

New Bioactive β -Resorcylic Acid Derivatives from the Alga-Derived Fungus *Penicillium antarcticum* KMM 4685

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Figure S58. ROESY spectrum for 1 in MeOD

Figure S59. ROESY spectrum for 2 in MeOD

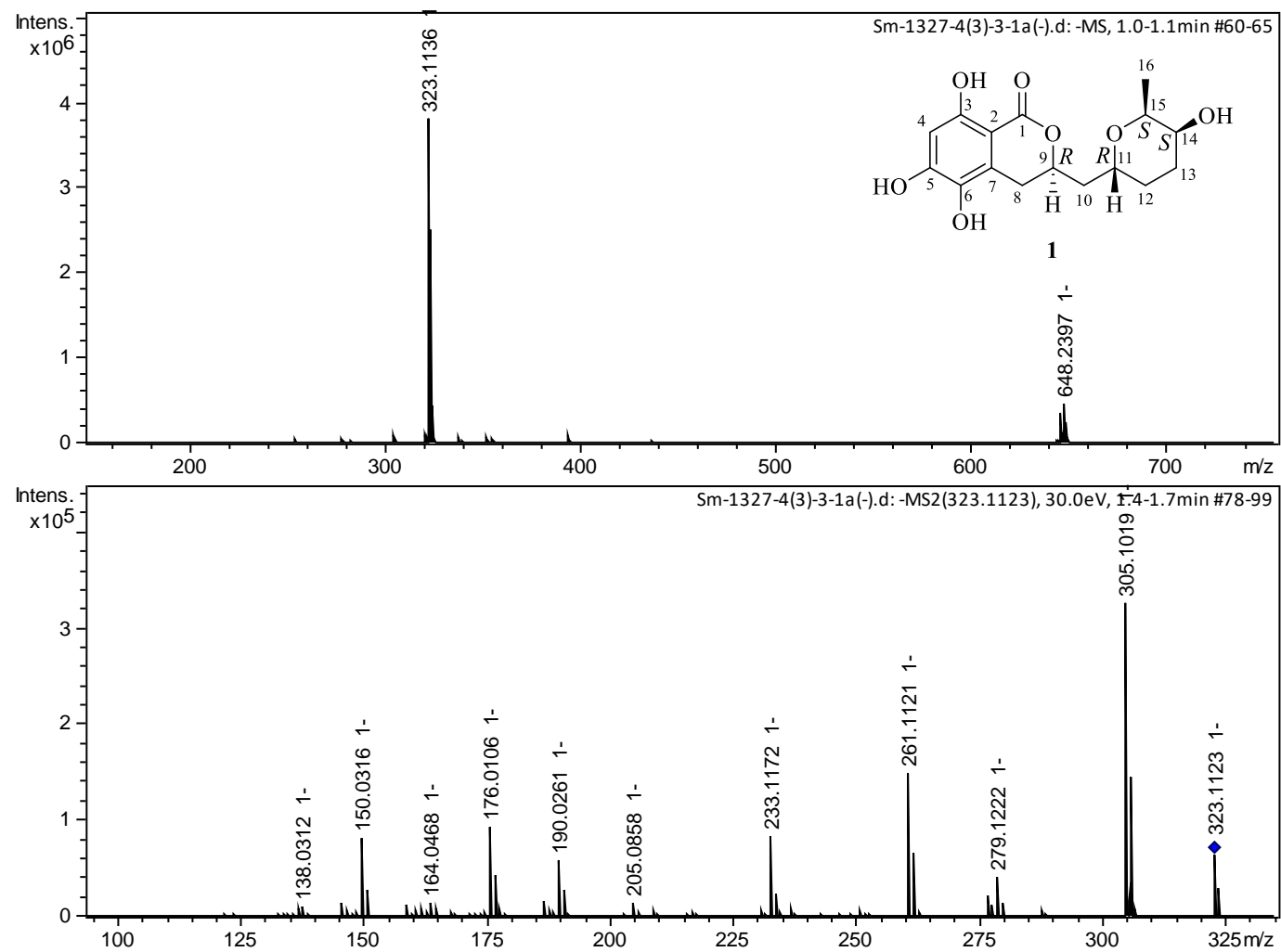
Figure S60. ROESY spectrum for 3 in MeOD

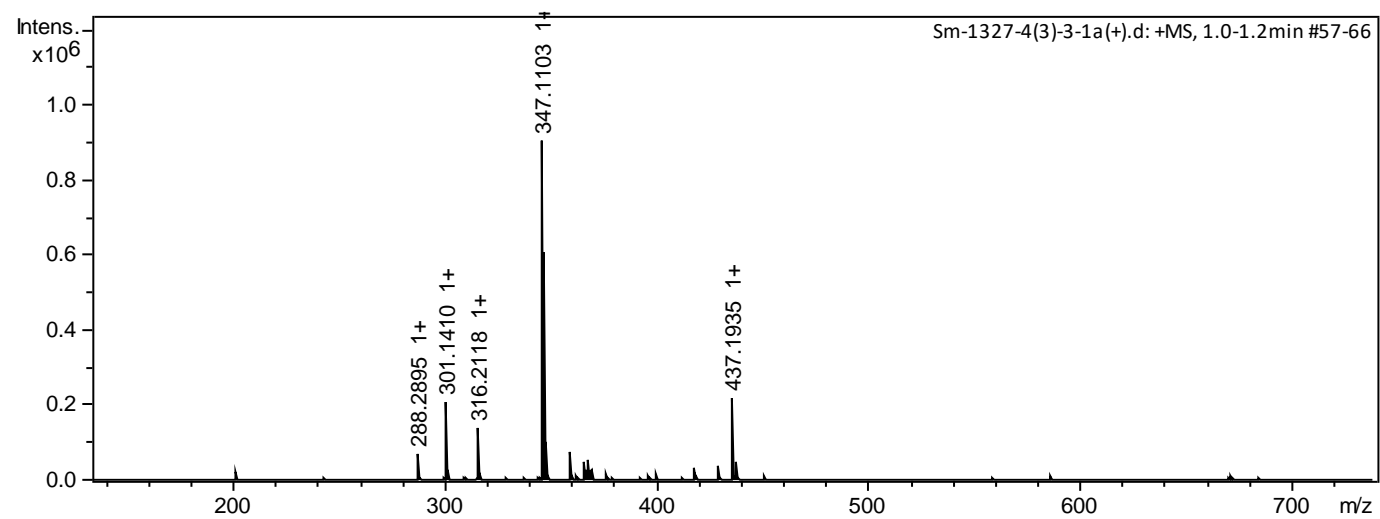
Figure S61. ROESY spectrum for 4 in MeOD

Figure S62. ROESY spectrum for 5 in MeOD

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Figure S1. HRESIMS for 1





	meas	calc	Δ (ppm)
[M-H] ⁻	323,1136	323,1136	0,2
[M+Na] ⁺	347,1103	347,1101	-0,4

Figure S2. ^1H NMR spectrum of **1** measured at 500 MHz in MeOD

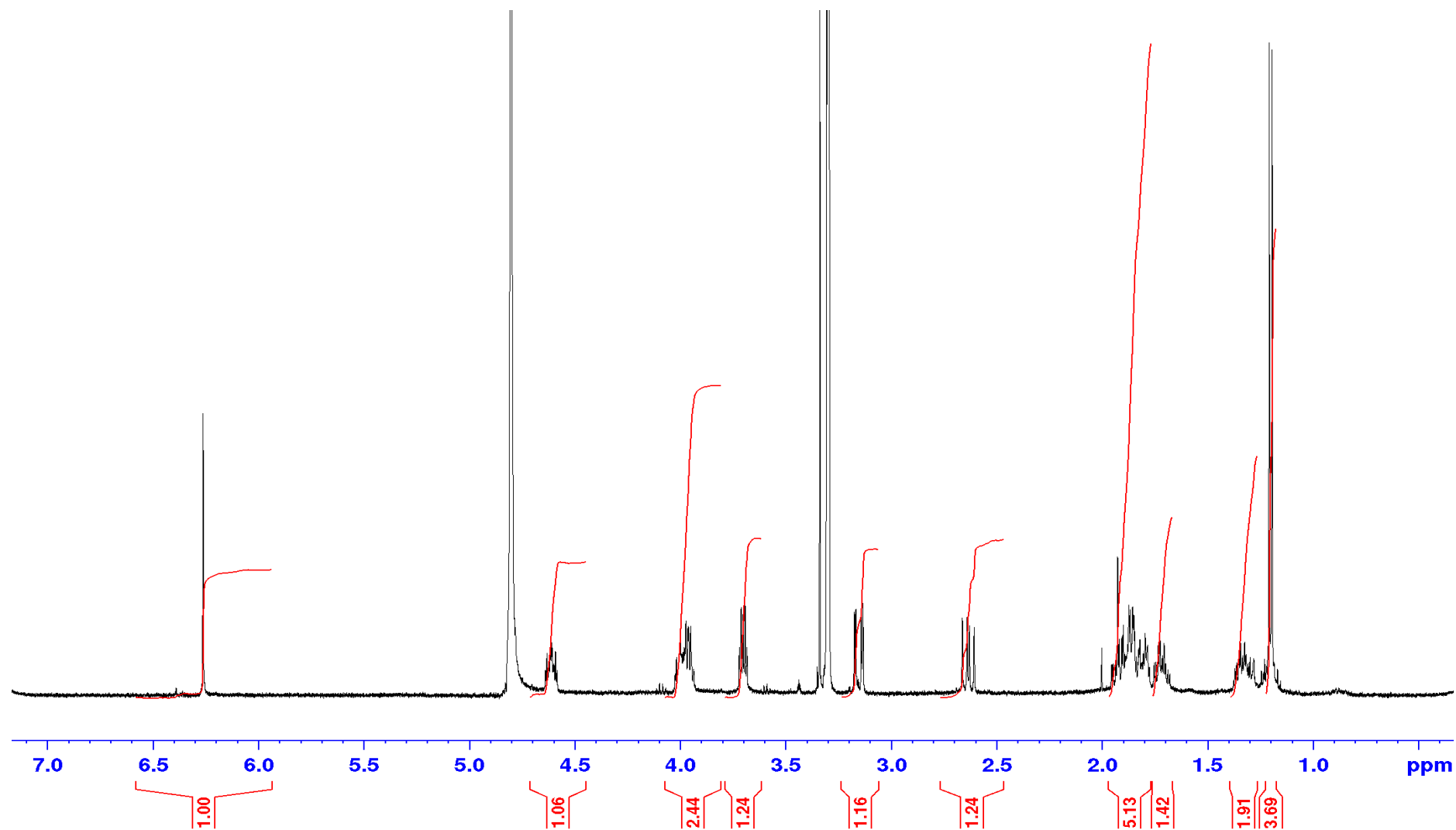


Figure S3. ^{13}C NMR spectrum of **1** measured at 125 MHz in MeOD

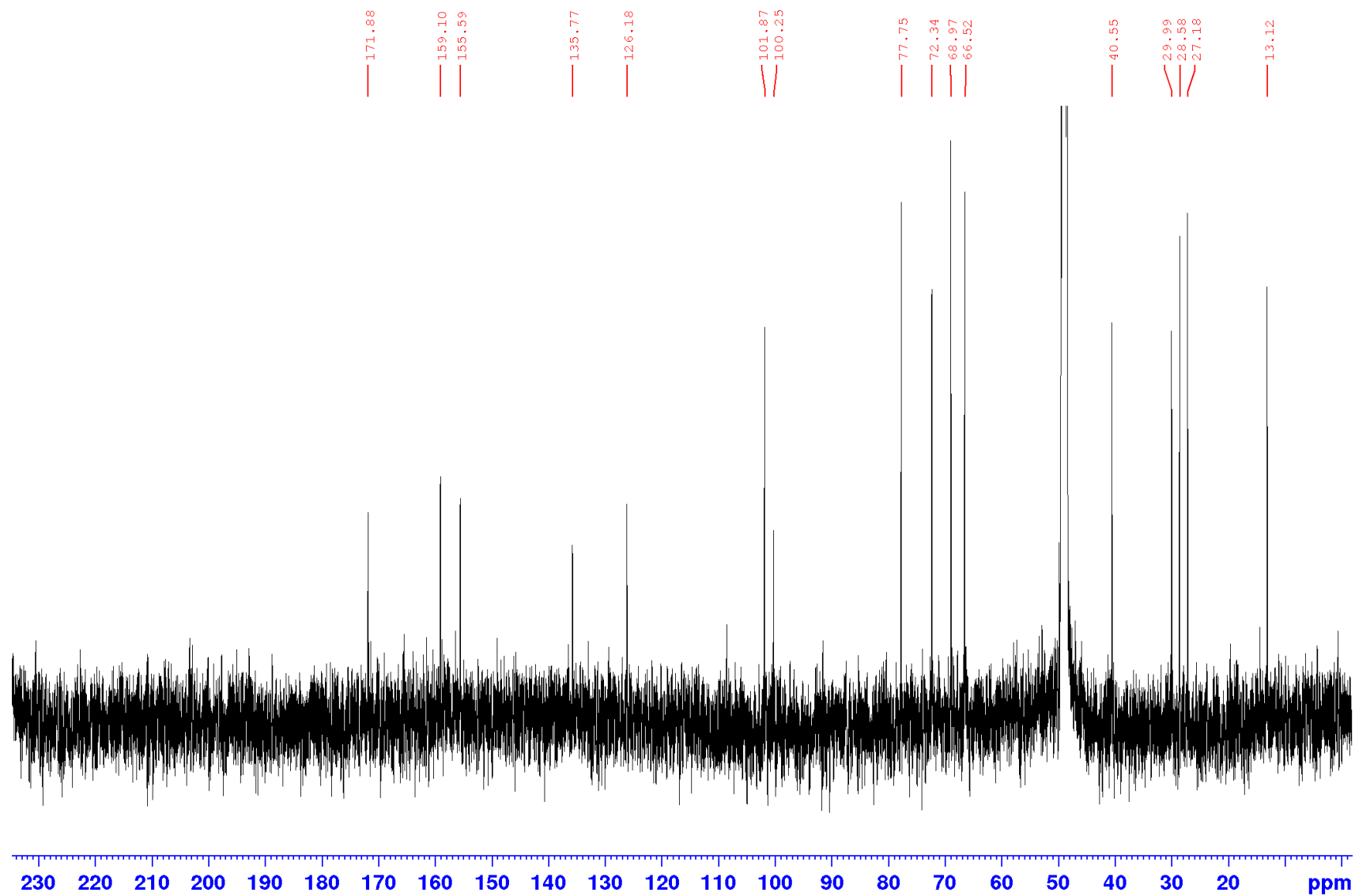


Figure S4. DEPT-135 spectrum of **1** measured at 125 MHz in MeOD

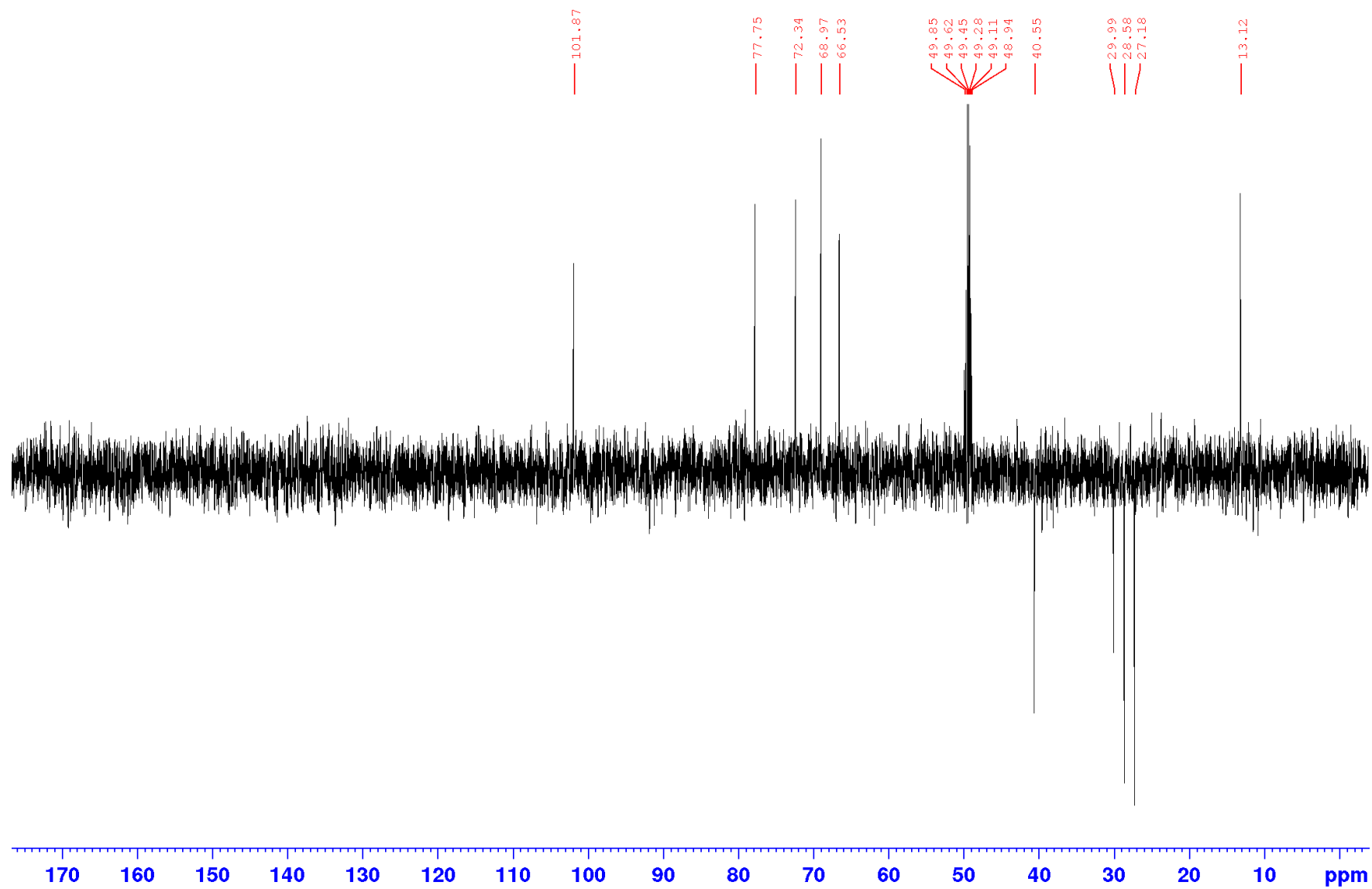


Figure S5. HSQC spectrum of 1 measured in MeOD

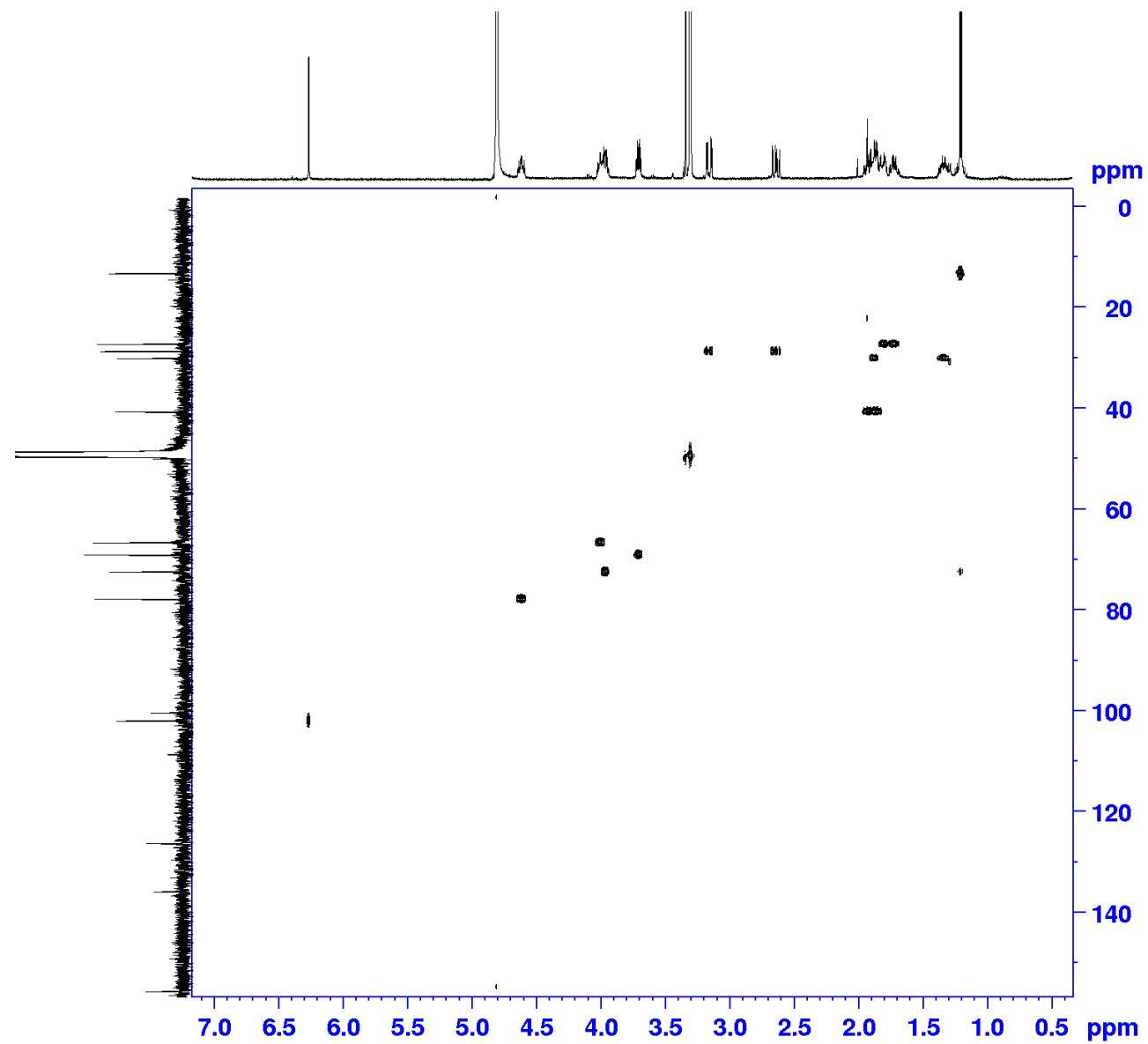


Figure S6. COSY spectrum of 1 measured in MeOD

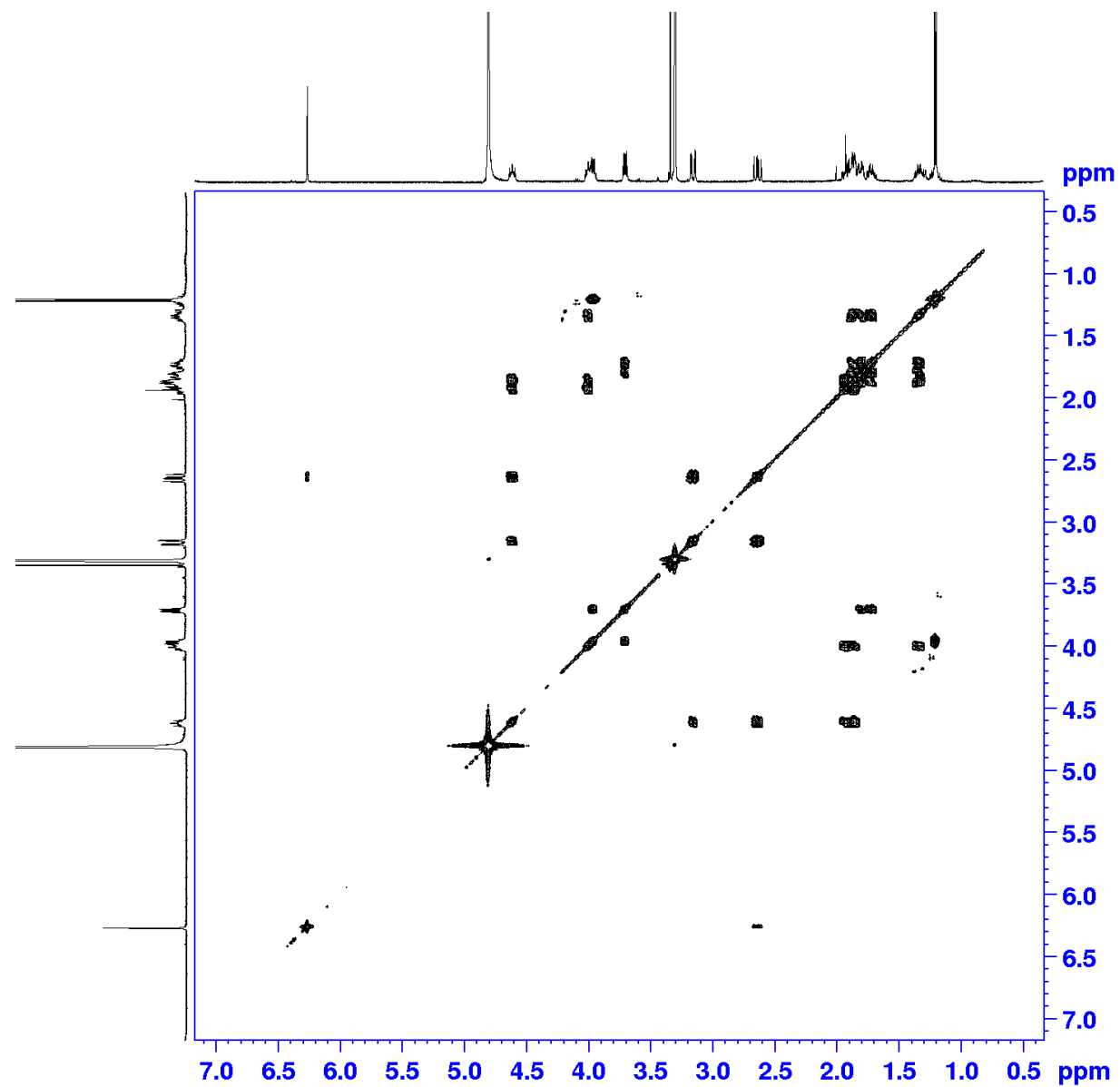


Figure S7. HMBC spectrum of 1 measured in MeOD

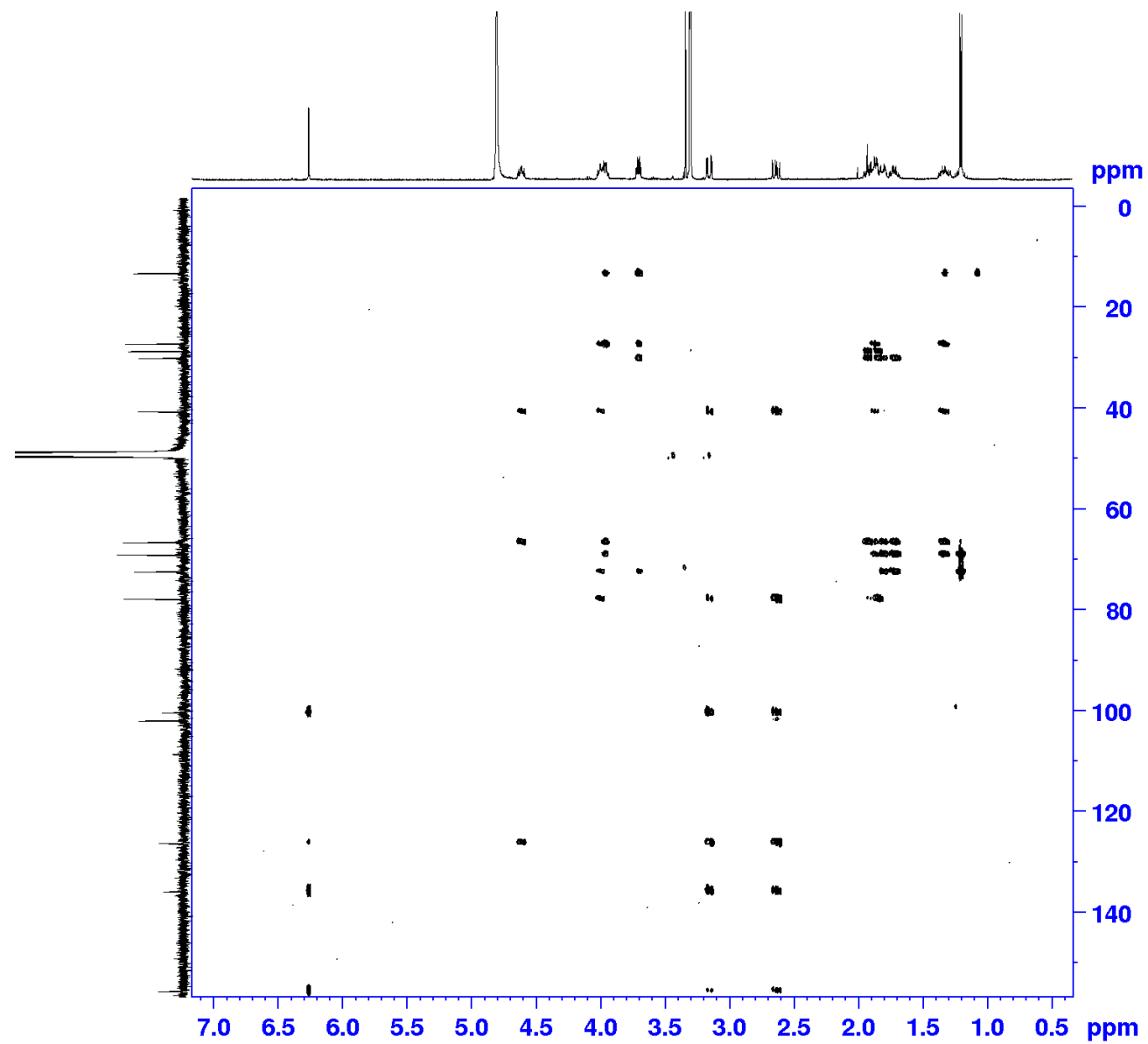
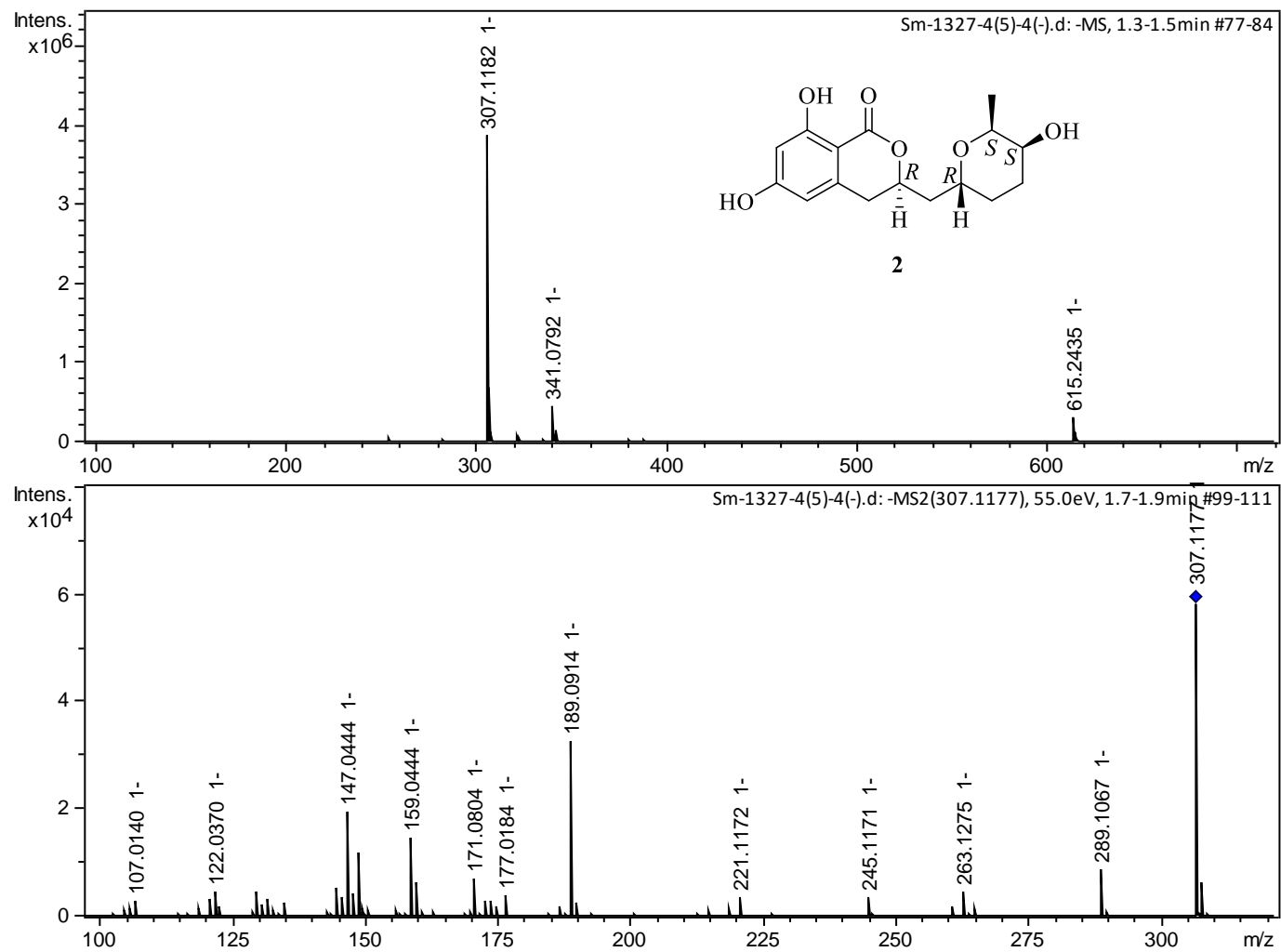


Figure S8. HRESIMS for 2



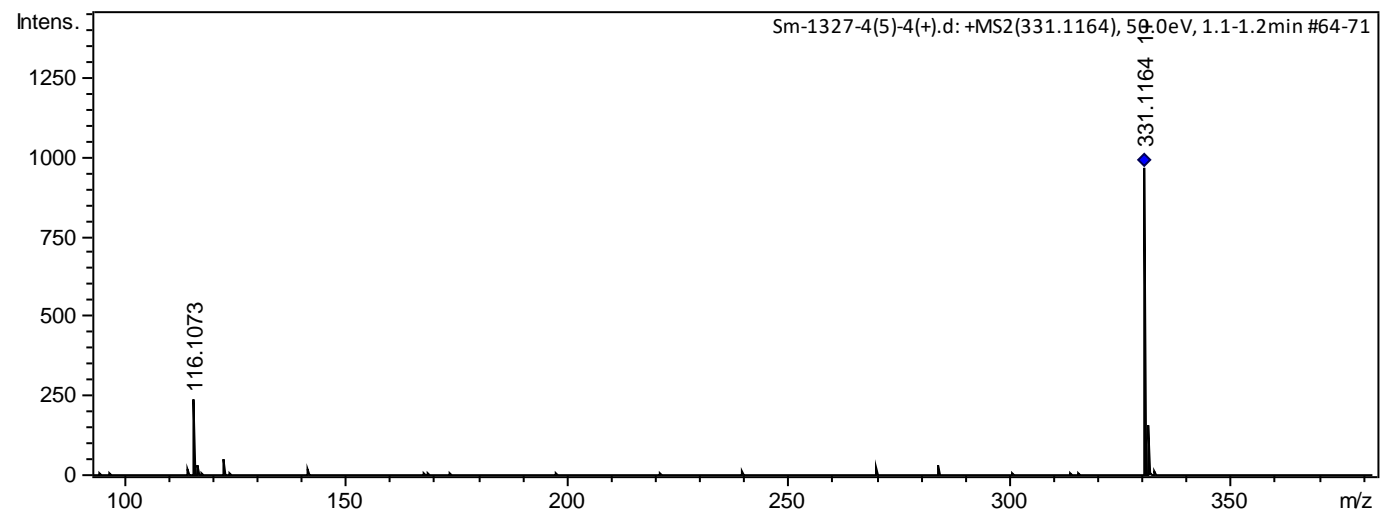
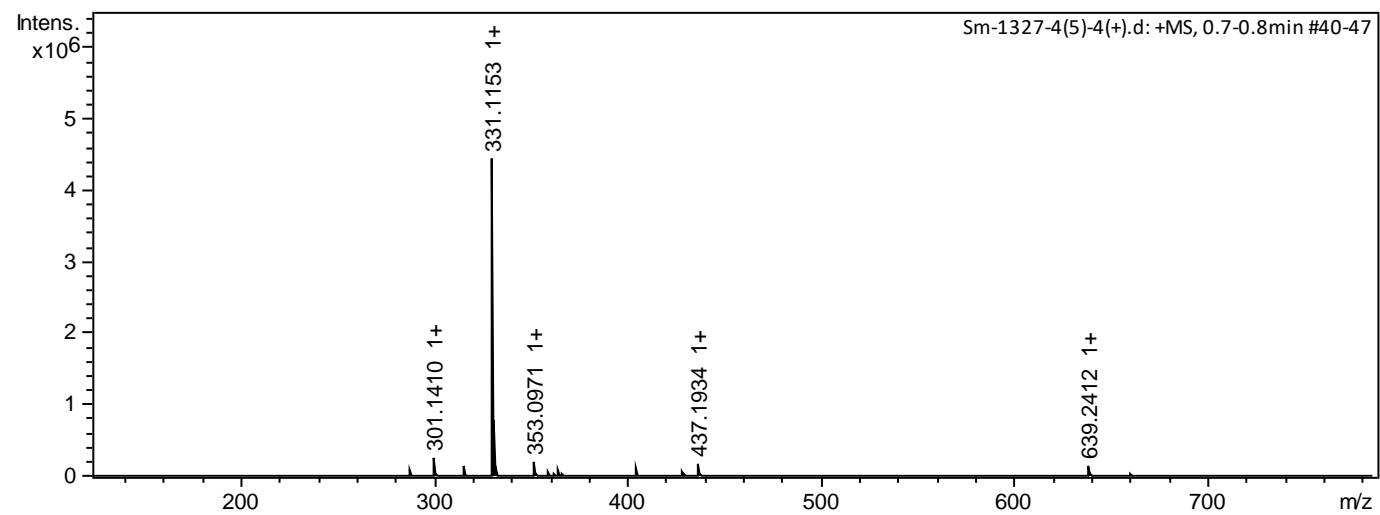


