

Supporting Information for

Bipodonines A-J, a new class of natural sesquiterpenes with 2-(tetrahydro-2*H*-pyran-2-yl)propan-2-ol system from the fungus *Bipolaris cynodontis* DJWT-01

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Table 1 ^1H NMR data of compounds 1-5.

No.	1 ^a	2 ^c	3 ^b	4 ^a	5 ^a
1	4.52 d (12.6)	4.12 dd (11.6, 7.9)	2.14 overlap 2.03 overlap	1.82 overlap 1.20 overlap	1.76 dd (6.9, 1.2) 1.10 overlap
2	1.86 d (11.8)	1.74 overlap	6.74 s	4.32 br s	4.14 m
4	1.46 m 1.92 m	1.76 m 1.87 m		2.49 dt (12.5, 3.9)	2.43 m
5	1.60 m 1.89 m	1.55 m 1.71 m	1.98 m 2.63 dd (16.9, 6.8)	1.86 m 1.93 m	1.50 m 1.96 dt (12.7, 4.1)
6	3.17 dd (12.0, 4.0)	3.18 dd (12.0, 3.8)	3.32 dd (10.7, 5.9)	3.13 dd (11.5, 3.9)	3.20 overlap
8	1.78 m 2.03 m	1.41 m 2.67 m	1.35 m 1.72 m	1.22 m 1.58 m	1.31 m 1.60 m
9	1.45 m 1.70 m	1.47 m 1.68 m	1.49 m 1.62 m	1.40 m 1.67 m	1.47 m 1.60 m
10	3.29 dd (12.0, 3.2)	3.25 dd (11.8, 2.7)	3.20 dd (8.0, 1.6)	3.21 dd (11.9, 2.9)	3.23 overlap
12	1.18 s 3H	1.17 s 3H	1.18 s 3H	1.18 s 3H	1.16 s 3H
13	1.17 s 3H	1.16 s 3H	1.17 s 3H	1.18 s 3H	1.14 s 3H
14	1.02 s 3H	1.06 s 3H	0.85 s 3H	1.15 s 3H	0.91 s 3H
15	1.43 s 3H	1.45 s 3H	2.30 s 3H	2.21 s 3H	2.19 s 3H
16		3.94 d (7.9)			

^a Recorded at 400 MHz, (δ , CDCl_3 , J in Hz); ^b Recorded at 600 MHz, (δ , CDCl_3 , J in Hz); ^c Recorded at 600 MHz, (δ , CD_3OD , J in Hz).

Table 2 ¹H NMR data of compounds **6-10**.

No.	6 ^a	7 ^b	8 ^b	9 ^b	10 ^b
1		10.01 d		2.30 overlap 2H	0.84 s 3H
2		2.07 s			
4	2.21 m	1.41 m	2.50 m	2.56 m 2H	2.47 m
	2.25 m	1.75 dt (14.3, 3.1)	2.63 m		2.59 m
5	1.73 t (6.3) 2H	1.45 m	1.69 m 2H	1.59 m	1.55 m
		1.66 m		1.85 m	1.81 m
6	3.29 dd (10.6, 2.7)	3.16 dd (11.9, 3.5)	3.65 dd (9.0, 3.6)	3.23 d (10.5)	2.98 dd (10.9, 1.9)
8	1.46 m	1.57 dd (12.6, 3.9)	1.86 dt (13.1, 3.2)	1.72 m 2H	1.35 m
	1.95 d (11.6)	1.91 m	1.98 m		1.50 m
9	1.49 m	1.50 m	1.52 m 2H	1.47 m	1.40 m
	1.62 m	1.84 m		1.57 m	1.51 m
10	3.22 dd (11.6, 2.5)	3.25 dd (11.7, 2.8)	3.18 dd (11.0, 3.4)	3.09 dd (11.5, 2.2)	3.06 dd (11.0, 2.2)
12	1.19 s 3H	1.18 s 3H	1.16 s 3H	1.18 s 3H	1.17 s 3H
13	1.18 s 3H	1.17 s 3H	1.20 s 3H	1.14 s 3H	1.13 s 3H
14	1.20 s 3H	1.23 s 3H	1.19 s 3H	1.03 s 3H	0.87 s 3H
15	1.79 s 3H	1.21 s 3H	2.15 s 3H	2.15 s 3H	2.15 s 3H

^a Recorded at 400 MHz, (δ , CDCl₃, *J* in Hz); ^b Recorded at 600 MHz, (δ , CDCl₃, *J* in Hz).

Table 3 ¹³C NMR data of compounds 1-10.

No.	1 ^a	2 ^c	3 ^b	4 ^a	5 ^a	6 ^a	7 ^b	8 ^a	9 ^a	10 ^b
1	68.7	72.8	40.6	43.5	44.6	173.8	207.2	181.0	44.5	27.2
2	59.3	54.2	138.5	66.7	66.5	133.6	64.8		176.4	
3	82.5	84.3	137.8	212.2	211.5	137.6	71.4	209.0	209.8	209.6
4	36.4	39.4	198.5	54.2	57.3	31.3	39.1	41.0	41.0	41.3
5	26.0	26.1	26.9	25.4	29.0	23.7	21.4	25.8	24.0	24.2
6	84.4	85.5	79.0	83.7	82.1	80.6	83.7	80.1	82.8	85.1
7	35.2	38.2	31.6	33.2	33.7	35.4	37.6	44.9	35.4	32.7
8	36.6	40.0	37.9	39.0	38.5	33.7	37.6	34.9	35.4	39.4
9	20.7	22.5	22.3	21.8	21.6	21.9	24.0	20.5	22.1	22.6
10	85.6	86.6	84.6	85.4	85.4	84.7	85.1	84.5	84.6	84.8
11	72.1	72.8	72.0	72.1	72.0	72.4	72.0	72.0	72.3	72.2
12	26.0	25.5	26.1	26.1	26.1	26.0	26.1	26.0	26.2	26.3
13	23.8	25.5	23.9	23.9	23.9	23.8	24.0	24.0	24.1	24.2
14	12.2	12.8	16.5	17.4	16.5	19.2	13.8	13.8	17.9	19.1
15	23.5	25.4	25.5	28.8	29.1	21.2	31.1	29.7	30.0	30.0
16	178.5	77.1								
17		175.4								

^a Recorded at 100 MHz, (δ , CDCl₃); ^b Recorded at 150 MHz, (δ , CDCl₃); ^c Recorded at 150 MHz, (δ , CD₃OD).

