

Supporting Information

Antimicrobial Spirotetronate Metabolites from Marine-derived

Micromonospora harpali SCSIO GJ089

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Table S1. ^1H (500 MHz) and ^{13}C (125 MHz) NMR data for compounds **3**, **6** and **10**.

position	3^a		6^b		10^a (tetrocarcin A)	
	δ_{C} type	δ_{H} mult. (<i>J</i> in Hz)	δ_{C} type	δ_{H} mult. (<i>J</i> in Hz)	δ_{C} type	δ_{H} mult. (<i>J</i> in Hz)
1	166.8, C		177.2, C		177.3, C	
2	100.9, C		98.9, C		98.8, C	
3	206.6, C		199.5, C		200.2, C	
4	51.3, C		52.8, C		52.8, C	
5	43.3, CH	2.0, m	45.5, CH	2.10, m	40.3, CH	2.04, m
6	31.3, CH	1.58, overlapped	32.6, CH	1.49, overlapped	32.6, CH	1.49, m
7 α	41.7, CH ₂	1.52, overlapped	43.3, CH ₂	1.49, overlapped	43.2, CH ₂	1.59, m
7 β		1.56, overlapped		1.59, m		1.47, m
8	34.7, CH	2.20, m	36.2, CH	2.20, m	36.2, CH	2.20, m
9	84.4, CH	3.45, m	86.6, CH	3.43, dd (10.1, 4.4)	86.7, CH	3.42, dd (10.9, 5.2)
10	38.6, CH	2.08, overlapped	40.4, CH	2.04, m	45.5, CH	2.1, t (9.7)
11	126.5, CH	5.75, d (10.5)	127.0, CH	5.76, d (10.1)	129.0, CH	5.39,ddd (10.0, 5.1, 2.4)
12	126.1, CH	5.41, ddd (9.8, 4.8, 2.1)	128.9, CH	5.40, m	126.9, CH	5.73, d (10.4)
13	54.3, CH	3.25, m	53.0, CH	3.64, overlapped	52.9, CH	3.64, m
14	136.1, C		138.4, C		138.2, C	
15	123.1, CH	5.15, d (9.1)	123.0, CH	5.21, d (5.3)	123.2, CH	5.23, m
16	30.8, CH ₂	2.22, m; 2.31, m	32.1, CH ₂	2.23, m; 2.32, m	32.2, CH ₂	2.22, m; 2.29, m
17	78.0, CH	4.27, br s	80.0, CH	4.27, br s	79.9, CH	4.20, br s
18	141.3, C		139.4, C		139.2, C	
19	118.7, CH	5.21, d (10.0)	122.3, CH	5.15, d (9.3)	122.0, CH	5.23, m
20	44.9, CH	3.0, t (9.7)	46.6, CH	2.80, t (9.5)	46.5, CH	2.81, t (9.5)
21	69.7, CH	4.72, dm (8.7)	72.2, CH	4.38, d (9.3)	71.4, CH	4.58, dm (9.3)
22	139.6, CH	6.35, s	140.8, CH	6.3, s	151.9, CH	6.87, s
23	130.9, C		134.3, C		139.3, C	
24 α	32.3, CH ₂	2.43, d (17.7)	33.4, CH ₂	2.26, overlapped	30.7, CH ₂	2.24, d (18.5)
24 β		2.88, d (17.7)		2.87, d (18.0)		2.75, dd (18.7, 2.6)
25	84.5, C		85.8, C		85.4, C	
26	201.9, C		200.5, C		200.8, C	
27	15.6, CH ₃	1.63, s	15.5, CH ₃	1.49, s	15.6, CH ₃	1.48, s
28	22.2, CH ₃	0.65, d (4.5)	23.2, CH ₃	0.66, d (3.9)	23.0, CH ₃	0.64, d (5.9)
29	14.1, CH ₃	1.08, d (7.0)	14.7, CH ₃	1.11, d (8.4)	14.7, CH ₃	1.10, d (7.0)
30	14.5, CH ₃	1.35, s	15.2, CH ₃	1.38, s	15.0, CH ₃	1.36, s
31	16.2, CH ₃	1.52, s	16.4, CH ₃	1.50, s	16.3, CH ₃	1.47, s
32	143.8, CH	7.18, d (16.2)	146.3, CH	7.30, d (16.0)	195.3, C	9.52, s
33	127.2, CH	6.07, d (16.2)	127.6, CH	6.22, d (16.1)		
34	198.4, C		201.2, C			
35	27.7, CH ₃	2.29, s	27.9, CH ₃	2.29, s		
NS1	96.6, CH	4.44, dd (9.8, 1.6)	96.6, CH	4.79, d (10.0)	98.1, CH	4.63, dd (9.6, 2.0)
NS2	36.1, CH ₂	1.64, m; 2.69, d (14.7)	37.8, CH ₂	1.79, m; 1.92, m	36.7, CH ₂	1.74, m; 2.72, m

NS3	91.6, C		58.0, C		92.2, C	
NS4	53.8, CH	4.36, d (9.8)	55.4, CH	3.62, br s	55.2, CH	4.34, br s
NS5	69.4, CH	3.48, m	68.9, CH	3.93, m	70.0, CH	3.57, m
NS6	17.9, CH ₃	1.16, d (6.1)	17.3, CH ₃	1.17, d (6.0)	17.9, CH ₃	1.12, d (6.1)
NS3-CH ₃	25.4, CH ₃	1.58, s	24.7, CH ₃	1.35, s	26.0, CH ₃	1.52, s
NS4-NHCO ₂ -	157.4, C		160.0, C		160.1, C	
NS4-NHCO ₂ CH ₃	52.9, CH ₃	3.70, s	52.9, CH ₃	3.68, s	53.0, CH ₃	3.68, s
DG1	98.6, CH	4.83, d (4.1)	99.9, CH	4.83, d (3.7)	99.9, CH	4.82, d (4.4)
DG2	31.6, CH ₂	1.77, m; 2.23, m	32.1, CH ₂	1.75, m; 2.30, m	32.2, CH ₂	1.75, m; 2.20, dd (15.1, 2.5)
DG3	66.8, CH	4.15, dt (3.0, 2.9)	67.8, CH	4.16, m	67.8, CH	4.16, dt (3.1, 3.0)
DG4	74.5, CH	4.58, dd (9.8, 2.8)	76.1, CH	4.54, dd (9.8, 2.3)	76.1, CH	4.53, dd (9.6, 3.1)
DG5	62.2, CH	4.35, dd (9.8, 1.4)	63.5, CH	4.39, m	63.5, CH	4.39, dq (9.6, 6.4)
DG6	18.2, CH ₃	1.13, d (6.3)	18.3, CH ₃	1.13, overlapped	18.2, CH ₃	1.13, d (6.4)
DG4-O ₂ C-	170.6, C		172.1, C		172.1, C	
DG4-O ₂ CCH ₃	21.2, CH ₃	2.08, s	21.1, CH ₃	2.09, s	21.0, CH ₃	2.08, s
AM/DG'1	92.7, CH	4.88, d (2.8)	93.7, CH	4.93, overlapped	92.9, CH	4.92, d (3.5)
AM/DG'2	29.7, CH ₂	1.75, m; 1.87, m	27.5, CH ₂	1.87, m; 1.99, m	28.3, CH ₂	1.73, m; 1.80, m
AM/DG'3	26.4, CH ₂	1.95, m; 2.0, m	30.4, CH ₂	1.86, m; 1.89, m	30.4, CH ₂	1.86, m; 1.89, m
AM/DG'4	81.3, CH	3.20, ddd (10.4, 4.7)	82.1, CH	3.21, ddd (9.8, 5.4)	82.1, CH	3.21, ddd (9.4, 4.5)
AM/DG'5	68.0, CH	3.70, m	69.3, CH	3.66, overlapped	69.3, CH	3.66, m
AM/DG'6	17.6, CH ₃	1.13, d (6.3)	17.4, CH ₃	1.13, overlapped	17.3, CH ₃	1.11, d (6.3)
DG''1	99.5, CH	4.89, dd (9.8, 1.8)	100.6, CH	4.93, overlapped	100.6, CH	4.93, d (9.0)
DG''2	37.1, CH ₂	1.67, m; 2.14, m	39.2, CH ₂	1.62, m; 2.01, m	39.2, CH ₂	1.62, m; 2.01, m
DG''3	64.0, CH	4.25, dt (3.1, 2.7)	64.0, CH	4.26, overlapped	64.0, CH	4.26, dt (3.1, 2.9)
DG''4	75.3, CH	3.44, m	76.4, CH	3.28, dd (9.5, 2.0)	76.4, CH	3.27, dd (9.5, 2.7)
DG''5	67.9, CH	3.85, dq (9.5, 6.3)	69.5, CH	3.91, m	69.5, CH	3.91, dq (9.5, 6.2)
DG''6	19.0, CH ₃	1.31, d (6.2)	19.3, CH ₃	1.29, d (6.2)	19.3, CH ₃	1.29, d (6.1)
AM'1	92.0, CH	4.92, br s	92.9, CH	4.92, br s	93.7, CH	4.93, br s
AM'2	27.5, CH ₂	1.72, m; 1.88, m	28.3, CH ₂	1.73, m; 1.80, m	27.5, CH ₂	1.87, m; 1.99, m
AM'3	29.8, CH ₂	1.80, m; 1.87, m	30.4, CH ₂	1.72, m; 1.75, m	30.4, CH ₂	1.72, m; 1.75, m
AM'4	71.8, CH	3.28, dd (4.3, 10.5)	72.6, CH	3.13, dd (9.7, 4.9)	72.6, CH	3.13, ddd (9.8, 4.5)
AM'5	70.4, CH	3.62, dq (9.1, 6.3)	71.4, CH	3.59, m	71.4, CH	3.59, m
AM'6	17.8, CH ₃	1.23, d (6.2)	18.4, CH ₃	1.20, d (6.1)	18.4, CH ₃	1.19, d (6.1)

^a Recorded in CDCl₃; ^b recorded in CD₃OD.

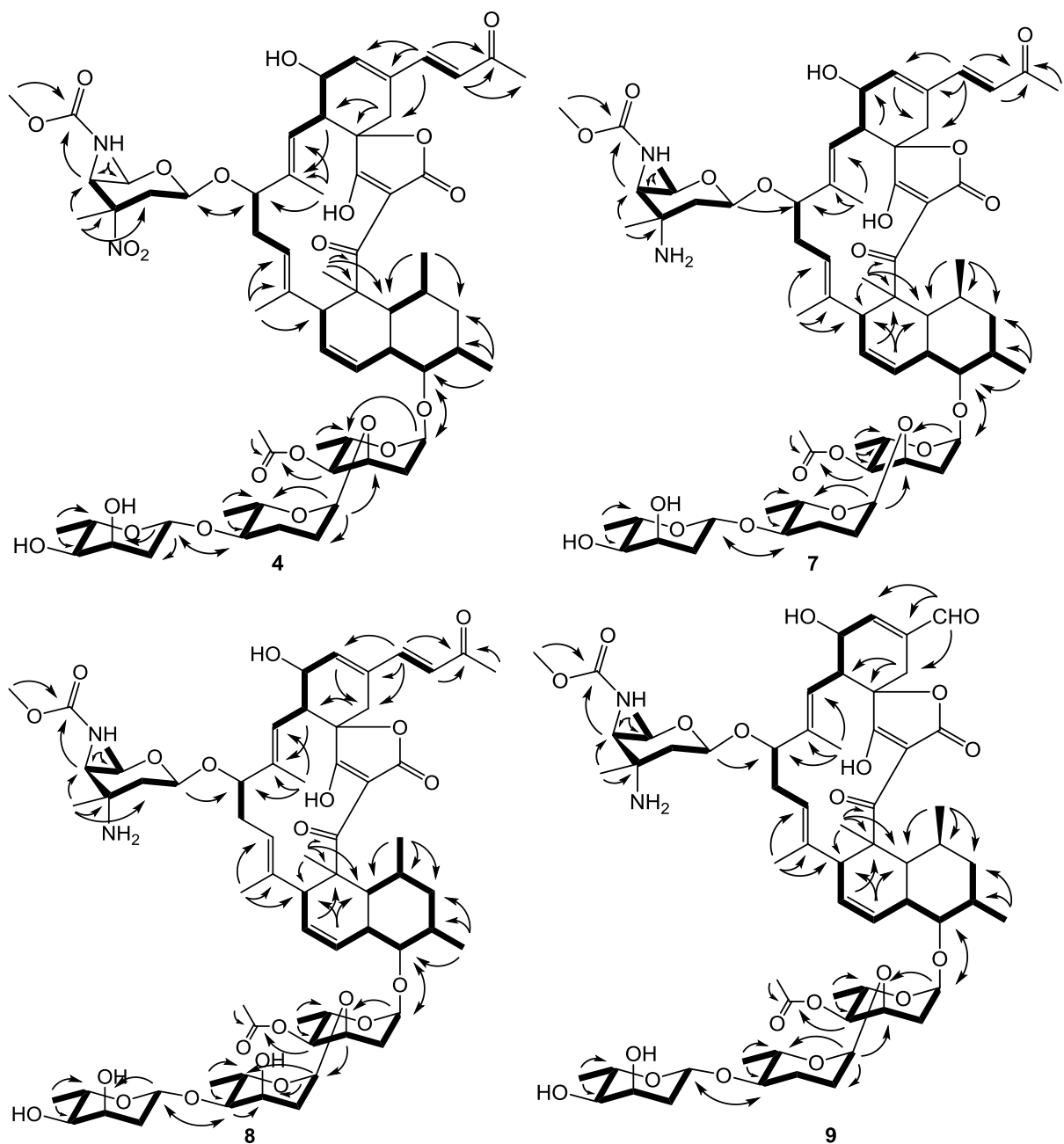


Figure S1. COSY (bold) and selected HMBC (arrow) correlations for microsporanates B, E–F, and tetrocarcin P (4, 7–8, and 9, respectively).

Figure S2. ^1H NMR (500 MHz) spectrum of compound **1** in CDCl_3 .

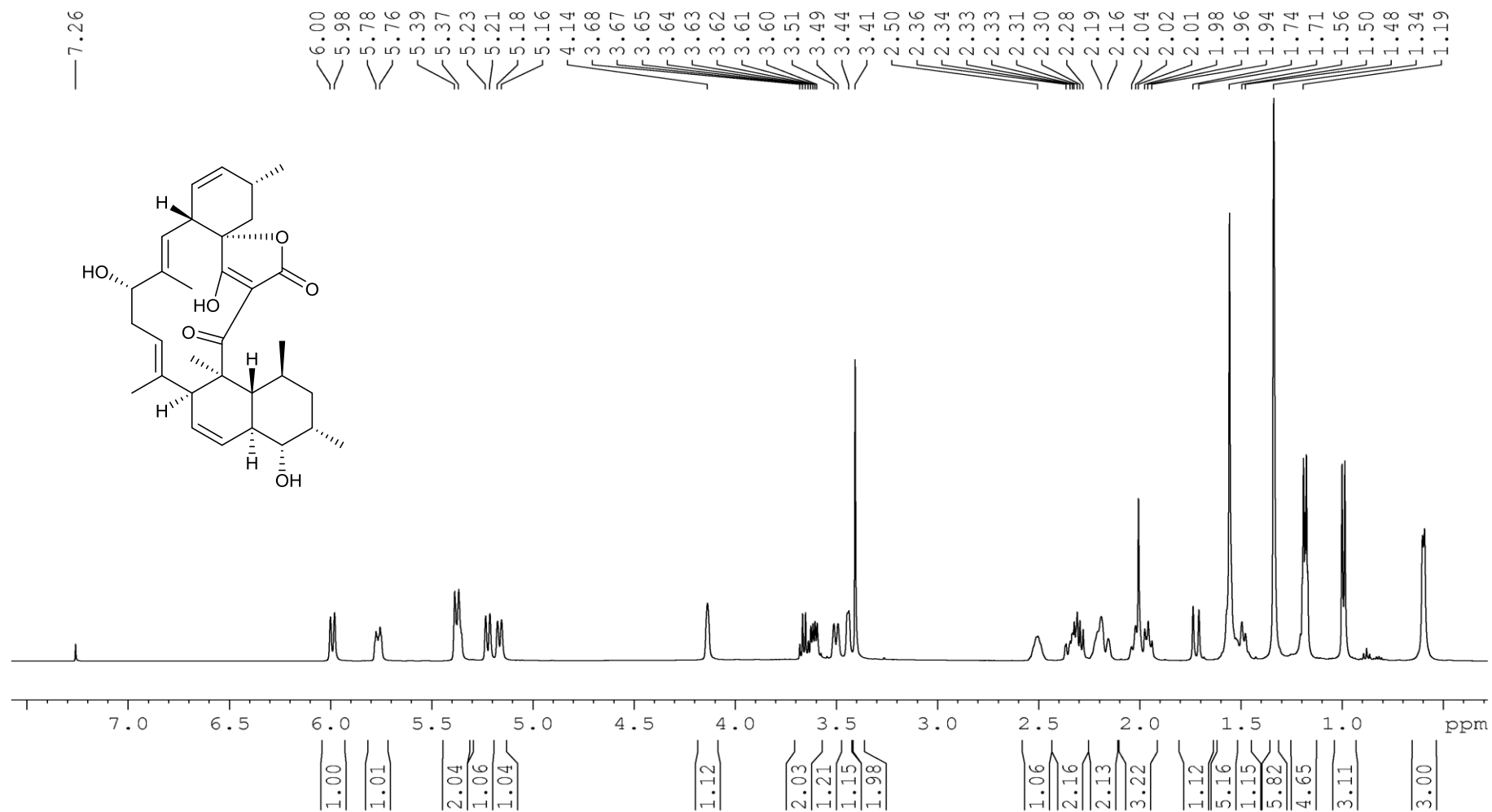


Figure S3. ^{13}C NMR (125 MHz) spectrum of compound **1** in CDCl_3 .

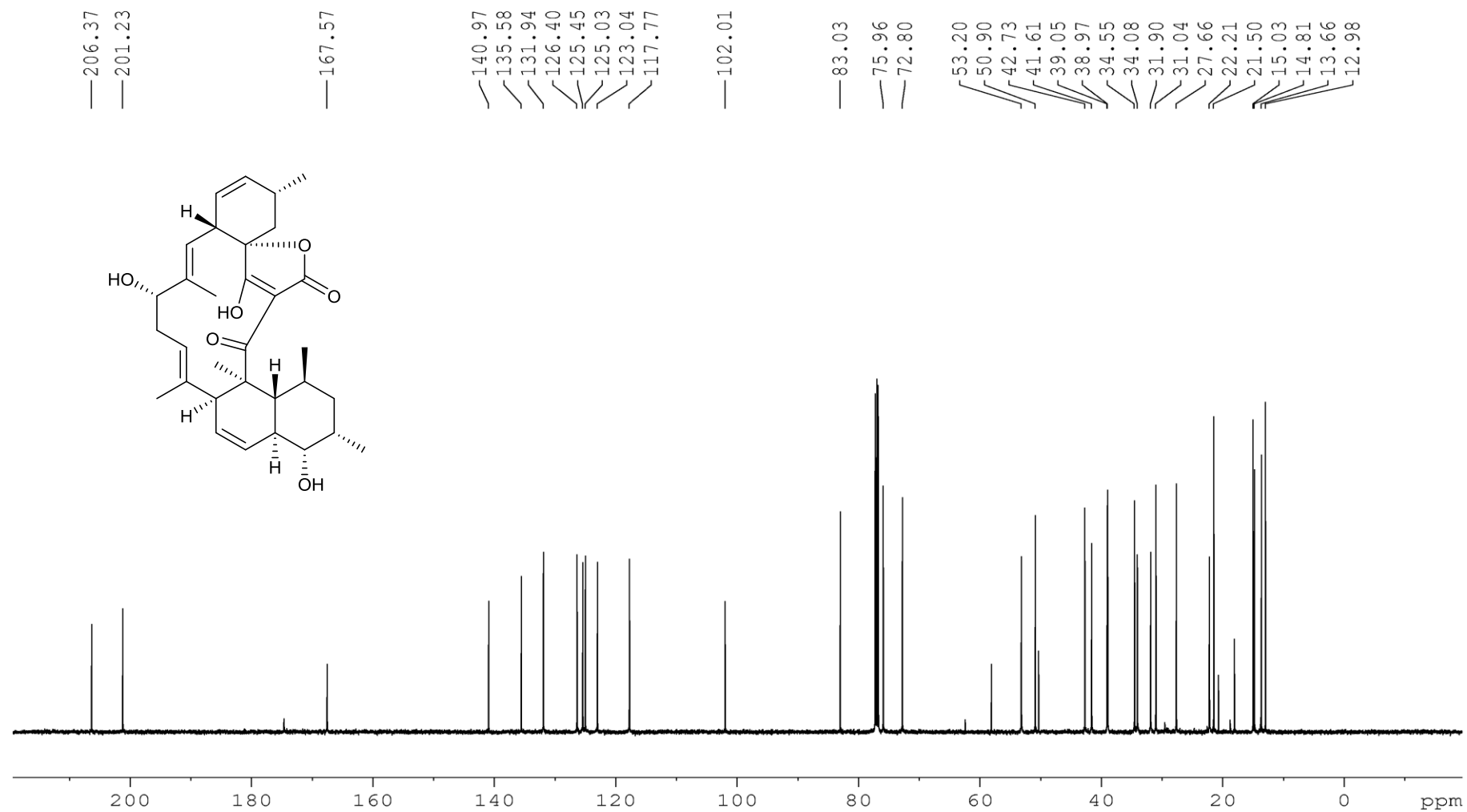


Figure S4. ^{13}C DEPT spectrum of compound **1** in CDCl_3 .

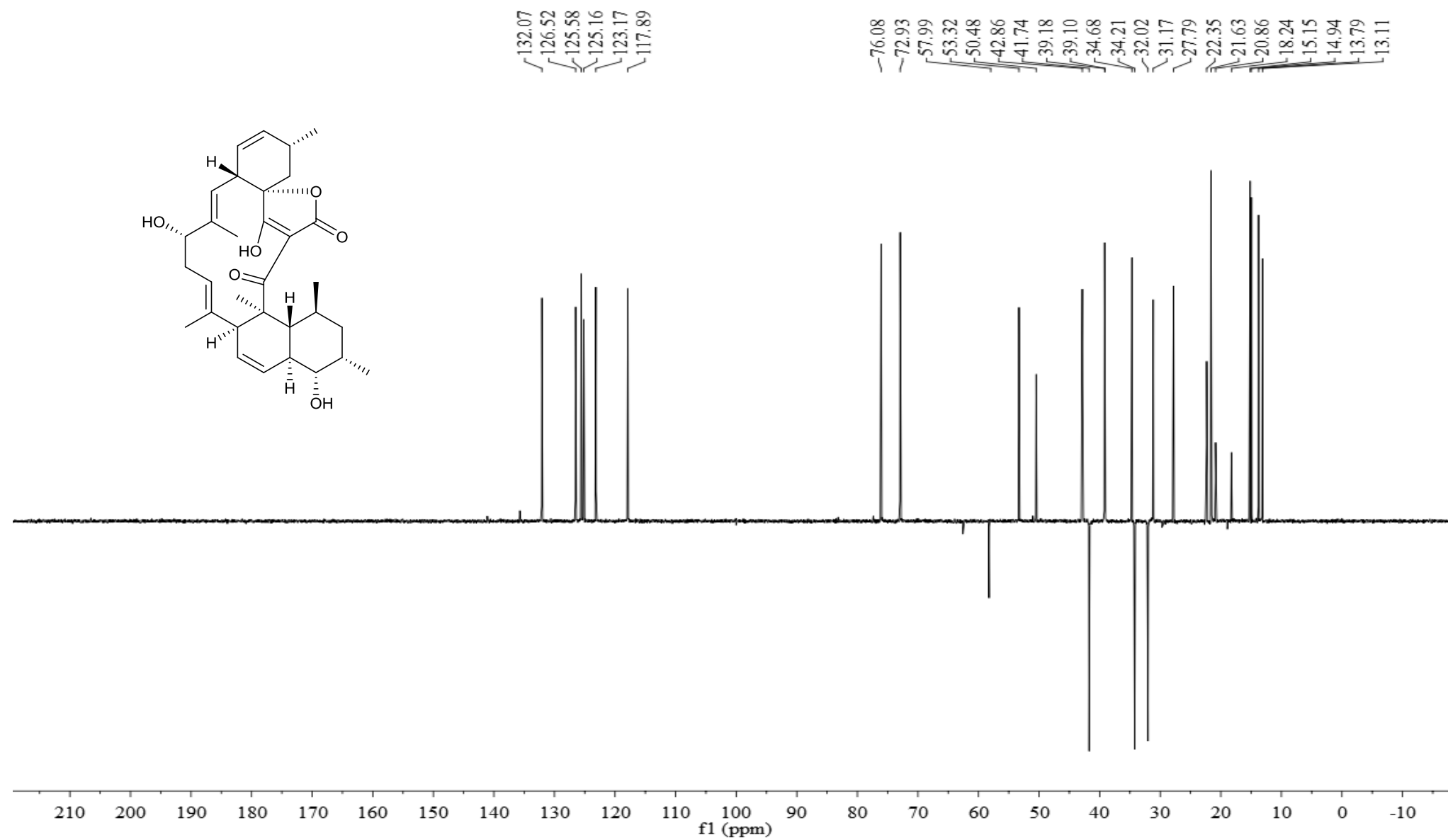


Figure S5. ^1H - ^1H COSY spectrum of compound **1** in CDCl_3 .

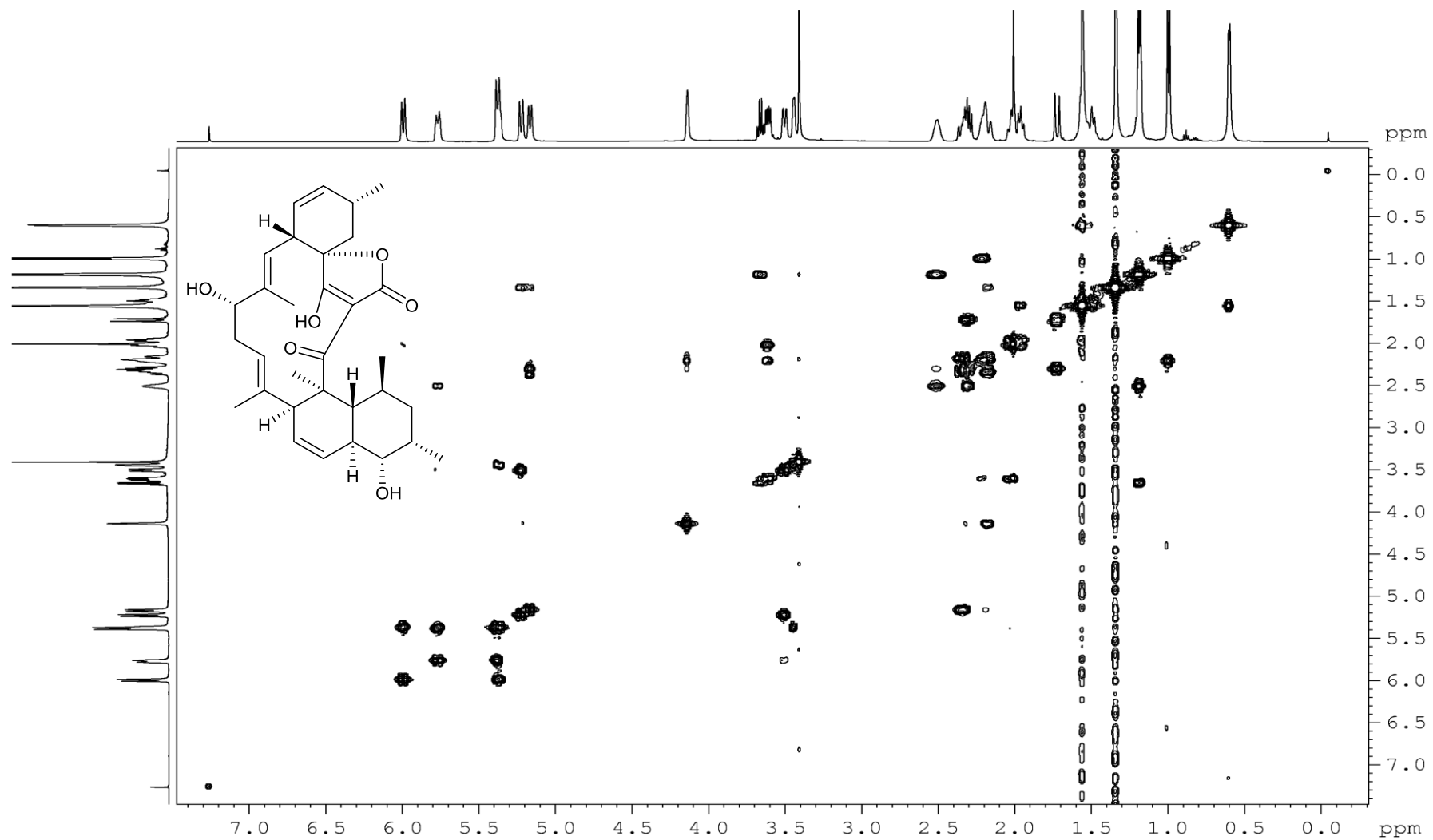


Figure S6. HSQC spectrum of compound **1** in CDCl₃.

