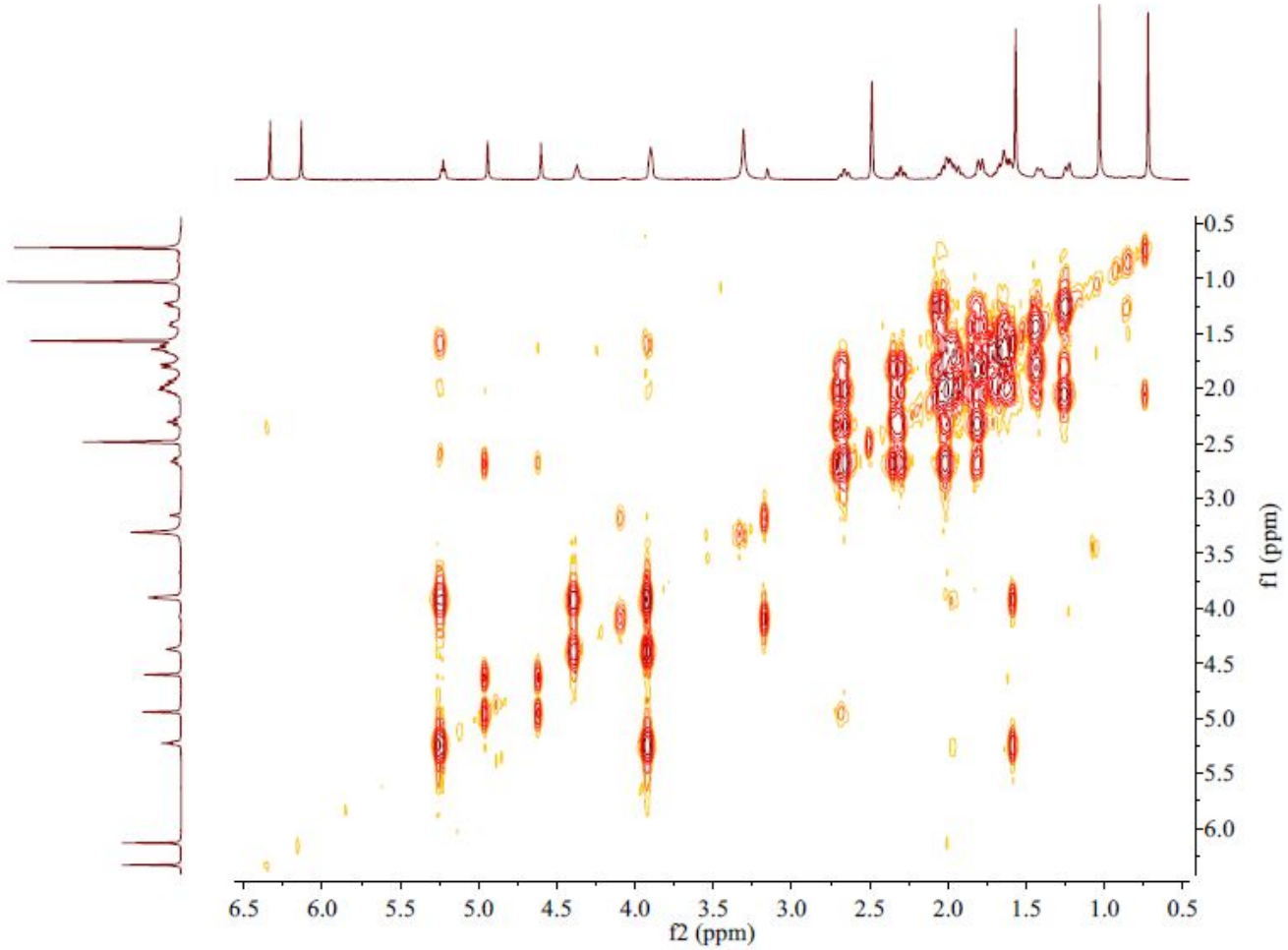

Figure S53. HSQC spectrum of compound **8**

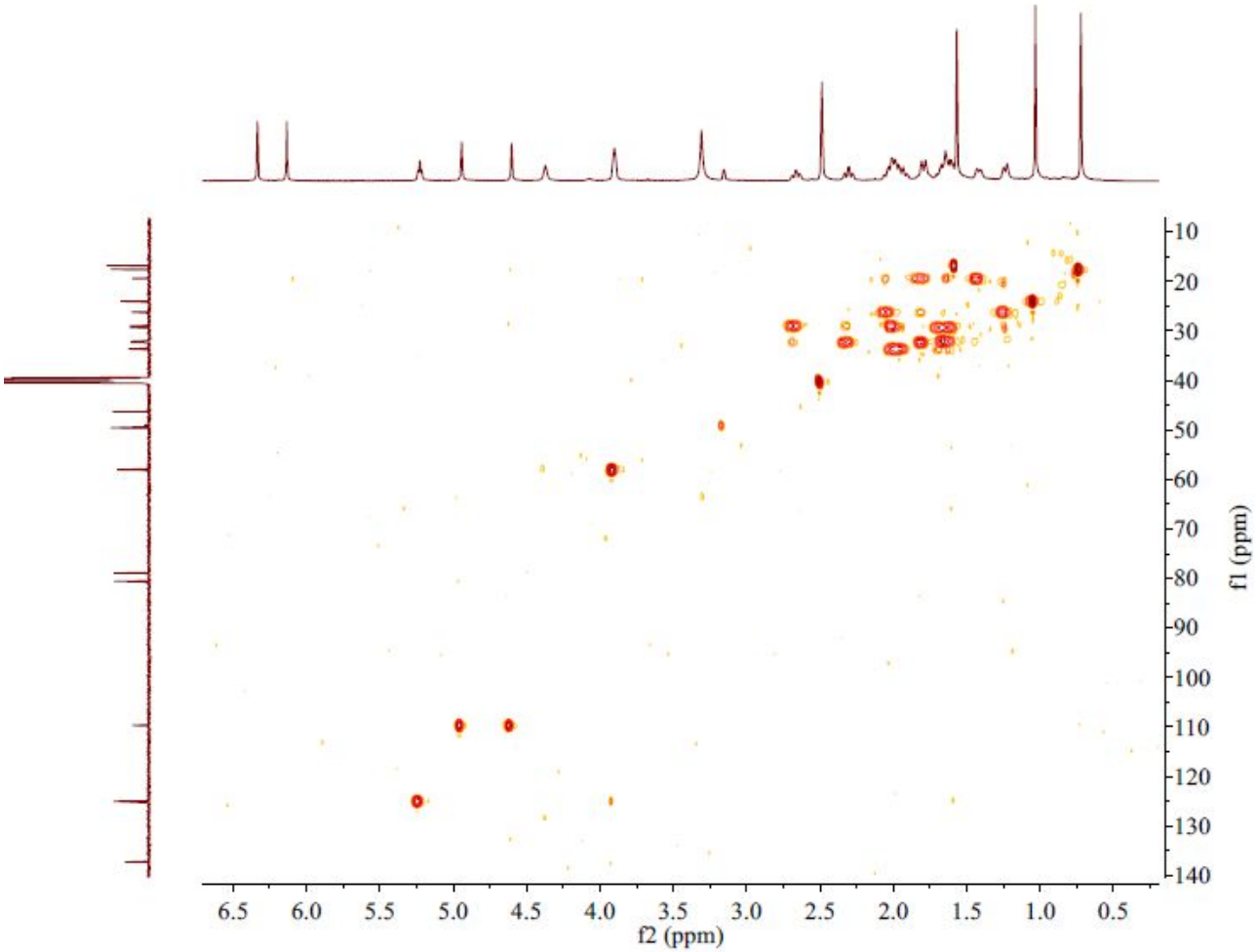

Figure S54. HMBC spectrum of compound **8**

