

ADDITIONAL FILE 2

Formation of Epoxy beyeranes during the Auto-oxidation of *Ent*-beyer-15-en-19-al isolated from the Essential oil of the Heartwood of *Erythroxylum monogynum* Roxb.

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Table of Content

- Table S1.** Comparison of reported and observed ^{13}C NMR spectroscopic data of *ent*-beyer-15-ene (**1**) and erythroxyol A (**2**)
- Table S2.** Comparison of reported ^1H (200 MHz) and ^{13}C (50 MHz) NMR Spectroscopic data with observed ^1H (400 MHz) and ^{13}C (100 MHz) NMR Spectroscopic Data and Selected HMBC correlations of **5**
- Table S3.** ^1H (400 MHz) and ^{13}C (100 MHz) NMR Spectroscopic Data and Selected HMBC correlations of **9**

For compound **3**

- Figure S4.** ^1H NMR Spectrum (400 MHz) of **3** in CDCl_3
- Figure S5.** ^{13}C NMR Spectrum (100 MHz) of **3** in CDCl_3
- Figure S6.** DEPT 135 Spectrum (100 MHz) of **3** in CDCl_3
- Figure S7.** HSQC Spectrum of **3** in CDCl_3
- Figure S8.** HMBC Spectrum of **3** in CDCl_3

For compound **4**

- Figure S9.** ^1H NMR Spectrum (400 MHz) of **4** in CDCl_3
- Figure S10.** ^1H NMR Spectrum (400 MHz) of **4** in CDCl_3 (Expansion δ 0.00 – 2.50)
- Figure S11.** ^{13}C NMR Spectrum (100 MHz) of **4** in CDCl_3
- Figure S12.** DEPT 135 Spectrum (100 MHz) of **4** in CDCl_3
- Figure S13.** HSQC Spectrum of **4** in CDCl_3
- Figure S14.** HMBC Spectrum of **4** in CDCl_3
- Figure S15.** 1D Selective Gradient NOESY spectrum (400 MHz) of **4** in CDCl_3 ; Irradiation at δ 3.433

For compound **5**

- Figure S16.** ^1H NMR Spectrum (400 MHz) of **5** in CDCl_3
- Figure S17.** ^1H NMR Spectrum (400 MHz) of **5** in CDCl_3 (Expansion δ 0.00 – 2.50)
- Figure S18.** ^{13}C NMR Spectrum (100 MHz) of **5** in CDCl_3
- Figure S19.** DEPT 135 Spectrum (100 MHz) of **5** in CDCl_3
- Figure S20.** HSQC Spectrum of **5** in CDCl_3
- Figure S21.** HMBC Spectrum of **5** in CDCl_3

For compound 6a and 6b

- Figure S22.** ^1H NMR Spectrum (400 MHz) of **6a** and **6b** in CDCl_3
- Figure S23.** ^1H NMR Spectrum (400 MHz) of **6a** and **6b** in CDCl_3 (Expansion δ 0.40 – 2.00)
- Figure S24.** ^{13}C NMR Spectrum (100 MHz) of **6a** and **6b** in CDCl_3
- Figure S25.** ^{13}C NMR Spectrum (100 MHz) of **6a** and **6b** in CDCl_3 (Expansion δ 0.00 – 65.00)
- Figure S26.** DEPT 135 Spectrum (100 MHz) of **6a** and **6b** in CDCl_3
- Figure S27.** HSQC Spectrum of **6a** and **6b** in CDCl_3
- Figure S28.** HMBC Spectrum of **6a** and **6b** in CDCl_3
- Figure S29.** 1D Selective Gradient NOESY spectrum (400 MHz) of **6a** and **6b** in CDCl_3 ; Irradiation at δ 0.924
- Figure S30.** 1D Selective Gradient NOESY spectrum (400 MHz) of **6a** and **6b** in CDCl_3 ; Irradiation at δ 1.134
- Figure S31.** 1D Selective Gradient NOESY spectrum (400 MHz) of **6a** and **6b** in CDCl_3 ; Irradiation at δ 1.296
- Figure S32.** ^1H NMR Spectrum (400 MHz) of **6a** in CDCl_3
- Figure S33.** ^1H NMR Spectrum (400 MHz) of **6a** in CDCl_3 (Expansion δ 0.40 – 3.50)
- Figure S34.** ^{13}C NMR Spectrum (100 MHz) of **6a** in CDCl_3
- Figure S35.** ^1H NMR Spectrum (400 MHz) of **6b** in CDCl_3
- Figure S36.** ^1H NMR Spectrum (400 MHz) of **6b** in CDCl_3 (Expansion δ 0.40 – 3.50)
- Figure S37.** ^{13}C NMR Spectrum (100 MHz) of **6b** in CDCl_3

For compound 7

- Figure S38.** ^1H NMR Spectrum (400 MHz) of **7** in CDCl_3
- Figure S39.** ^{13}C NMR Spectrum (100 MHz) of **7** in CDCl_3
- Figure S40.** DEPT 135 Spectrum (100 MHz) of **7** in CDCl_3
- Figure S41.** HSQC Spectrum of **7** in CDCl_3
- Figure S42.** HMBC Spectrum of **7** in CDCl_3
- Figure S43.** 1D Selective Gradient NOESY spectrum (400 MHz) of **7** in CDCl_3 ; Irradiation at δ 0.856
- Figure S44.** 1D Selective Gradient NOESY spectrum (400 MHz) of **7** in CDCl_3 ; Irradiation at δ 1.282

For compound 8

Figure S45. ^1H NMR Spectrum (400 MHz) of **8** in CDCl_3

Figure S46. ^{13}C NMR Spectrum (100 MHz) of **8** in CDCl_3

Figure S47. DEPT 135 Spectrum (100 MHz) of **8** in CDCl_3

Figure S48. HSQC Spectrum of **8** in CDCl_3

Figure S49. HMBC Spectrum of **8** in CDCl_3

Figure S50. 1D Selective Gradient NOESY spectrum (400 MHz) of **8** in CDCl_3 ; Irradiation at δ 0.740

Figure S51. 1D Selective Gradient NOESY spectrum (400 MHz) of **8** in CDCl_3 ; Irradiation at δ 1.117

For compound 9

Figure S52. ^1H NMR Spectrum (400 MHz) of **9** in CDCl_3

Figure S53. ^{13}C NMR Spectrum (100 MHz) of **9** in CDCl_3

Figure S54. DEPT 135 Spectrum (100 MHz) of **9** in CDCl_3

Figure S55. HSQC Spectrum of **9** in CDCl_3

Figure S56. HMBC Spectrum of **9** in CDCl_3

Figure S57. 1D Selective Gradient NOESY spectrum (400 MHz) of **9** in CDCl_3 ; Irradiation at δ 1.136

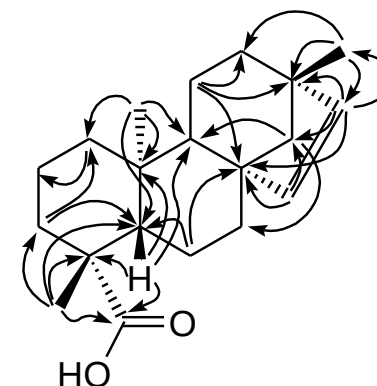
Figure S58. 1D Selective Gradient NOESY spectrum (400 MHz) of **9** in CDCl_3 ; Irradiation at δ 0.709

S1. Comparison of reported and observed ^{13}C NMR spectroscopic data of *ent*-beyer-15-ene (**1**) and erythroxyol A (**2**) in CDCl_3

C	<i>Ent</i> -beyer-15-ene (1)		Erythroxyol A (2)	
	δ (reported) at 20 MHz	δ (observed) at 100 MHz	δ (reported) at 20 MHz	δ (observed) at 100 MHz
1	39.3	39.3	39.2	39.2
2	18.7	18.7	18.3	18.3
3	42.2	42.2	35.7	35.6
4	33.3	33.2	38.5	38.5
5	56.1	56.1	56.8	56.8
6	20.3	20.2	20.1	20.2
7	37.4	37.36 or 37.41	37.3	37.7 or 37.2
8	49.1	49.1	49.0	49.0
9	53.0	52.9	53.0	52.9
10	37.4	37.36 or 37.41	37.3	37.7 or 37.2
11	20.5	20.3	20.3	20.3
12	33.7	33.3	33.2	33.2
13	43.6	43.7	43.6	43.6
14	61.3	61.3	61.2	61.1
15	135.2	135.4	135.0	135.0
16	136.1	136.3	136.0	136.5
17	25.0	25.1	24.9	24.9
18	33.8	33.8	27.0	27.0
19	22.0	22.1	65.5	65.5
20	15.1	15.1	15.6	15.8

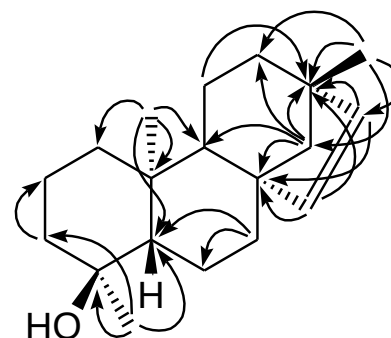
S2. Comparison of reported ^1H (200 MHz) and ^{13}C (50 MHz) NMR Spectroscopic data with observed ^1H (400 MHz) and ^{13}C (100 MHz) NMR Spectroscopic Data and Selected HMBC correlations of **5**

C	Type	δ_{H} (Rep)	δ_{C} (Rep)	δ_{H} (Obs)	δ_{C} (Obs)	HMBC
1	CH_2		39.6	0.90 m, 1.69 m	39.5	2
2	CH_2		19.3	1.41 m, 1.80 m	19.2	
3	CH_2		38.0	1.01 m, 2.15 m	37.9	1, 5
4	C		43.9	-	43.8	
5	CH		57.2	1.10 m	57.0	4, 9, 10, 19
6	CH_2		21.6	1.82 m	21.6	5, 8
7	CH_2		37.7	1.29 m, 1.66 m	37.7	
8	C		49.2	-	49.1	
9	CH		52.4	0.97 m	52.3	
10	C		37.7	-	37.9	
11	CH_2		20.5	1.53 m, 1.25	20.4	8, 12, 13
12	CH_2		33.2	1.25 m	33.1	
13	C		43.7	-	43.7	
14	CH_2		61.1	1.01 m, 1.45 m	61.0	7, 9
15	CH	5.47 d ($J=5.7$ Hz)	134.8	5.73 d ($J=5.7$ Hz)	134.8	8, 14
16	CH	5.76 d ($J=5.7$ Hz)	136.5	5.45 d ($J=5.7$ Hz)	136.5	8, 13, 14, 17
17	CH_3	1.01 s	24.9	0.99 s	24.9	16, 12, 13
18	CH_3	1.26 s	29.1	1.24 s	29.1	3, 4, 5, 19
19	C		184.3	-	183.8	
20	CH_3	0.69 s	13.8	0.67 s	13.8	1, 5, 9, 10

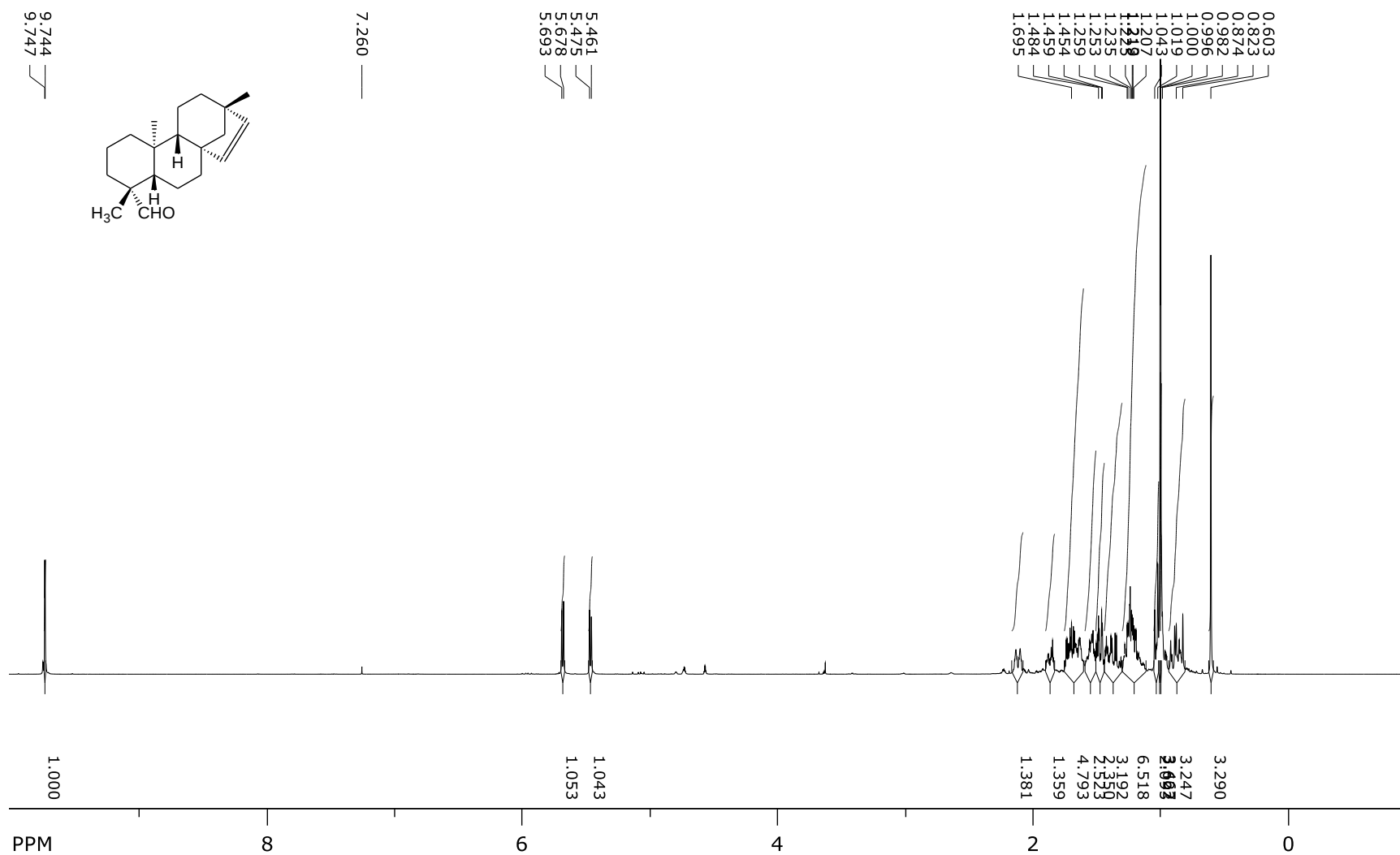


S3. ^1H (400 MHz) and ^{13}C (100 MHz) NMR Spectroscopic Data and Selected HMBC correlations of **9**

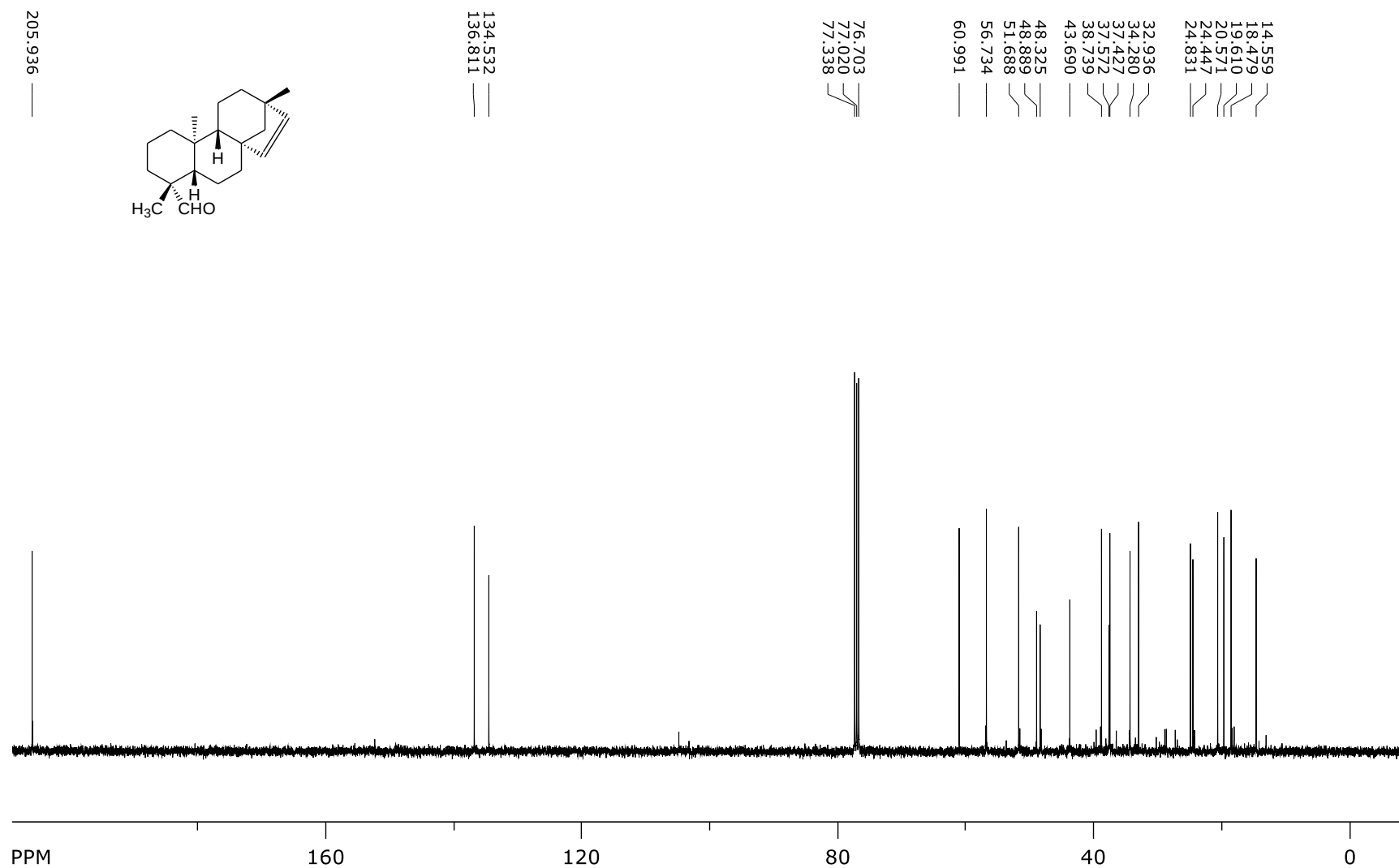
C	δ_{H}	δ_{C}	HMBC
1	0.89 m, 1.57 m	38.4	CH_2
2	1.51 m	19.9	CH_2
3	1.33 m, 1.76 m	43.0	CH_2 2
4	-	72.4	C
5	1.13 m	57.6	CH
6	1.38 m, 1.75 m	19.1	CH_2
7	1.37 m, 1.66 m	36.7	CH_2 5, 6
8	-	49.0	C
9	1.05 m	52.6	CH
10	-	38.0	C
11	0.83 m, 1.27 m	20.4	CH_2 13
12	1.27 m	33.1	CH_2 14
13	-	43.7	C
14	1.04 m, 1.45 m	61.1	CH_2 8, 9, 12, 13
15	5.68 d ($J= 5.7$ Hz)	135.0	CH 8, 13, 14, 16
16	5.46 d ($J= 5.7$ Hz)	136.5	CH 8, 13, 14, 15
17	1.00 s	24.9	CH_3 12, 13, 14, 16
18	-	-	
19	1.14 s	23.3	CH_3 3, 4, 5,
20	0.71 s	14.5	CH_3 1, 5, 9, 10



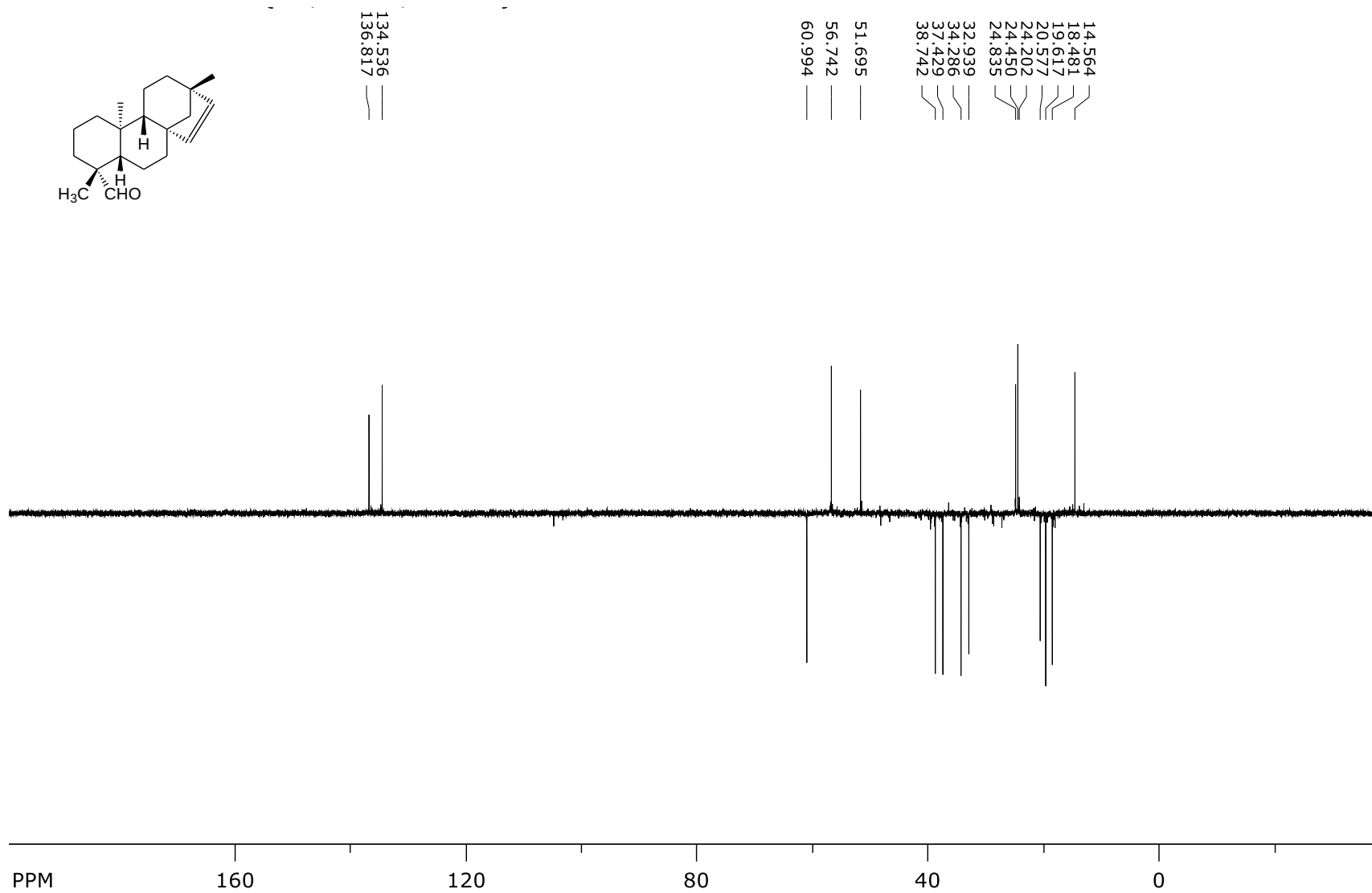
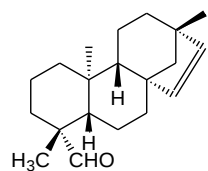
S4. ^1H NMR Spectrum (400 MHz) of **3** in CDCl_3



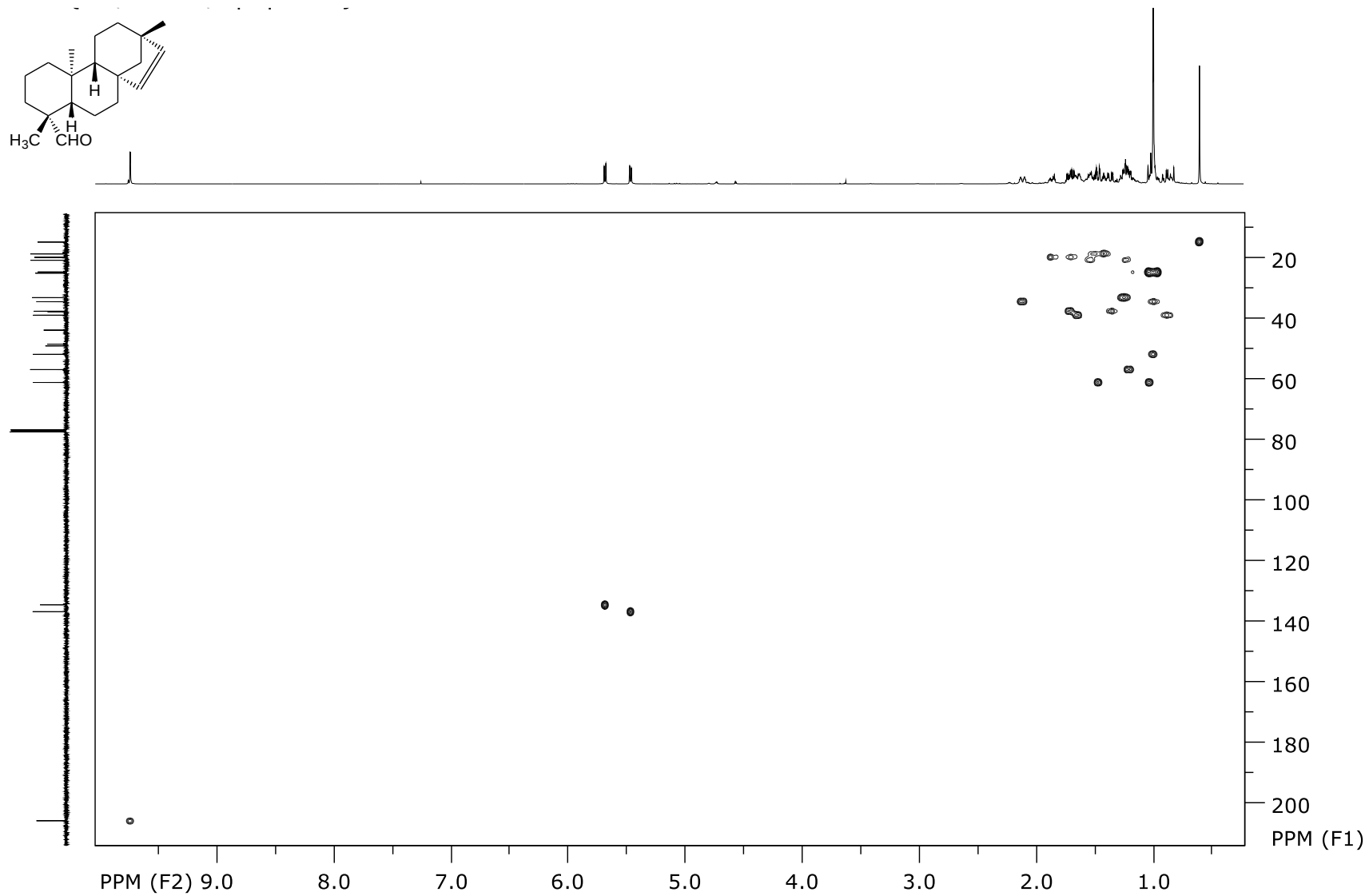
S5. ^{13}C NMR Spectrum (100 MHz) of **3** in CDCl_3