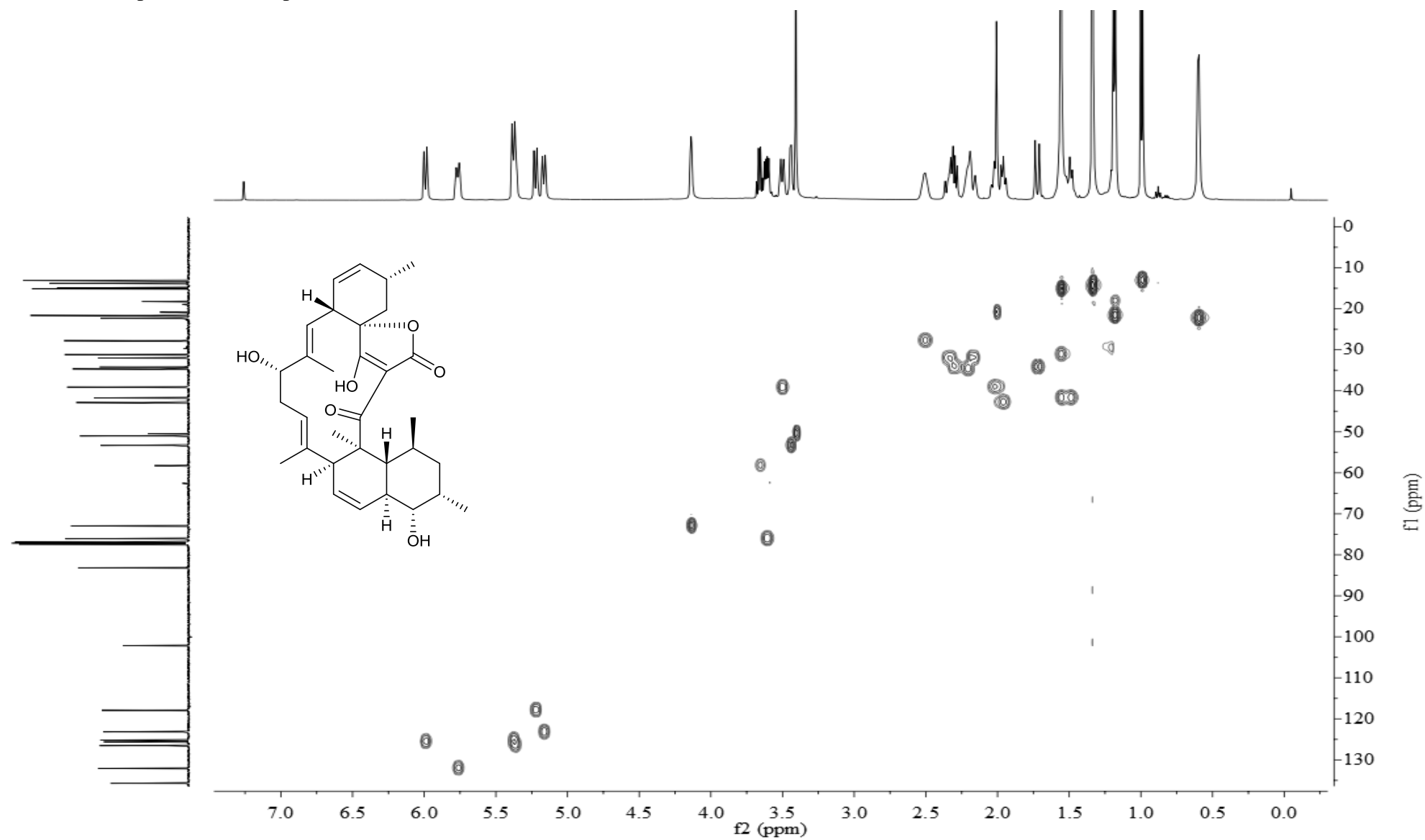


Figure S7. HMBC spectrum of compound **1** in CDCl₃.

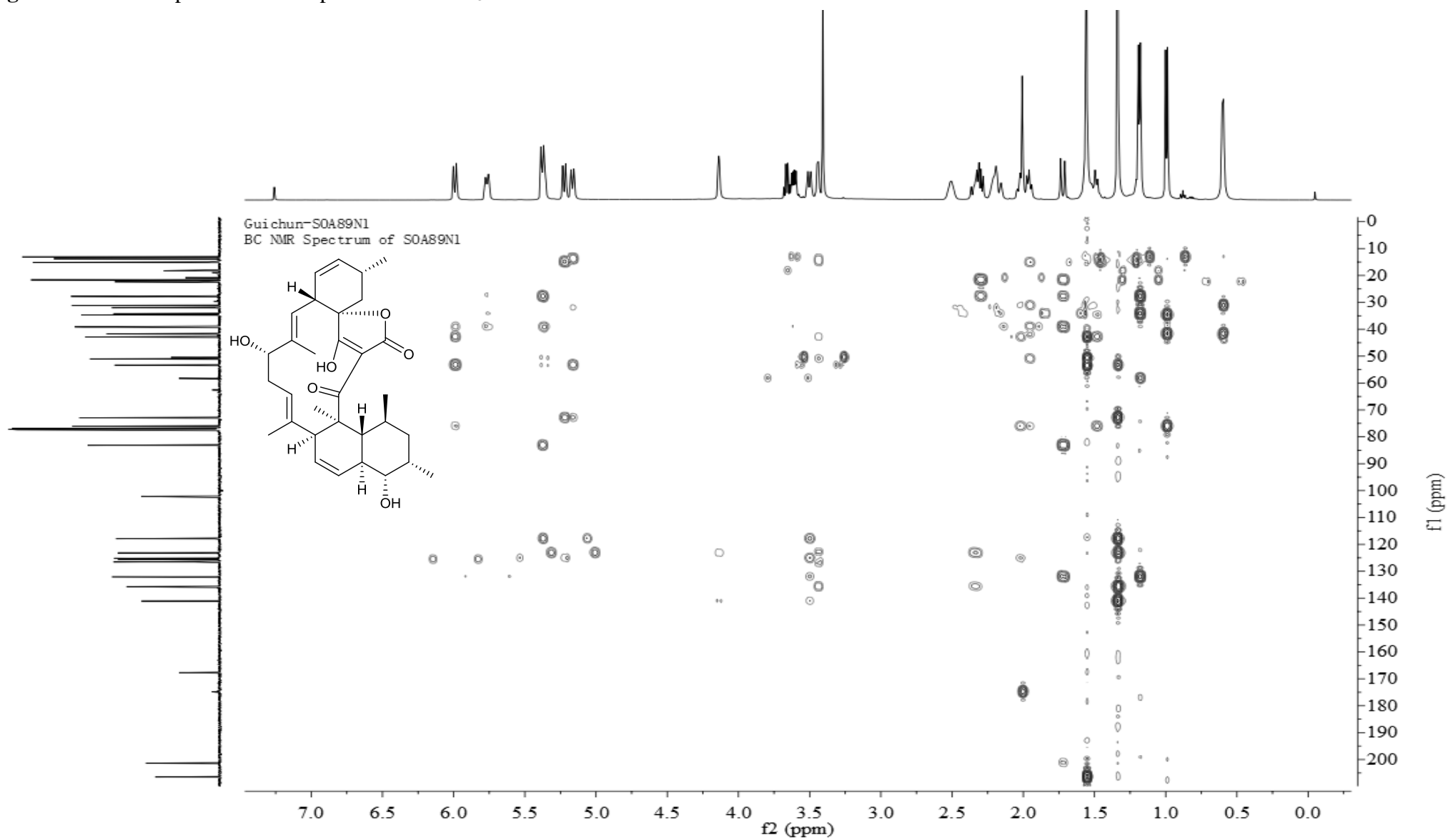


Figure S8. NOESY spectrum of compound **1** in CDCl₃.

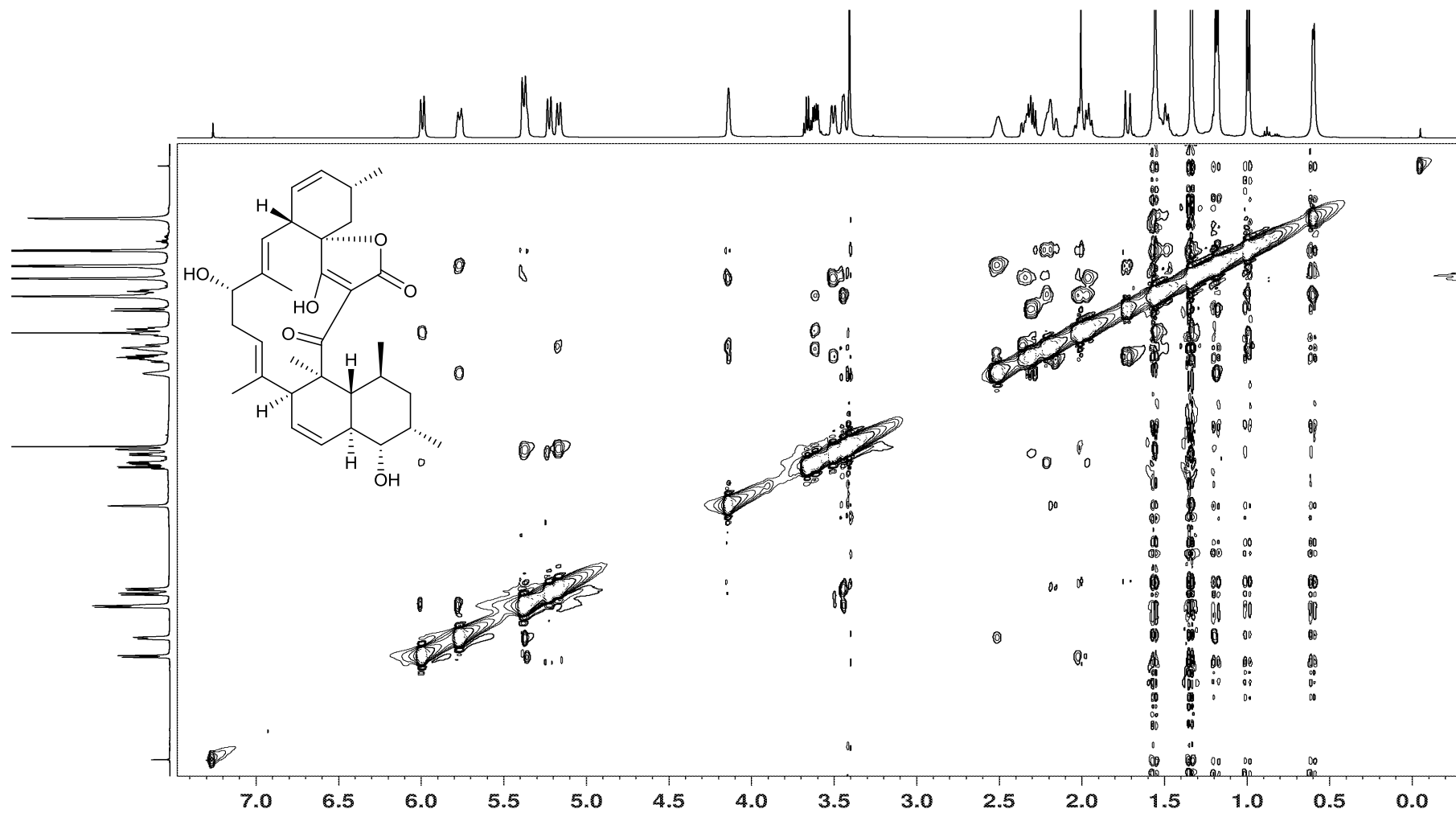


Figure S9. ^1H NMR (500 MHz) spectrum of compound **2** in CDCl_3 / CD_3OD .

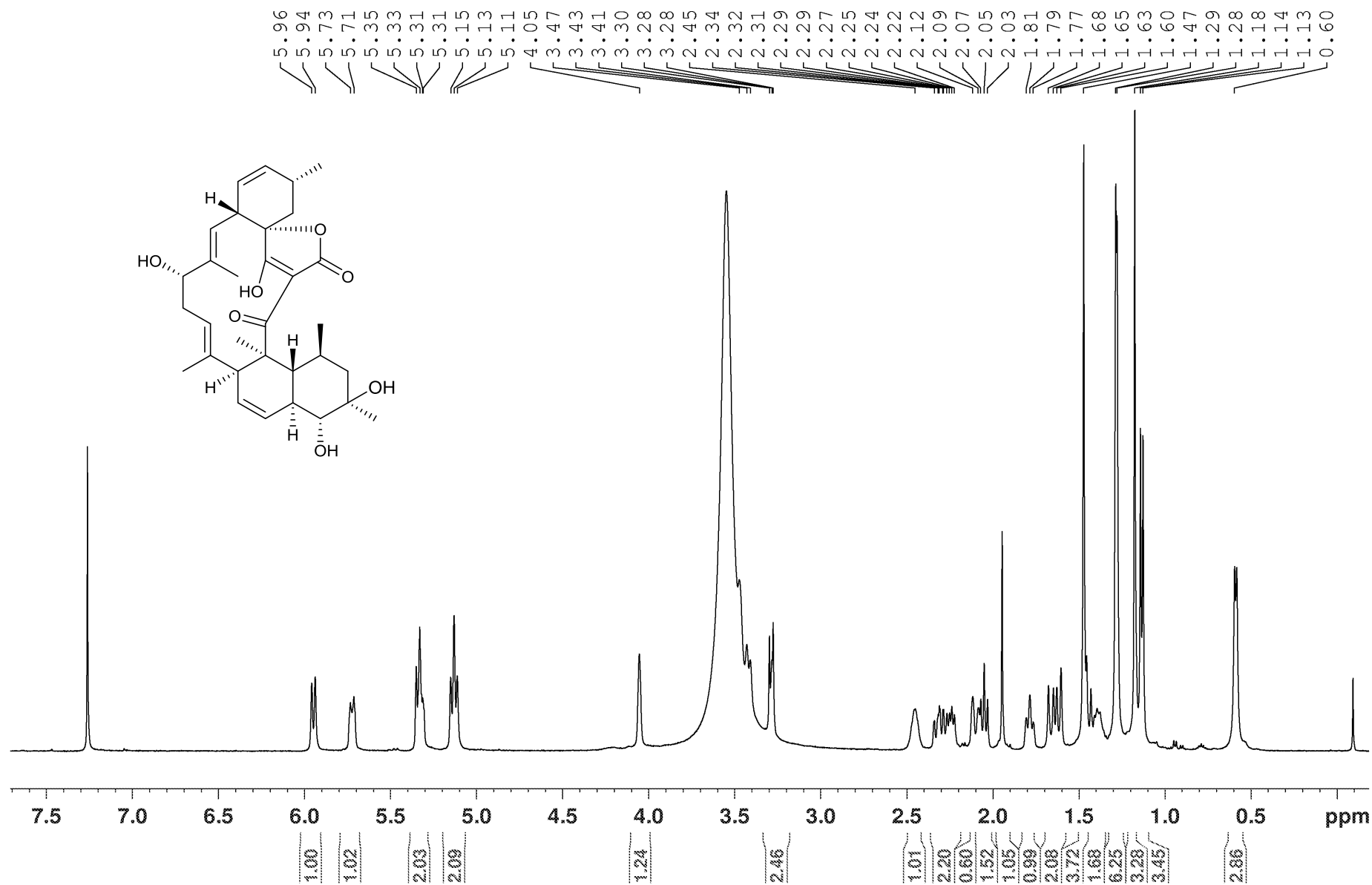


Figure S10. ^{13}C NMR (125 MHz) spectrum of compound **2** in $\text{CDCl}_3/\text{CD}_3\text{OD}$.

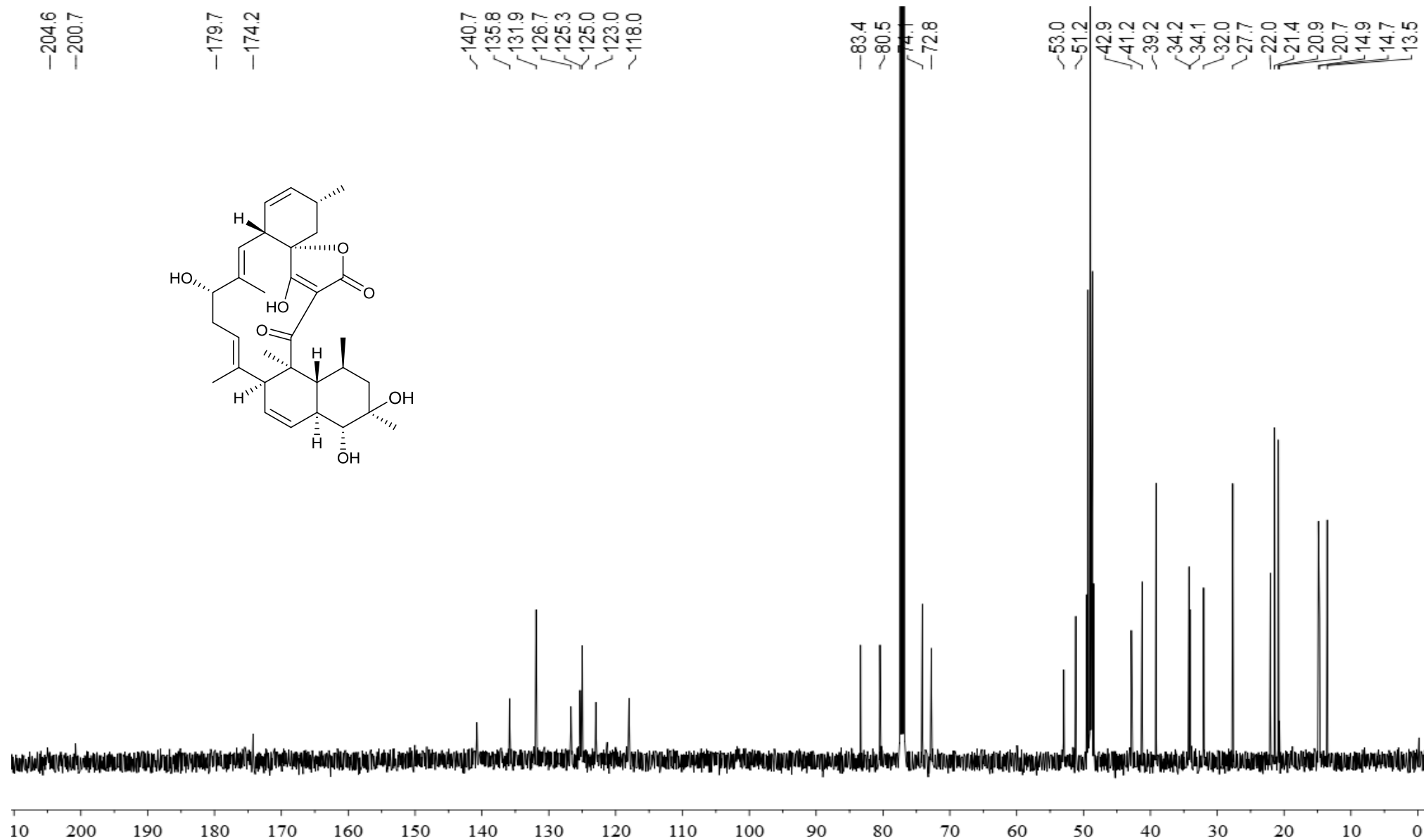


Figure S11. ^{13}C DEPT spectrum of compound **2** in $\text{CDCl}_3/\text{CD}_3\text{OD}$.

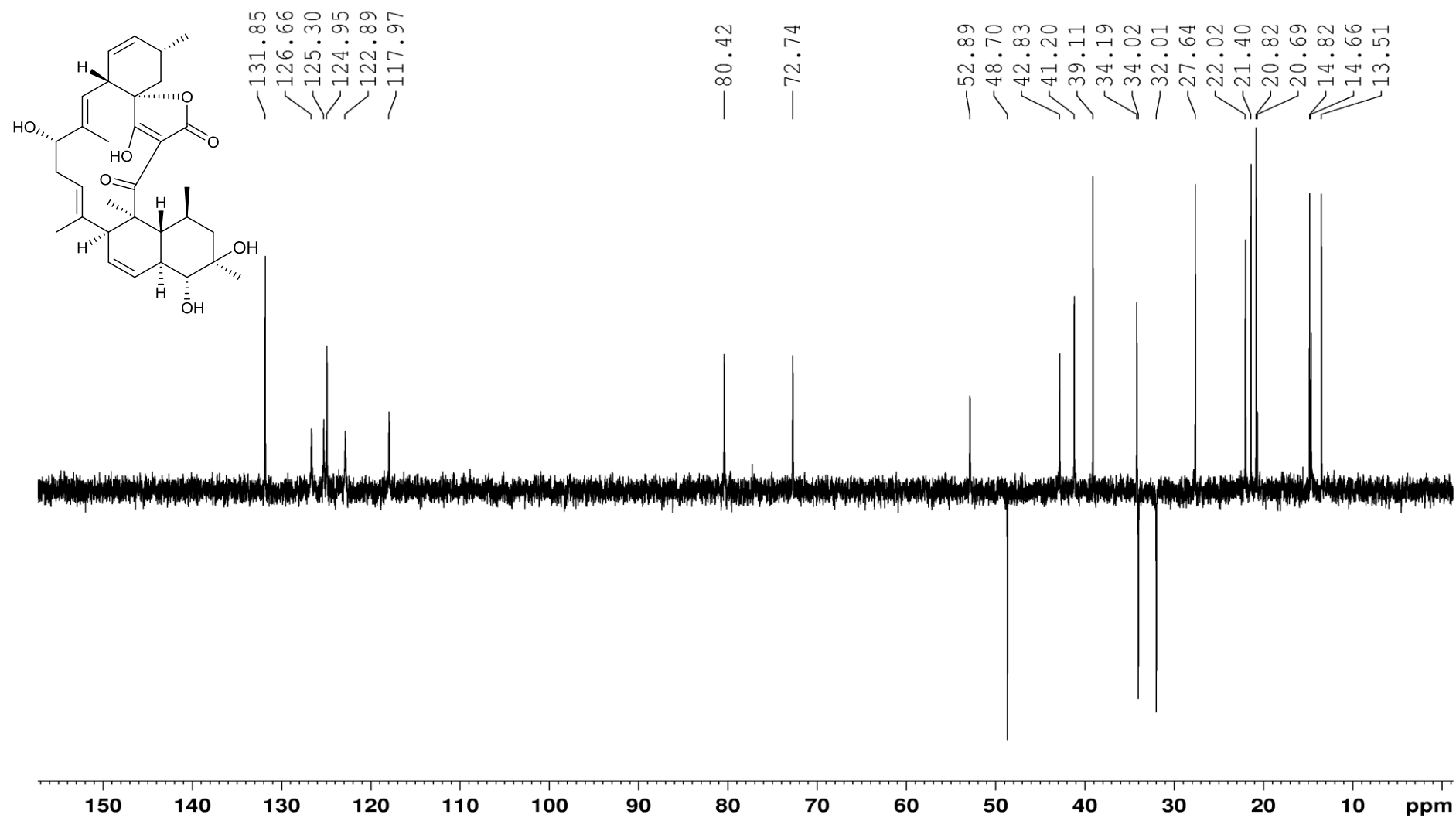


Figure S12. ^1H - ^1H COSY spectrum of compound **2** in $\text{CDCl}_3/\text{CD}_3\text{OD}$.

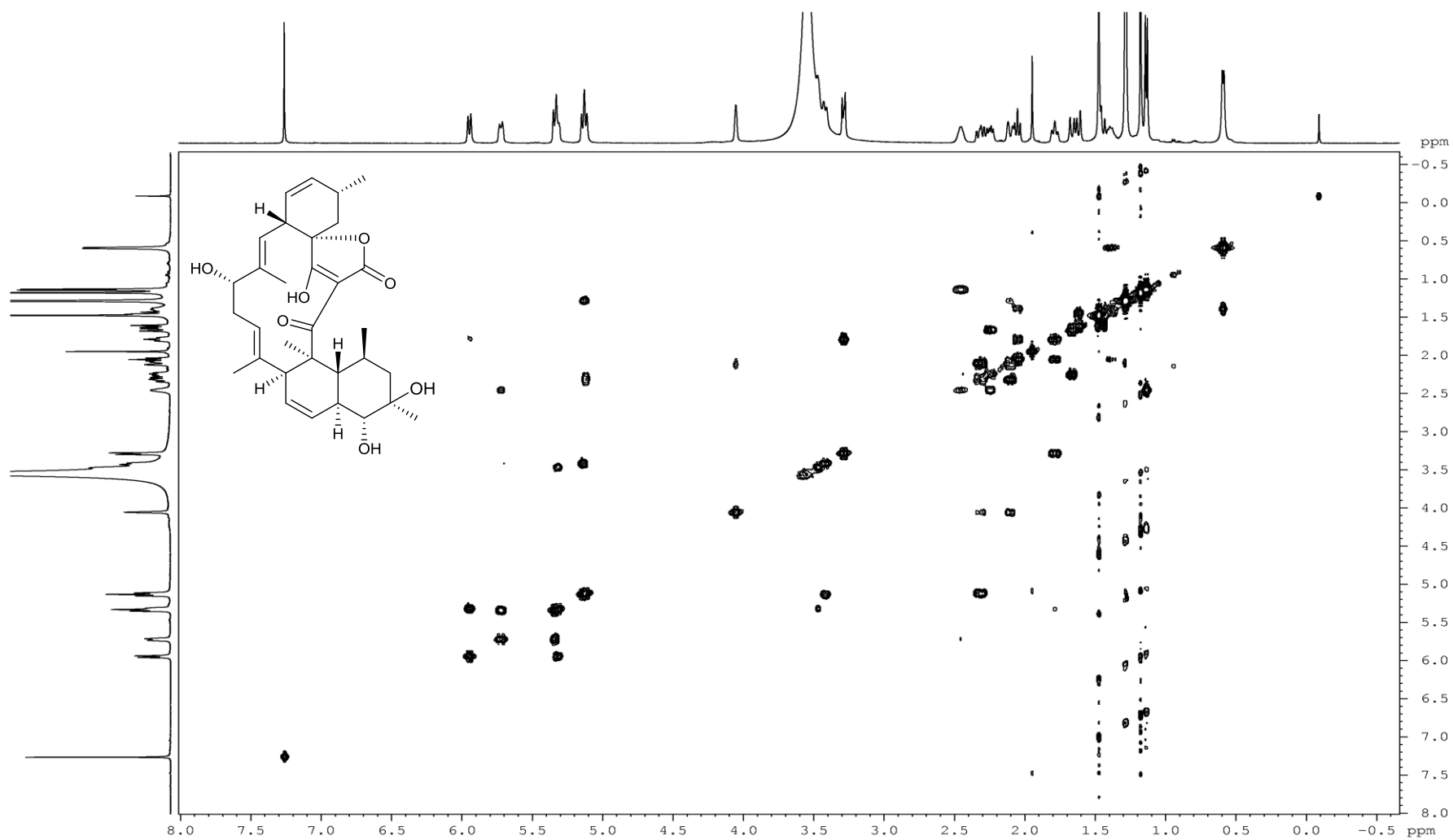


Figure S13. HSQC spectrum of compound **2** in CDCl₃/CD₃OD.

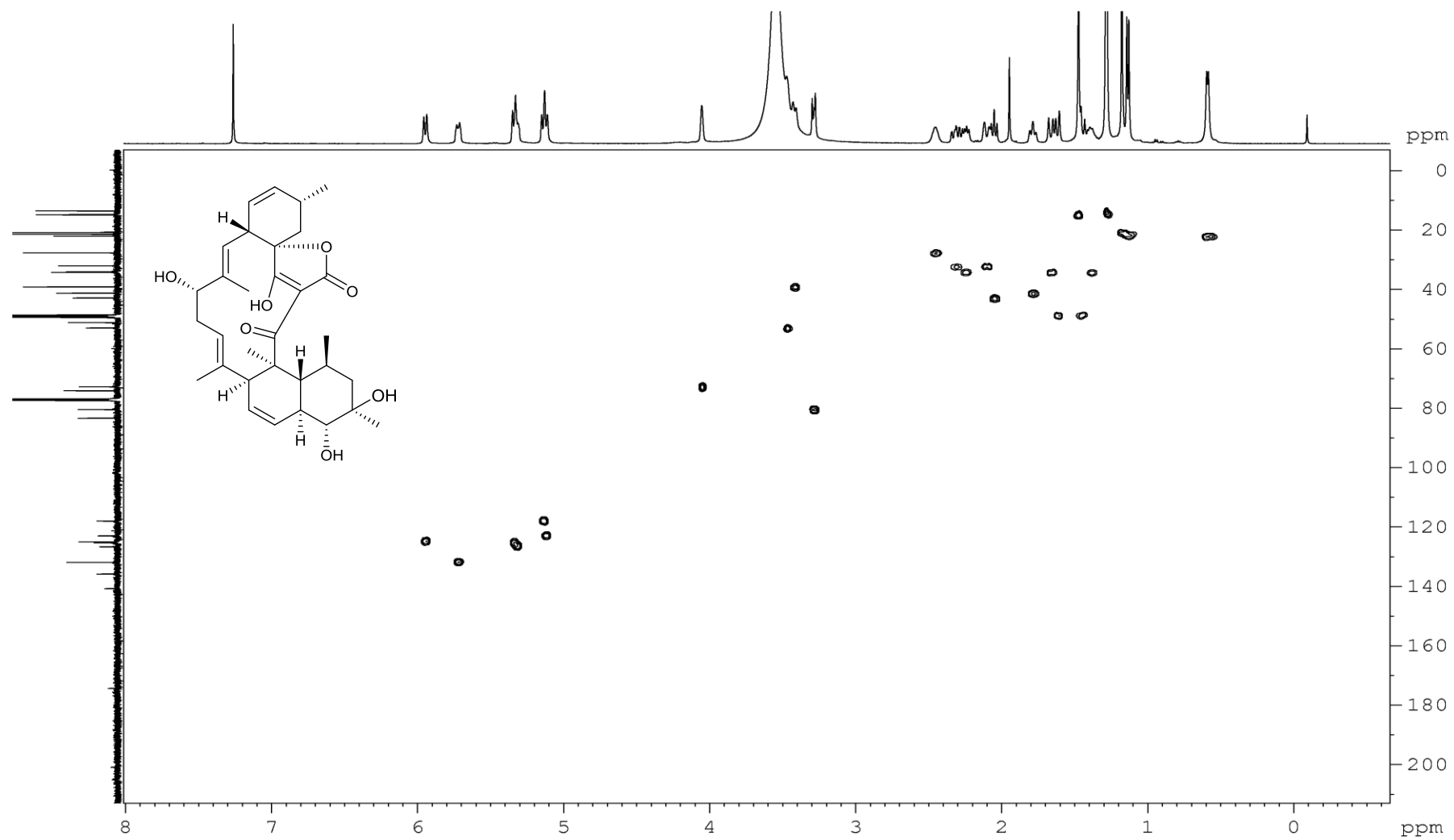


Figure S14. HMBC spectrum of compound **2** in CDCl₃/CD₃OD.