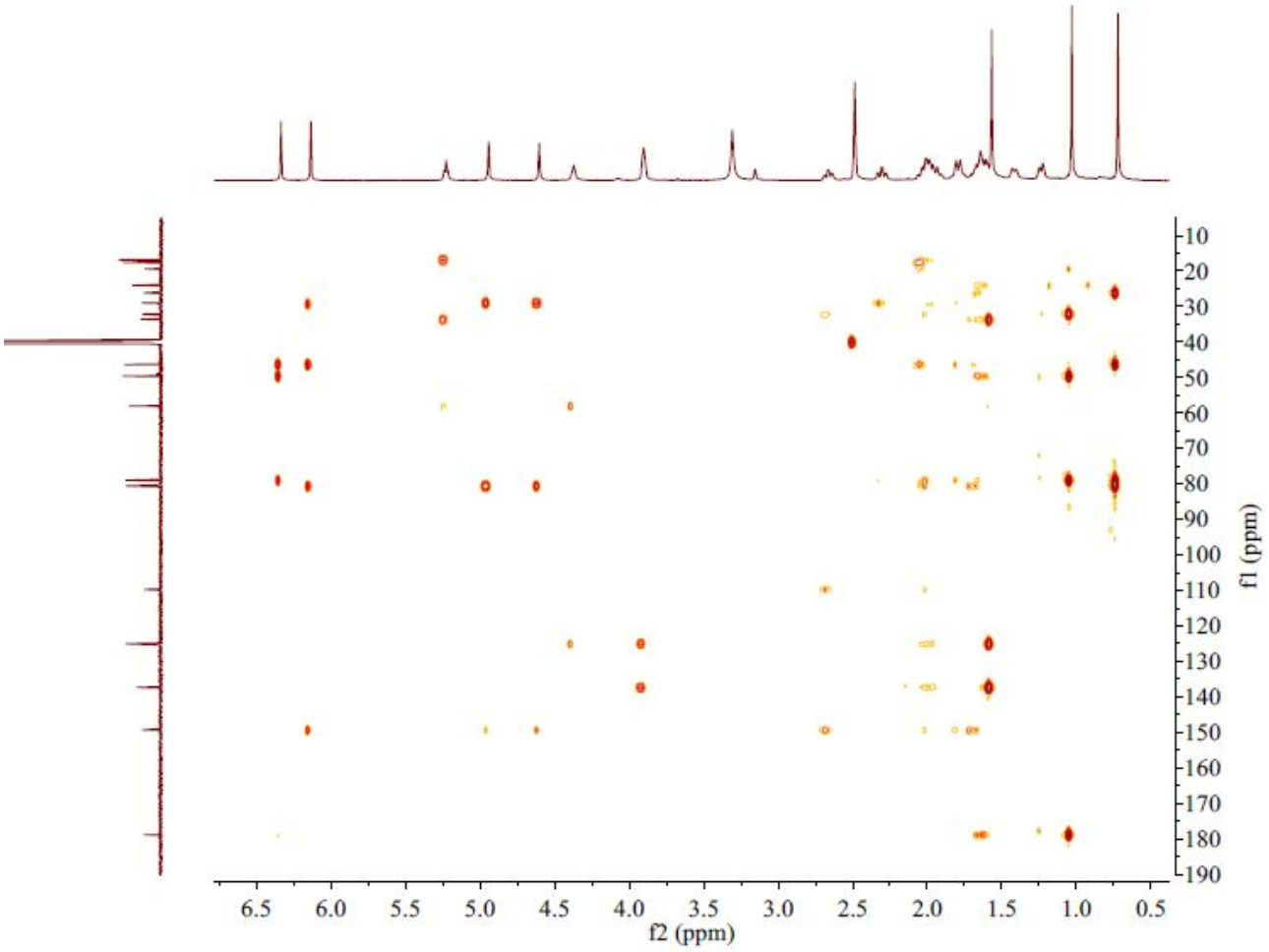

Figure S55. NOESY spectrum of compound **8**

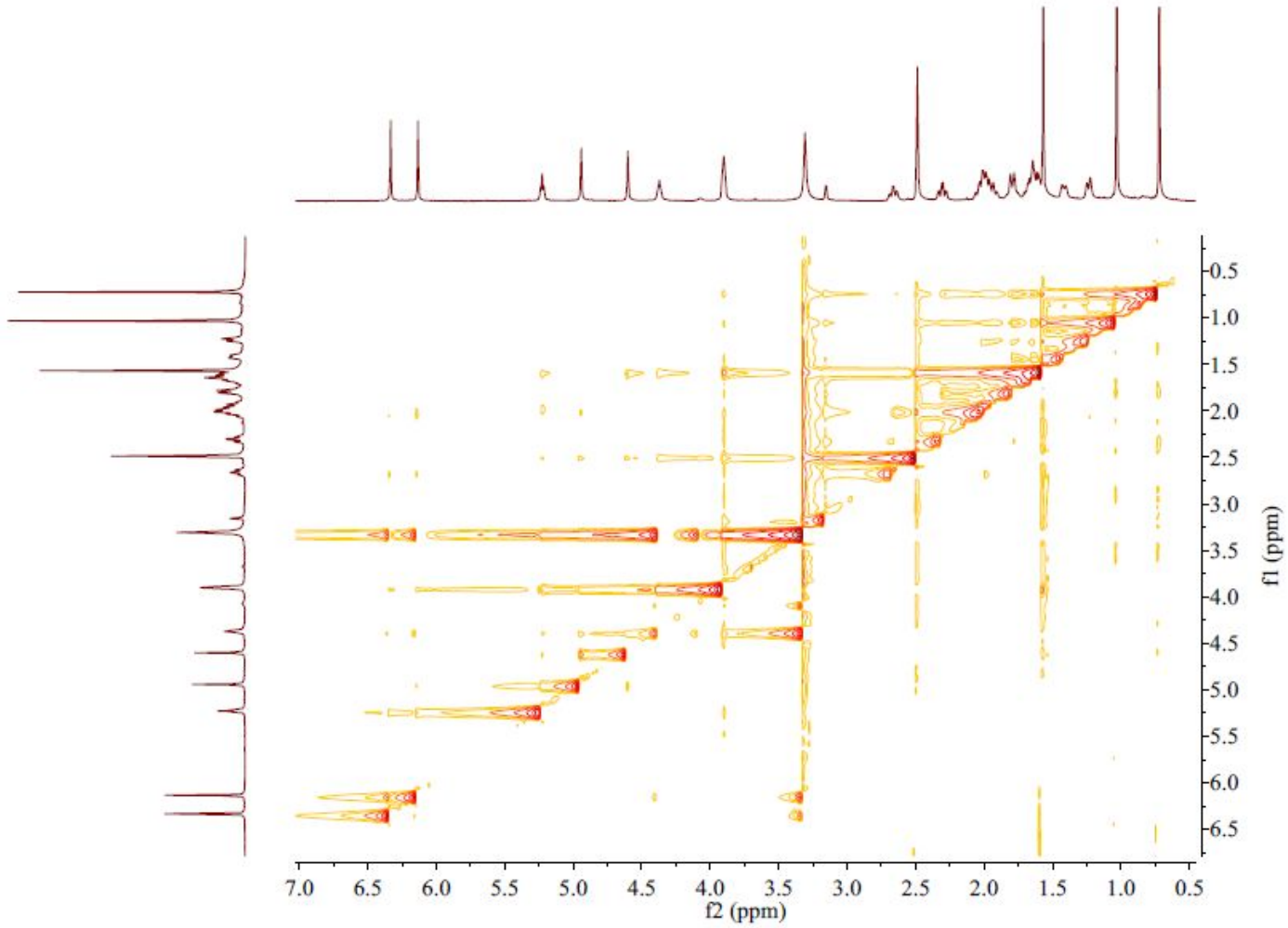

Figure S56. ECD spectrum of compound **8**