Figure S9. ^1H NMR spectrum of **2** measured at 500 MHz in MeOD

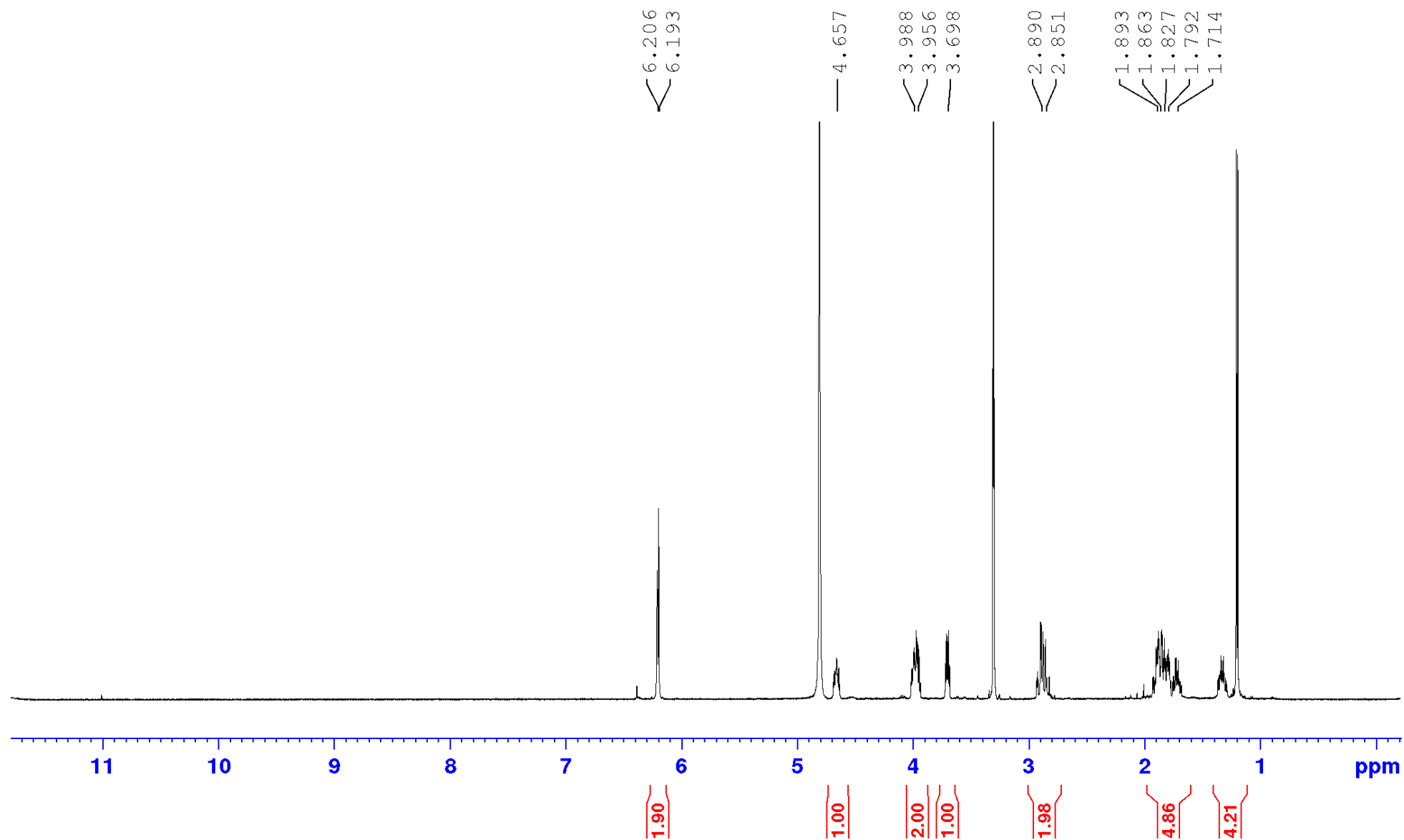


Figure S10. ^{13}C NMR spectrum of **2** measured at 125 MHz in MeOD

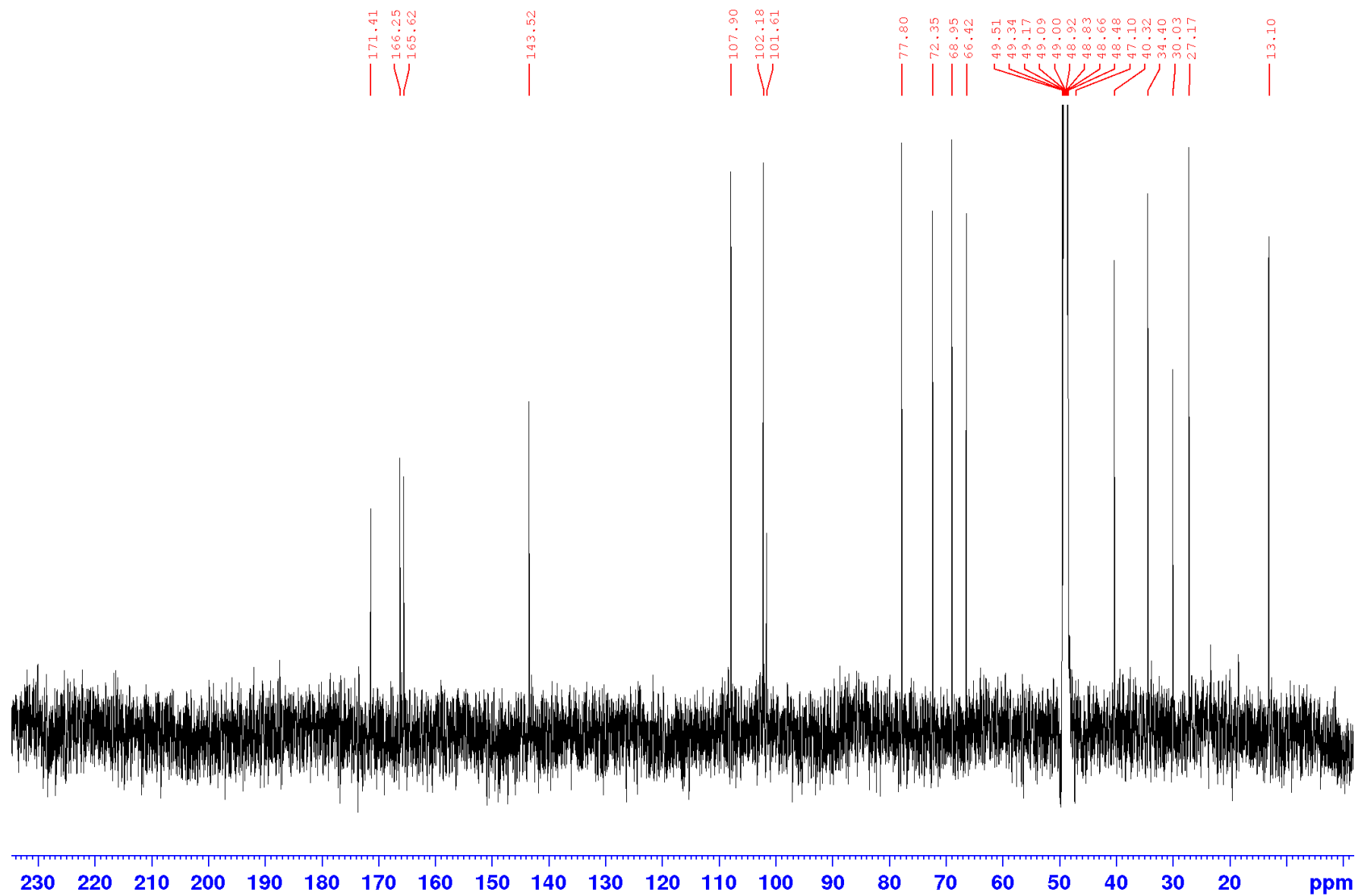


Figure S11. DEPT-135 spectrum of 2 measured at 125 MHz in MeOD

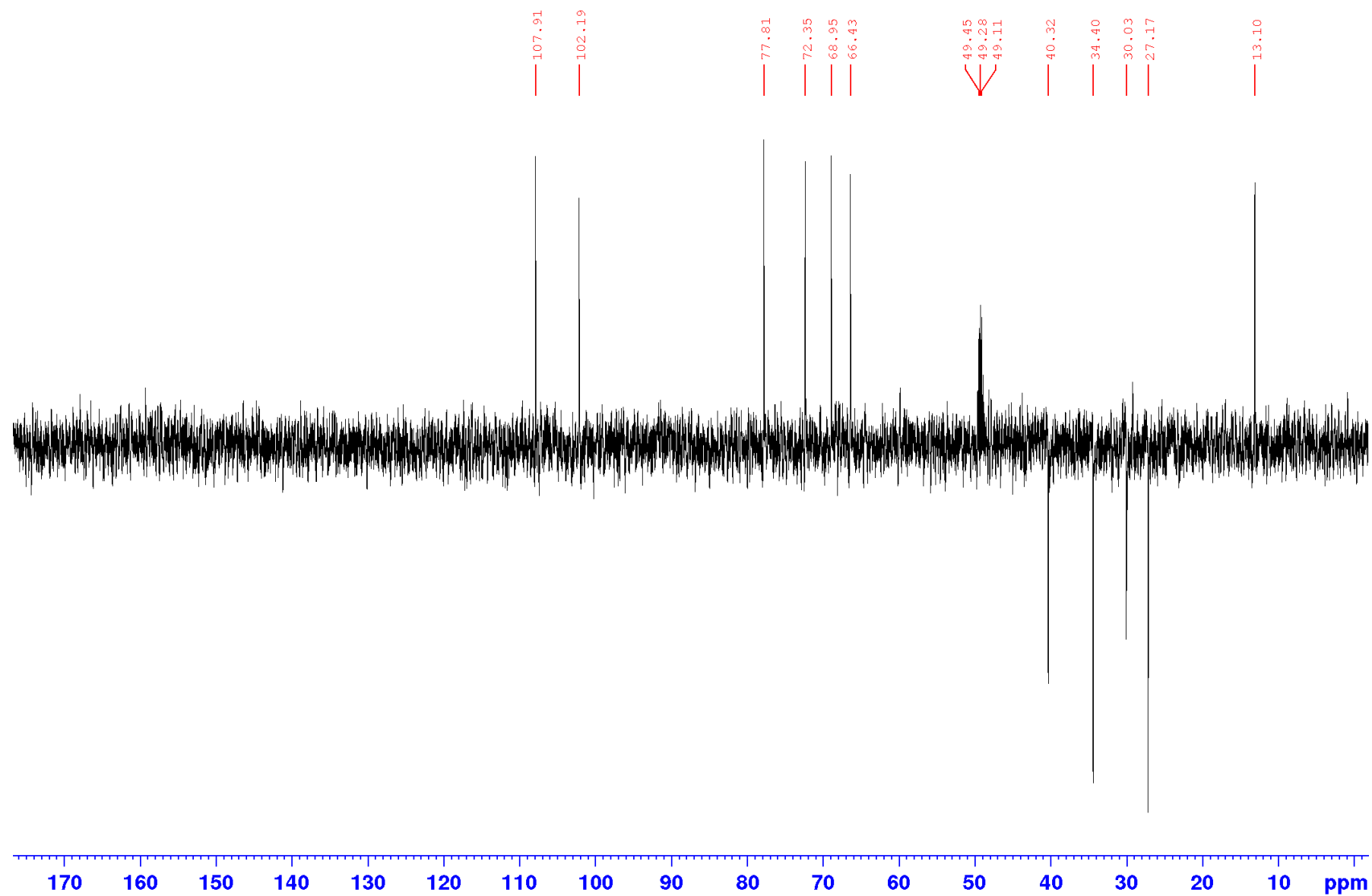


Figure S12. HSQC spectrum of 2 measured in MeOD

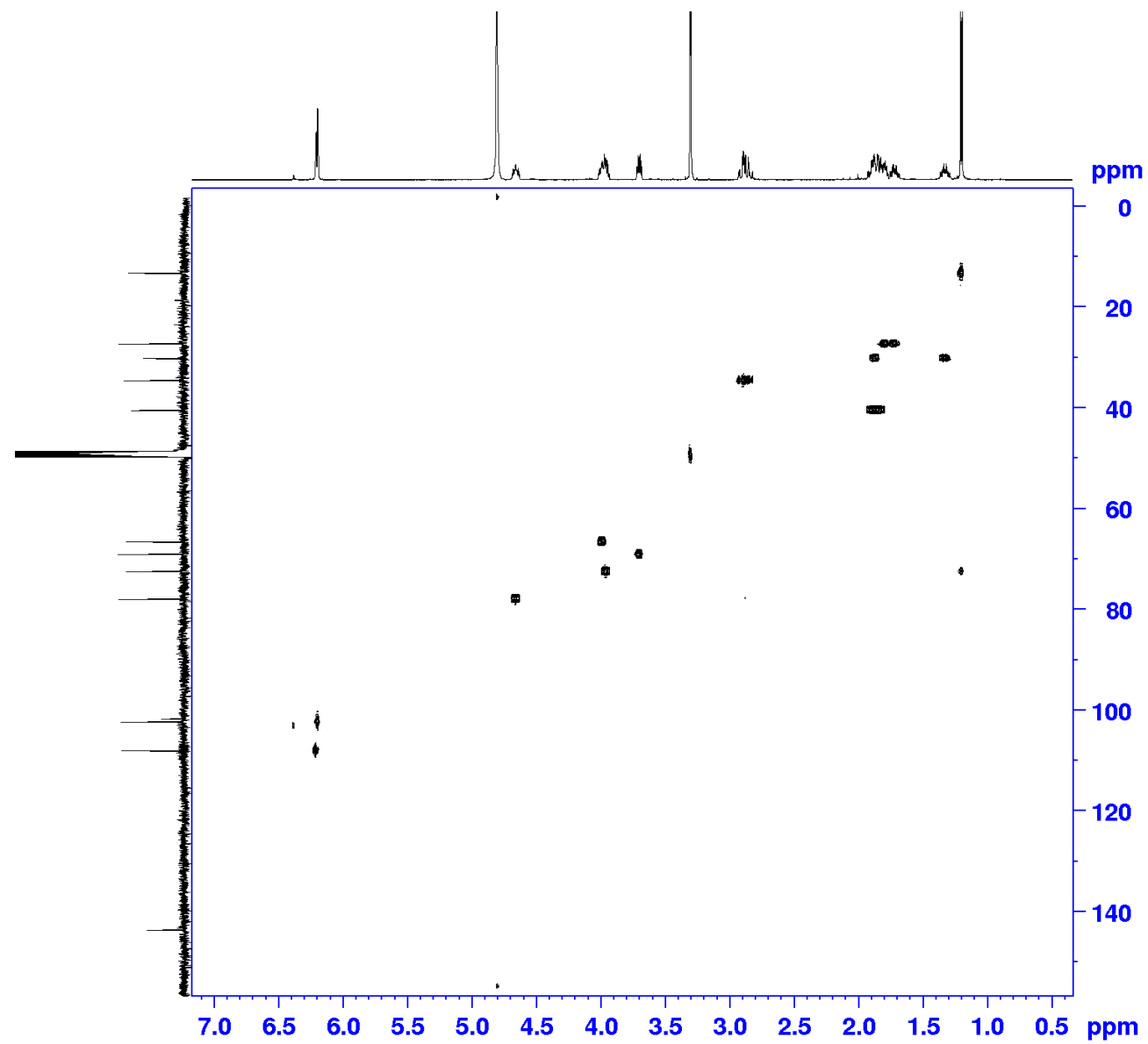


Figure S13. COSY spectrum of 2 measured in MeOD

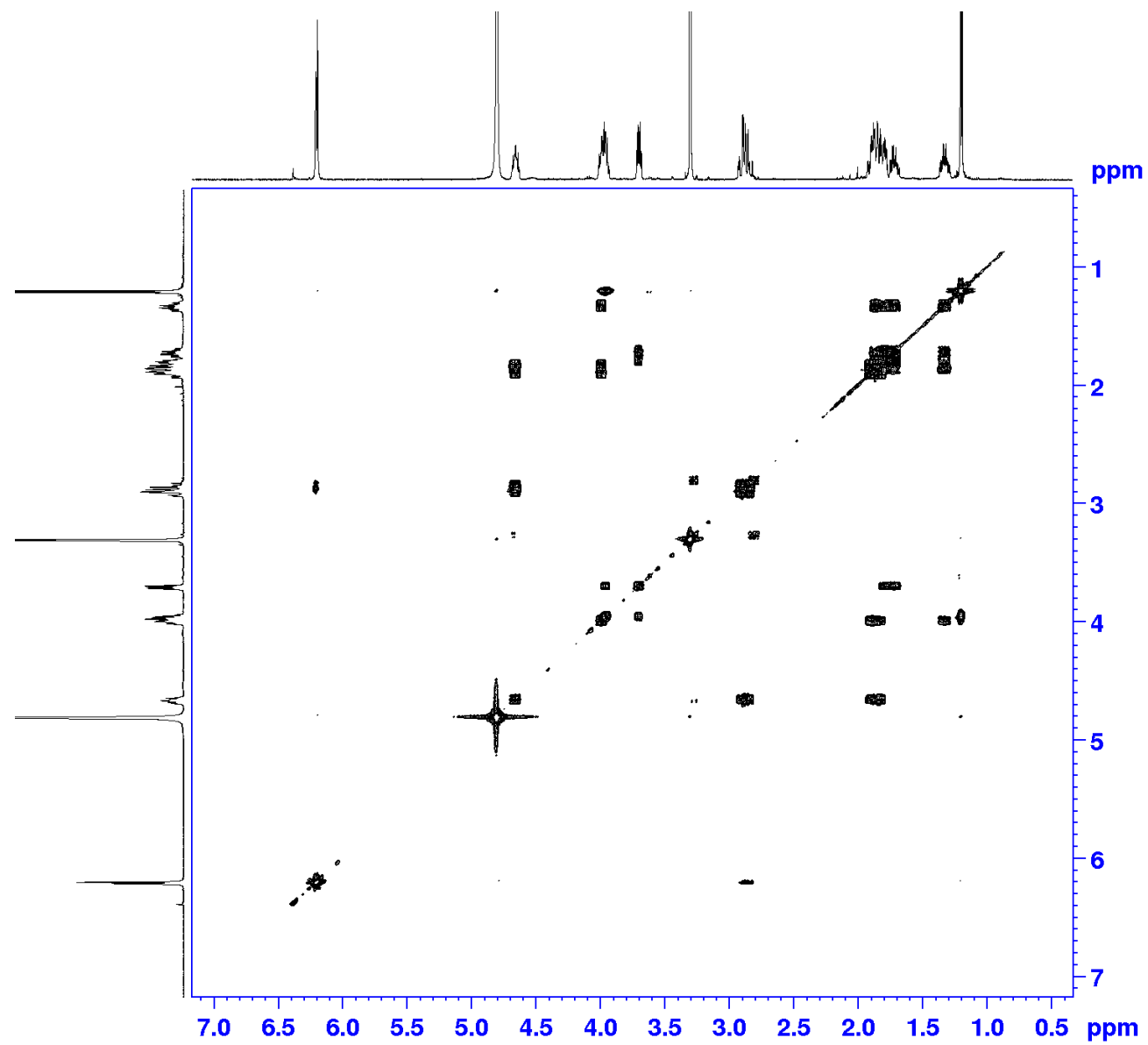


Figure S14. HMBC spectrum of 2 measured in DMSO-d6

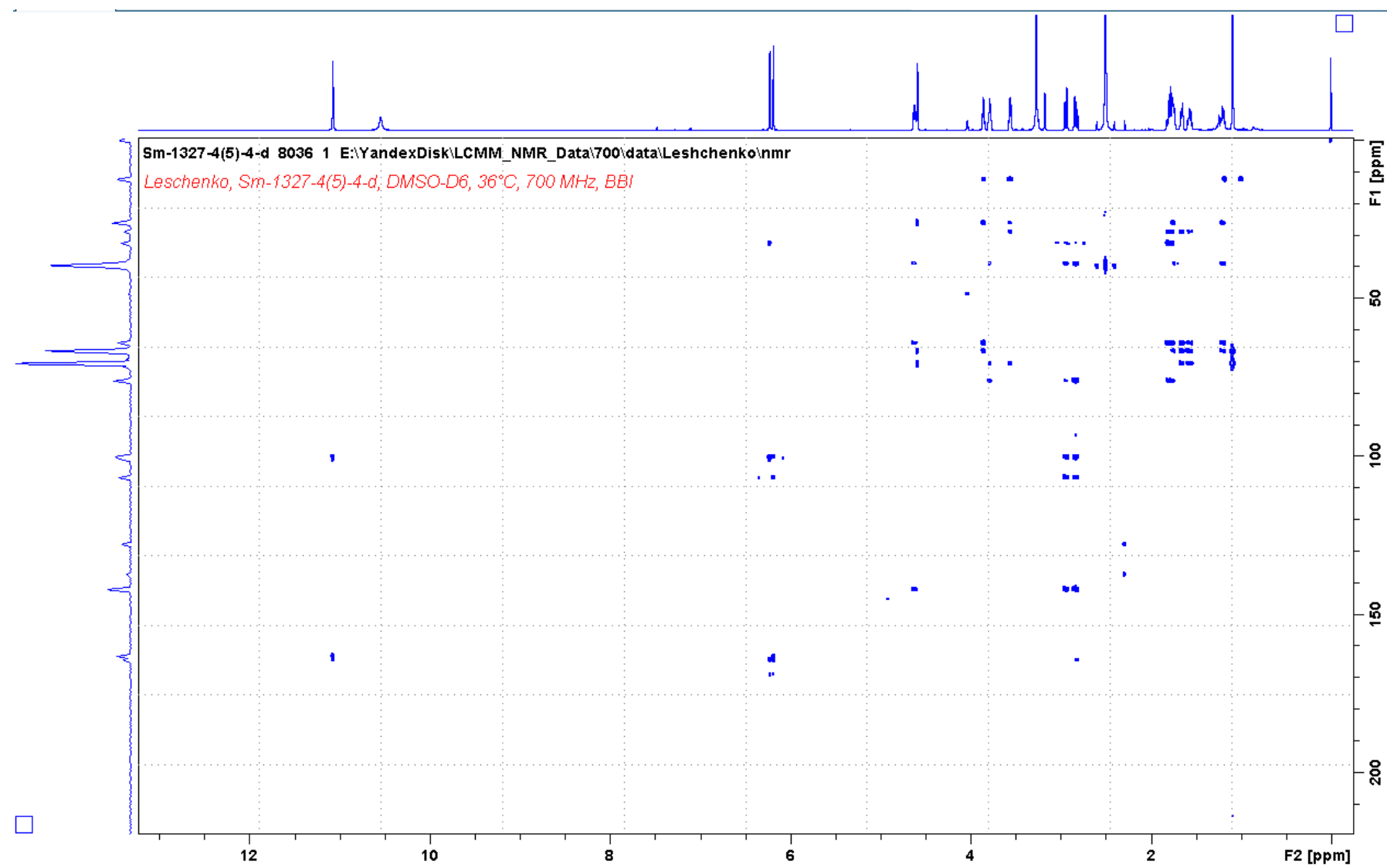
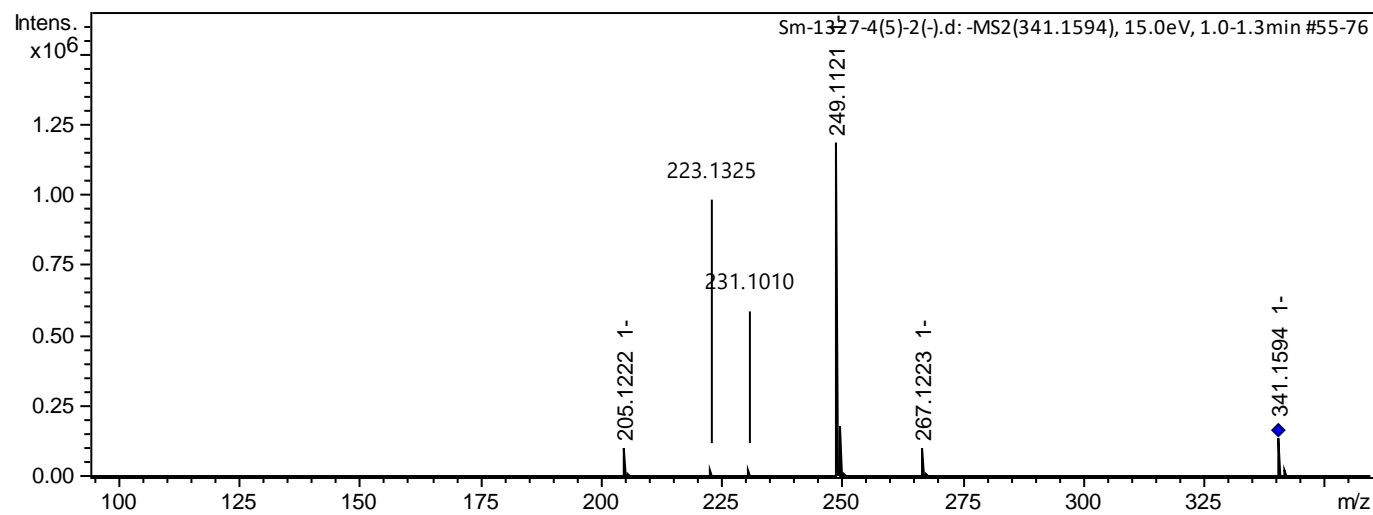
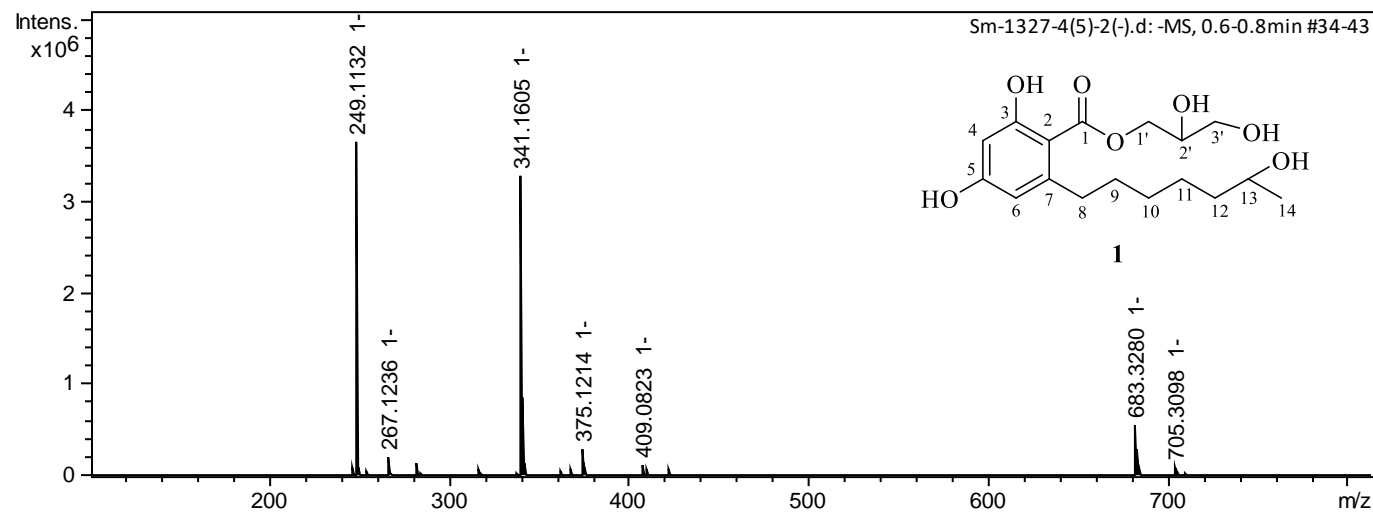
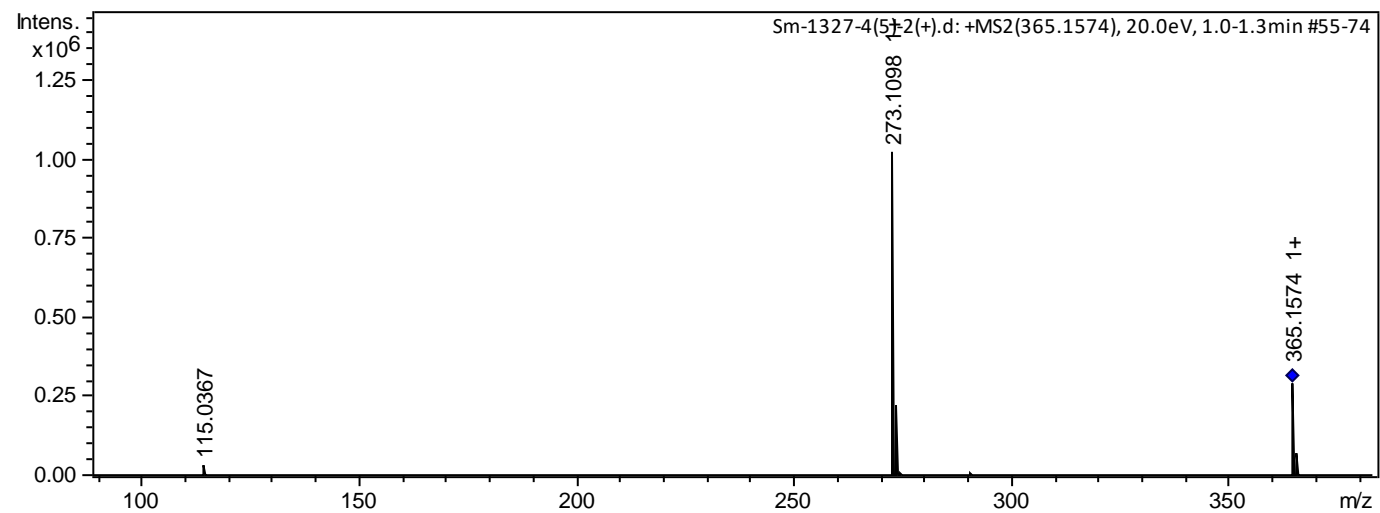
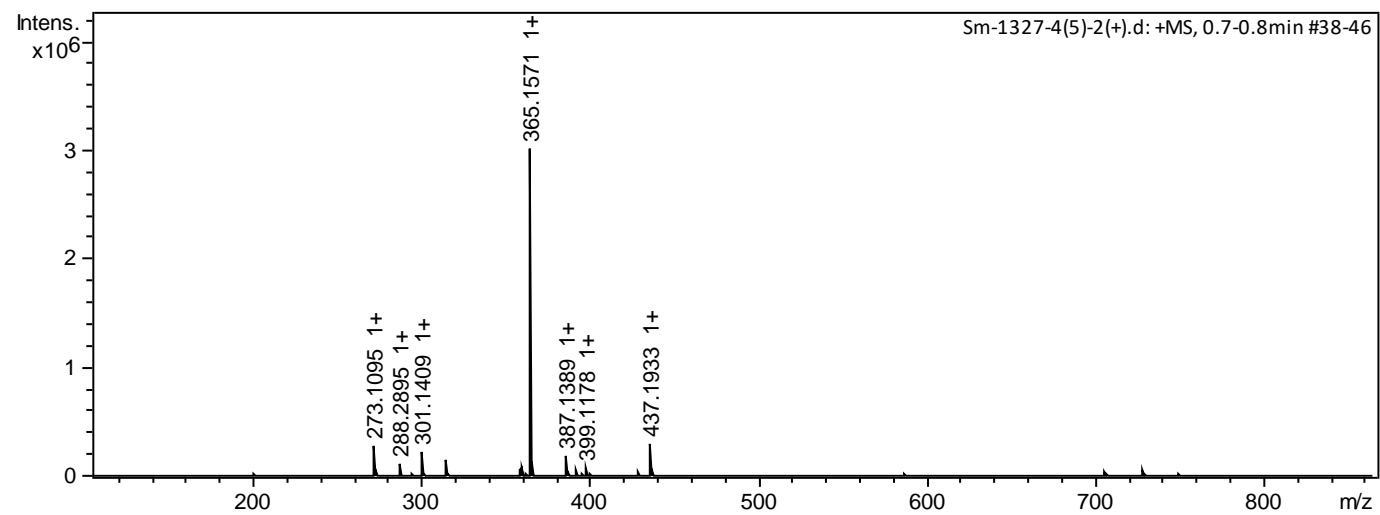