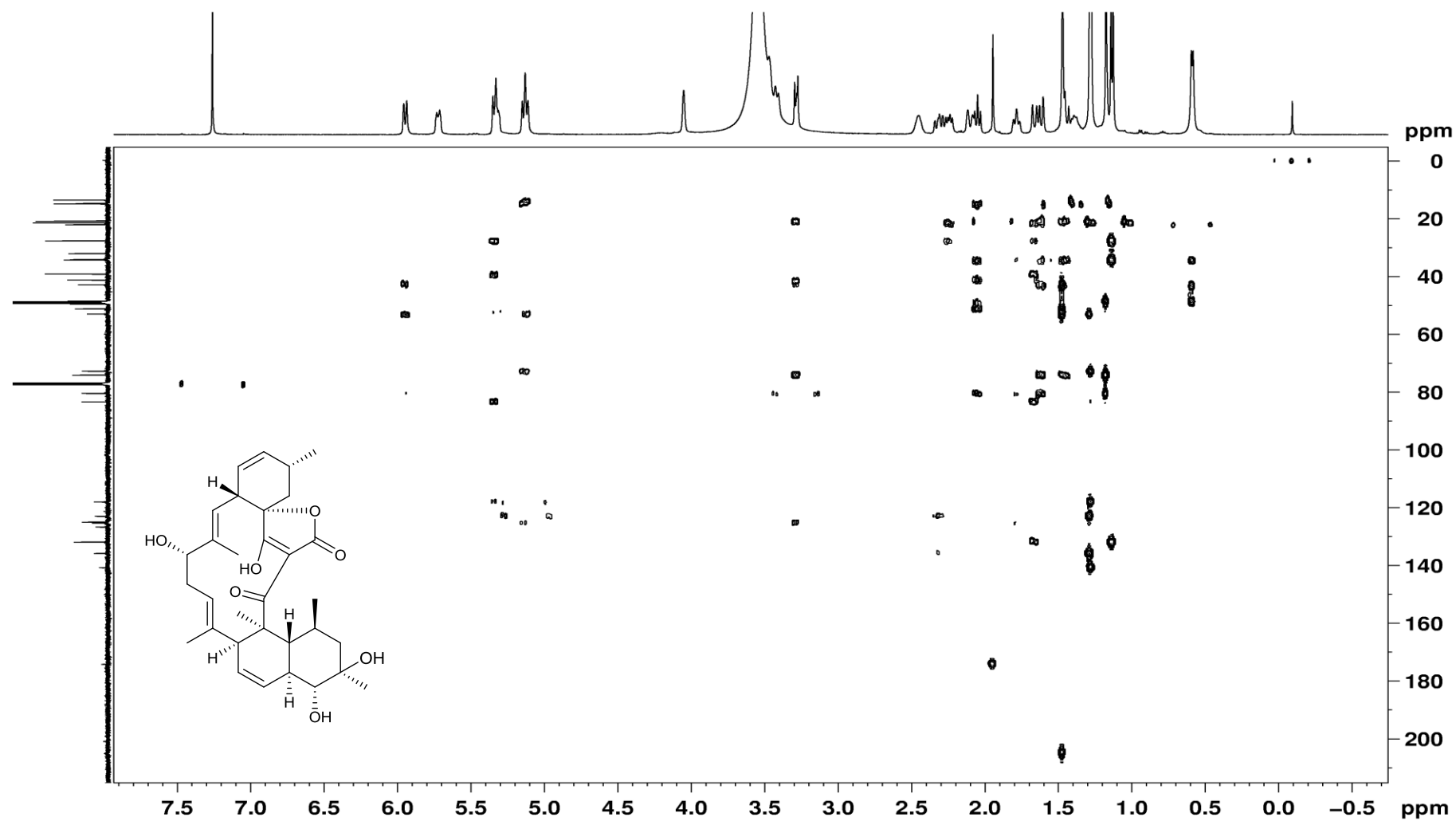


Figure S15. NOESY spectrum of compound **2** in CDCl₃/CD₃OD.

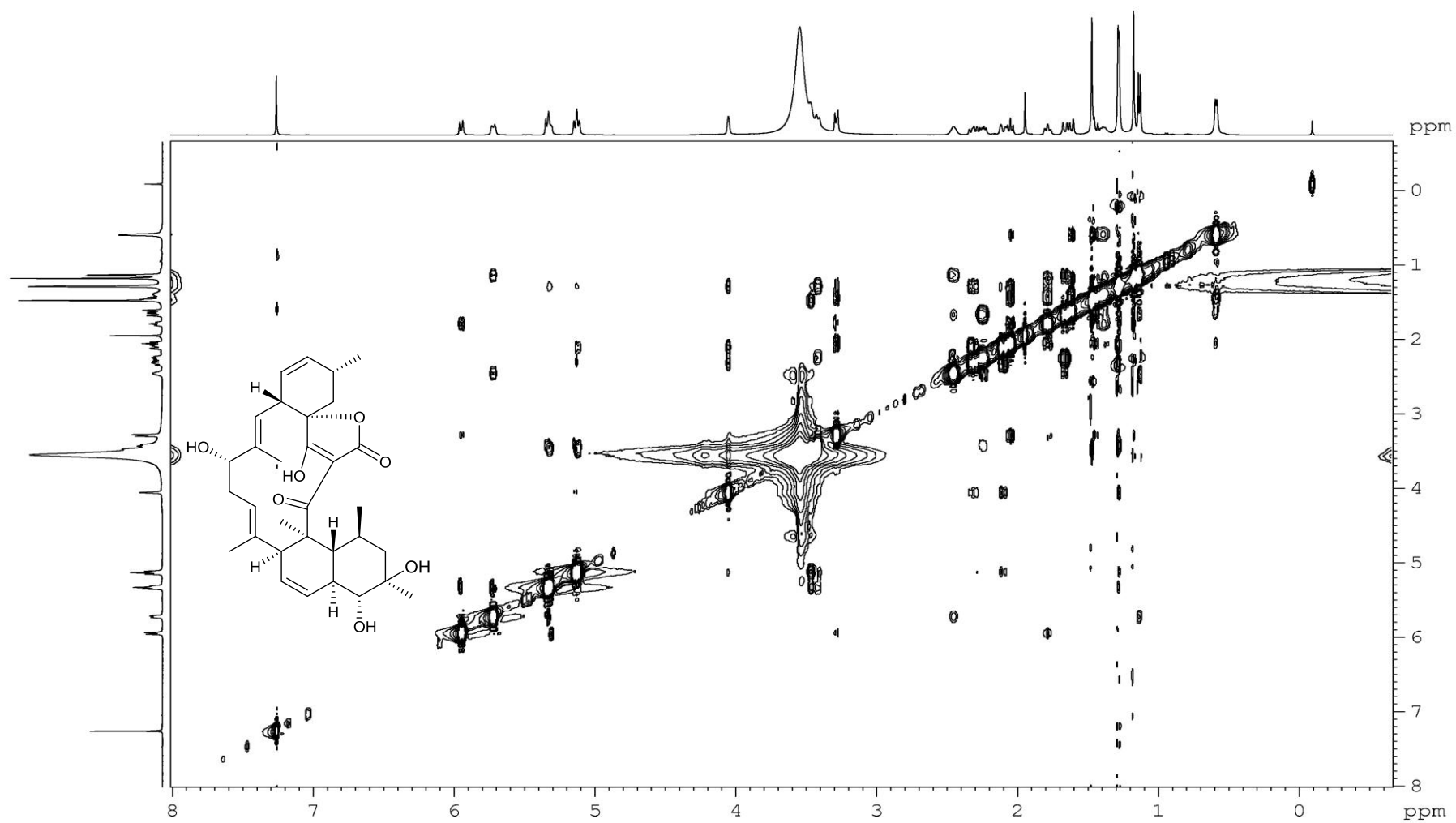


Figure S16. ^1H NMR (500 MHz) spectrum of compound **3** in CDCl_3 .

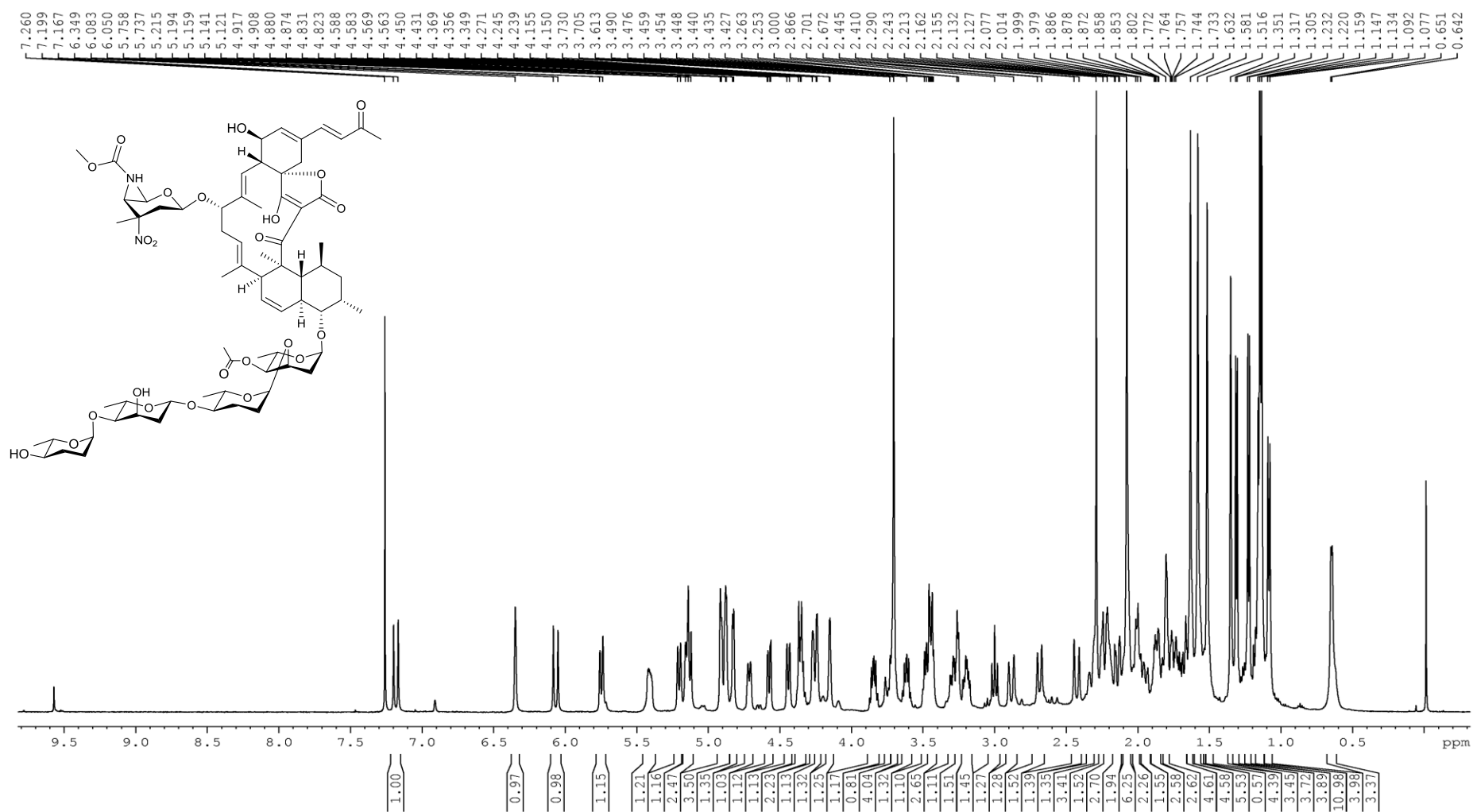


Figure S17. ^{13}C NMR (125 MHz) spectrum of compound **3** in CDCl_3 .

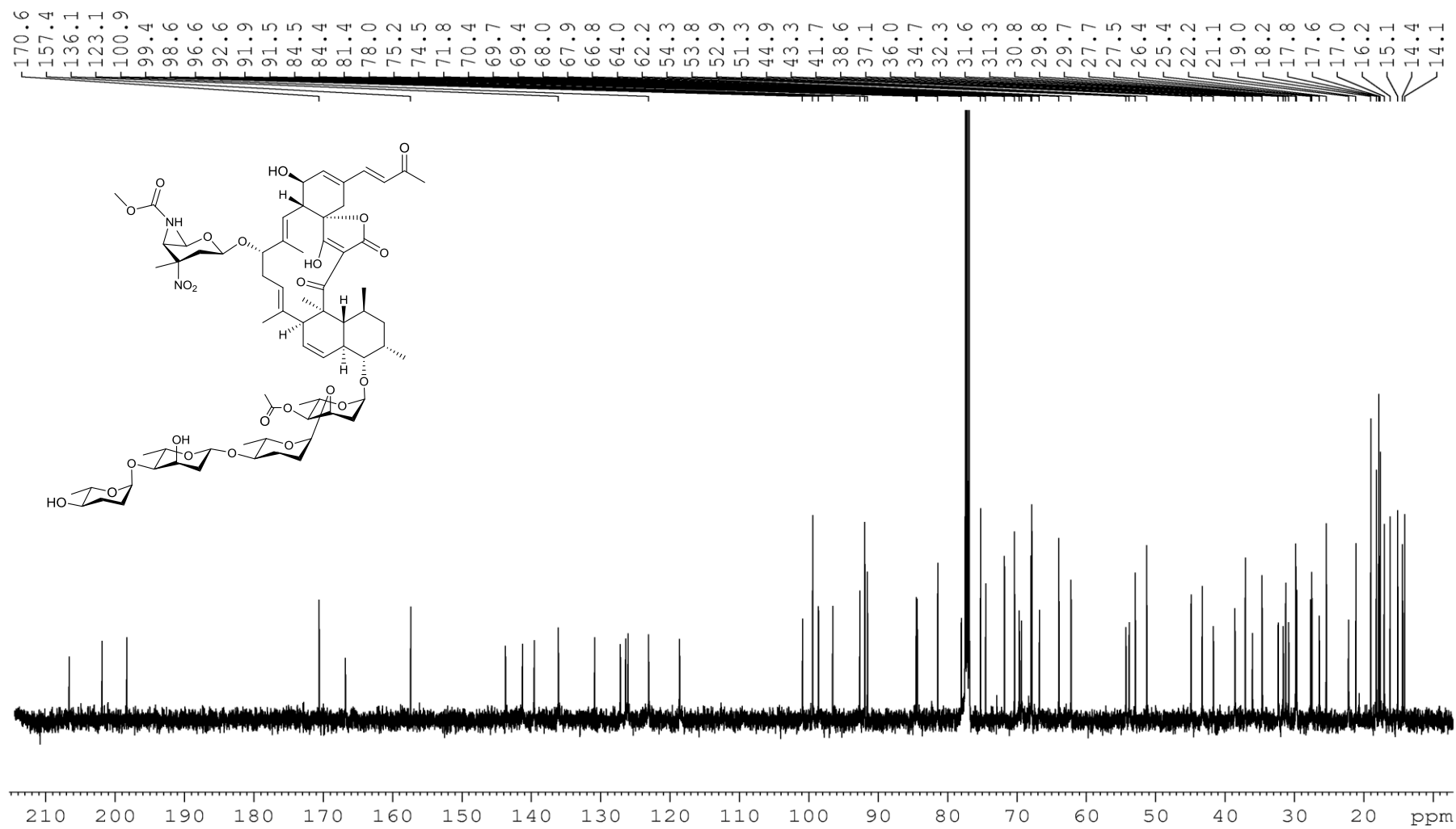


Figure S18. ^{13}C DEPT spectrum of compound **3** in CDCl_3 .

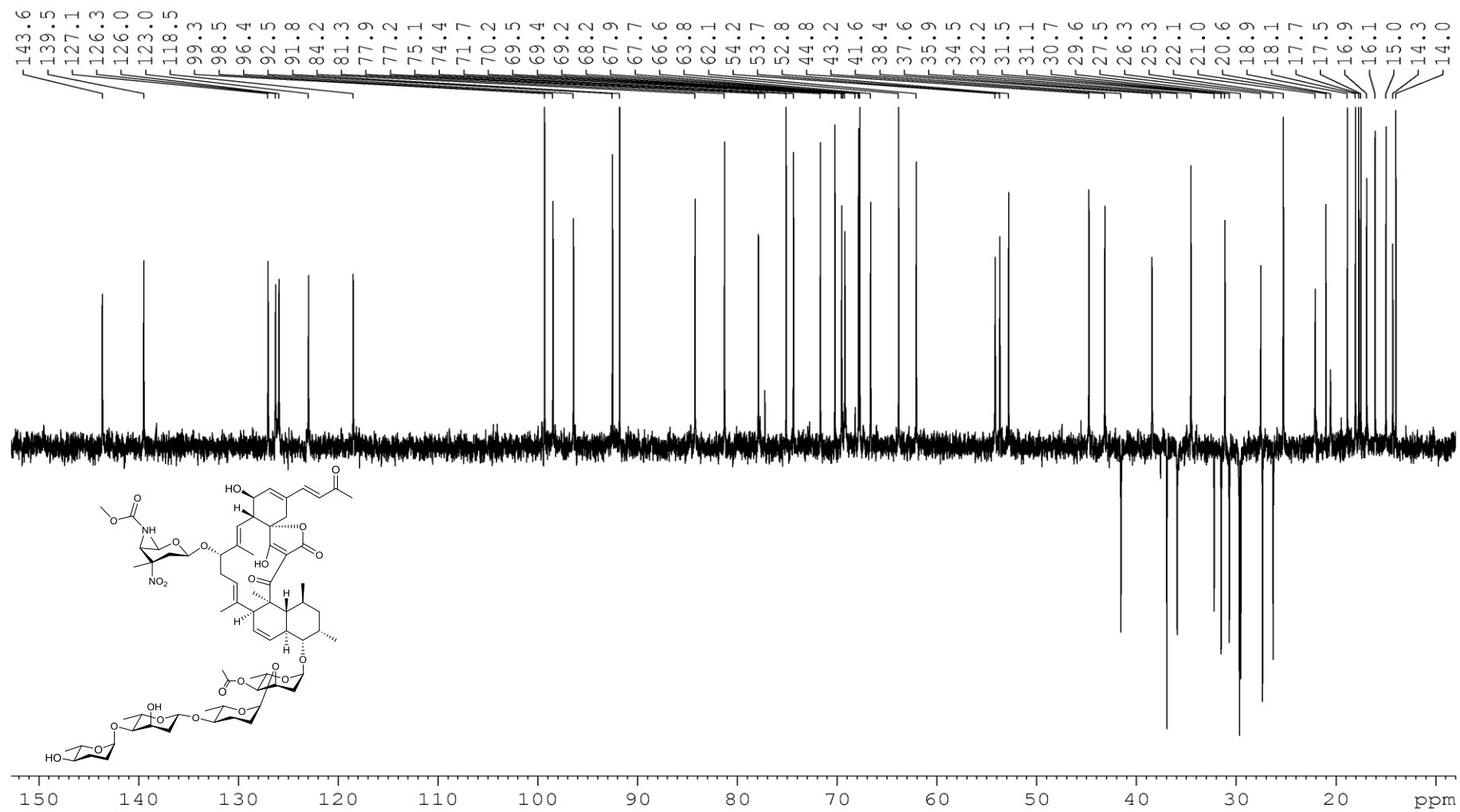


Figure S19. ^1H - ^1H COSY spectrum of compound **3** in CDCl_3 .

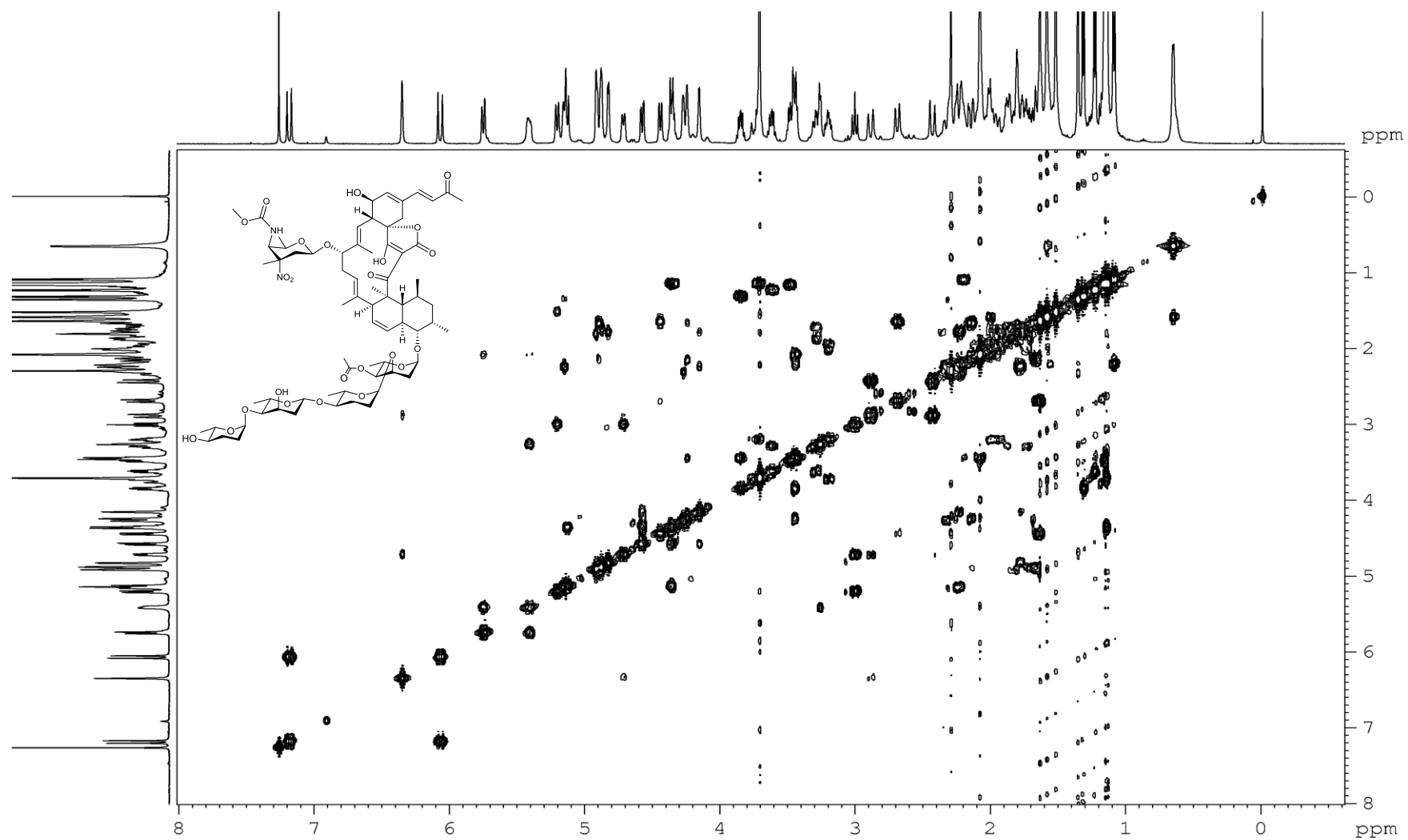


Figure S20. HSQC spectrum of compound **3** in CDCl₃.

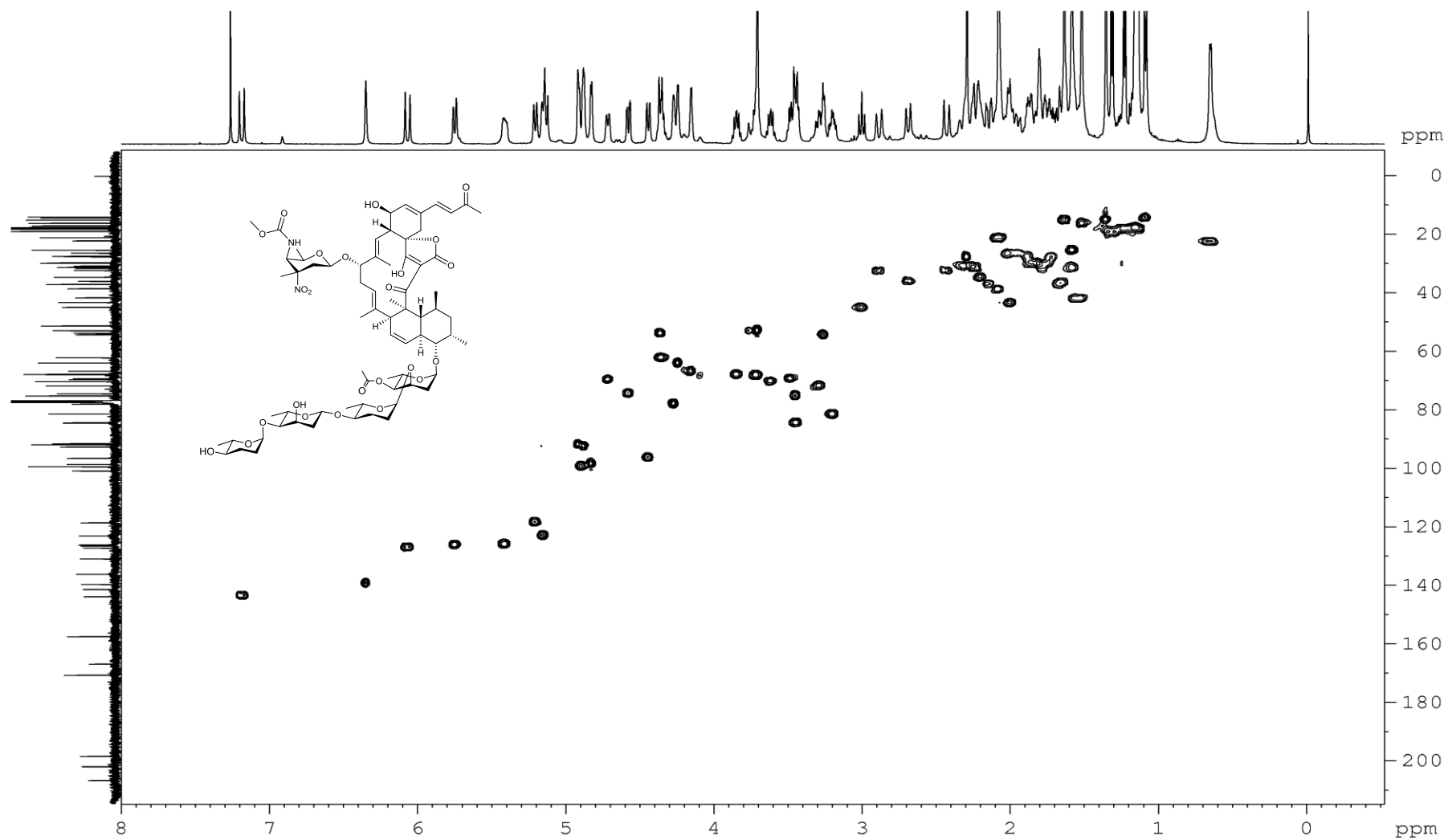


Figure S21. HMBC spectrum of compound **3** in CDCl₃.

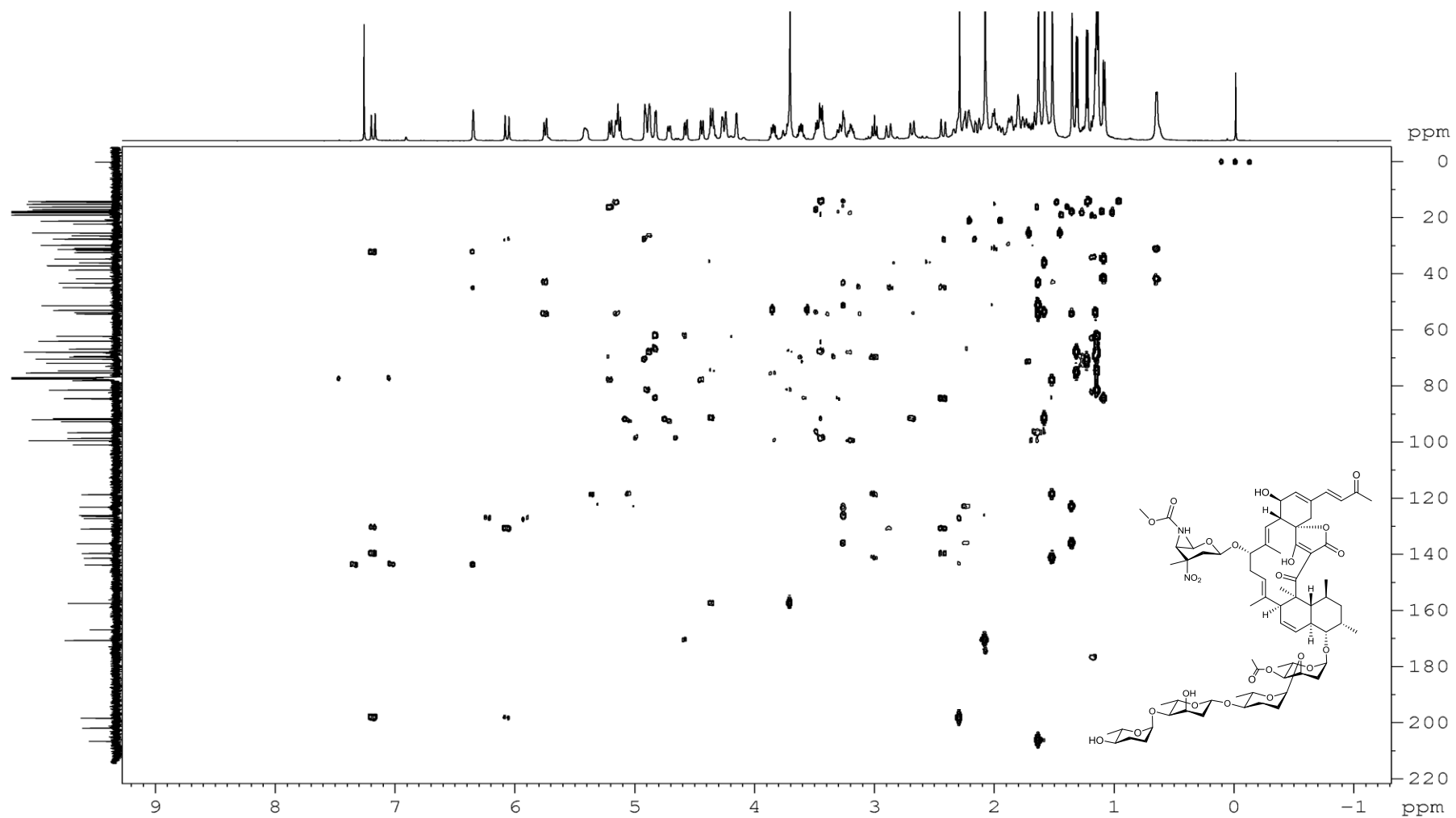


Figure S22. NOESY spectrum of compound **3** in CDCl₃.