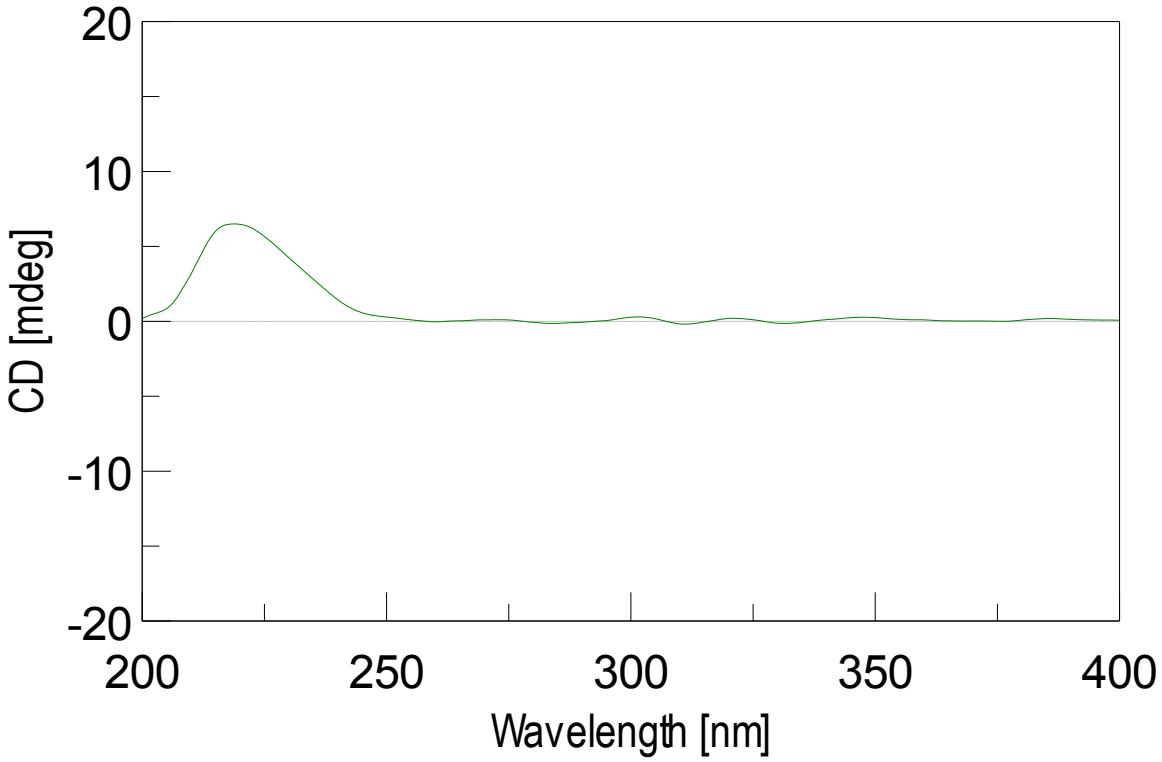

Figure S57.Crystal packing of compound **1** at 300(2) K

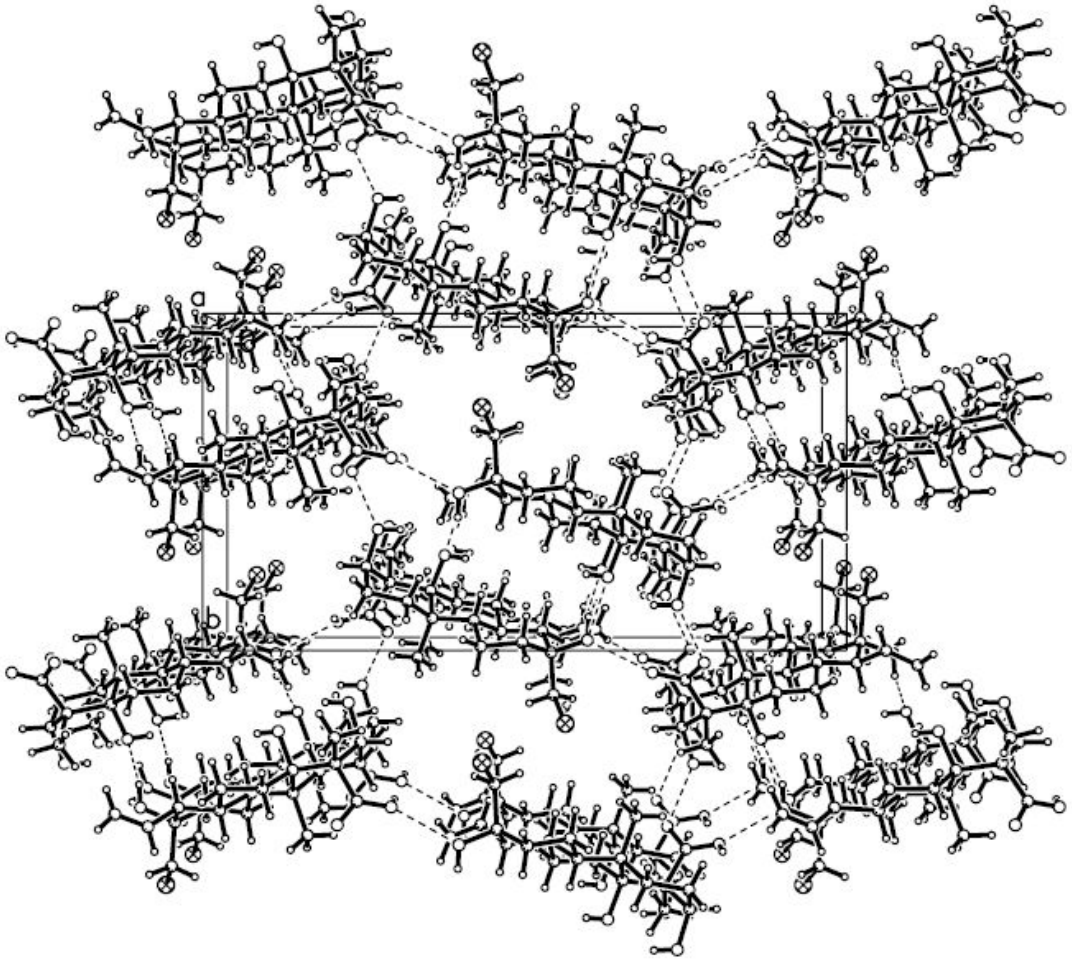

Figure S58.Crystal packing