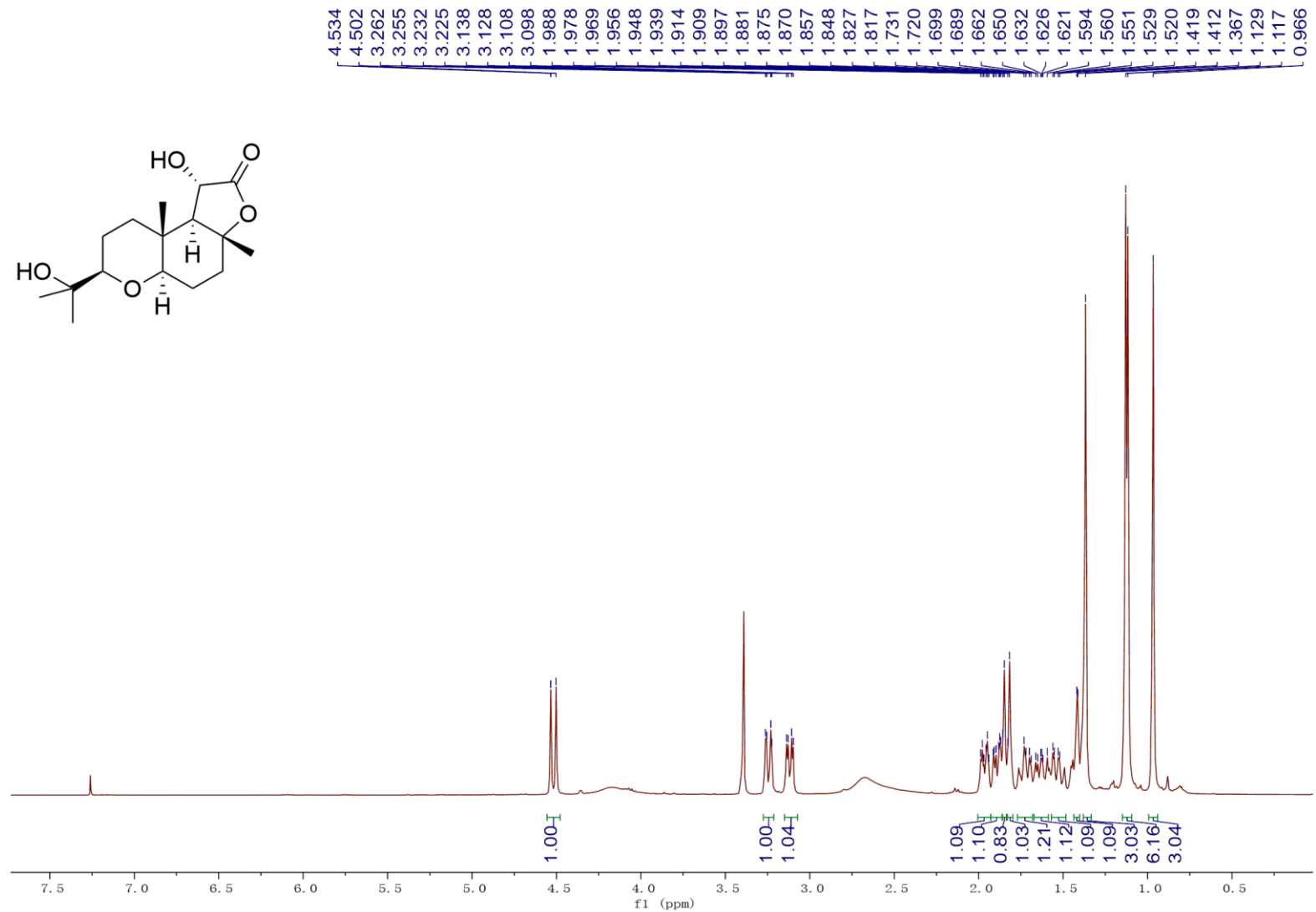


Fig. S1. ¹H NMR spectrum (CDCl₃, 400 MHz) of **1**

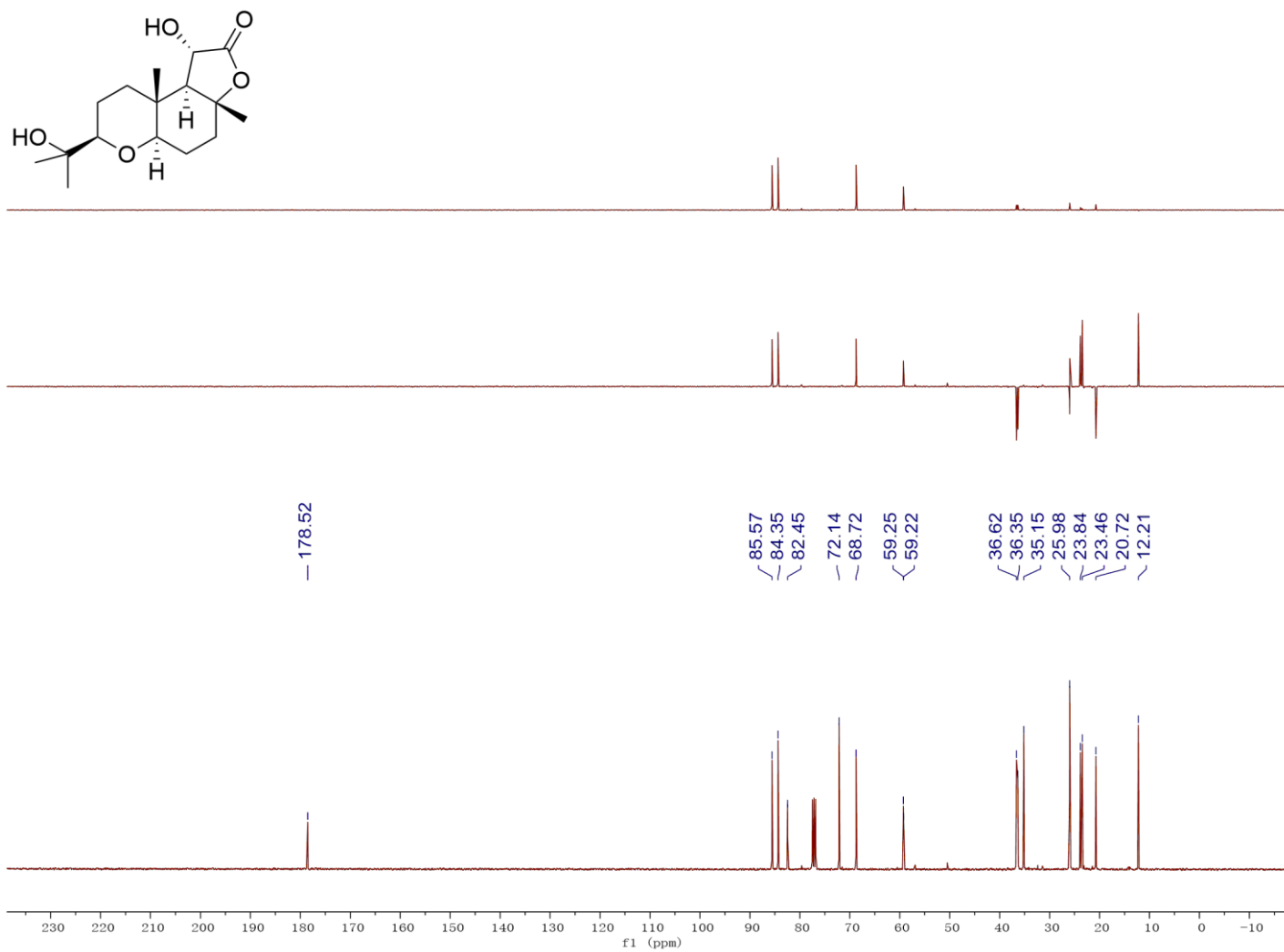


Fig. S2. ^{13}C and DEPT spectra (CDCl_3 , 100 MHz) of **1**

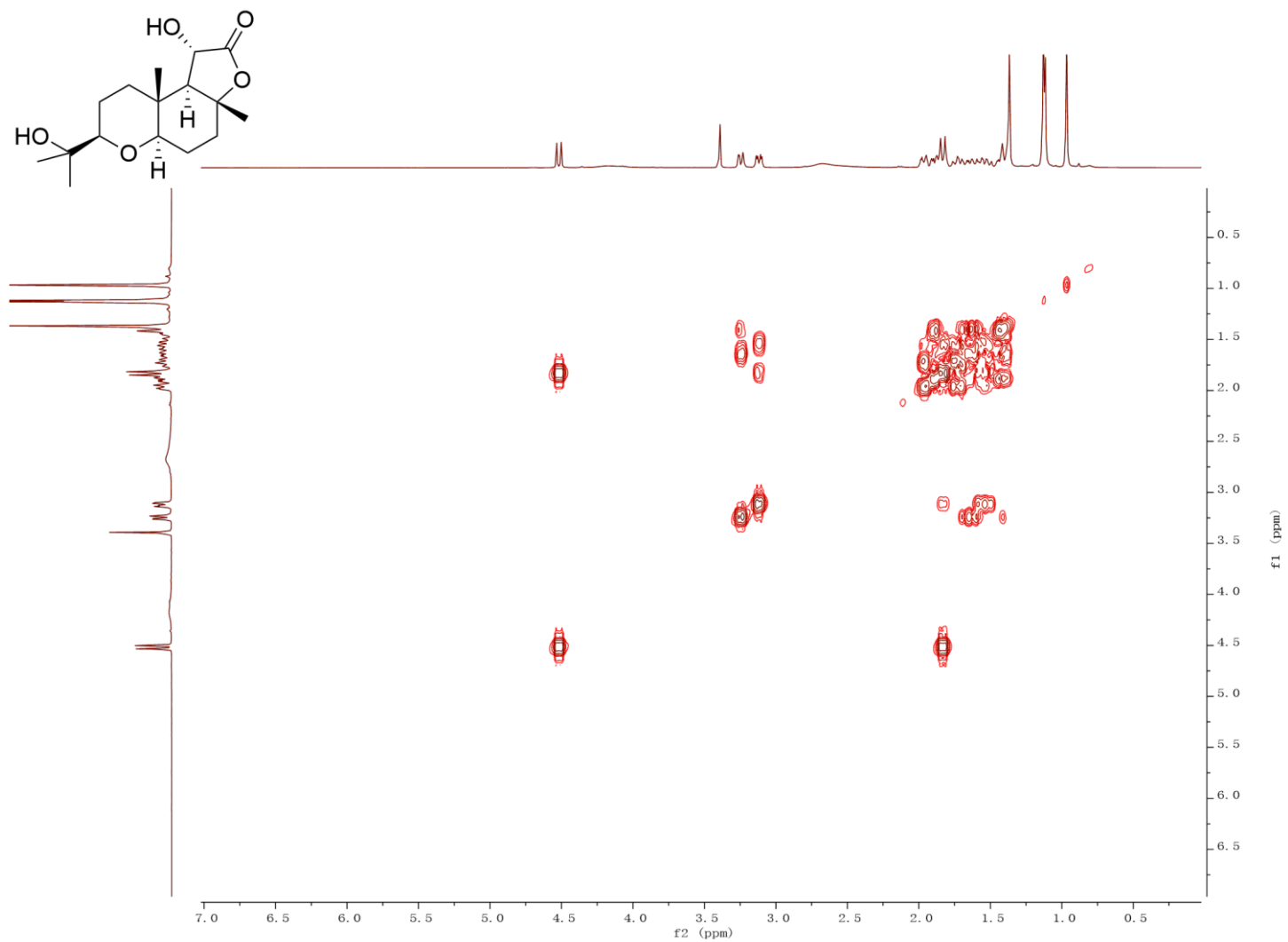


Fig. S3. ^1H - ^1H COSY spectrum (CDCl_3 , 400 MHz) of **1**

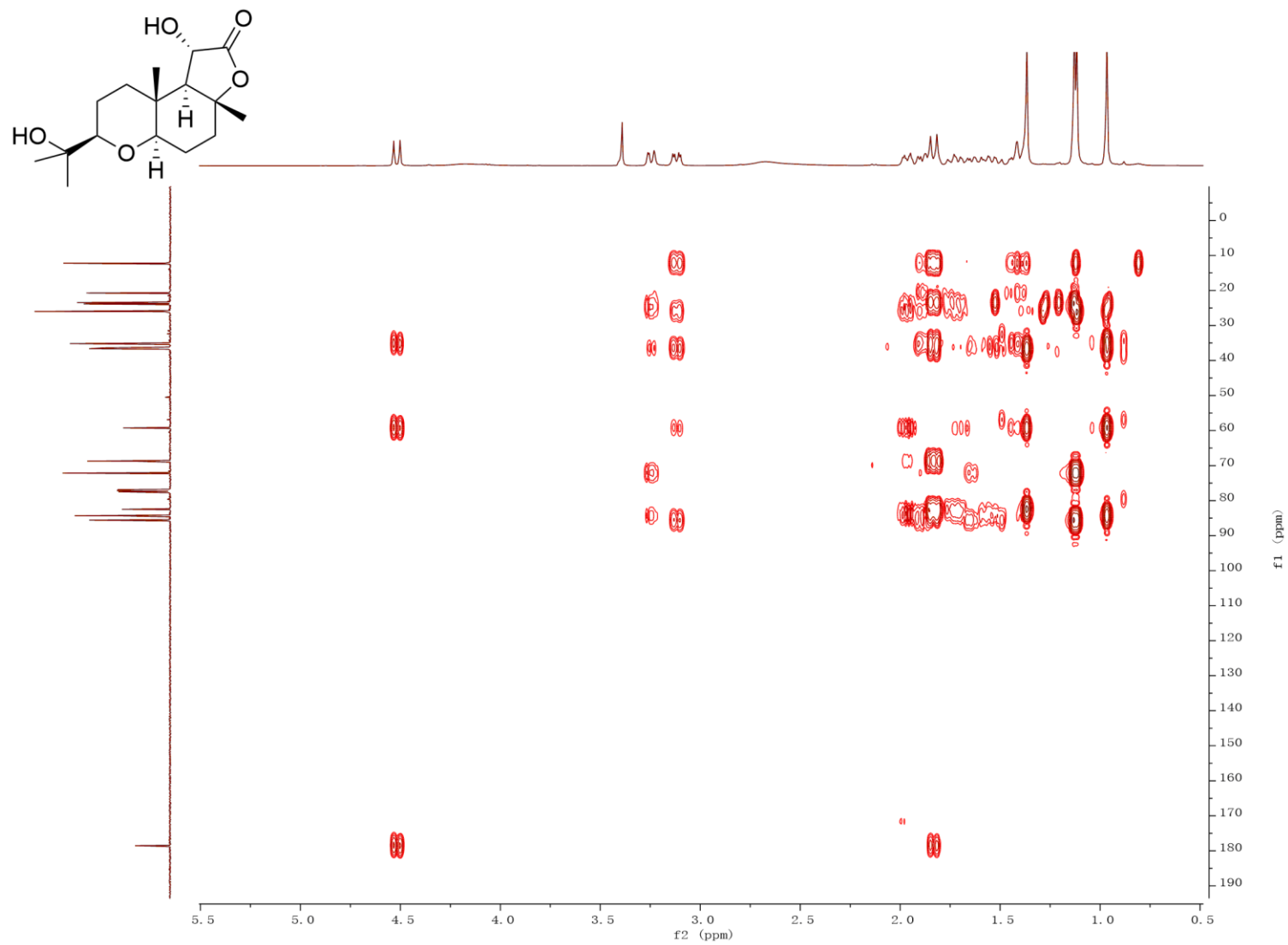