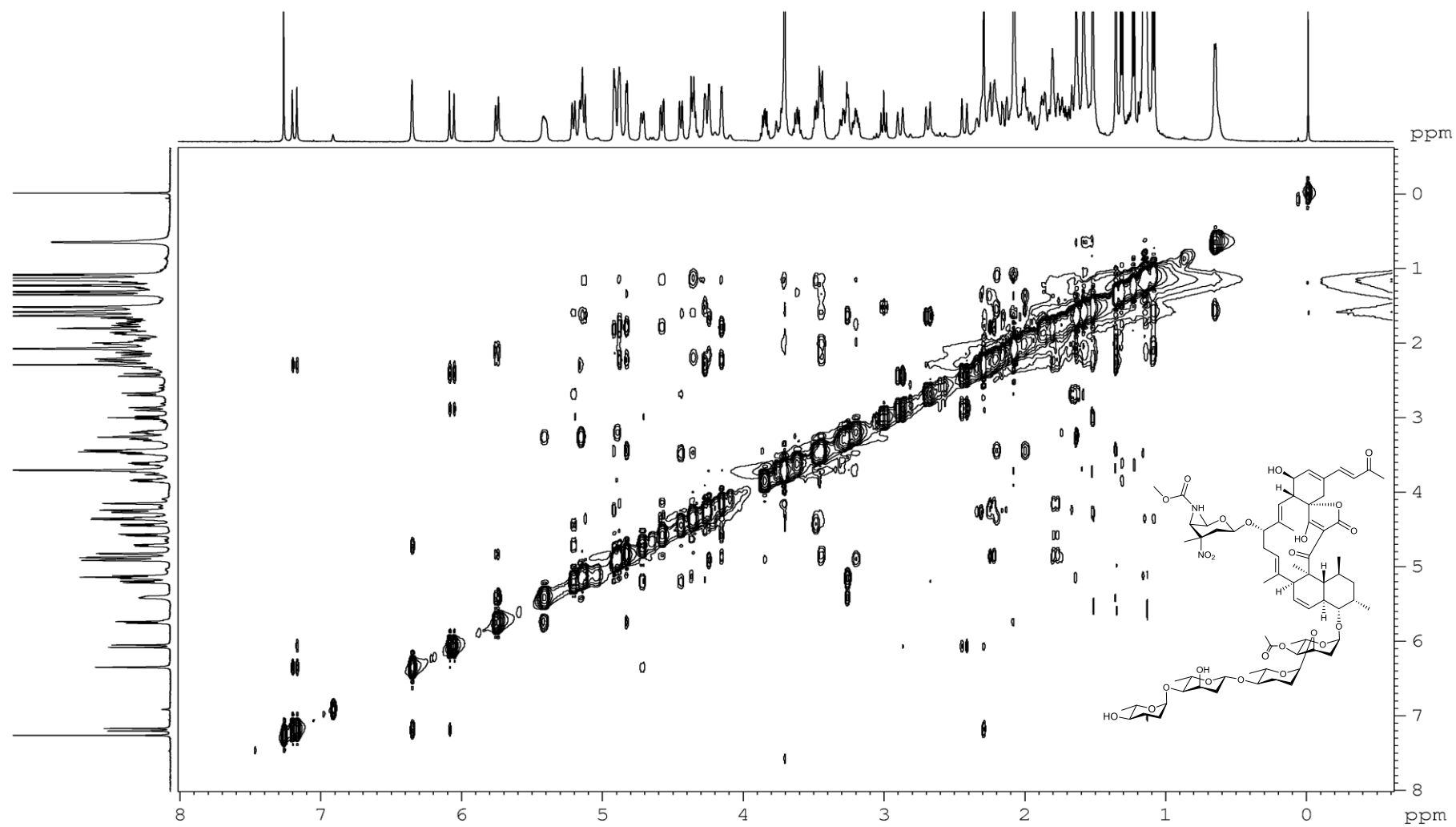


Figure S23. ^1H NMR (500 MHz) spectrum of compound **4** in CDCl_3 .

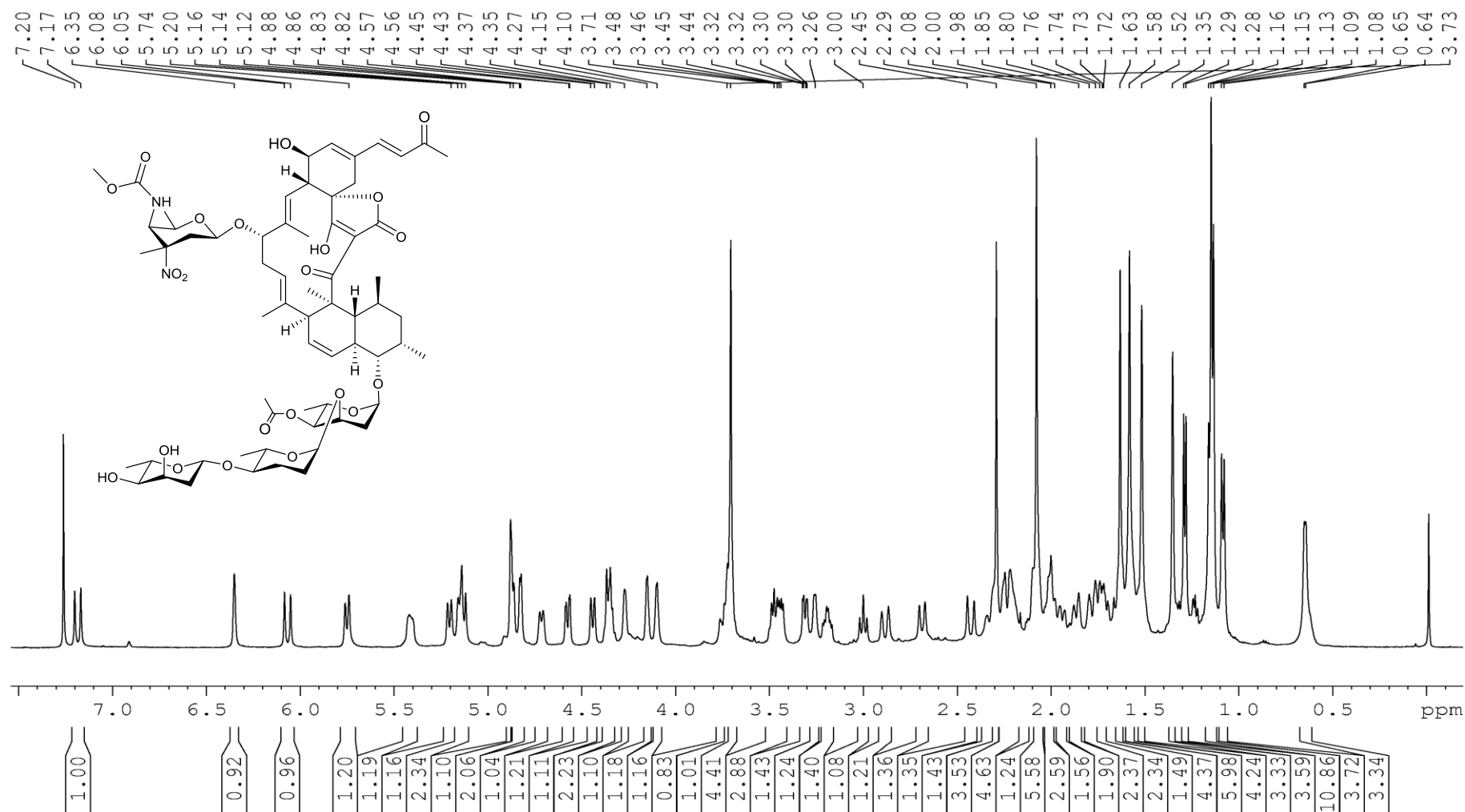
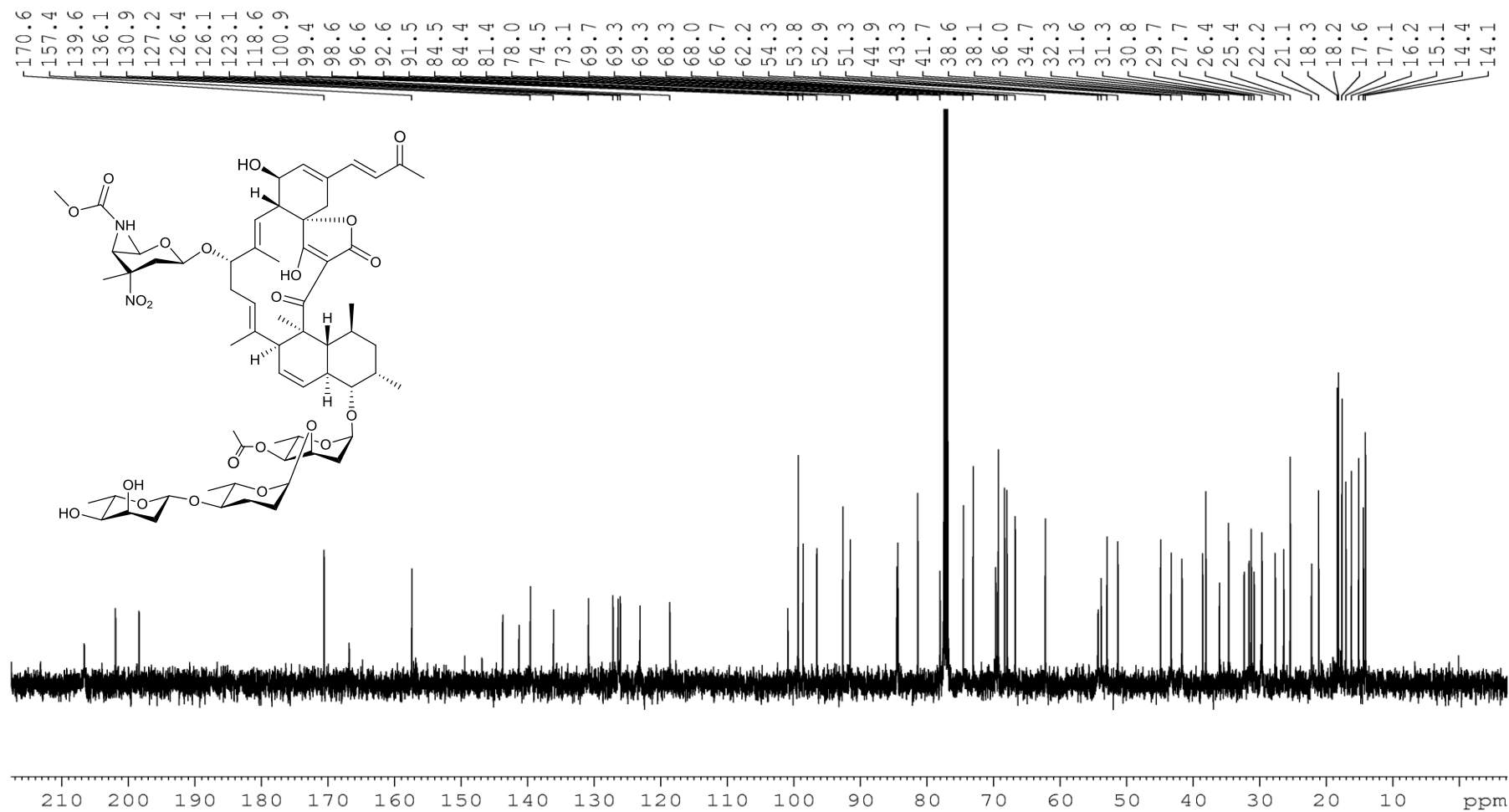


Figure S24. ^{13}C NMR (125 MHz) spectrum of compound **4** in CDCl_3 .



Chemical structure of compound 1 is shown in the top left corner. The structure is a complex polycyclic molecule with multiple sugar units and a nitro group. The ^{13}C NMR spectrum is displayed below the structure, with peaks labeled with their chemical shifts in ppm. The peaks are:

- 143.6
- 139.5
- 127.1
- 126.3
- 126.0
- 123.0
- 118.5
- 99.2
- 98.5
- 96.4
- 92.5
- 84.3
- 81.3
- 77.9
- 77.2
- 74.4
- 72.9
- 69.5
- 69.2
- 69.2
- 68.2
- 67.9
- 66.6
- 62.1
- 54.2
- 53.7
- 52.8
- 44.8
- 43.2
- 41.6
- 38.4
- 38.0
- 35.9
- 34.5
- 32.2
- 31.5
- 31.1
- 30.7
- 29.6
- 27.5
- 26.3
- 25.3
- 22.1
- 21.0
- 18.2
- 18.1

Figure S26. ^1H - ^1H COSY spectrum of compound **4** in CDCl_3 .

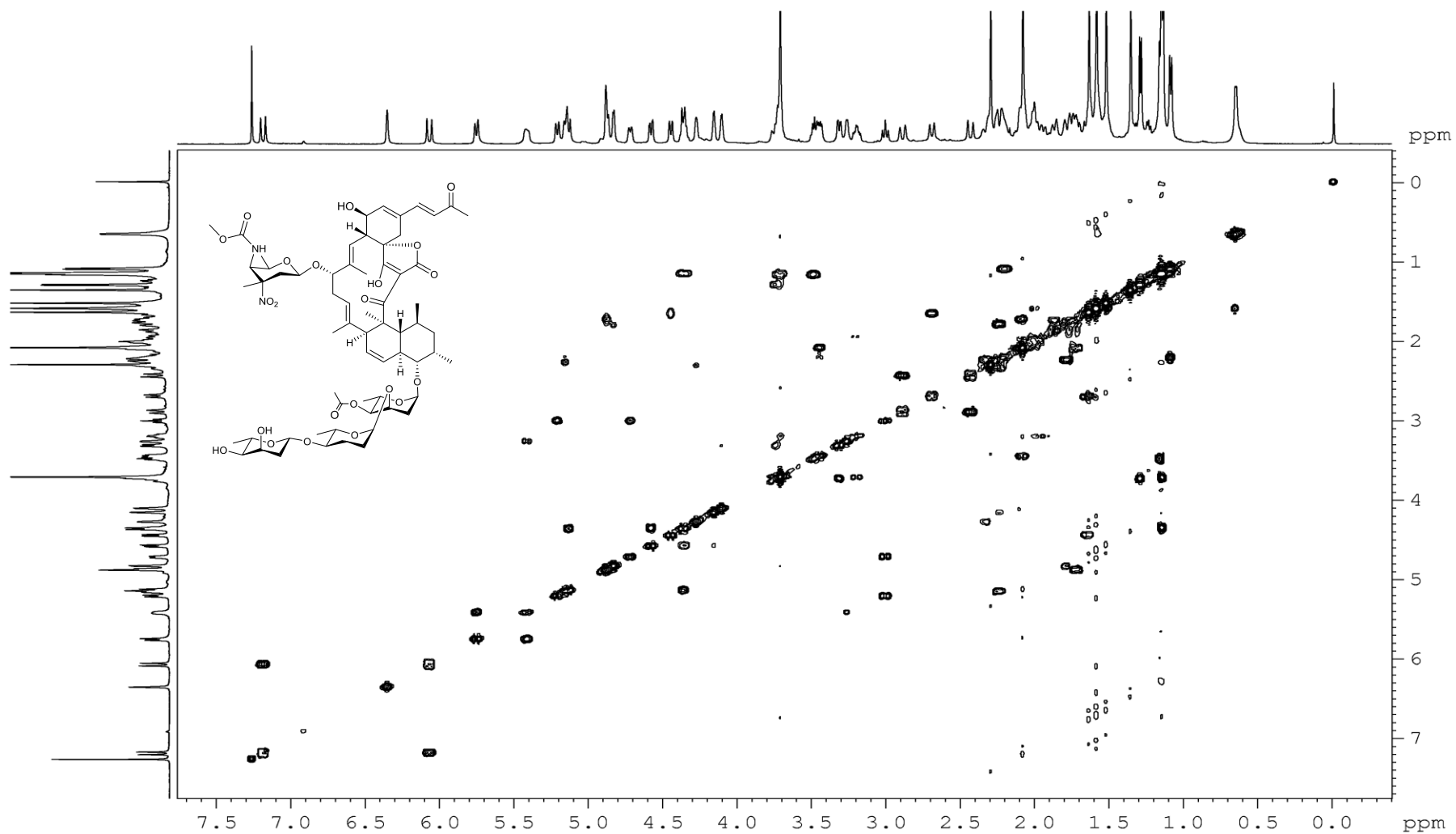


Figure S27. HSQC spectrum of compound **4** in CDCl₃.

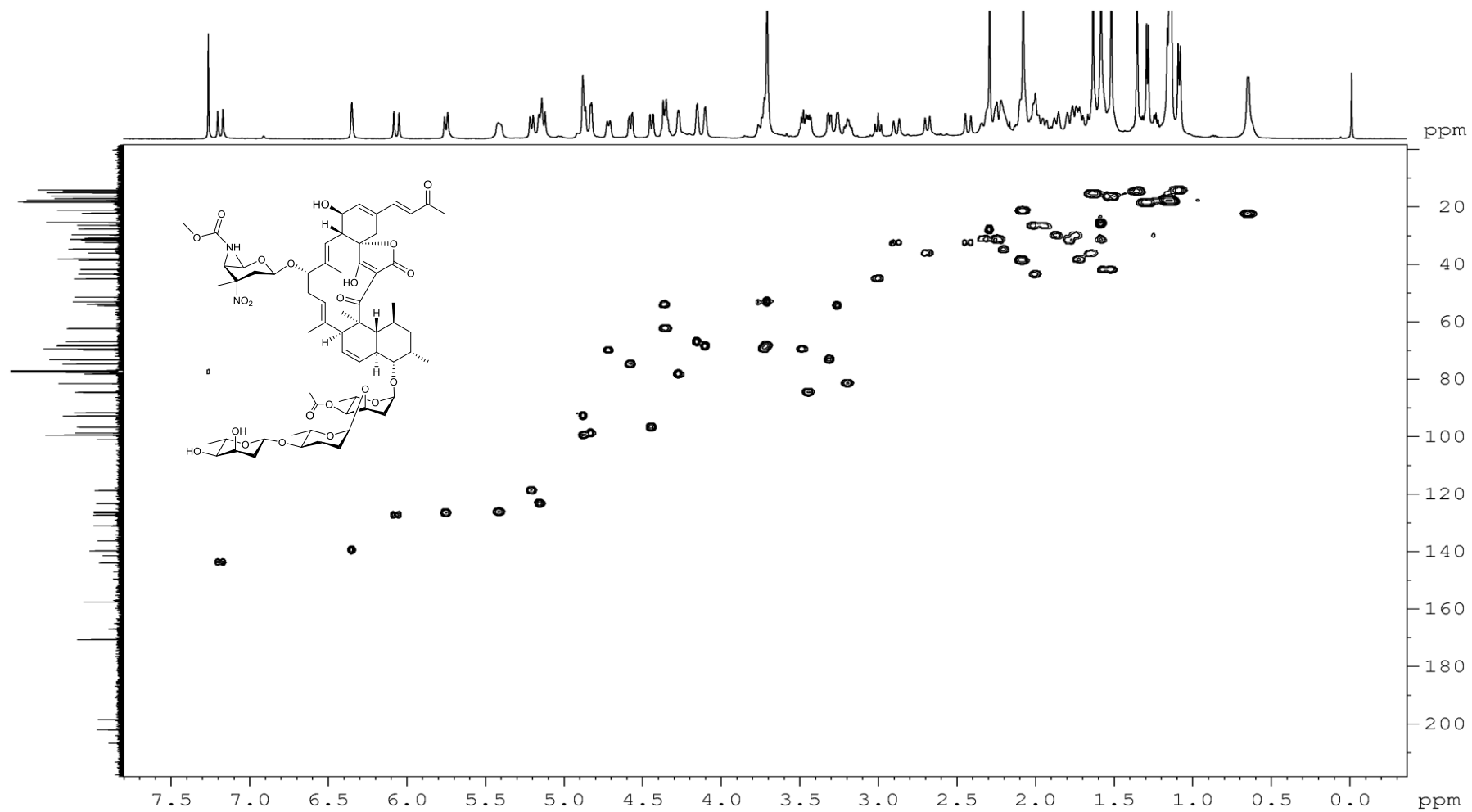


Figure S28. HMBC spectrum of compound **4** in CDCl₃.

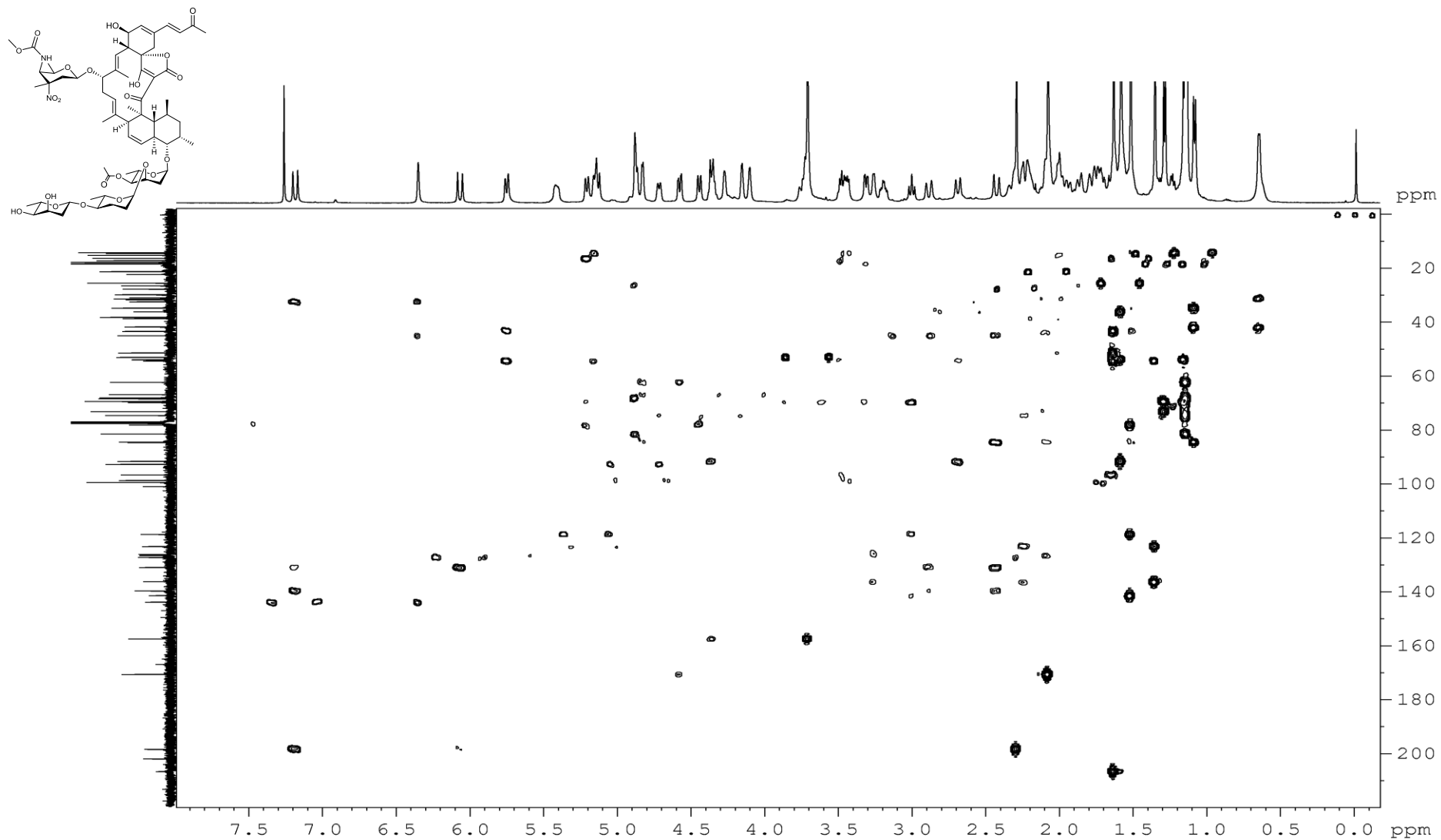


Figure S29. NOESY spectrum of compound **4** in CDCl₃.

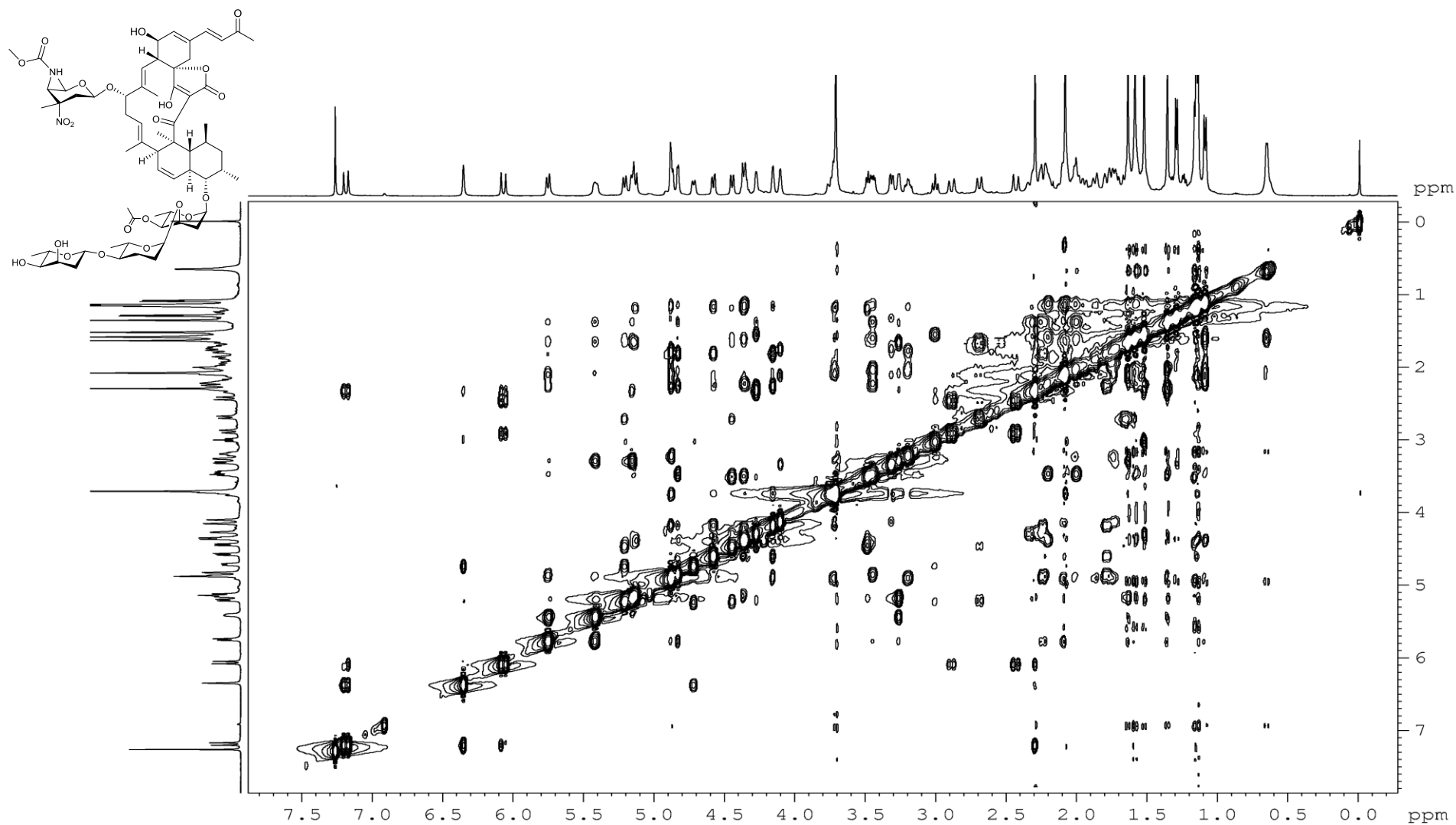


Figure S30. ^1H NMR (500 MHz) spectrum of compound **5** in CDCl_3 .

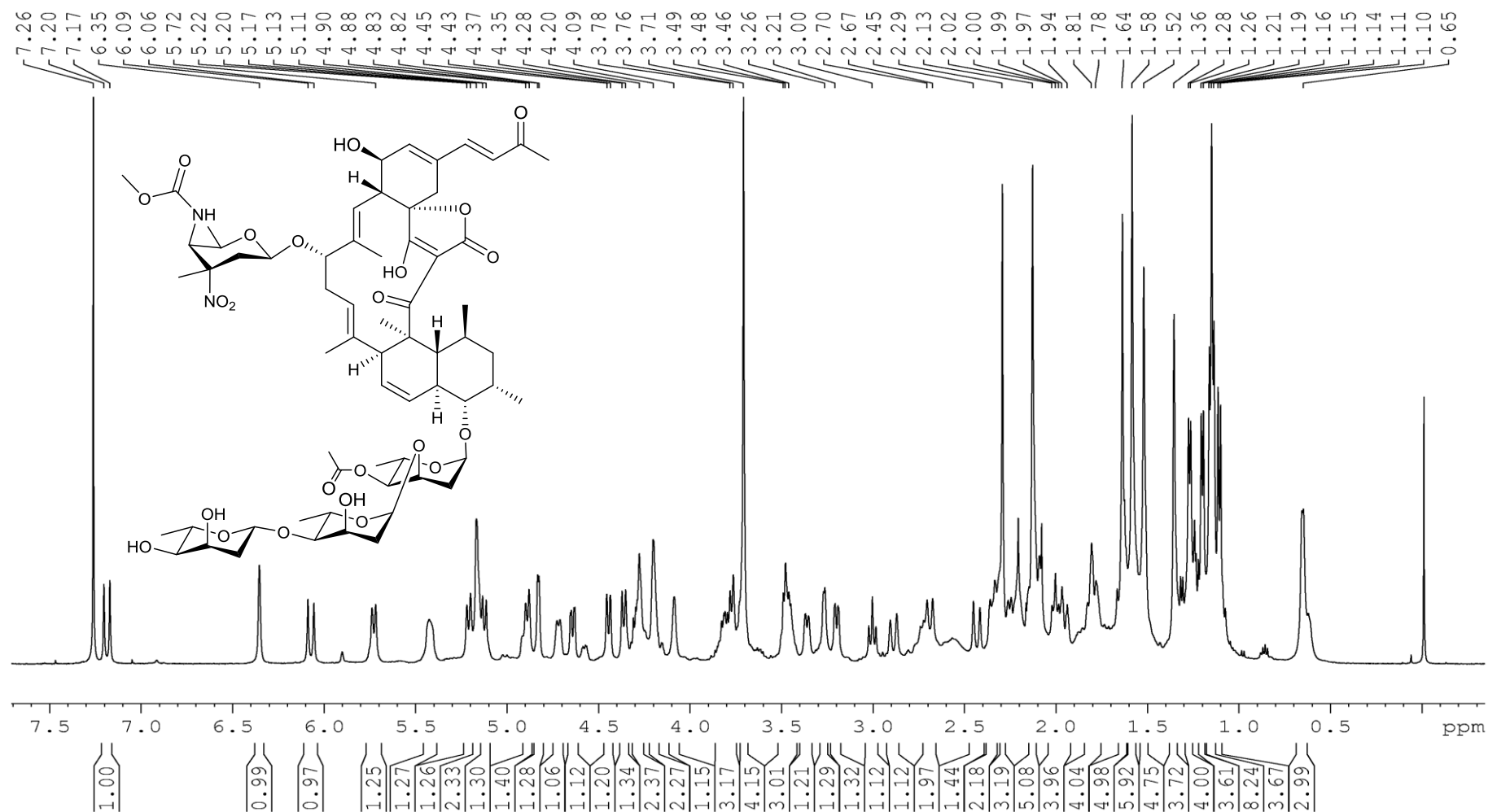


Figure S31. ^{13}C NMR (125 MHz) spectrum of compound **5** in CDCl_3 .