of compound **2** at 297(2) K

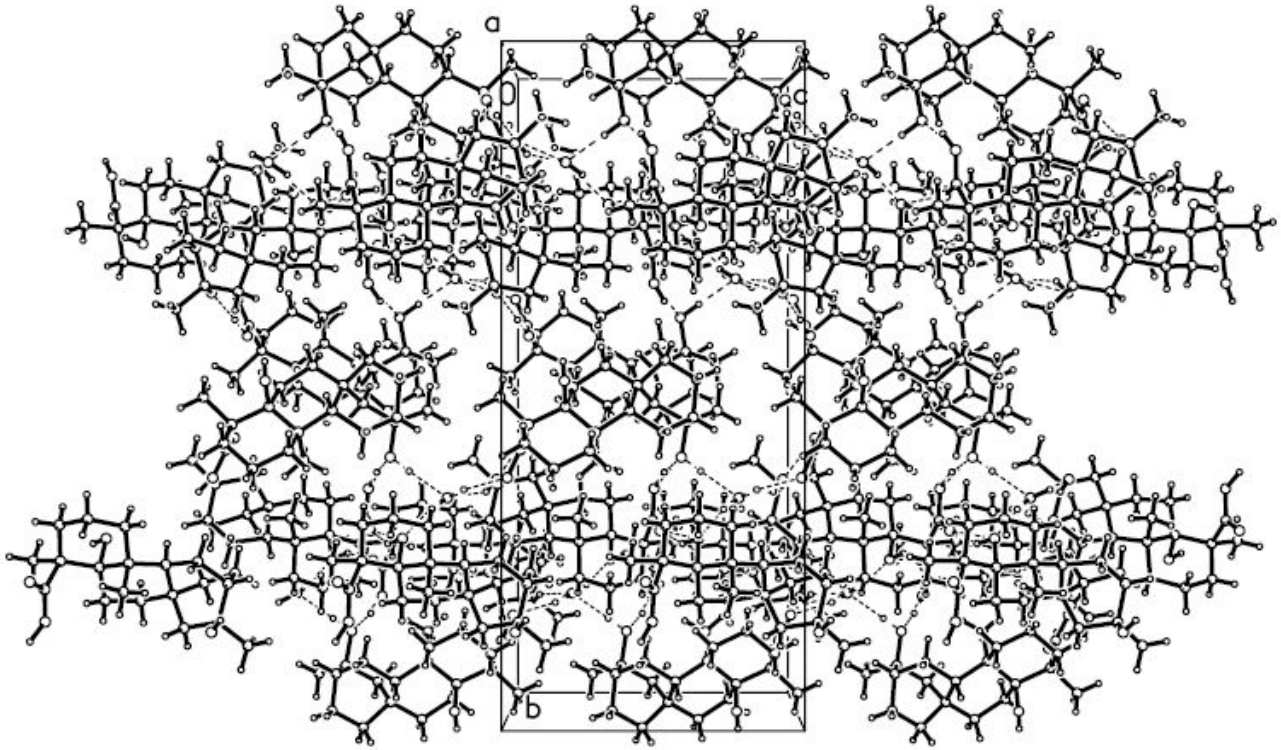

Figure S59.Crystal packing of compound **3** at 293(2) K

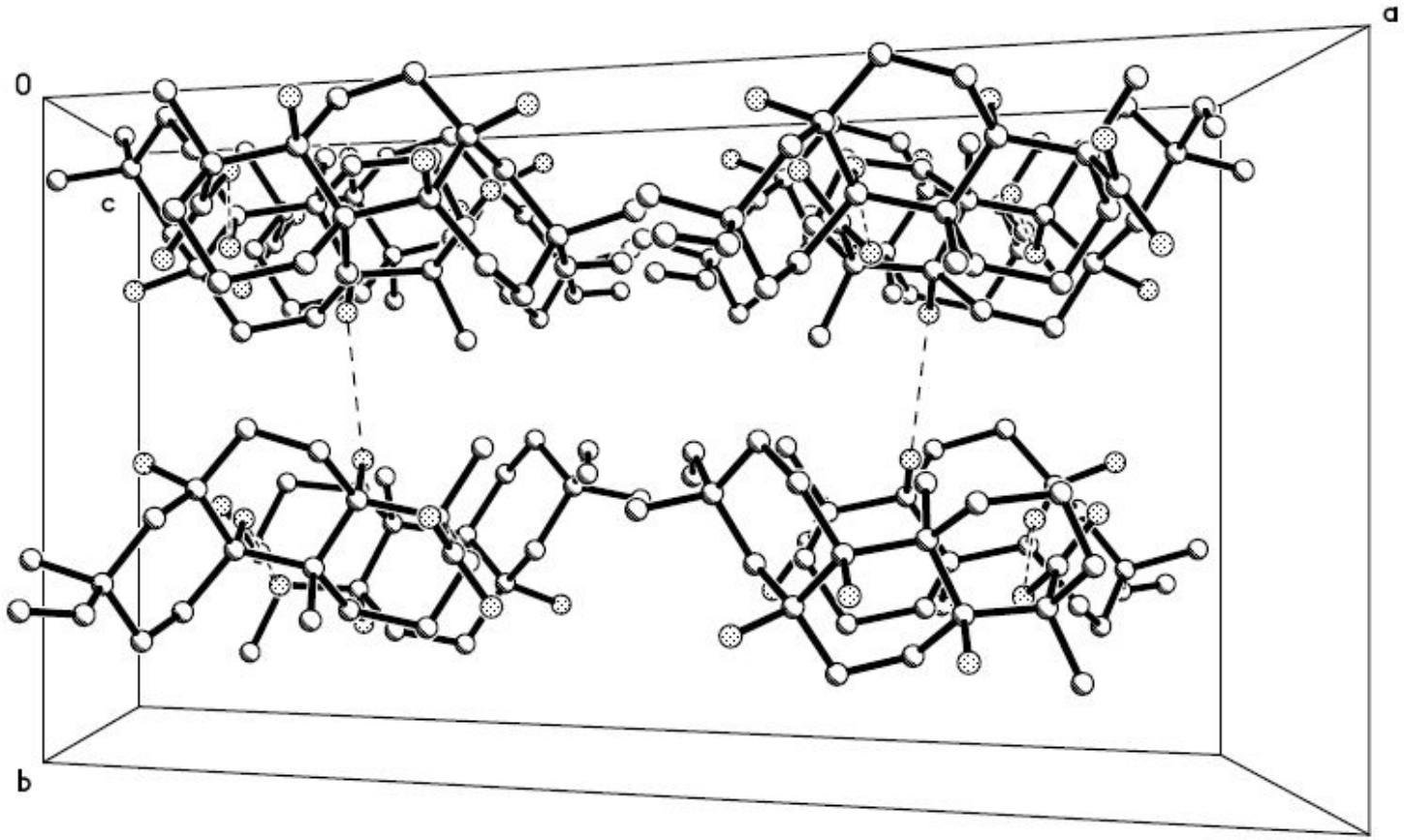