Fig. S4. HMBC spectrum (CDCl₃, 400 MHz) of **1**

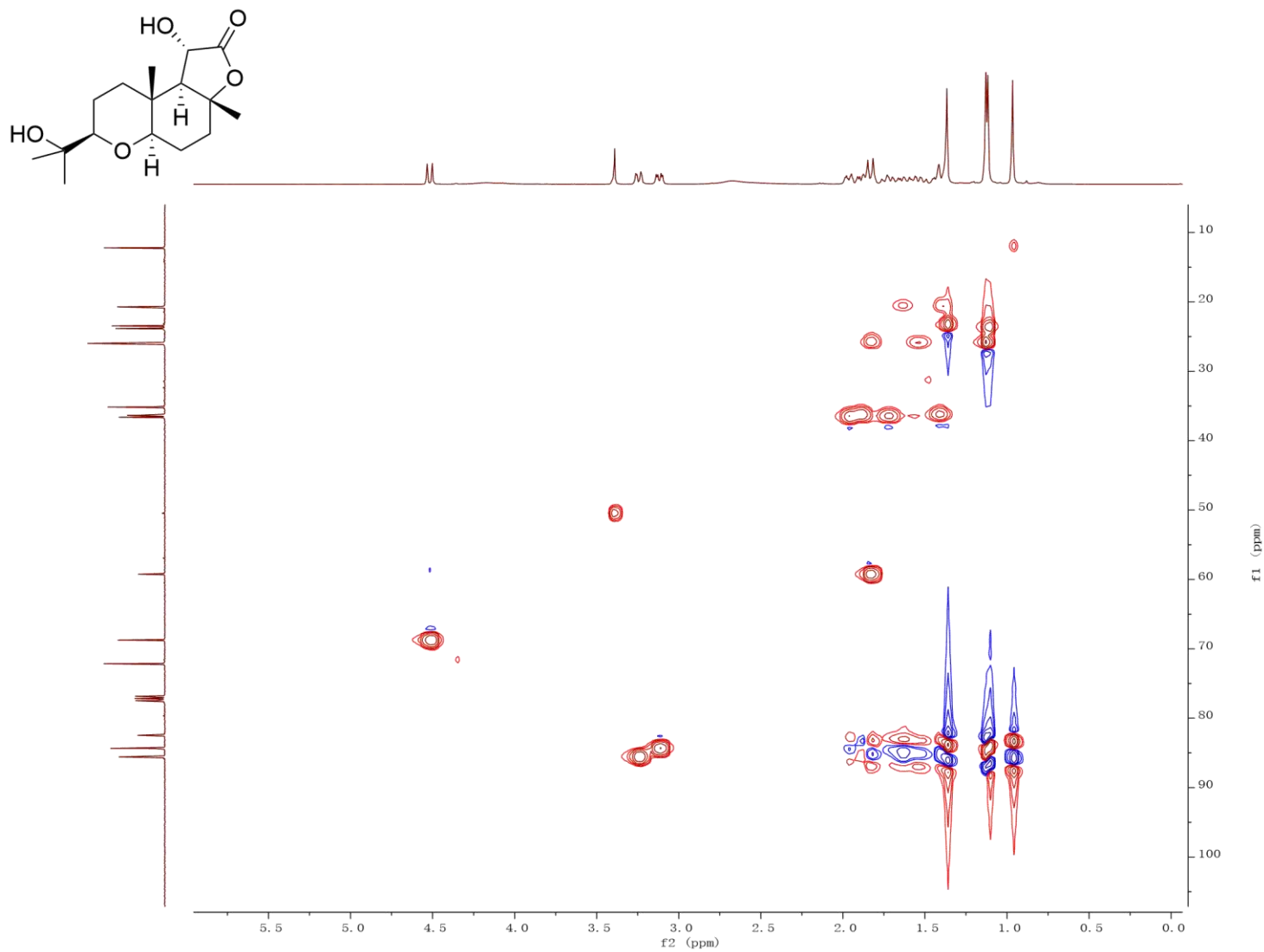


Fig. S5. HSQC spectrum (CDCl₃, 400 MHz) of **1**

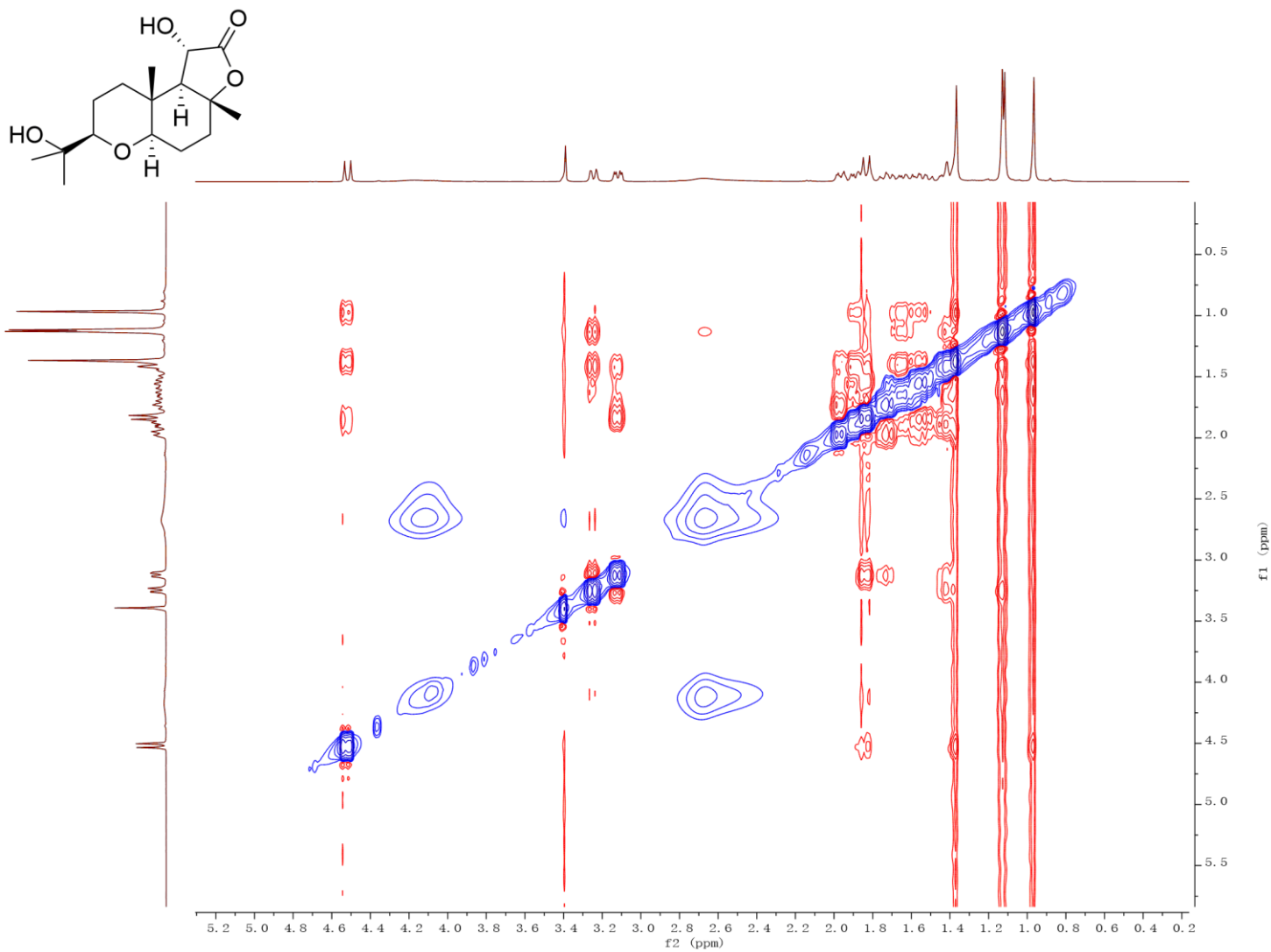


Fig. S6. NOESY spectrum (CDCl₃, 400 MHz) of **1**

DJ1-VA-292 #47 RT: 0.96 AV: 1 NL: 4.42E7
T: FTMS + c ESI Full ms [100.00-850.00]