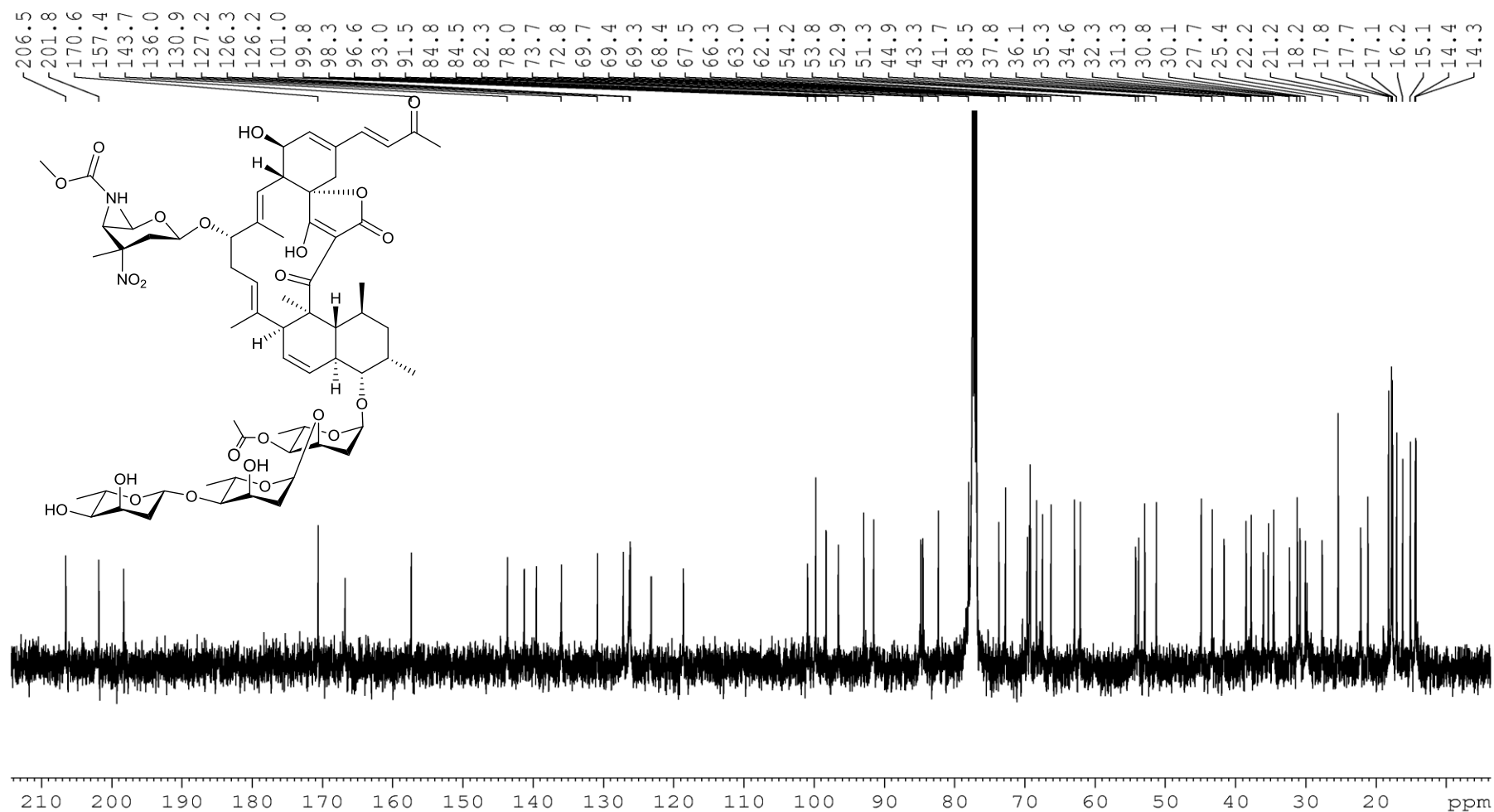


Figure S32. ^{13}C DEPT spectrum of compound **5** in CDCl_3 .

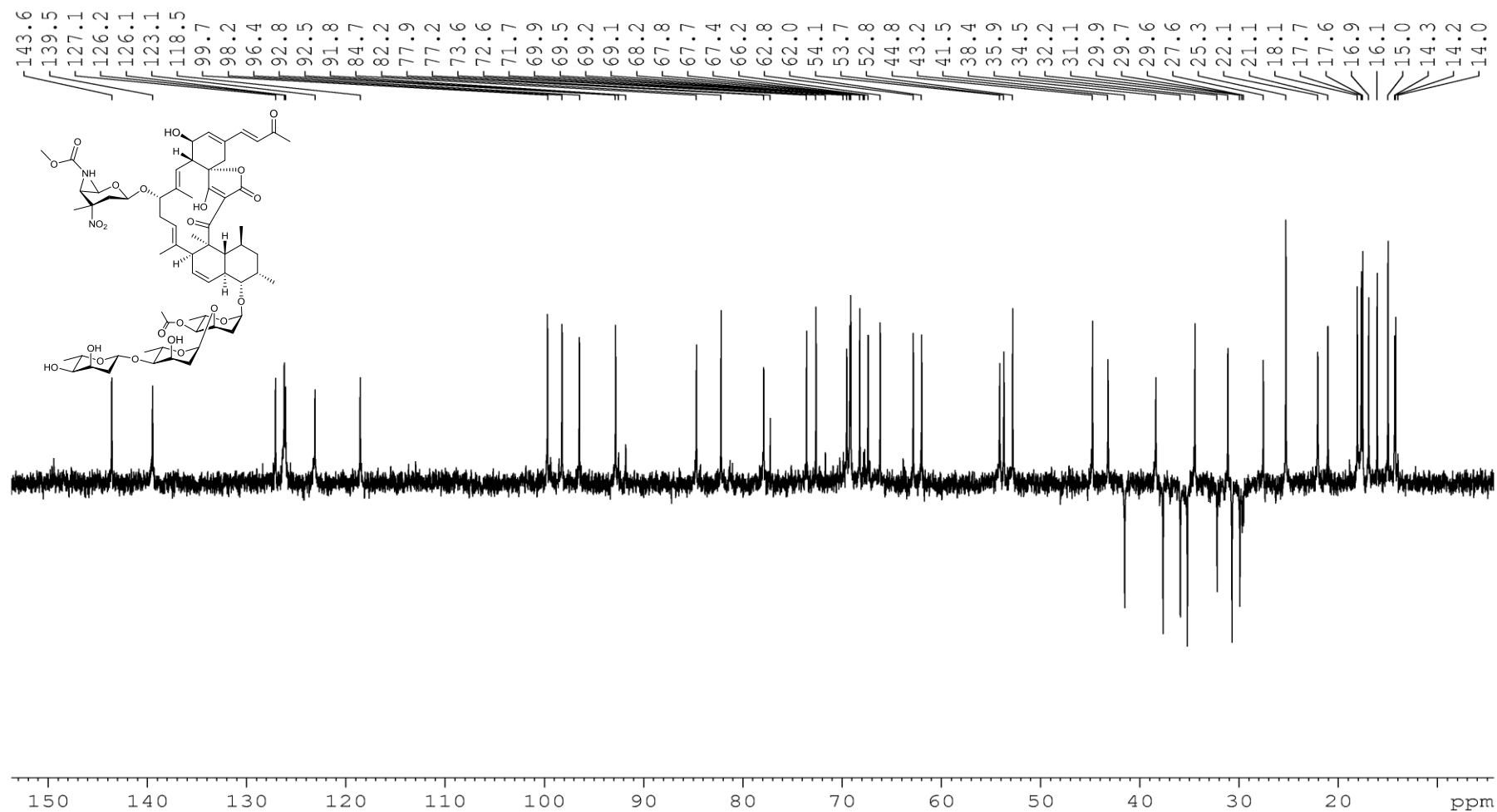


Figure S33. ^1H - ^1H COSY spectrum of compound **5** in CDCl_3 .

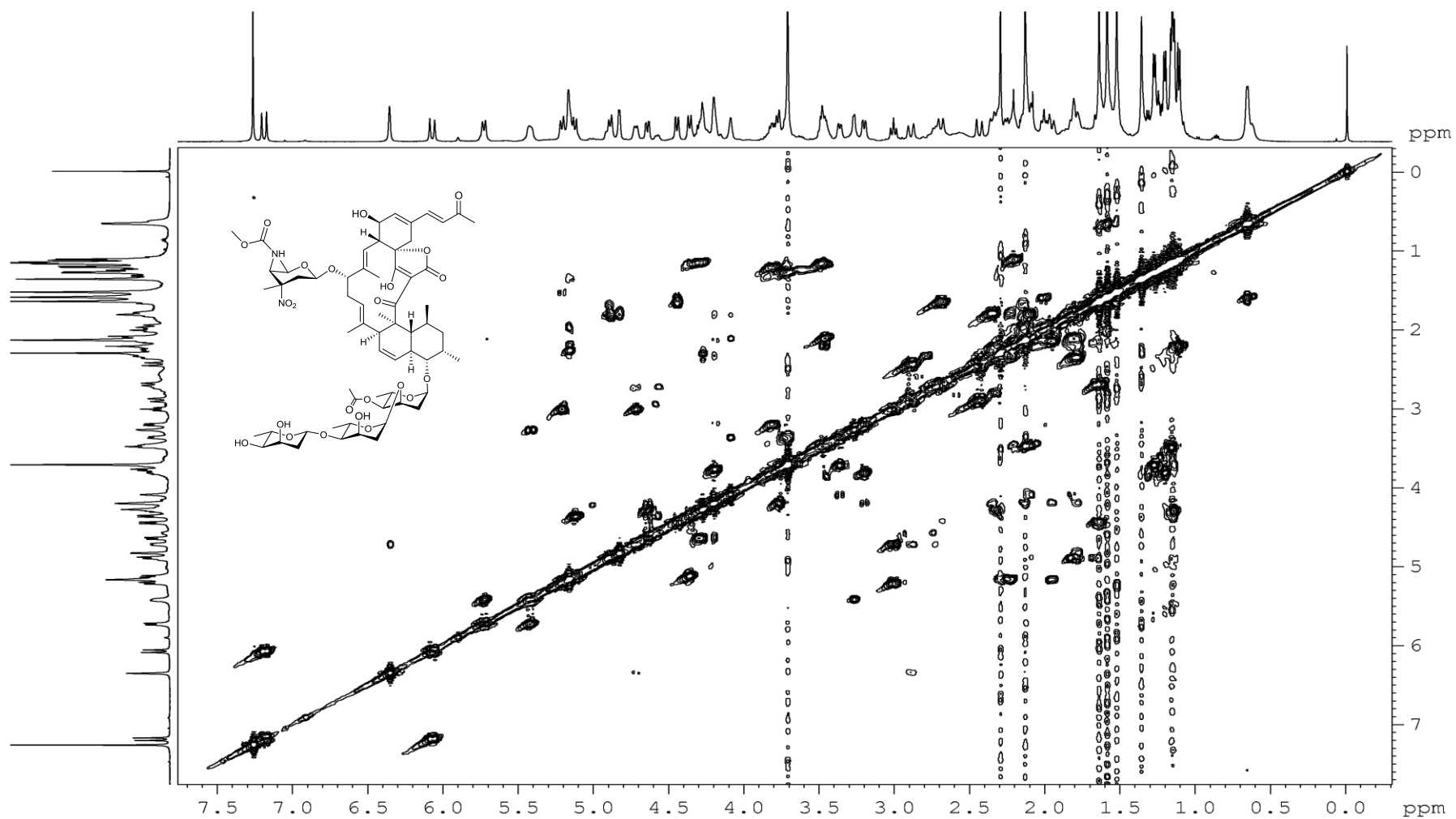


Figure S34. HSQC spectrum of compound **5** in CDCl₃.

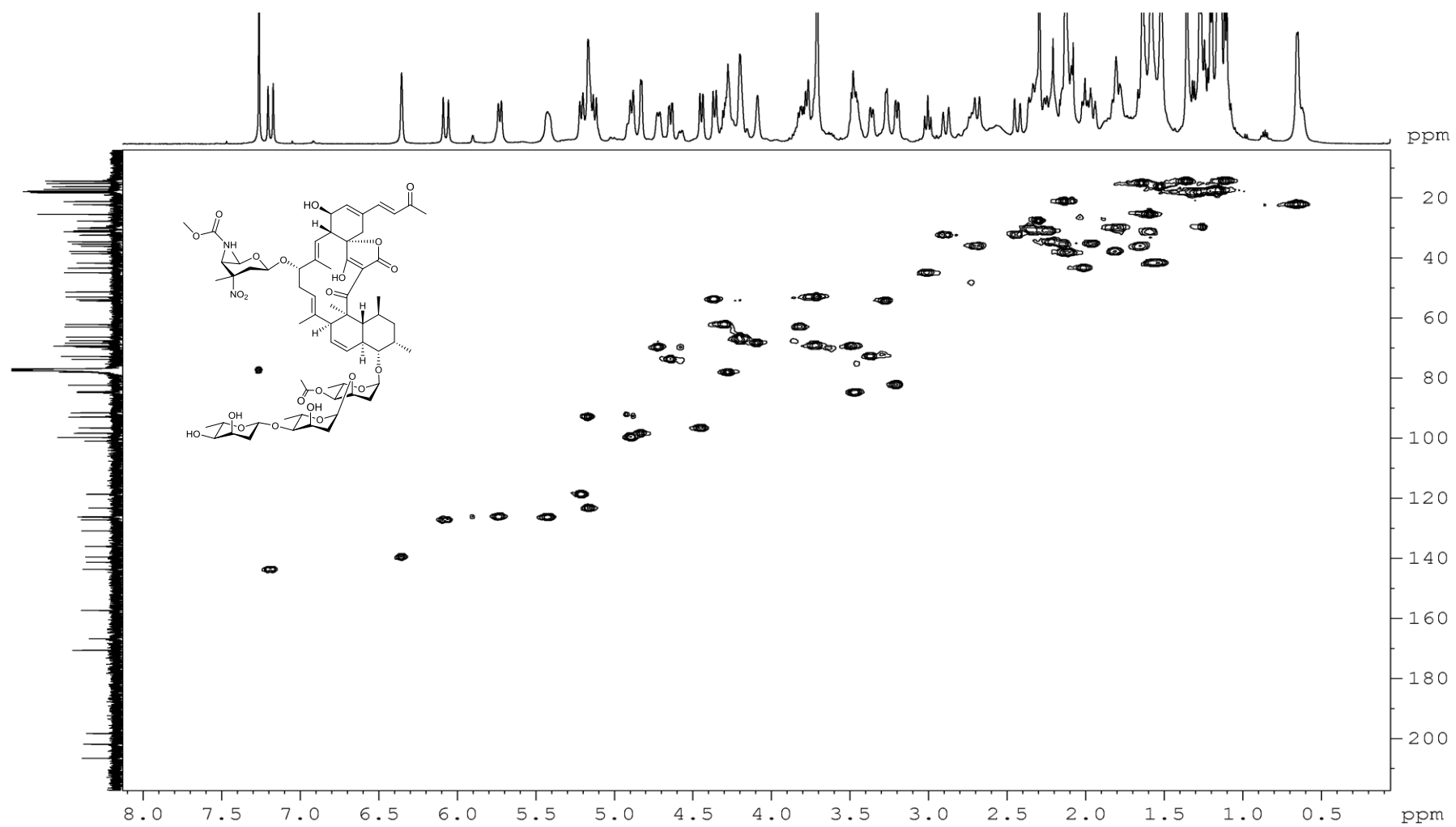


Figure S35. HMBC spectrum of compound **5** in CDCl₃.

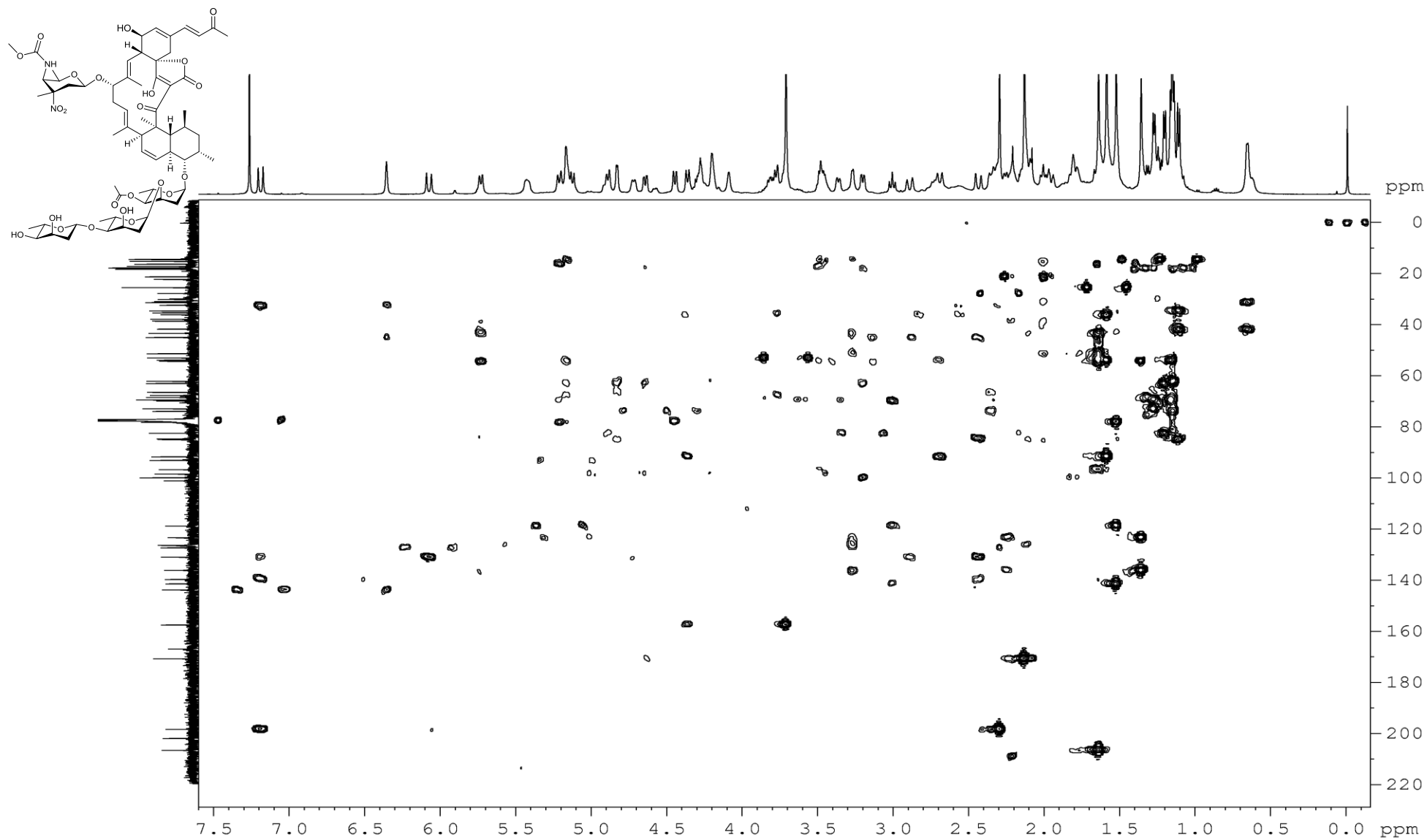


Figure S36. NOESY spectrum of compound **5** in CDCl₃.

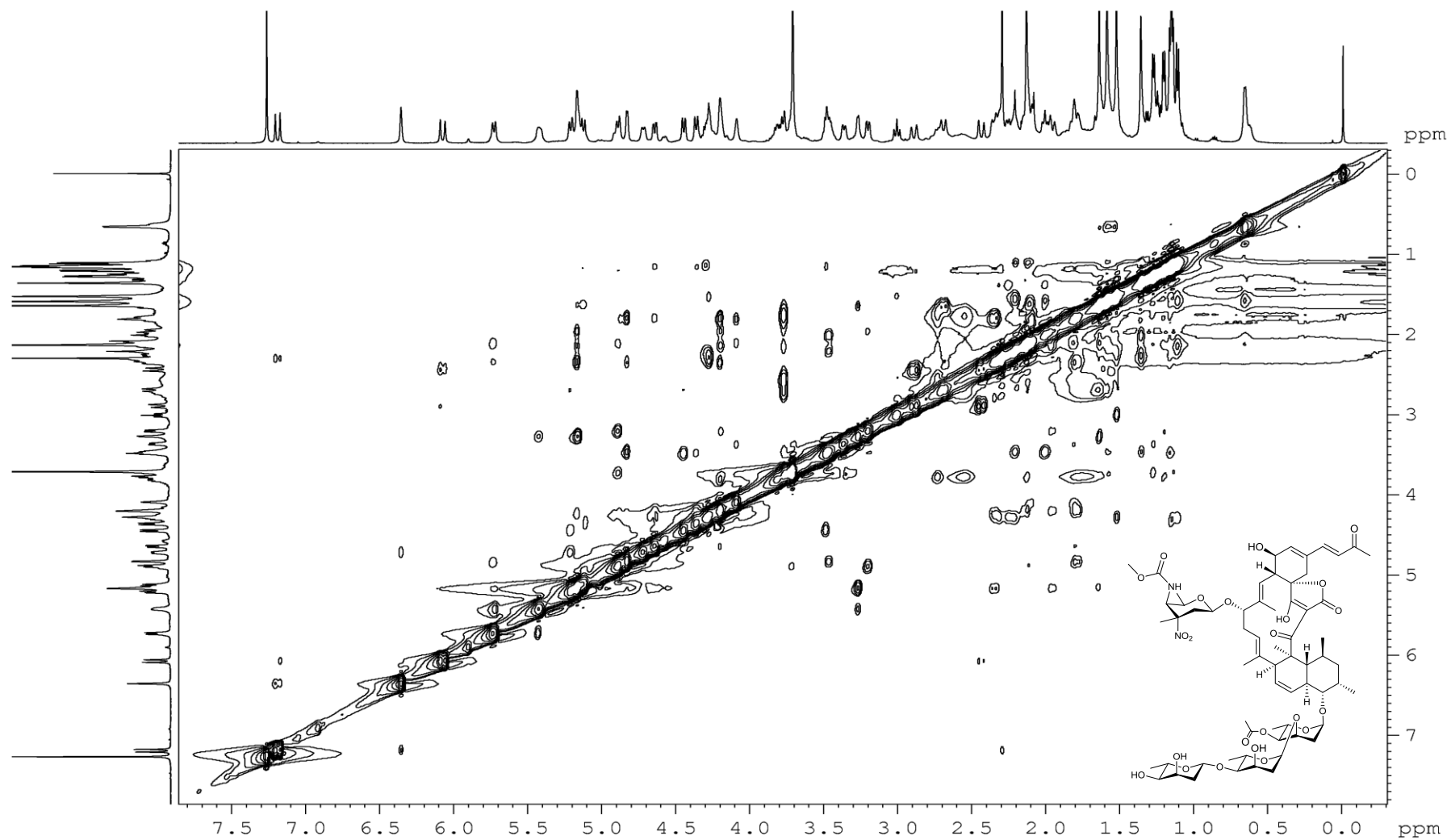


Figure S37. ^1H NMR (500 MHz) spectrum of compound **6** in CD_3OD .

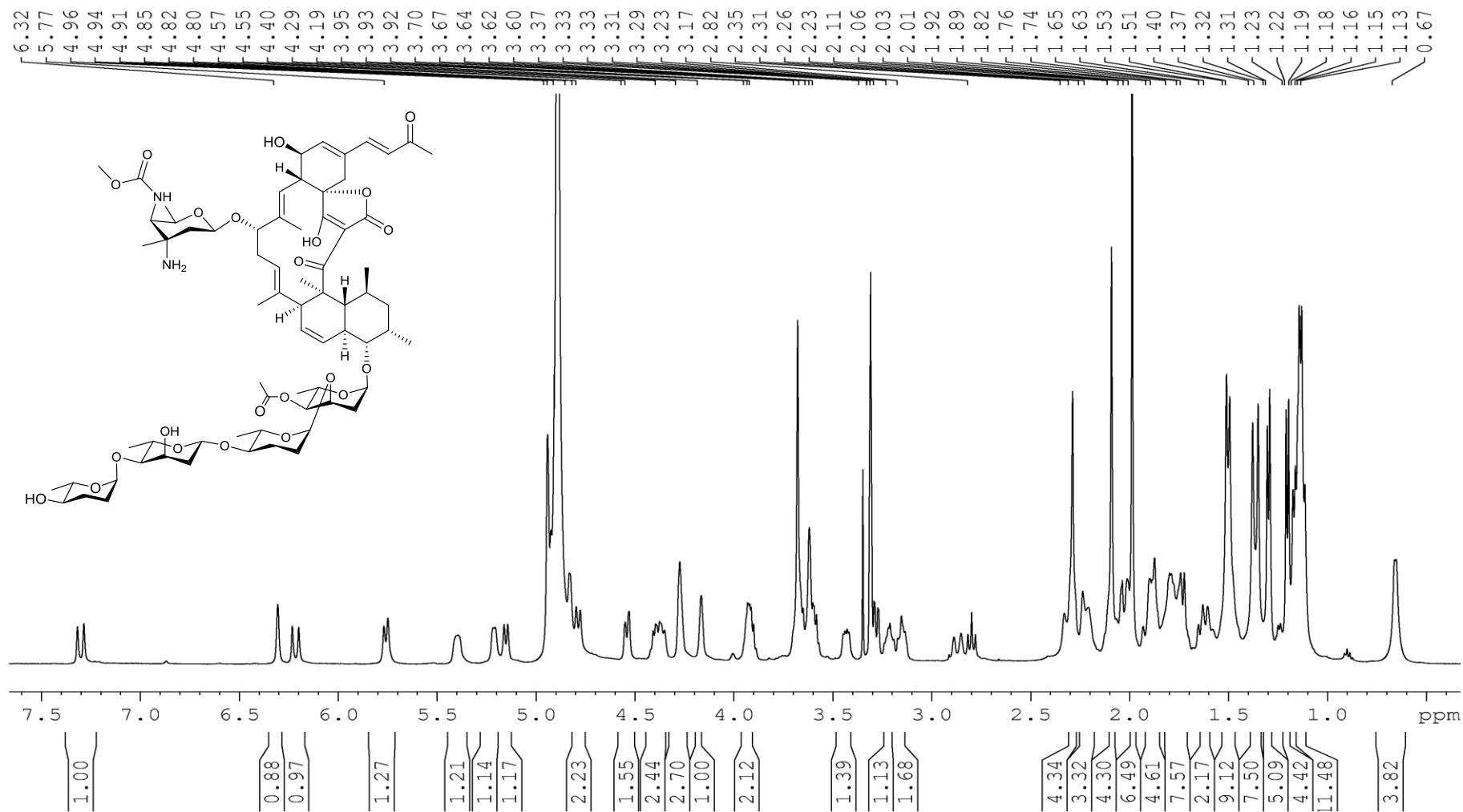
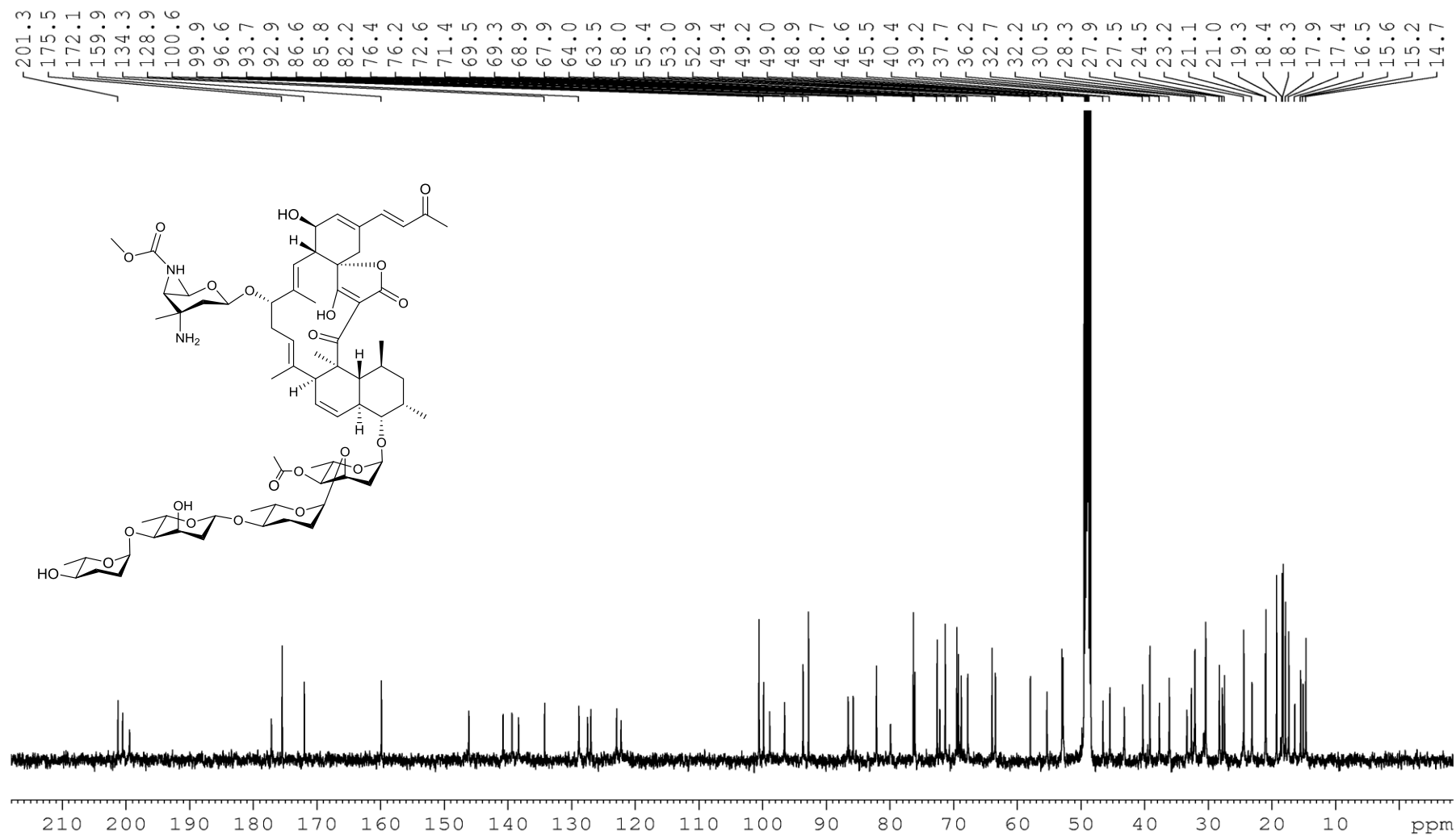


Figure S38. ^{13}C NMR (125 MHz) spectrum of compound **6** in CD_3OD .



The figure displays the chemical structure of compound 1 and its corresponding ¹³C NMR spectrum. The chemical structure is a complex polycyclic molecule with multiple stereocenters and functional groups, including a carboxamide, a ketone, and several hydroxyl groups. The ¹³C NMR spectrum shows a range of peaks from approximately 15 to 155 ppm. The peak assignments are as follows:

Chemical Shift (ppm)
144.8
139.4
127.5
126.2
125.6
121.6
120.9
99.2
98.5
95.2
92.3
91.4
85.2
80.8
78.5
74.9
74.7
71.2
70.0
68.1
67.9
67.4
66.4
62.6
62.1
54.0
51.6
51.5
45.2
44.1
41.8
38.9
37.8
36.3
34.8
32.0
31.3
30.7
29.1
29.0
26.9
26.4
26.1
23.0
21.8
19.7
19.6
17.9
17.6

The chemical structure shows a complex molecule with a central aglycone core. The aglycone is a polycyclic system with several functional groups, including hydroxyl groups, a ketone, and a double bond. It is linked to a series of sugar units (glucose and galactose) via glycosidic bonds. The structure is highly detailed, showing stereochemistry and various substituents.