Figure S15. HRESIMS for 3





	meas	calc	Δ (ppm)
[M-H] ⁻	341,1605	341,1606	0,1
[M+Na] ⁺	365,1571	365,1571	-0,1

Figure S16. ^1H NMR spectrum of **3** measured at 500 MHz in MeOD

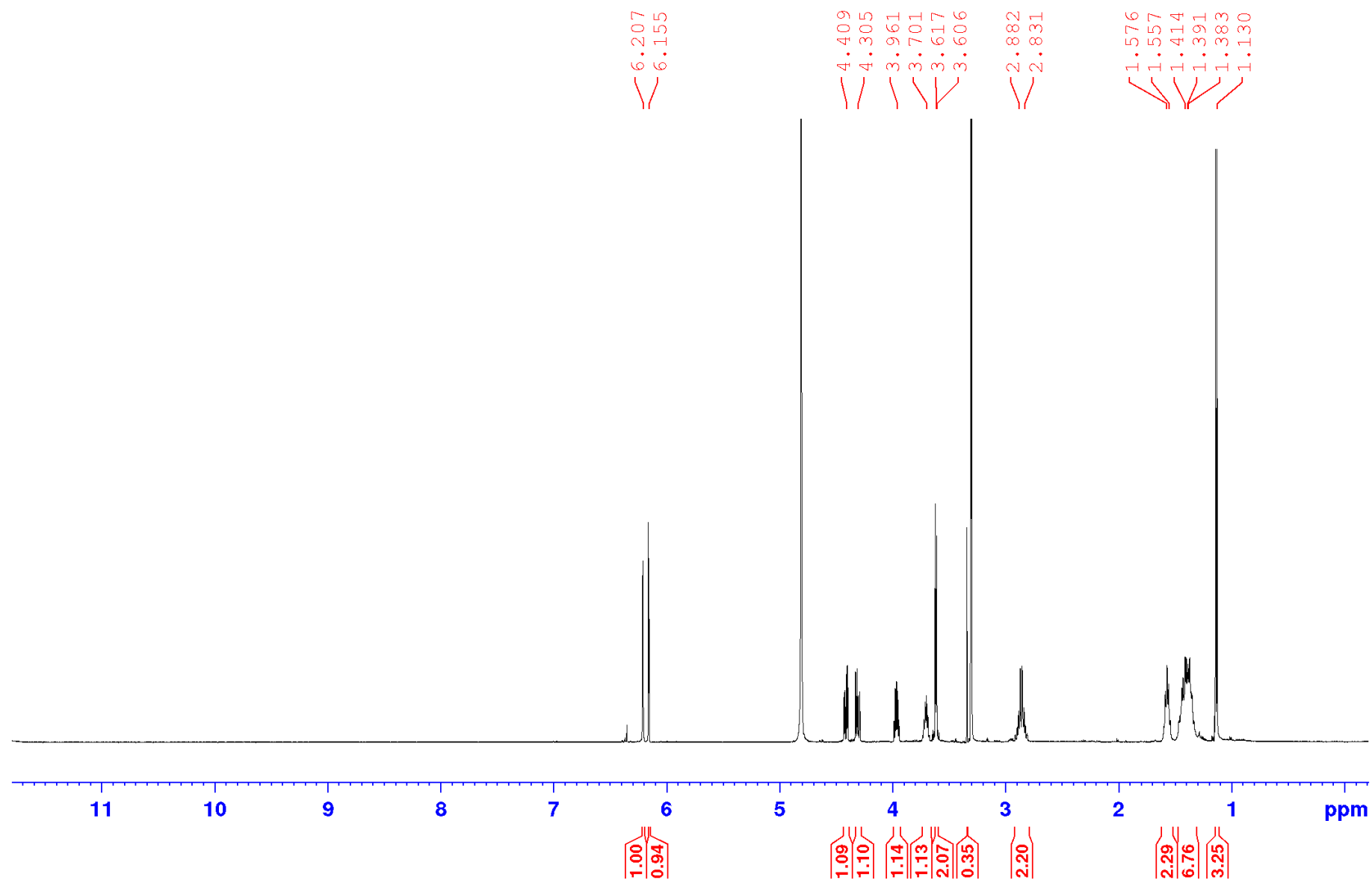


Figure S17. ^{13}C NMR spectrum of 3 measured at 75 MHz in MeOD

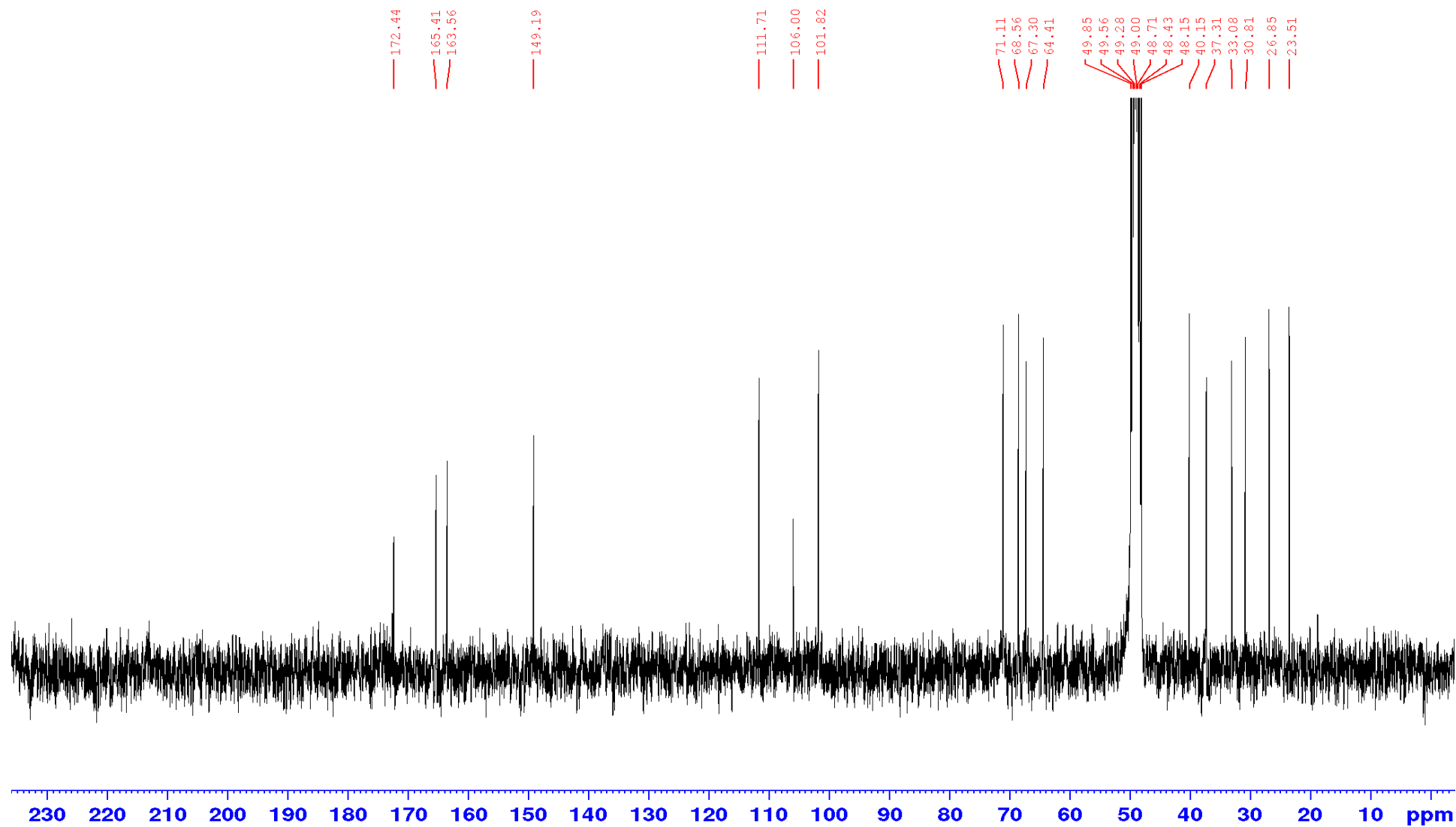


Figure S18. DEPT-135 spectrum of 3 measured at 75 MHz in MeOD

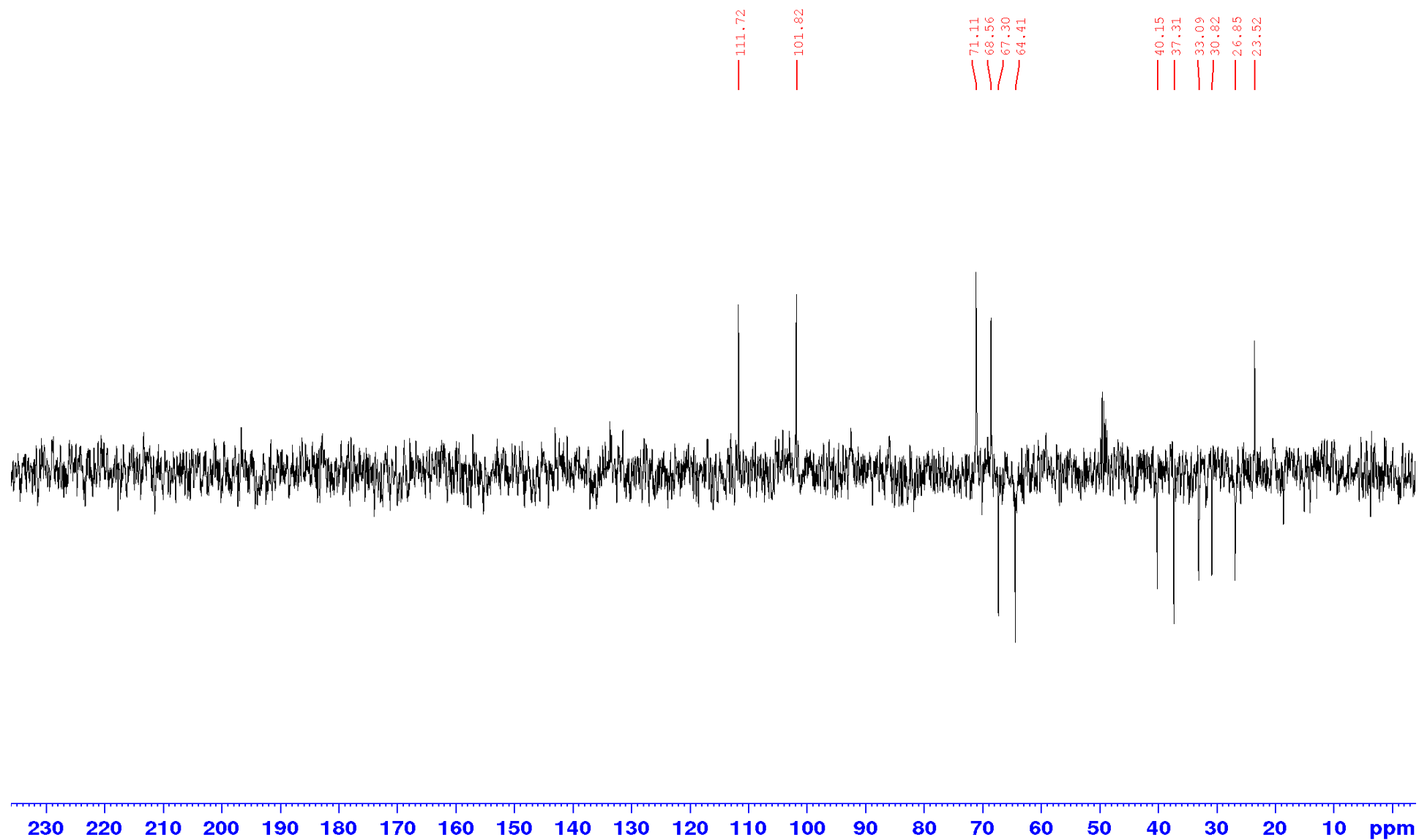


Figure S19. HSQC spectrum of 3 measured in MeOD

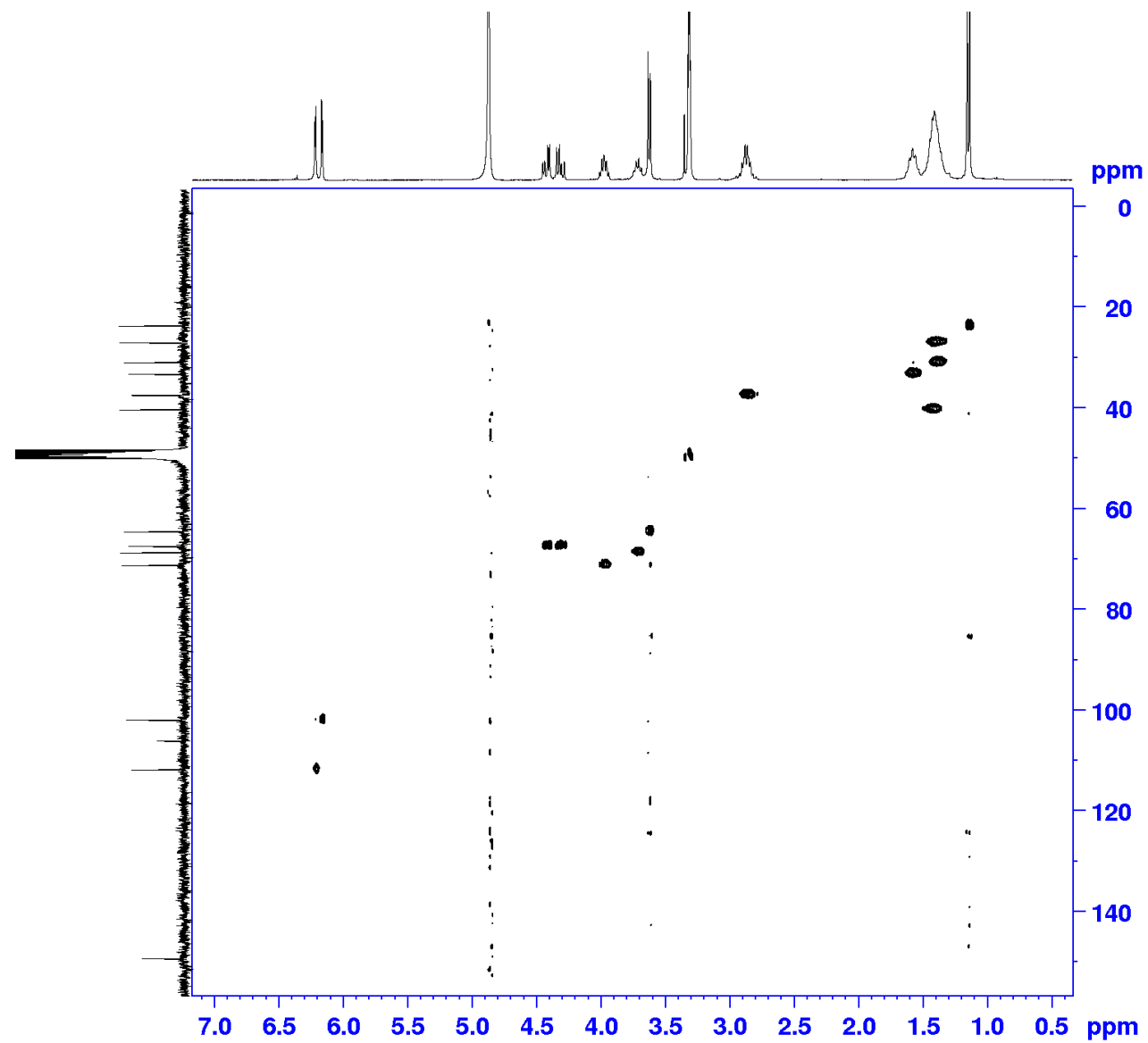


Figure S20. COSY spectrum of 3 measured in MeOD

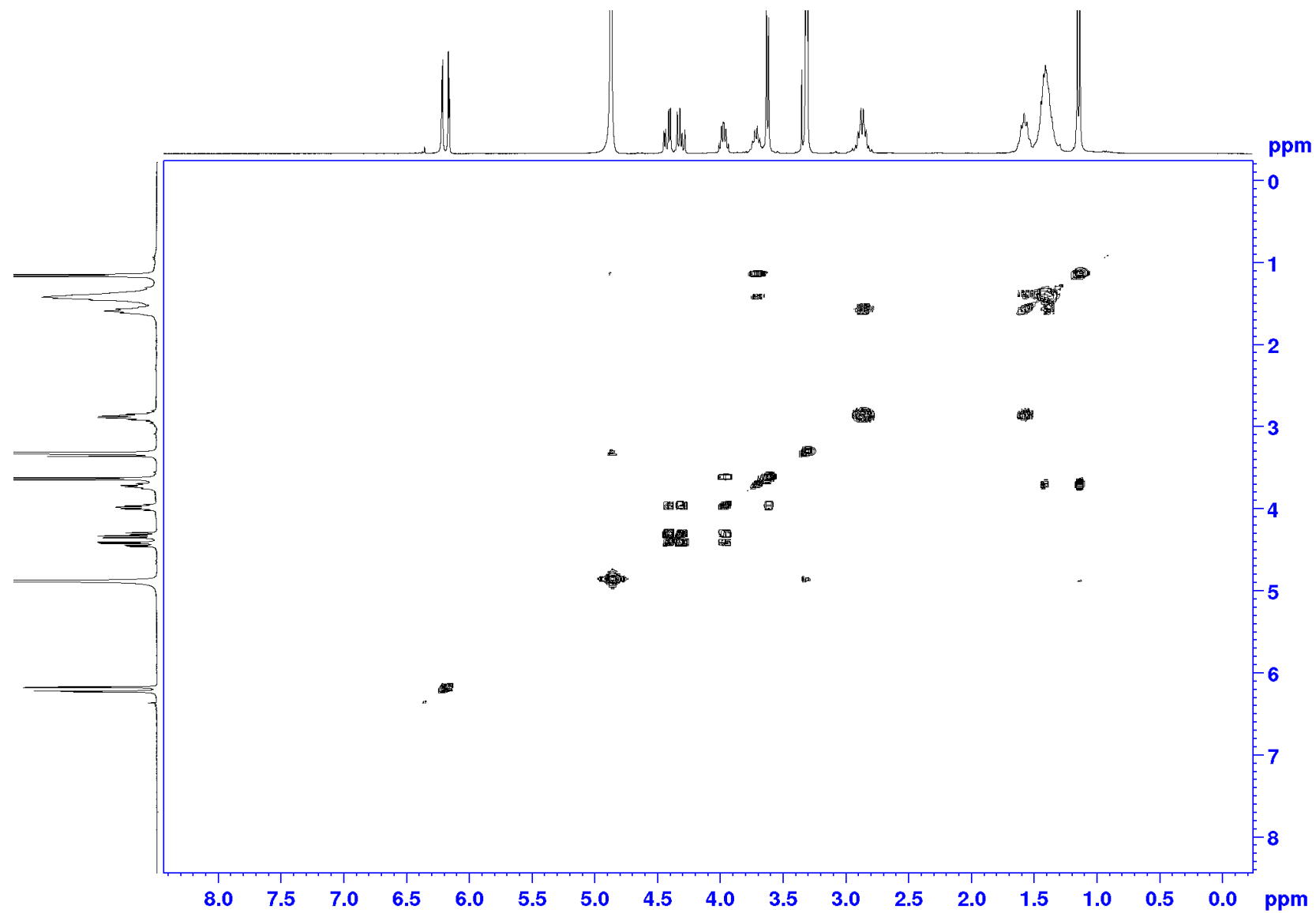


Figure S21. HMBC spectrum of 3 measured in MeOD

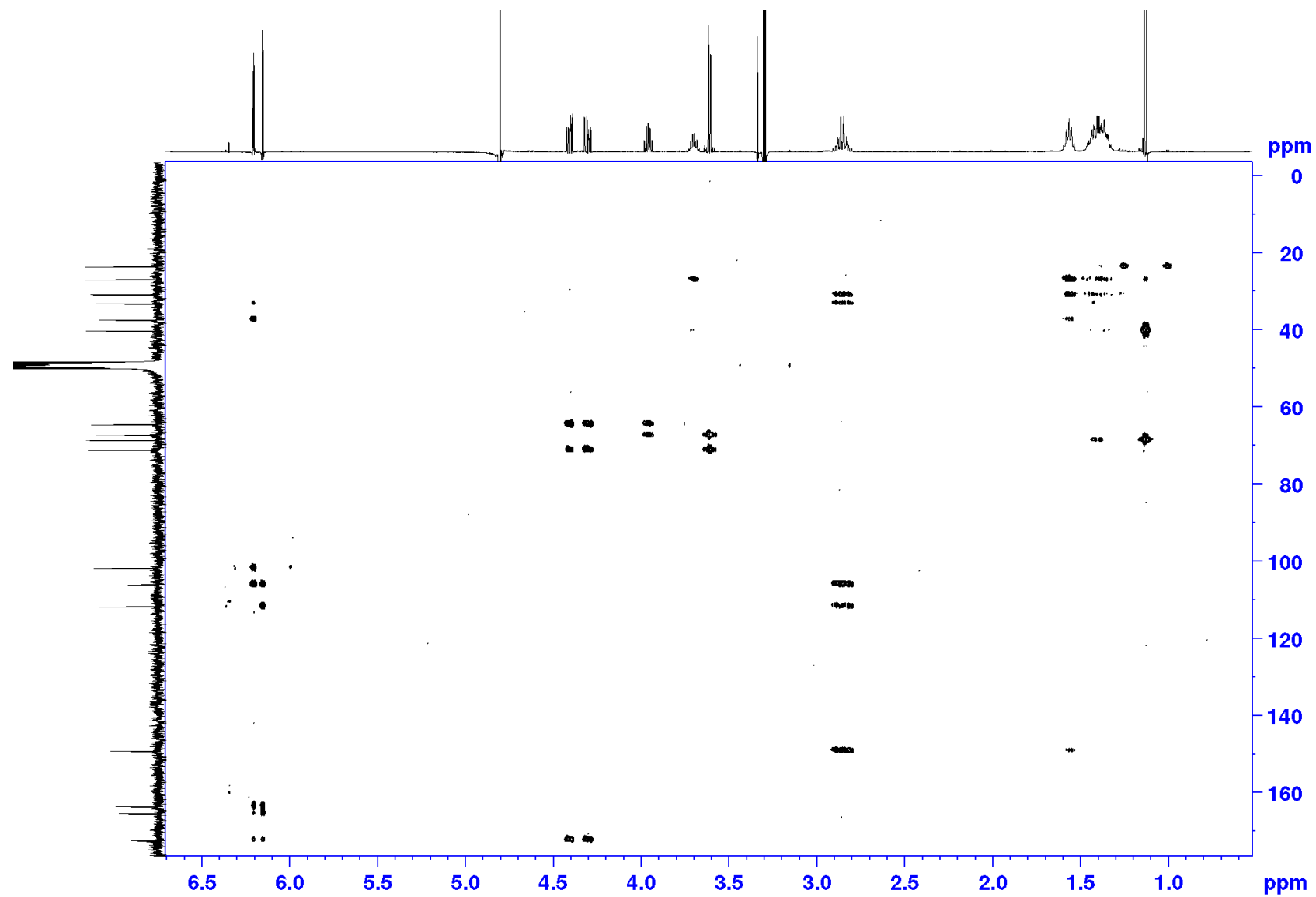
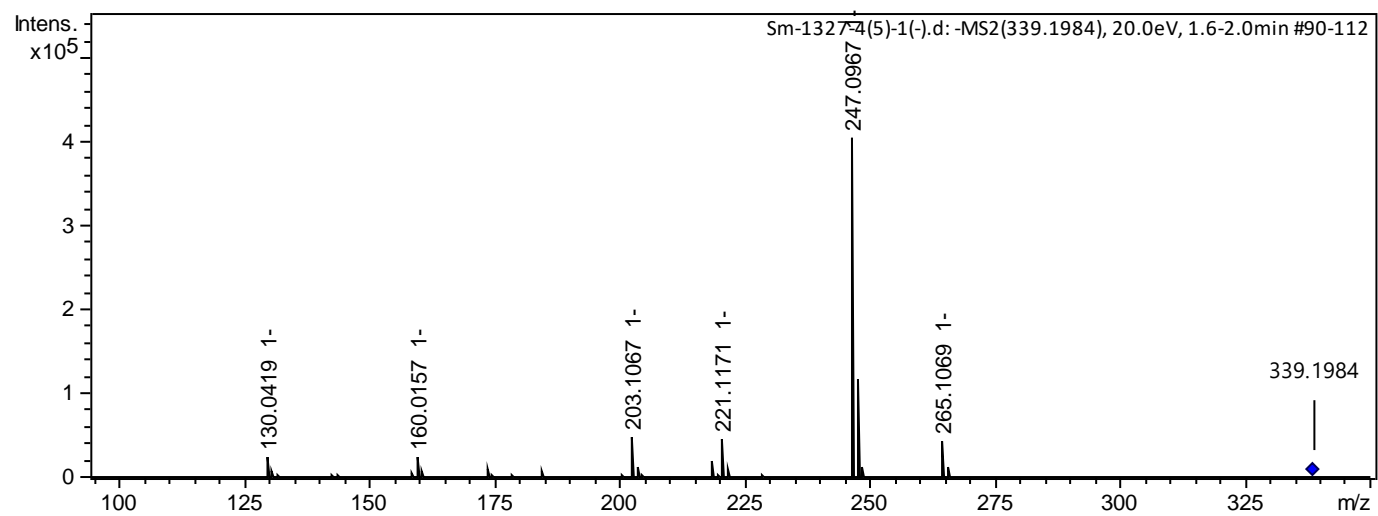
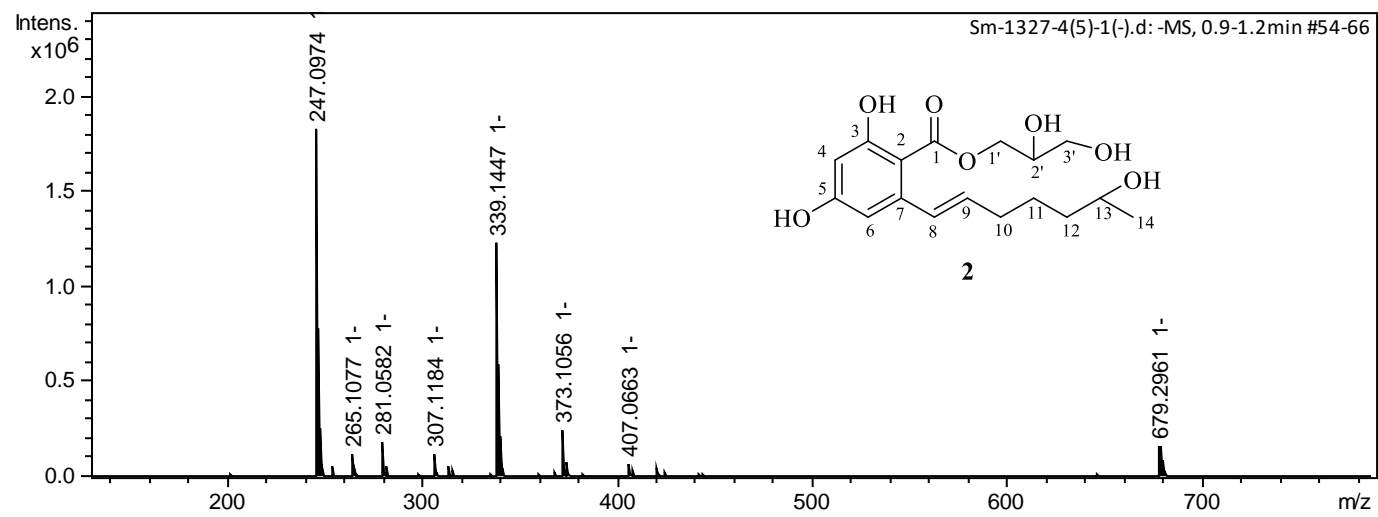
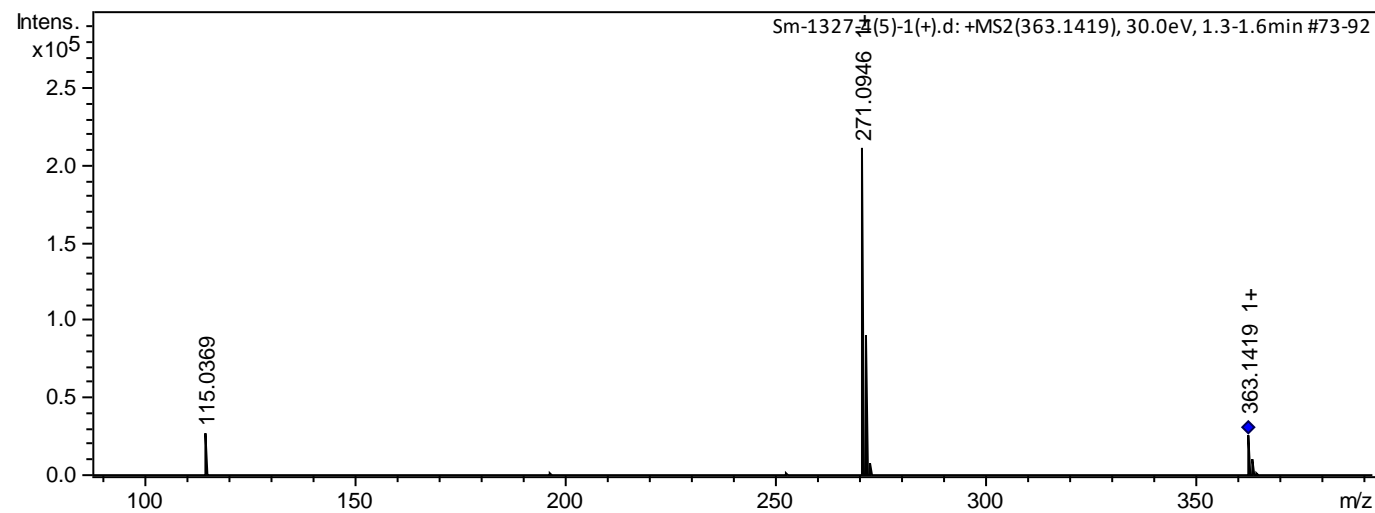
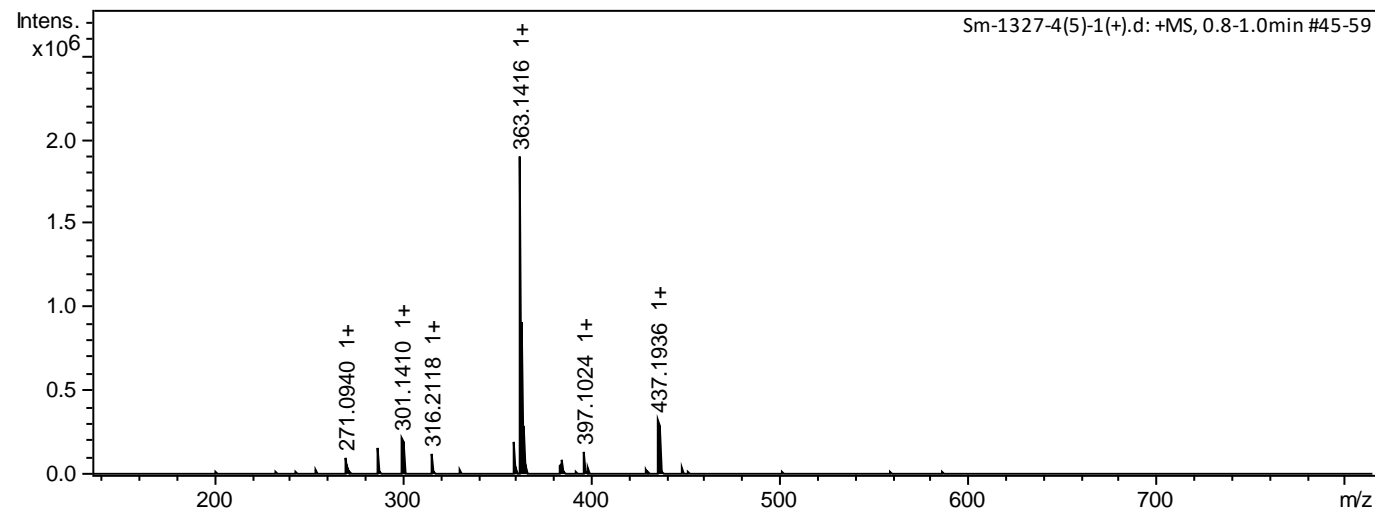