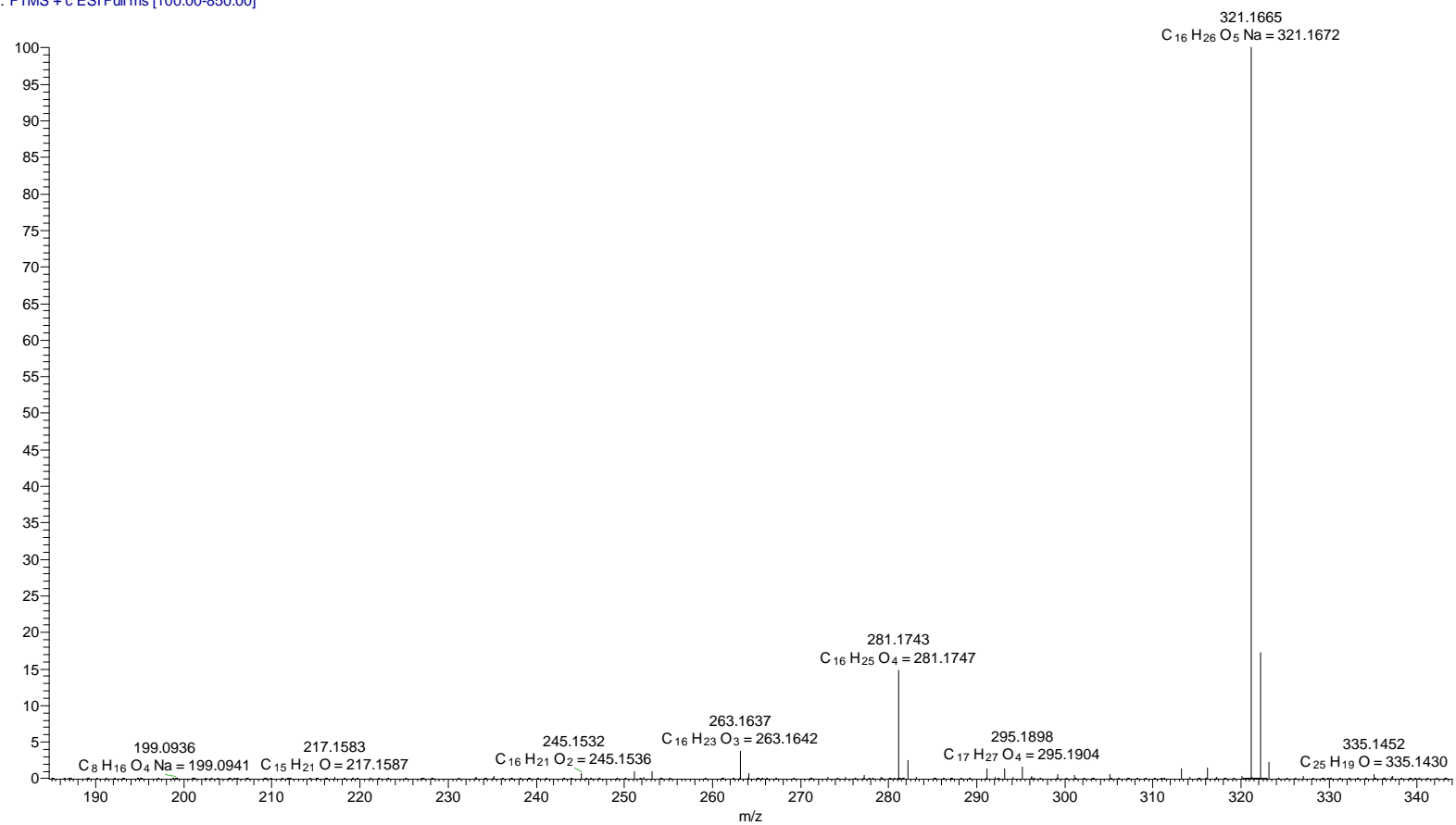


Fig. S7. (+)-HR-ESI-MS (positive mode) of **1**

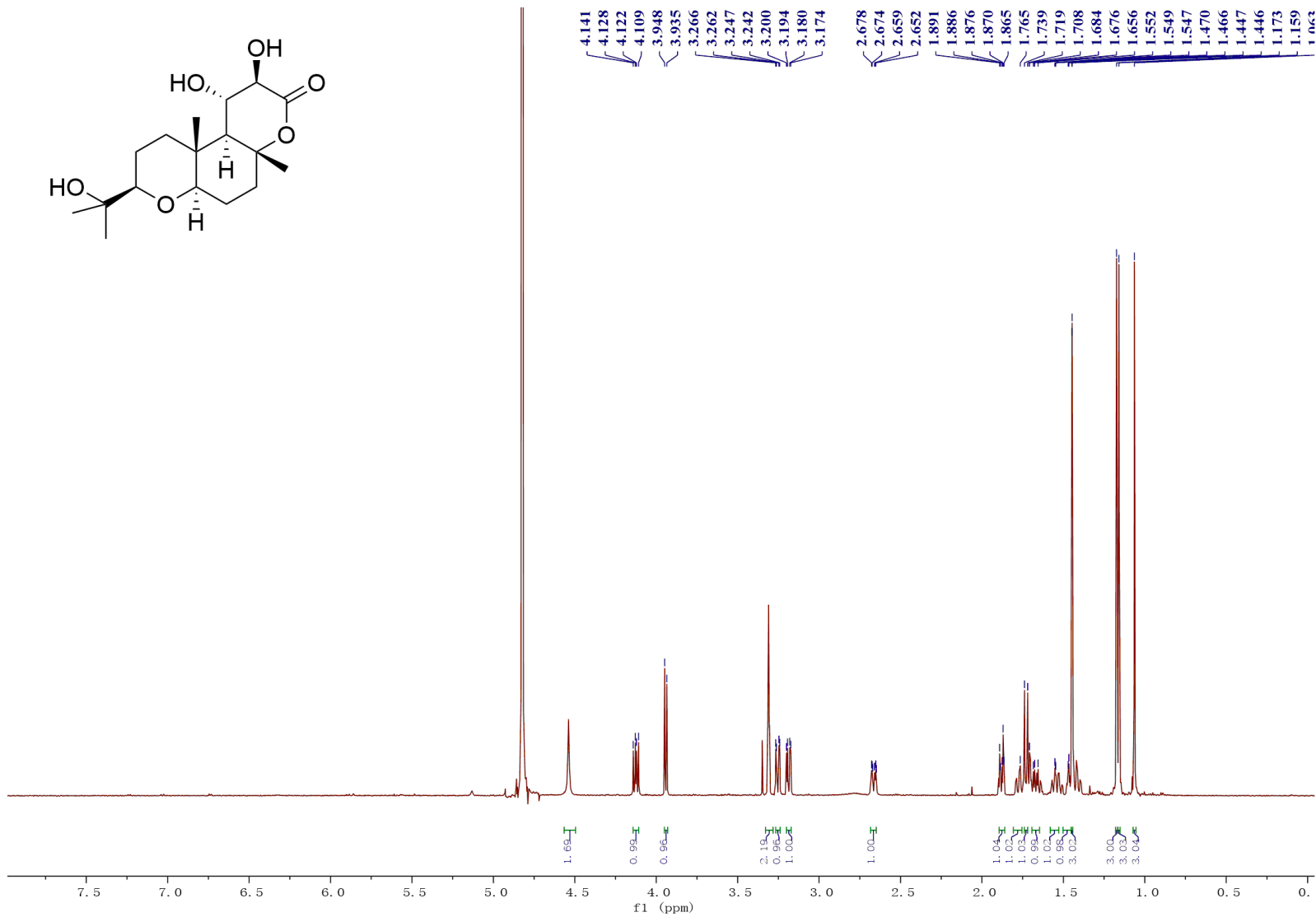


Fig. S8. ¹H NMR spectrum (MeOD, 600 MHz) of 2

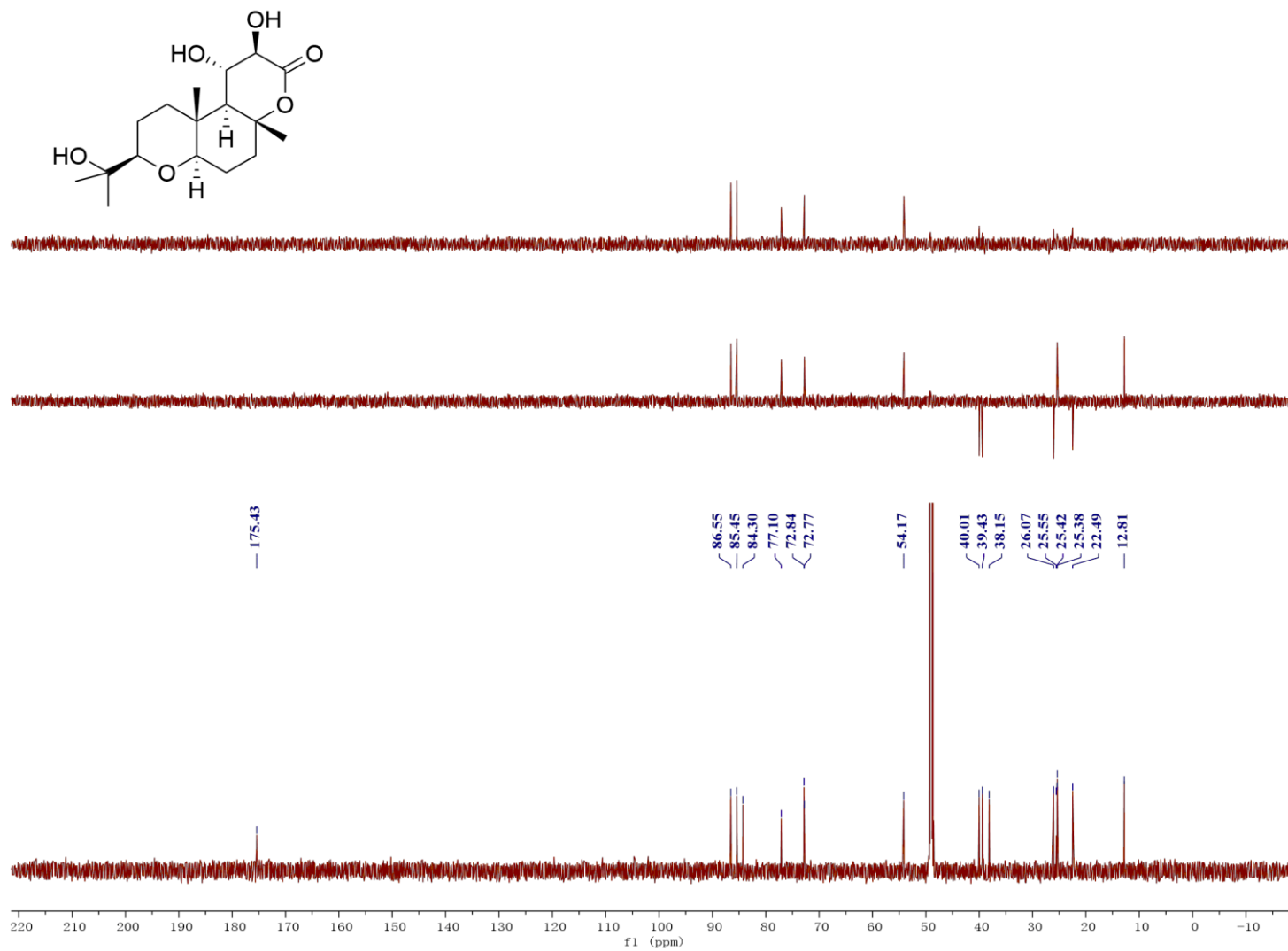


Fig. S9. ^{13}C and DEPT spectra (MeOD, 150 MHz) of **2**

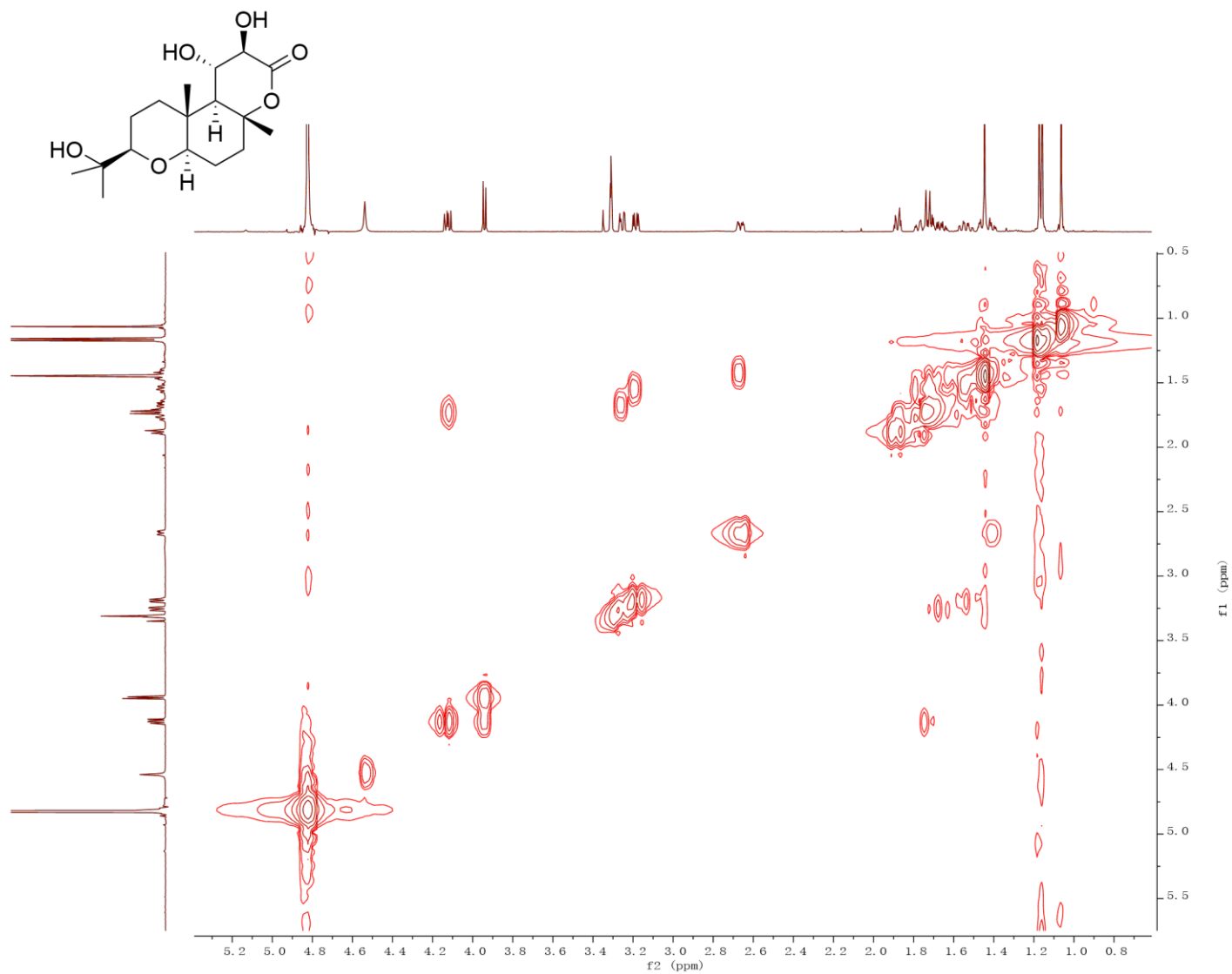


Fig. S10. ^1H - ^1H COSY spectrum (MeOD, 600 MHz) of **2**