Figure S60.Crystal packing of compound **4** at 293(2) K

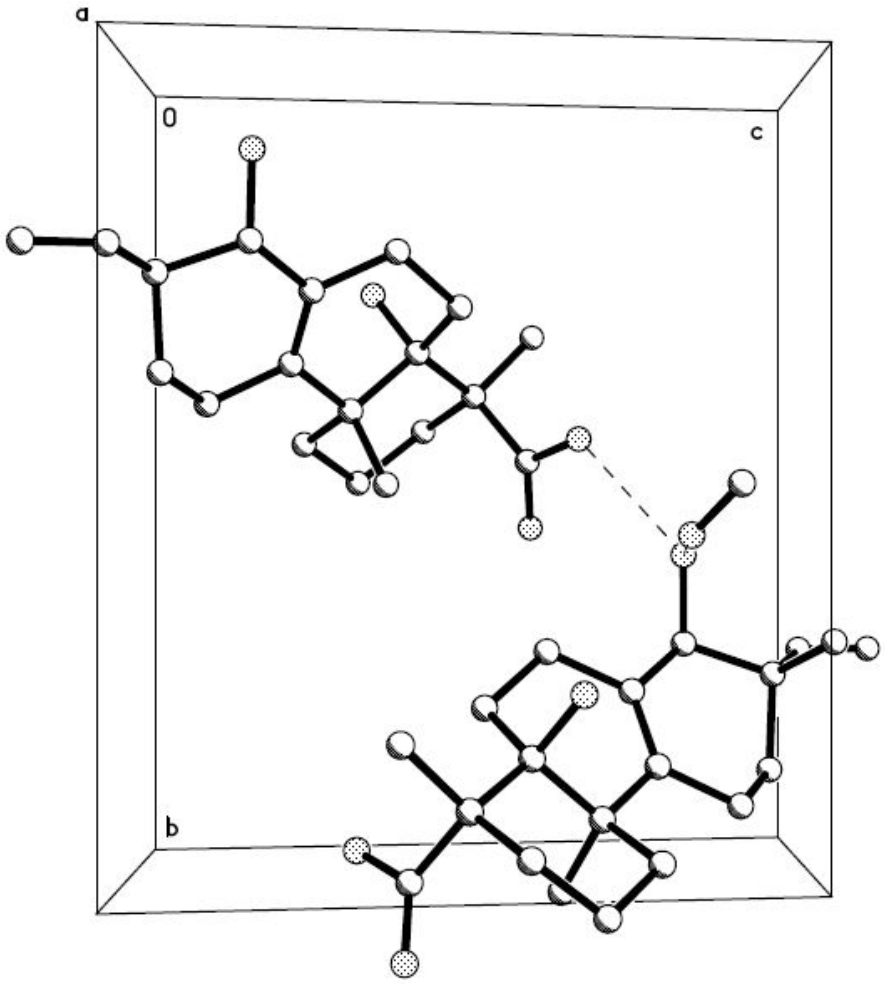
a
0
c
b

Figure S61.Crystal packing of compound **5** at 298(2) K