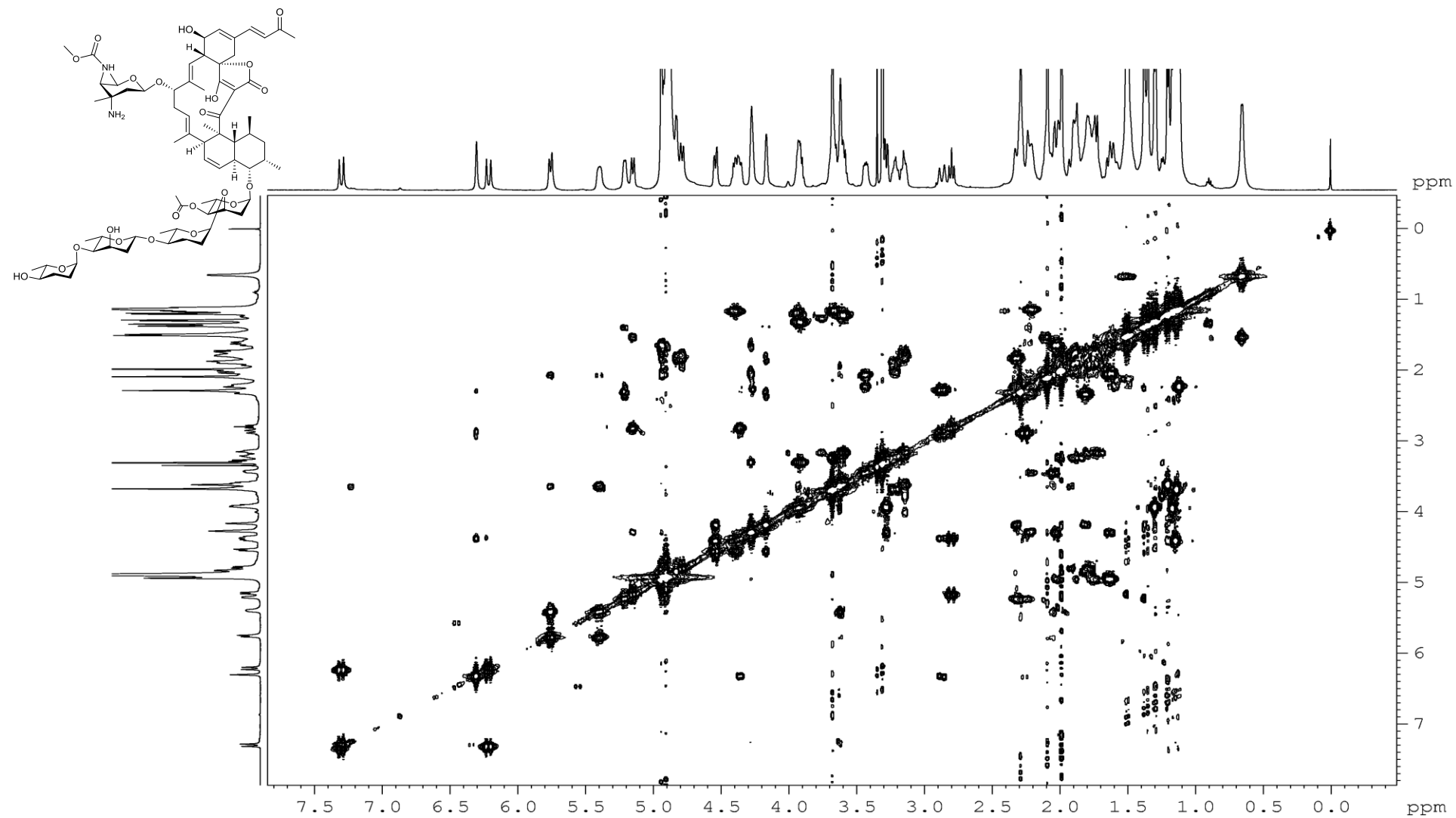


Figure S41. HSQC spectrum of compound **6** in CD₃OD.

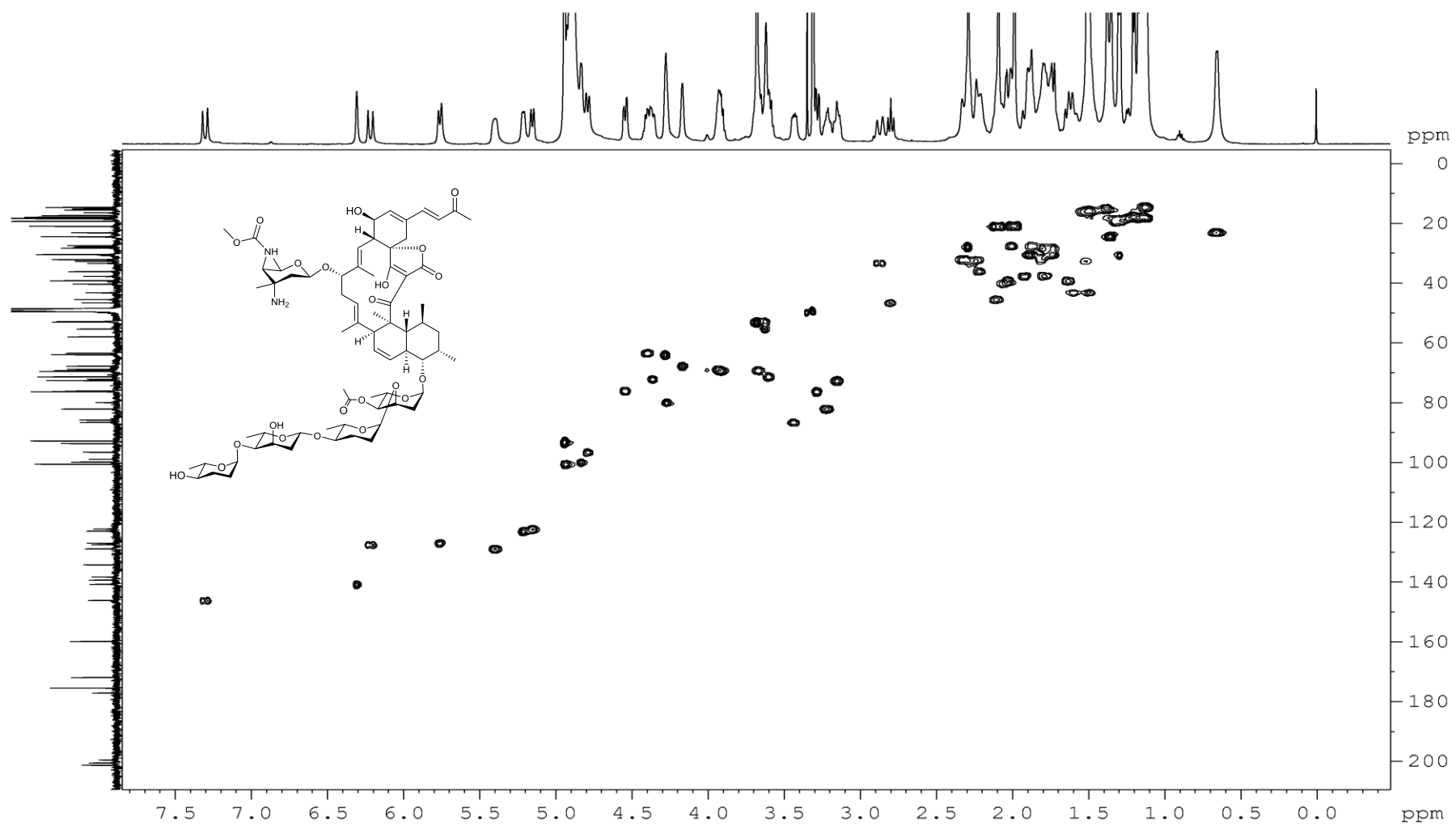


Figure S42. HMBC spectrum of compound **6** in CD₃OD.

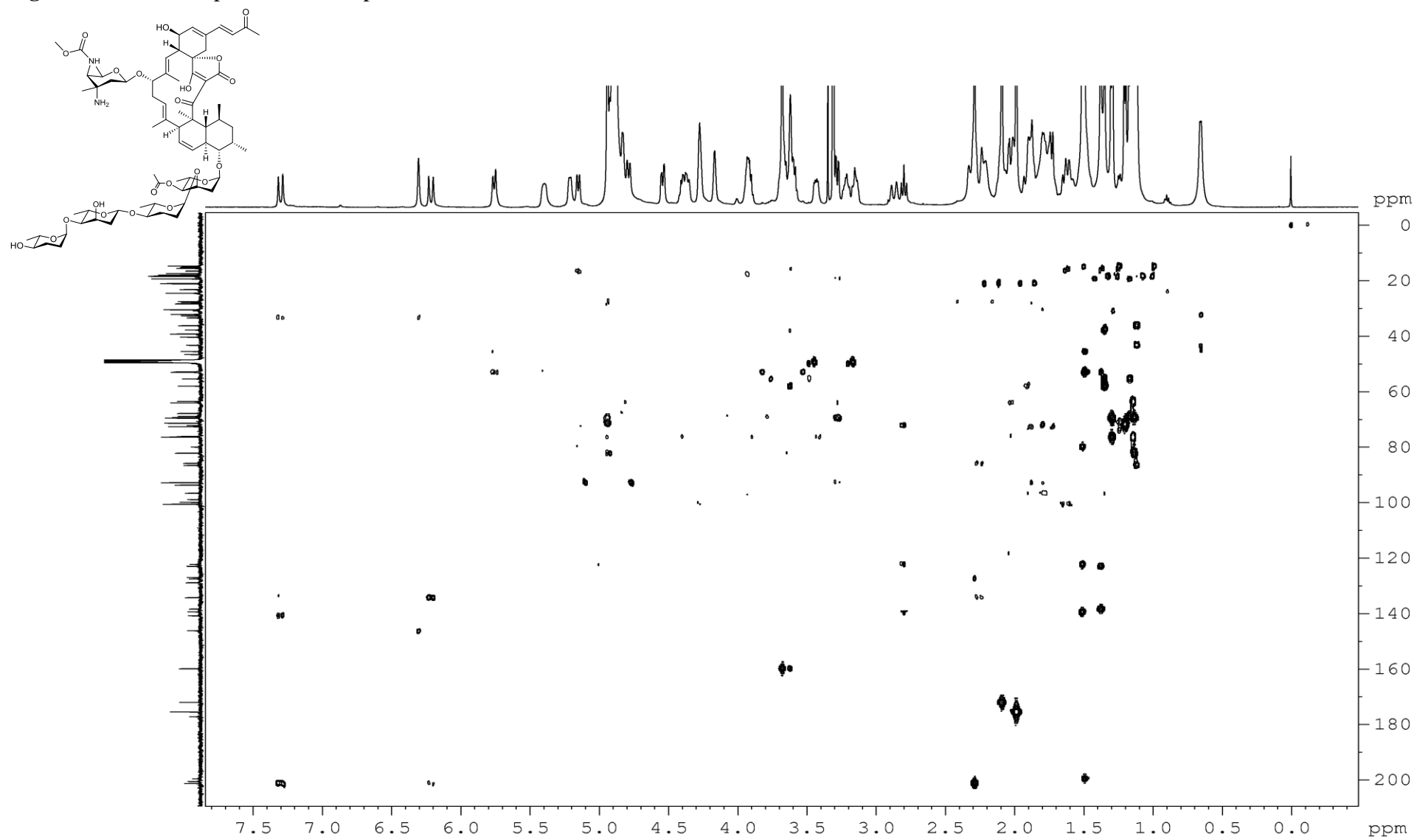


Figure S43. ^1H NMR (500 MHz) spectrum of compound **7** in CD_3OD .

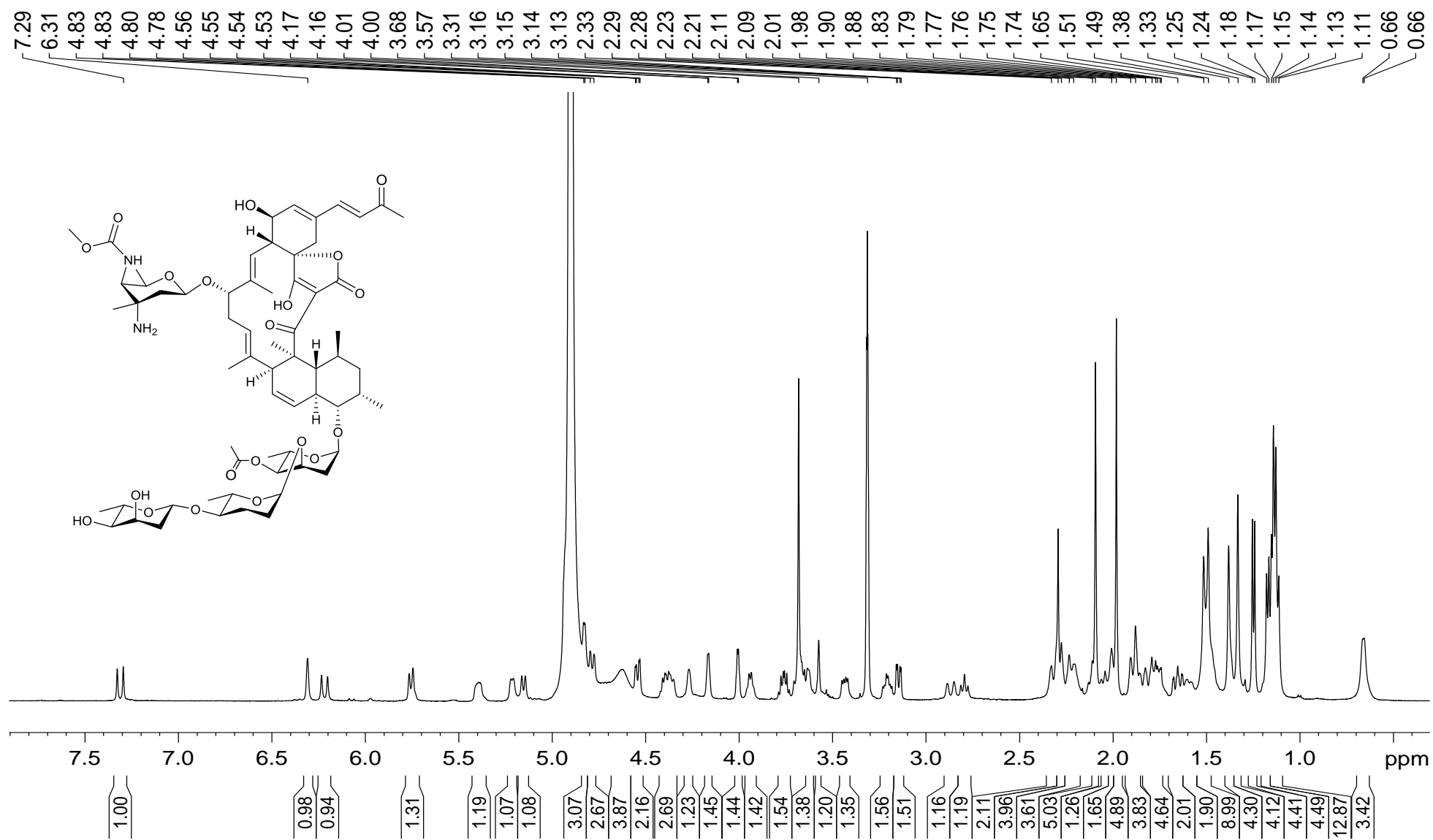


Figure S44. ^{13}C NMR (125 MHz) spectrum of compound **7** in CD_3OD .

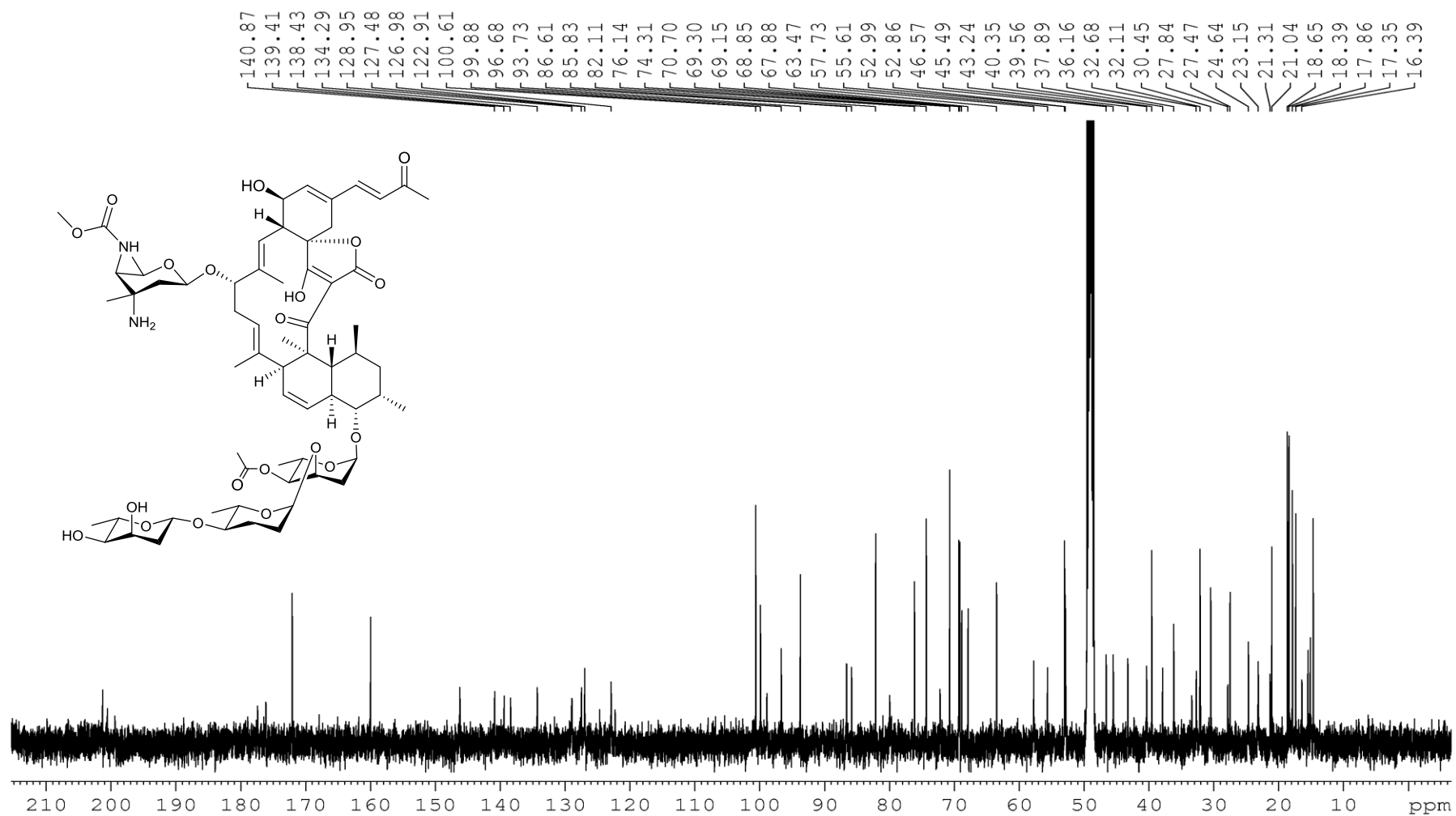


Figure S45. ^{13}C DEPT spectrum of compound **7** in CD_3OD .

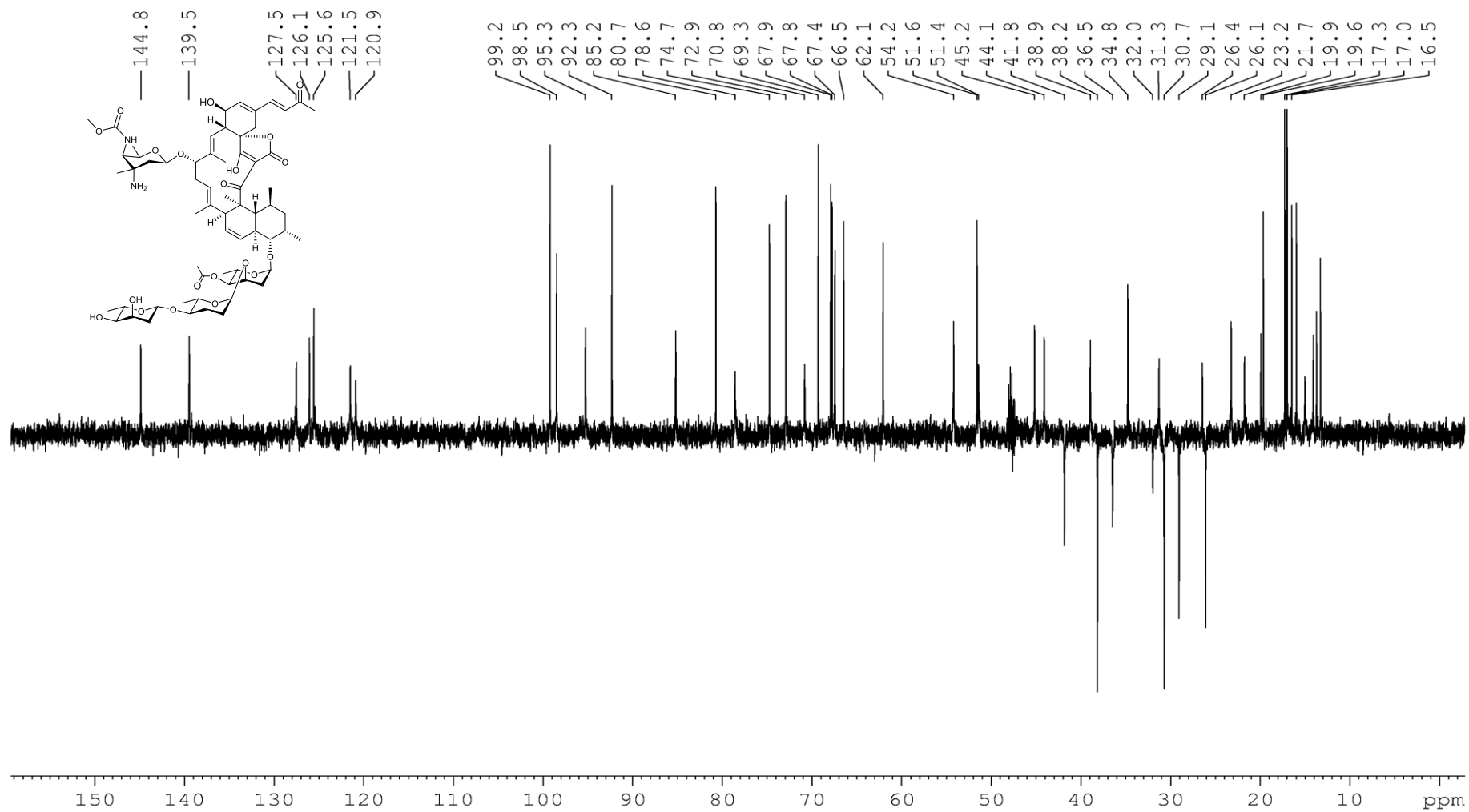


Figure S46. ^1H - ^1H COSY spectrum of compound **7** in CD_3OD .

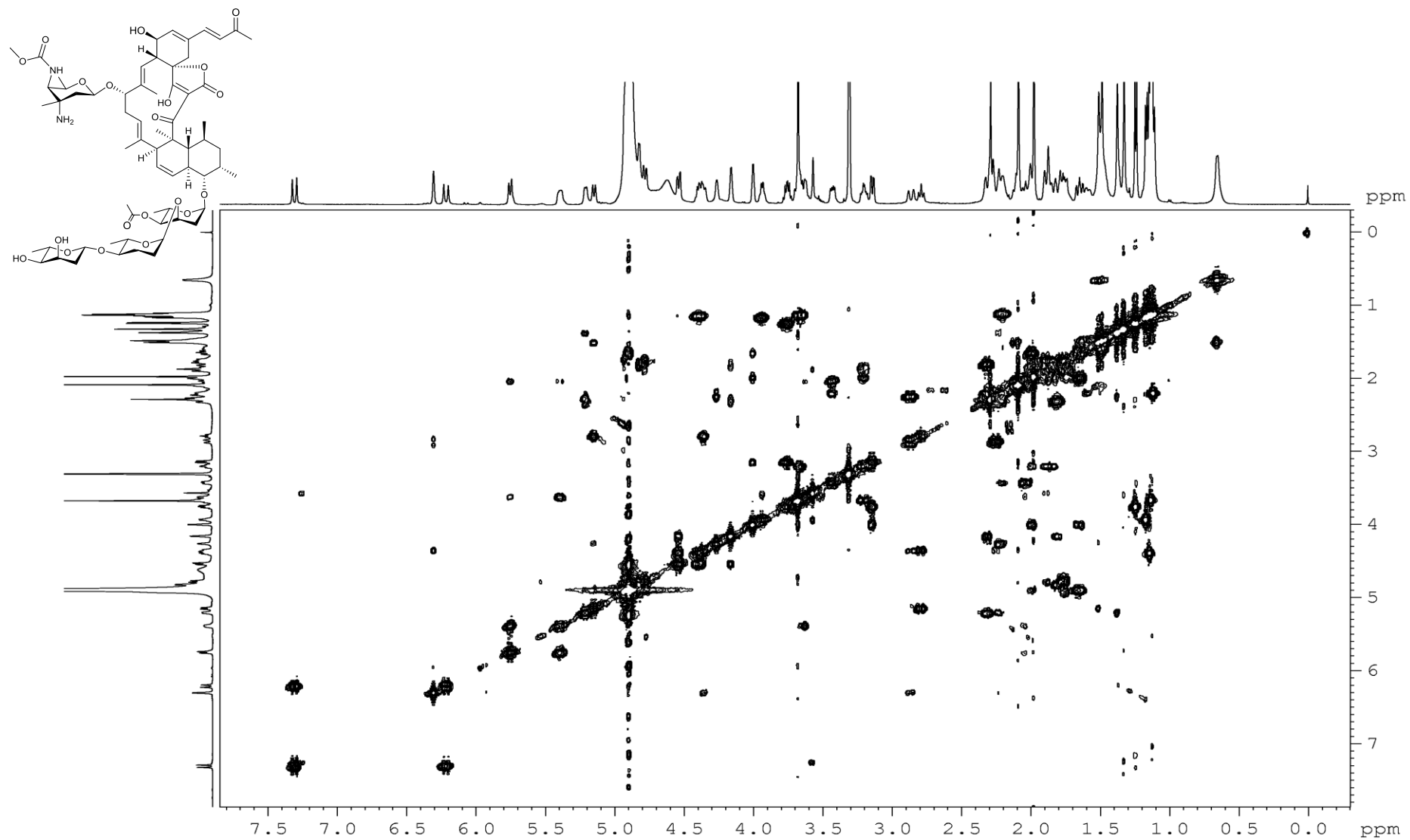


Figure S47. HSQC spectrum of compound **7** in CD₃OD.

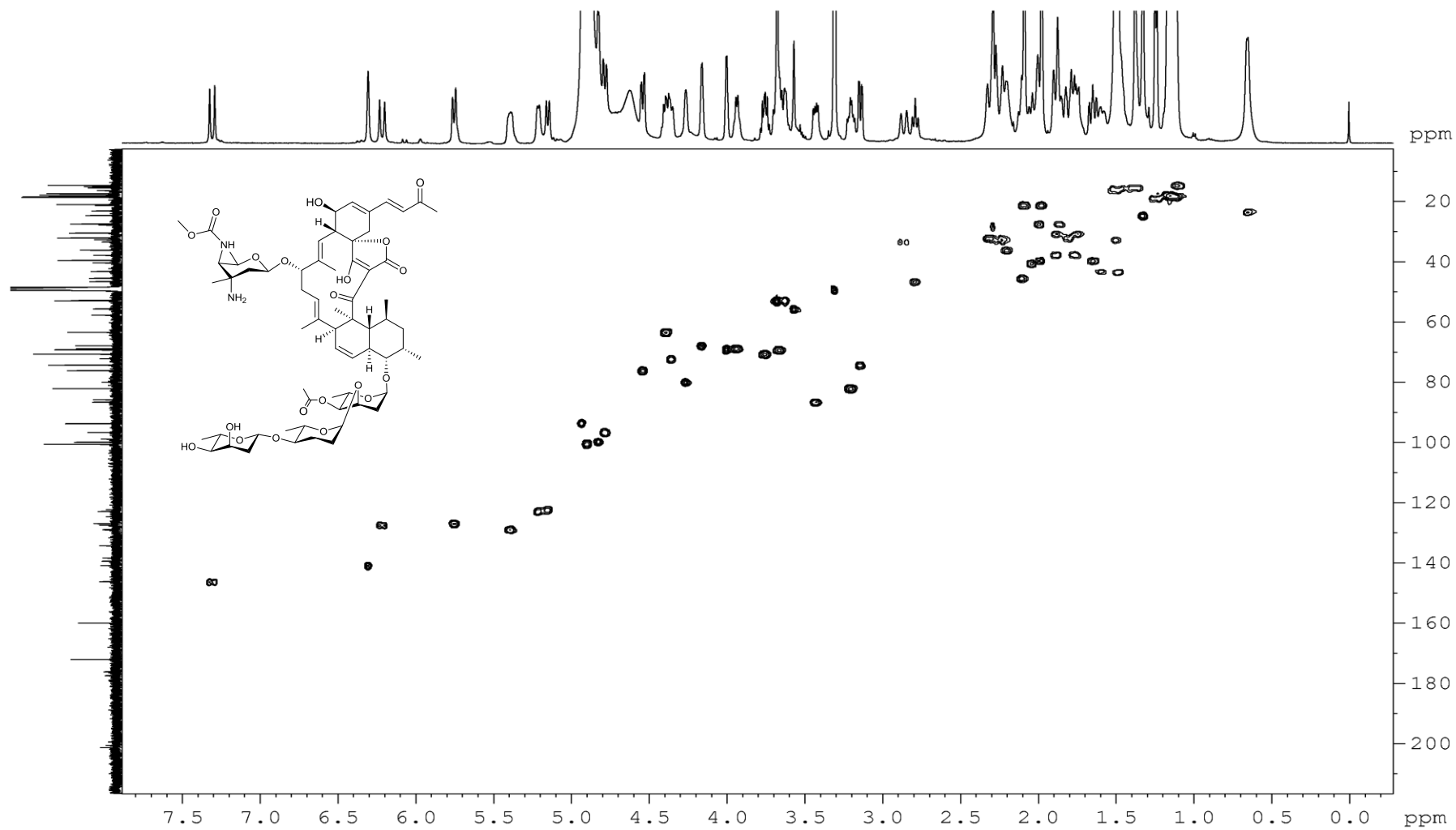


Figure S48. HMBC spectrum of compound **7** in CD₃OD.