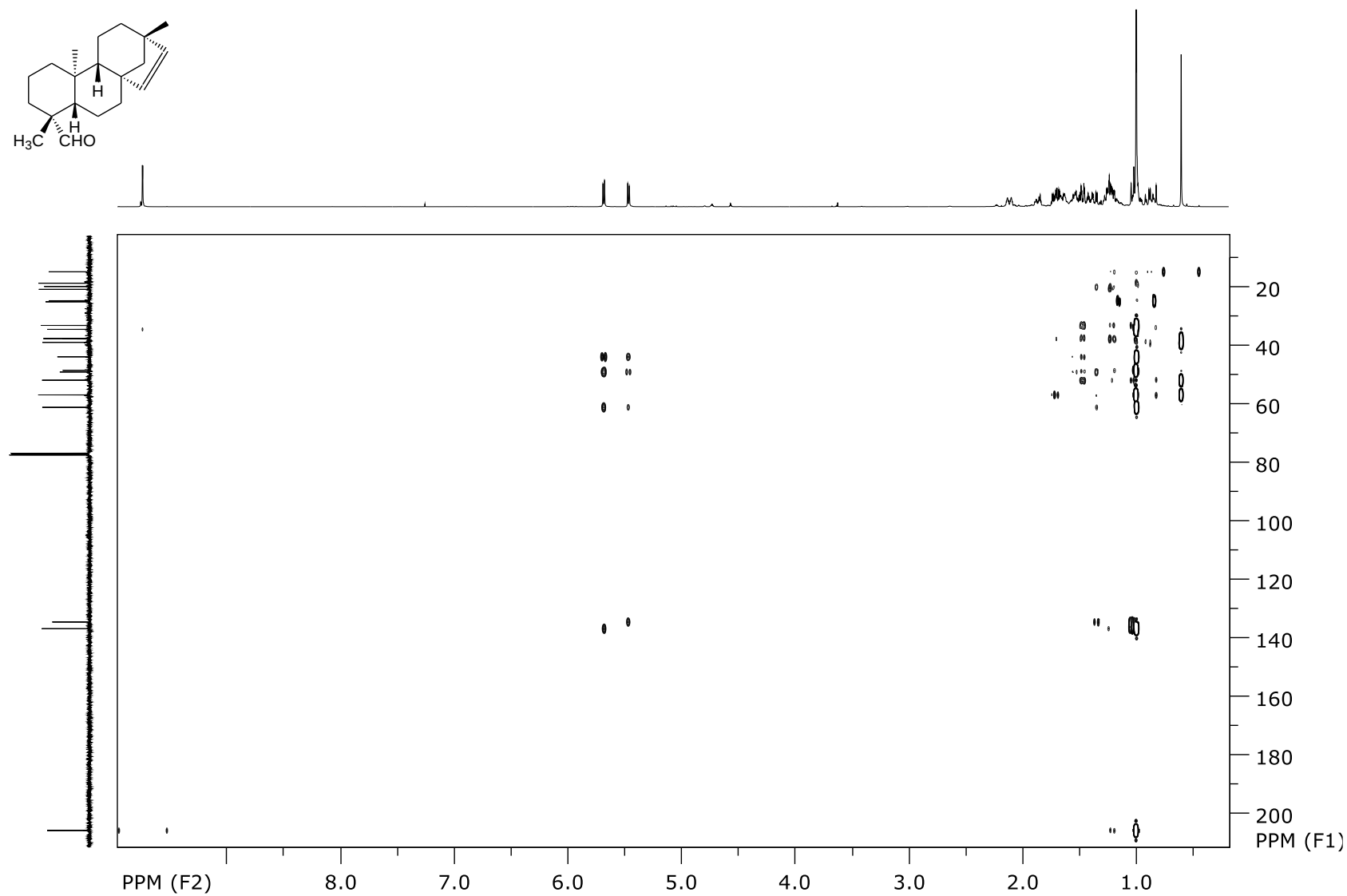
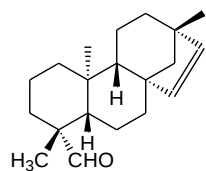
S6. DEPT 135 Spectrum (100 MHz) of **3** in CDCl₃



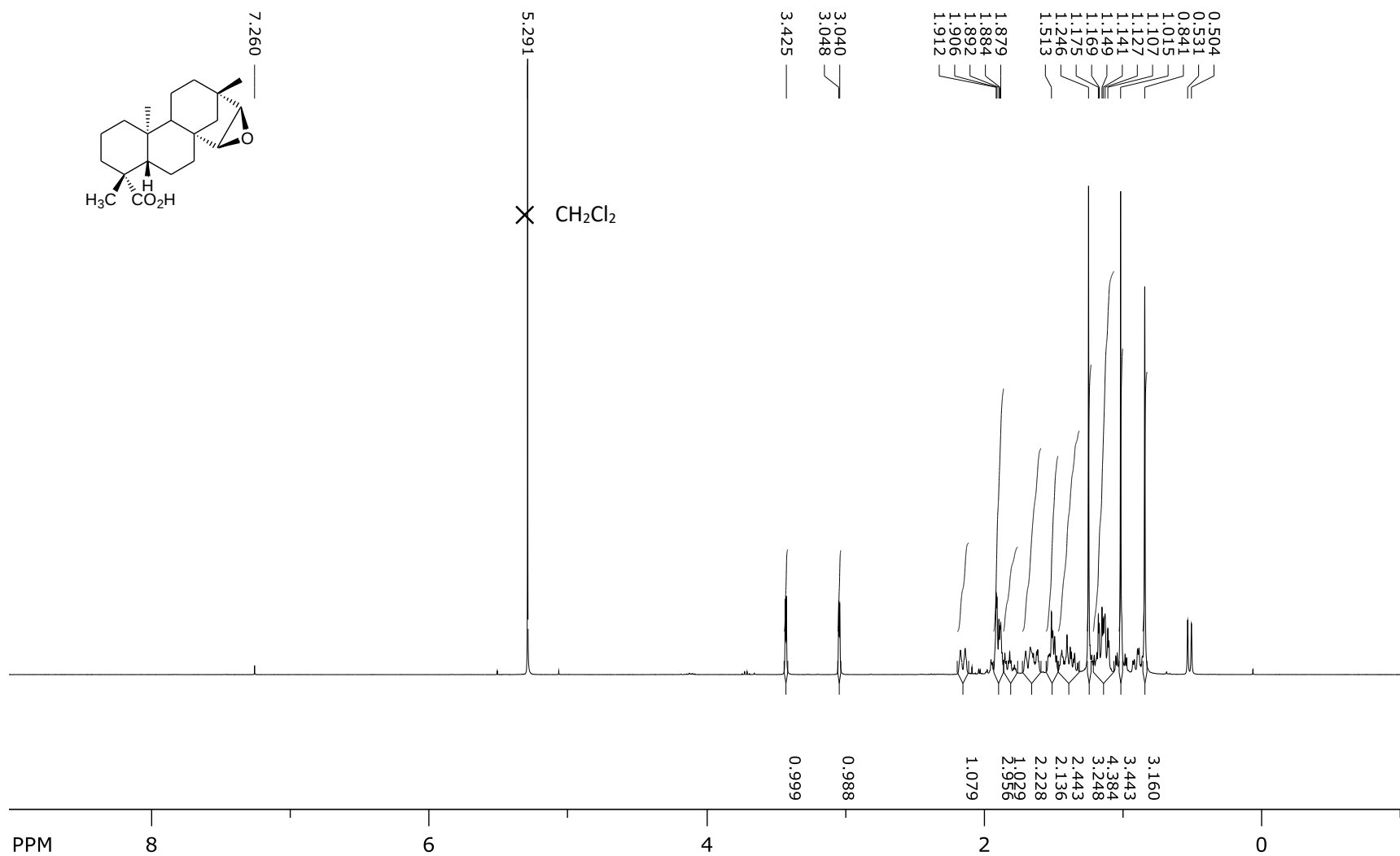
S7. HSQC Spectrum of **3** in CDCl₃



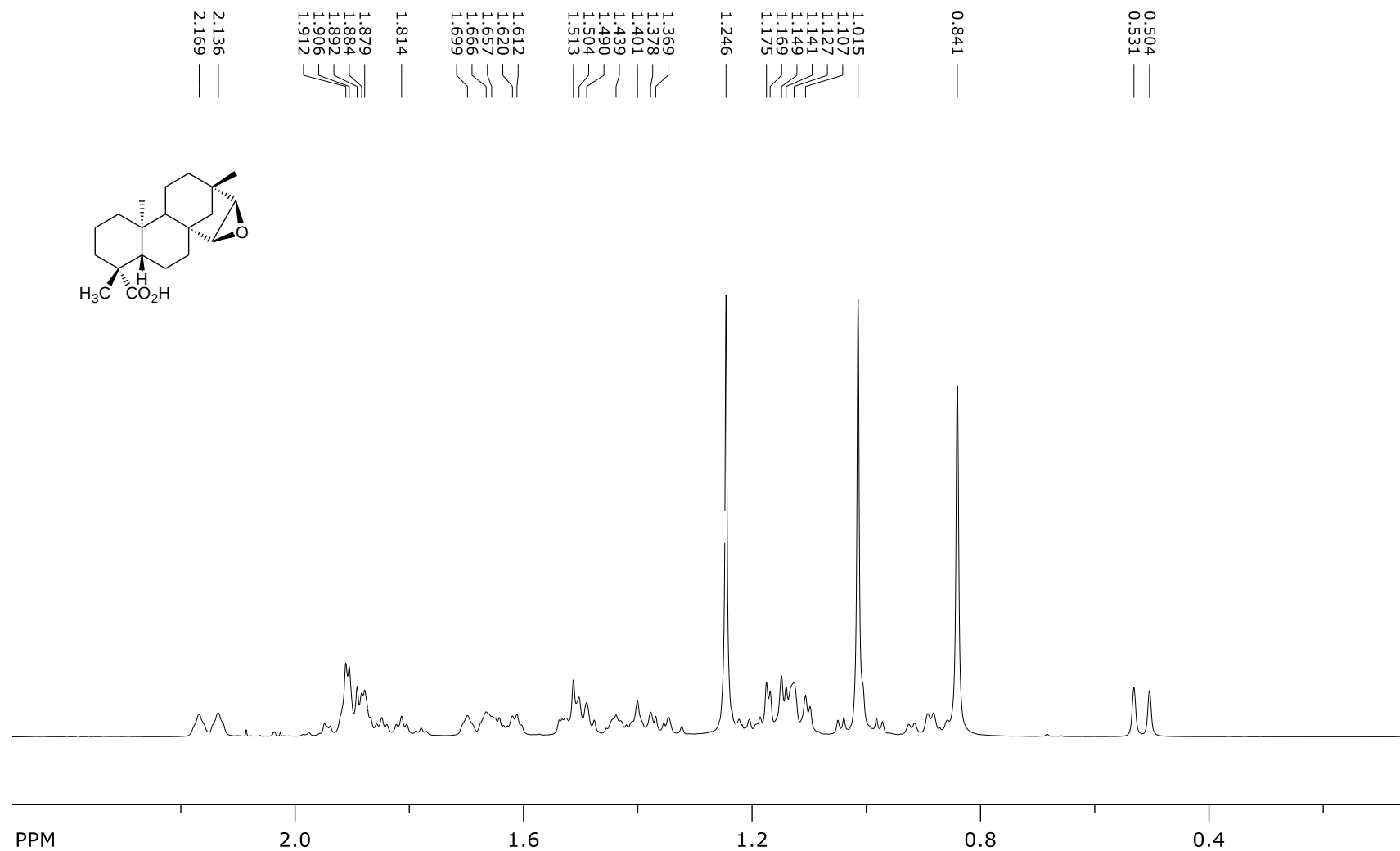
S8. HMBC Spectrum of **3** in CDCl₃



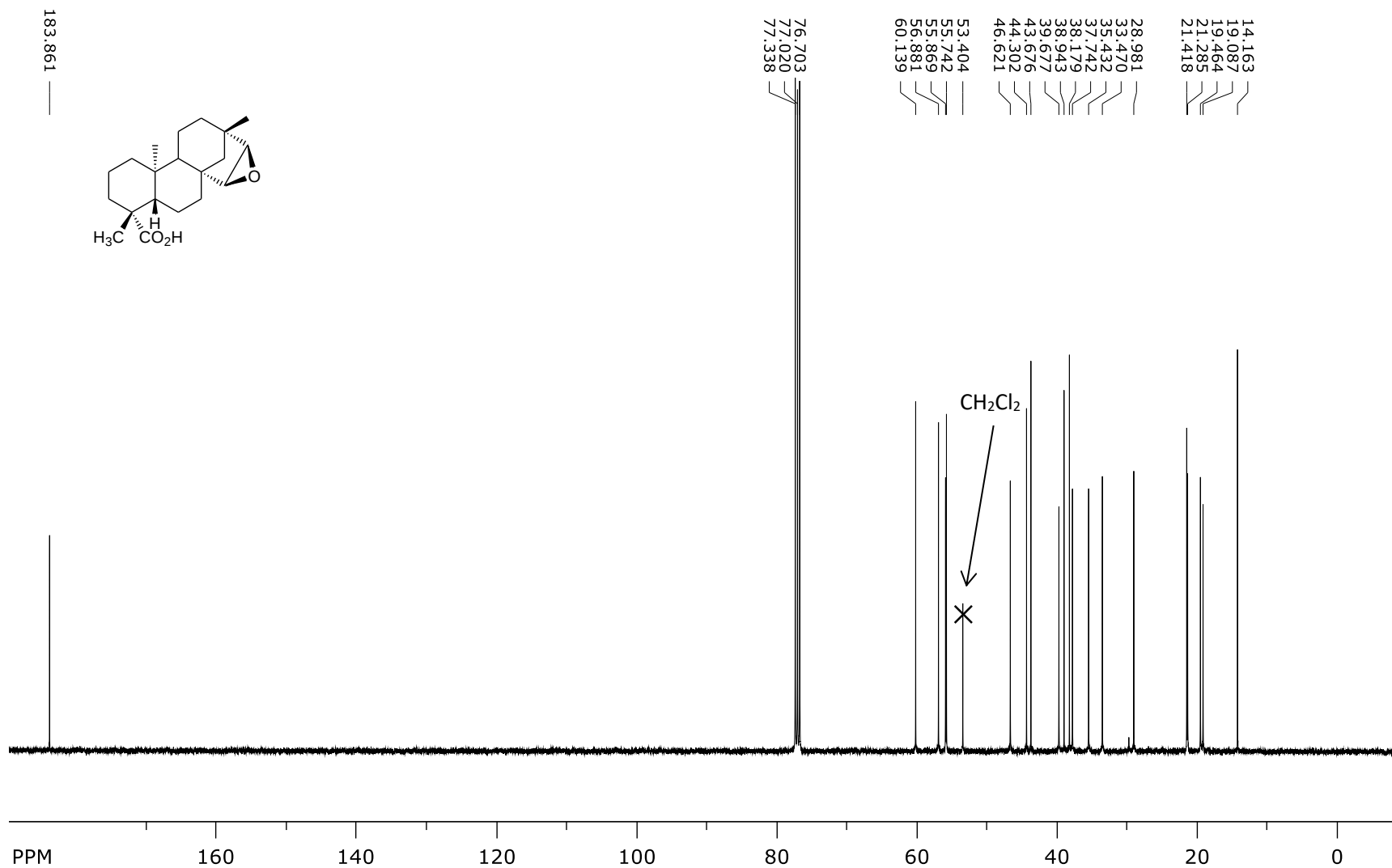
S9. ^1H NMR Spectrum (400 MHz) of **4** in CDCl_3



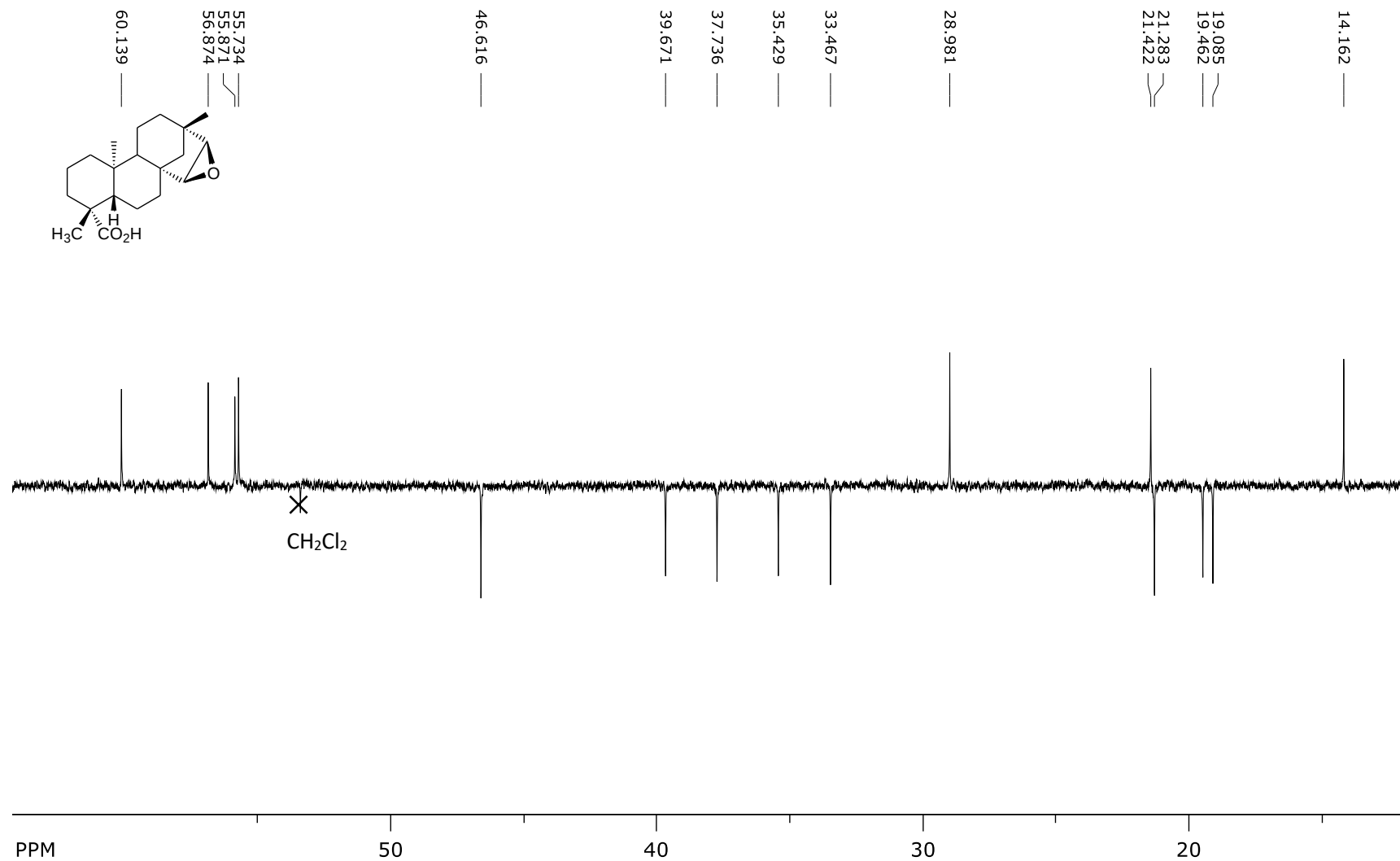
S10. ^1H NMR Spectrum (400 MHz) of **4** in CDCl_3 (Expansion δ 0.00 – 2.50)



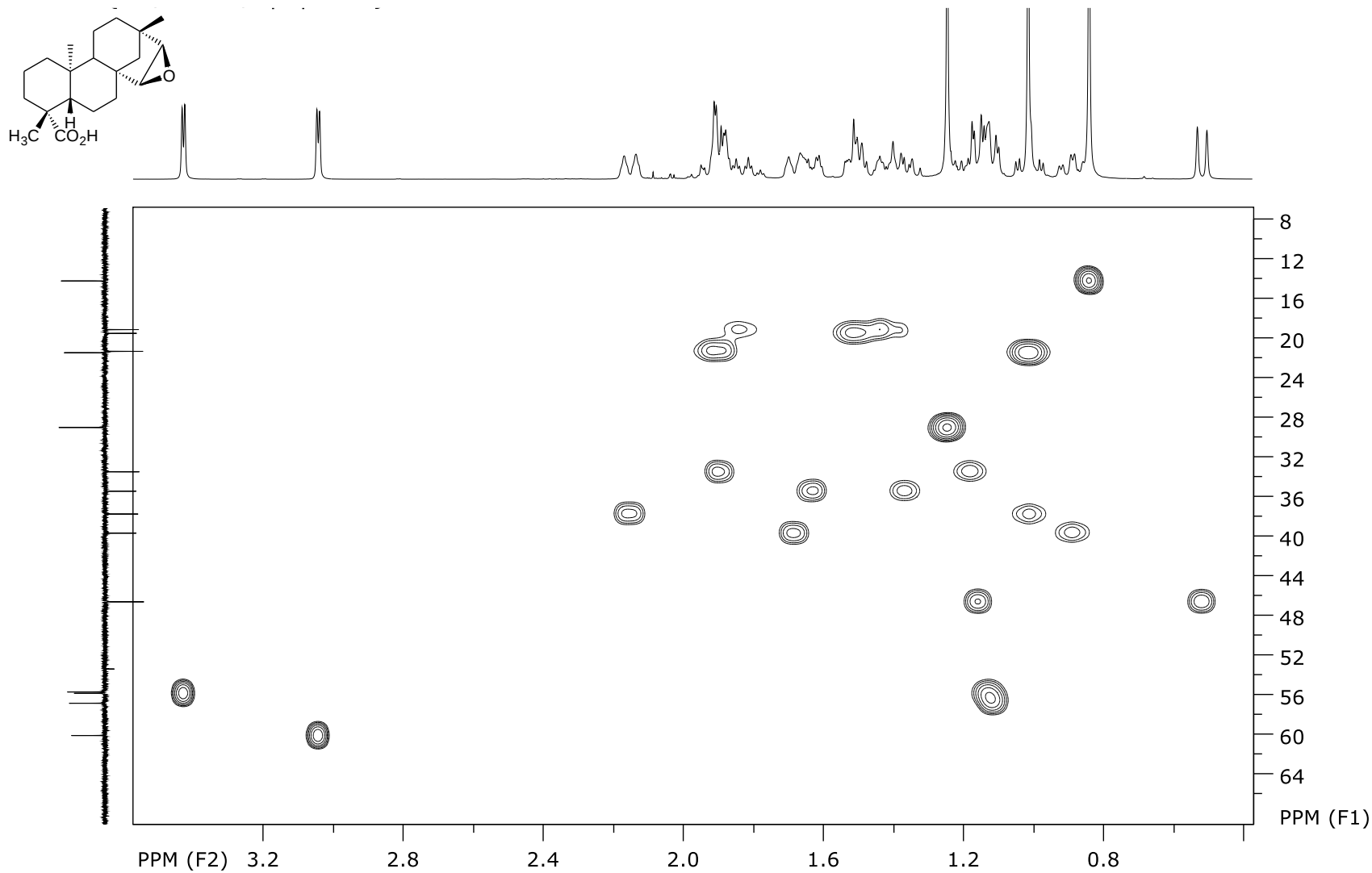
S11. ^{13}C NMR Spectrum (100 MHz) of **4** in CDCl_3



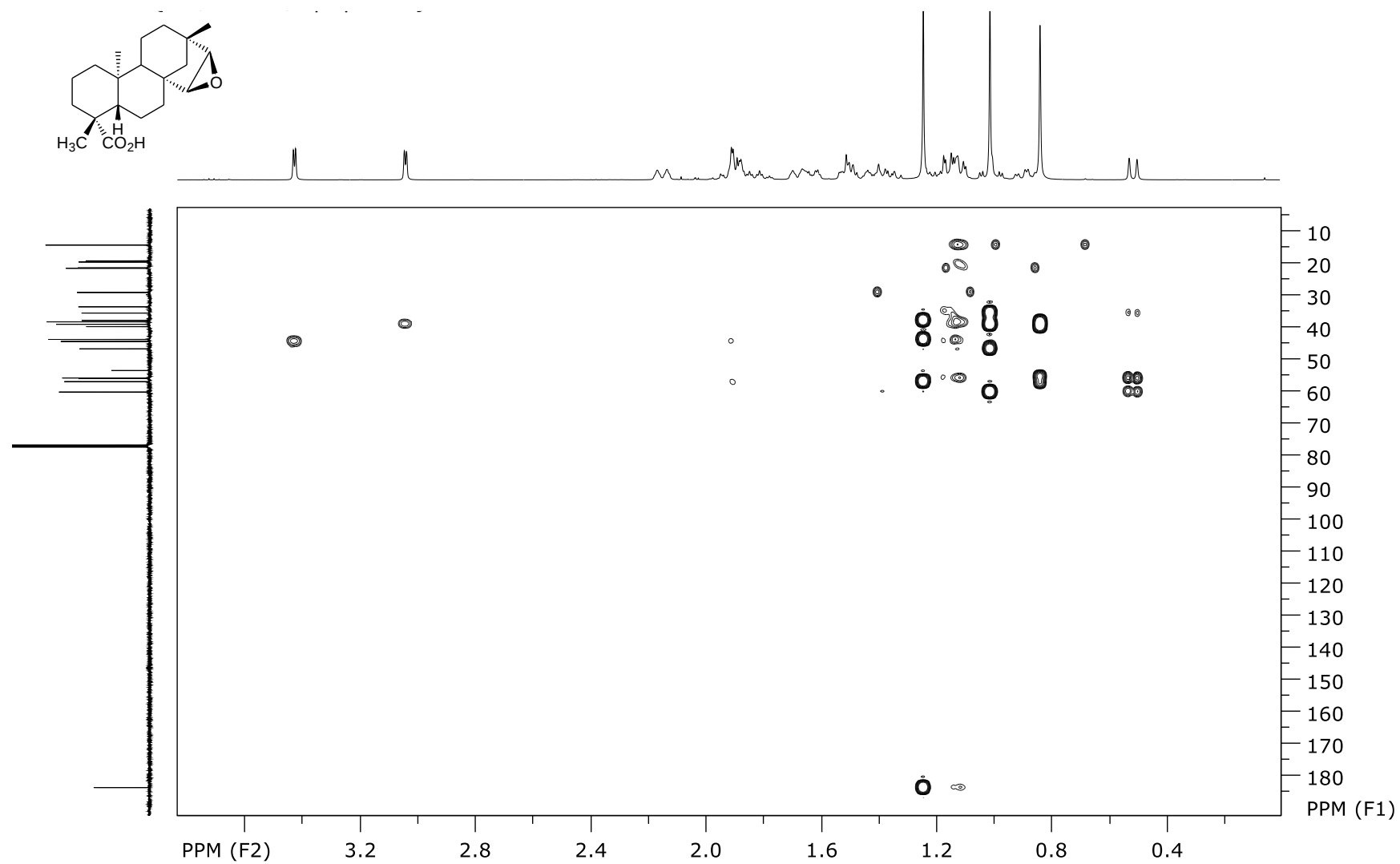
S12. DEPT135 Spectrum (100 MHz) of **4** in CDCl₃