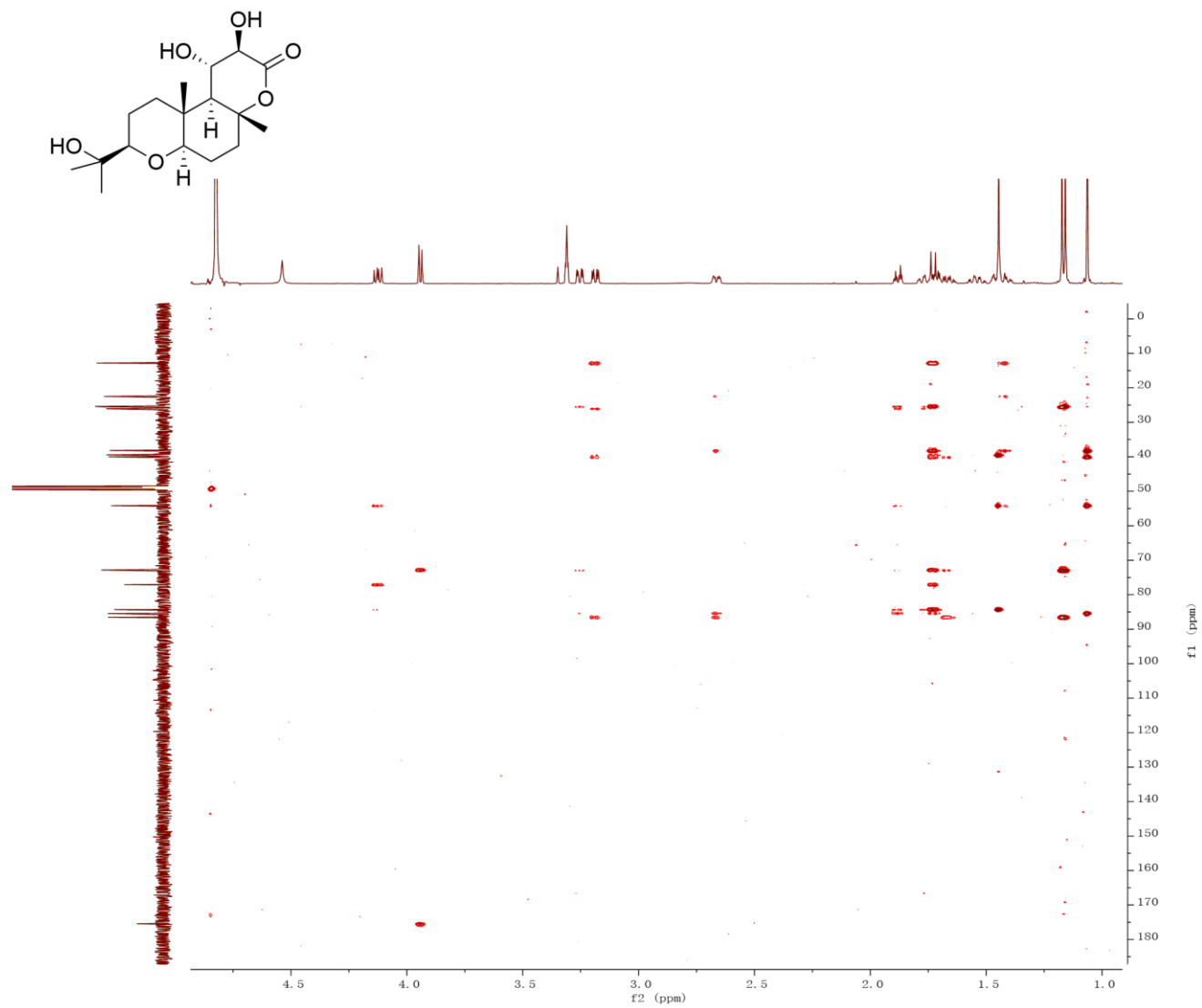


Fig. S11. HMBC spectrum (MeOD, 600 MHz) of **2**

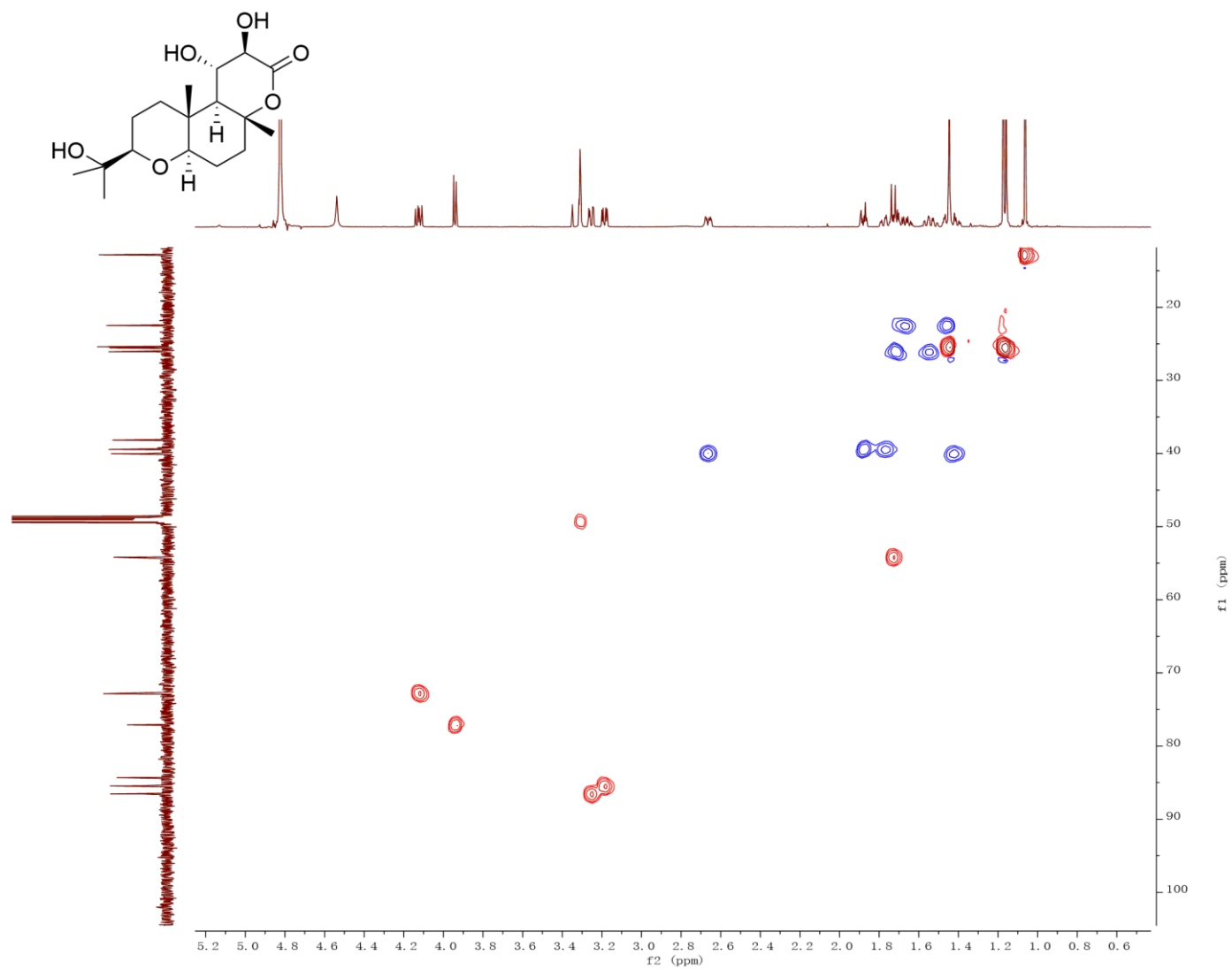


Fig. S12. HSQC spectrum (MeOD, 600 MHz) of **2**

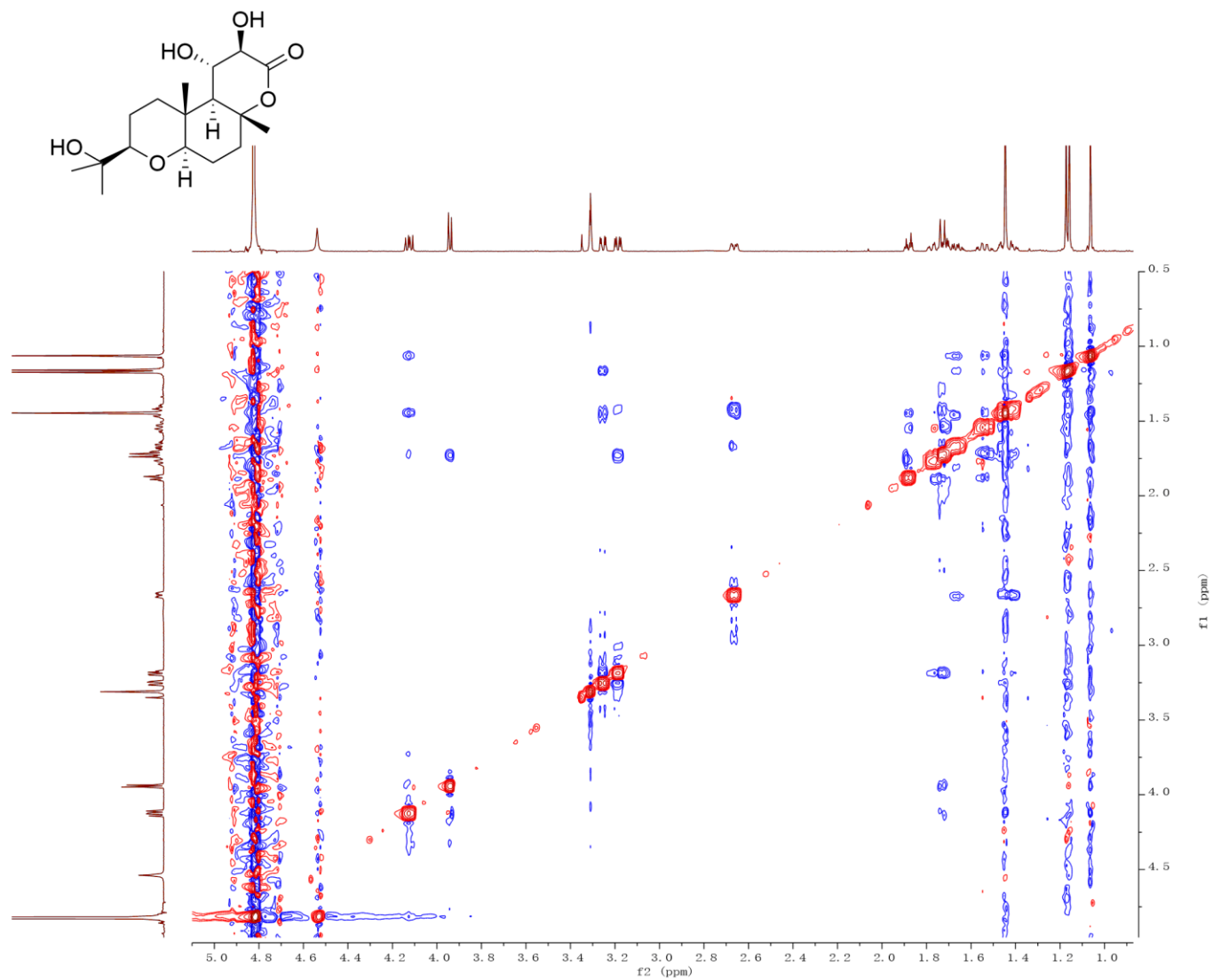


Fig. S13. NOESY spectrum (MeOD, 600 MHz) of **2**

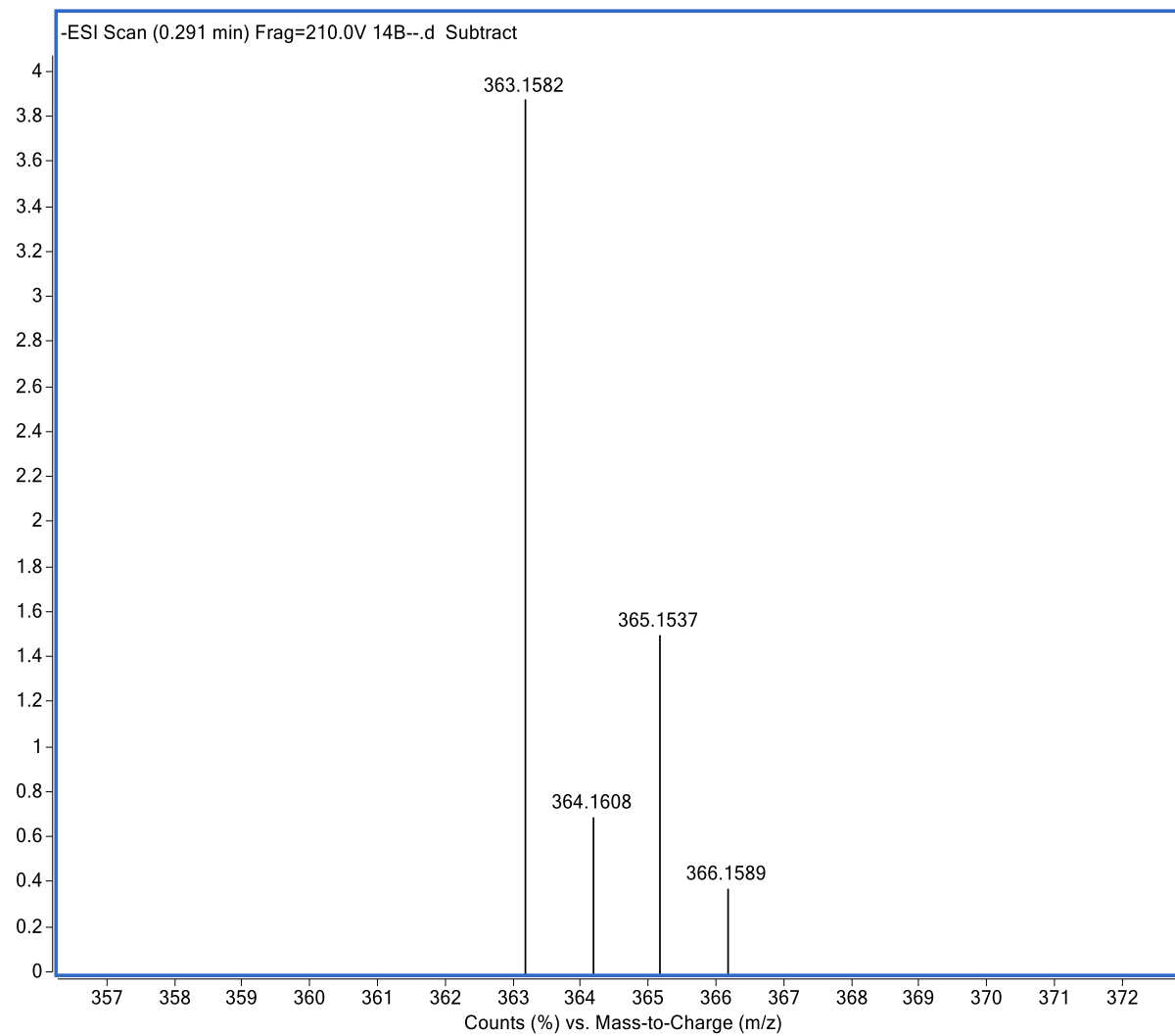


Fig. S14. (+)-HR-ESI-MS (positive mode) of **2**.