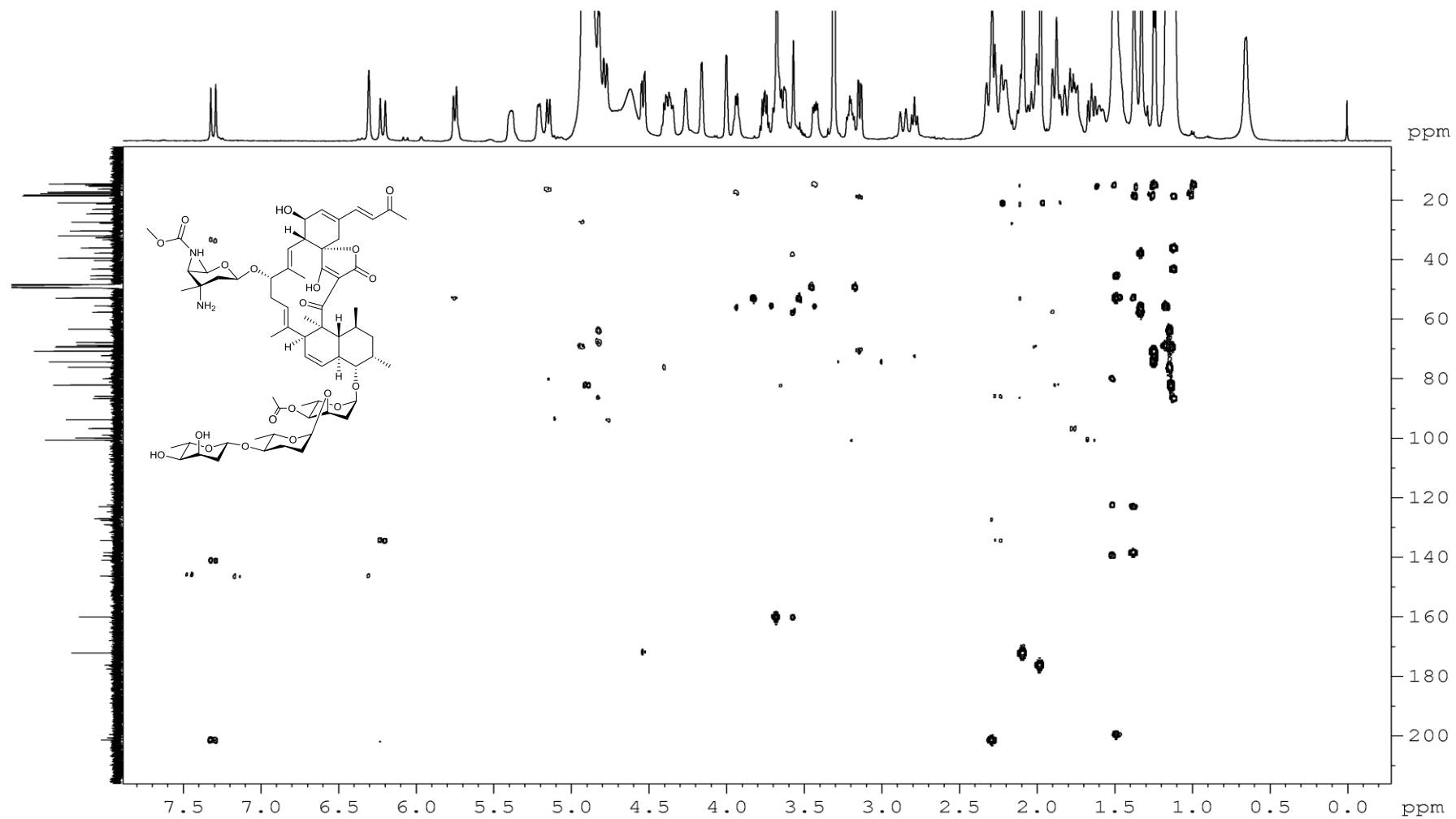


Figure S49. NOESY spectrum of compound **7** in CD₃OD.

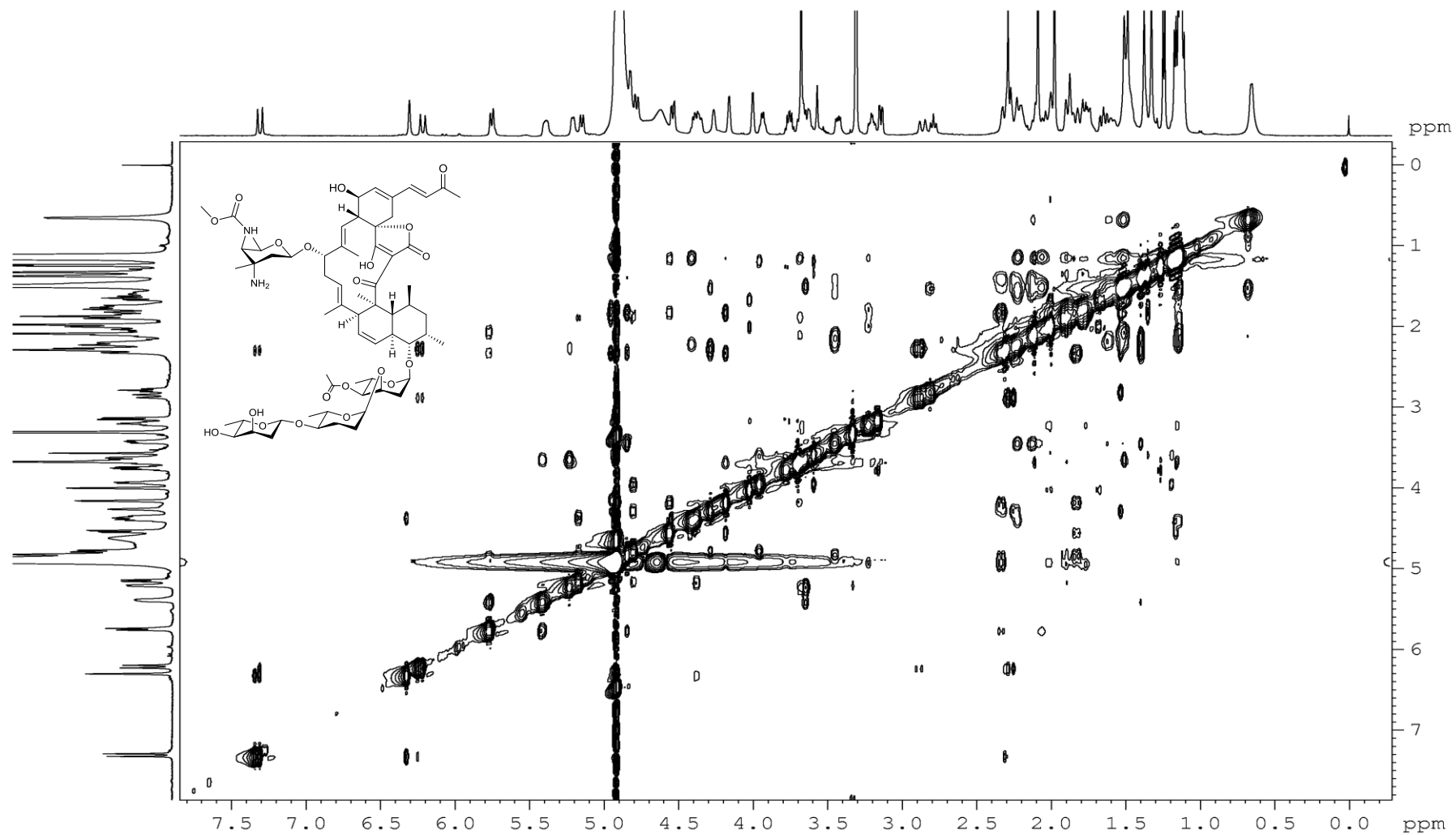


Figure S50. ^1H NMR (700 MHz) spectrum of compound **8** in CD_3OD .

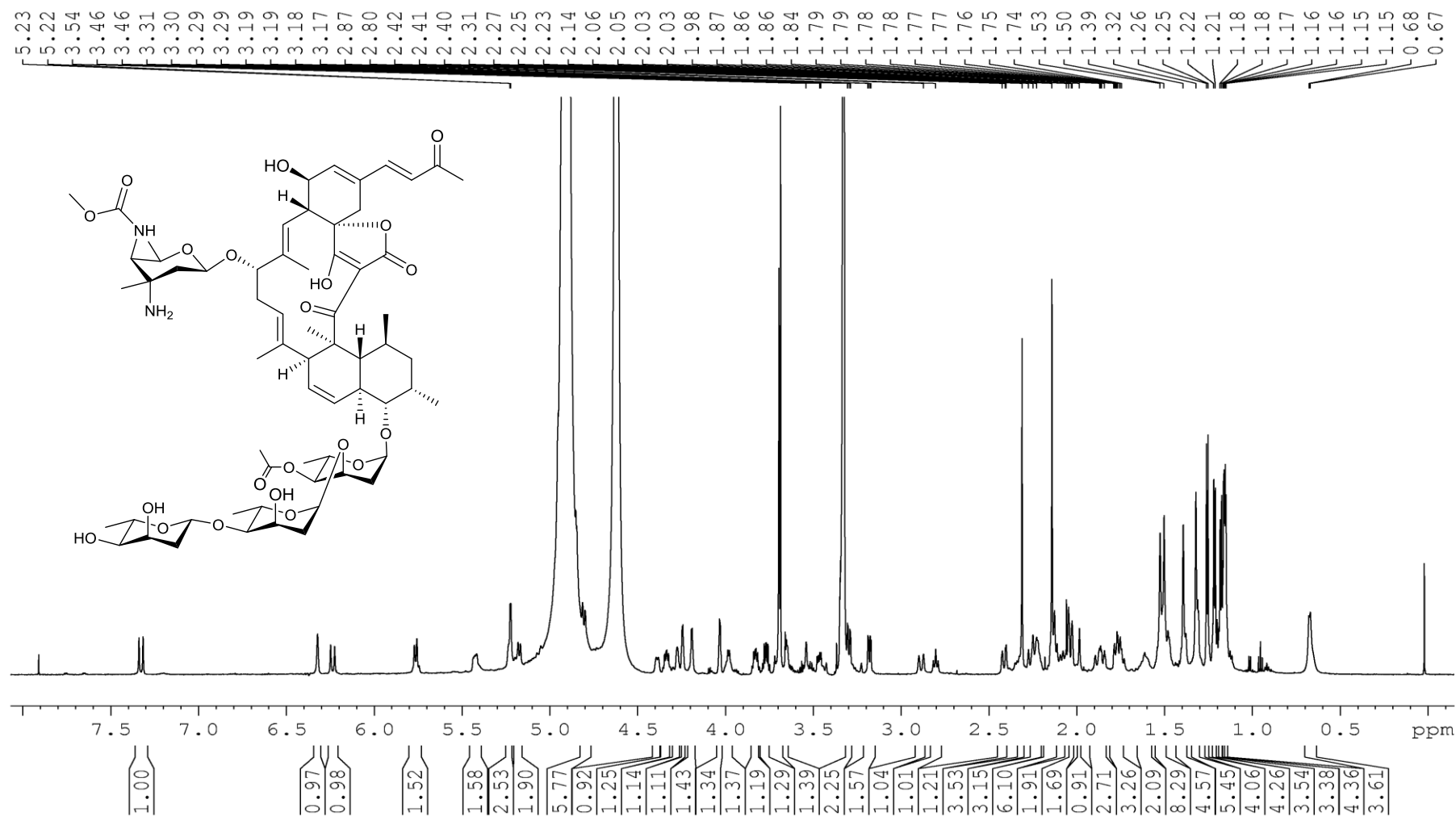
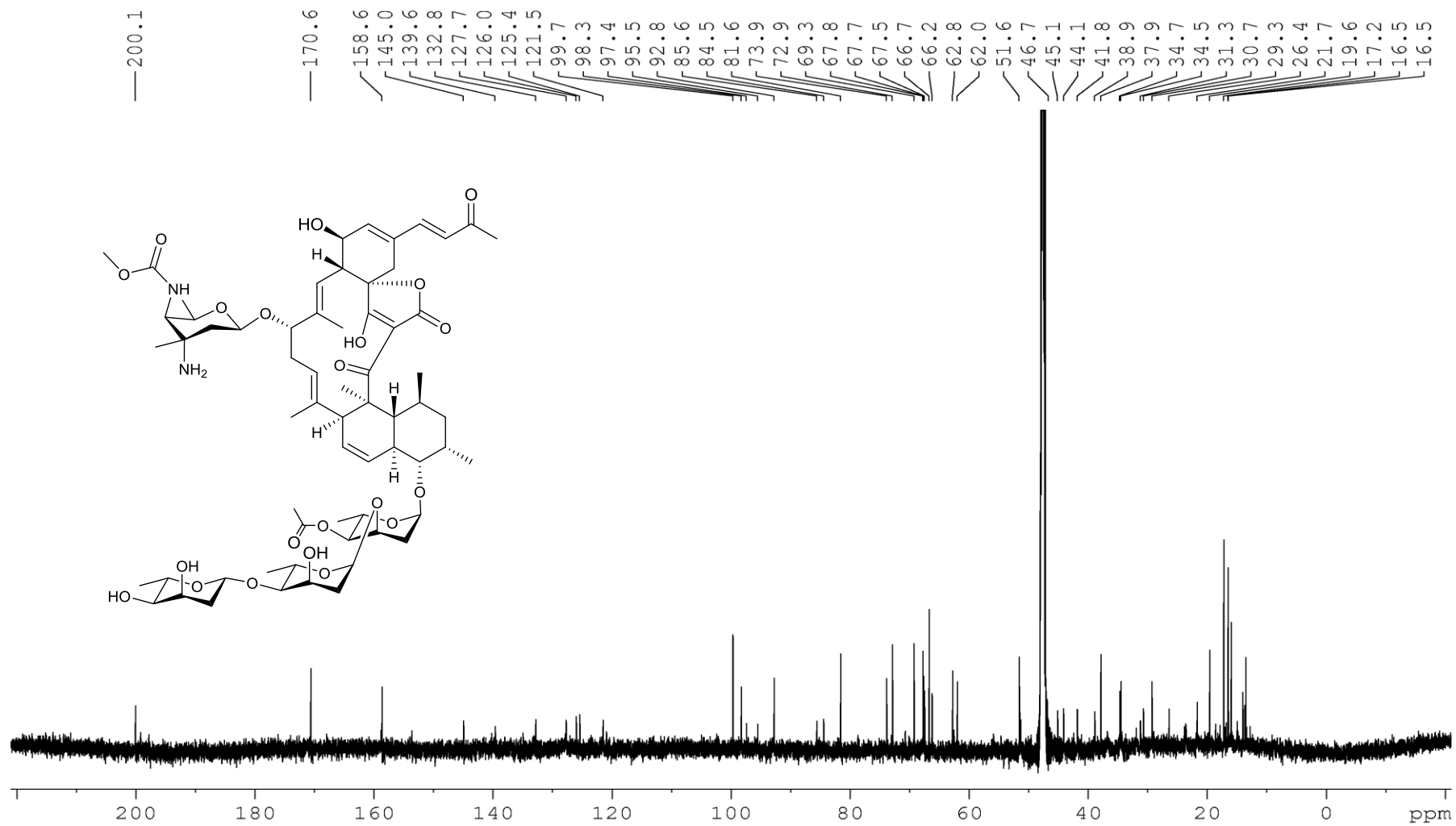


Figure S51. ^{13}C NMR (176 MHz) spectrum of compound **8** in CD_3OD .



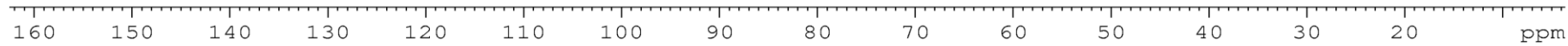


Figure S53. ^1H - ^1H COSY spectrum of compound **8** in CD_3OD .

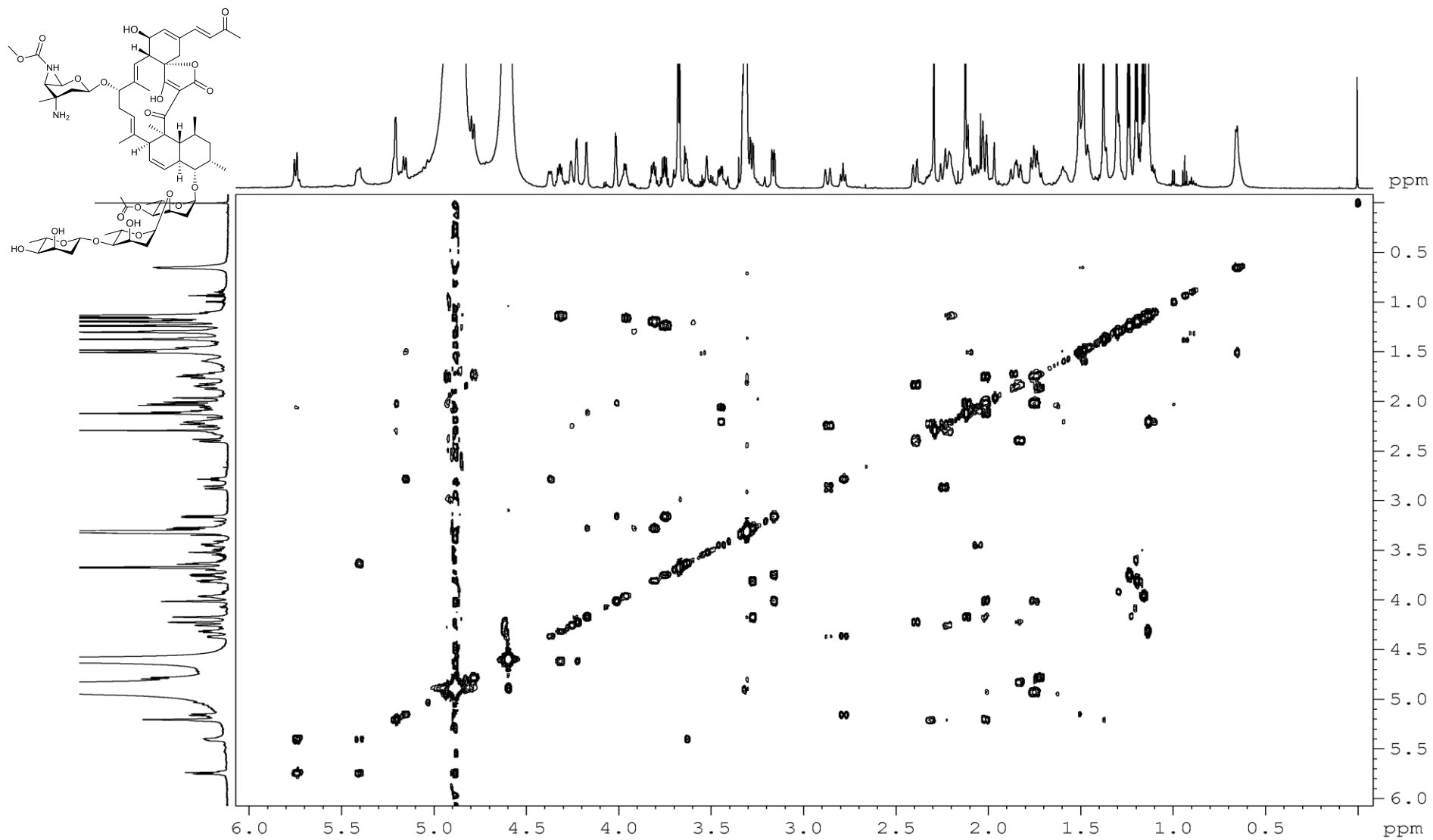


Figure S54. HSQC spectrum of compound **8** in CD₃OD.

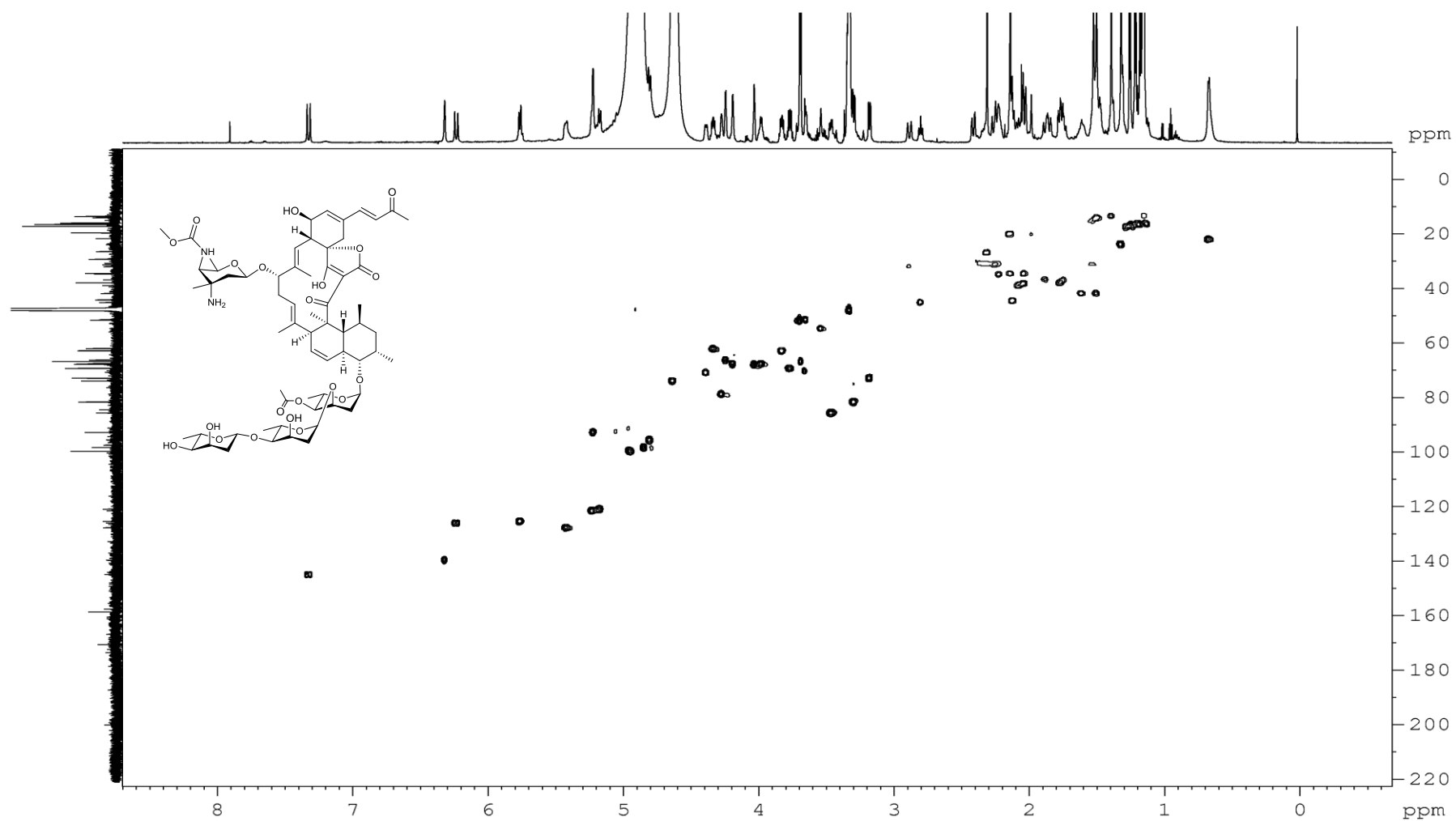


Figure S55. HMBC spectrum of compound **8** in CD₃OD.

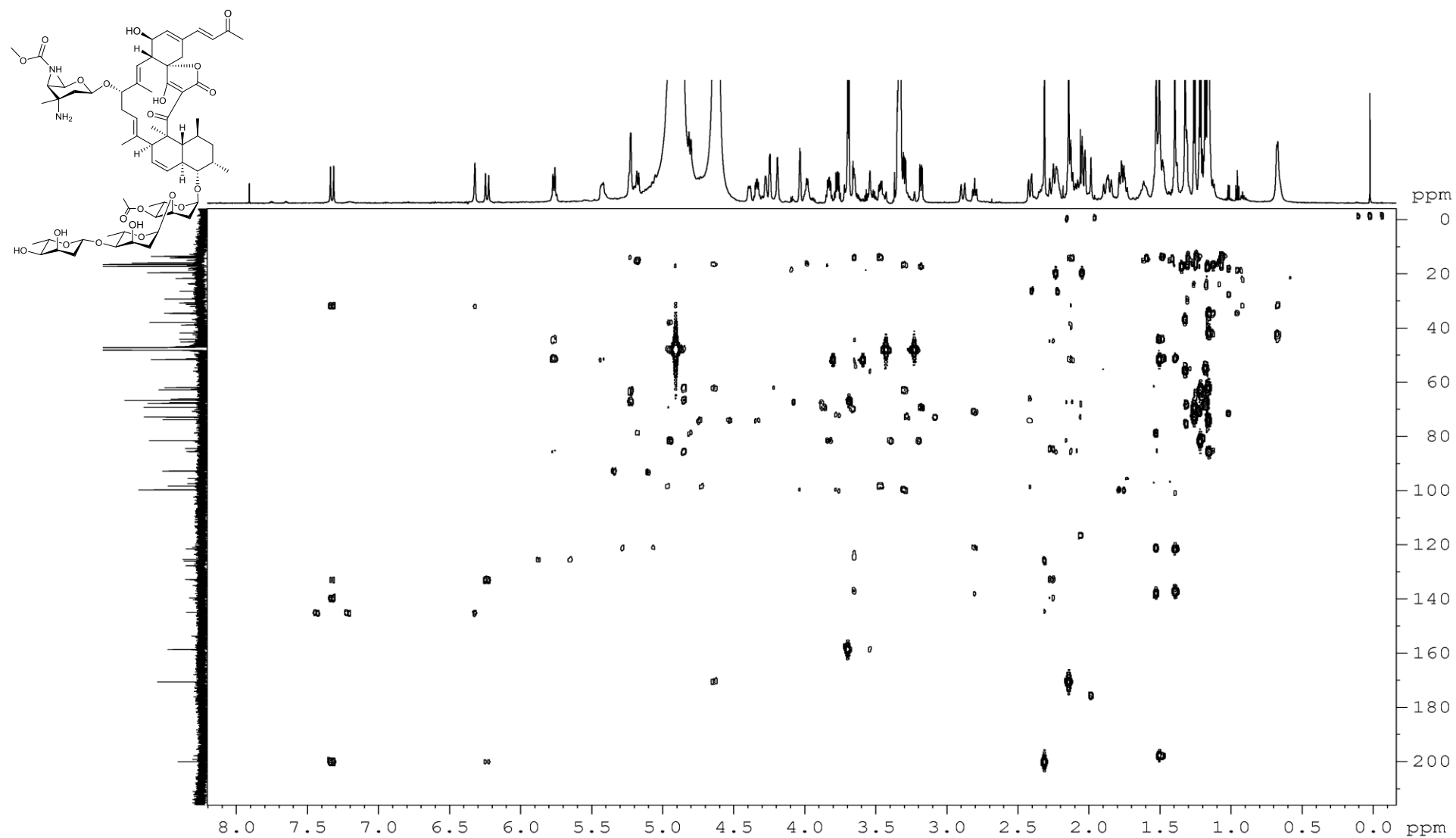


Figure S56. NOESY spectrum of compound **8** in CD₃OD.

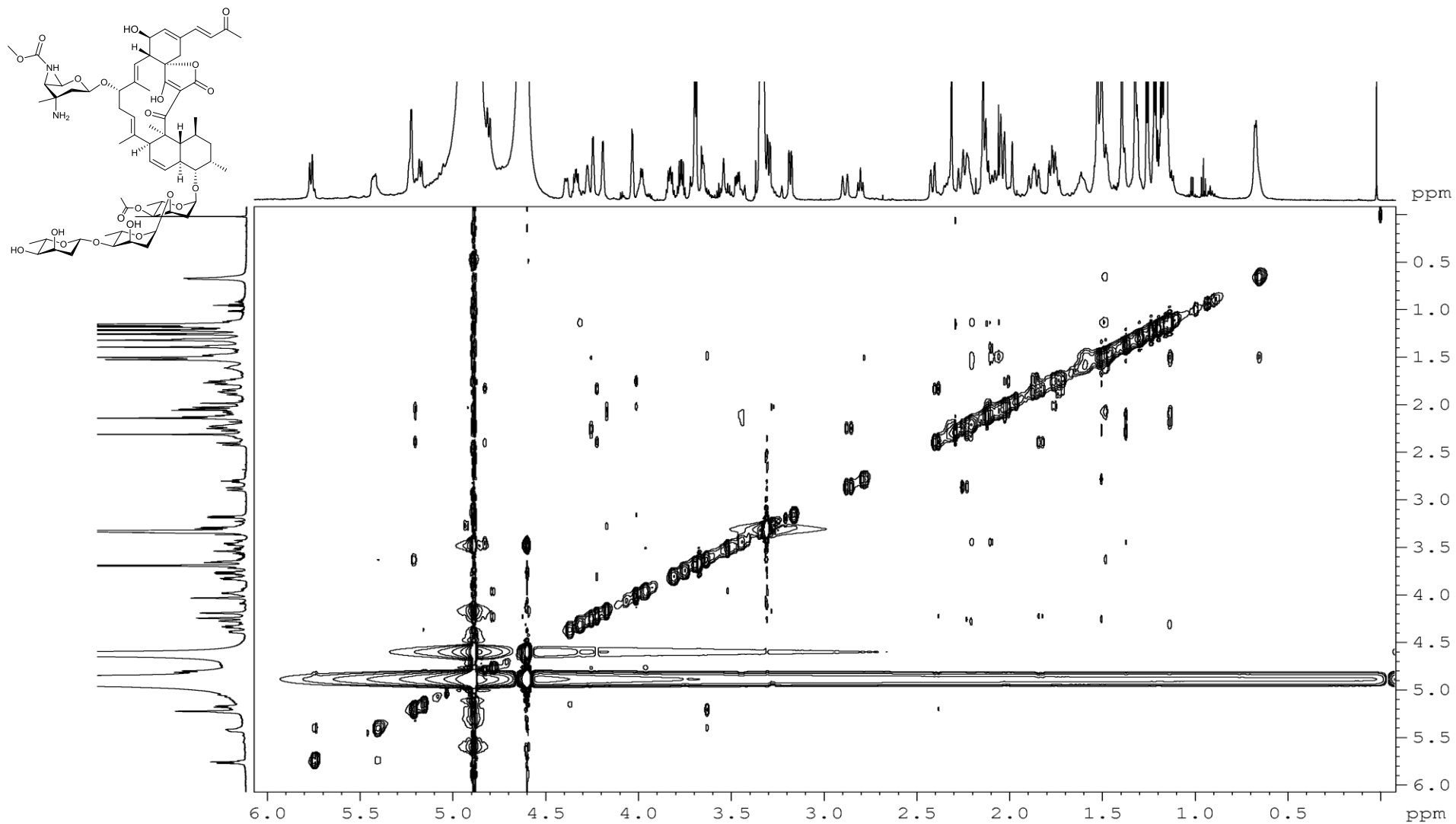


Figure S57. ^1H NMR (700 MHz) spectrum of compound **9** in CD_3OD .