S13. HSQC spectrum of **4** in CDCl₃

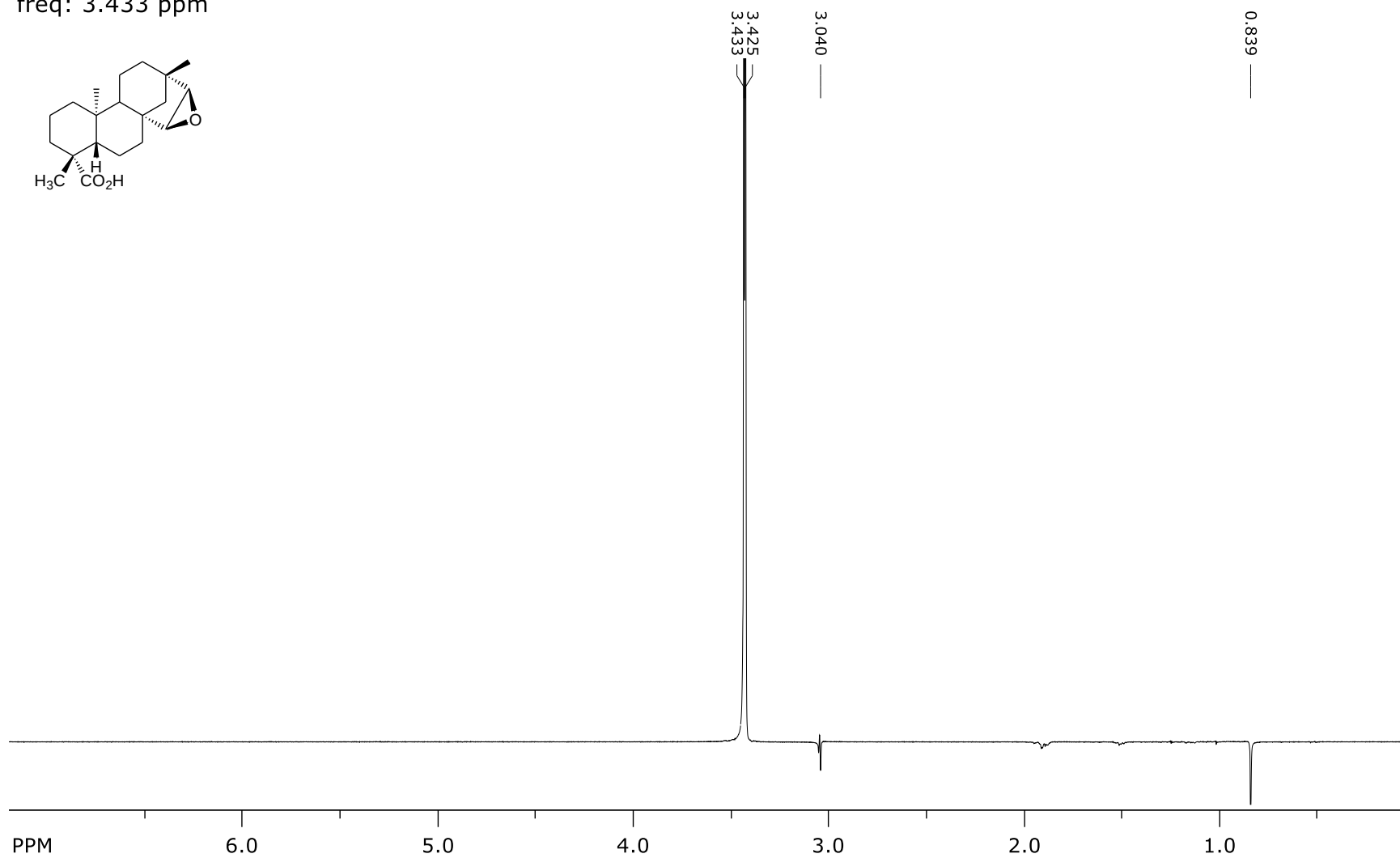
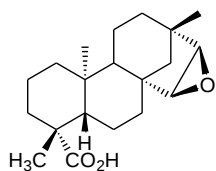


S14. HMBC spectrum of **4** in CDCl₃

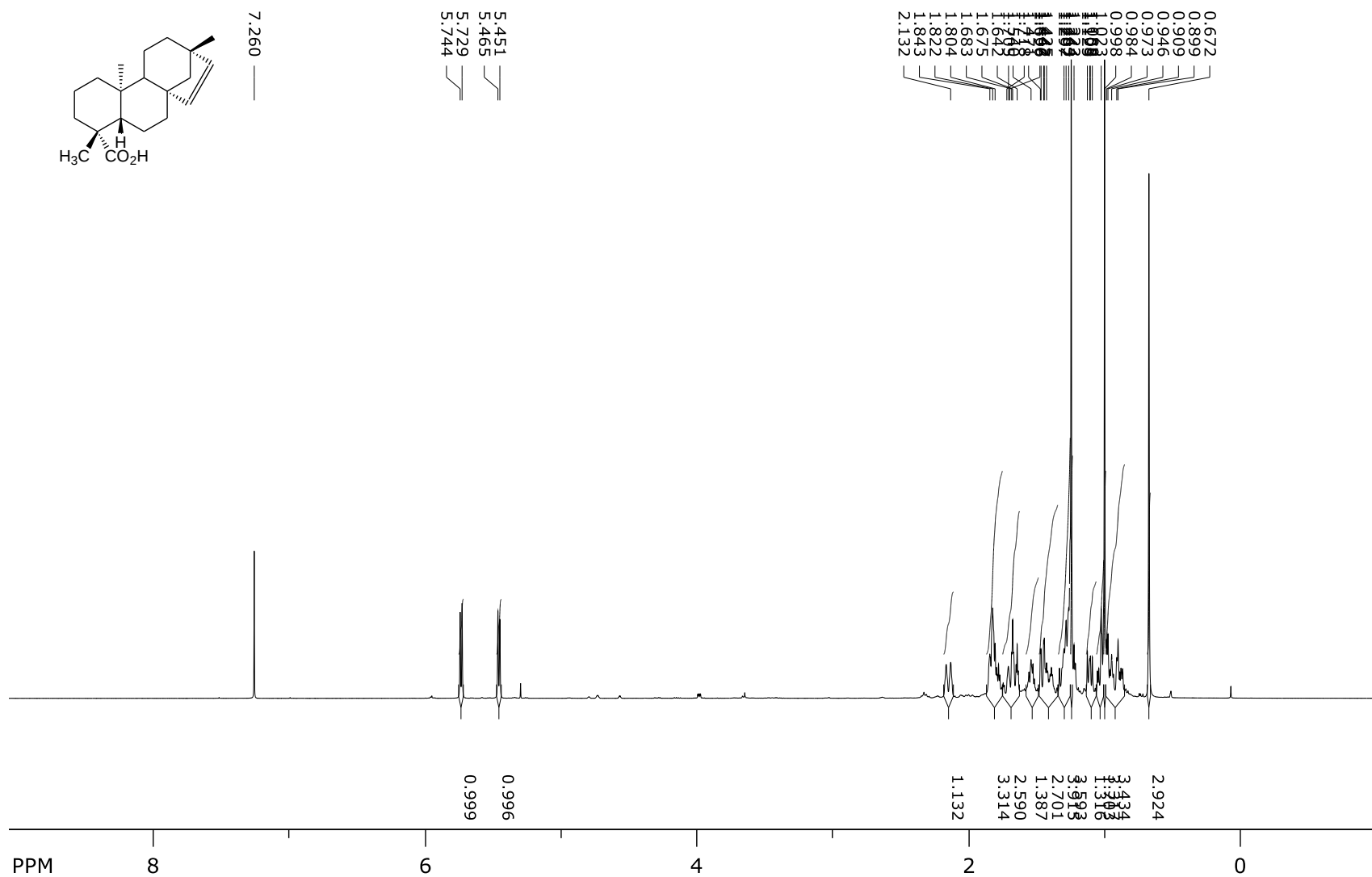


S15. 1D Selective Gradient NOESY spectrum (400 MHz) of **4** in CDCl₃; Irradiation at δ 3.433

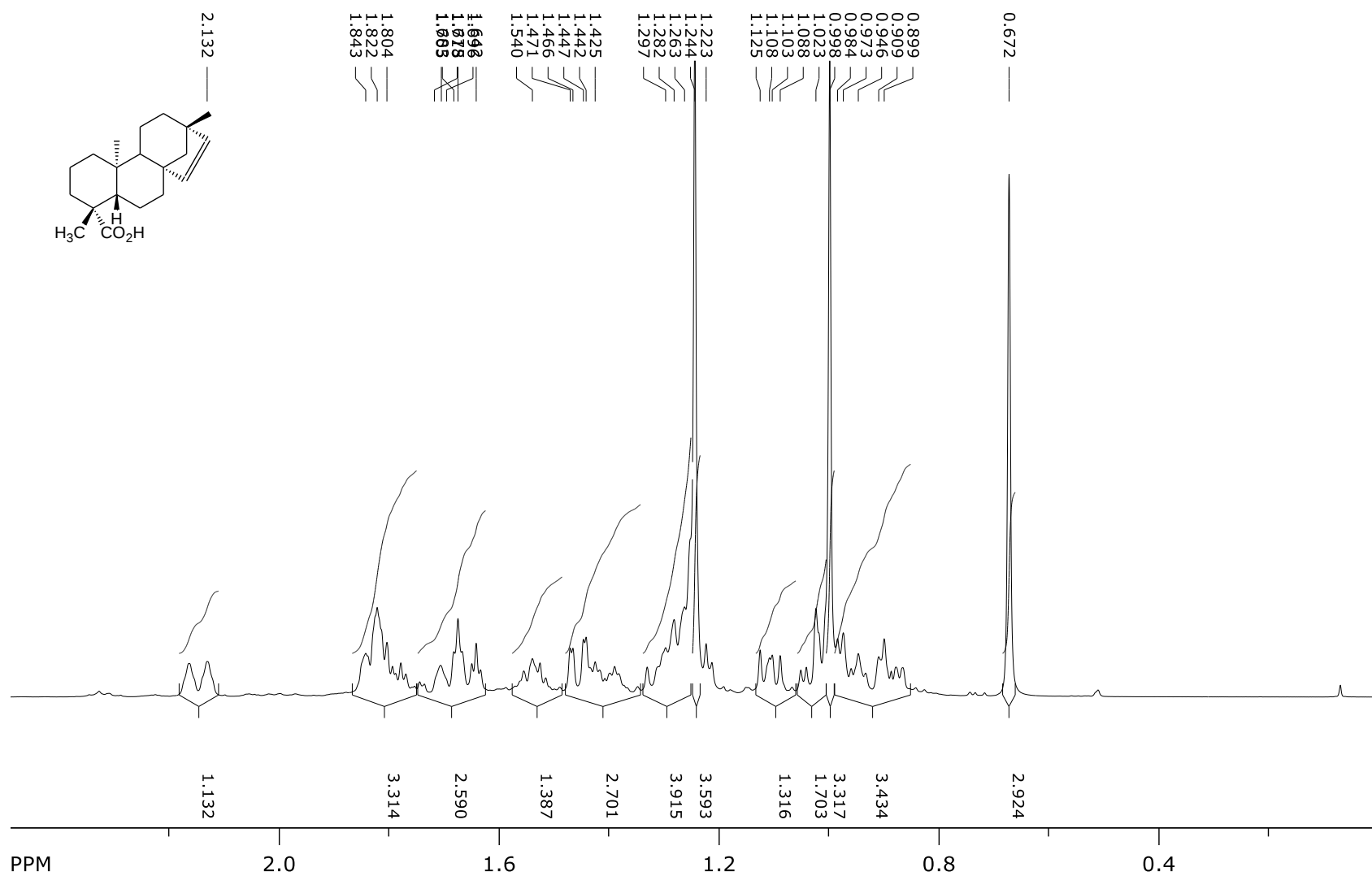
1D Selective Gradient NOESY
freq: 3.433 ppm



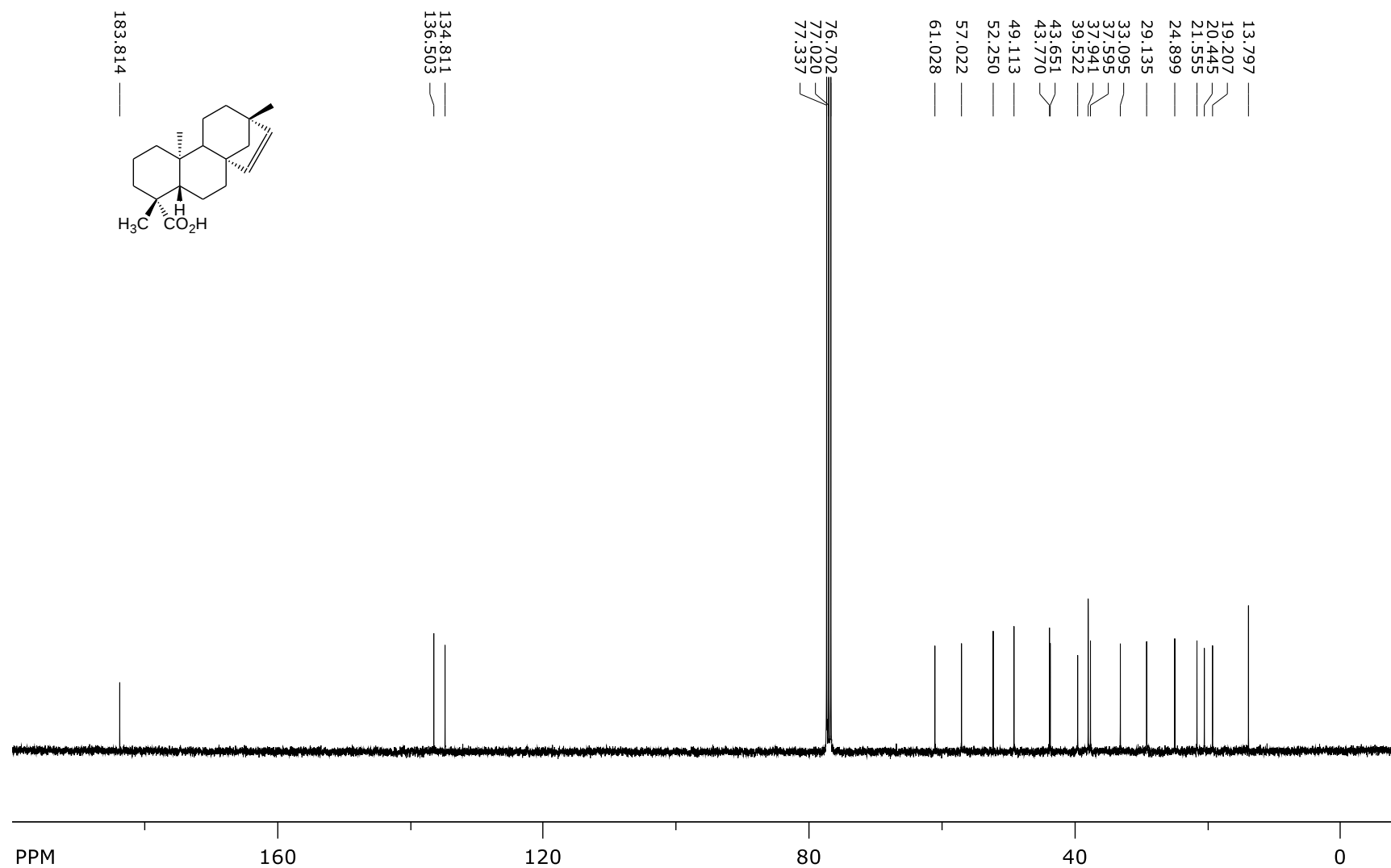
S16. ^1H NMR Spectrum (400 MHz) of **5** in CDCl_3



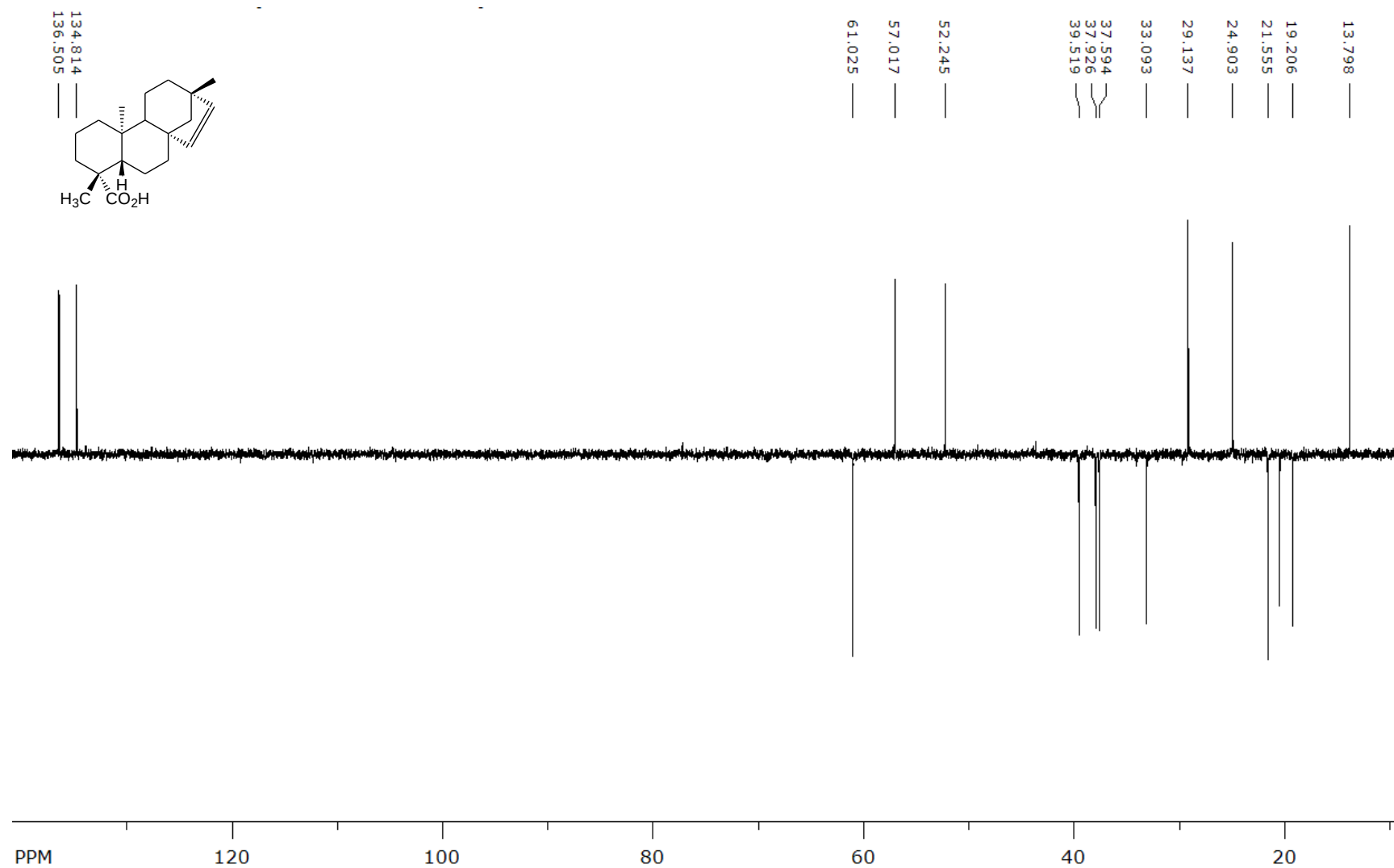
S17. ^1H NMR Spectrum (400 MHz) of 5 in CDCl_3 (Expansion δ 0.00 – 2.50)



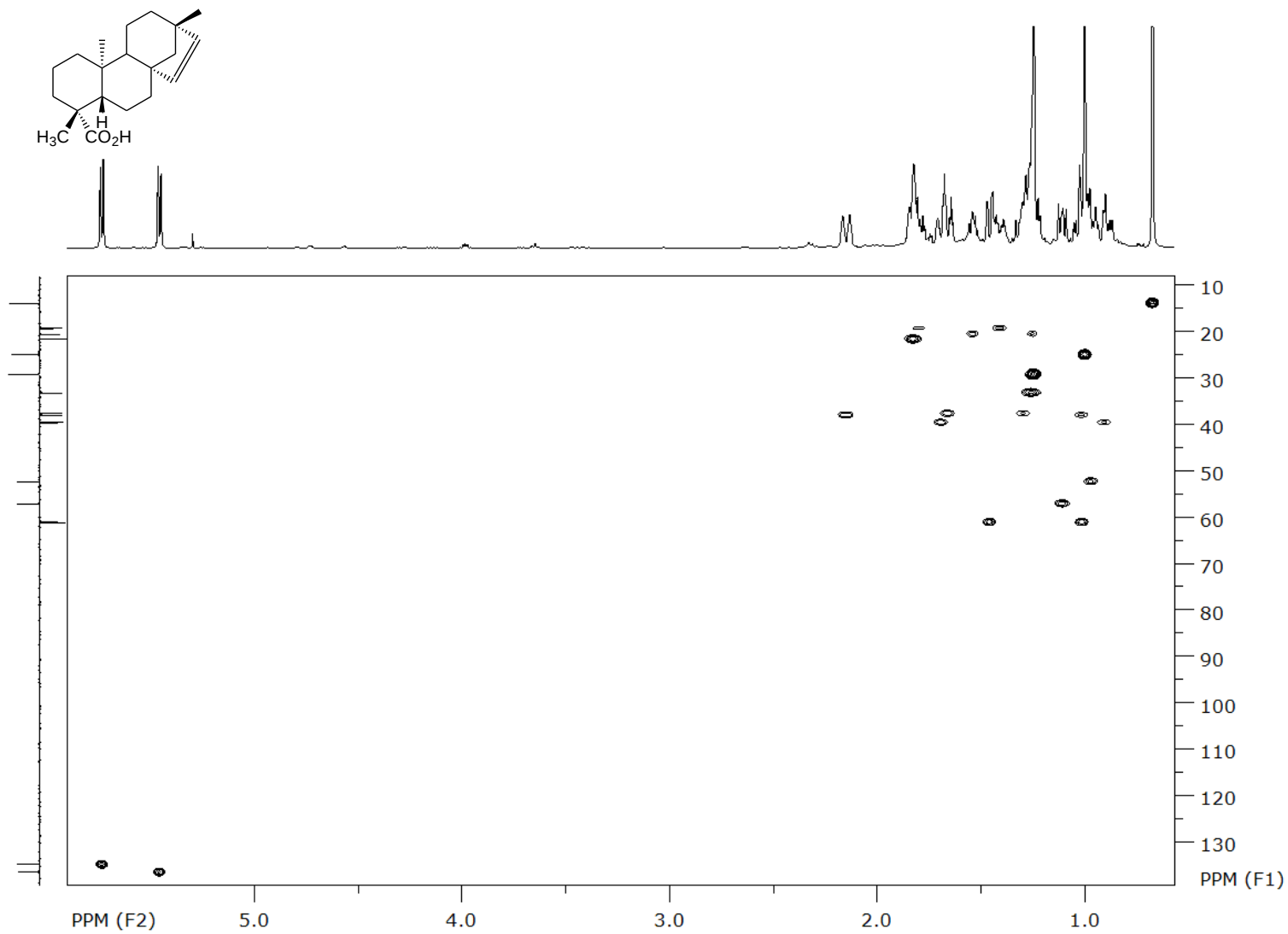
S18. ^{13}C NMR Spectrum (100 MHz) of **5** in CDCl_3



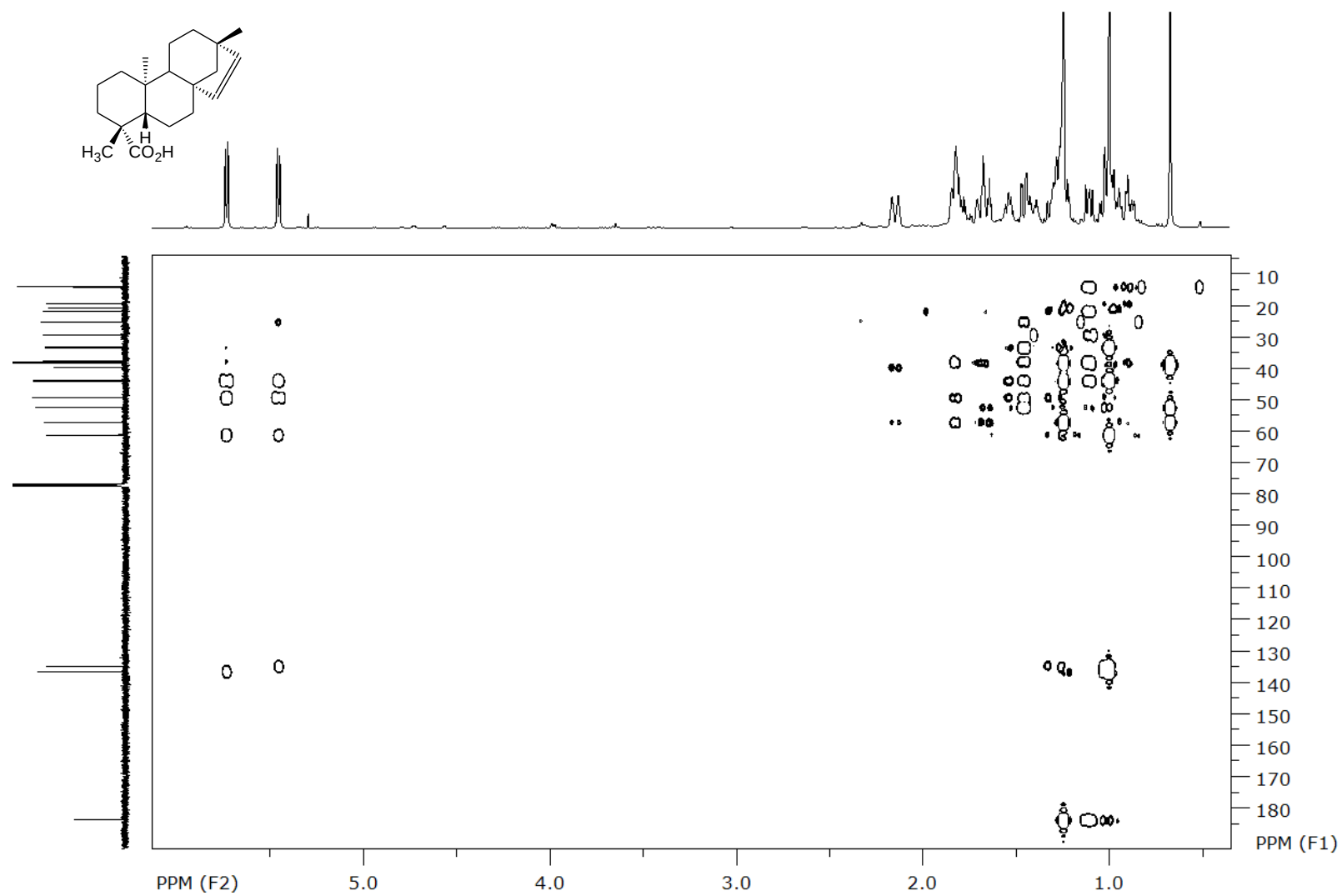
S19. DEPT 135 Spectrum (100 MHz) of **5** in CDCl₃