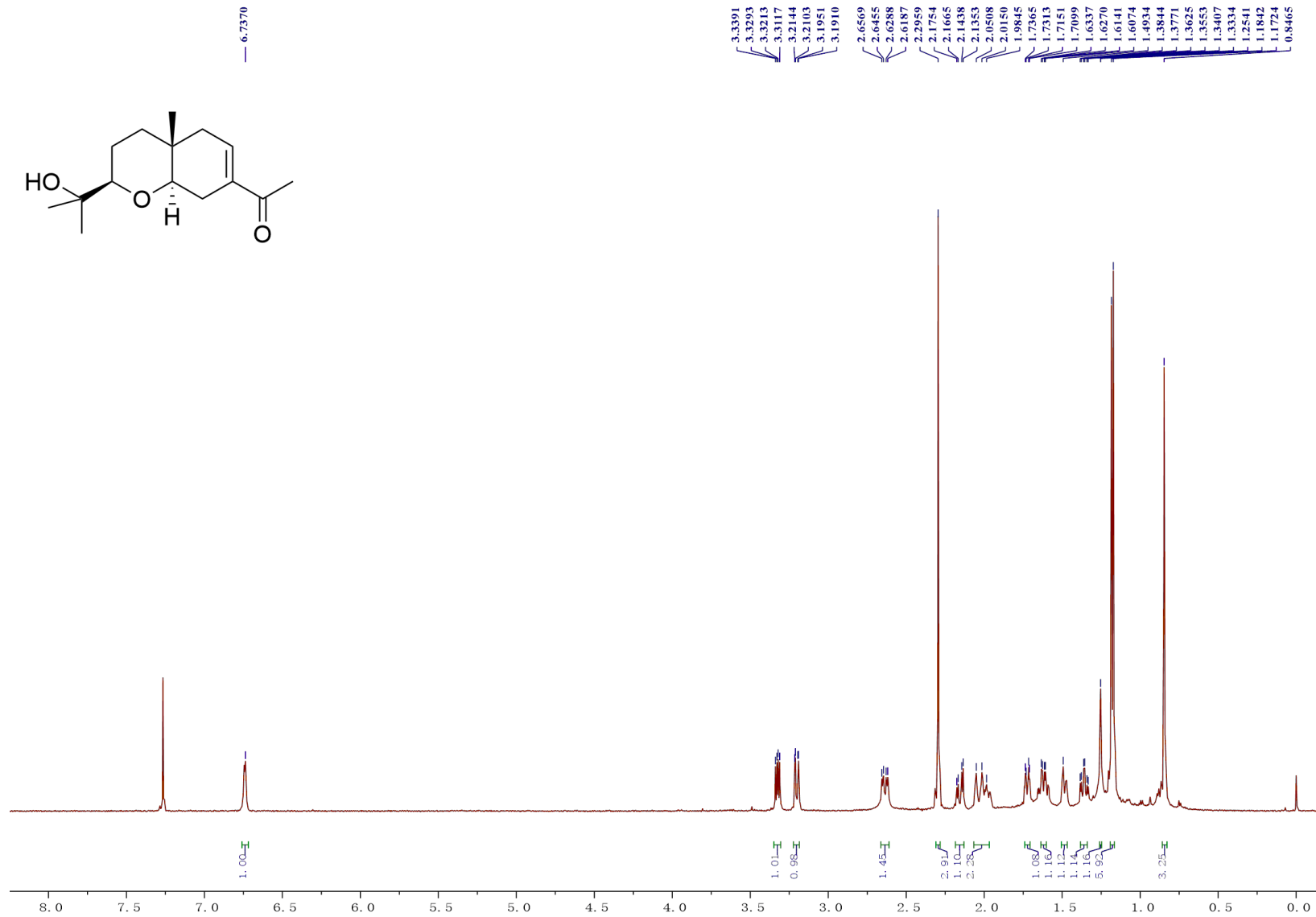


Fig. S15. ¹H NMR spectrum (CDCl₃, 600 MHz) of 3

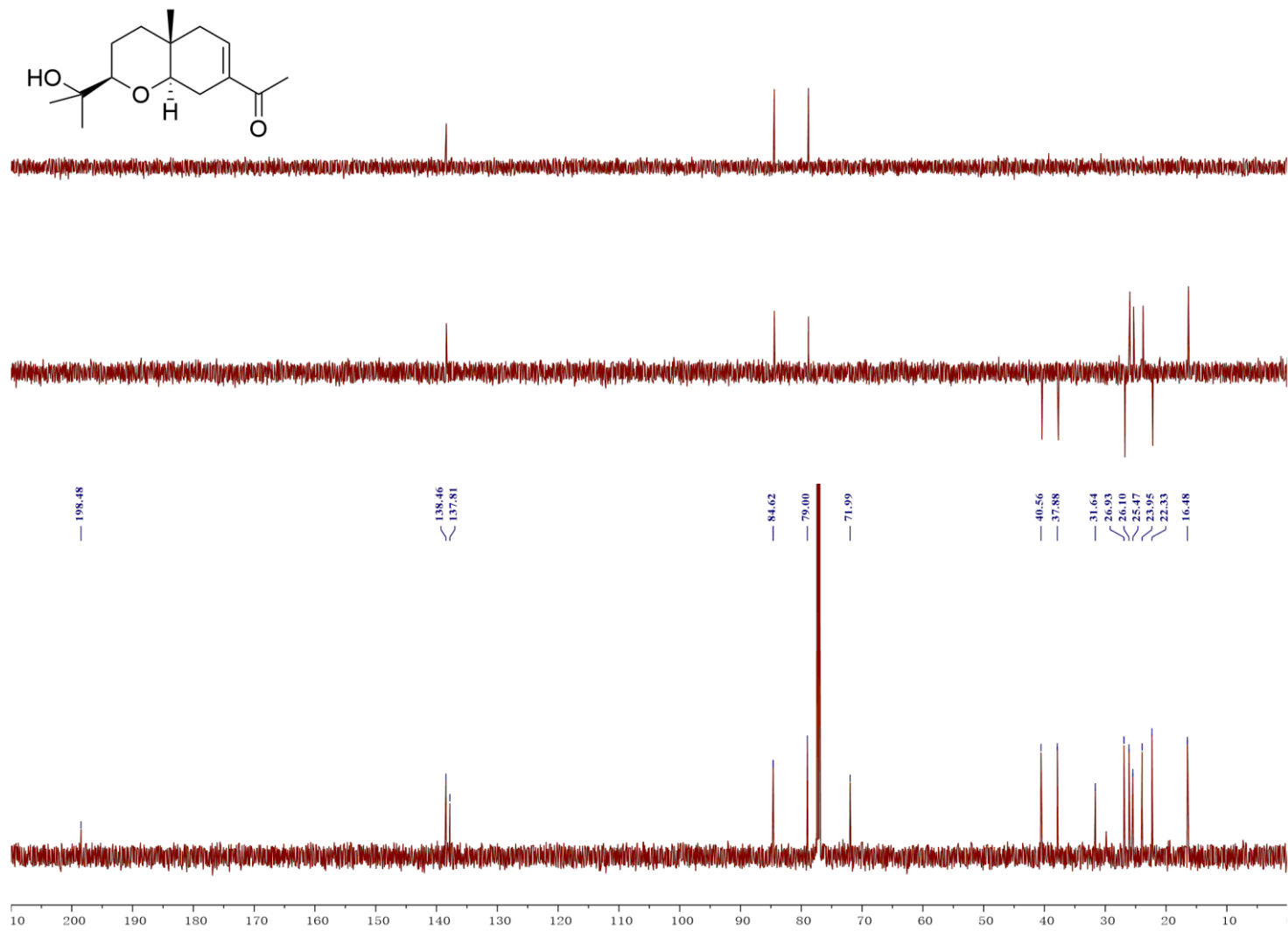


Fig. S16. ¹³C and DEPT spectra (CDCl₃, 150 MHz) of **3**

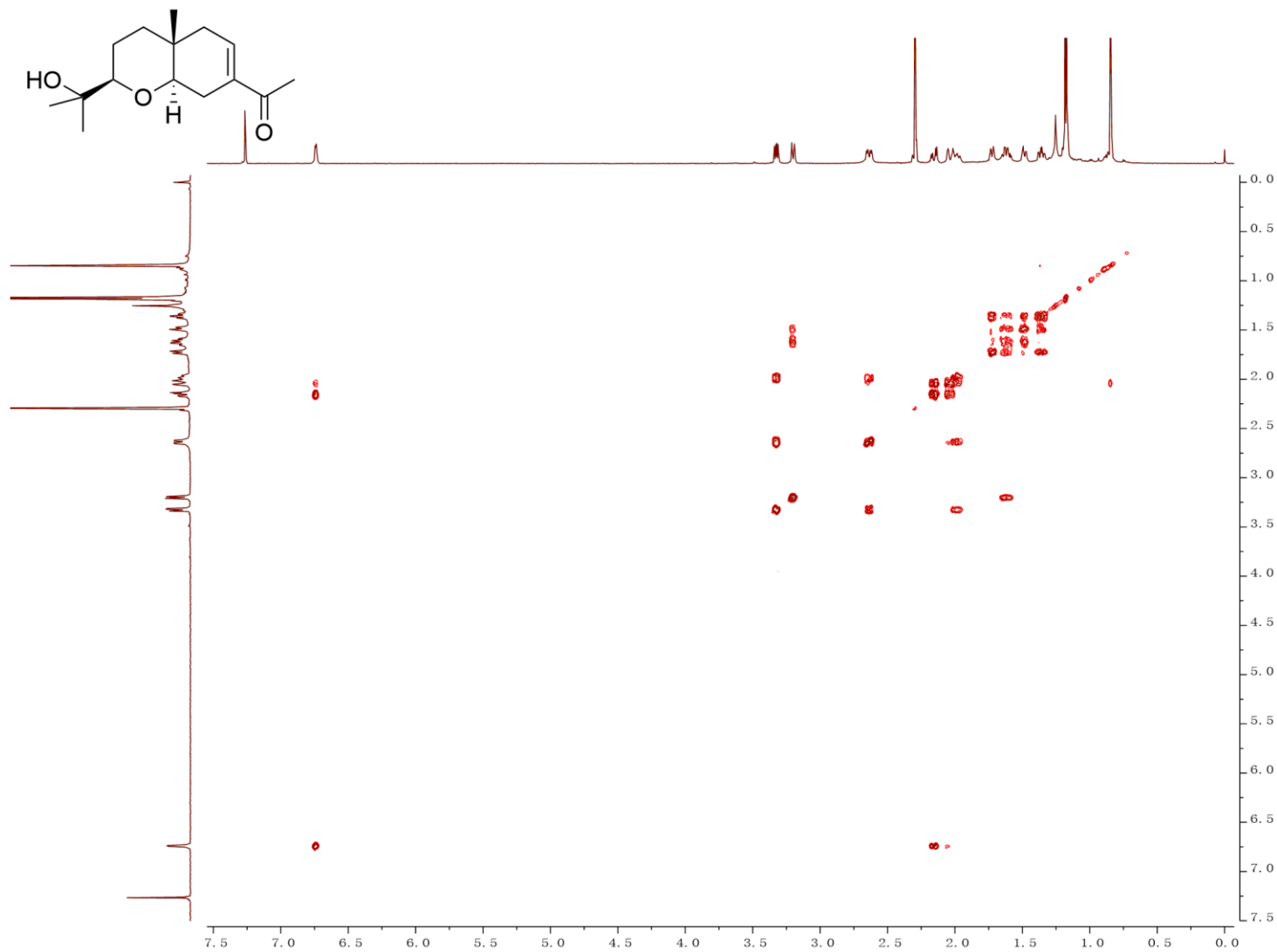