Figure S22. HRESIMS for 4





	meas	calc	Δ (ppm)
[M-H] ⁻	339,1447	339,1449	0,6
[M+Na] ⁺	363,1416	363,1414	-0,5

Figure S23. ^1H NMR spectrum of **4** measured at 500 MHz in MeOD

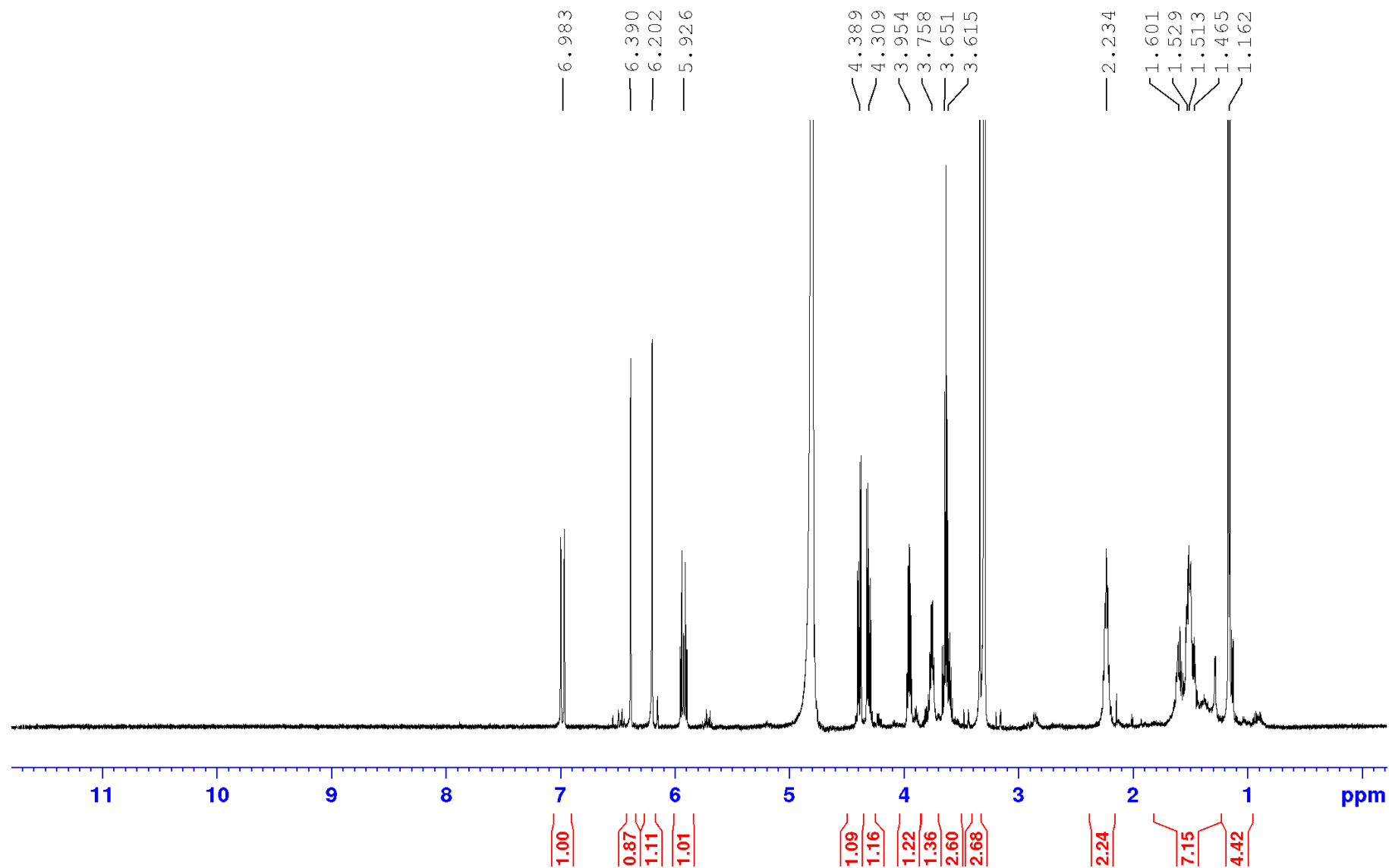


Figure S23. ^{13}C NMR spectrum of **4** measured at 75 MHz in MeOD

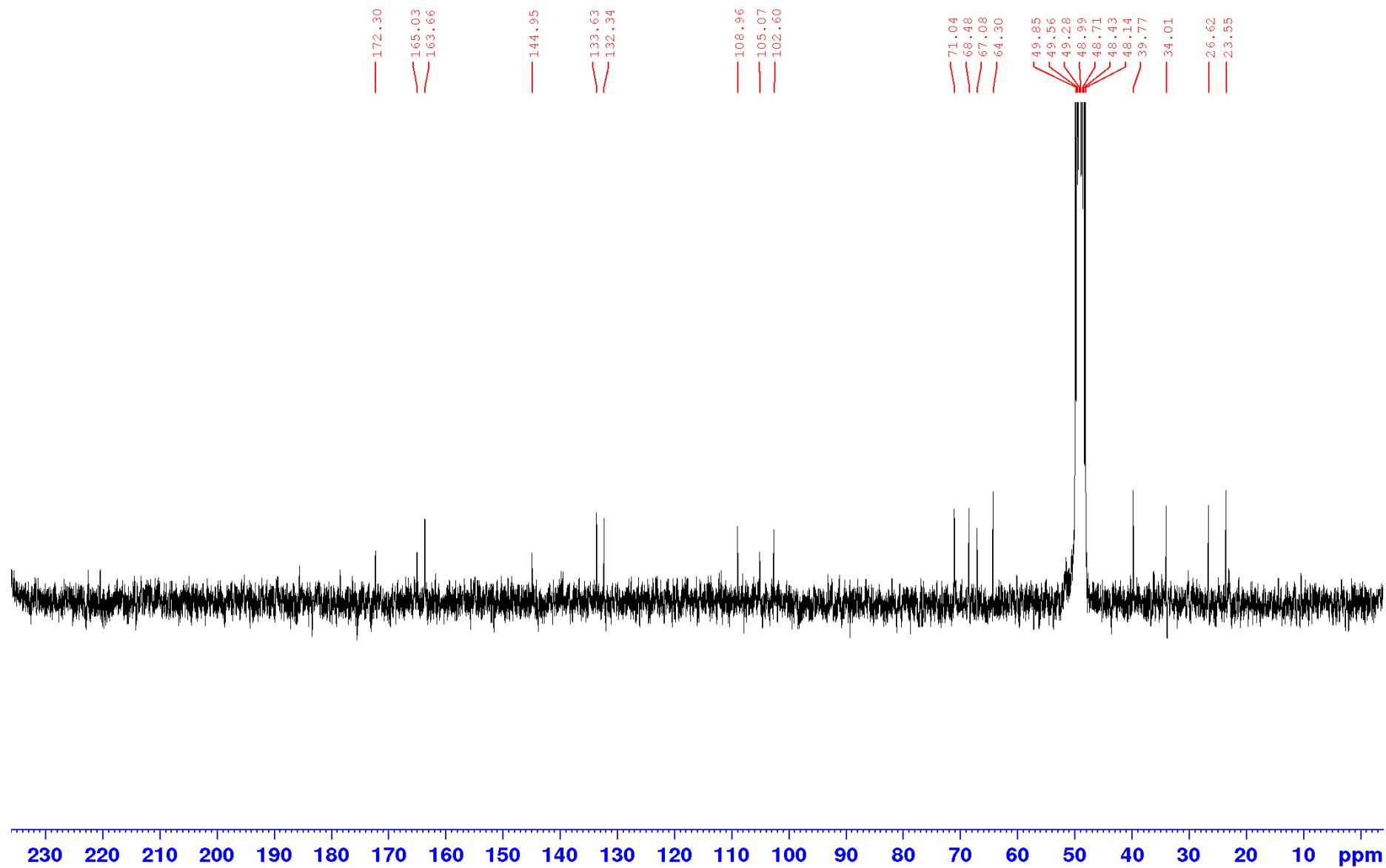


Figure S25. ^{13}C NMR spectrum of **4** measured at 75 MHz in MeOD

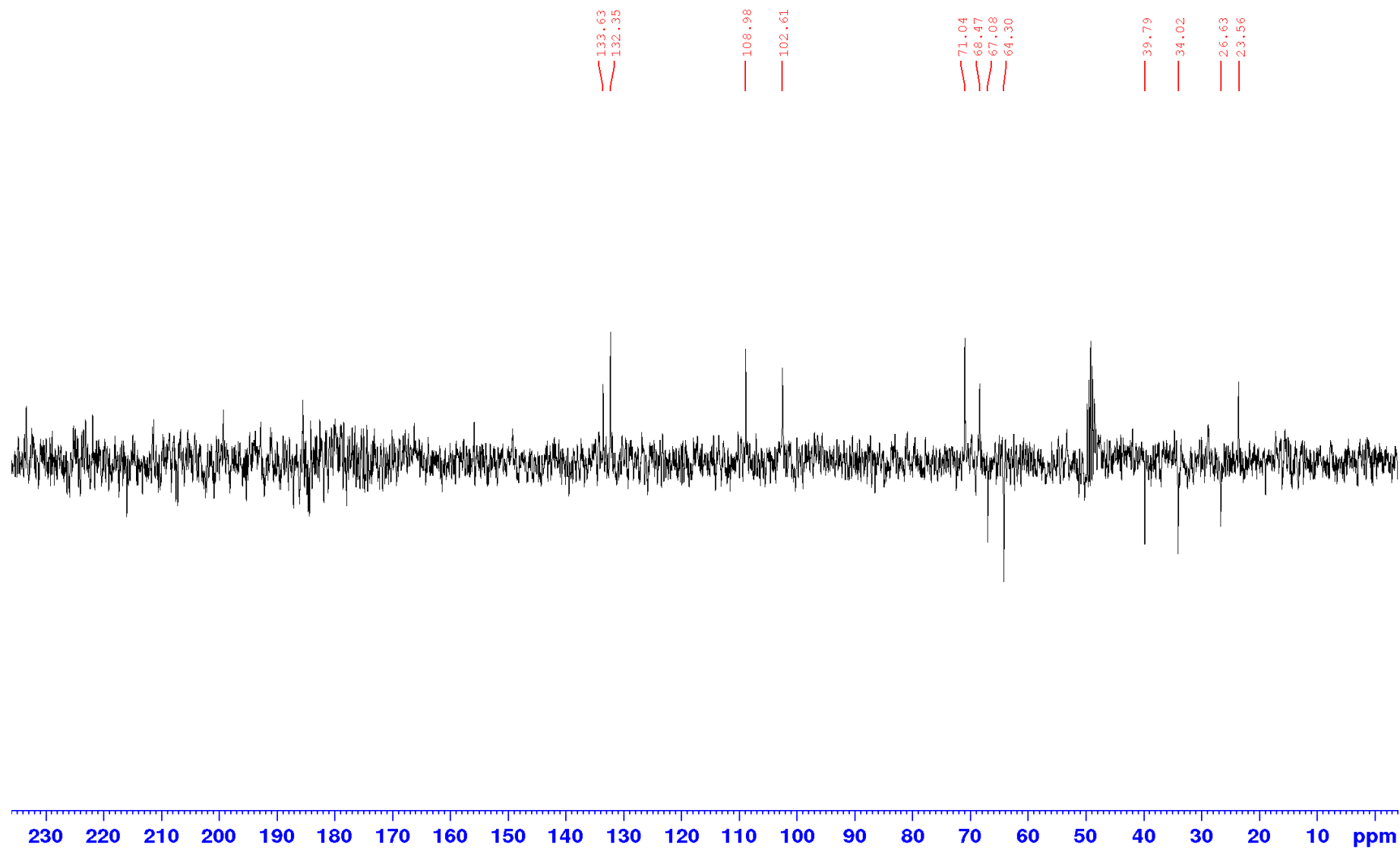


Figure S26. HSQC spectrum of 4 measured in MeOD

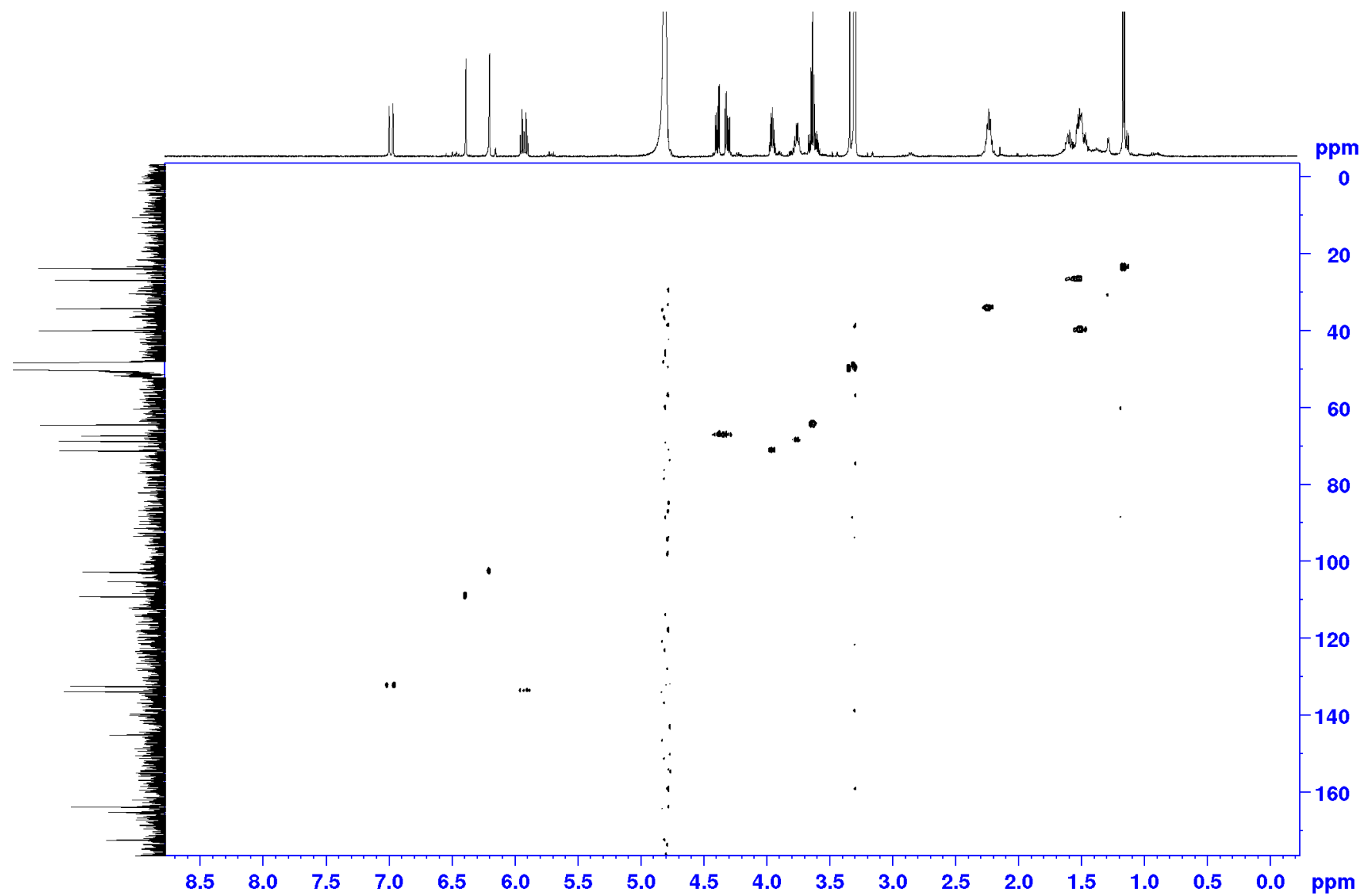


Figure S27. COSY spectrum of 4 measured in MeOD

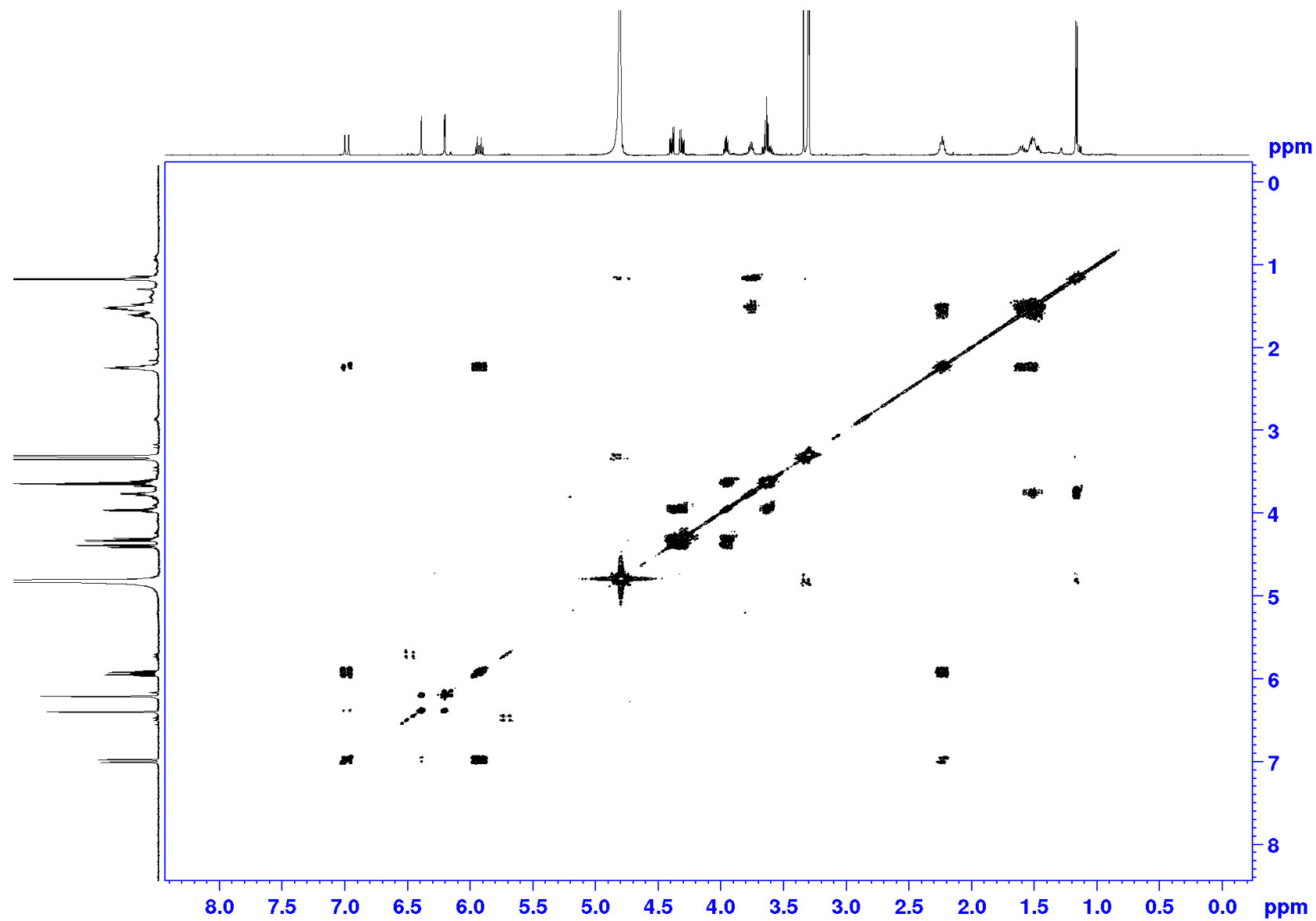


Figure S28. HMBC spectrum of 4 in MeOD

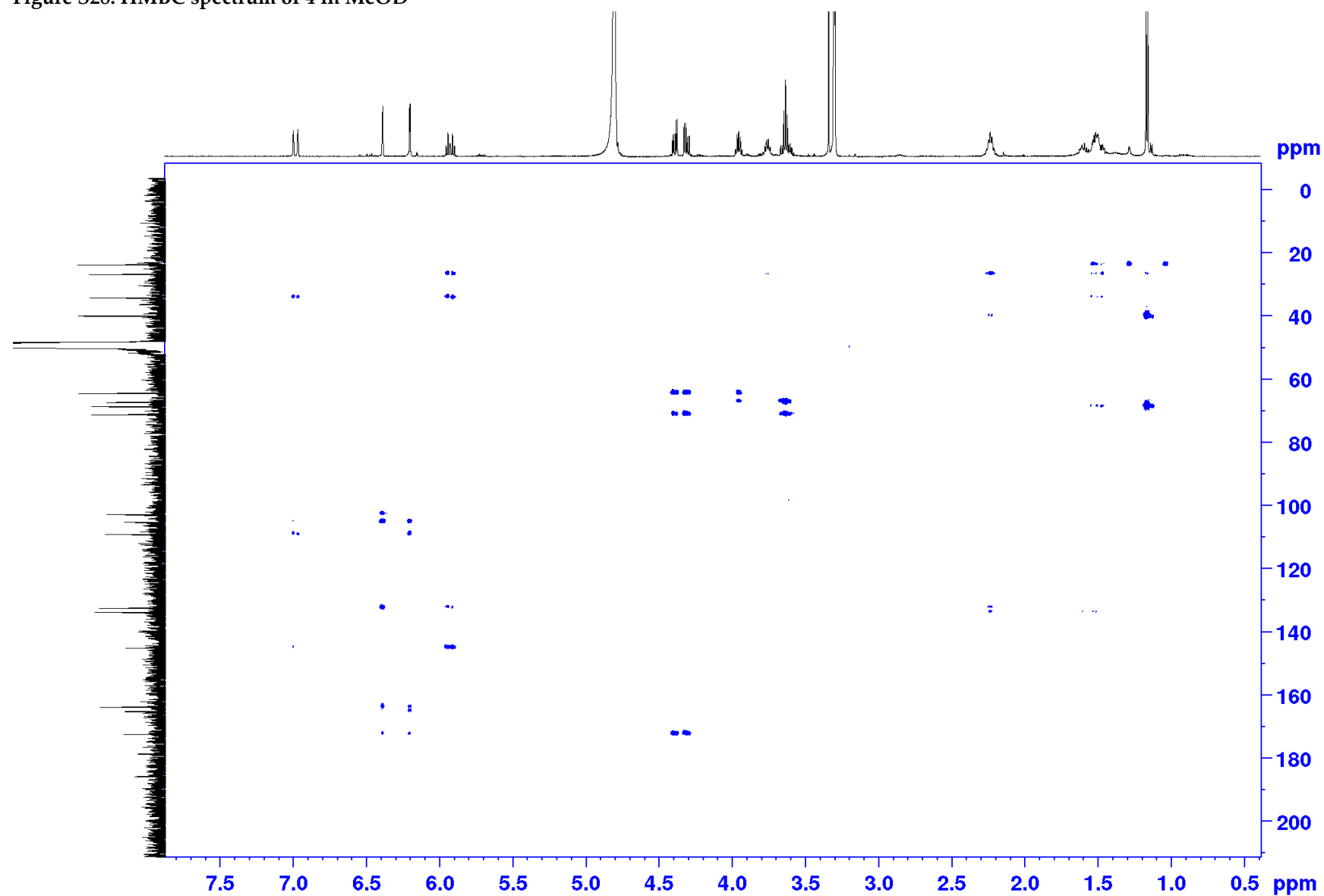
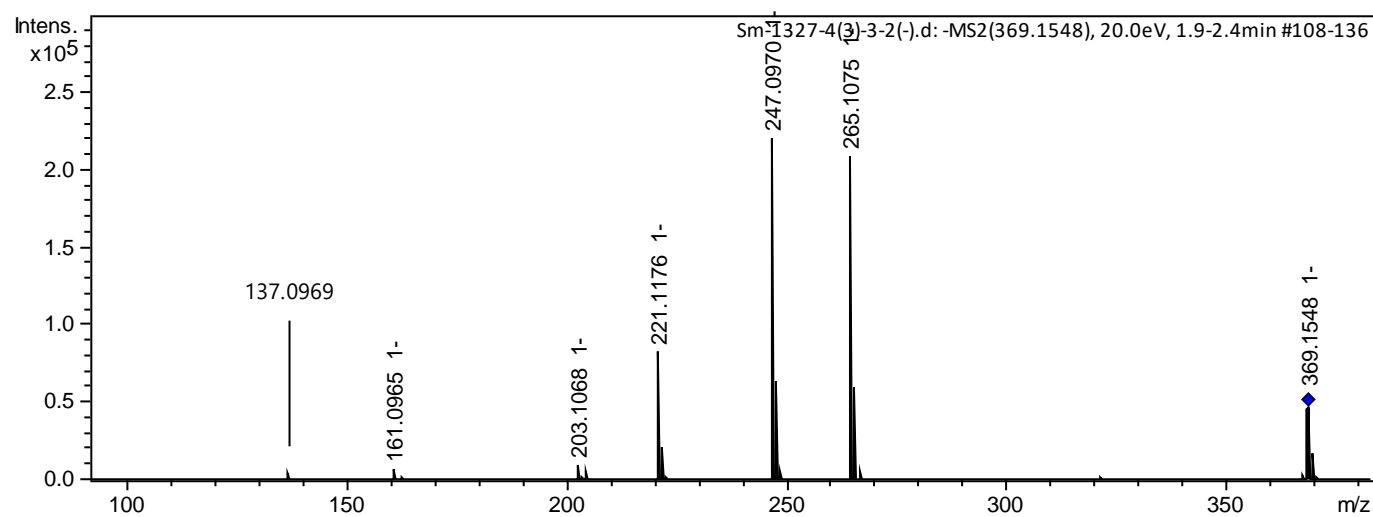
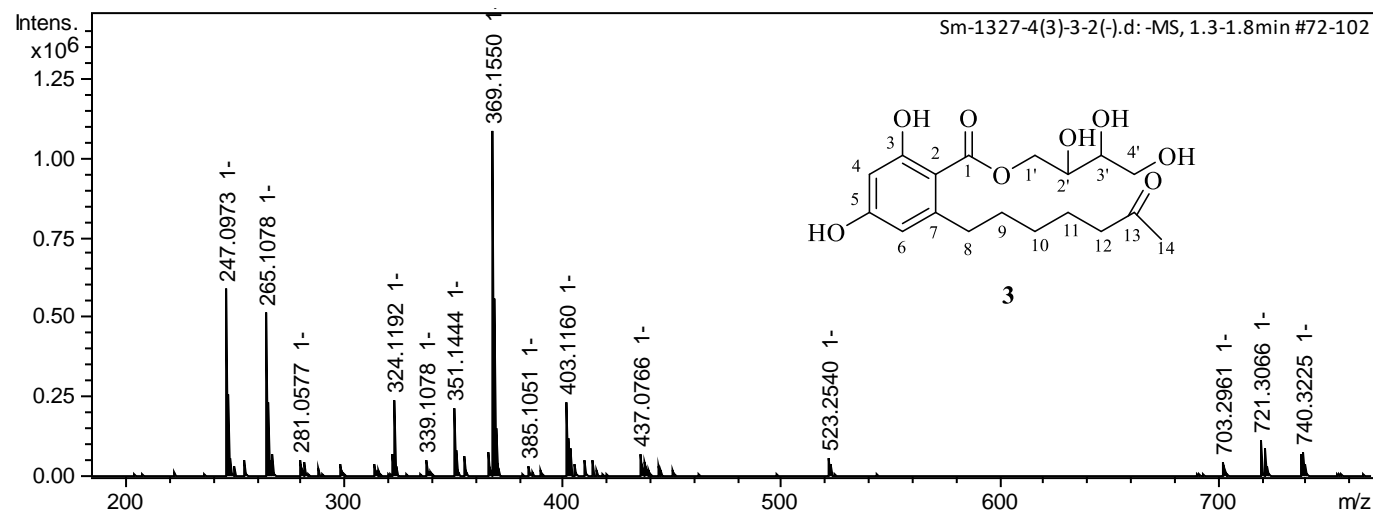
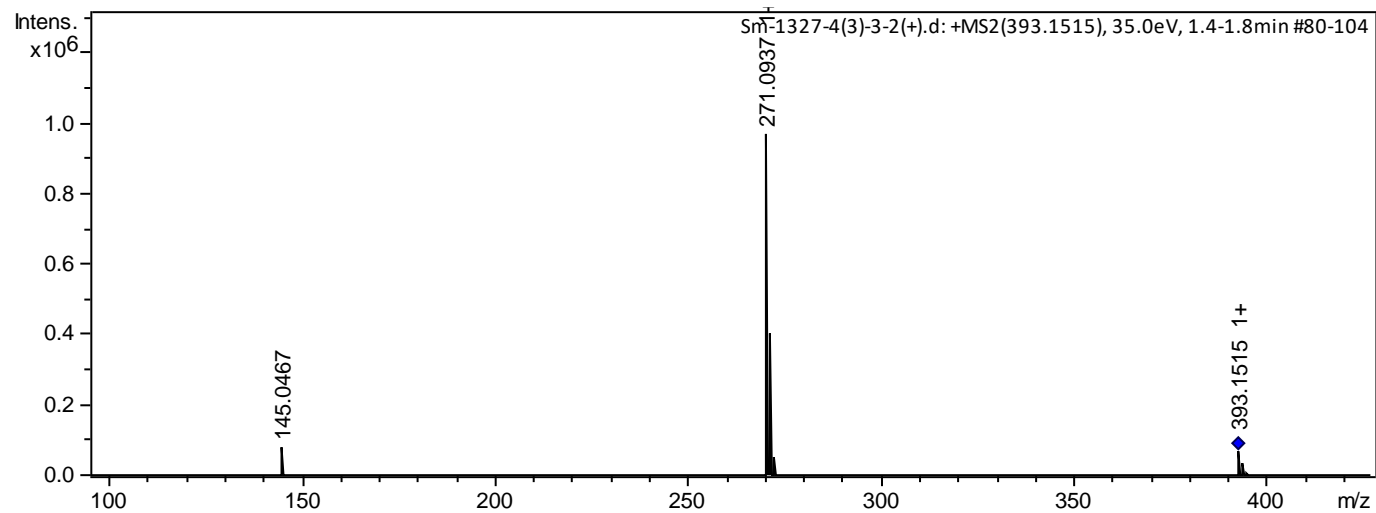
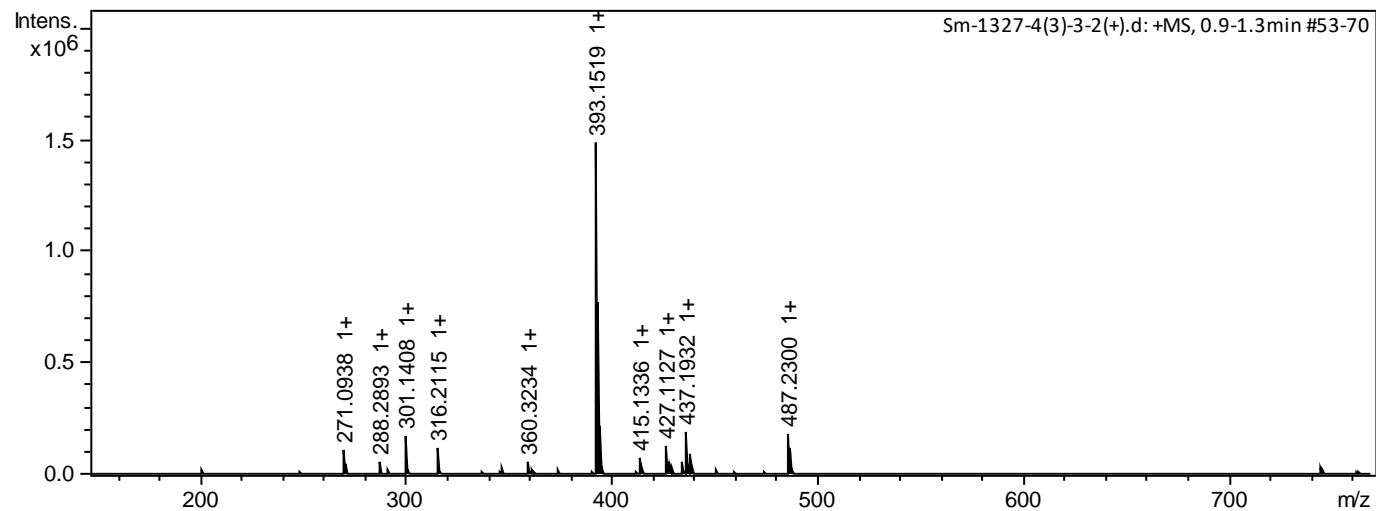