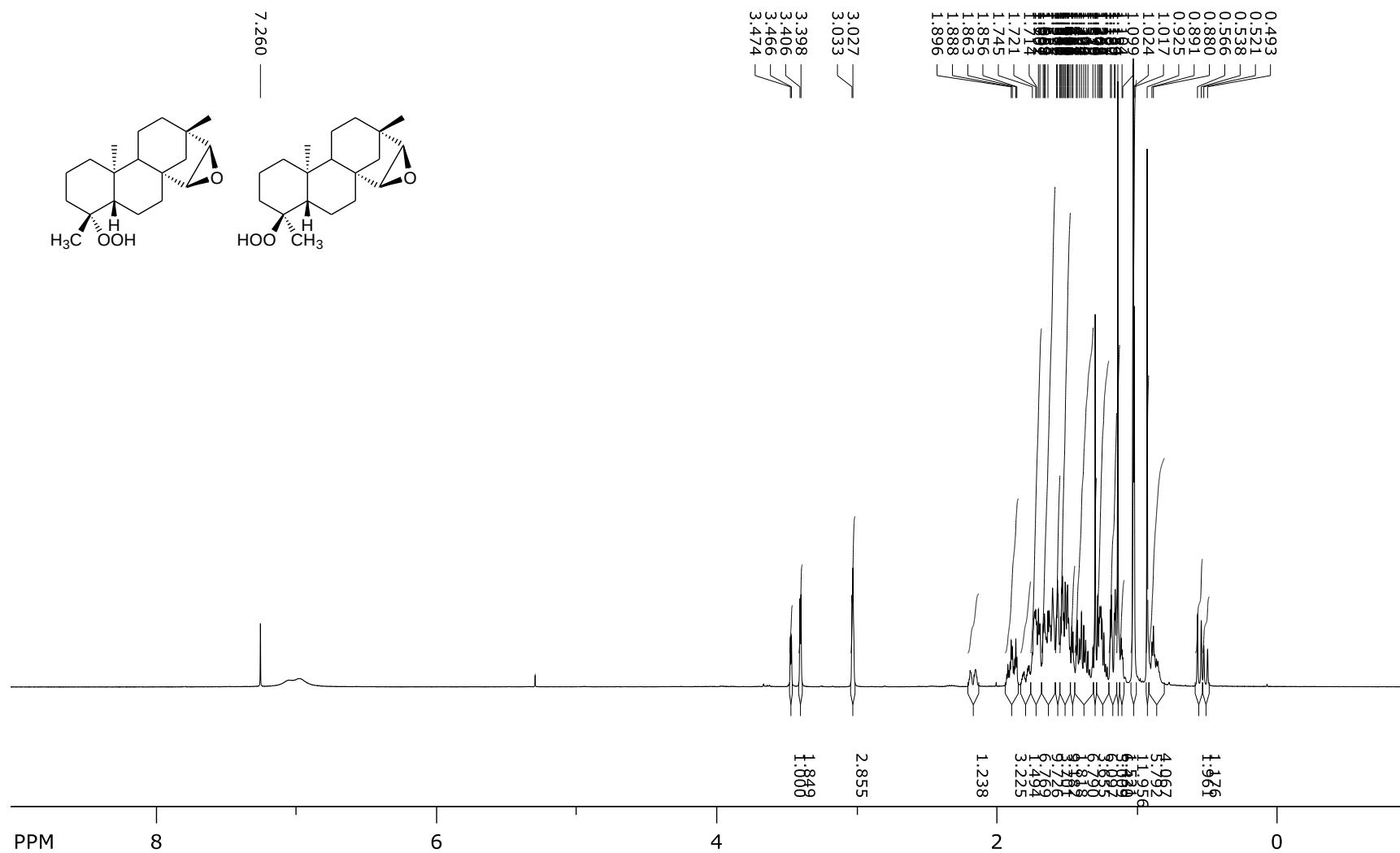
S20. HSQC Spectrum of **5** in CDCl₃



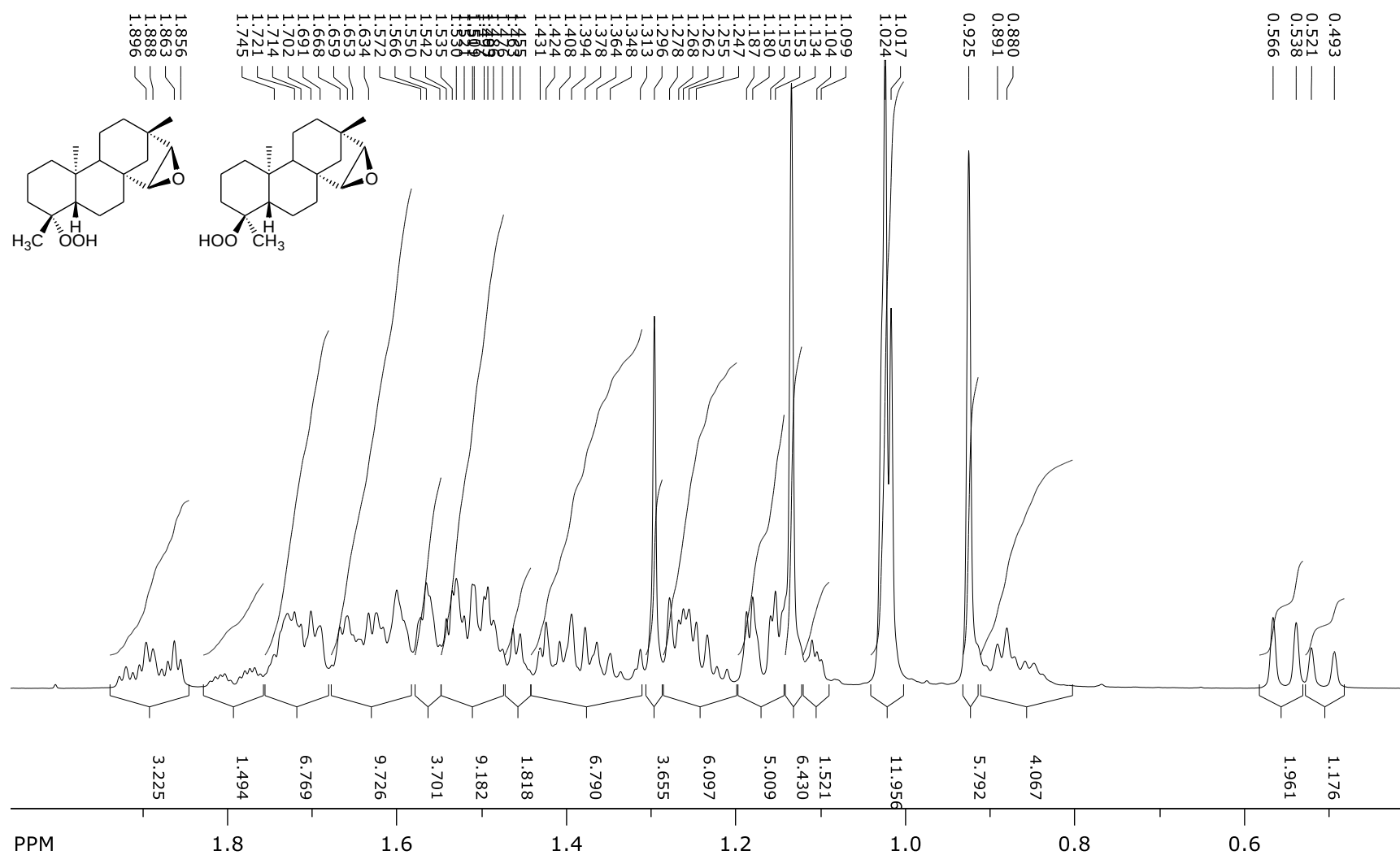
S21. HMBC Spectrum of 5 in CDCl₃



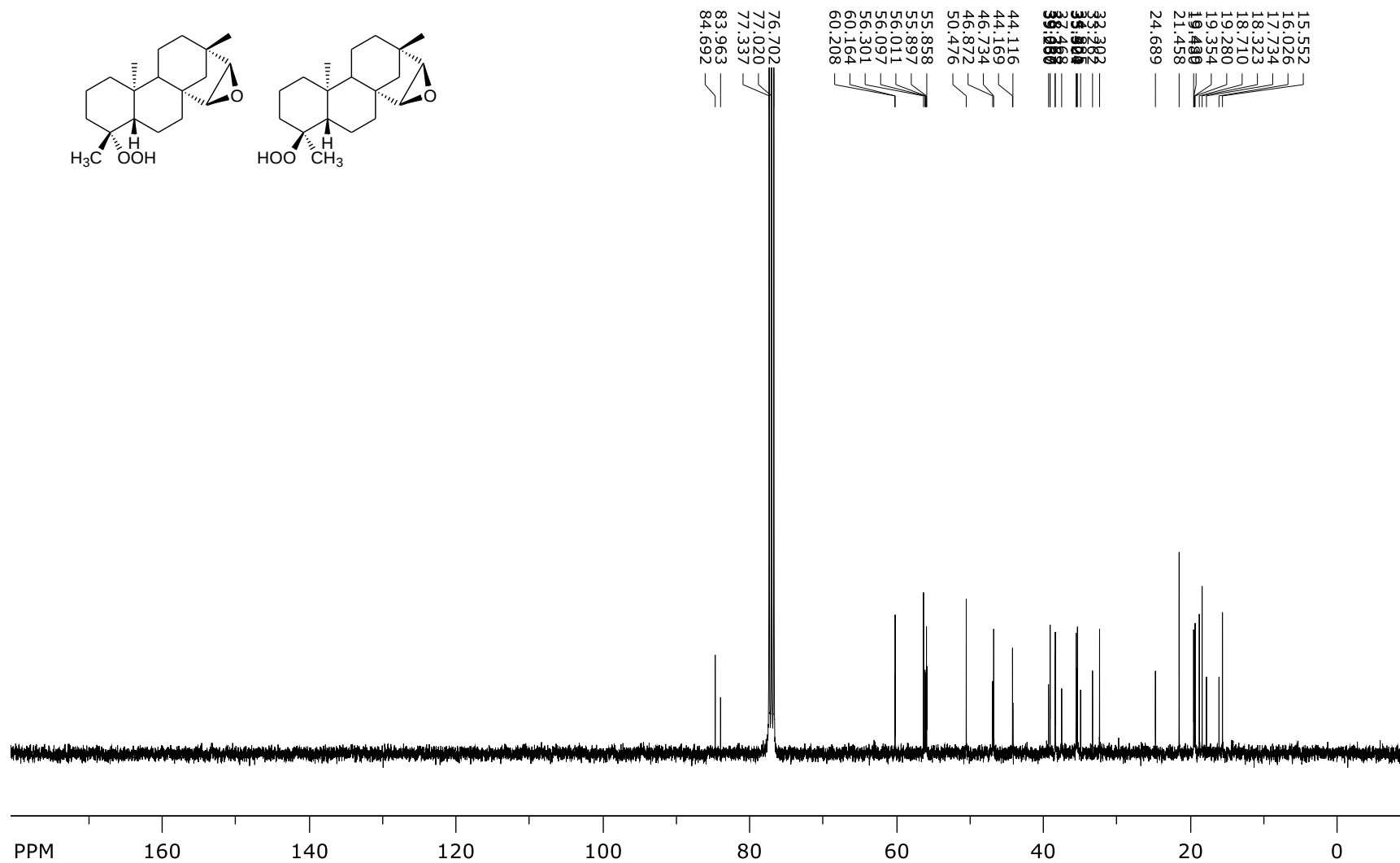
S22. ^1H NMR Spectrum (400 MHz) of **6a** and **6b** in CDCl_3



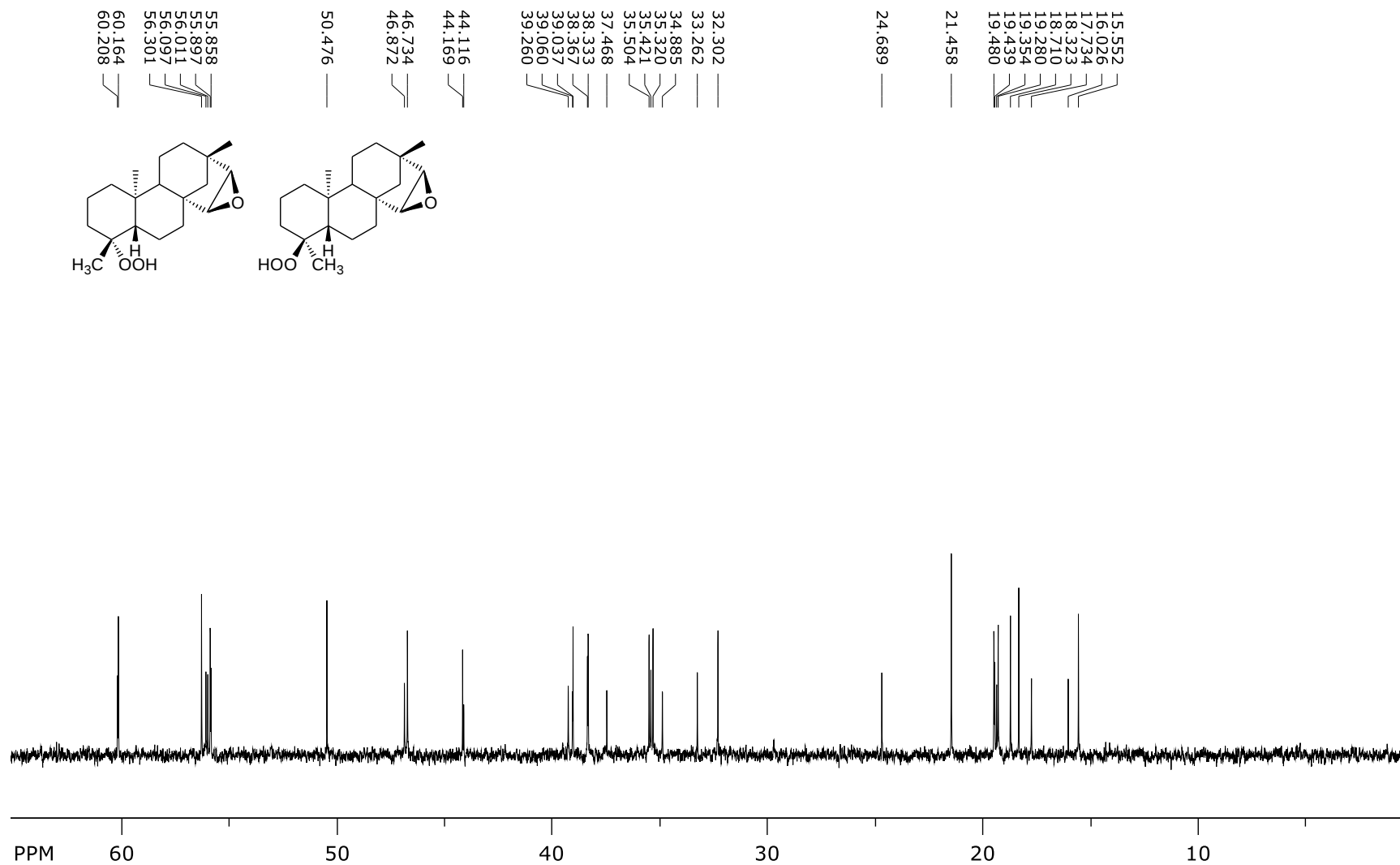
S23. ^1H NMR Spectrum (400 MHz) of **6a** and **6b** in CDCl_3 (Expansion δ 0.40 – 2.00)



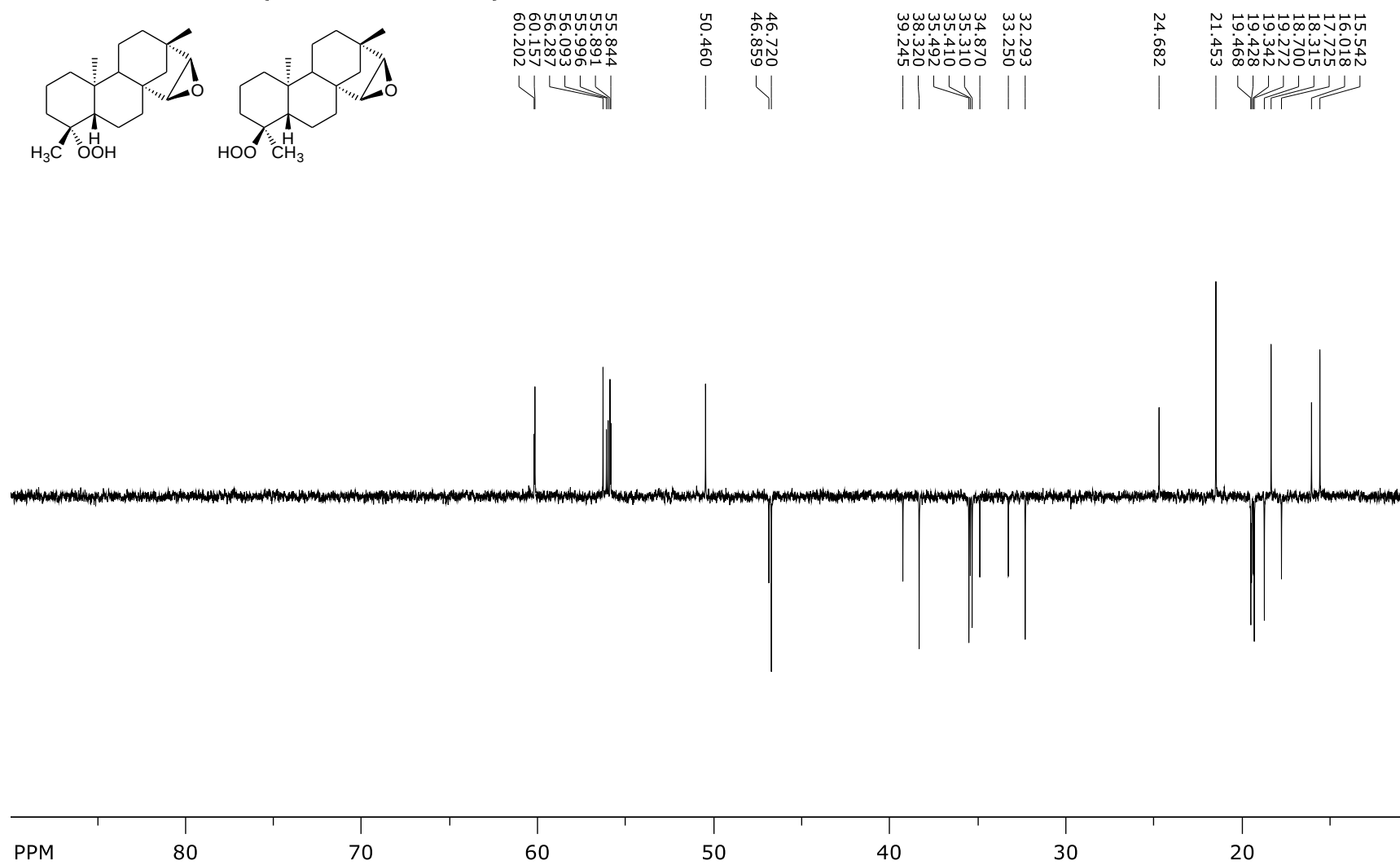
S24. ^{13}C NMR Spectrum (100 MHz) of **6a** and **6b** in CDCl_3



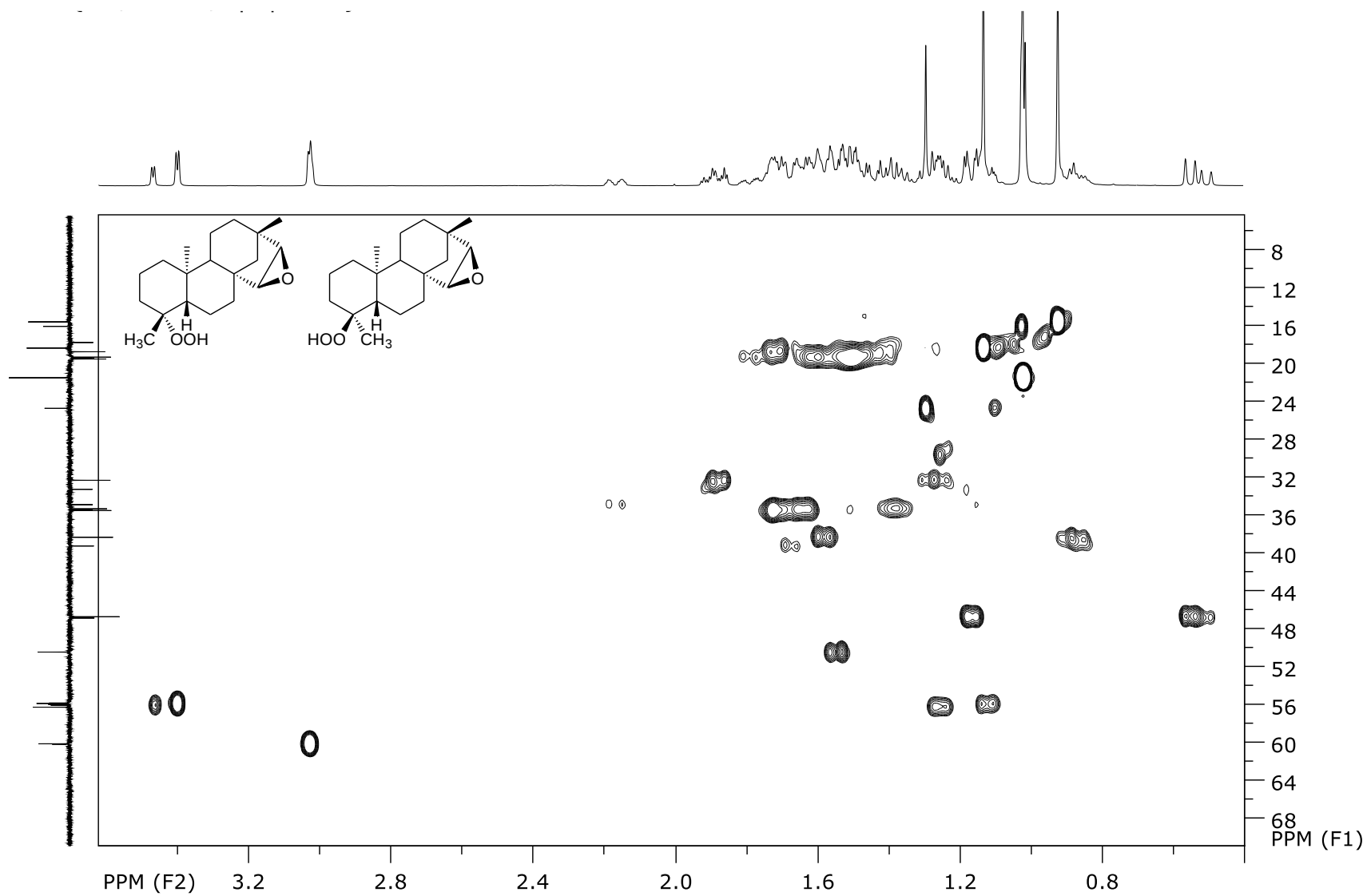
S25. ^{13}C NMR Spectrum (100 MHz) of **6a** and **6b** in CDCl_3 (Expansion δ 0.00 – 65.00)



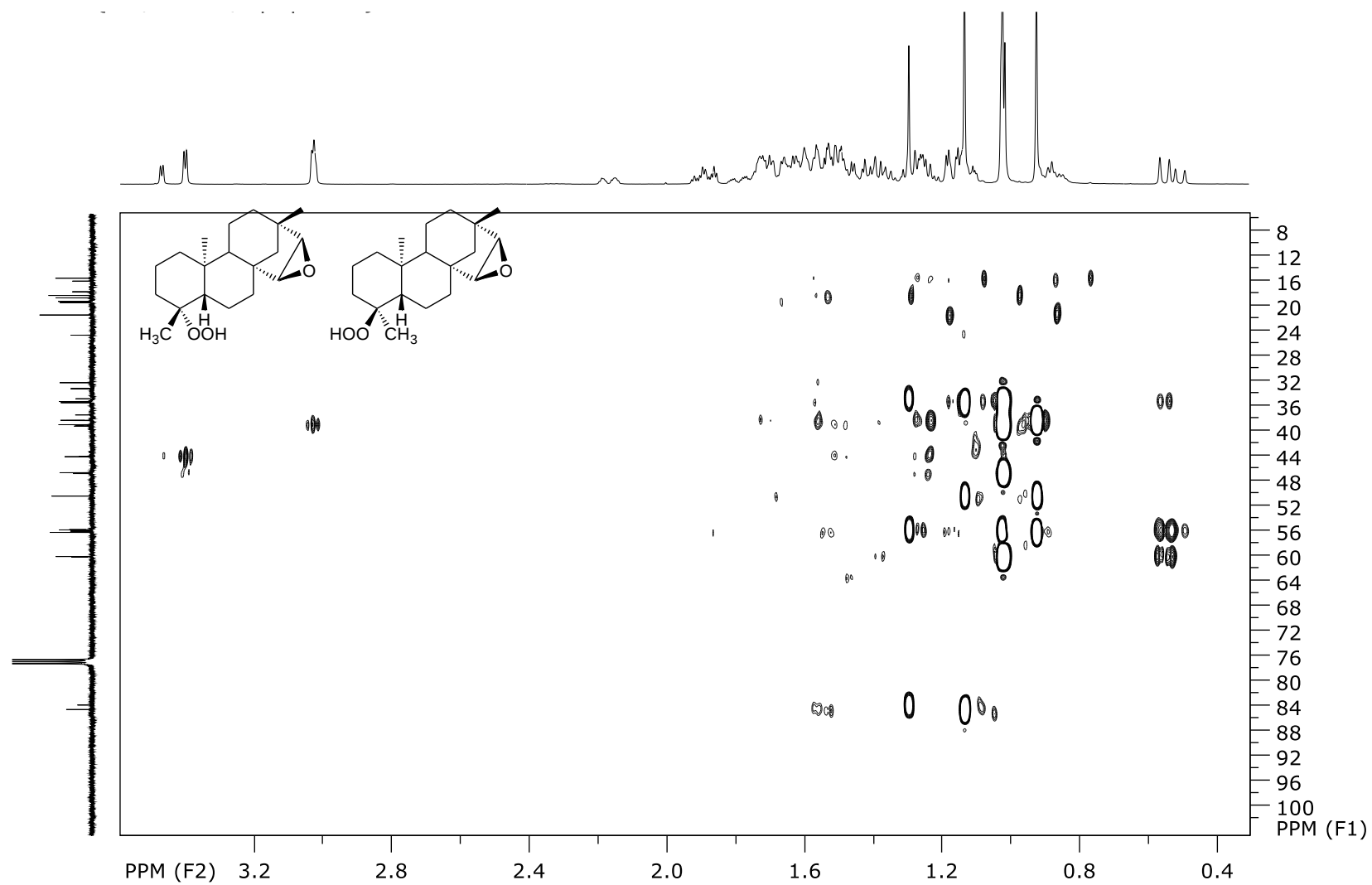
S26. DEPT 135 Spectrum (100 MHz) of **6a** and **6b** in CDCl₃