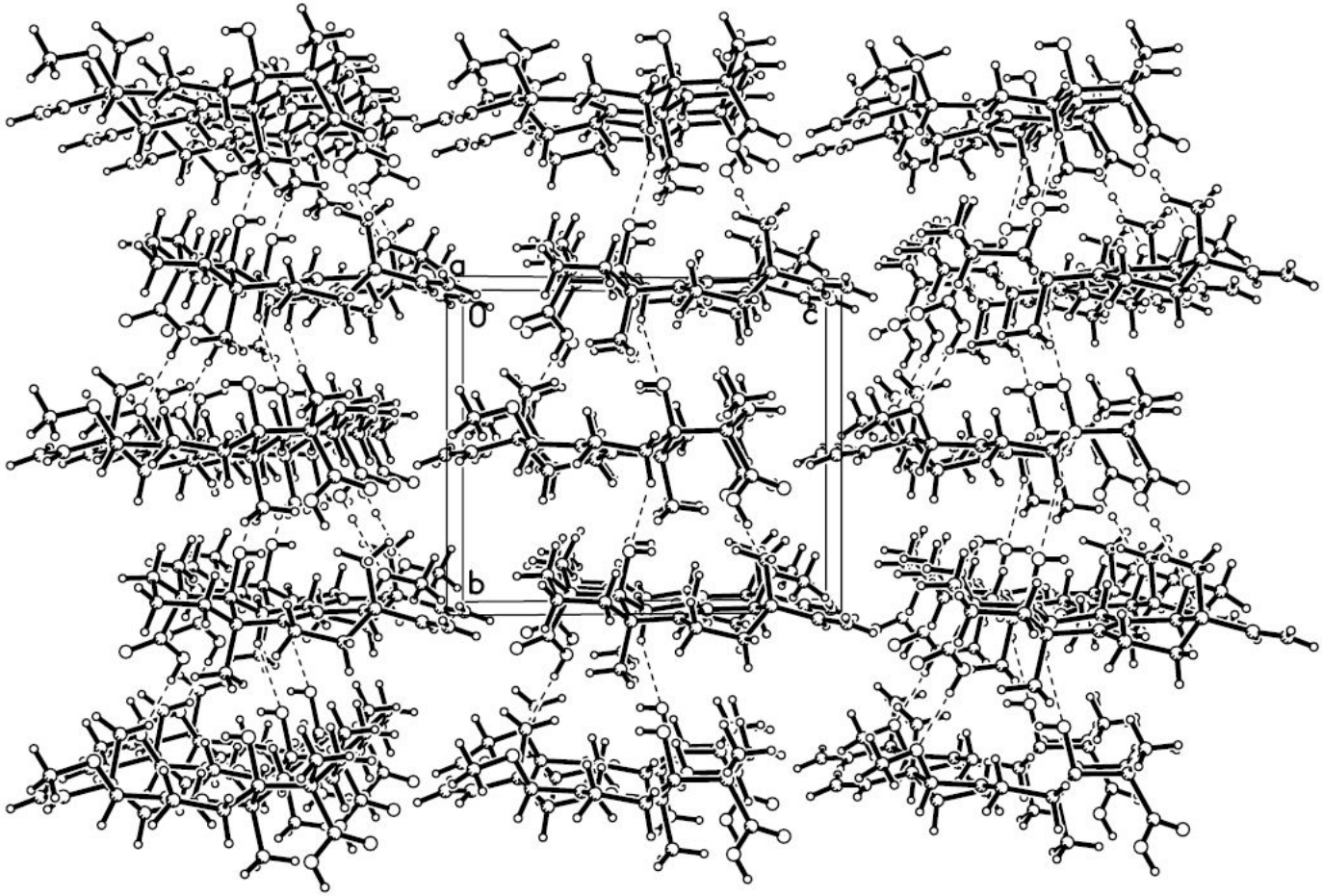

Figure S62.Crystal packing of compound **7** at 293(2) K

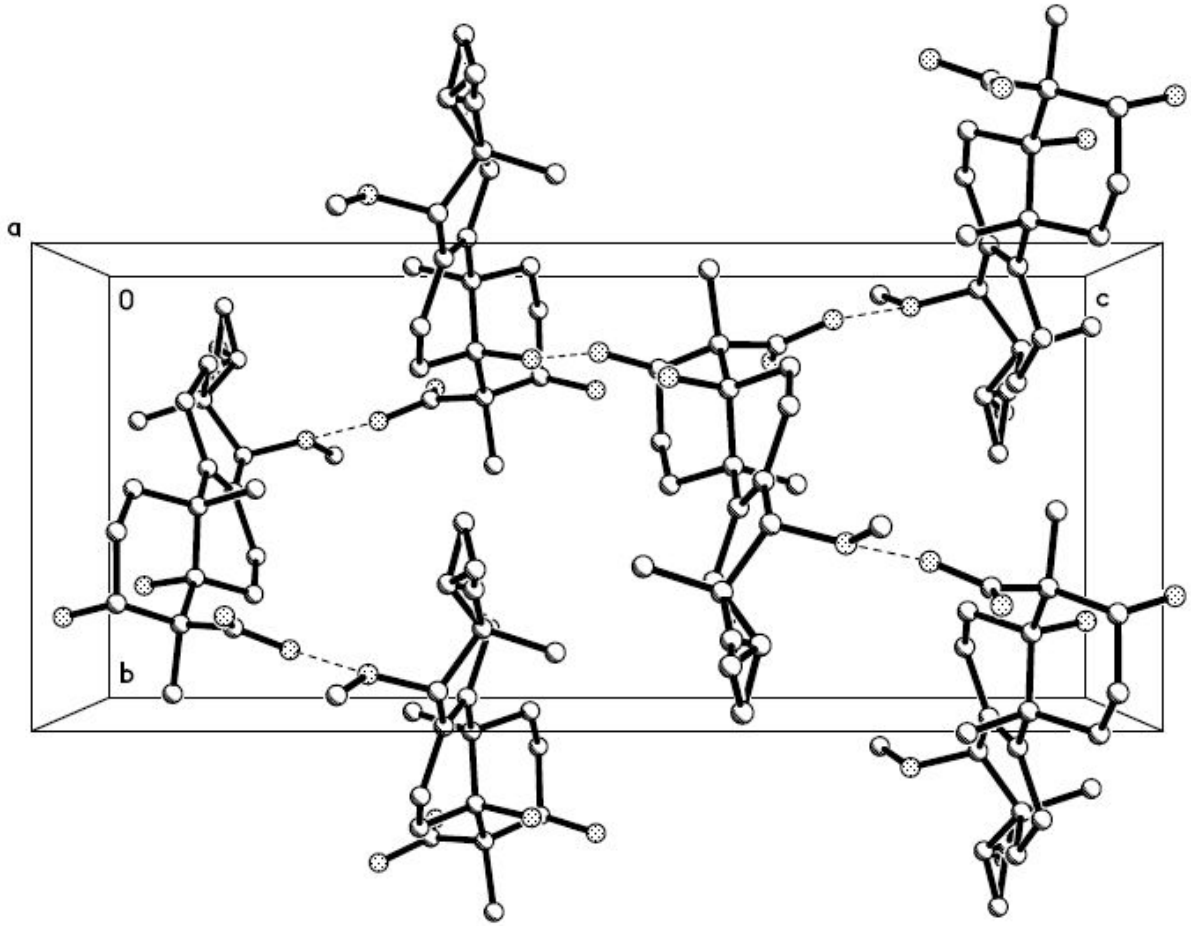

Figure S63. Key NOESY correlations of