Figure S29. HRESIMS for 5





	meas	calc	Δ (ppm)
[M-H] ⁻	369,1550	369,1555	1,3
[M+Na] ⁺	393,1519	393,152	0,3

Figure S30. ^1H NMR spectrum of **5** measured at 500 MHz in MeOD

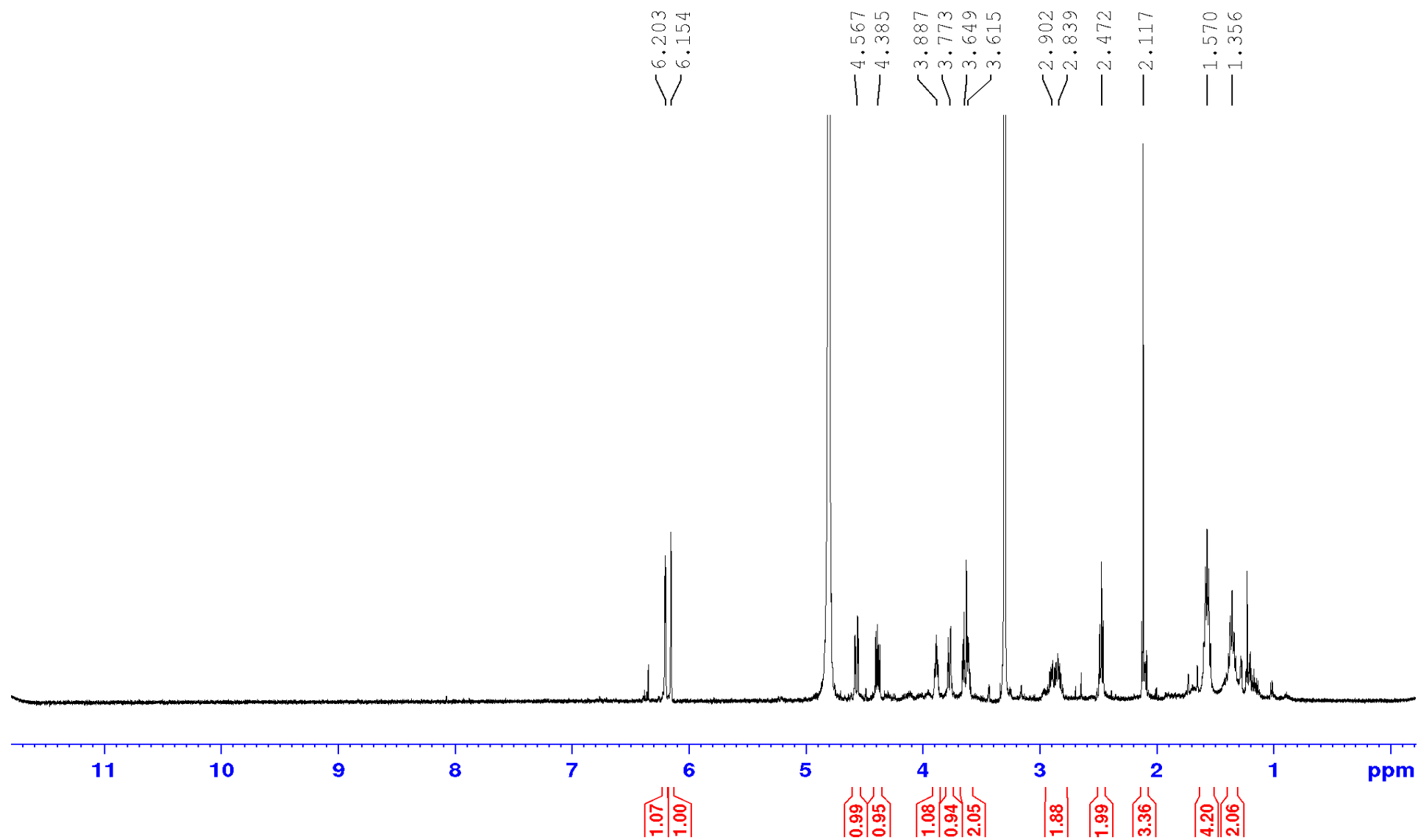


Figure S31. ^{13}C NMR spectrum of **5** measured at 125 MHz in MeOD

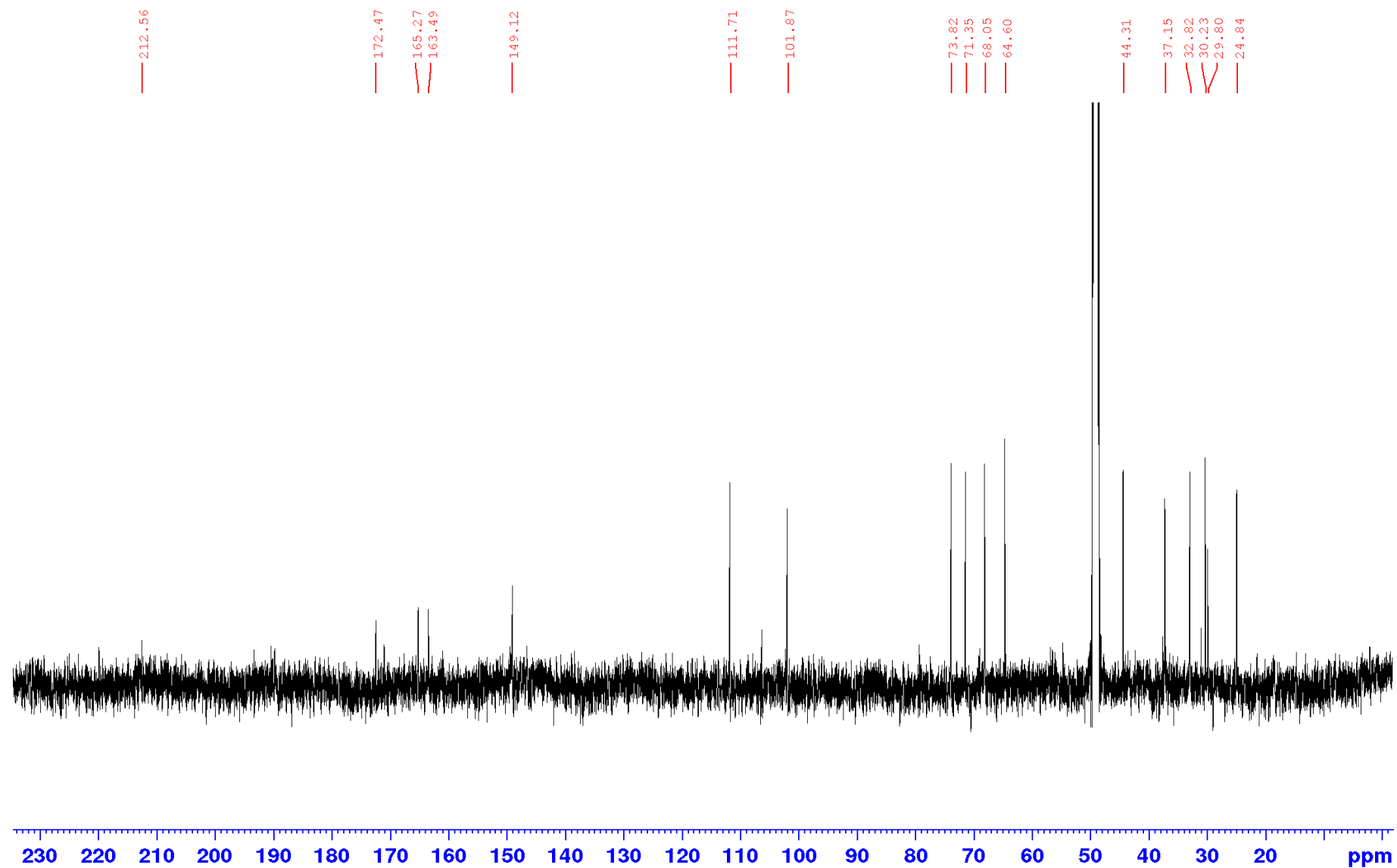


Figure S32. DEPT spectrum of 5 measured at 125 MHz in MeOD

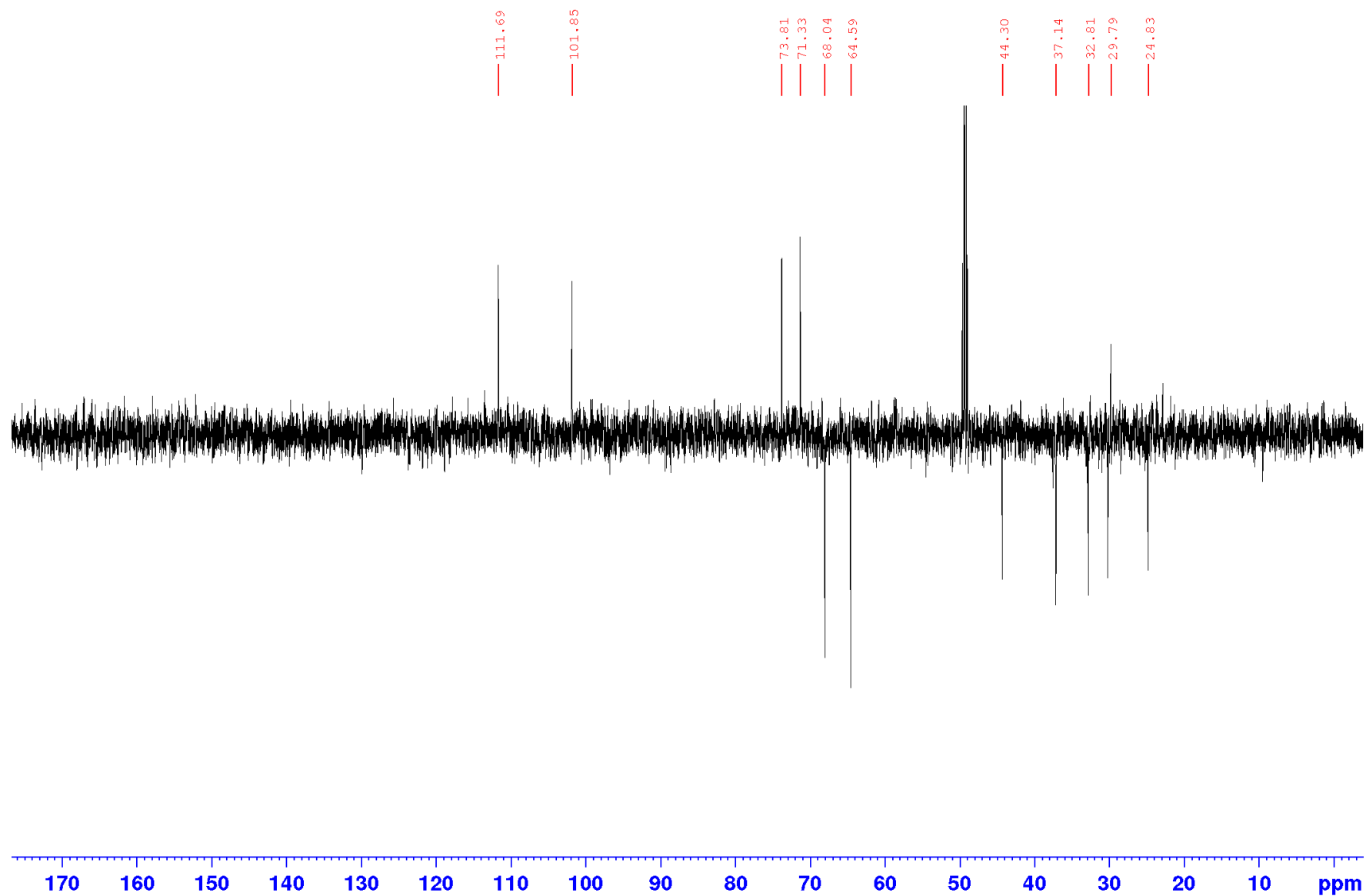


Figure S33. HSQC spectrum of 5 measured in MeOD

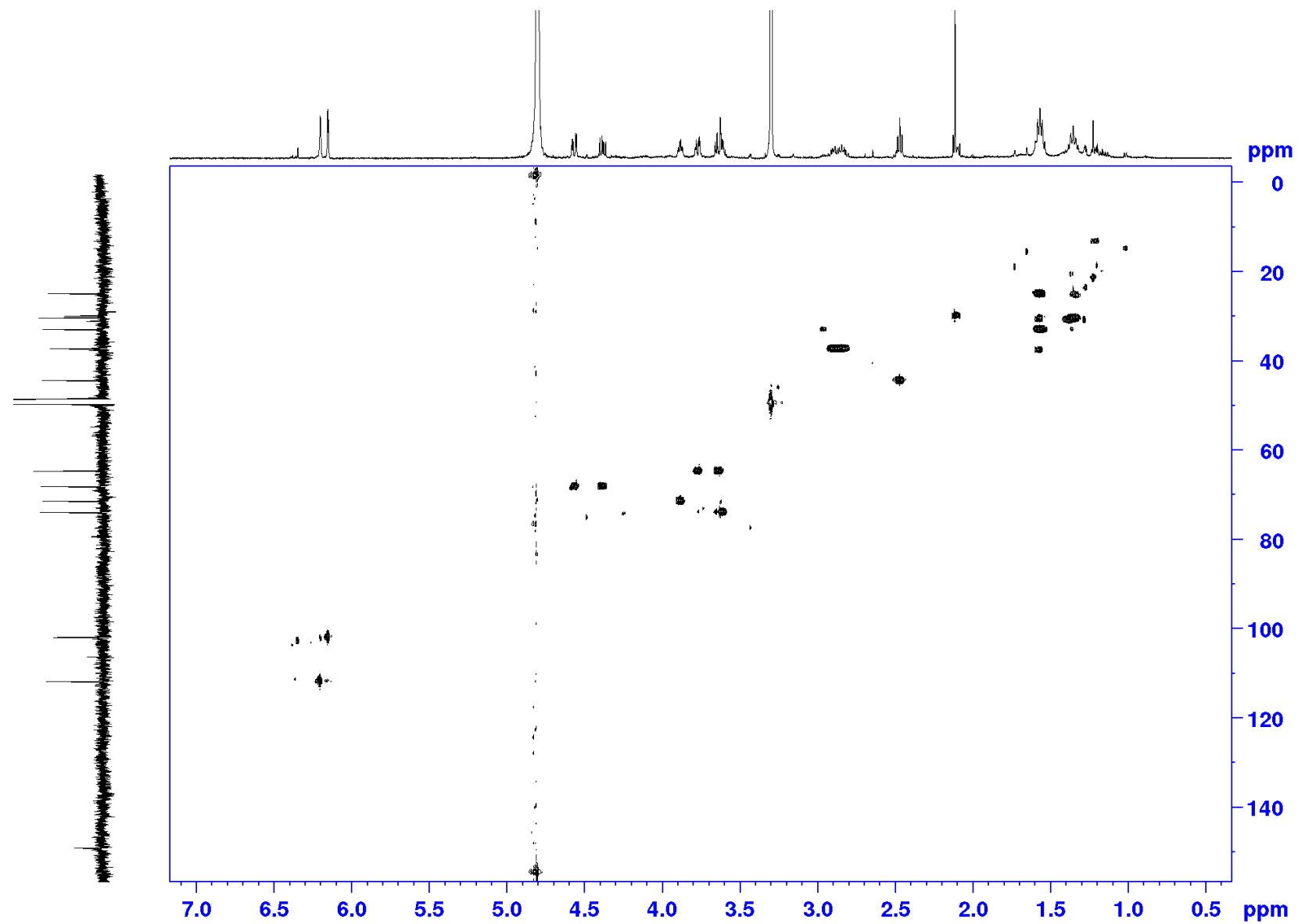


Figure S34. HMBC spectrum of 5 measured in MeOD

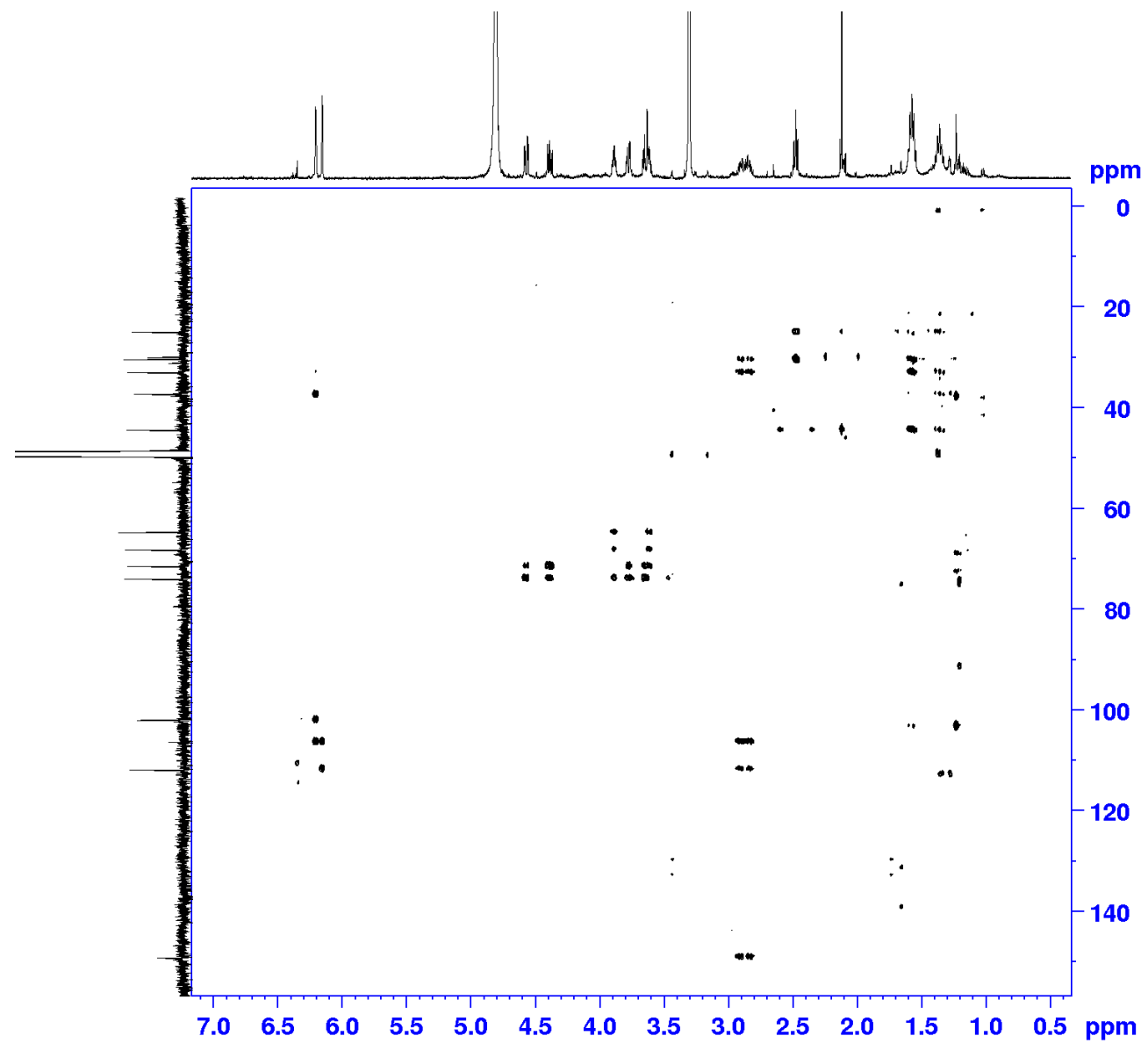


Figure S35. COSY spectrum of 5 measured in MeOD

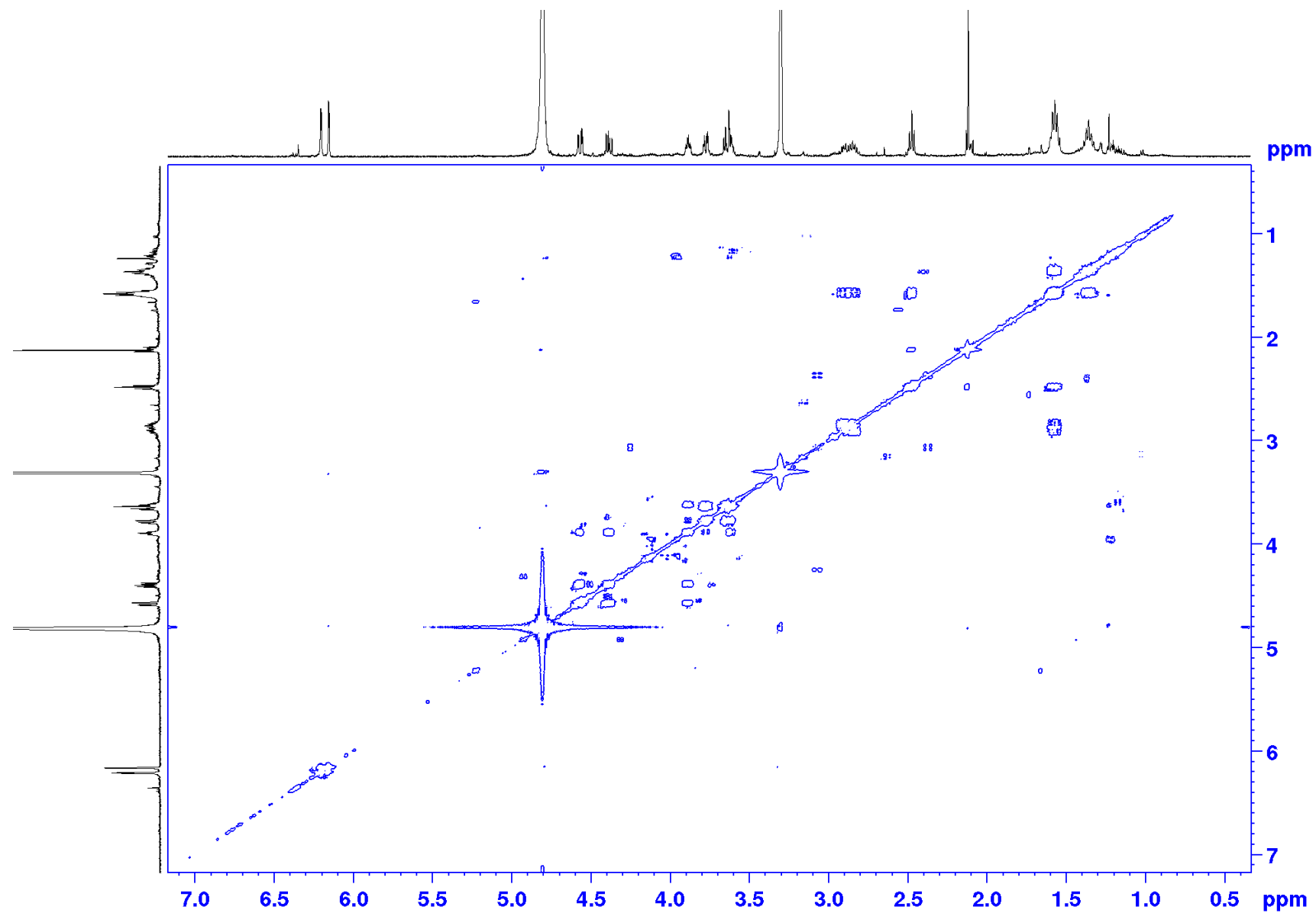
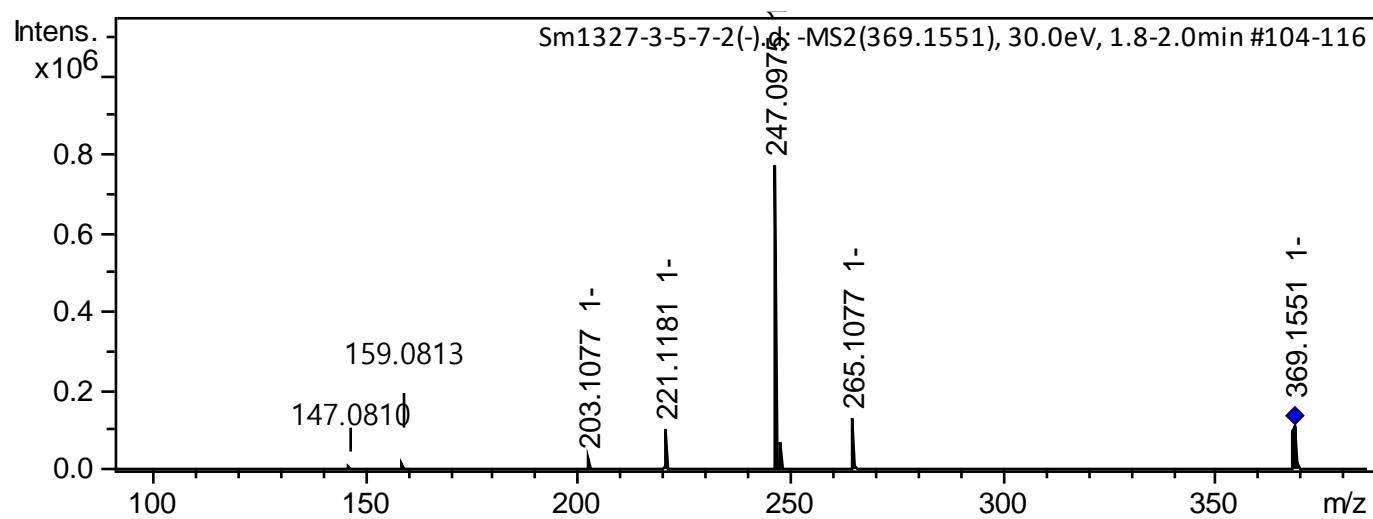
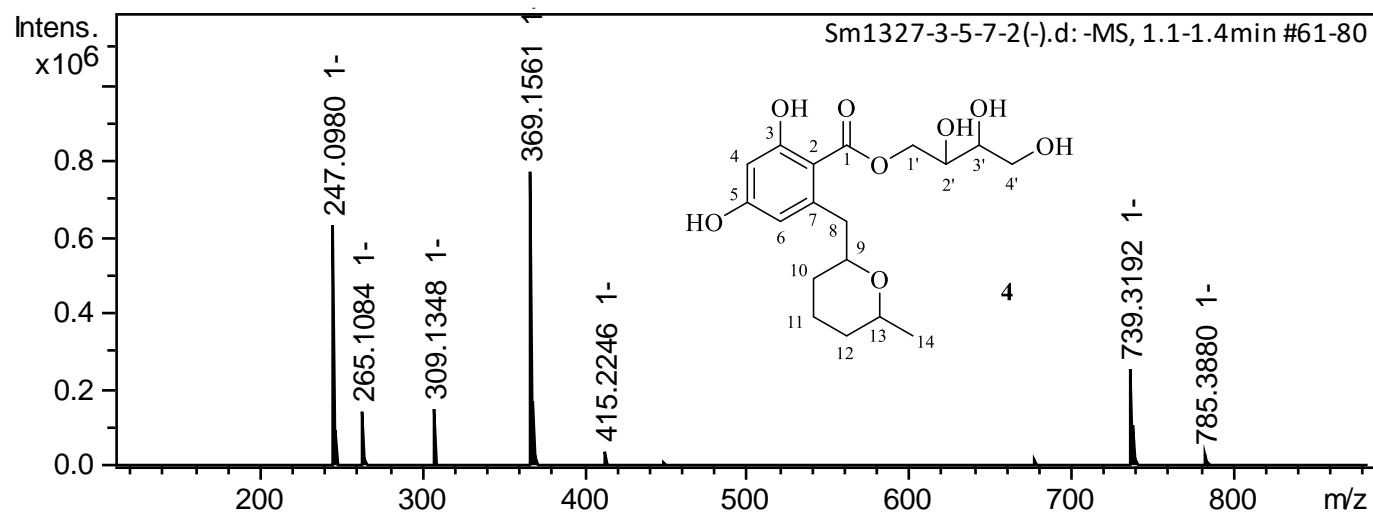
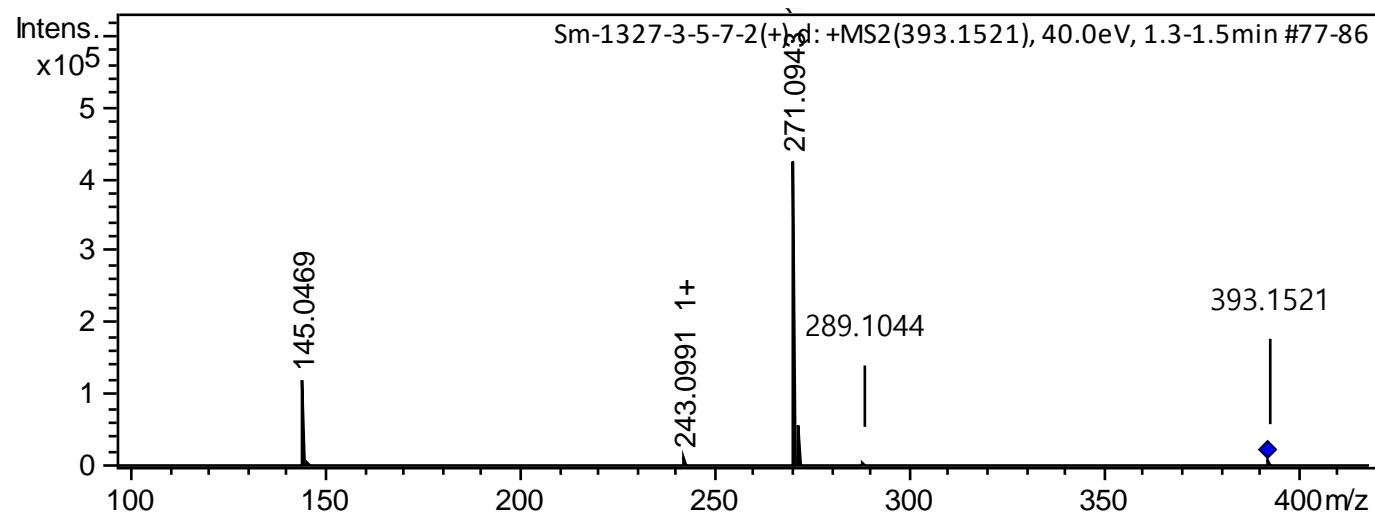
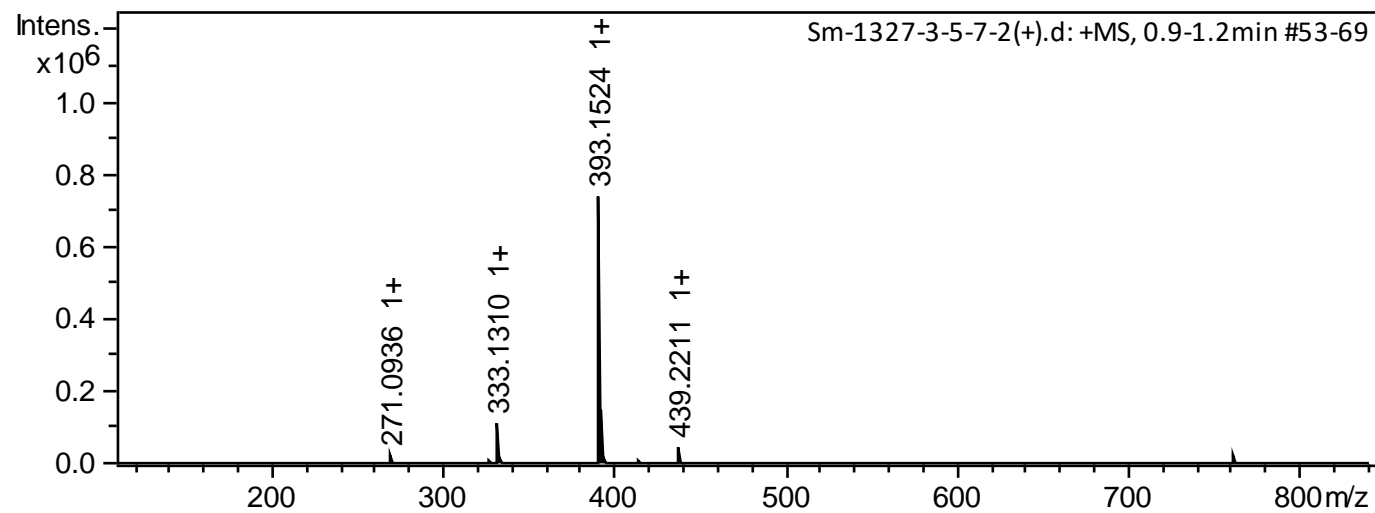