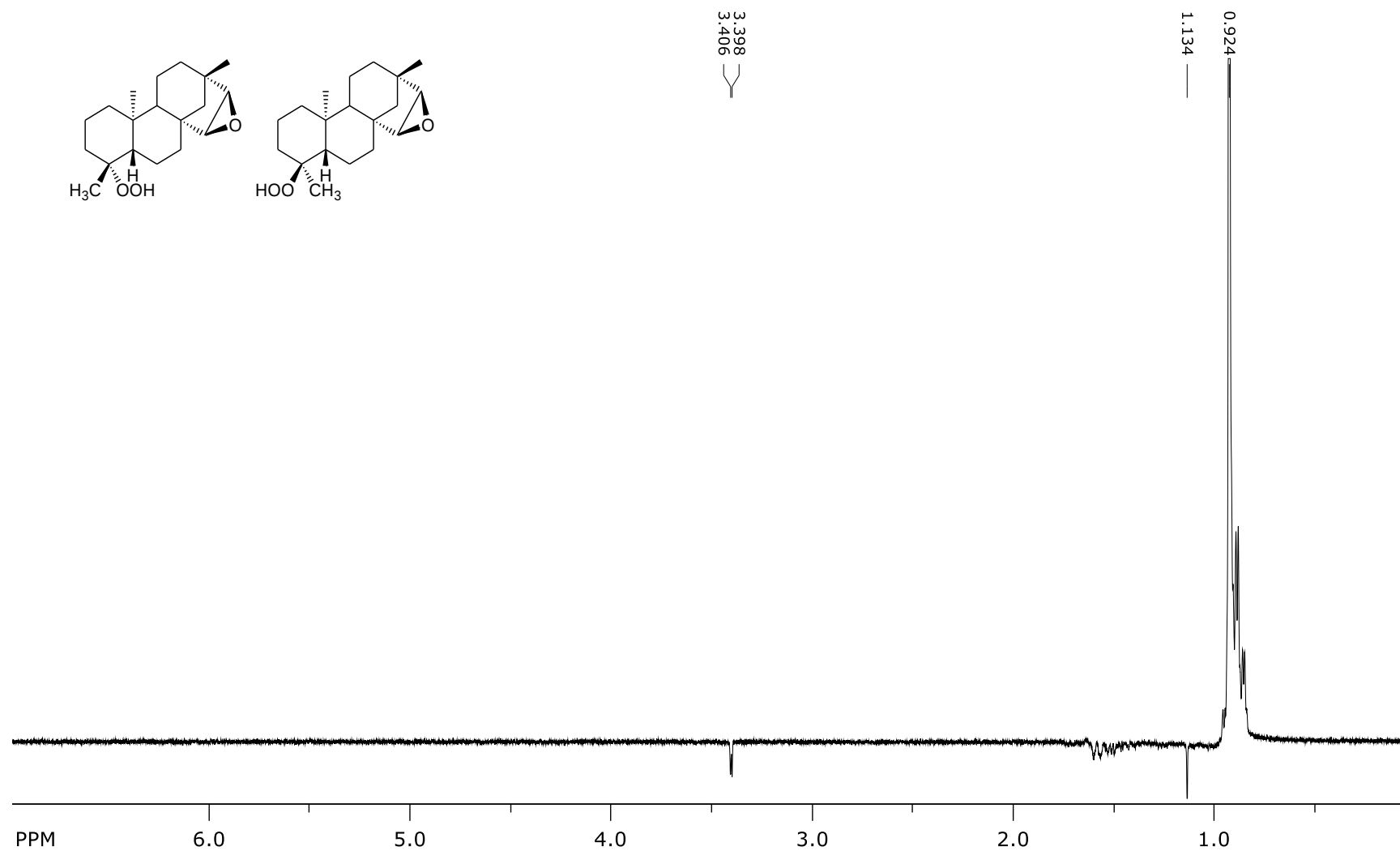
S27. HSQC Spectrum of **6a** and **6b** in CDCl₃



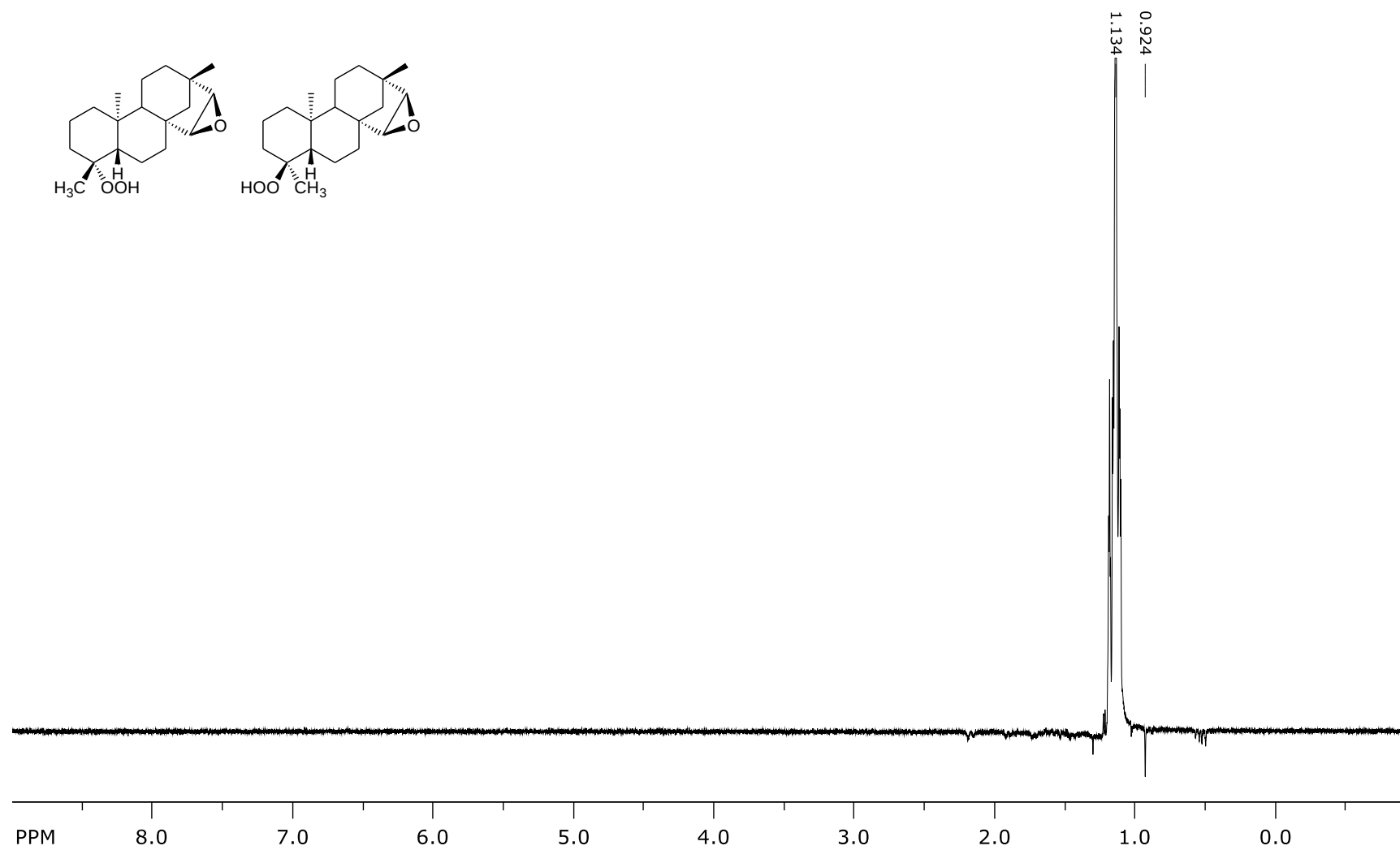
S28. HMBC Spectrum of **6a** and **6b** in CDCl₃



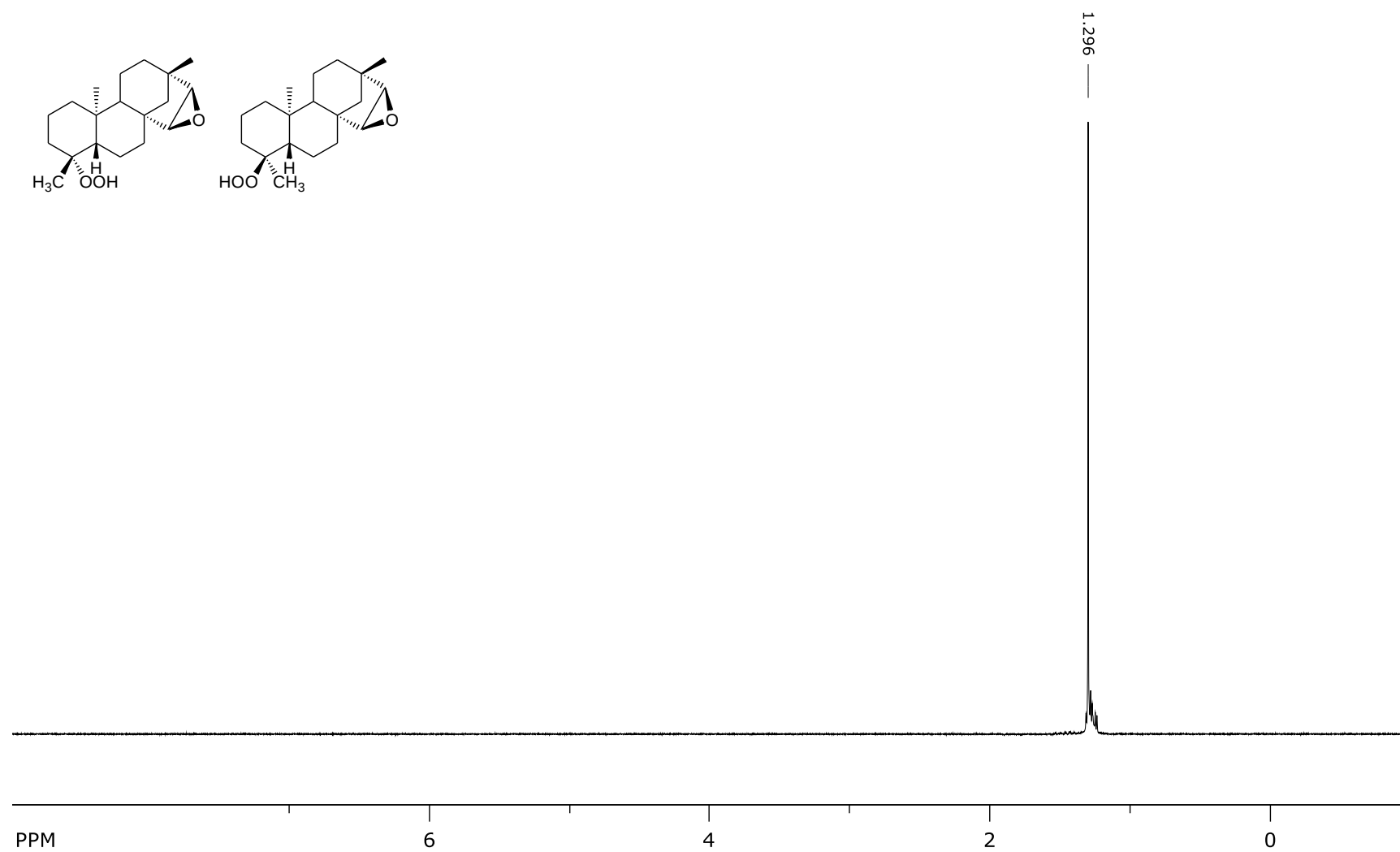
S29. 1D Selective Gradient NOESY spectrum (400 MHz) of **6a** and **6b** in CDCl₃; Irradiation at δ 0.924



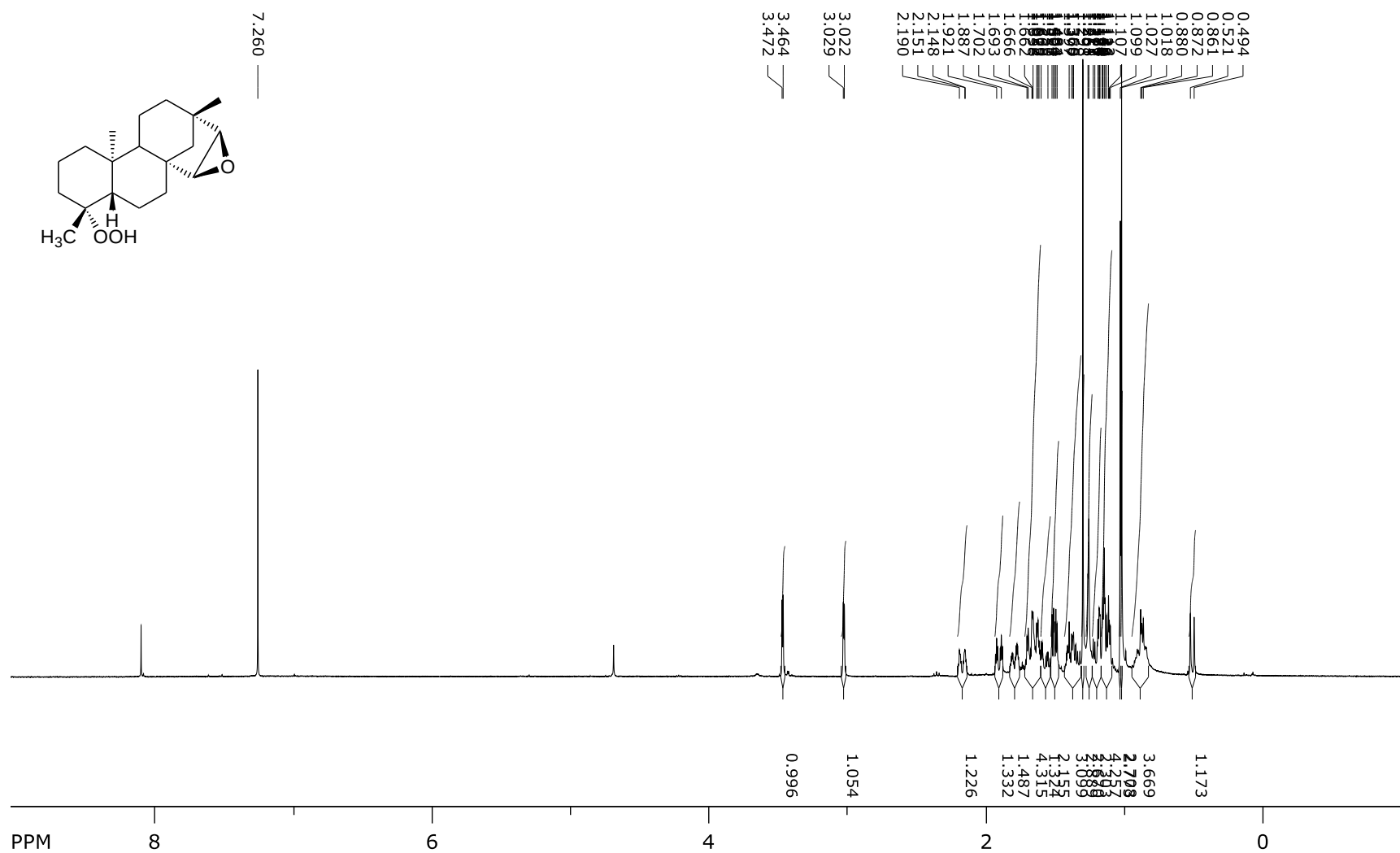
S30. 1D Selective Gradient NOESY spectrum (400 MHz) of **6a** and **6b** in CDCl₃; Irradiation at δ 1.134



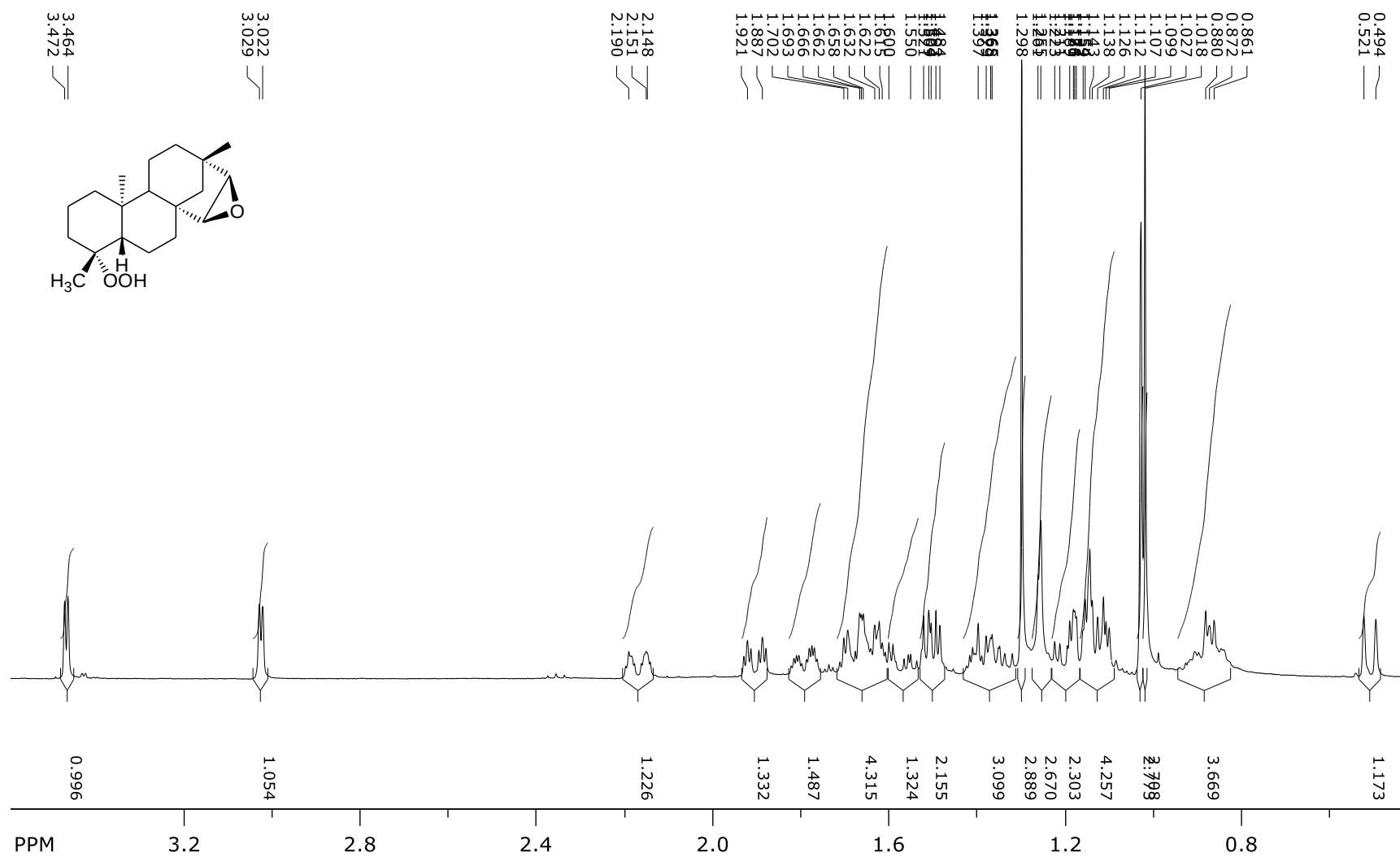
S31. 1D Selective Gradient NOESY spectrum (400 MHz) of **6a** and **6b** in CDCl₃; Irradiation at δ 1.296



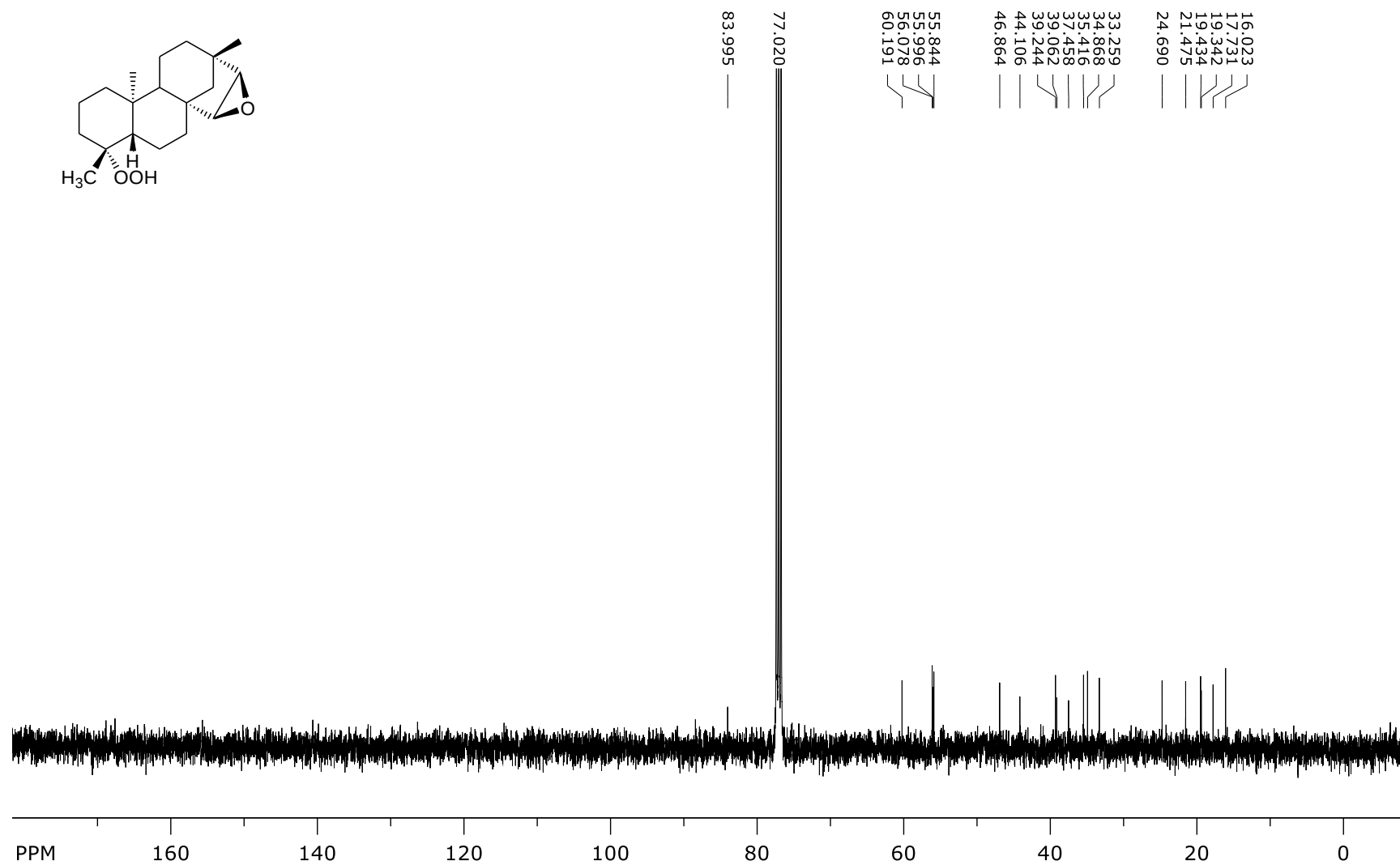
S32. ^1H NMR Spectrum (400 MHz) of **6a** in CDCl_3



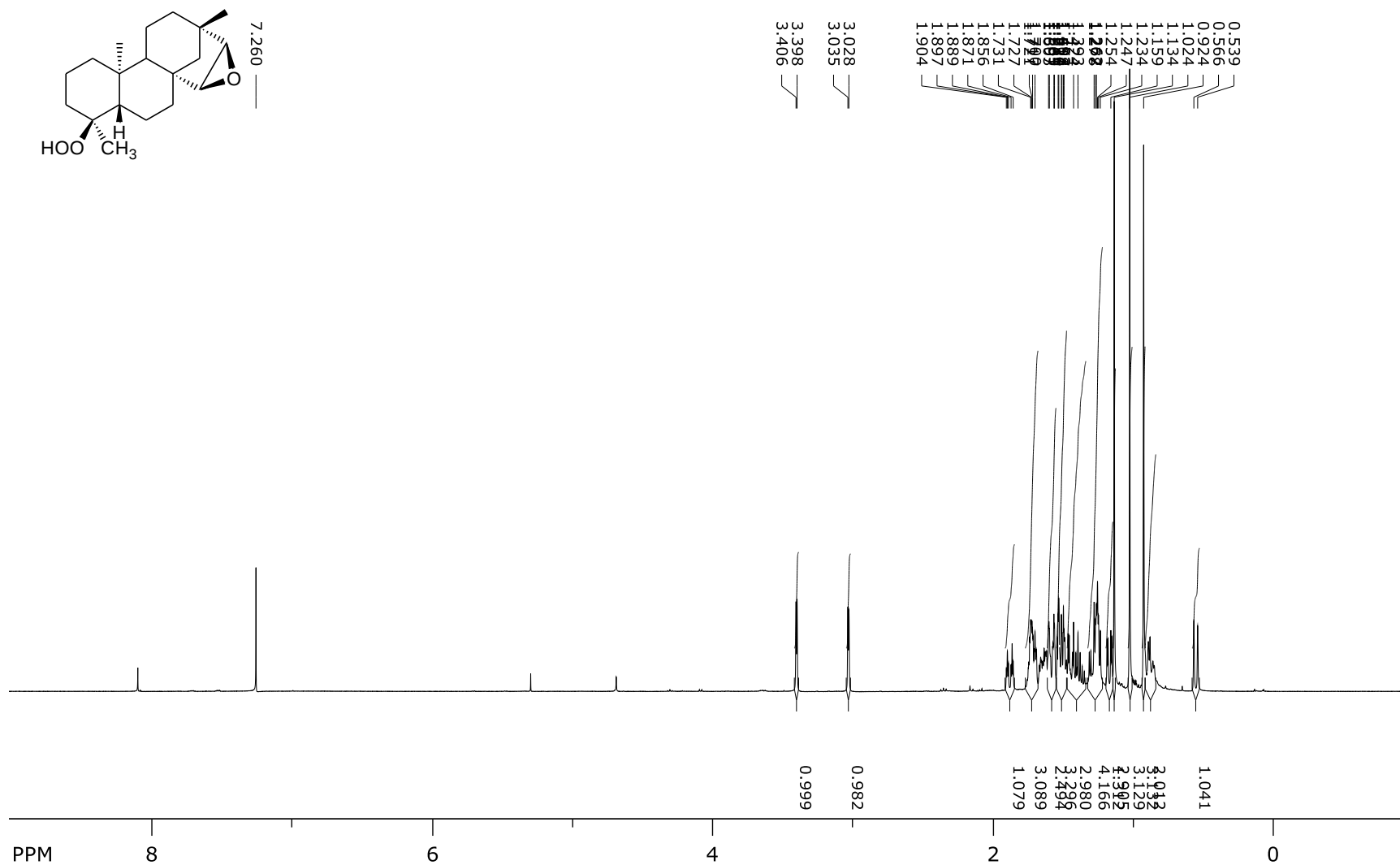
S33. ^1H NMR Spectrum (400 MHz) of **6a** in CDCl_3 (Expansion δ 0.40 – 3.50)



S34. ^{13}C NMR Spectrum (100 MHz) of **6a** in CDCl_3



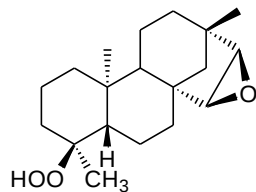
S35. ^1H NMR Spectrum (400 MHz) of **6b** in CDCl_3



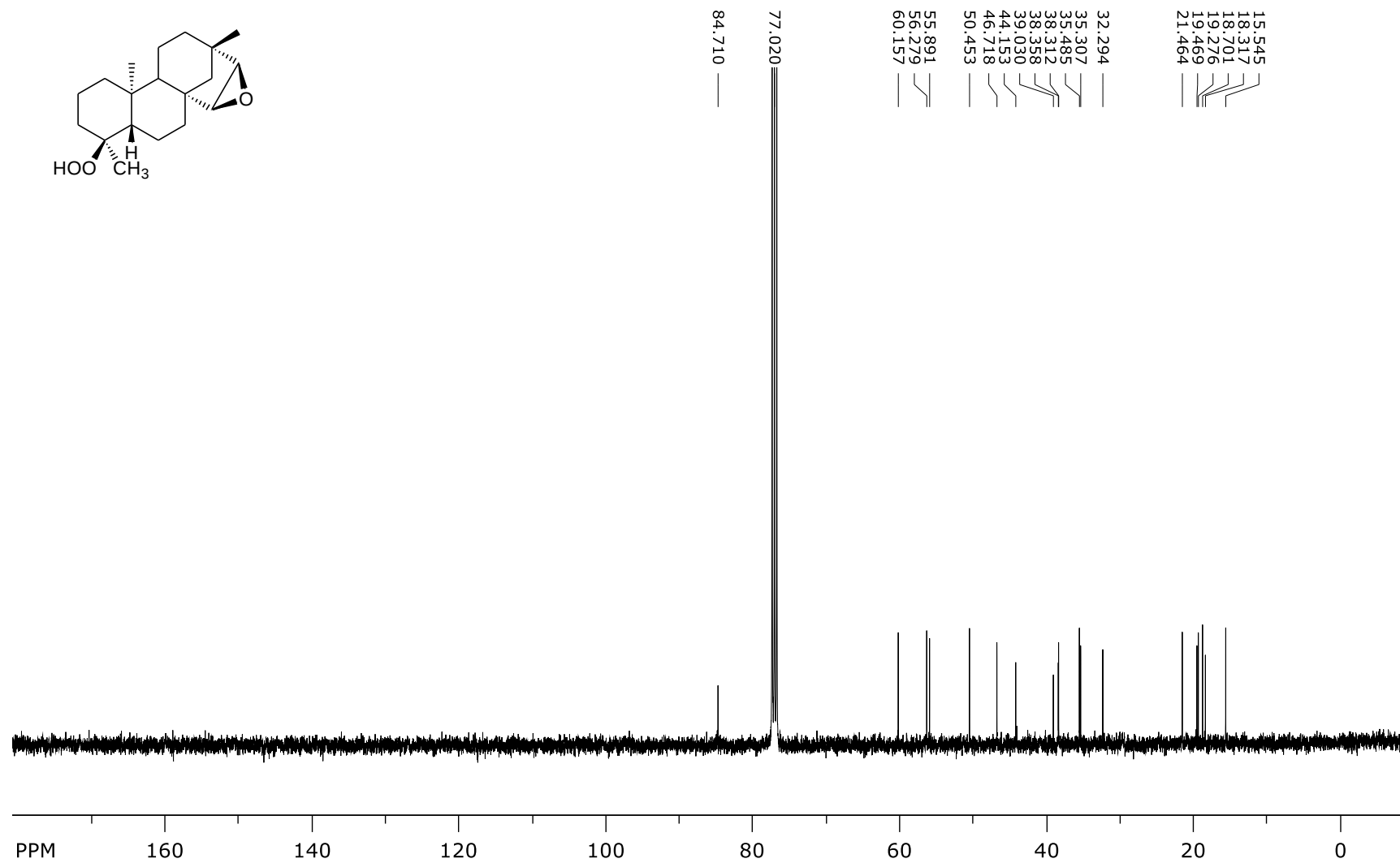
Chemical structure of 10-acetoxycyclohexylidene-1,2,3,4-tetrahydronaphthalene-1-carboxylic acid is shown in the top right corner.