Fig. S17. ^1H - ^1H COSY spectrum (CDCl_3 , 600 MHz) of **3**

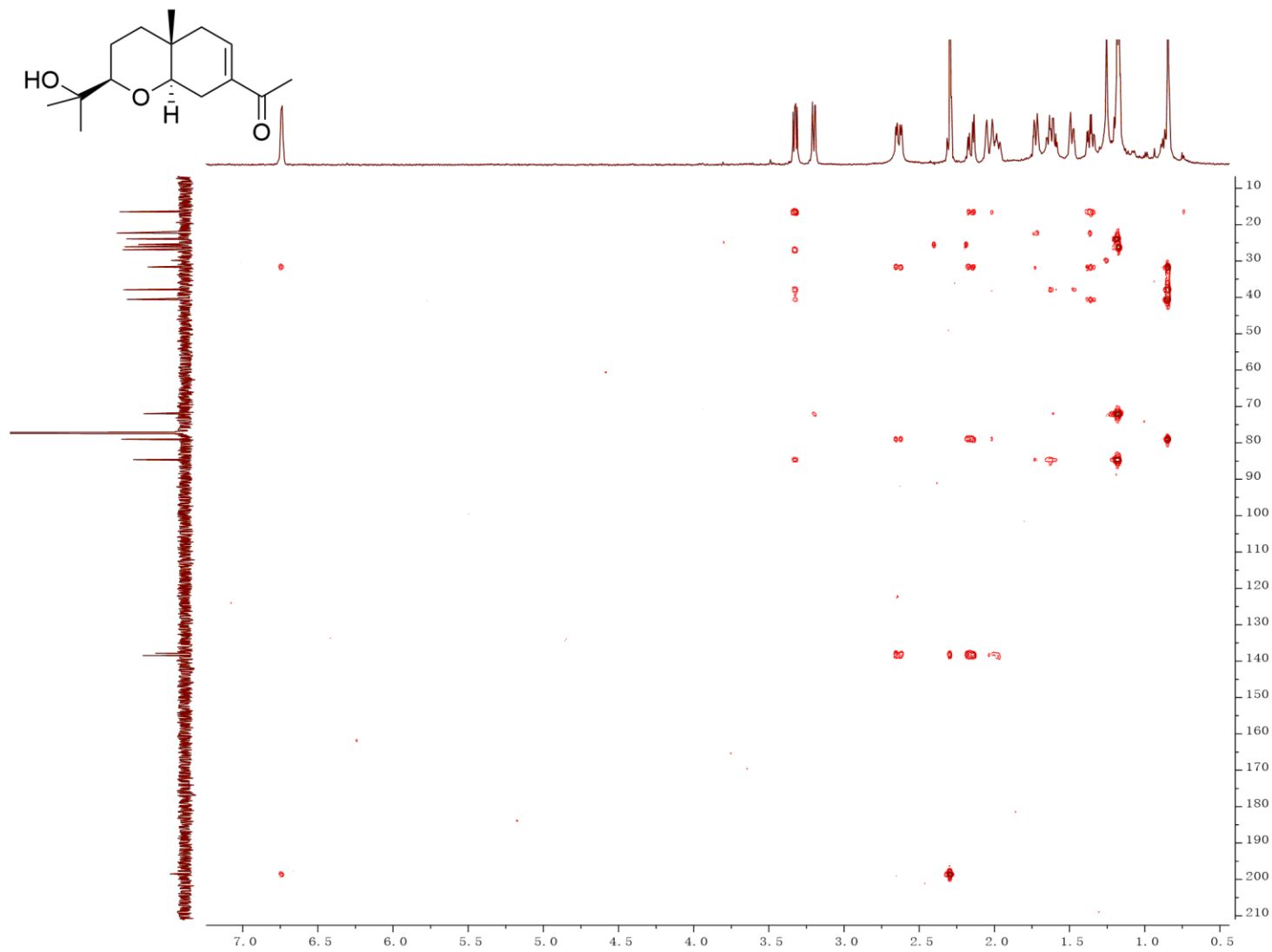


Fig. S18. HMBC spectrum (CDCl₃, 600 MHz) of **3**

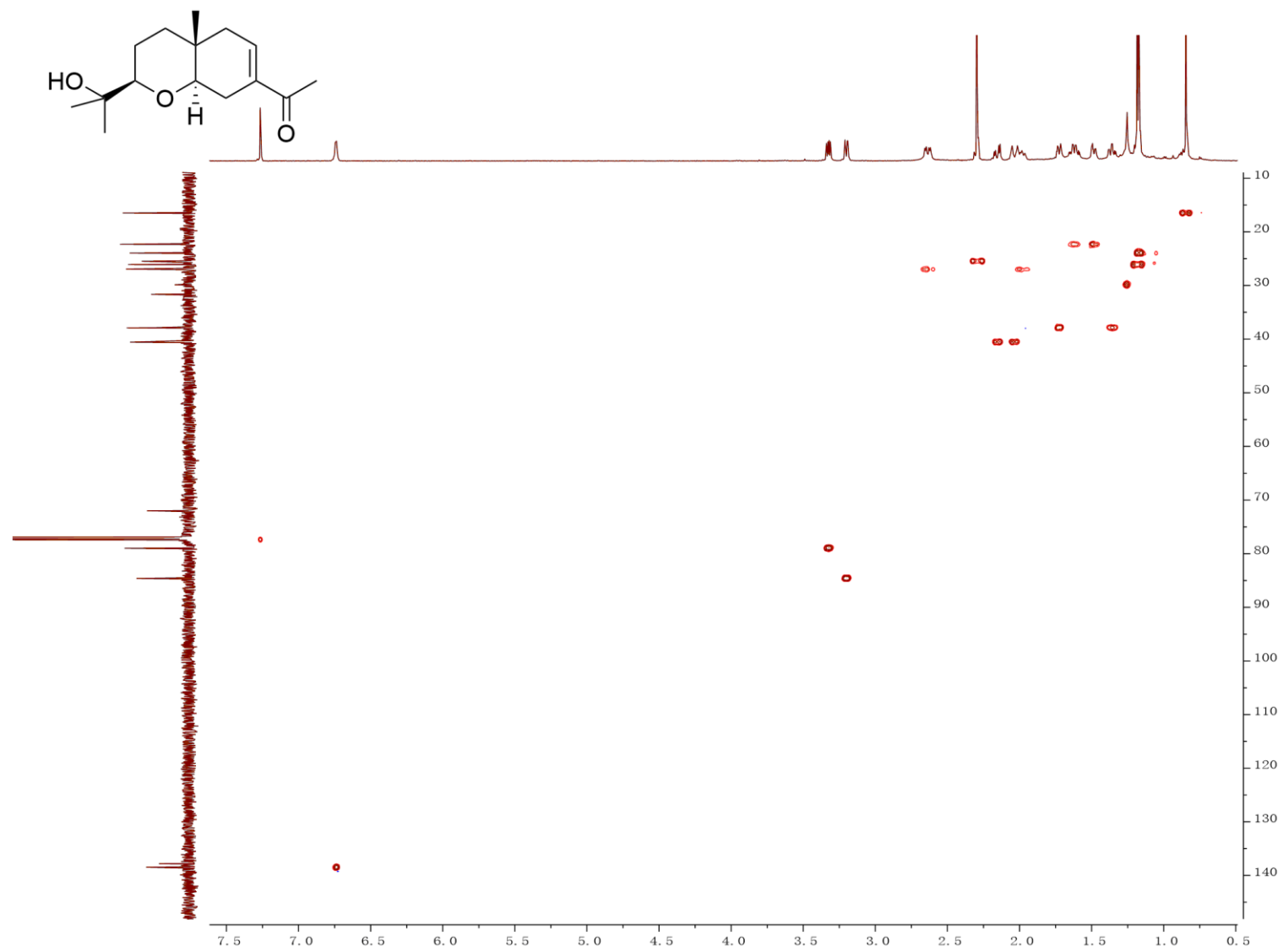


Fig. S19. HSQC spectrum (CDCl₃, 600 MHz) of **3**

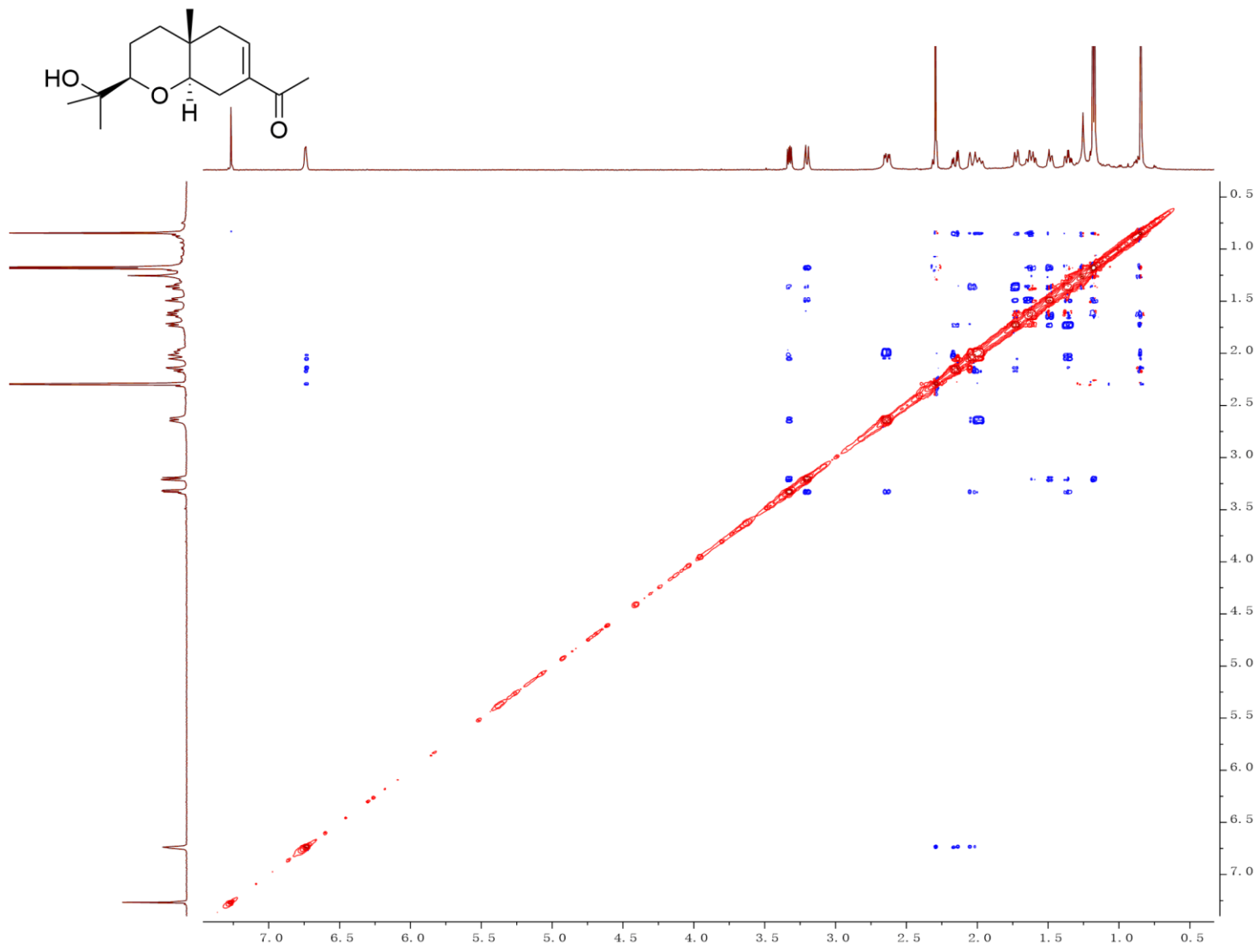