Figure S36. HRESIMS for 6





	meas	calc	Δ (ppm)
[M-H] ⁻	369,1561	369,1555	-1,7
[M+Na] ⁺	393,1524	393,152	-0,9

Figure S37. ^1H NMR spectrum of **6** measured at 700 MHz in acetone- d_6

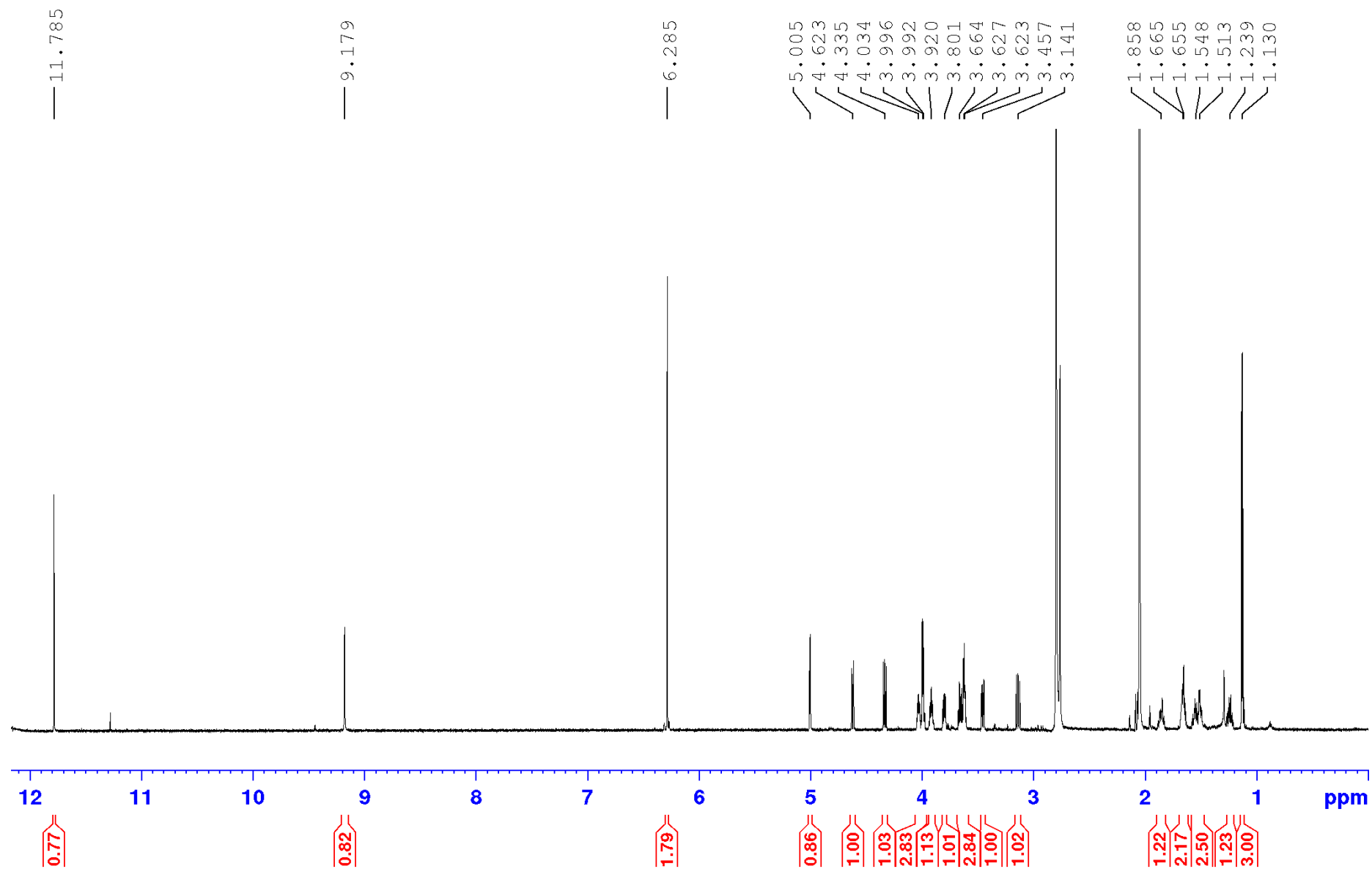


Figure S38. ^{13}C NMR spectrum of 6 measured at 175 MHz in acetone- d_6

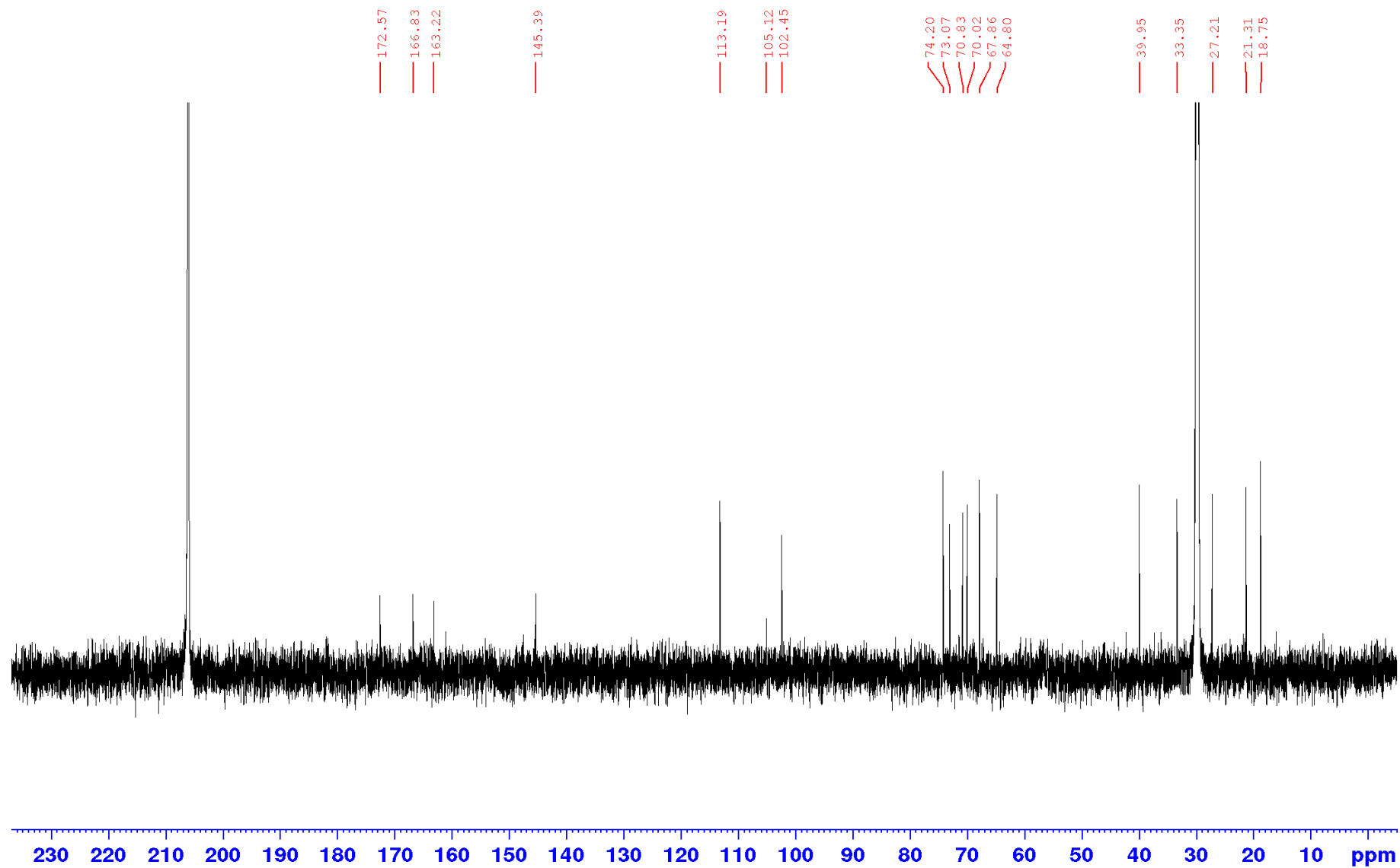


Figure S39. DEPT spectrum of 6 measured at 175 MHz in MeOD

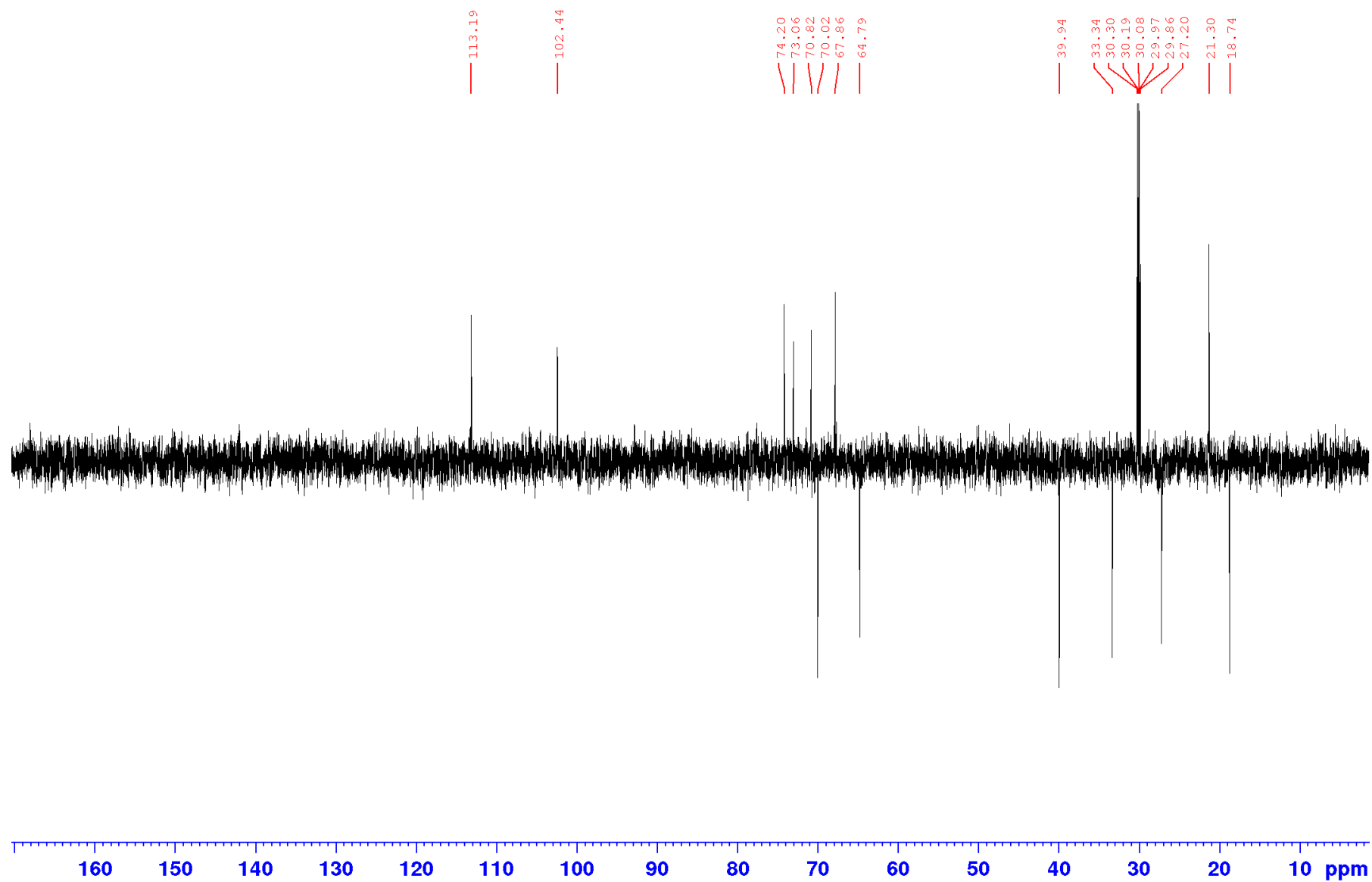


Figure S40. HSQC spectrum of 6 measured in acetone-d₆

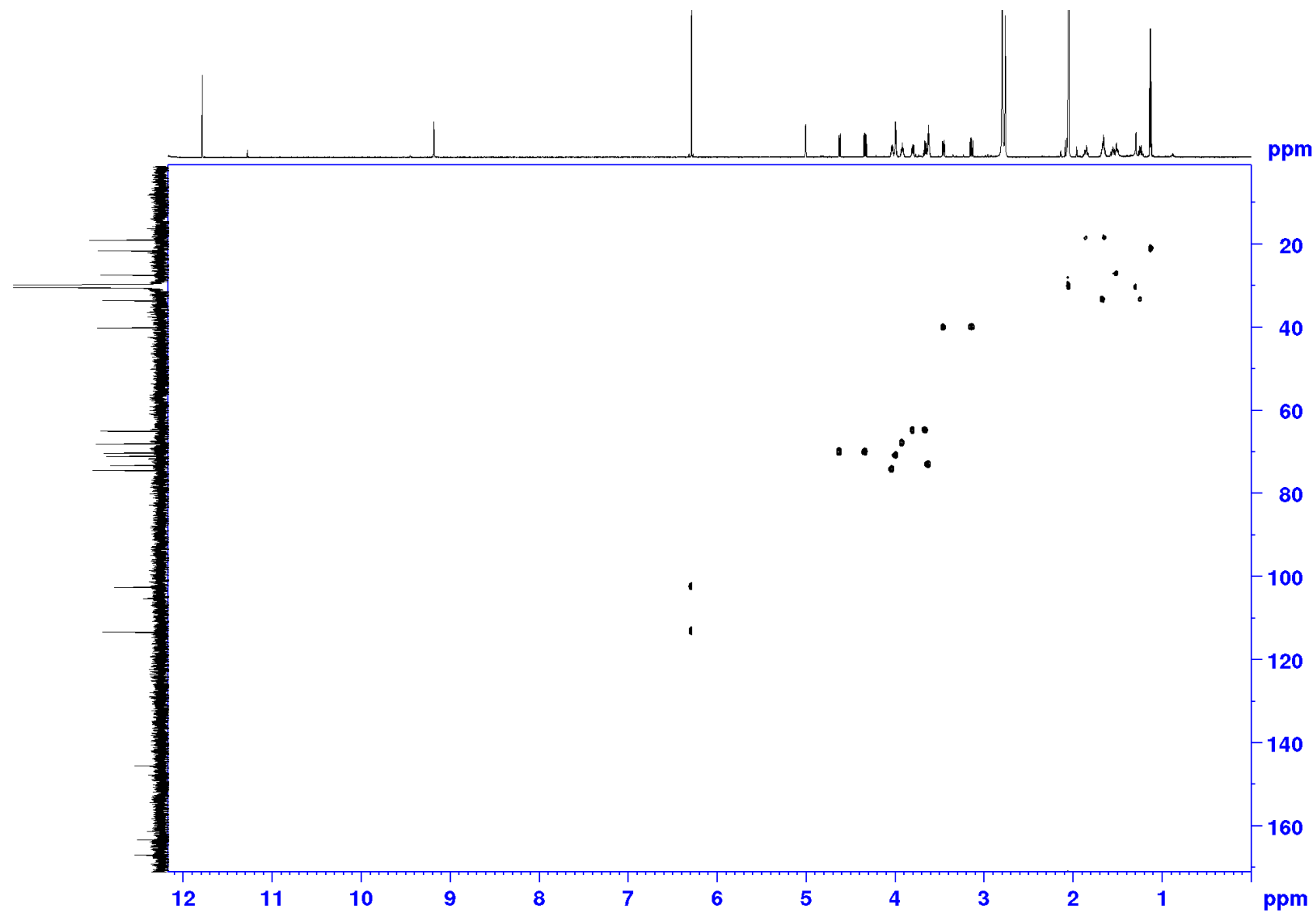


Figure S41. COSY spectrum of 6 measured in acetone- d_6

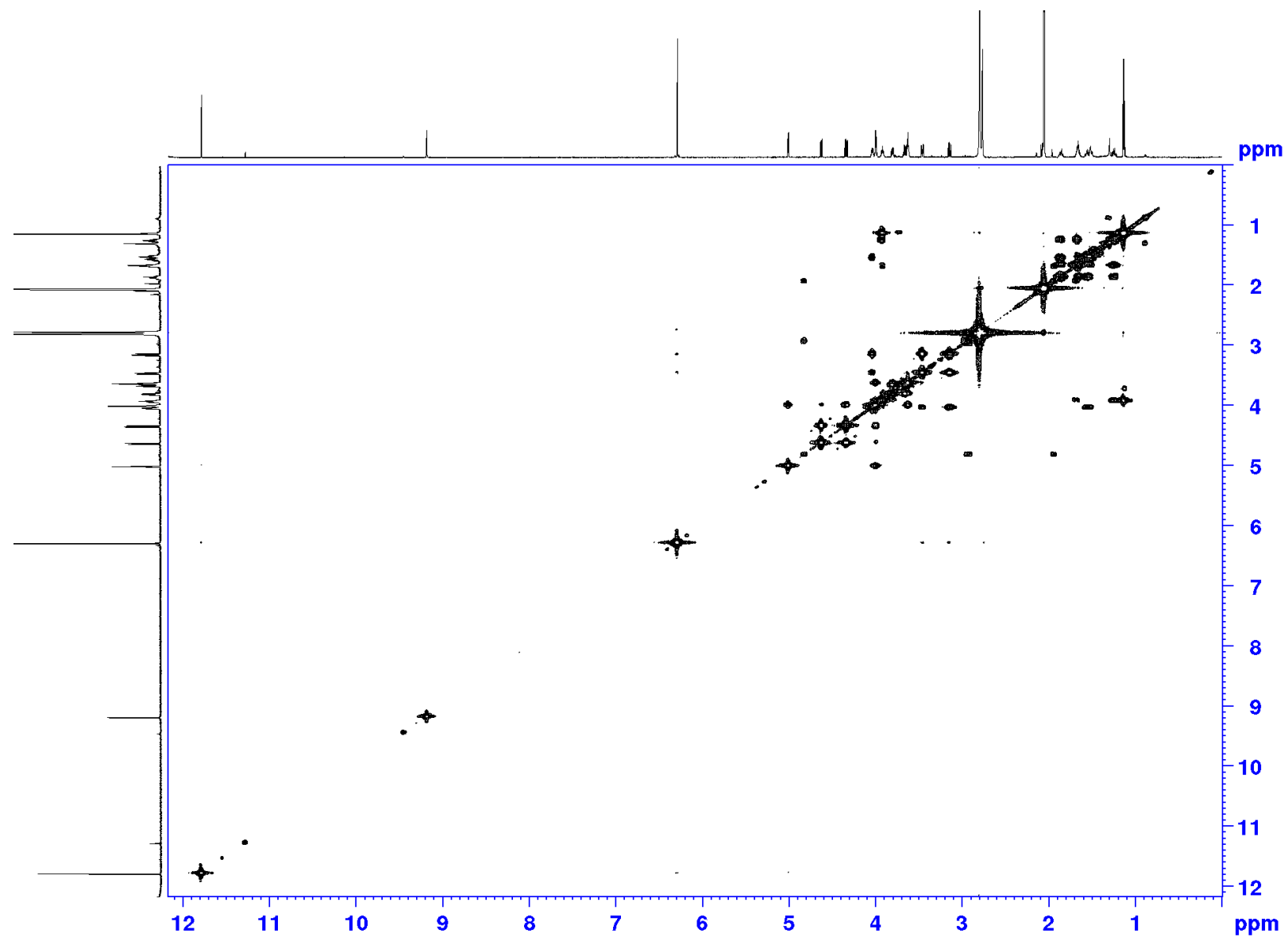


Figure S42. HMBC spectrum of 6 measured in acetone- d_6

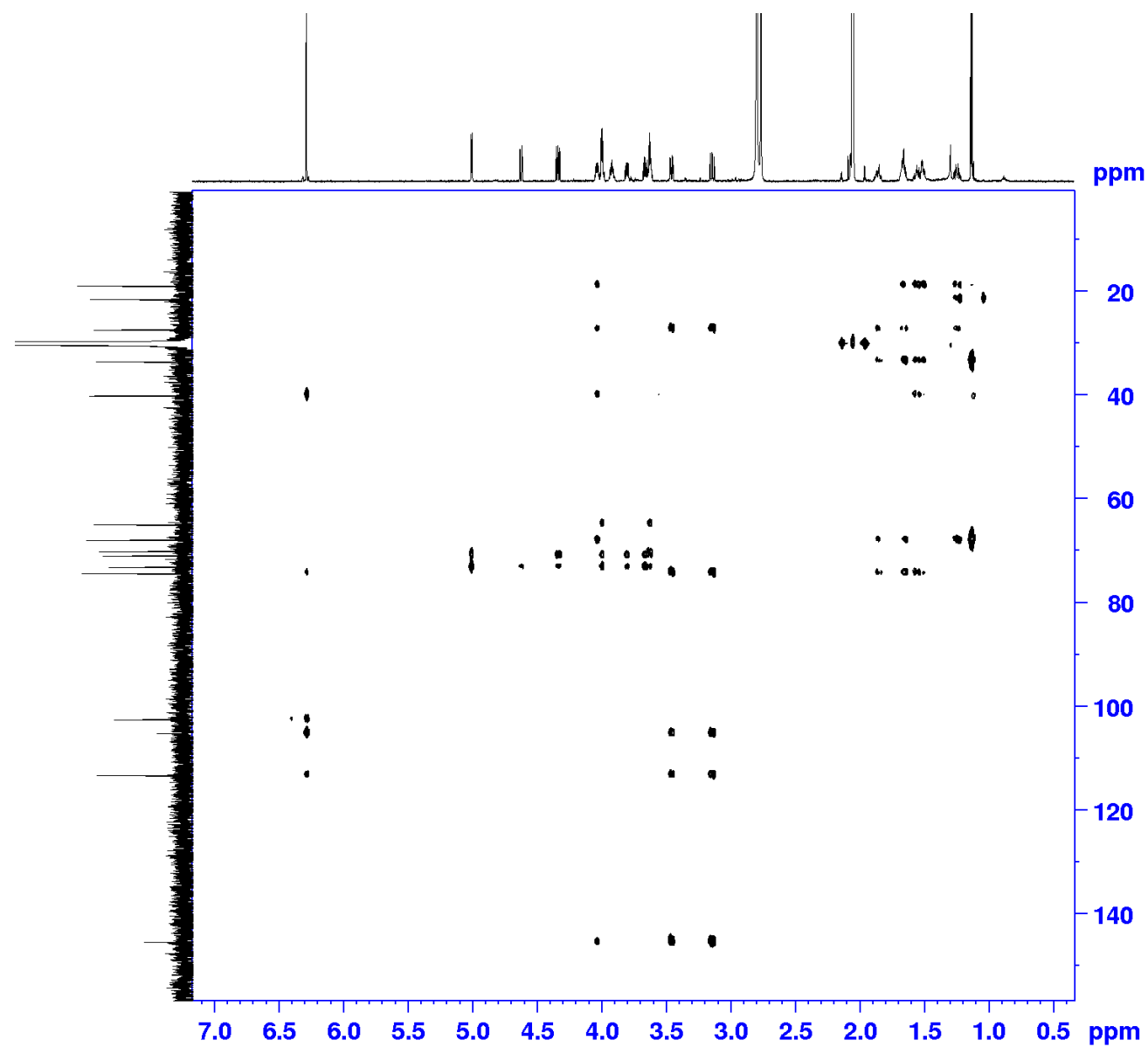
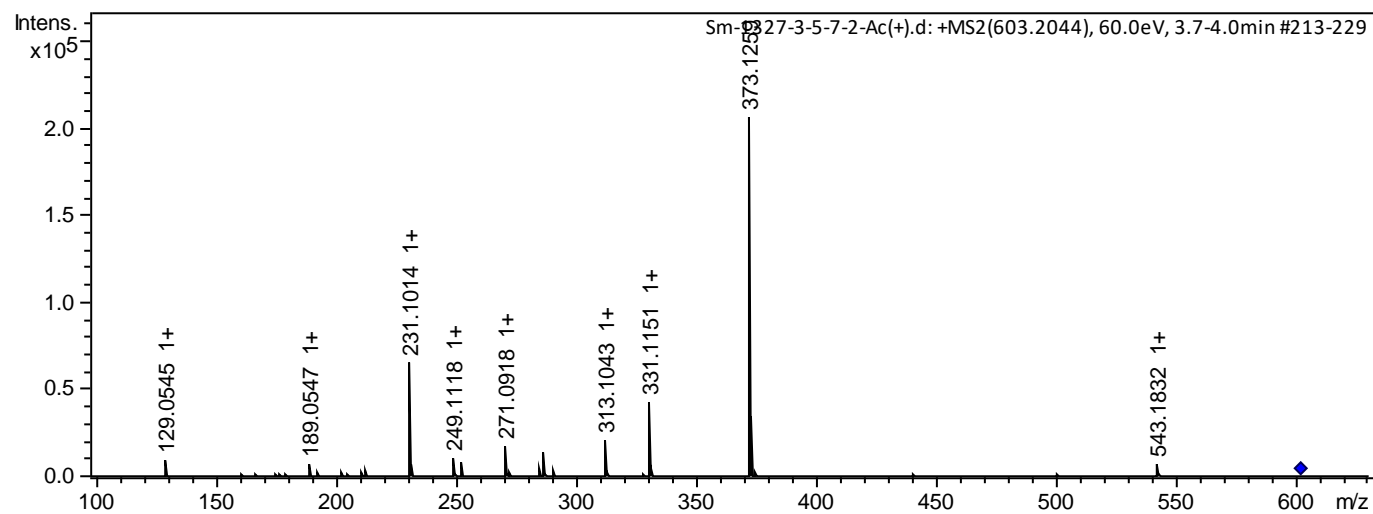
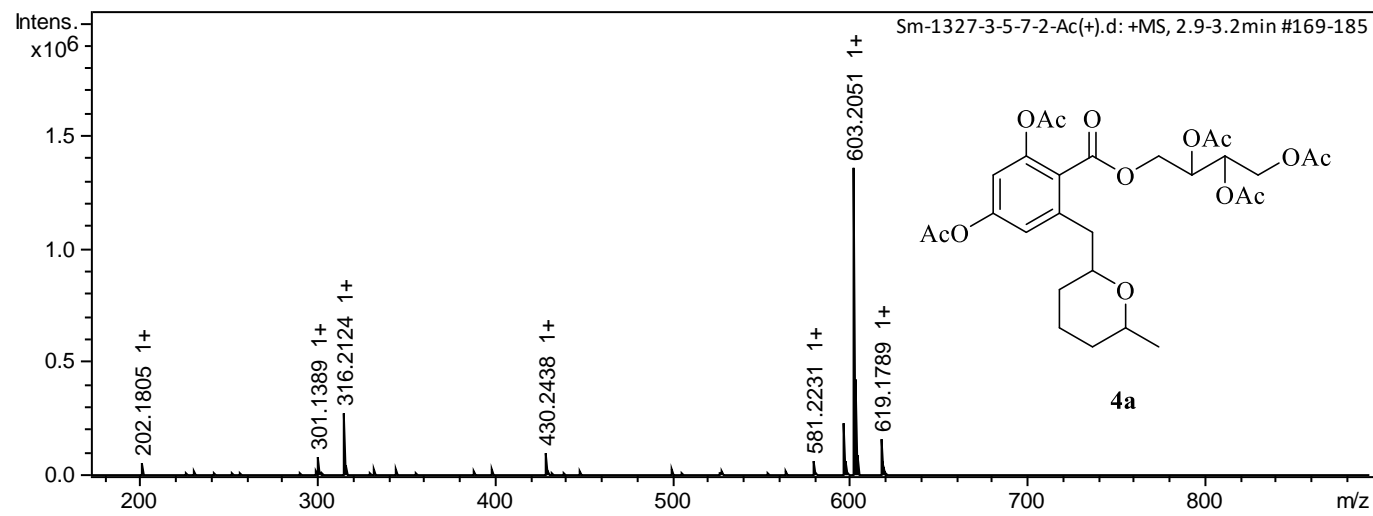
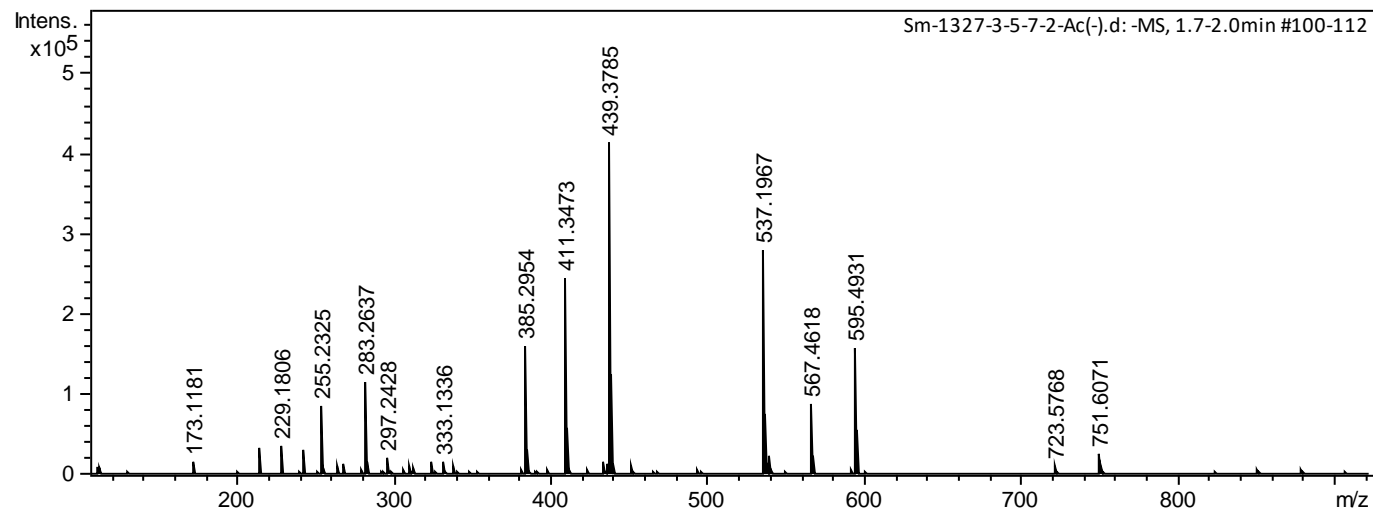


Figure S43. HRESIMS for 6a





	meas	calc	Δ (ppm)
[M+Na] ⁺	603,2051	603,2048	-0,4

Meas. m/z	Ion Formula	m/z	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
129,0545	C ₆ H ₉ O ₃	129,0546	1	4,7	3	even	ok
189,0547	C ₁₁ H ₉ O ₃	189,0546	-0,2	11,2	8	even	ok
231,1014	C ₁₄ H ₁₅ O ₃	231,1016	0,8	28,9	8	even	ok
249,1118	C ₁₄ H ₁₇ O ₄	249,1121	1,2	26,4	7	even	ok
271,0918	C ₁₄ H ₁₆ NaO ₄	271,0941	8,4	27,6	7	even	ok
285,1092	C ₁₅ H ₁₈ NaO ₄	285,1097	1,9	16	7	even	ok
287,1251	C ₁₅ H ₂₀ NaO ₄	287,1254	1,1	29,4	6	even	ok
313,1043	C ₁₆ H ₁₈ NaO ₅	313,1046	1,1	27,9	8	even	ok
331,1151	C ₁₆ H ₂₀ NaO ₆	331,1152	0,3	30,4	7	even	ok
373,1259	C ₁₈ H ₂₂ NaO ₇	373,1258	-0,3	20,4	8	even	ok
441,1515	C ₂₂ H ₂₆ NaO ₈	441,152	1,1	30	10	even	ok

485,1786	C ₂₄ H ₃₀ NaO ₉	485,1782	-0,9	n.a.	10	even	ok
501,1725	C ₂₄ H ₃₀ NaO ₁₀	501,1731	1,2	28,2	10	even	ok
543,1832	C ₂₆ H ₃₂ NaO ₁₁	543,1837	0,9	30,8	11	even	ok
603,2044	C ₂₈ H ₃₆ NaO ₁₃	603,2048	0,7	39,4	11	even	ok
253,0681	C ₁₀ H ₁₄ NaO ₆	253,0683	0,6	7,7	4	even	ok

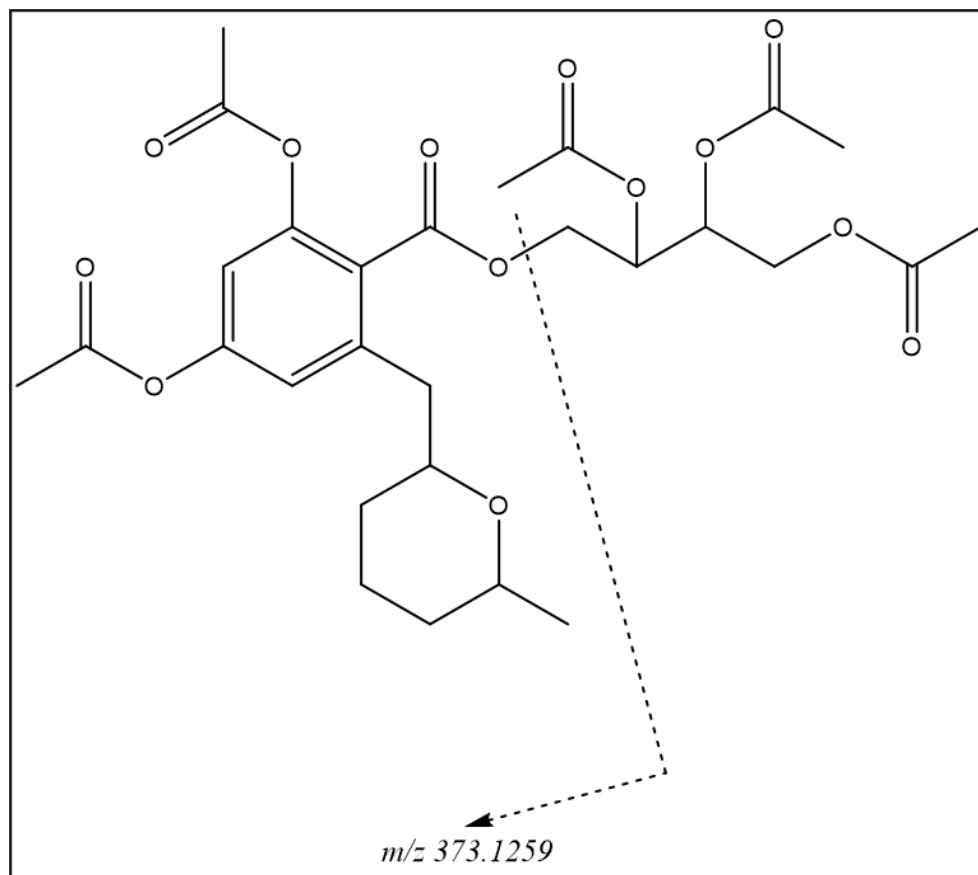


Figure S44. ^1H NMR spectrum of 6a measured at 700 MHz in acetone- d_6

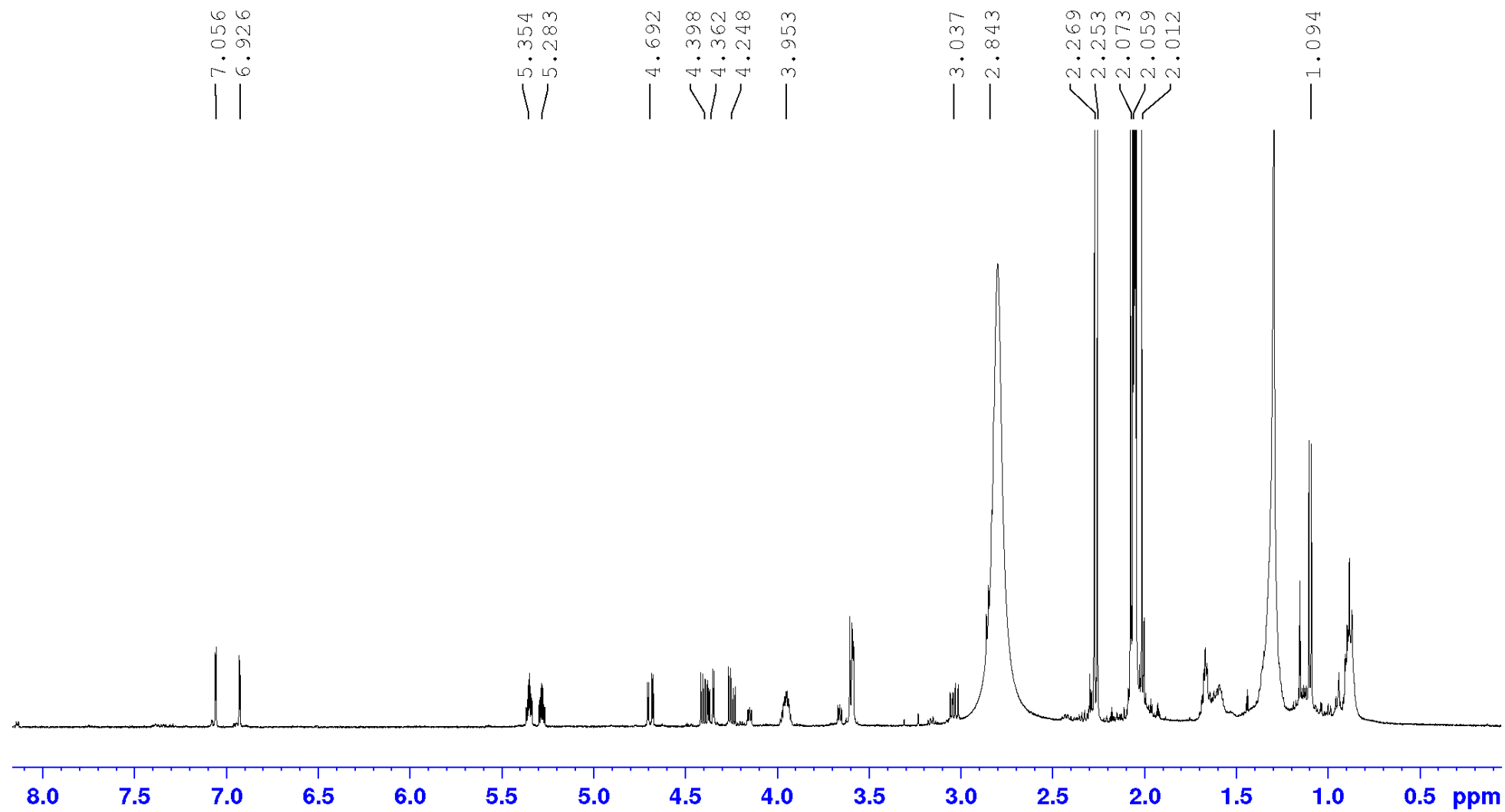


Figure S45. ^{13}C NMR spectrum of 6a measured at 175 MHz in acetone- d_6

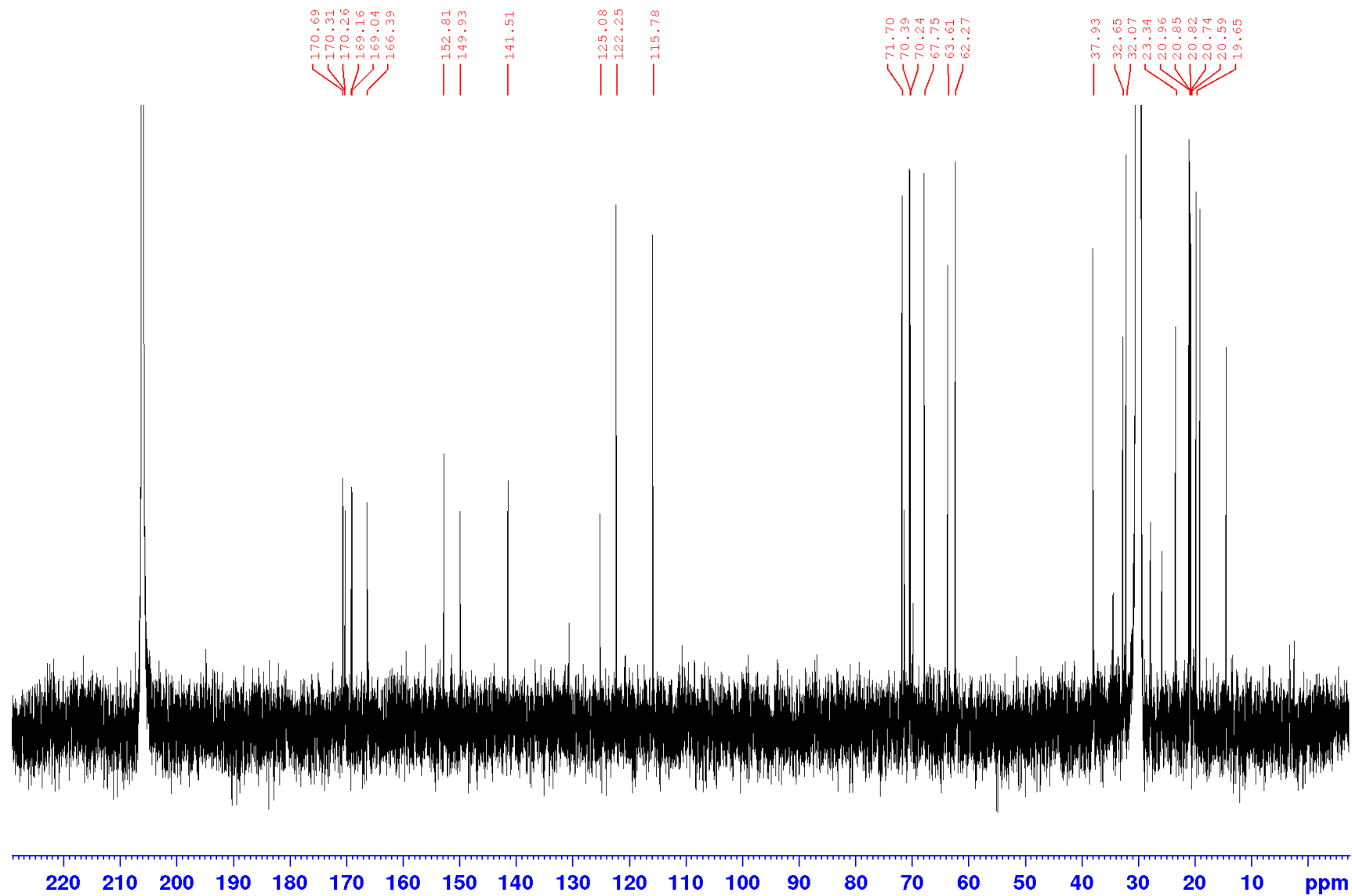


Figure S46. HSQC spectrum of 6a measured in acetone-d₆

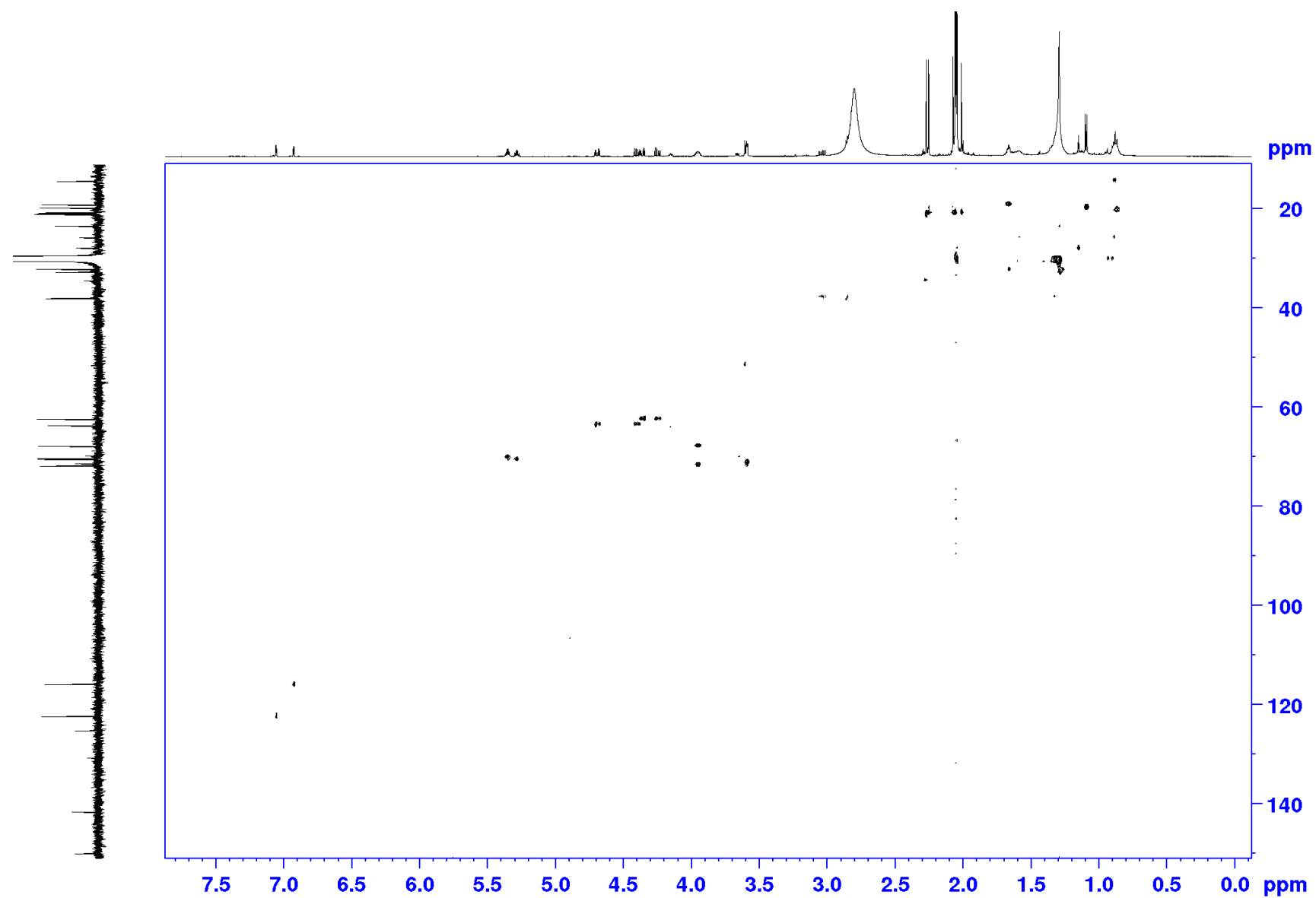


Figure S47. COSY spectrum of 6a measured in acetone-d6

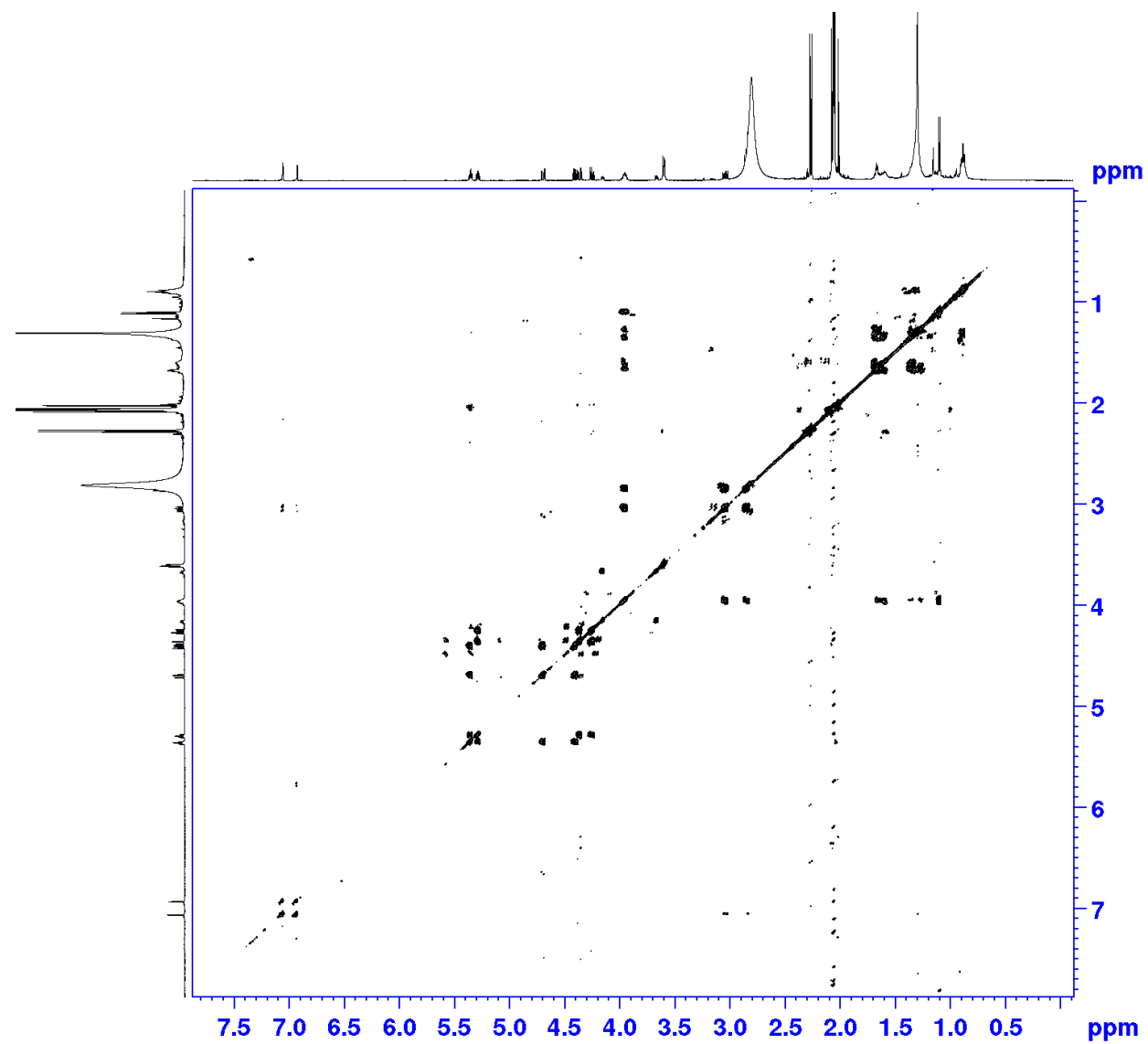
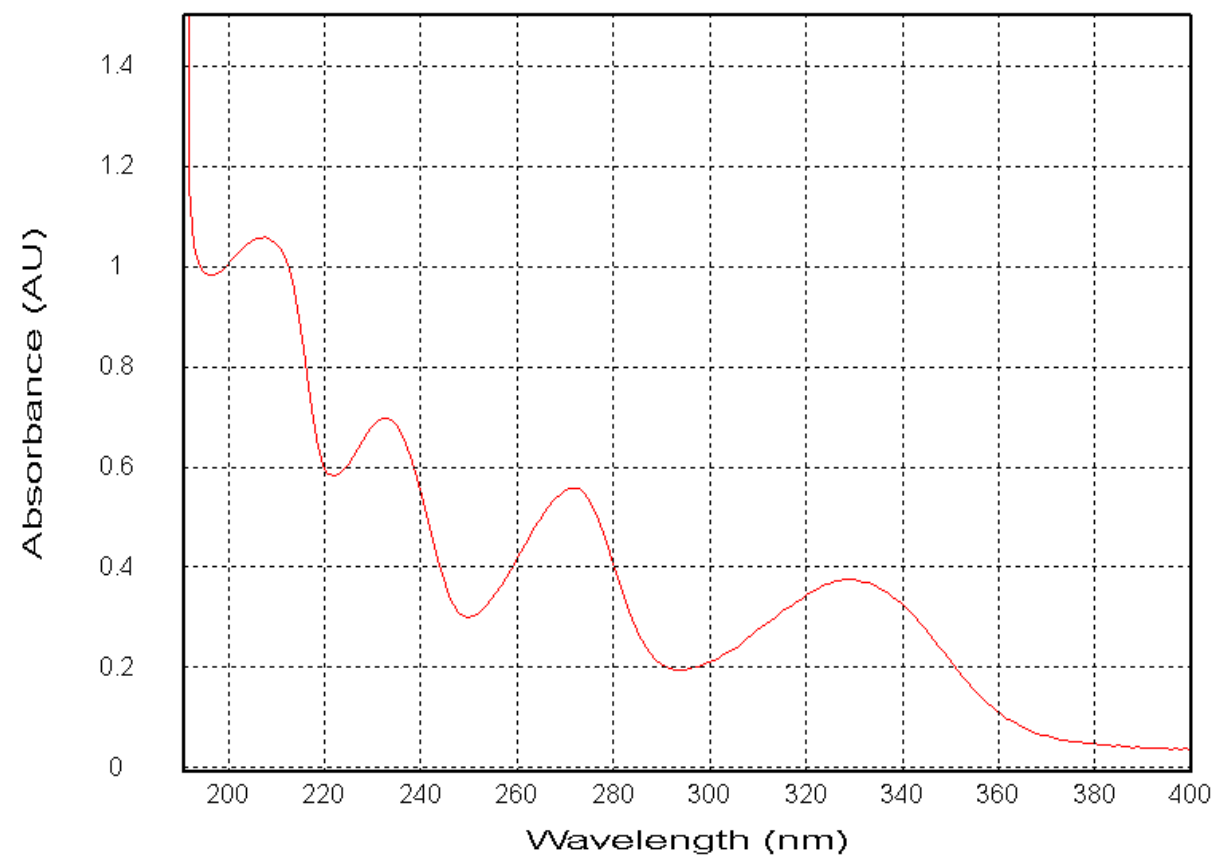