¹H NMR spectrum (400 MHz, CDCl₃) showing peaks and integration values:

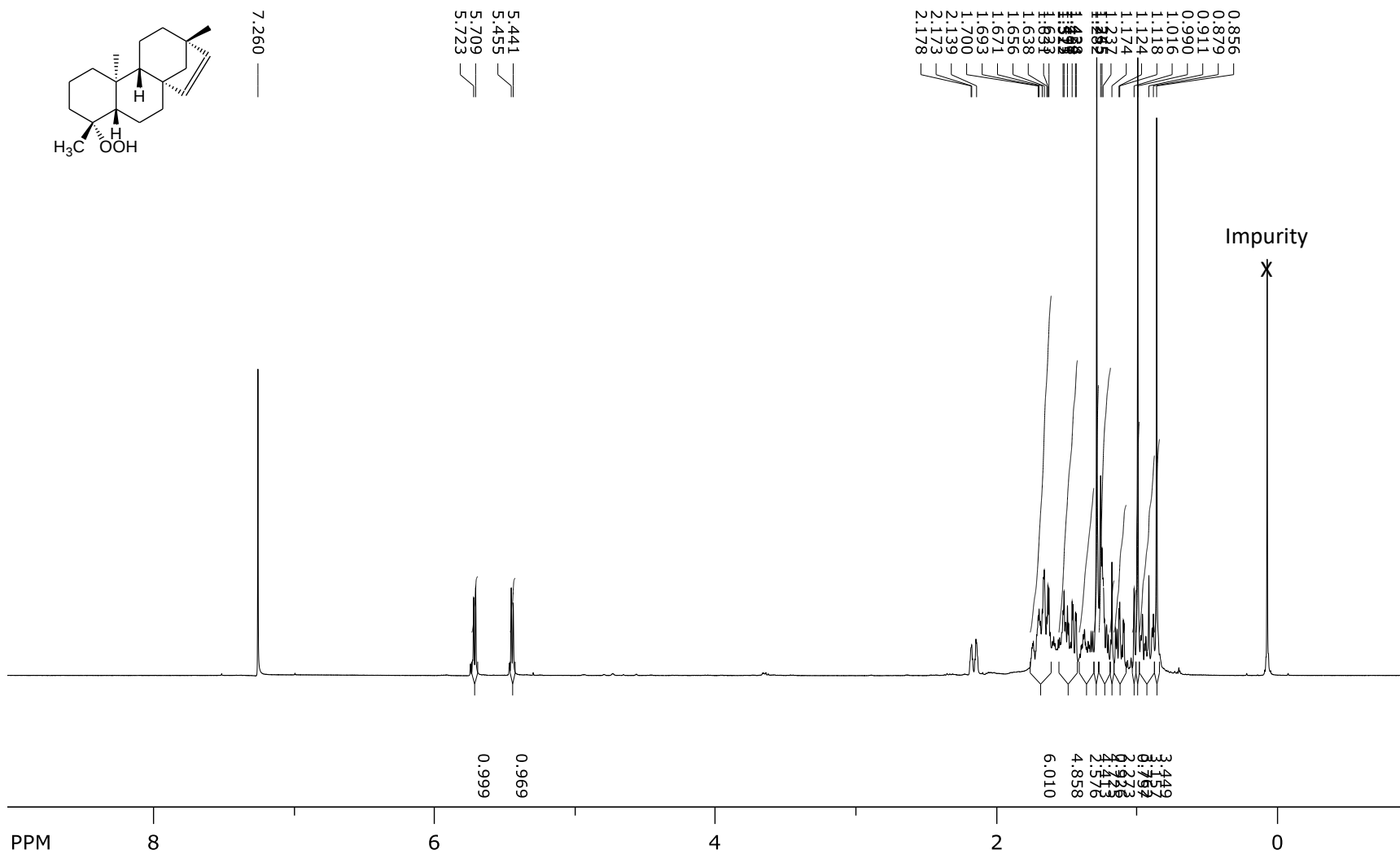
Chemical Shift (ppm)	Integration
0.539, 0.566	1.041
0.924	2.012
1.024, 1.134, 1.134, 1.159, 1.234, 1.247, 1.254, 1.262, 1.267, 1.278	3.129
1.393, 1.424, 1.453, 1.497, 1.508, 1.519, 1.561, 1.565, 1.597, 1.603, 1.700, 1.717, 1.721, 1.721, 1.731, 1.856, 1.871, 1.889, 1.897, 1.904	2.905
1.278	4.166
1.393, 1.424, 1.453, 1.497, 1.508, 1.519, 1.561, 1.565, 1.597, 1.603, 1.700, 1.717, 1.721, 1.721, 1.731, 1.856, 1.871, 1.889, 1.897, 1.904	2.980
1.393, 1.424, 1.453, 1.497, 1.508, 1.519, 1.561, 1.565, 1.597, 1.603, 1.700, 1.717, 1.721, 1.721, 1.731, 1.856, 1.871, 1.889, 1.897, 1.904	3.296
1.393, 1.424, 1.453, 1.497, 1.508, 1.519, 1.561, 1.565, 1.597, 1.603, 1.700, 1.717, 1.721, 1.721, 1.731, 1.856, 1.871, 1.889, 1.897, 1.904	2.494
1.393, 1.424, 1.453, 1.497, 1.508, 1.519, 1.561, 1.565, 1.597, 1.603, 1.700, 1.717, 1.721, 1.721, 1.731, 1.856, 1.871, 1.889, 1.897, 1.904	3.089
1.393, 1.424, 1.453, 1.497, 1.508, 1.519, 1.561, 1.565, 1.597, 1.603, 1.700, 1.717, 1.721, 1.721, 1.731, 1.856, 1.871, 1.889, 1.897, 1.904	1.079
3.028, 3.035	0.982
3.398, 3.406	0.999



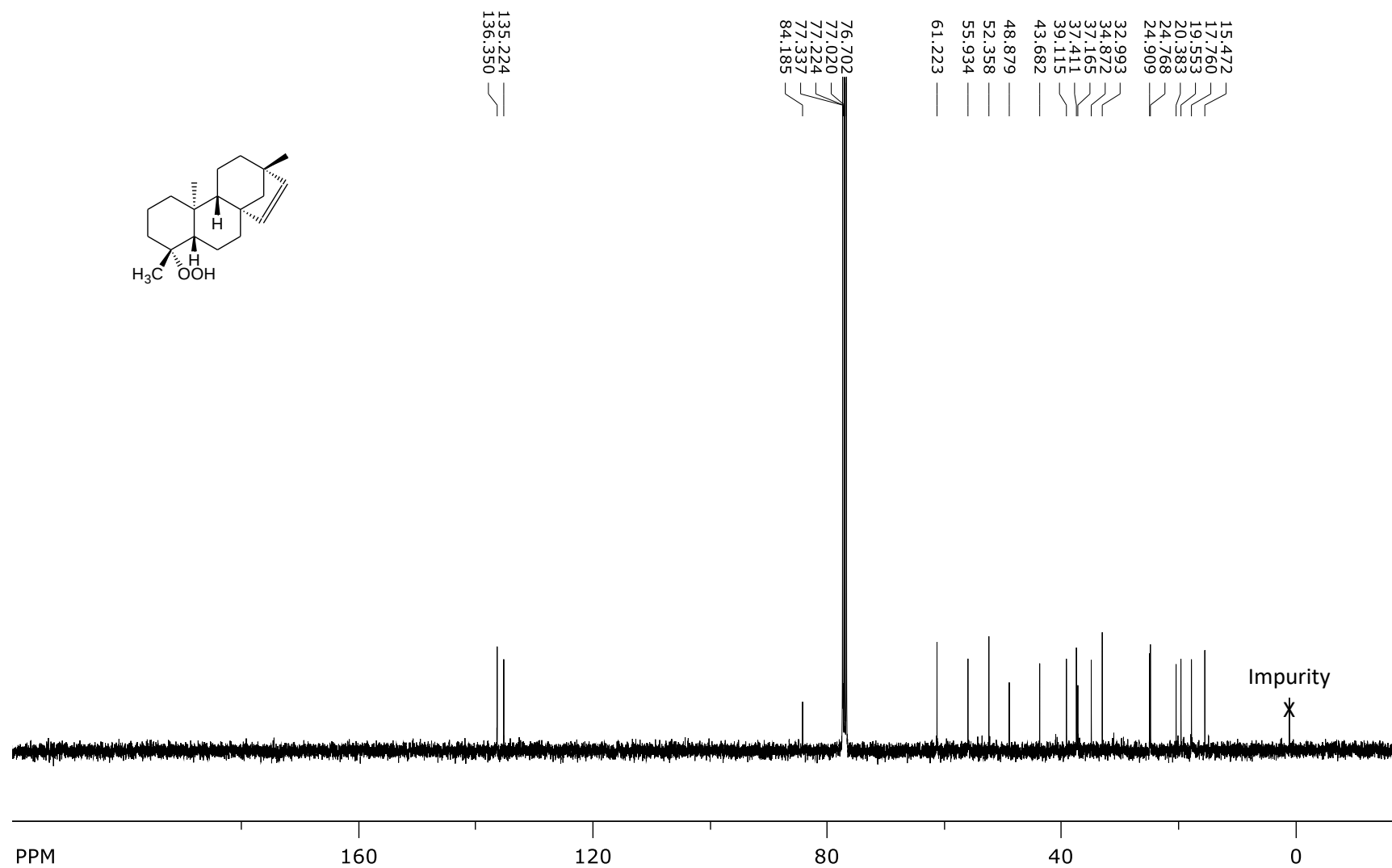
S37. ^{13}C NMR Spectrum (100 MHz) of **6b** in CDCl_3



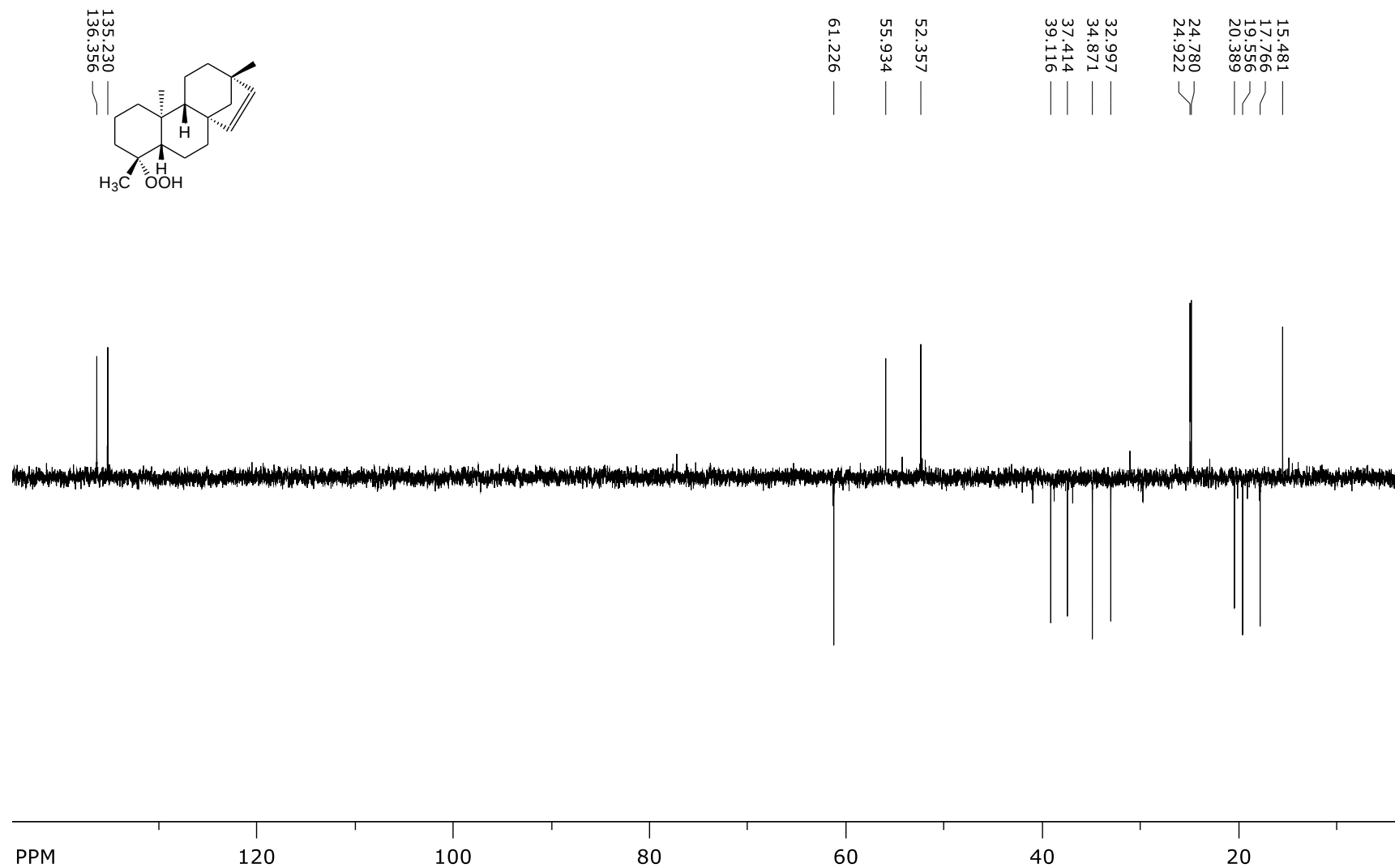
S38. ^1H NMR Spectrum (400 MHz) of **7** in CDCl_3



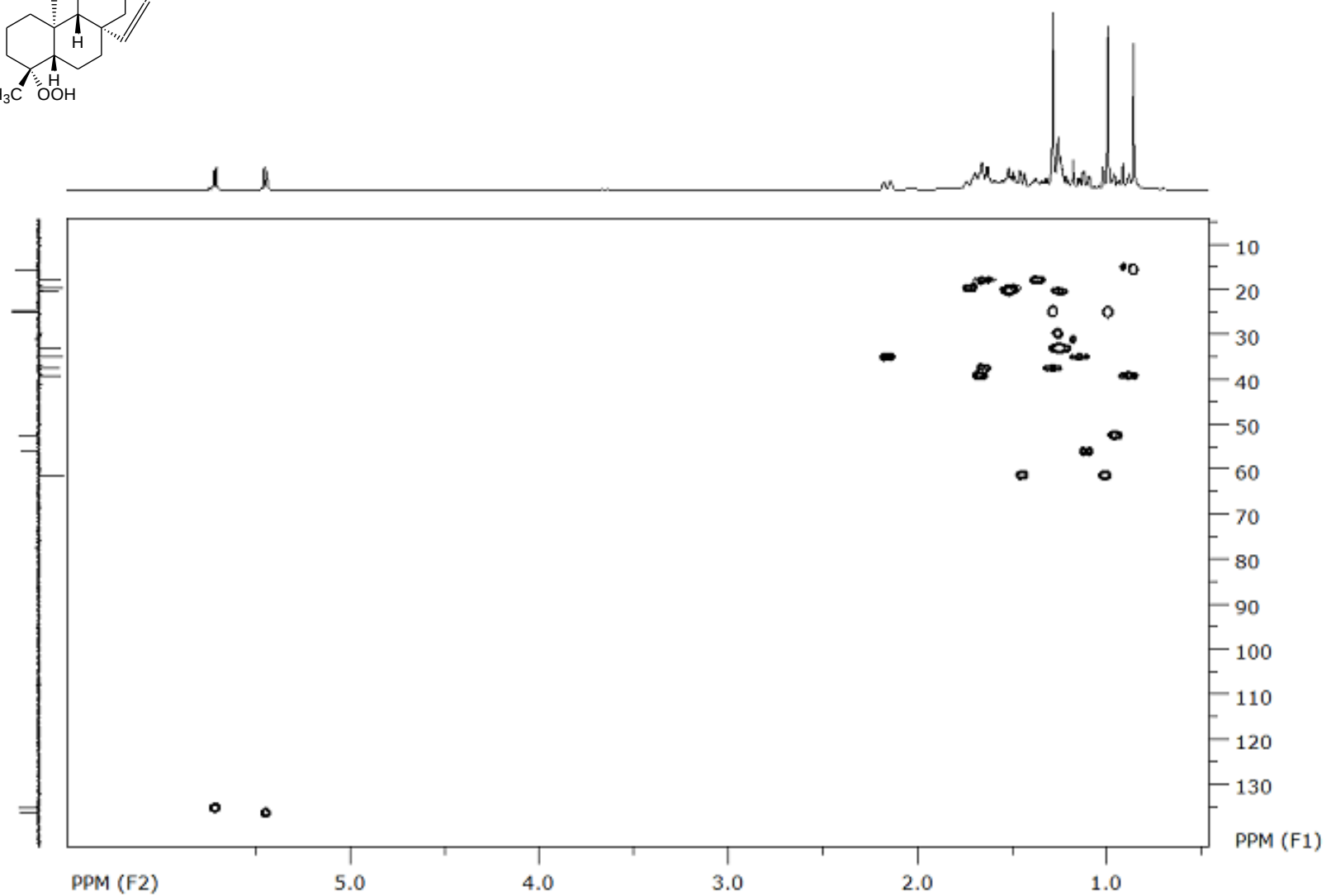
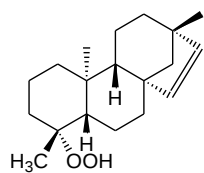
S39. ^{13}C NMR Spectrum (100 MHz) of **7** in CDCl_3



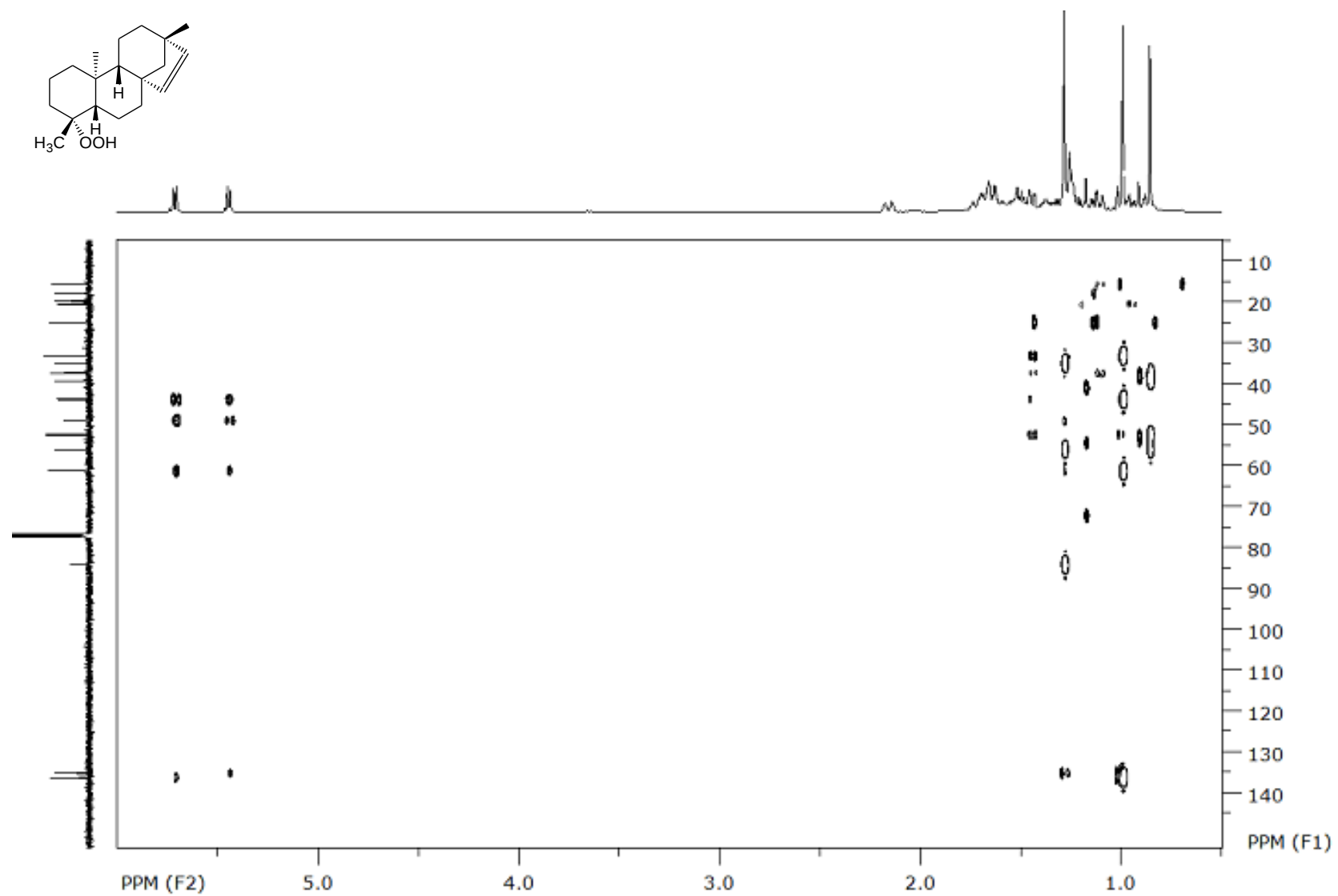
S40. DEPT 135 Spectrum (100 MHz) of **7** in CDCl₃



S41. HSQC Spectrum of **7** in CDCl₃

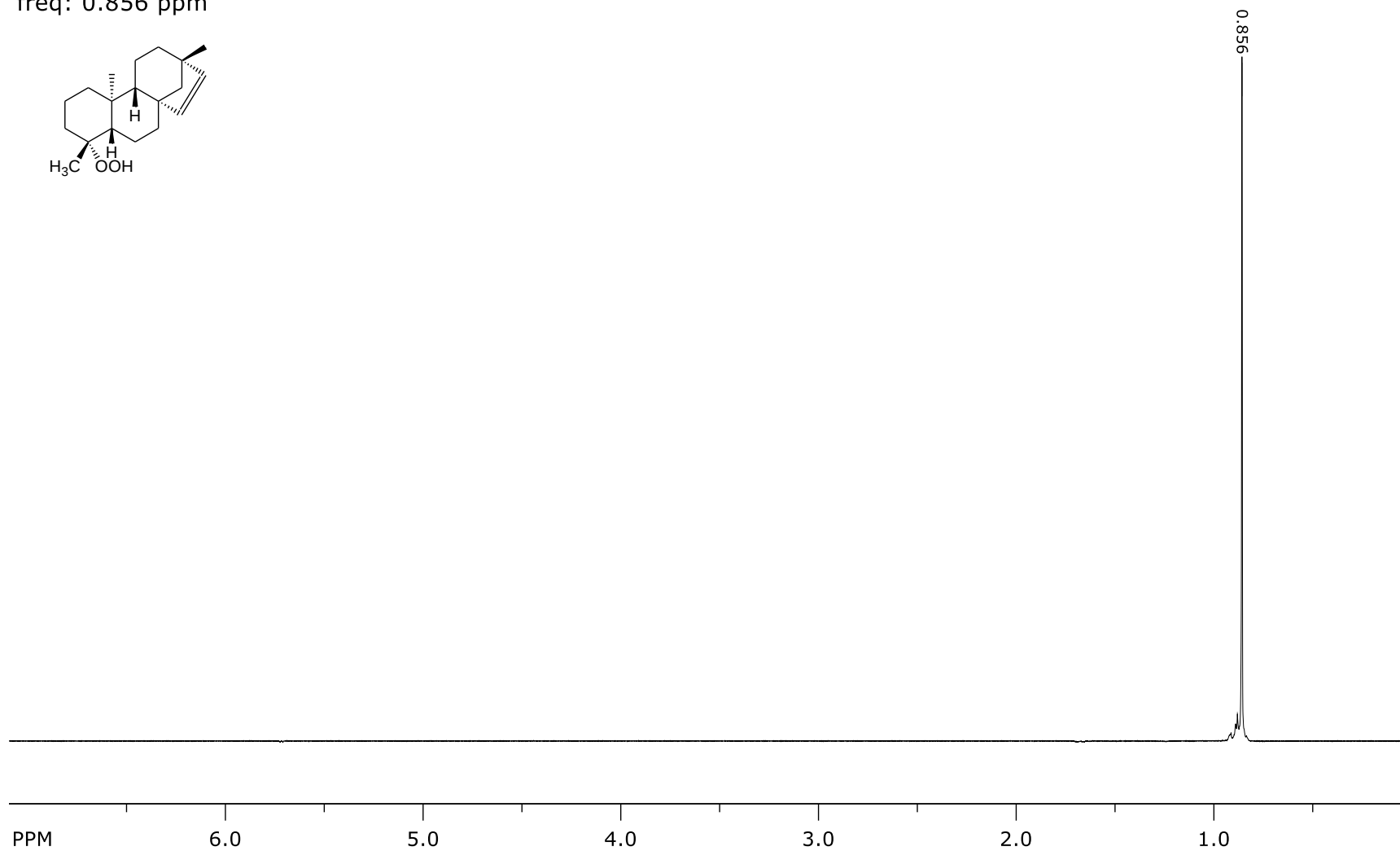
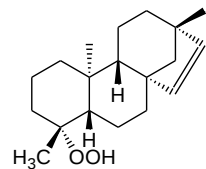