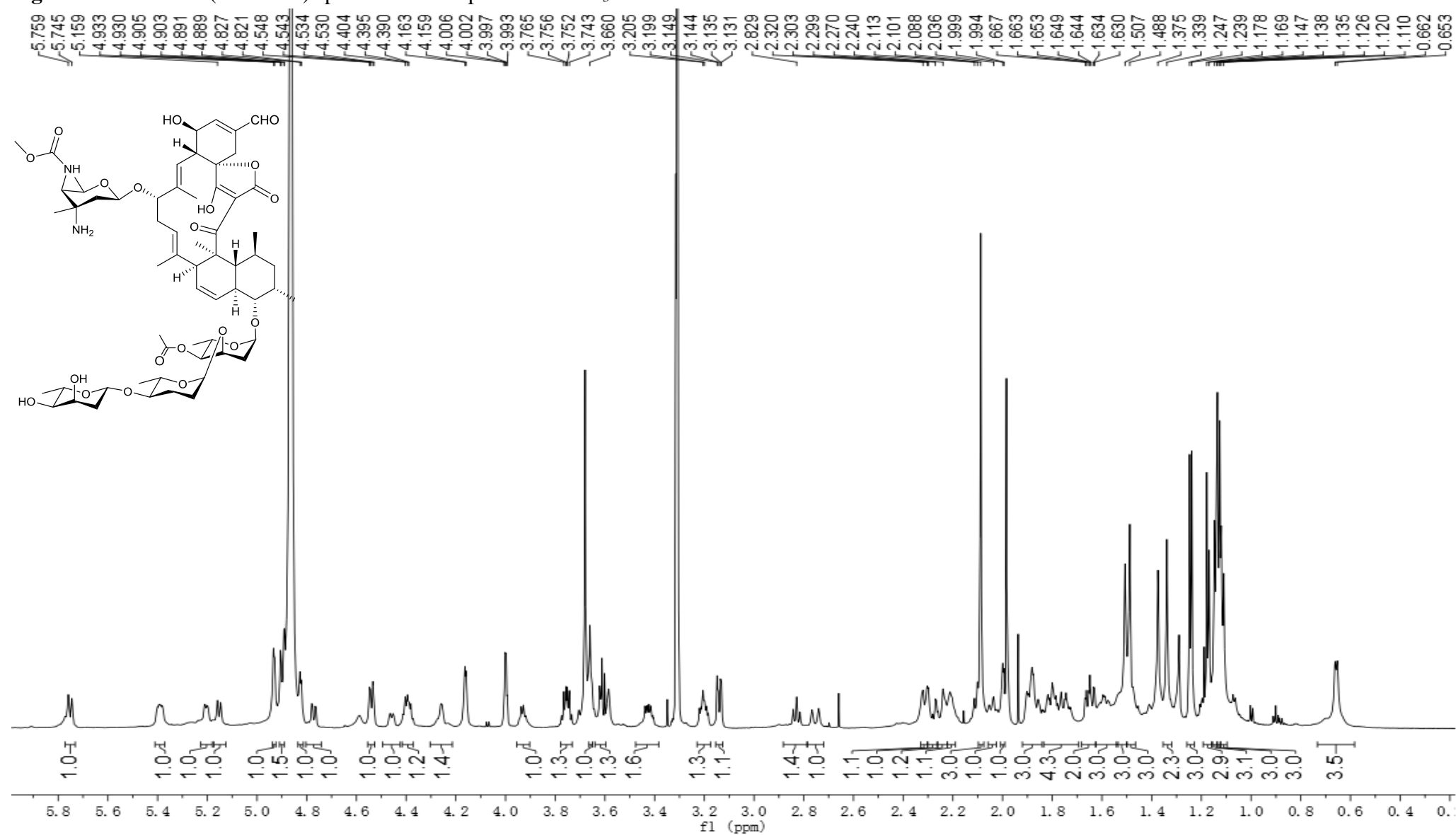


Figure S58. ^{13}C NMR (176 MHz) spectrum of compound **9** in CD_3OD .

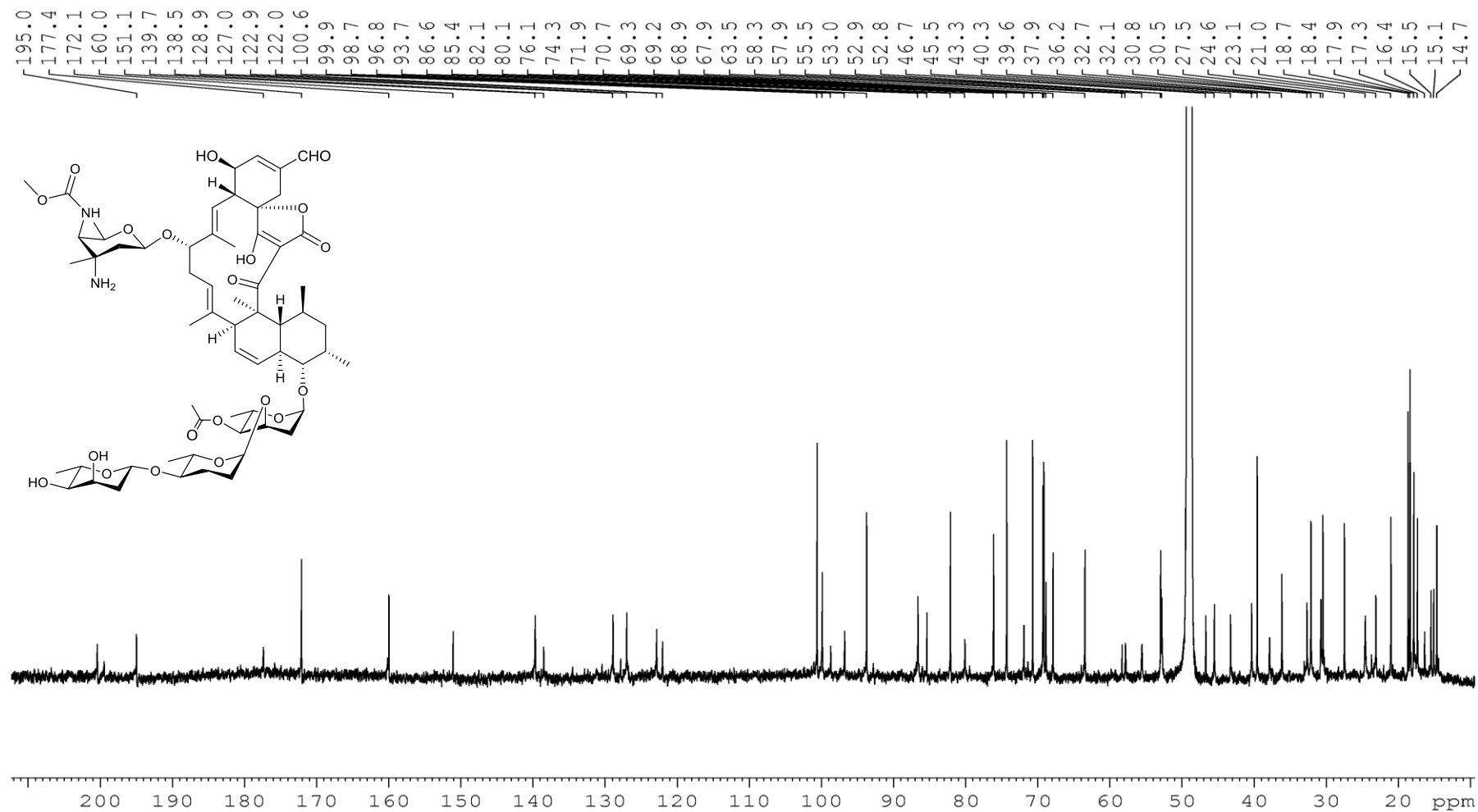


Figure S59. ^{13}C DEPT spectrum of compound **9** in CD_3OD .

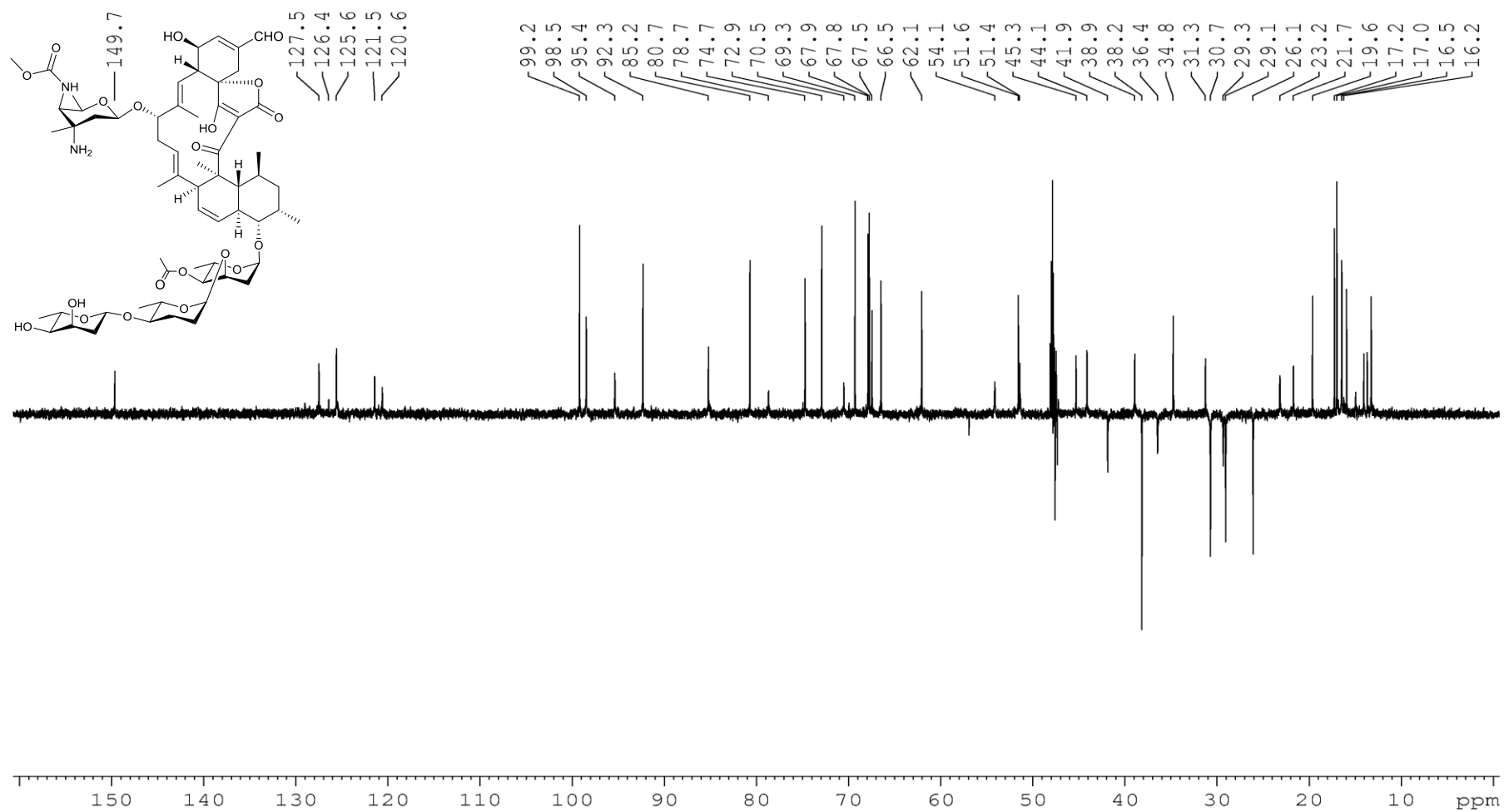


Figure S60. ^1H - ^1H COSY spectrum of compound **9** in CD_3OD .

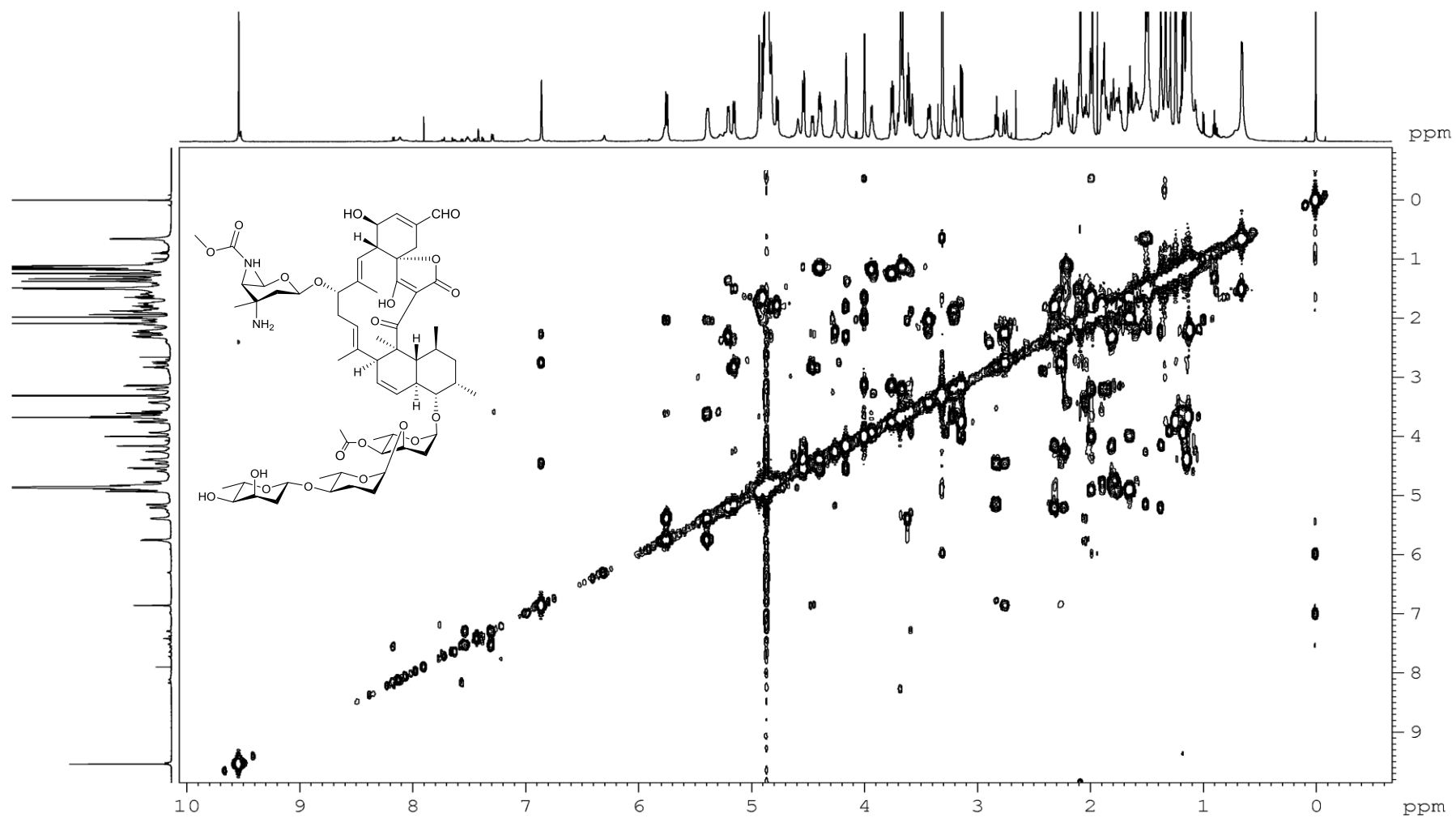


Figure S61. HSQC spectrum of compound **9** in CD₃OD.

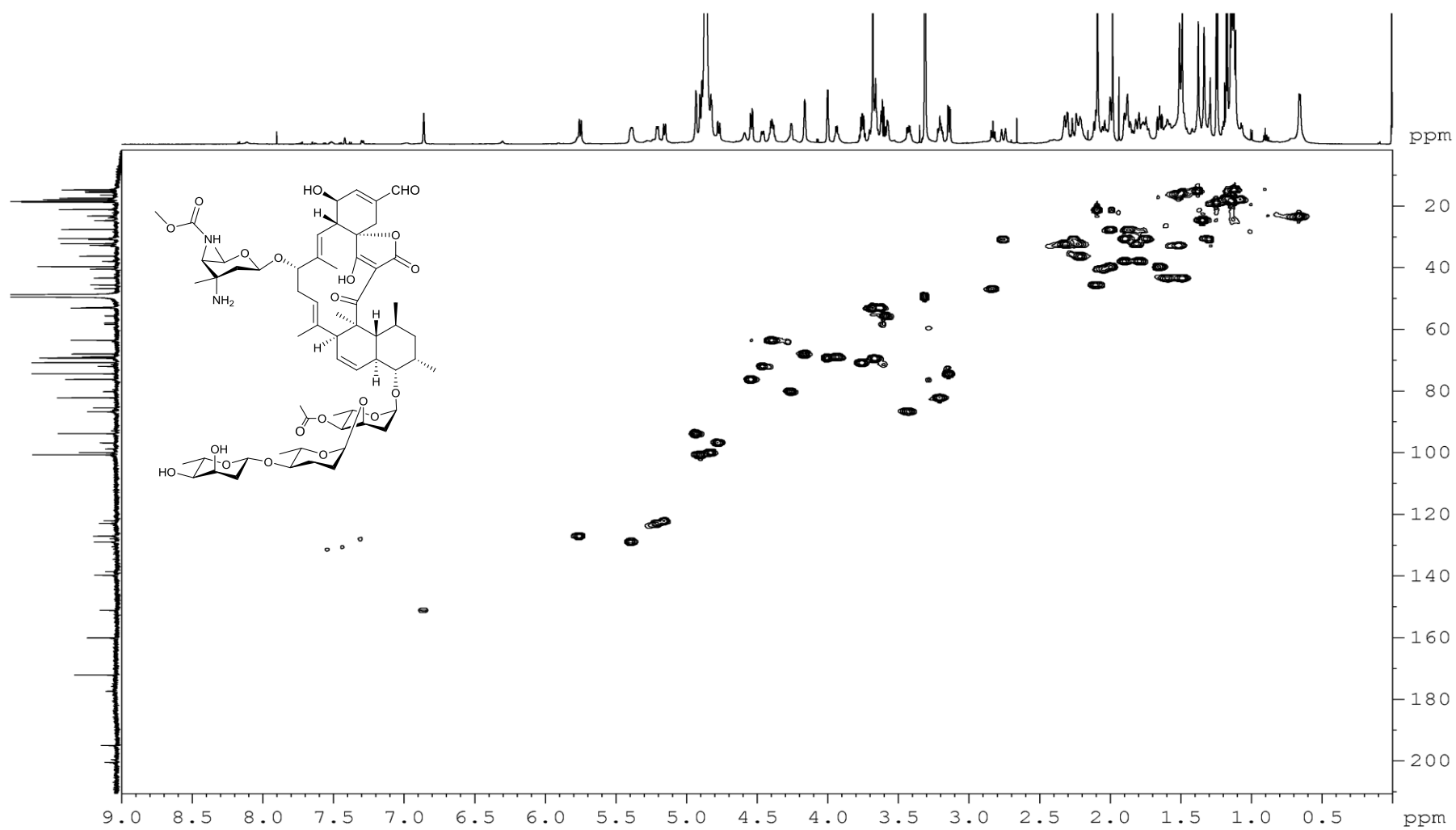


Figure S62. HMBC spectrum of compound **9** in CD₃OD.

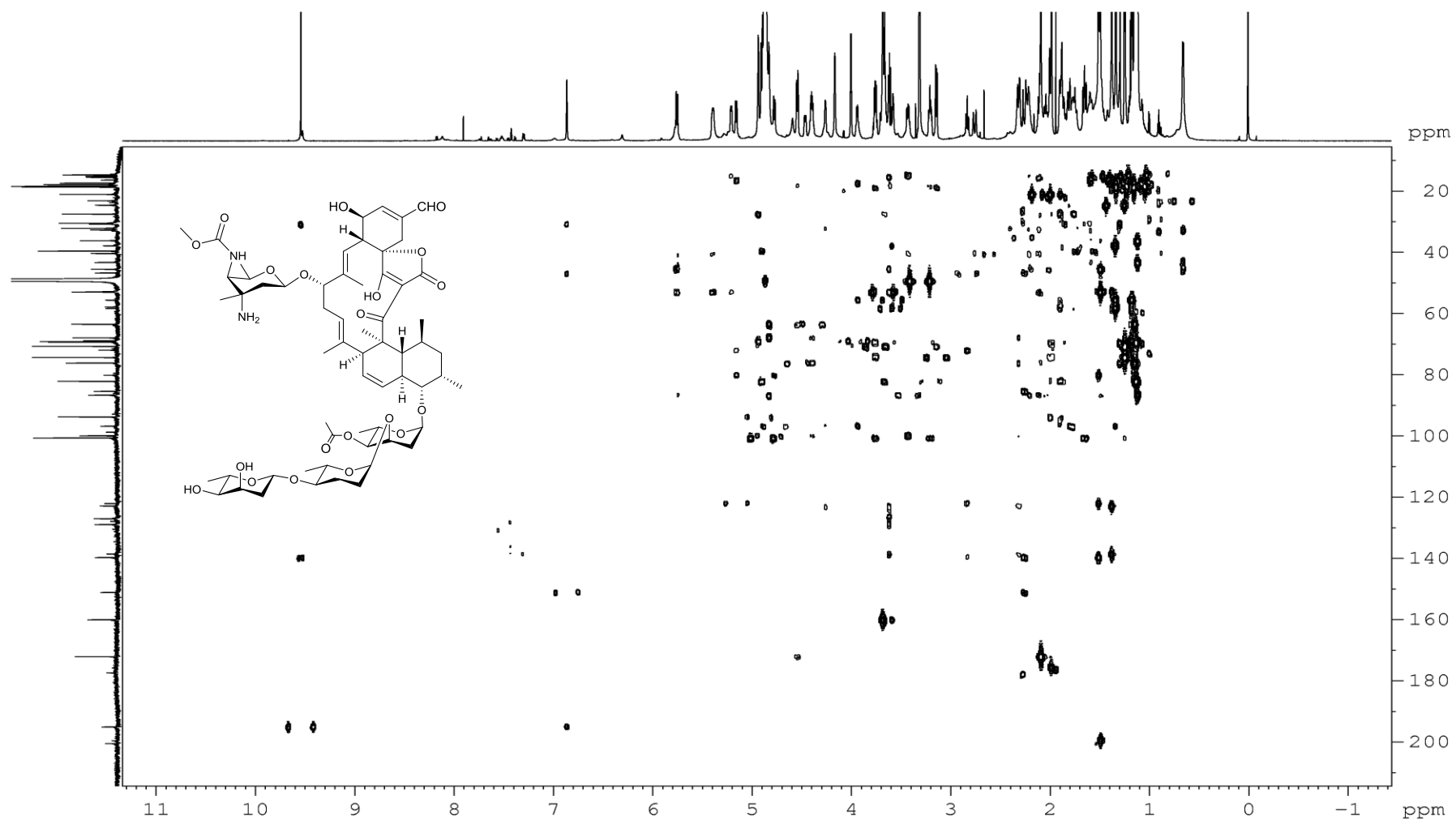
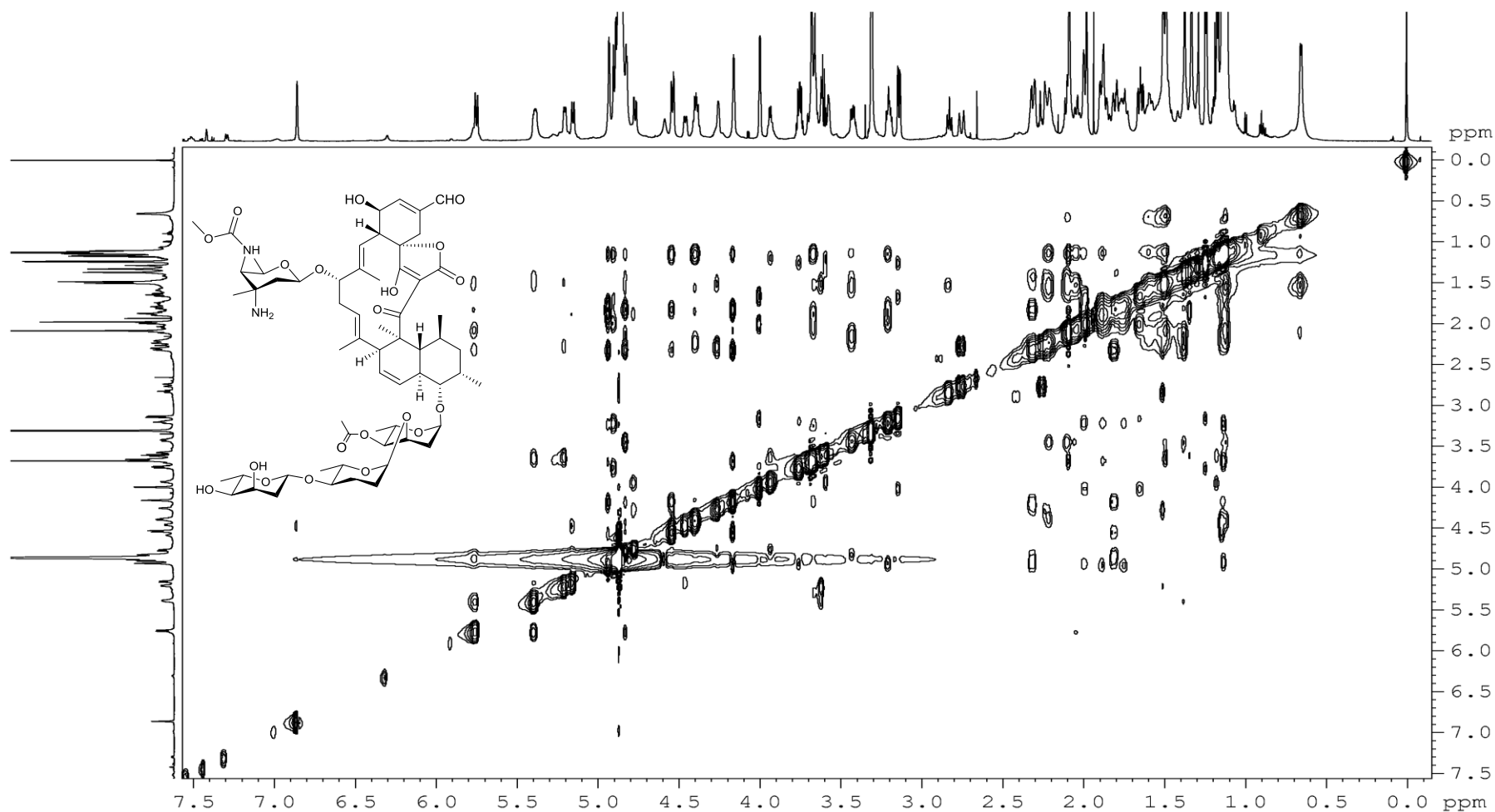


Figure S63. NOESY spectrum of compound **9** in CD₃OD.



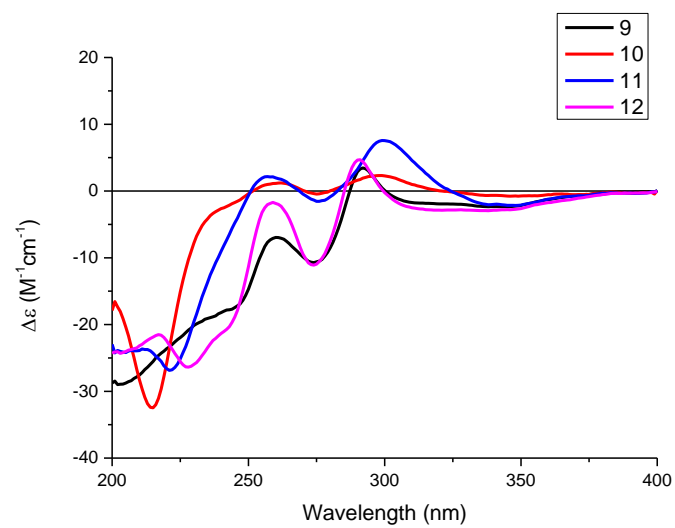
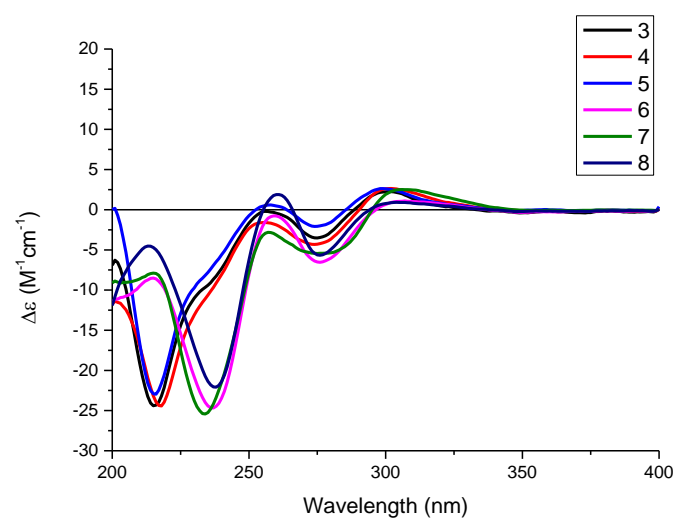
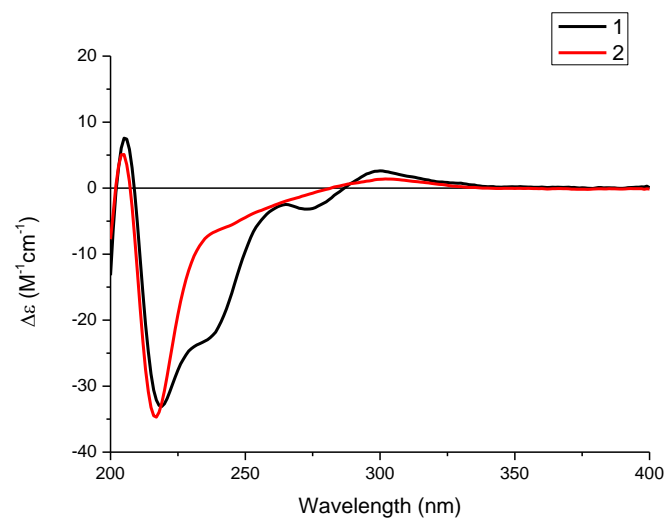


Figure S64. The CD spectra of compounds 1–12.