compounds **1**–**5** and **7**

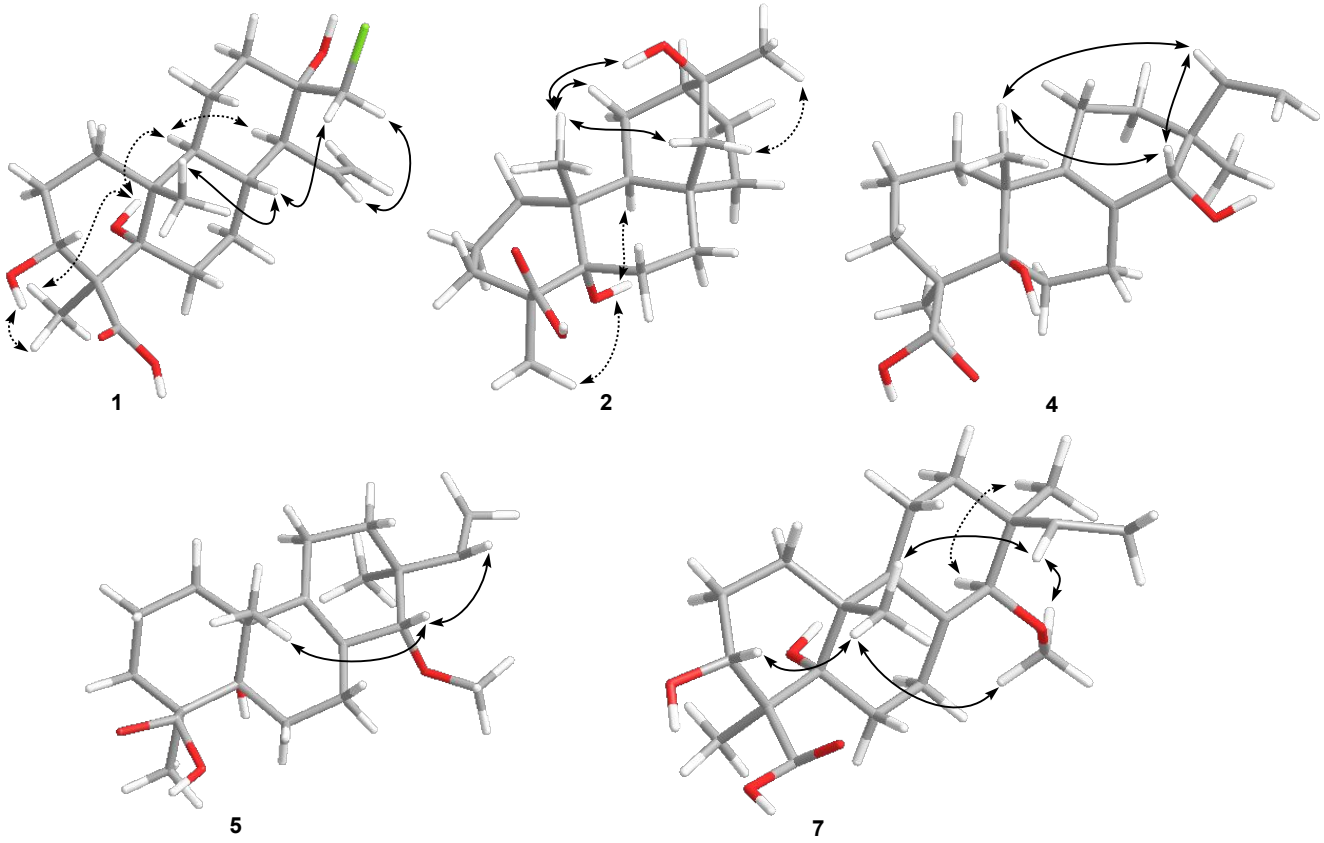
1
2
4
5
7

Table S1. Crystal data and structure refinement for compounds **1**–**5** and **7**.