S42. HMBC Spectrum of 7 in CDCl₃



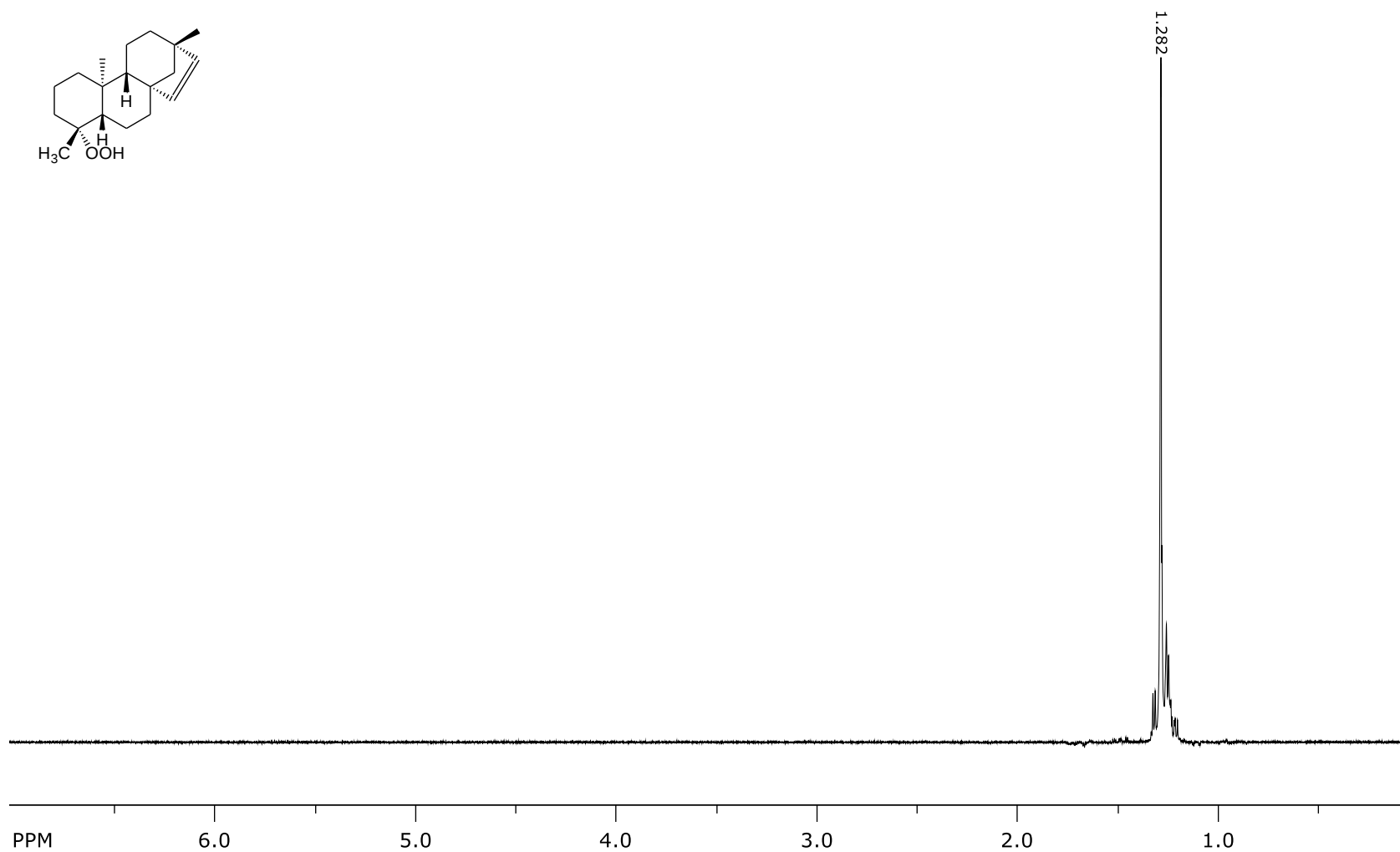
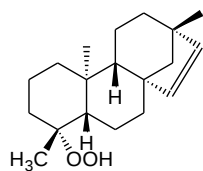
S43. 1D Selective Gradient NOESY spectrum (400 MHz) of **7** in CDCl₃; Irradiation at δ 0.856

1D Selective Gradient NOESY
freq: 0.856 ppm

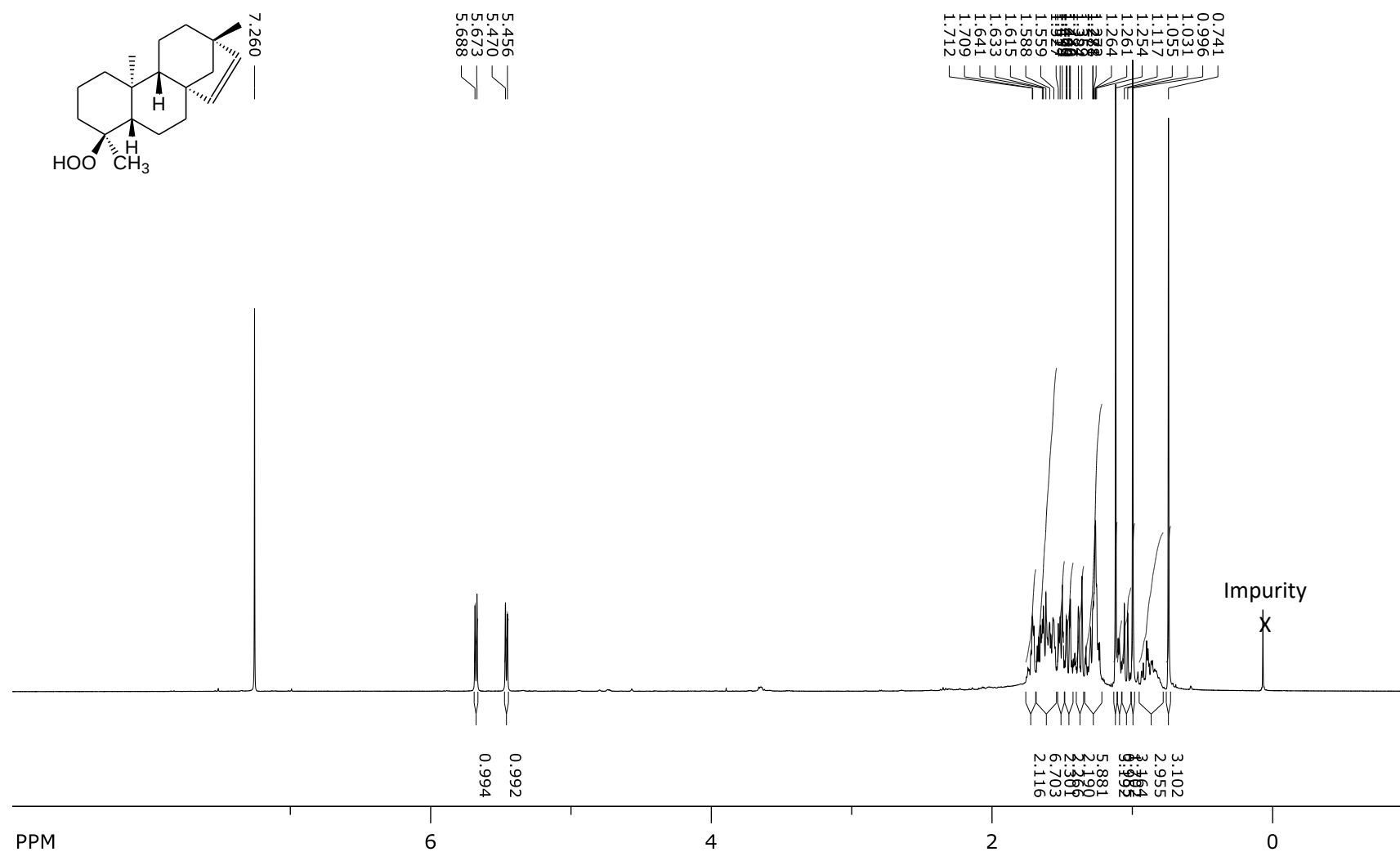


S44. 1D Selective Gradient NOESY spectrum (400 MHz) of **7** in CDCl₃; Irradiation at δ 1.282

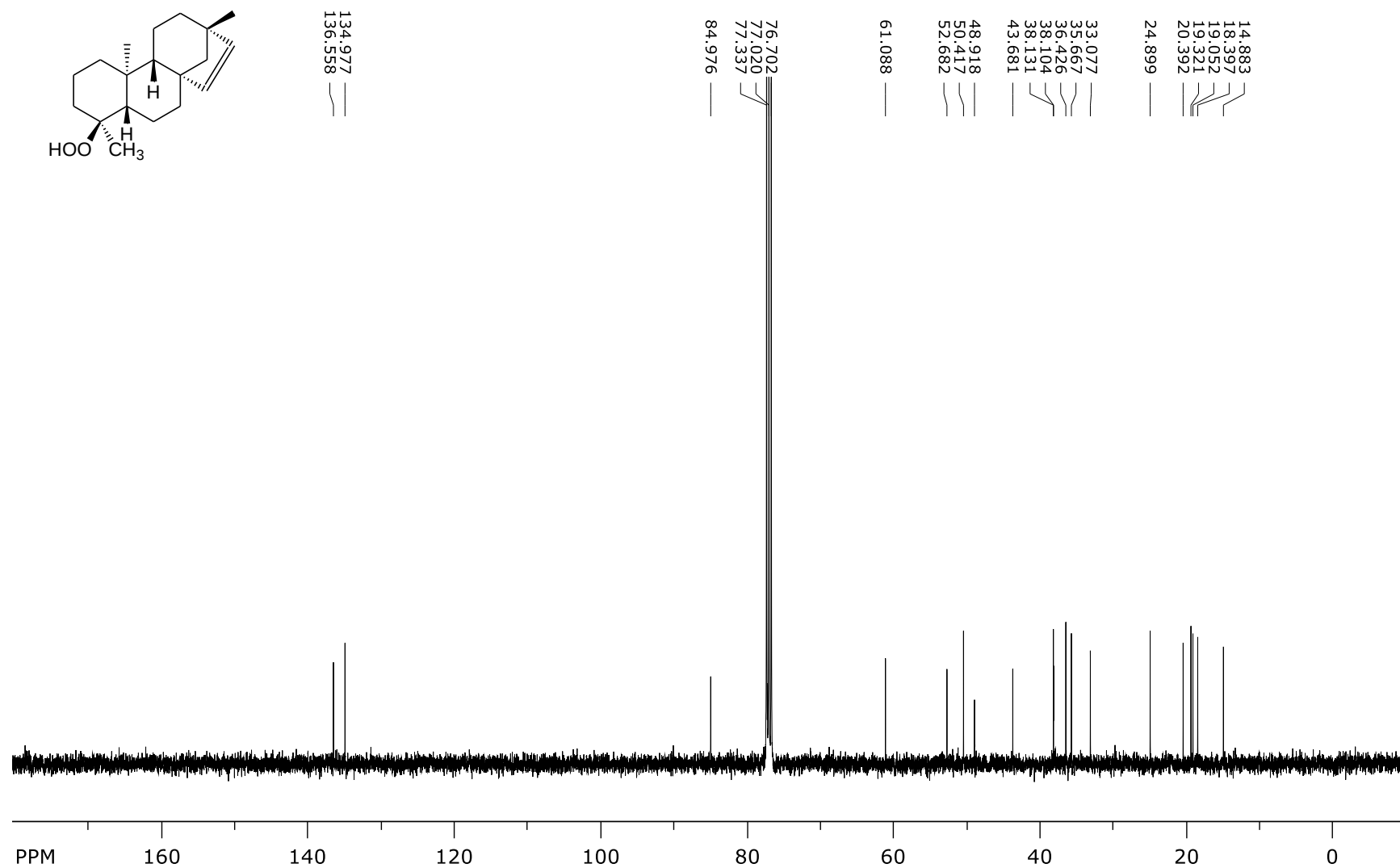
1D Selective Gradient NOESY Freq: 1.282



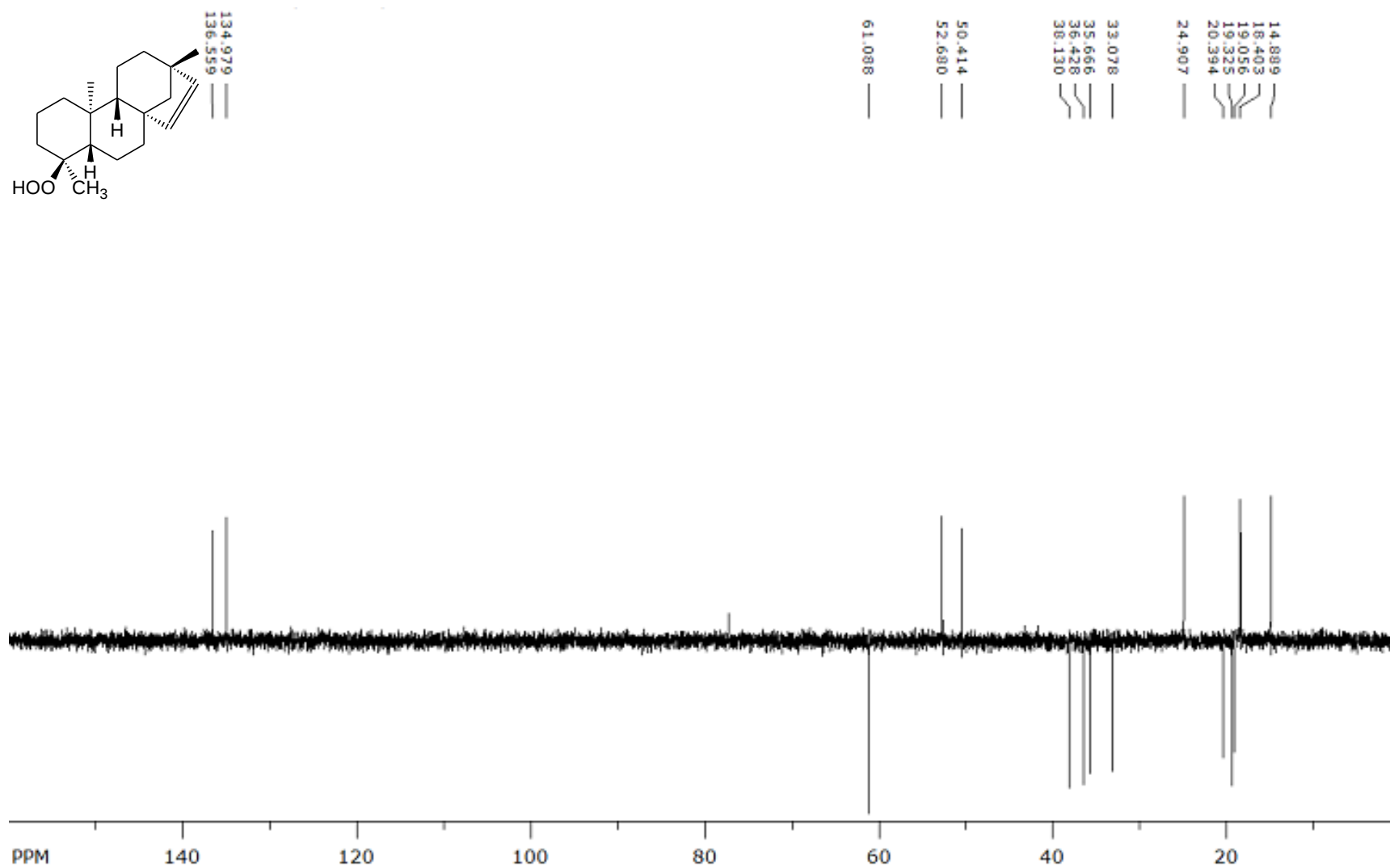
S45. ^1H NMR Spectrum (400 MHz) of **8** in CDCl_3



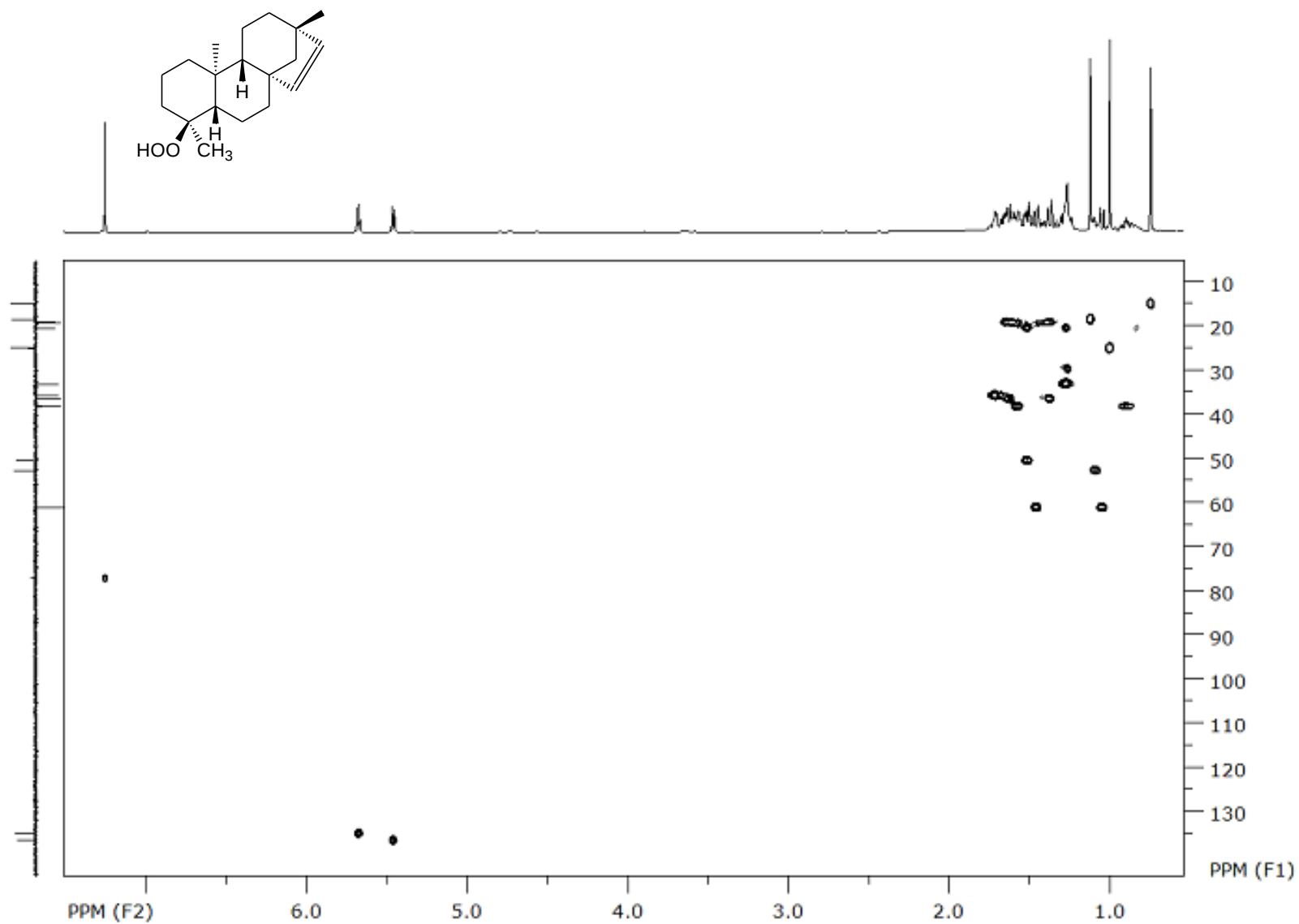
S46. ^{13}C NMR Spectrum (100 MHz) of **8** in CDCl_3



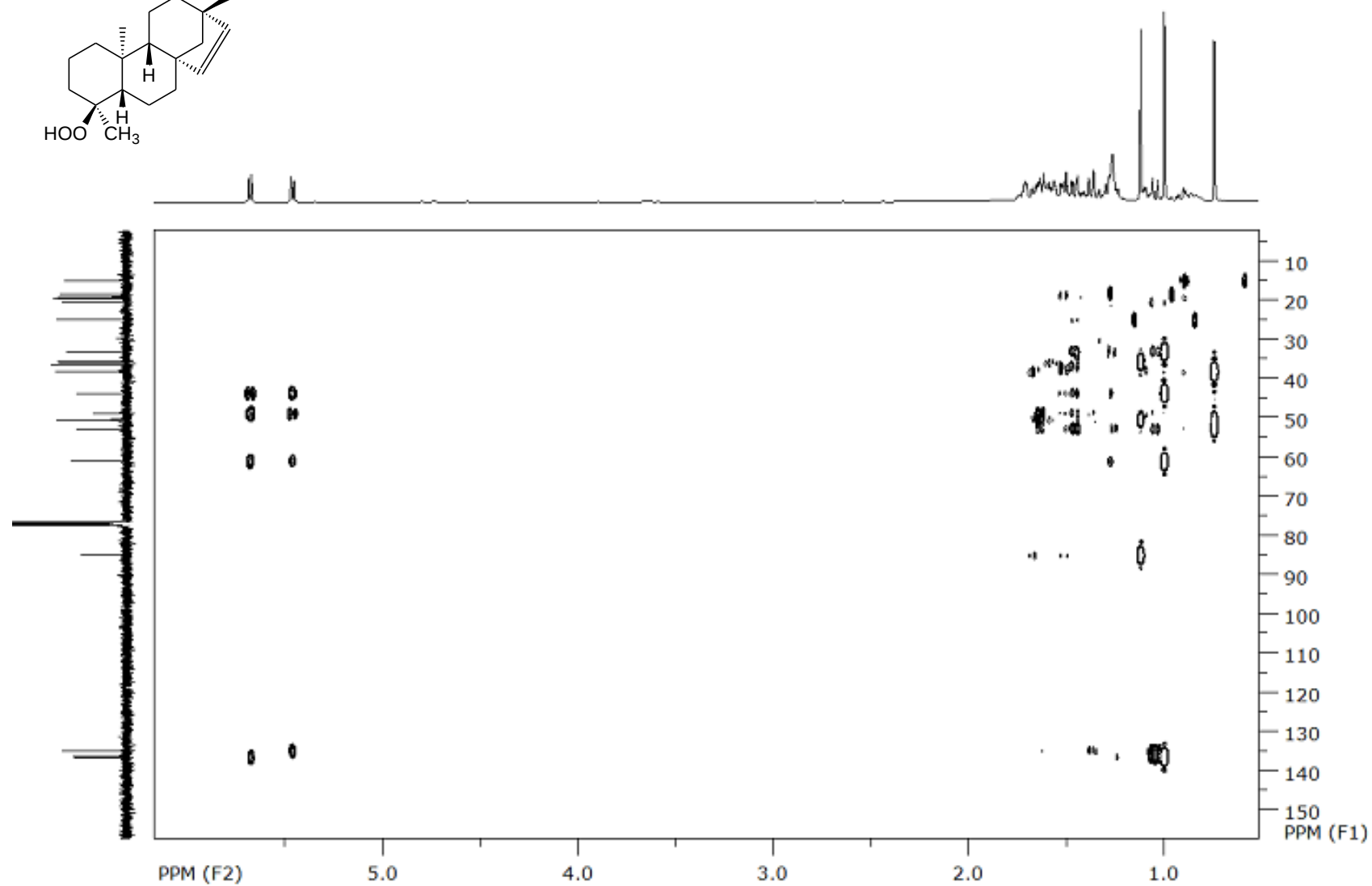
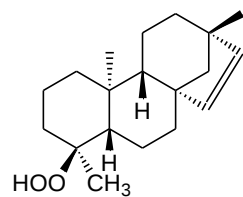
S47. DEPT135 Spectrum (100 MHz) of **8** in CDCl₃



S48. HSQC Spectrum of **8** in CDCl₃

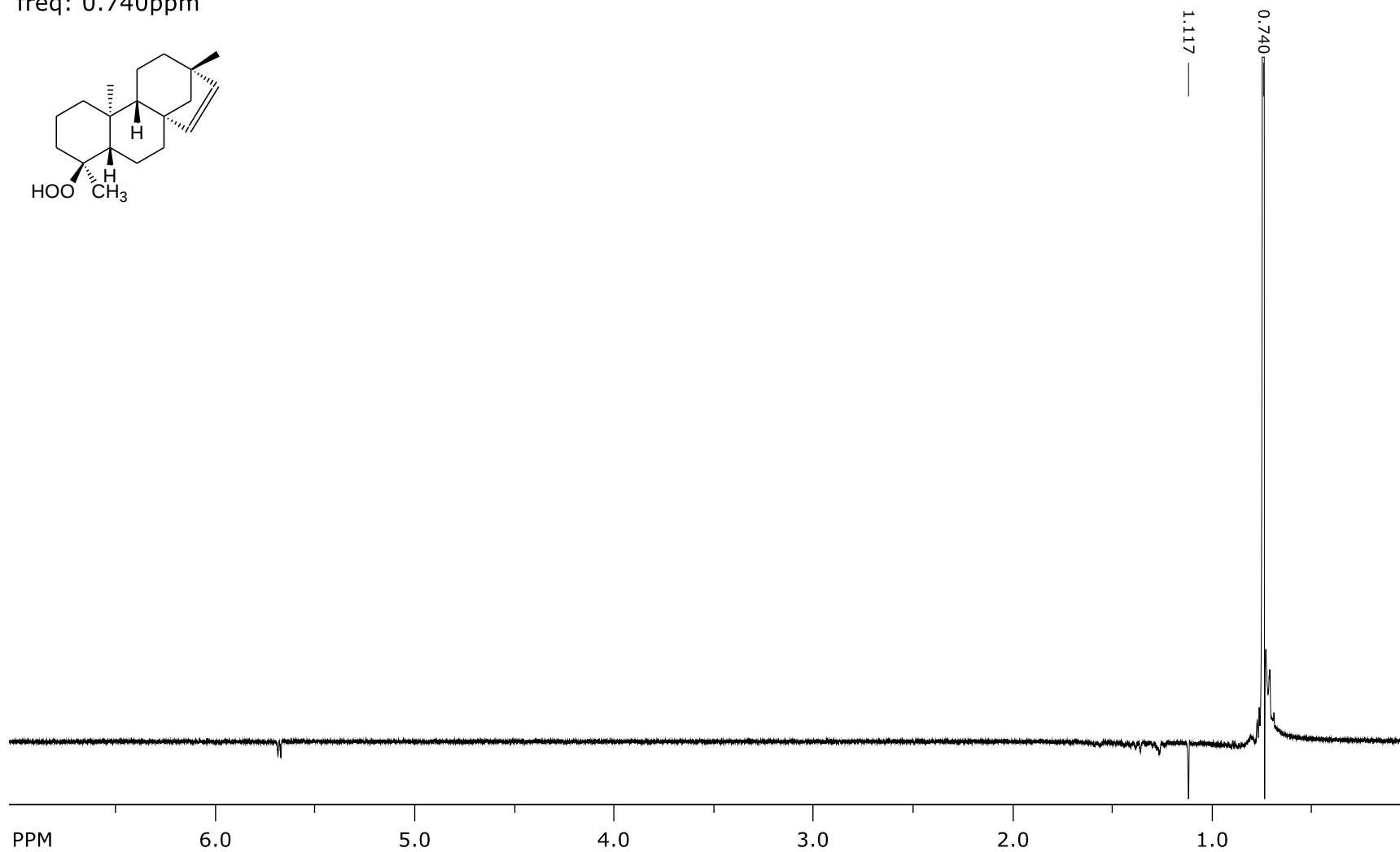


S49. HMBC Spectrum of **8** in CDCl₃



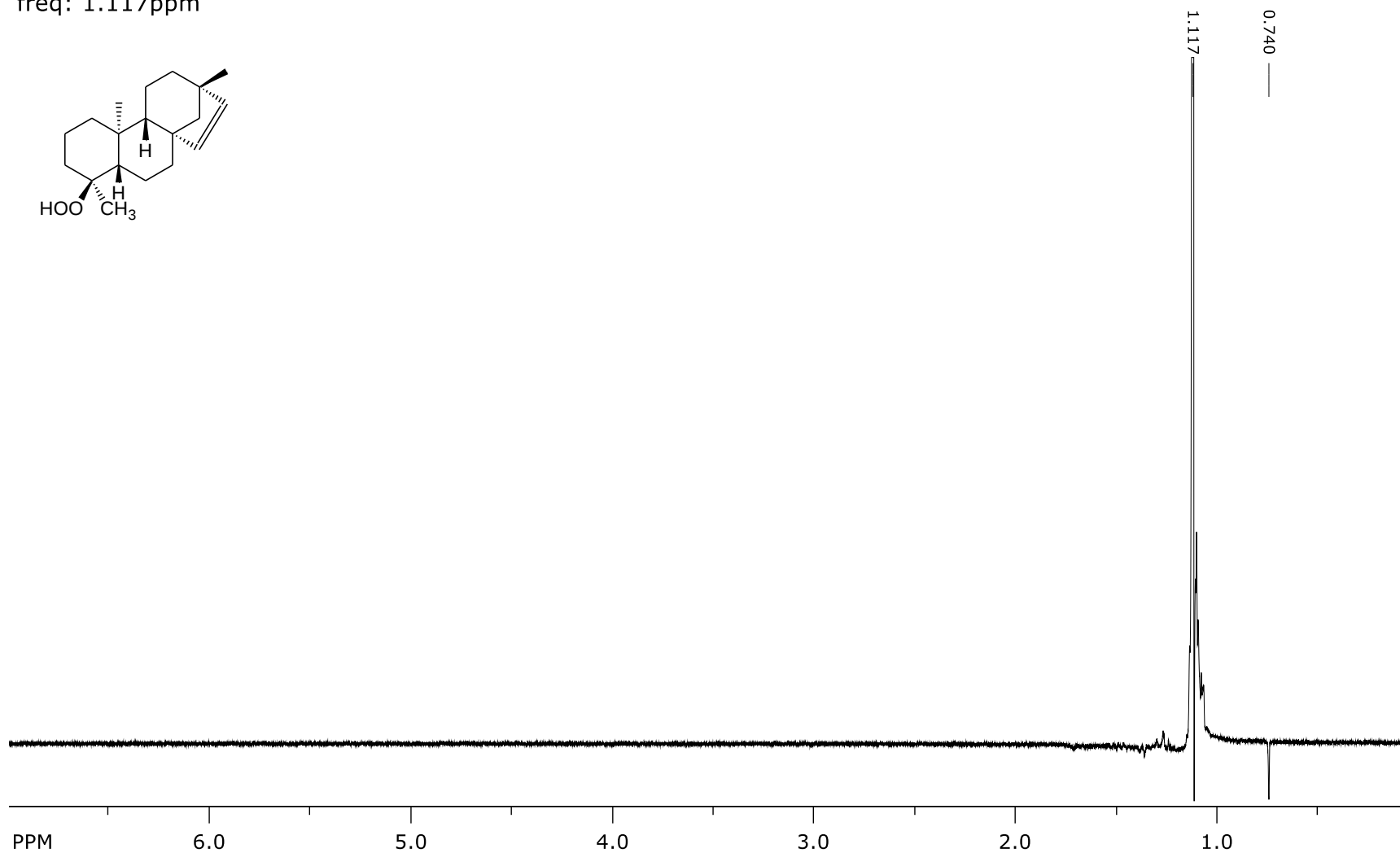
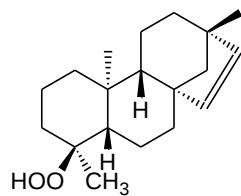
S50. 1D Selective Gradient NOESY spectrum (400 MHz) of **8** in CDCl₃; irradiation at δ 0.740