Figure S48. UV and CD data for 1



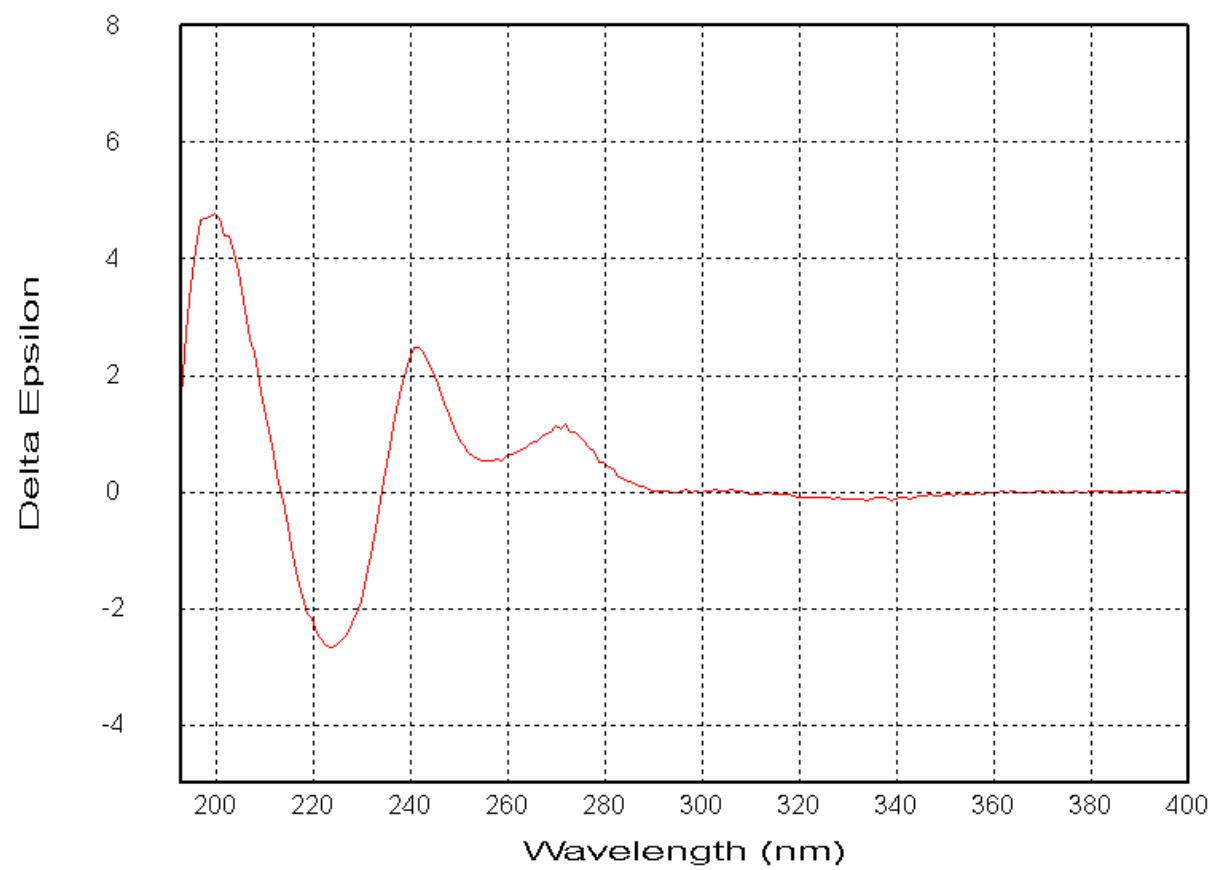
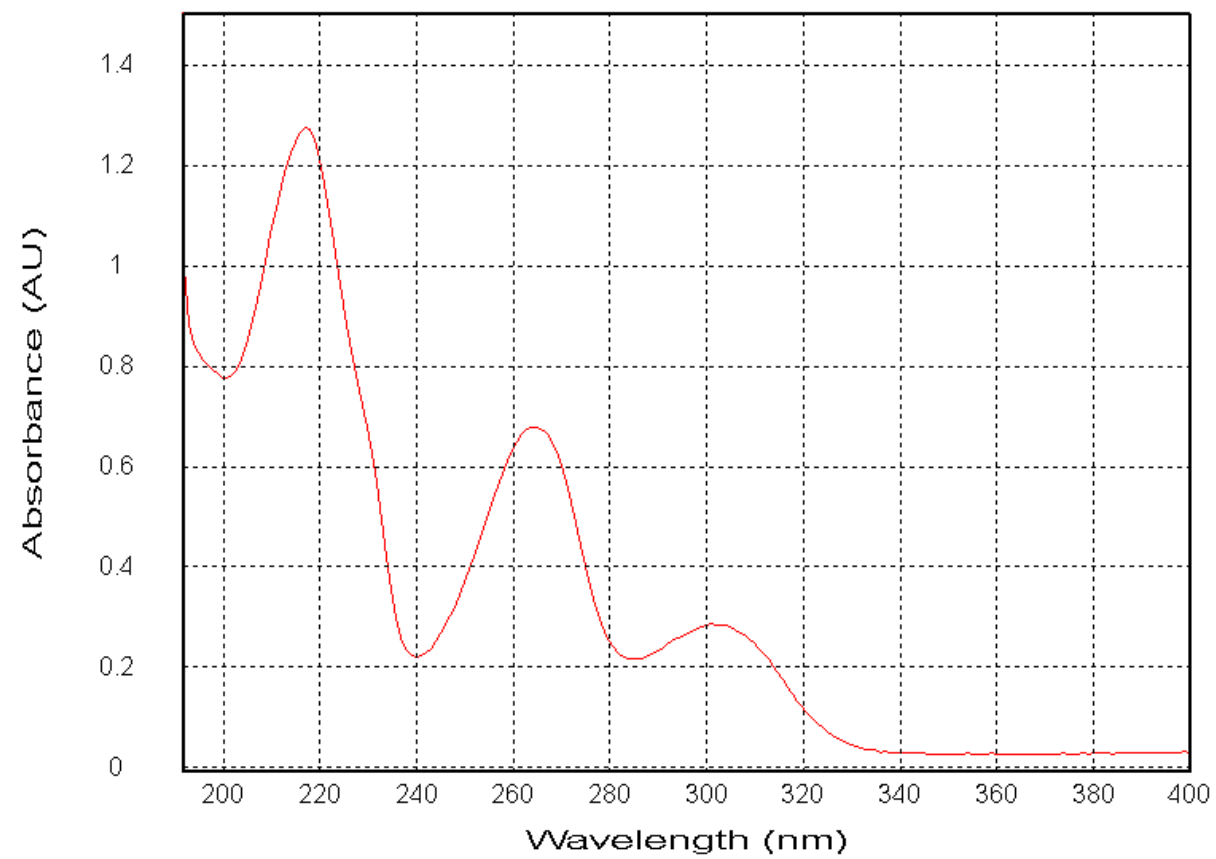


Figure S49. UV and CD data for 3



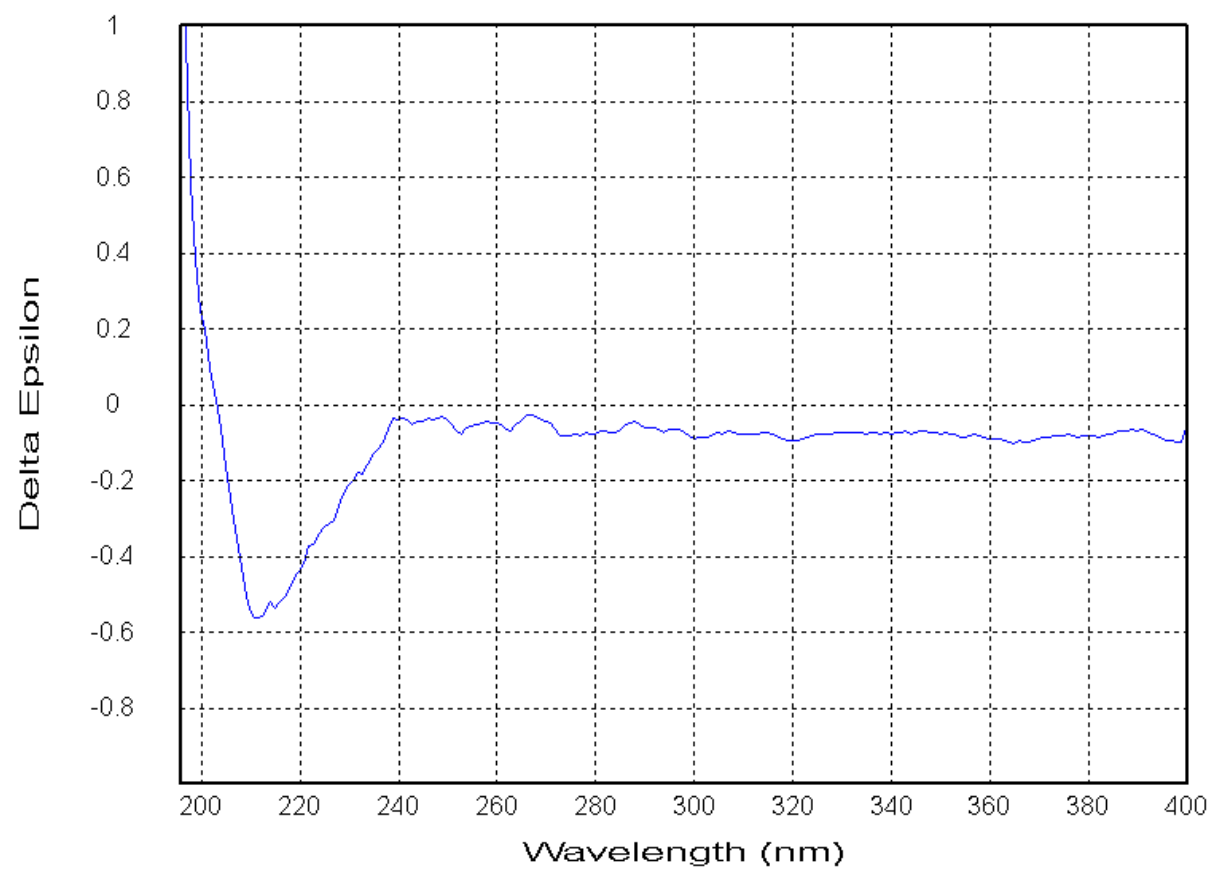
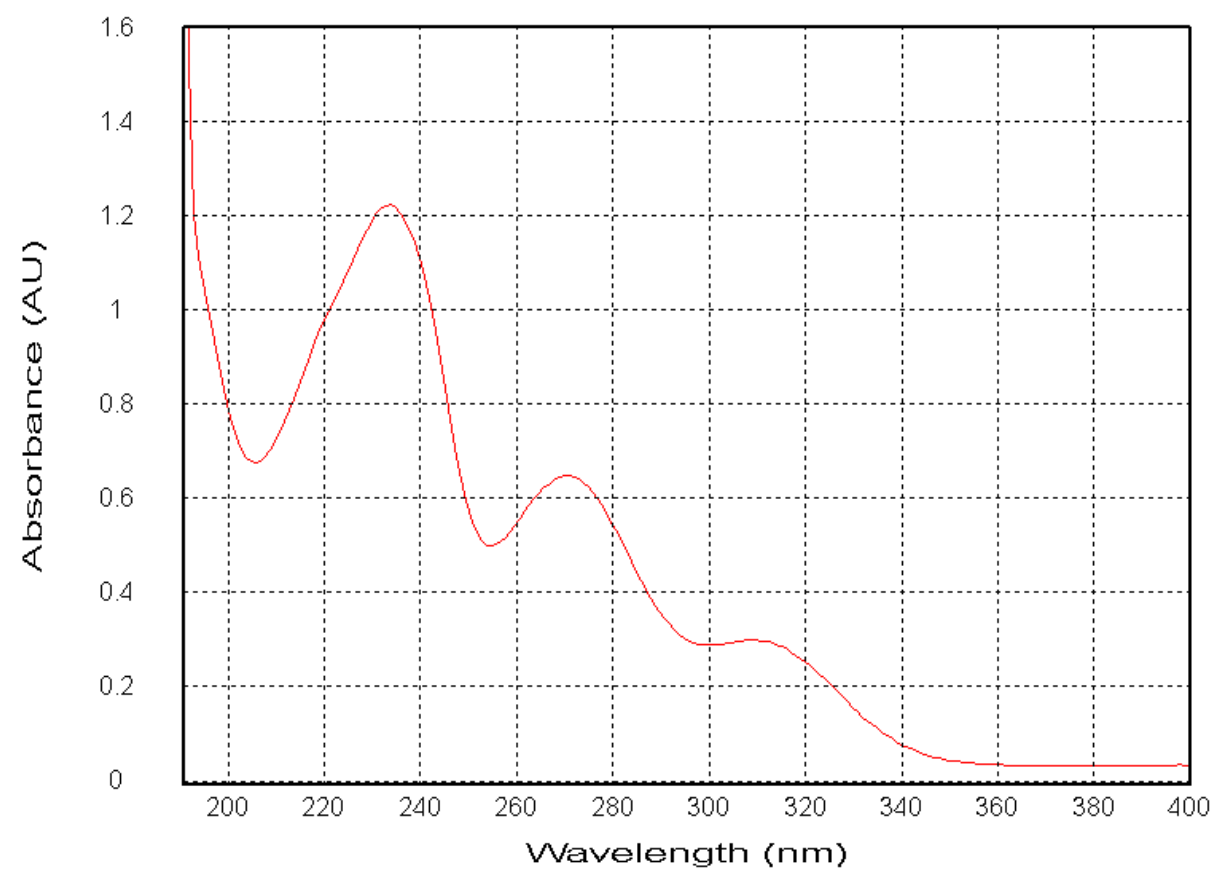


Figure S50. UV and CD data for 4



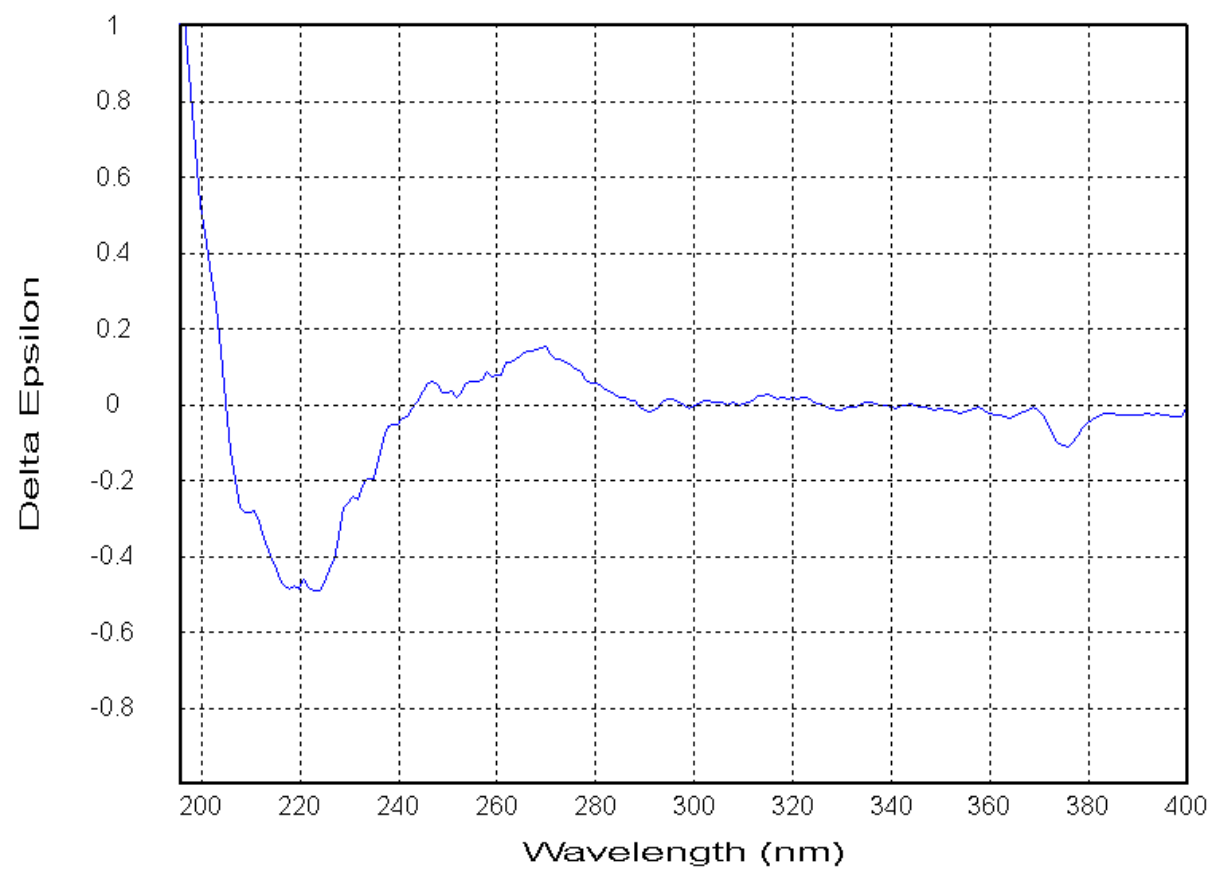
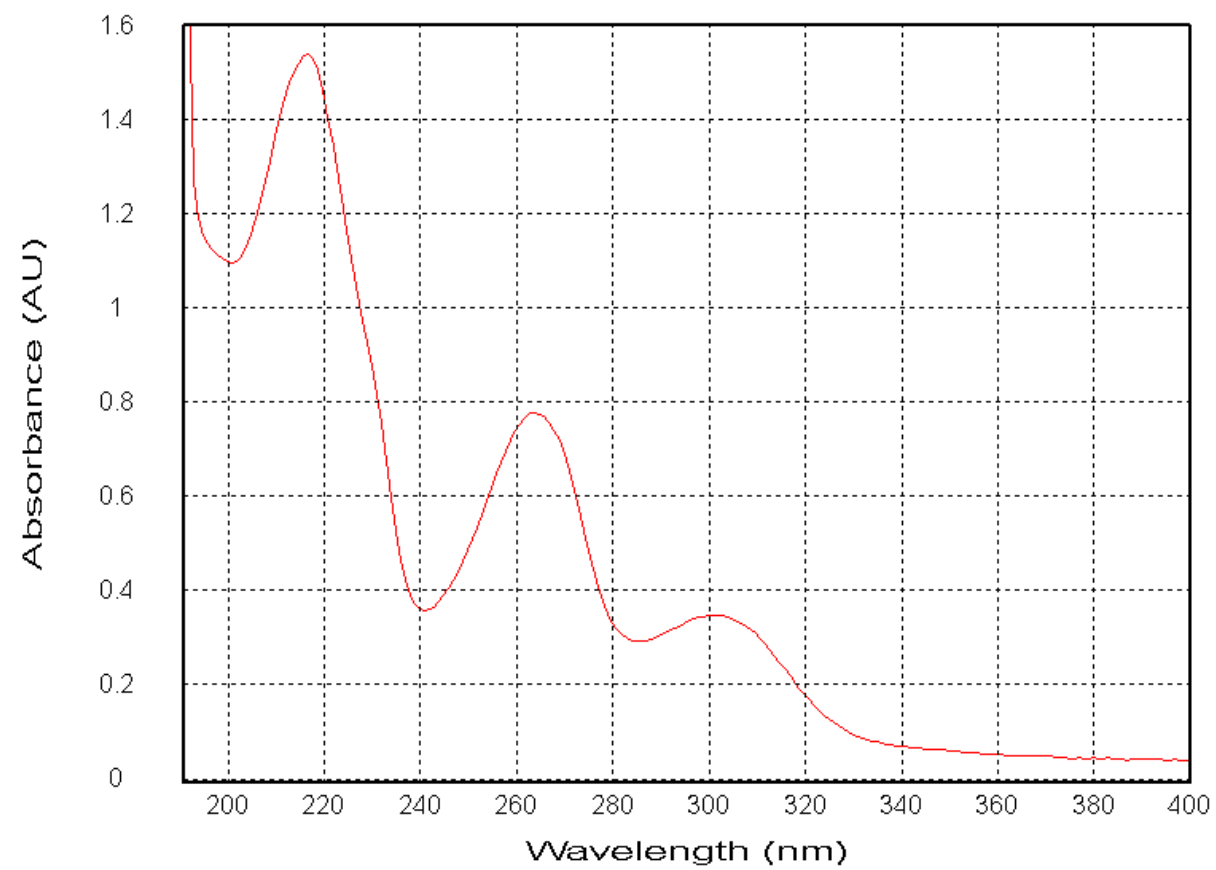


Figure S51. UV and CD data for 5



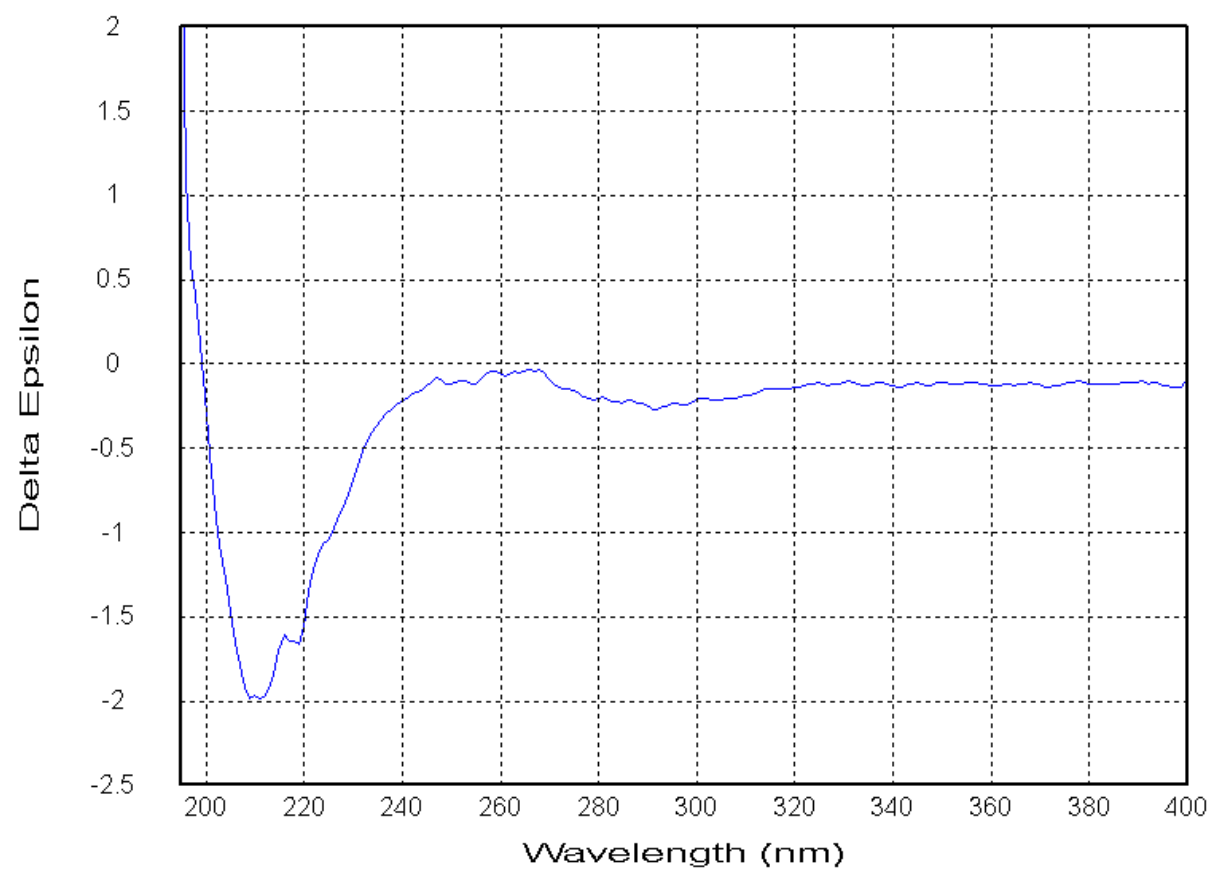
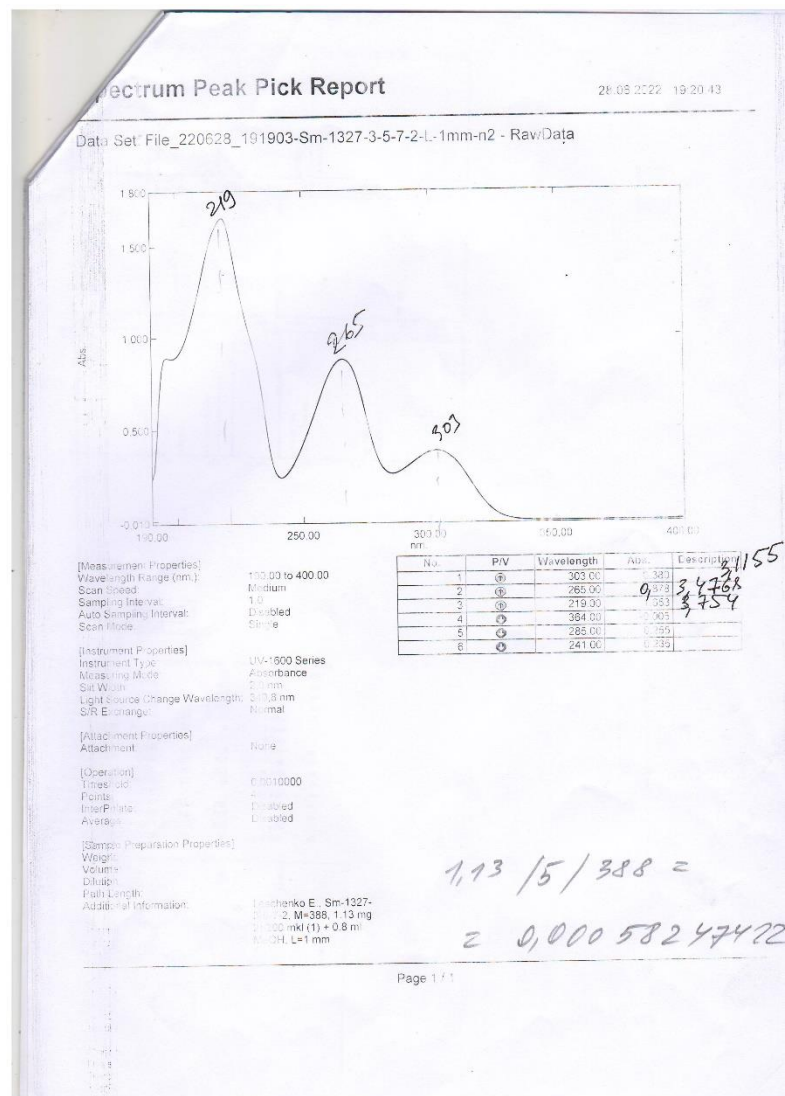


Figure S52. UV and CD data for 6



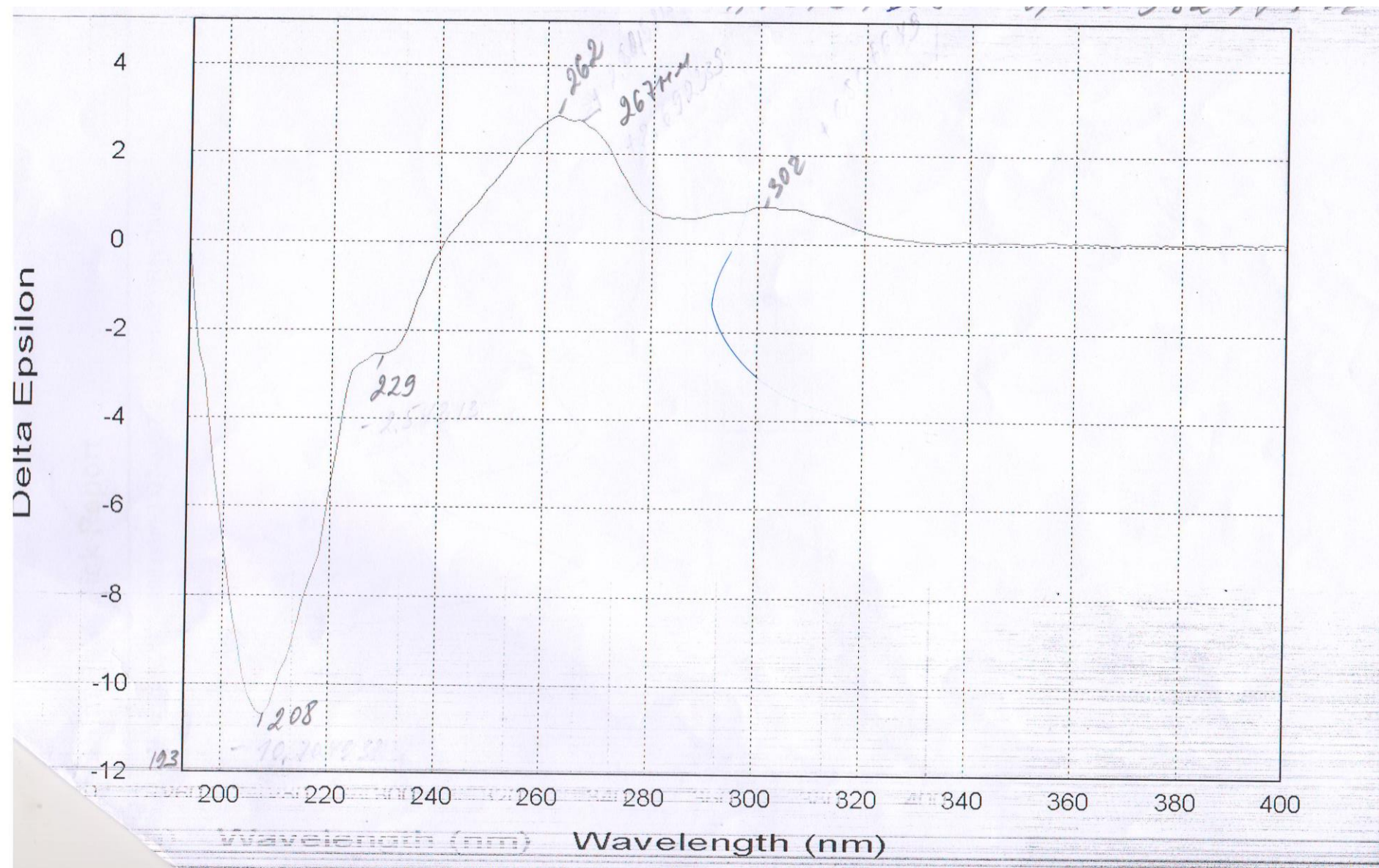


Figure S53. ¹H NMR spectrum for MTPA-2a (S)

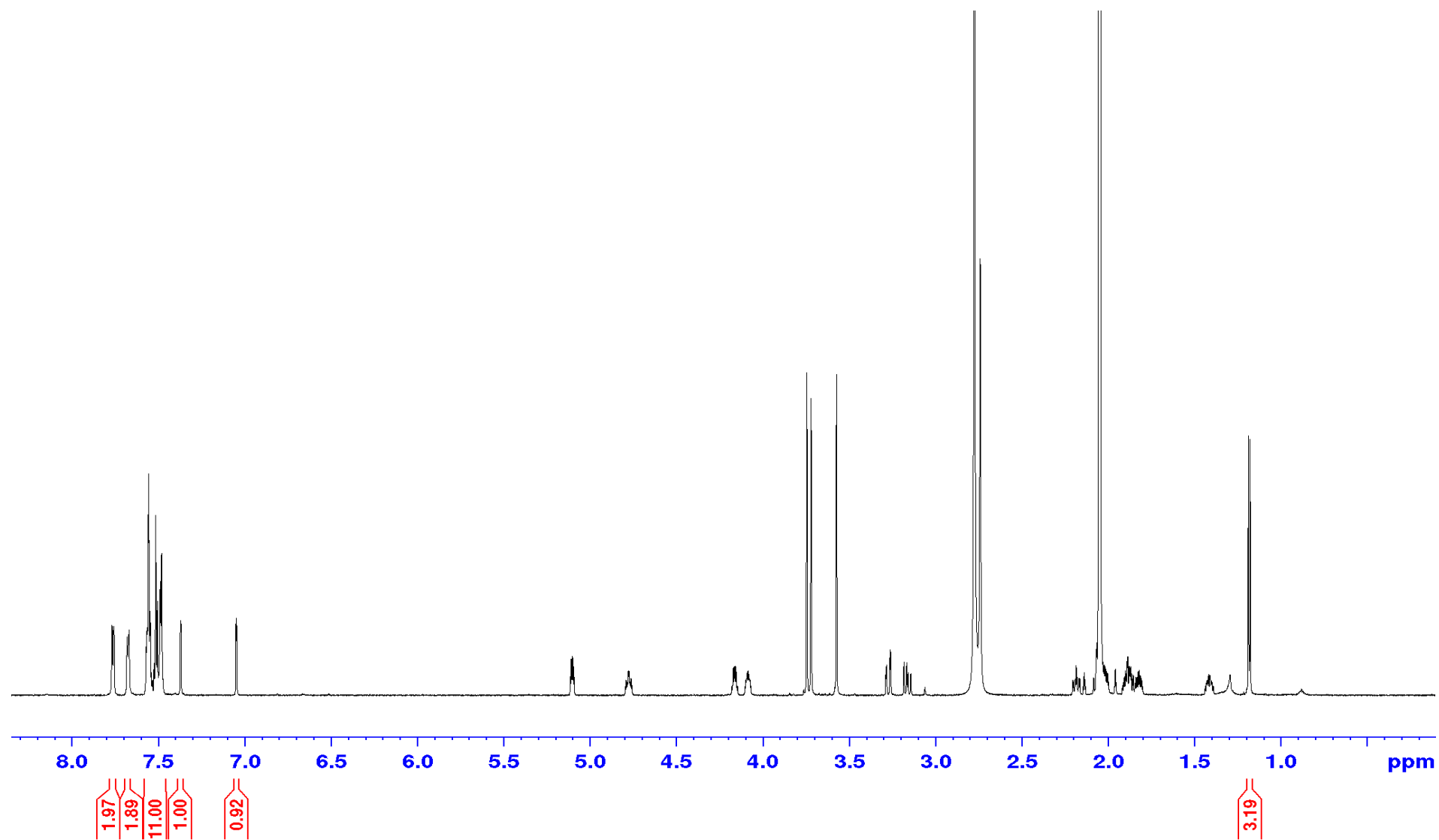


Figure S54. ^1H NMR spectrum for MTPA-2b (R)