Identification code	Compound 1	Compound 2	Compound 3	Compound 4	Compound 5	Compound 7
Empirical formula	C20H31ClO5	C20H32O4	C40H66O11	C21H34O5	C21H32O4	C21H32O5
Formula weight	386.90	336.45	722.92	366.48	348.47	364.47
Temperature	300(2) K	297(2) K	293(2) K	293(2) K	298(2) K	293(2) K
Wavelength	1.54178 Å	1.54178 Å	1.54178 Å	1.54178 Å	1.54178 Å	1.54178 Å
Crystal system, space group	Orthorhombic, P2(1)2(1)2(1)	Orthorhombic, P2(1)2(1)2	Monoclinic, C2	Monoclinic, P2(1)	Monoclinic, P2(1)	Orthorhombic, P2(1)2(1)2(1)
Unit cell dimensions	a = 7.6170 (2) Å, alpha = 90 deg. b = 11.8104 (3) Å, beta = 90 deg. c = 22.6071 (6) Å, gamma = 90 deg.	a = 12.7945 (18) Å, alpha = 90 deg. b = 26.092 (4) Å, beta = 90 deg. c = 11.4869 (16) Å, gamma = 90 deg.	a = 25.917(3) Å, alpha = 90 deg. b = 12.6548(16) Å, beta = 118.868(4) deg. c = 13.9501(15) Å, gamma = 90 deg.	a = 7.2621(8) Å, alpha = 90 deg. b = 12.6474(10) Å, beta = 99.188(2) deg. c = 10.7864(12) Å, gamma = 90 deg.	a = 7.7113(2) Å, alpha = 90 deg. b = 10.3066(2) Å, beta = 97.2150(10) deg. c = 12.1791(3) Å, gamma = 90 deg.	a = 9.4565(5) Å, alpha = 90 deg. b = 9.5803(7) Å, beta = 90 deg. c = 22.1890(14) Å, gamma = 90 deg.
Volume	2033.73(9) Å^3	3834.7(9) Å^3	4006.7(8) Å ^3	977.98(17) Å ^3	960.30(4) Å ^3	2010.2(2) Å ^3
Z, Calculated density	4, 1.264 Mg/m^3	8, 1.166 Mg/m^3	4, 1.198 Mg/m^3	2, 1.245 Mg/m^3	2, 1.205 Mg/m^3	4, 1.204 Mg/m^3
Absorption coefficient	1.884 mm^-1	0.633 mm^-1	0.697 mm^-1	0.701 mm^-1	0.651 mm^-1	0.682 mm^-1
F(000)	832	1472	1576	400	380	792
Crystal size	0.160 x 0.150 x 0.120 mm	0.180 x 0.160 x 0.140 mm	0.26 x 0.15 x 0.10 mm	0.23 x 0.20 x 0.18 mm	0.180 x 0.160 x 0.150 mm	0.38 x 0.20 x 0.12 mm
Theta range for data collection	4.223 to 68.207 deg.	3.388 to 65.104 deg.	3.62 to 66.03 deg.	4.15 to 66.05 deg.	5.642 to 68.222 deg.	3.98 to 66.03 deg.

Limiting indices	-9<=h<=9, -14<=k<=14, -27<=l<=26	-14<=h<=15, -30<=k<=30, -13<=l<=13	-30<=h<=30, -14<=k<=14, -14<=l<=16	-8<=h<=8, -14<=k<=14, -12<=l<=12	-9<=h<=9, -12<=k<=12, -14<=l<=14	-11<=h<=7, -7<=k<=11, -24<=l<=26
Reflections collected / unique	33394 / 3696 [R(int) = 0.0436]	41676 / 6516 [R(int) = 0.0776]	12865/6638 [R(int) = 0.0628]	5856/2915 [R(int) = 0.0676]	13464/3523 [R(int) = 0.0361]	6843/3437 [R(int) = 0.0319]
Completeness to theta = 67.679	99.4 %	99.7 %	99.7 %	99.8 %	99.8 %	100 %
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents
Data / restraints / parameters	3696 / 2 / 248	6516 / 1 / 455	6638/1/468	2915/8/240	3523/3/236	3437/4/250
Goodness-of-fit on F^2	1.083	1.056	1.067	1.042	1.127	1.032
Final R indices [I>2sigma(I)]	R1 = 0.0467, wR2 = 0.1338	R1 = 0.0539, wR2 = 0.1447	R1 = 0.1038, wR2 = 0.2491	R1 = 0.0627, wR2 = 0.1366	R1 = 0.0519, wR2 = 0.1372	R1 = 0.0459, wR2 = 0.1116
R indices (all data)	R1 = 0.0487, wR2 = 0.1366	R1 = 0.0679, wR2 = 0.1565	R1 = 0.1521, wR2 = 0.3021	R1 = 0.0904, wR2 = 0.1571	R1 = 0.0565, wR2 = 0.1420	R1 = 0.0583, wR2 = 0.1212
Absolute structure parameter	0.08(3)	0.0(3)	0.0(5)	0.0(5)	0.0(3)	0.0(3)
Extinction coefficient	n/a	n/a	n/a	n/a	n/a	n/a
Largest diff. peak and hole	0.263 and -0.299 e.A^-3	0.419 and -0.190 e.A^-3	0.422 and -0.363 e.A^-3	0.159 and -0.174 e.A^-3	0.461 and -0.209 e.A^-3	0.158 and -0.150 e.A^-3