1D Selective Gradient NOESY
freq: 0.740ppm

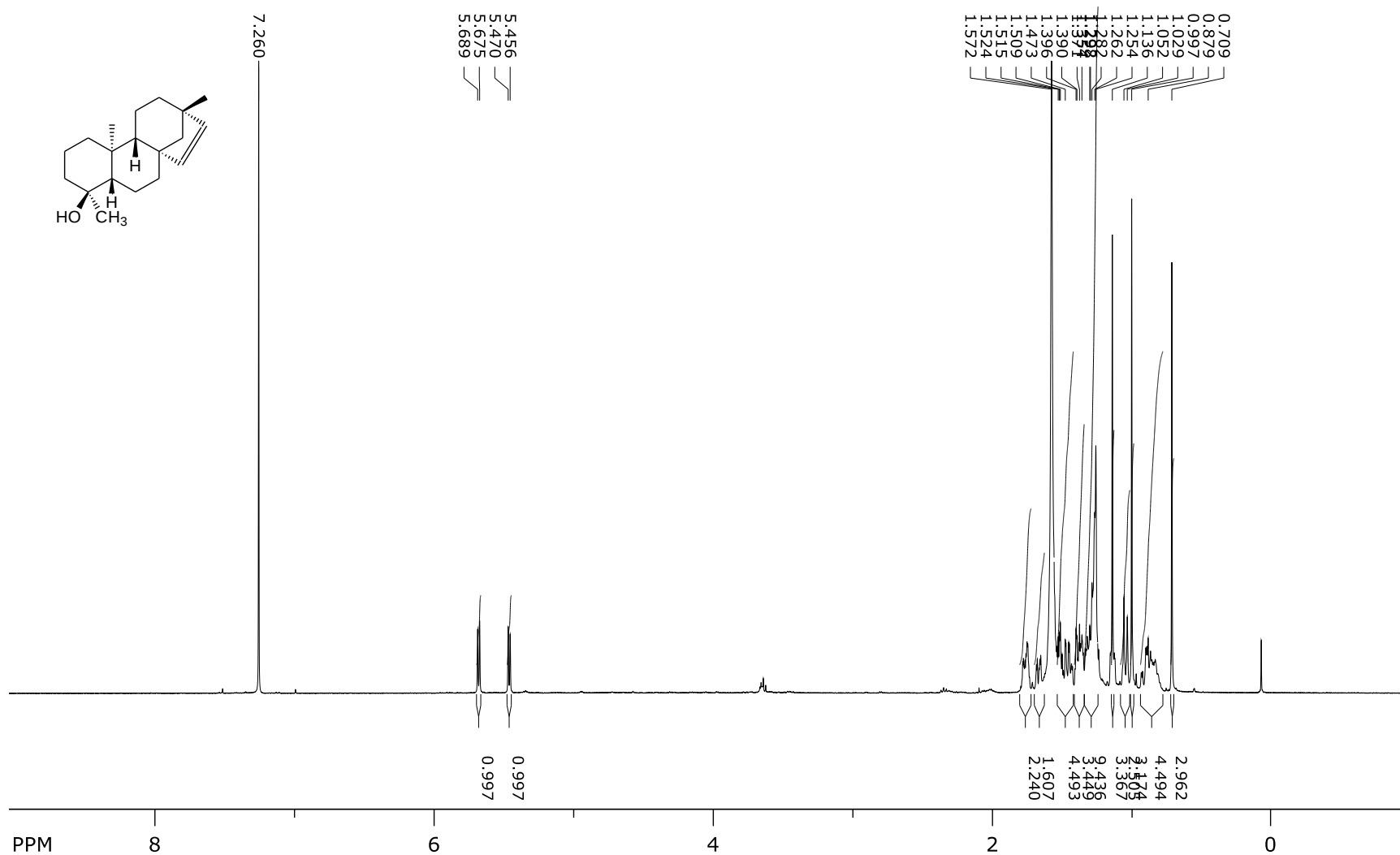


S51. 1D Selective Gradient NOESY spectrum (400 MHz) of **8** in CDCl₃; Irradiation at δ 1.117

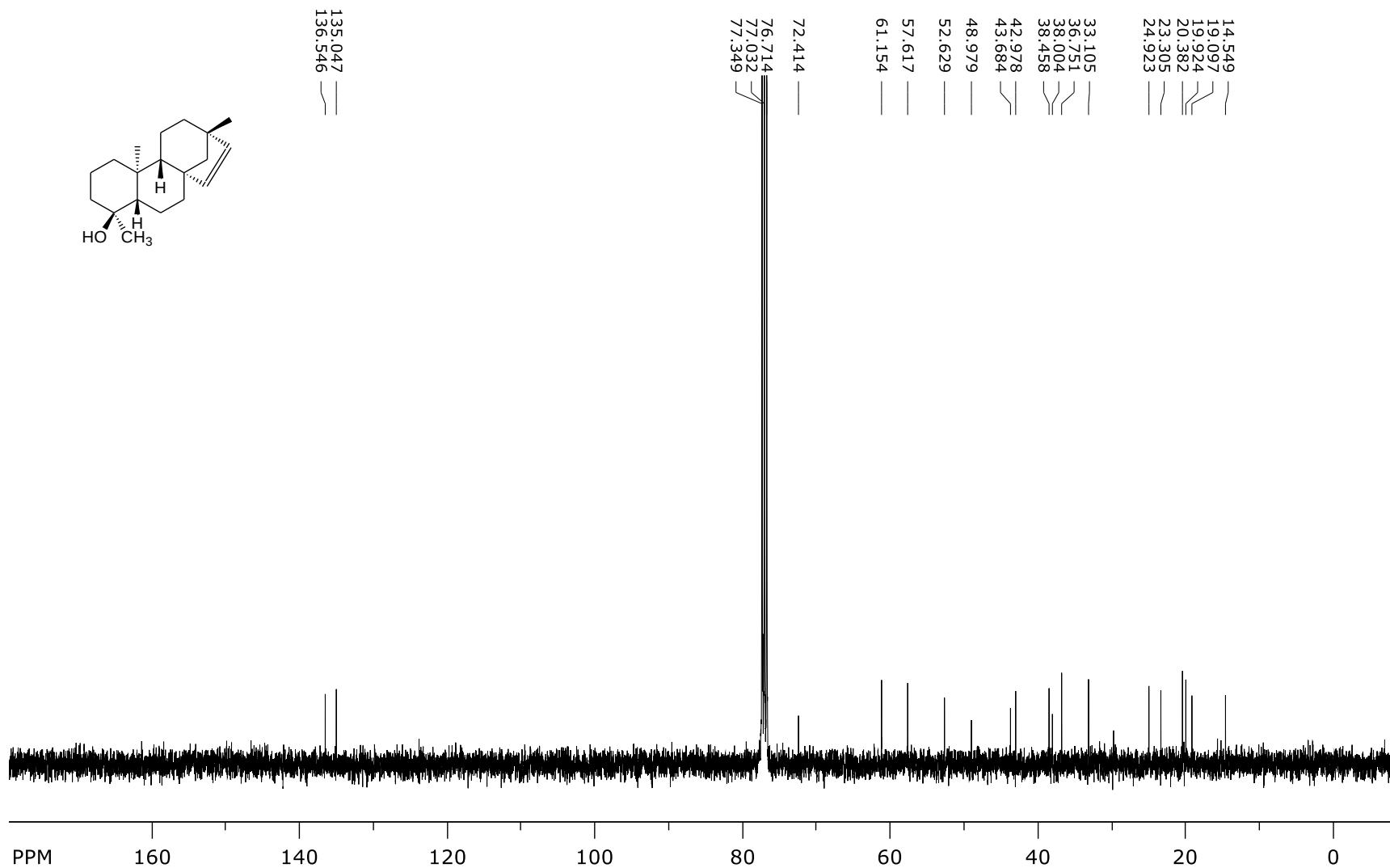
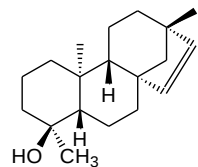
1D Selective Gradient NOESY
freq: 1.117ppm



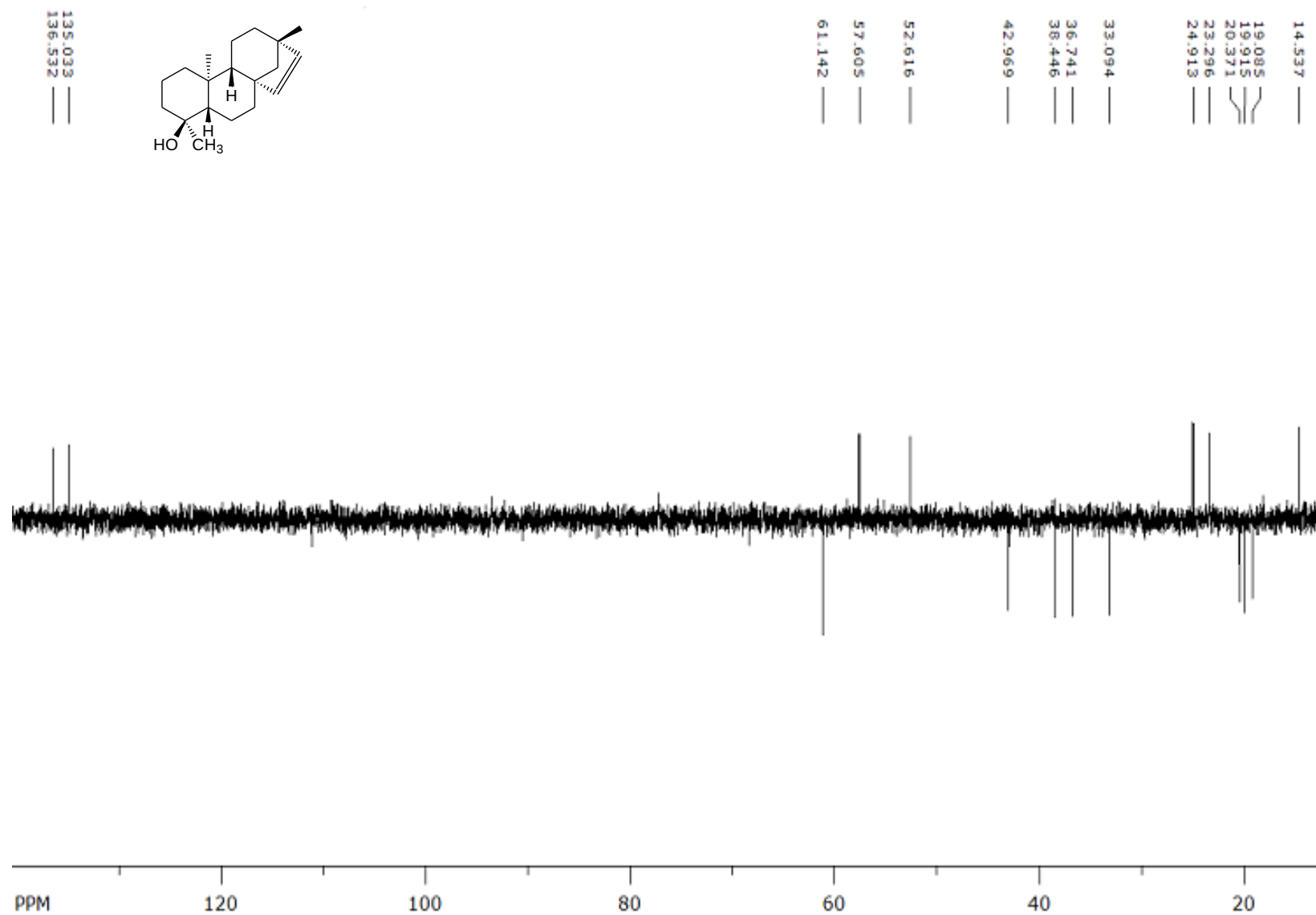
S52. ^1H NMR Spectrum (400 MHz) of **9** in CDCl_3



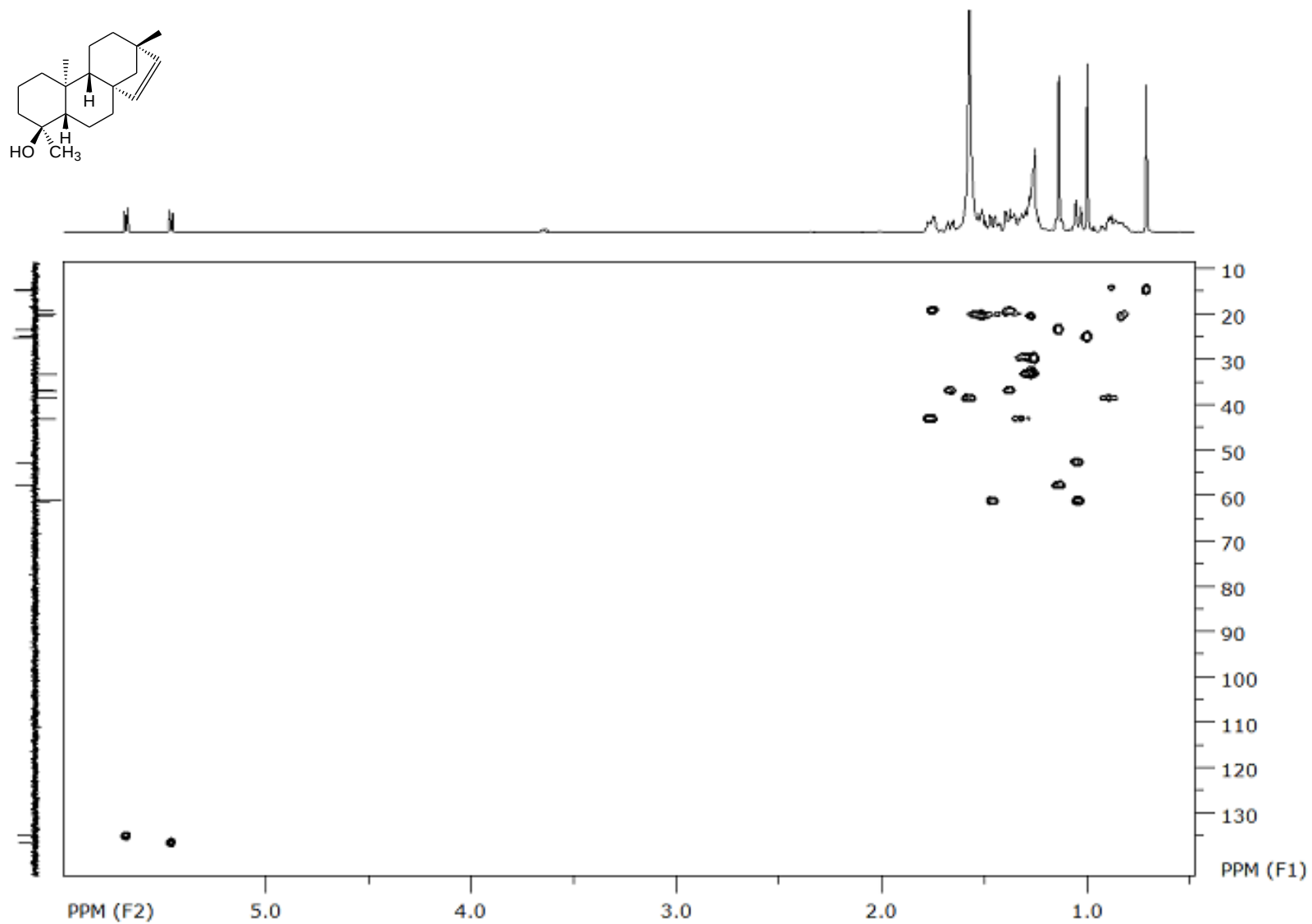
S53. ^{13}C NMR Spectrum (100 MHz) of **9** in CDCl_3



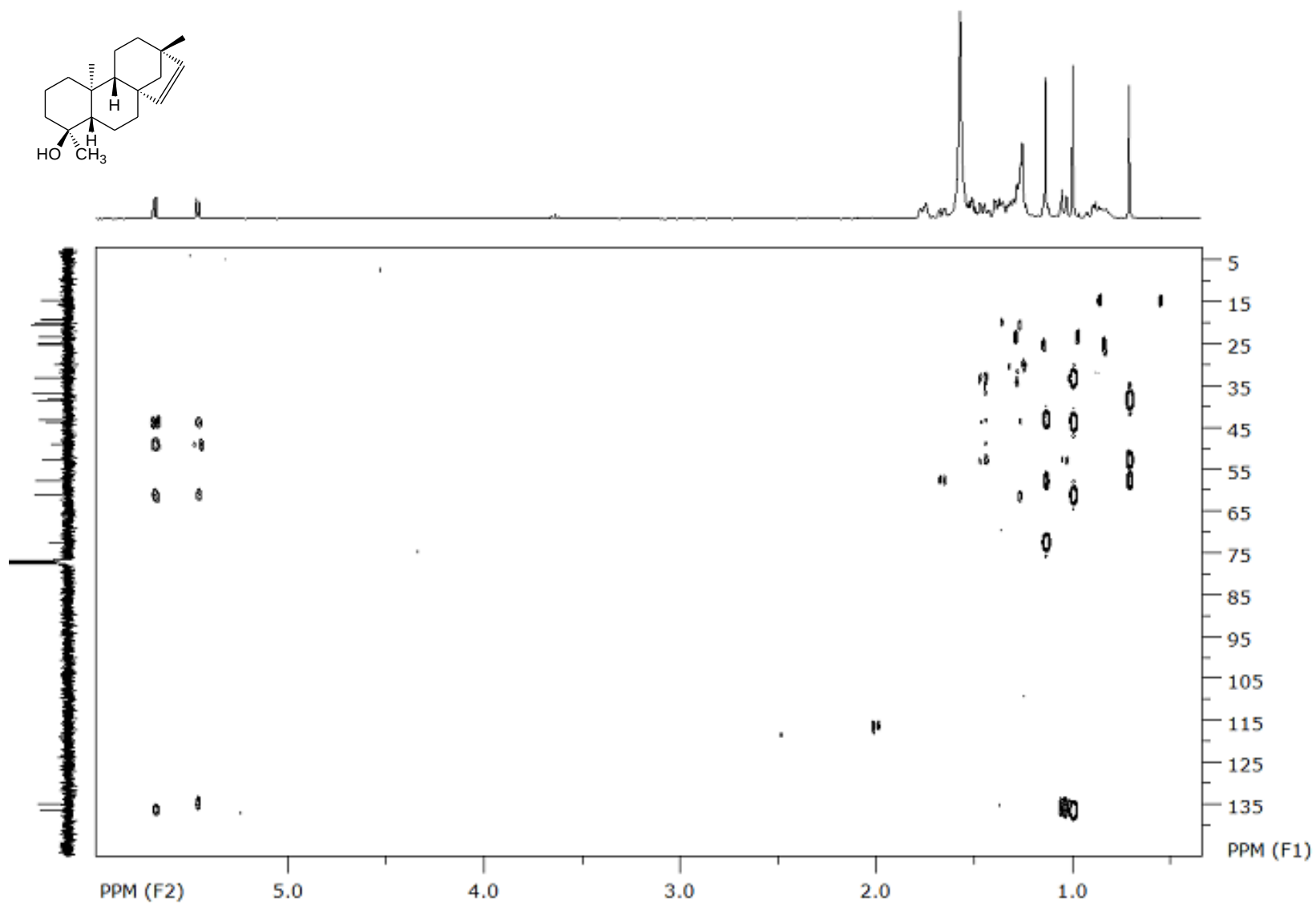
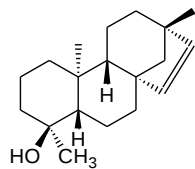
S54. DEPT135 Spectrum (100 MHz) of **9** in CDCl₃



S55. HSQC Spectrum of **9** in CDCl₃

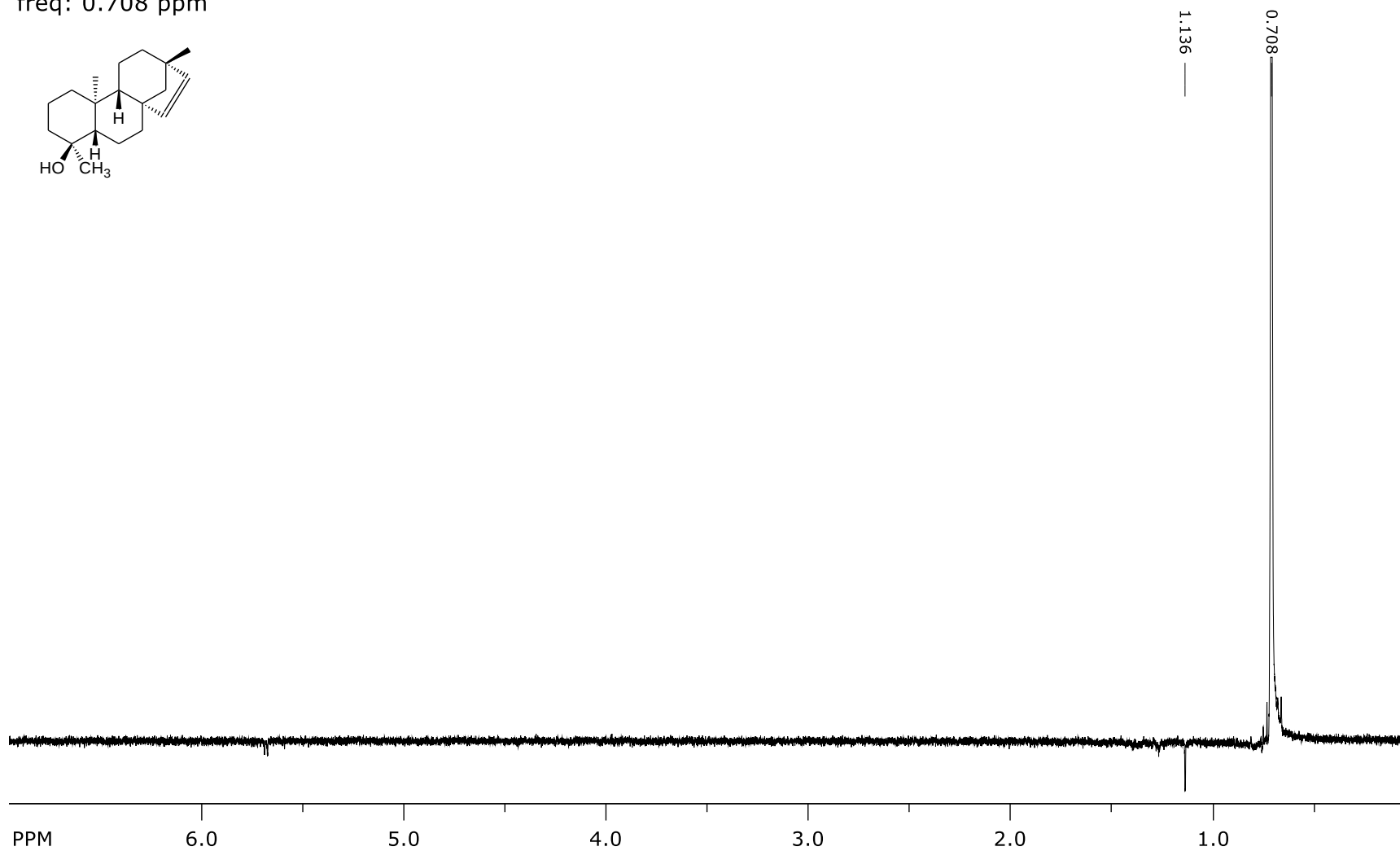
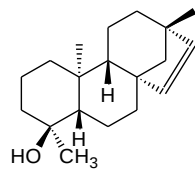


S56. HMBC Spectrum of **9** in CDCl₃



S57. 1D Selective Gradient NOESY spectrum (400 MHz) of **9** in CDCl₃; Irradiation at δ 0.708

1D Selective Gradient NOESY
freq: 0.708 ppm



S58. 1D Selective Gradient NOESY spectrum (400 MHz) of **9** in CDCl₃; Irradiation at δ 1.135

1D Selective Gradient NOESY
freq: 1.136 ppm