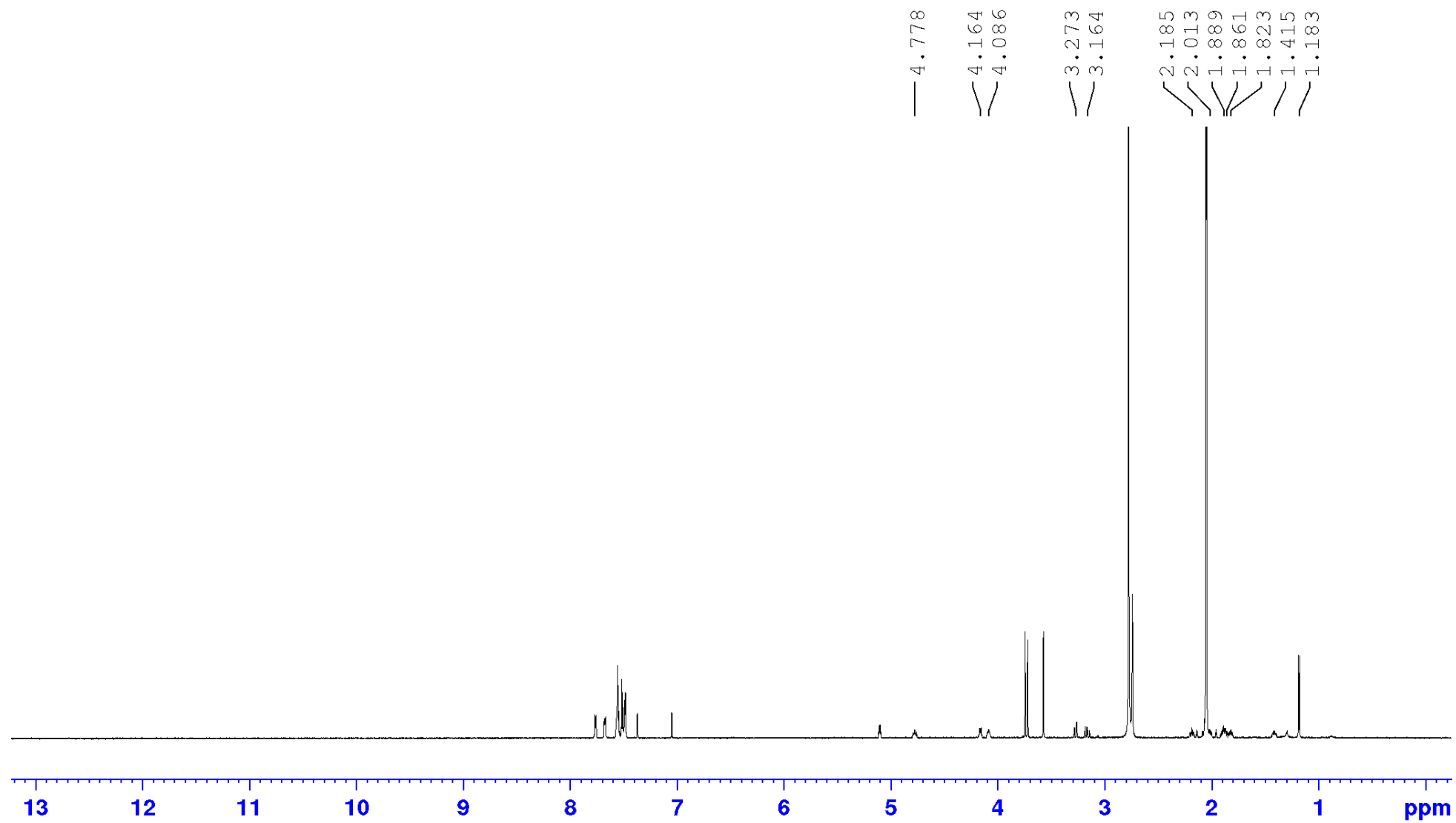


Figure S55. COSY spectrum for MTPA-2b (R)

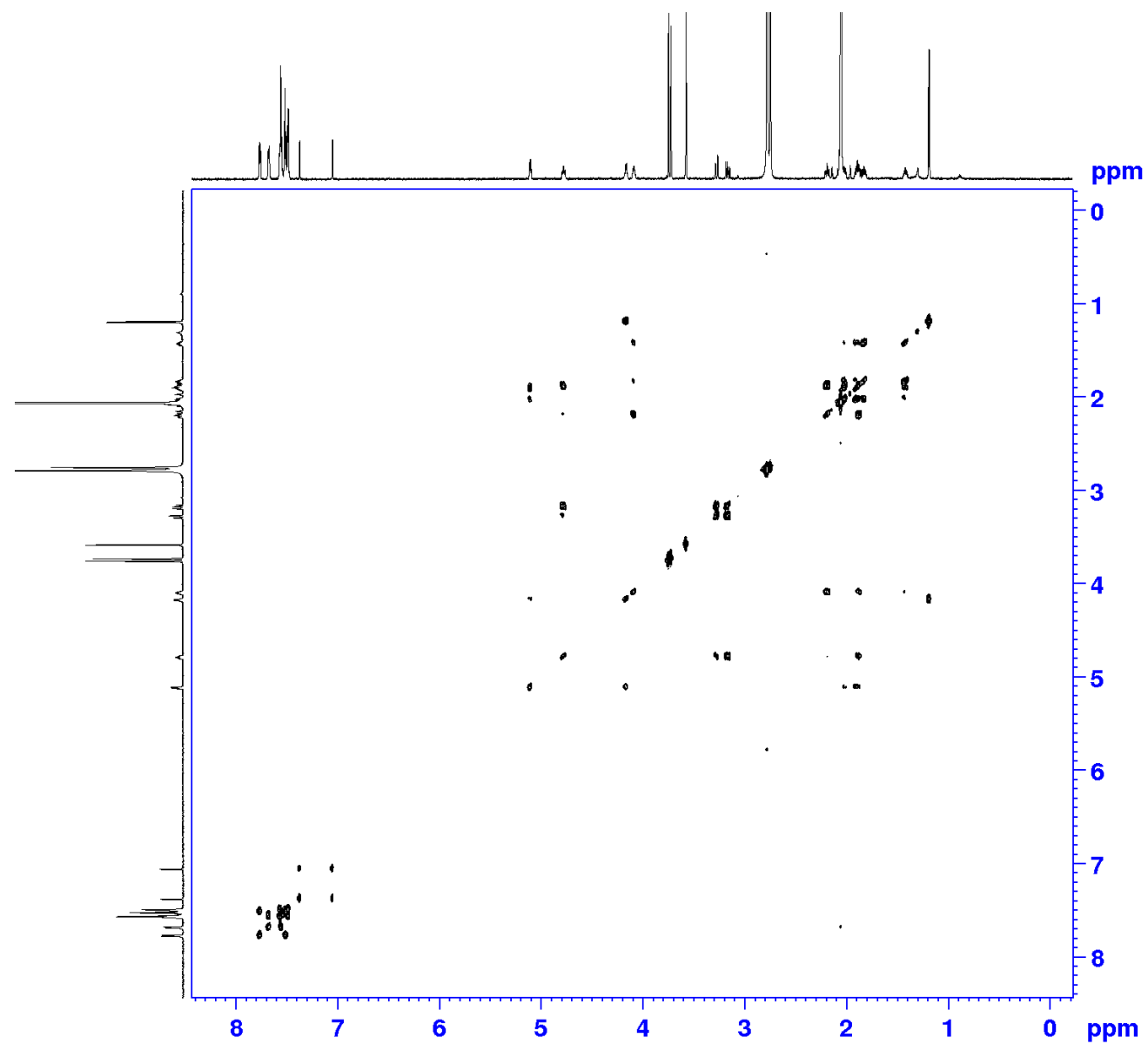


Figure S56. HSQC spectrum for MTPA-2b (R)

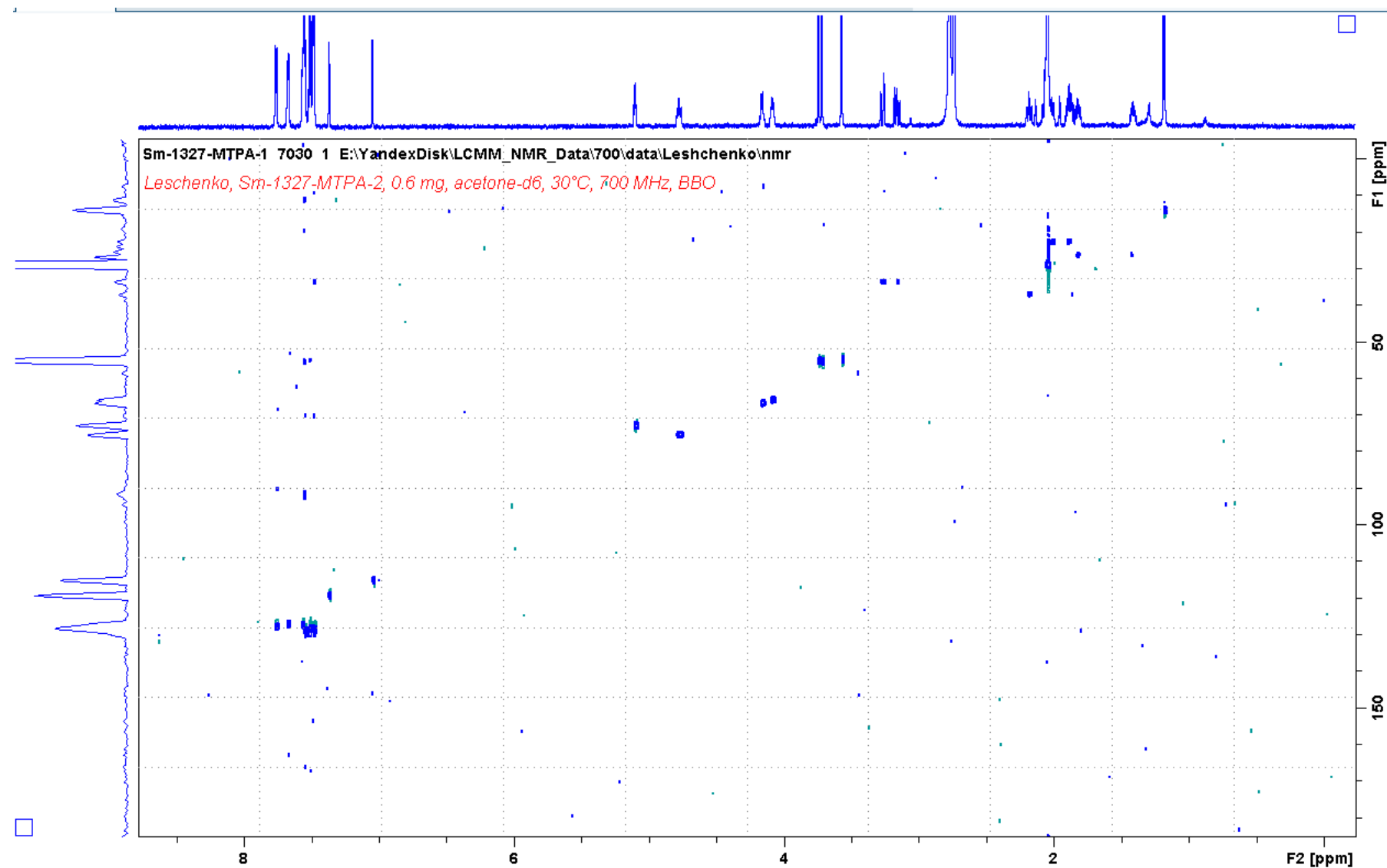


Figure S57. Scheme of isolation compounds 1-6.

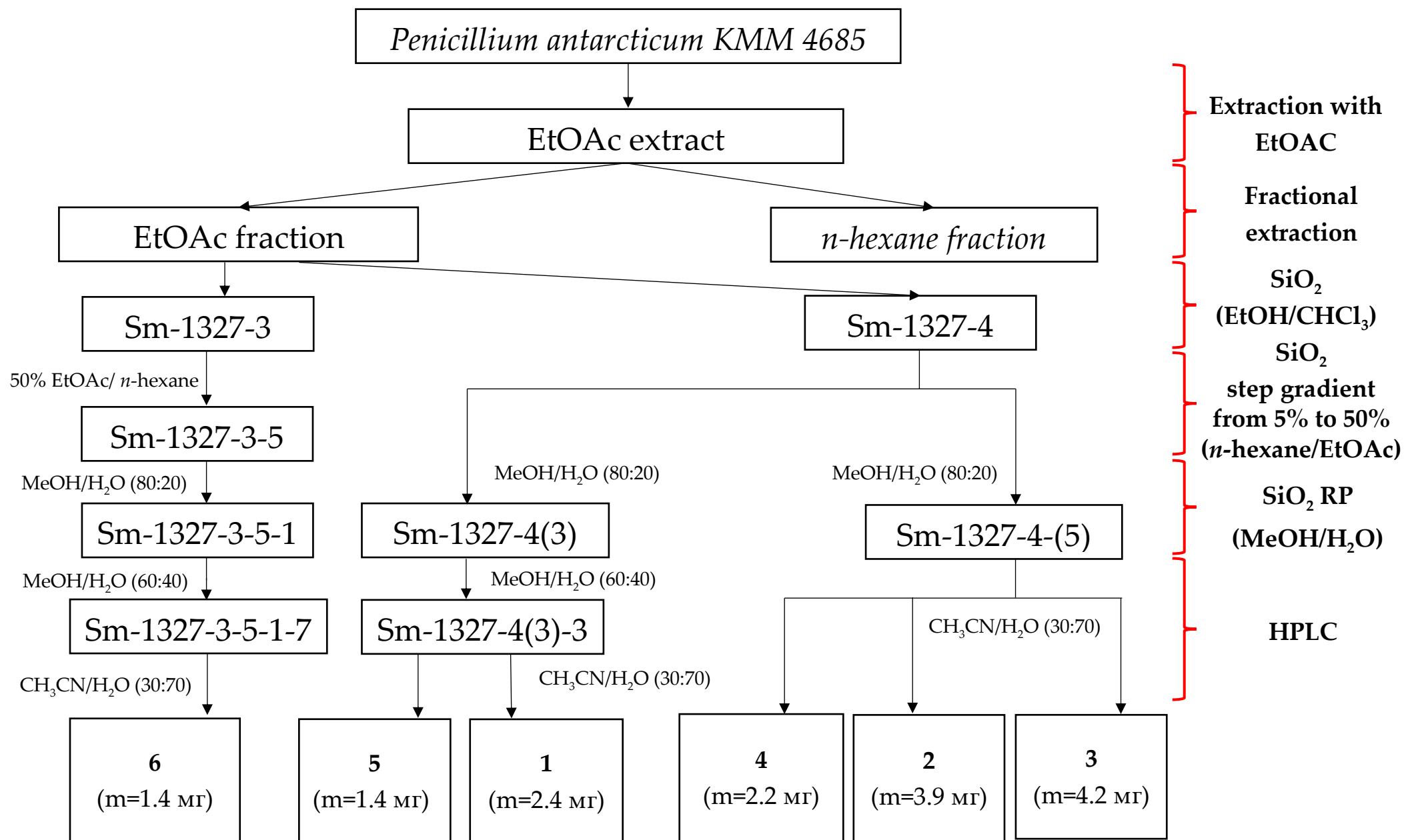


Figure S58. ROESY spectrum for 1

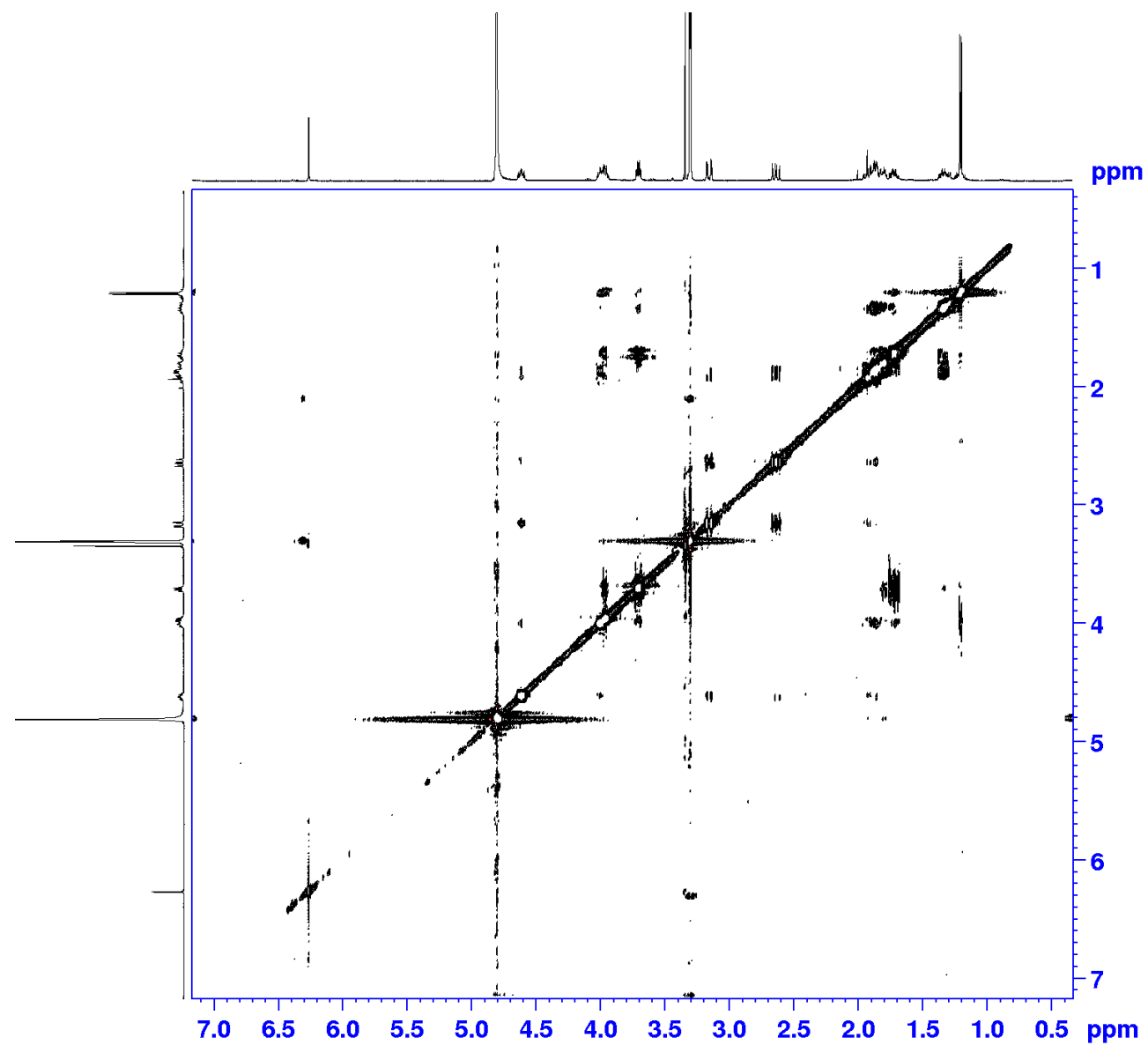


Figure S59. ROESY spectrum for 2

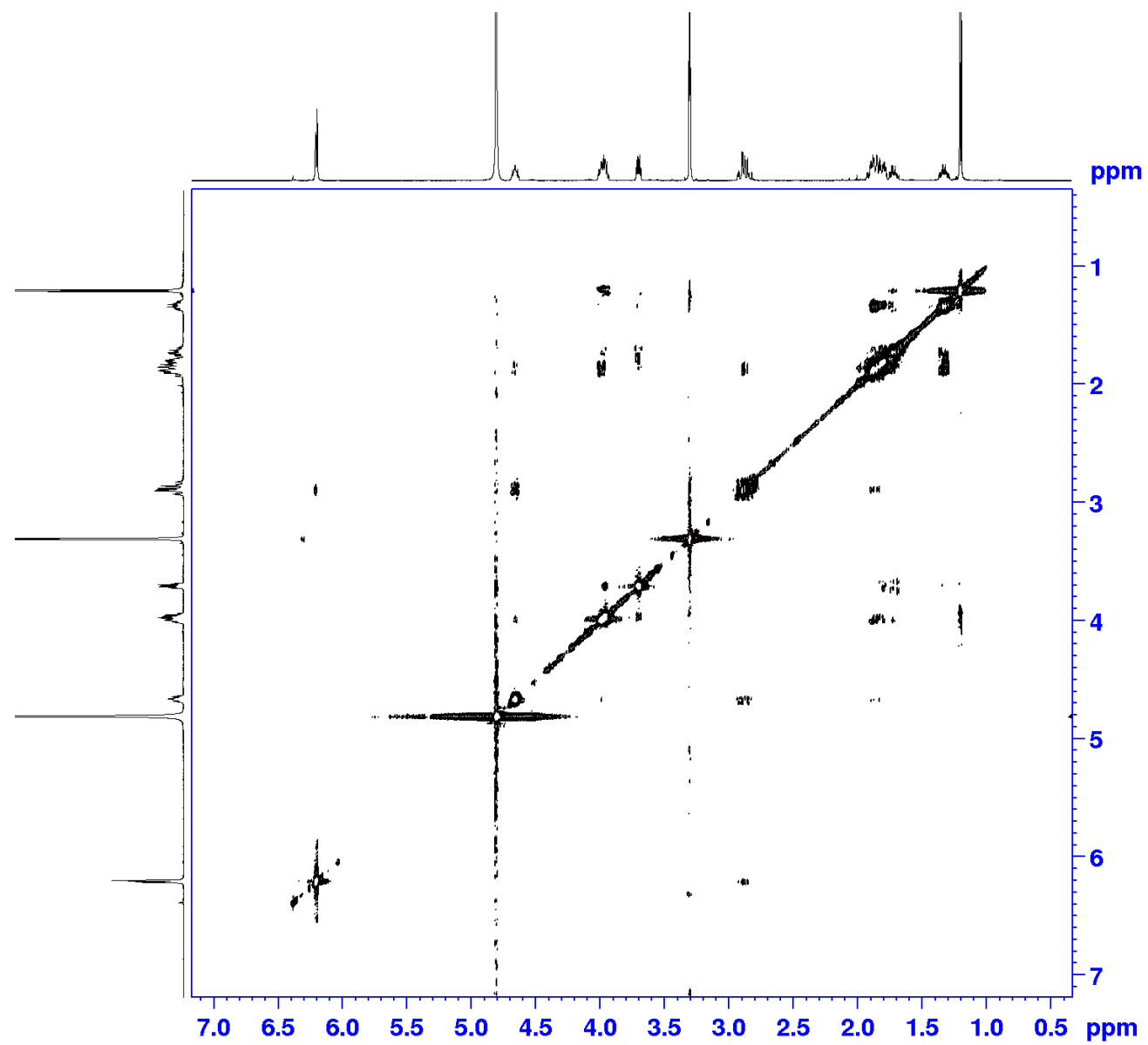


Figure S60. ROESY spectrum for 3

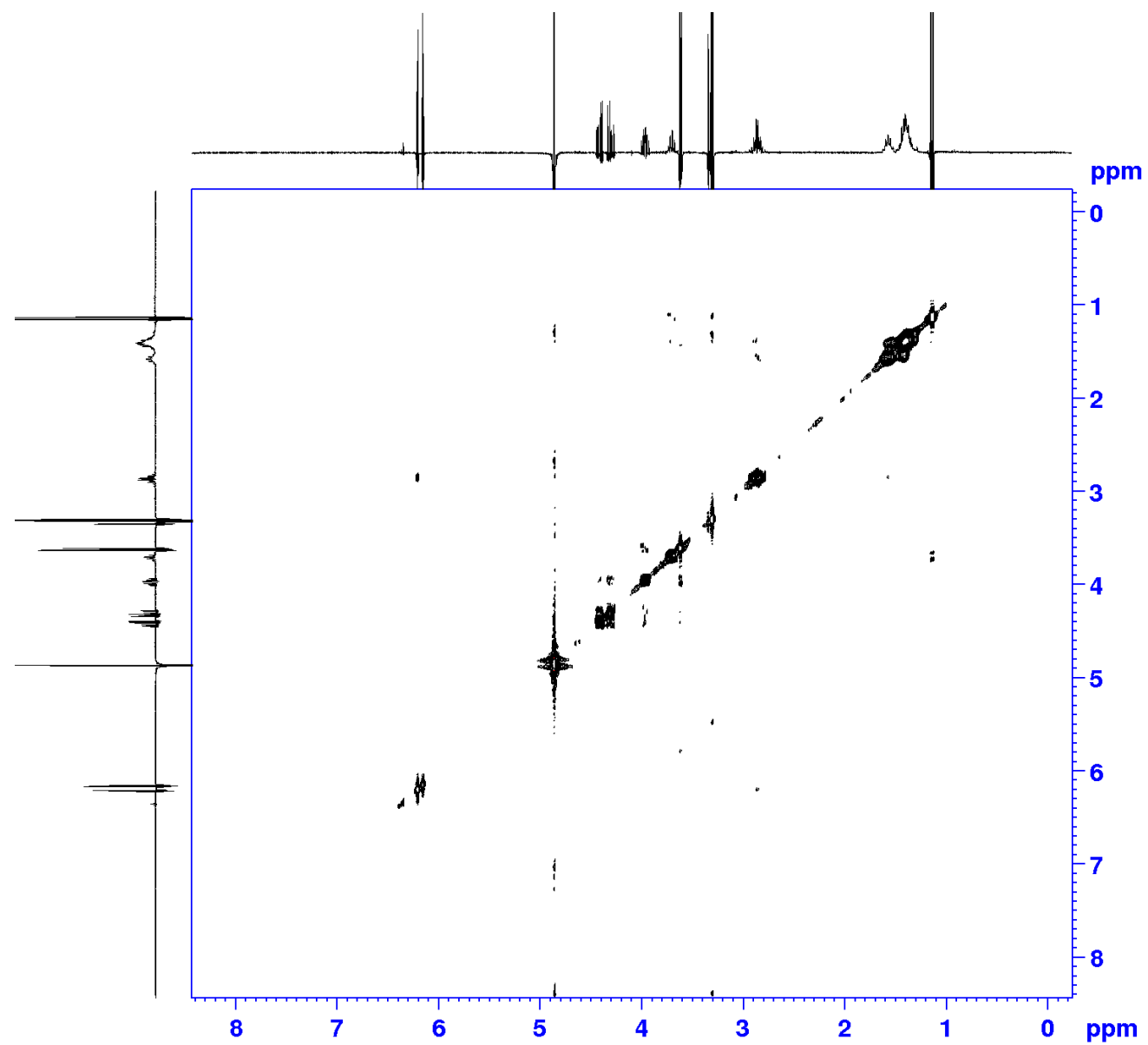


Figure S61. ROESY spectrum for 4

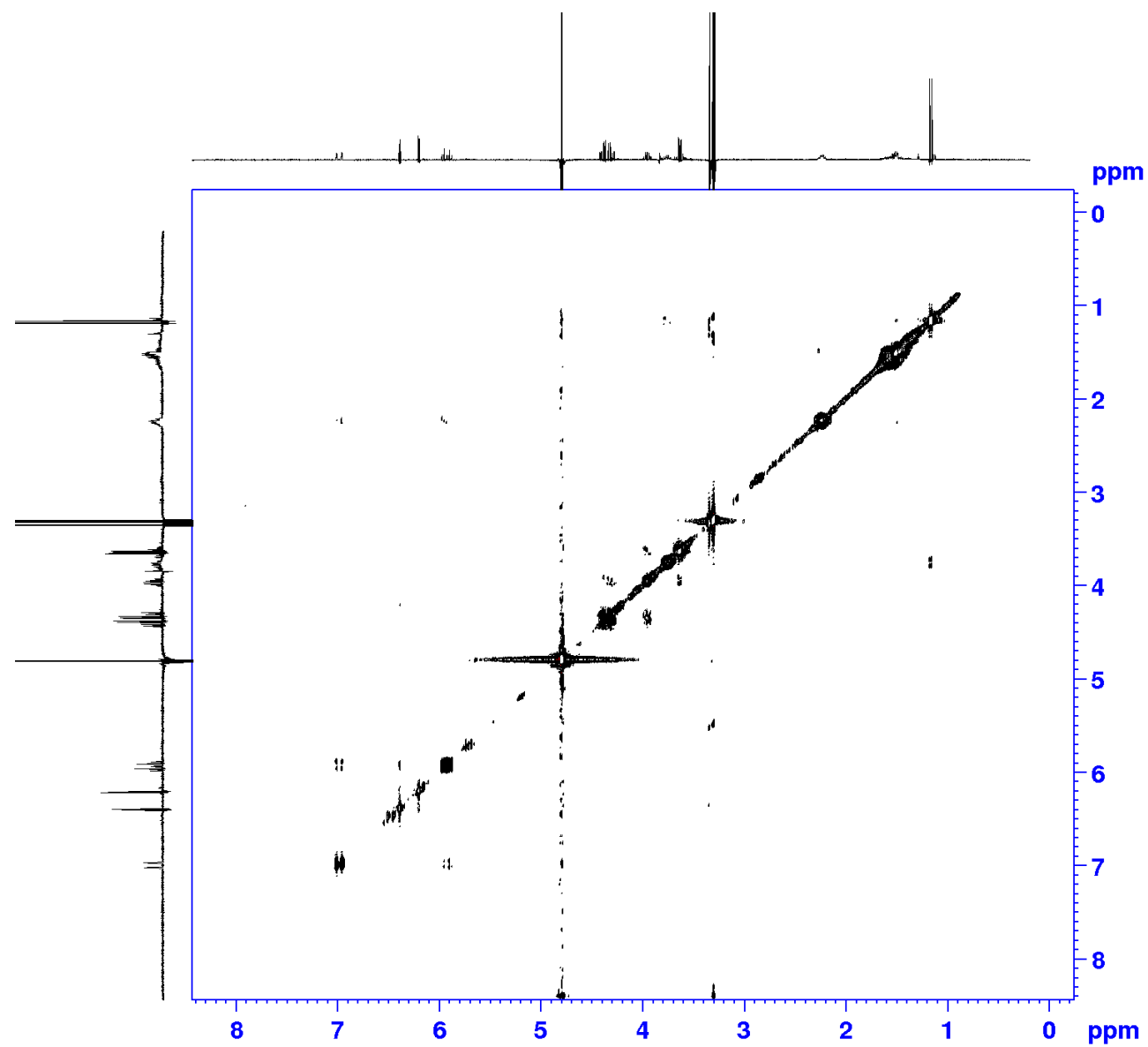


Figure S62. ROESY spectrum for 5

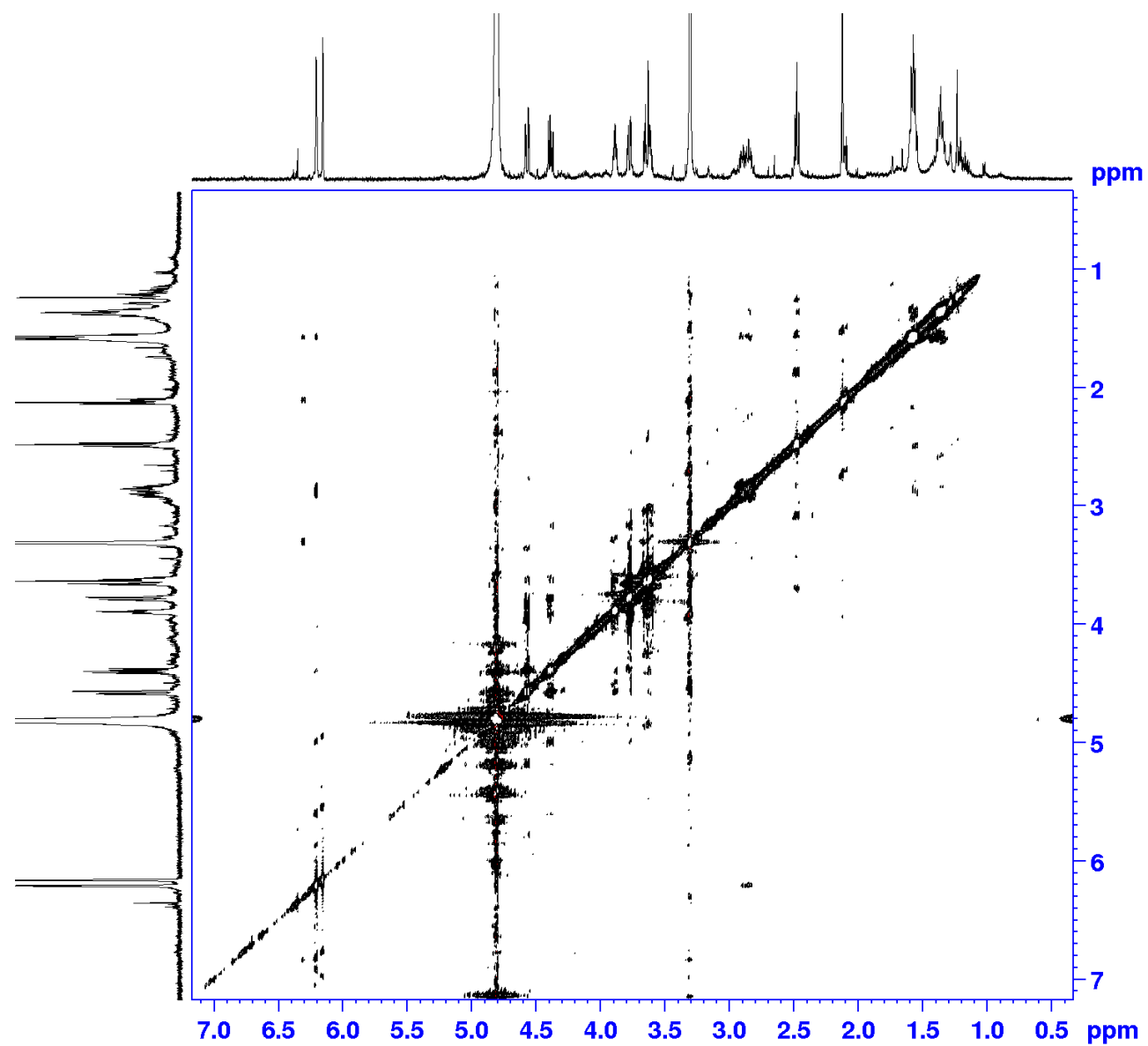
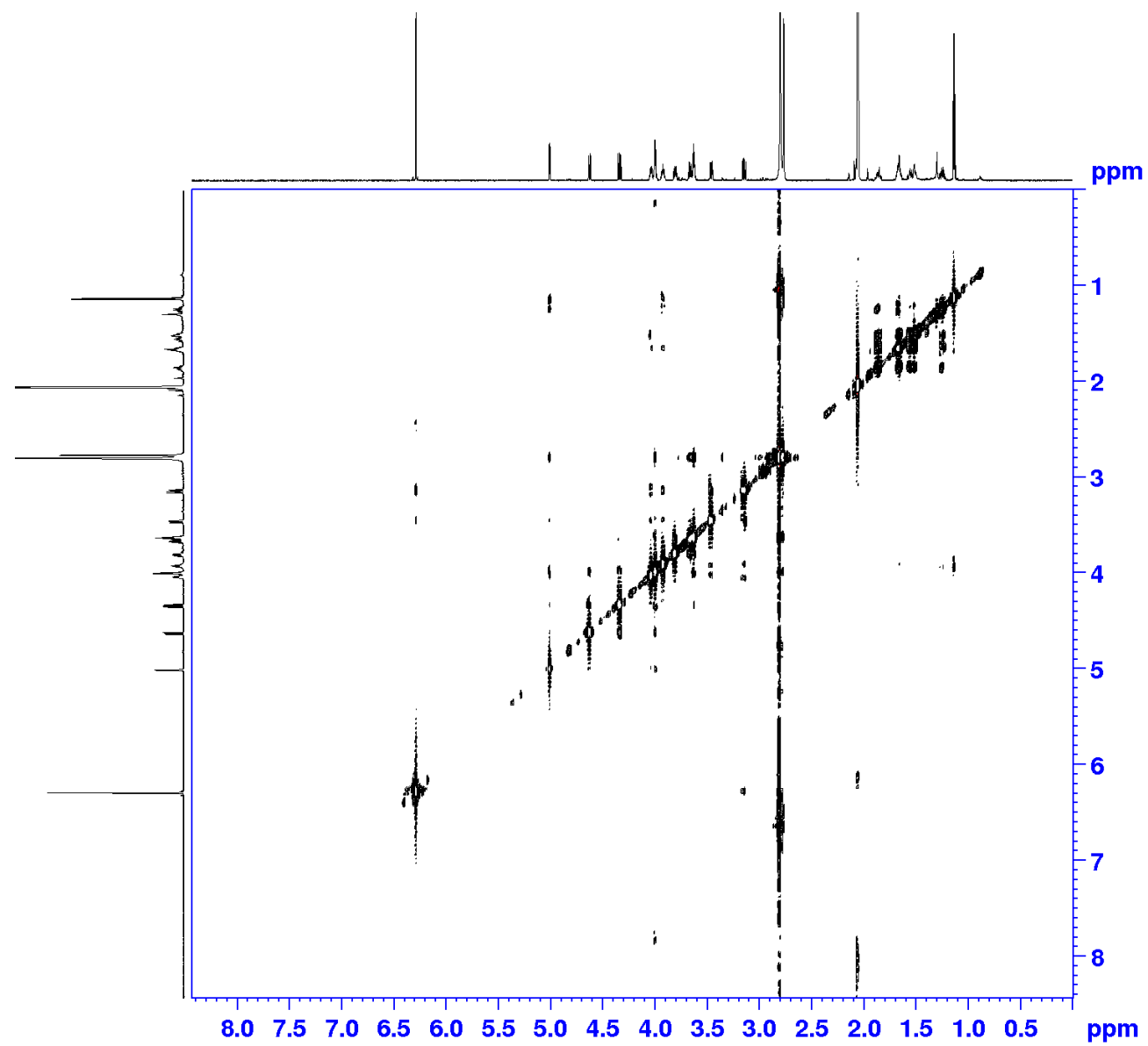


Figure S63. ROESY spectrum for 6



Sm-1327-3-5-7-2 23 1 E:\YandexDisk\LCMM_NMR_Data\700\data\Leshchenko\mr

Sm-1327-3-5-7-2. 1.4 mg, Acetone

col : 3.9148 ppm / 2740.3652 Hz Index = 1390

row : 1.859 ppm / 1301.372 Hz Index = 868

Value = -1459

4.0

3.9

3.8

F2 [ppm]