Fig. S20. NOESY spectrum (CDCl₃, 600 MHz) of **3**

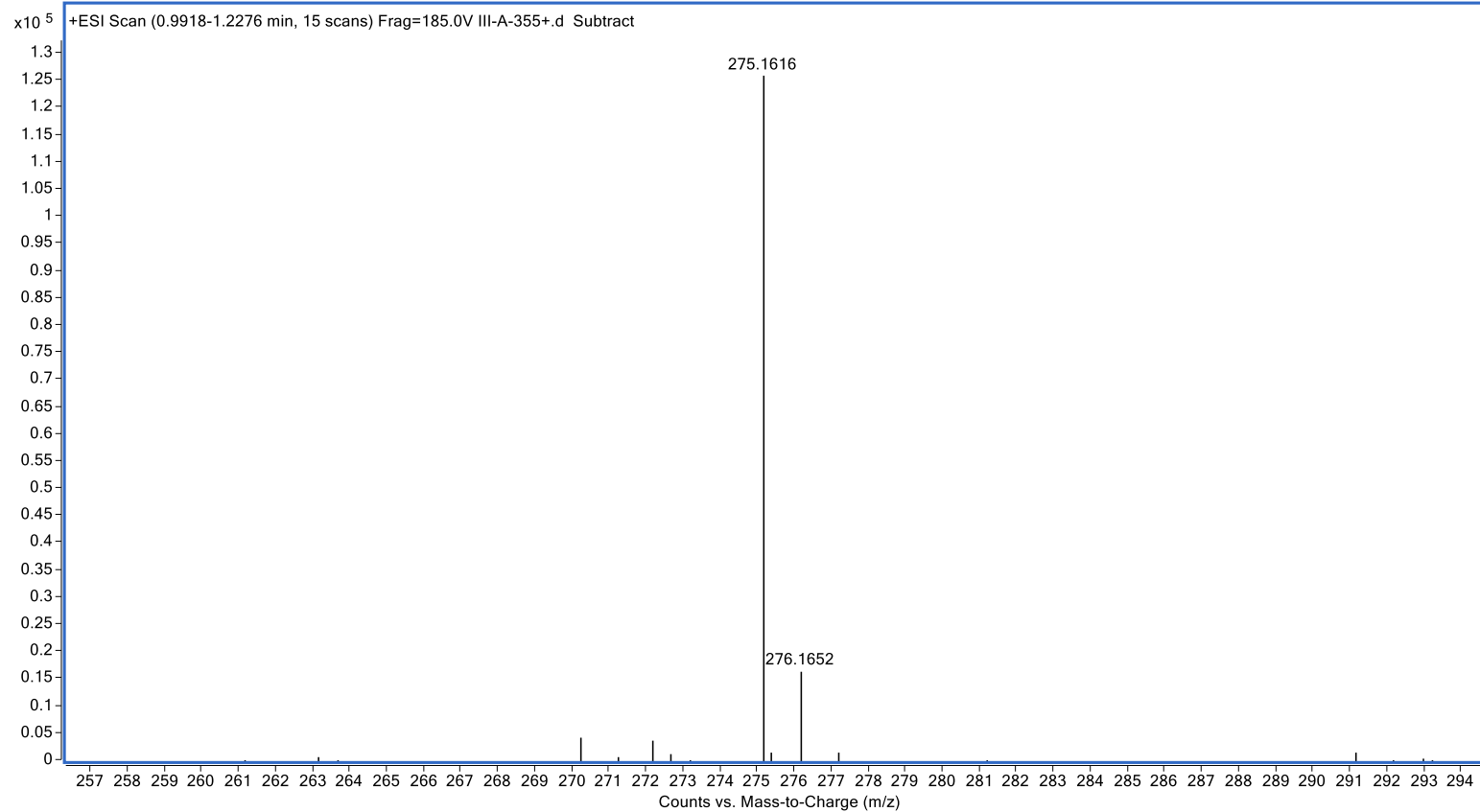


Fig. S21. (+)-HR-ESI-MS (positive mode) of **3**

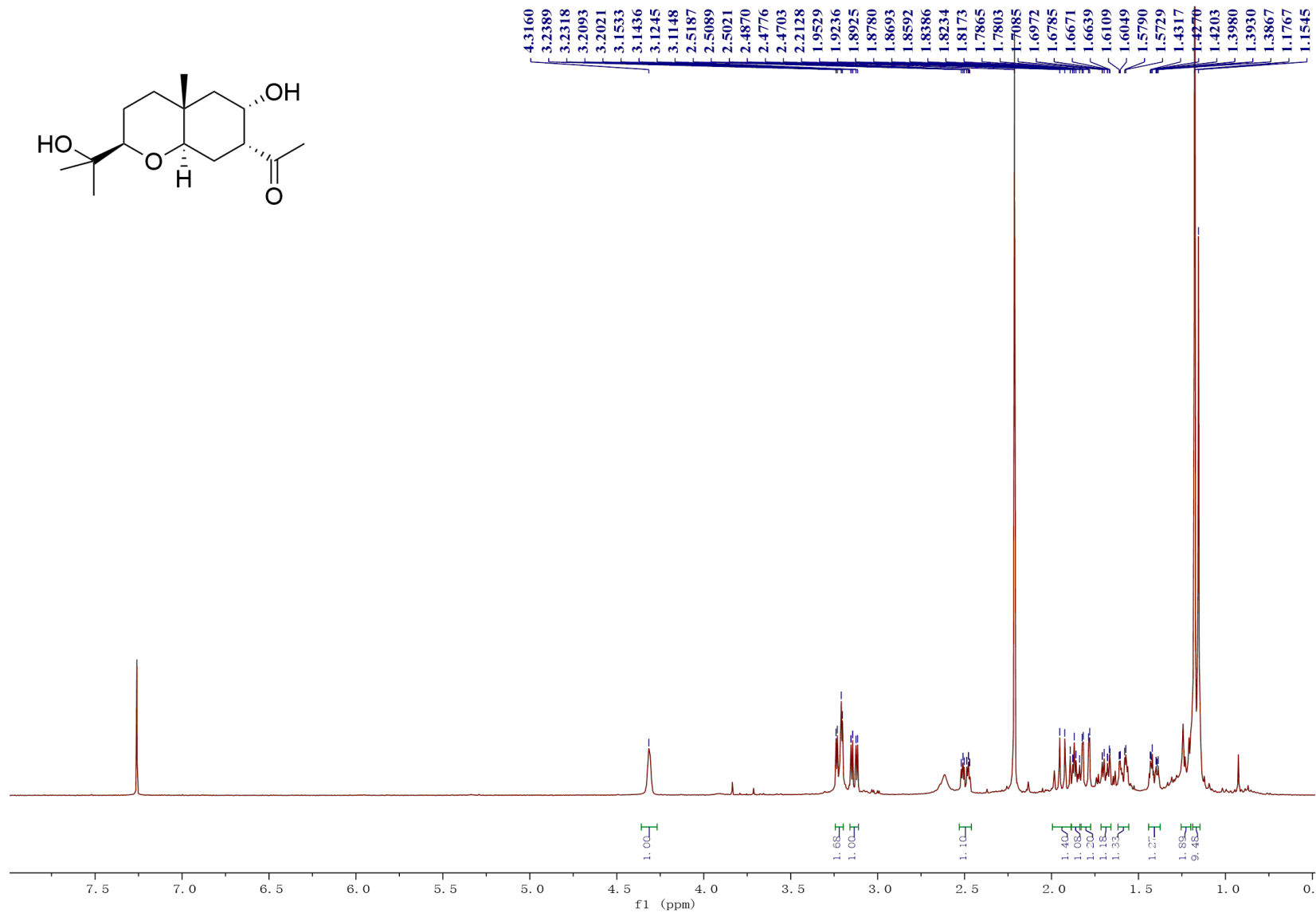


Fig. S22. ¹H NMR spectrum (CDCl₃, 400 MHz) of 4

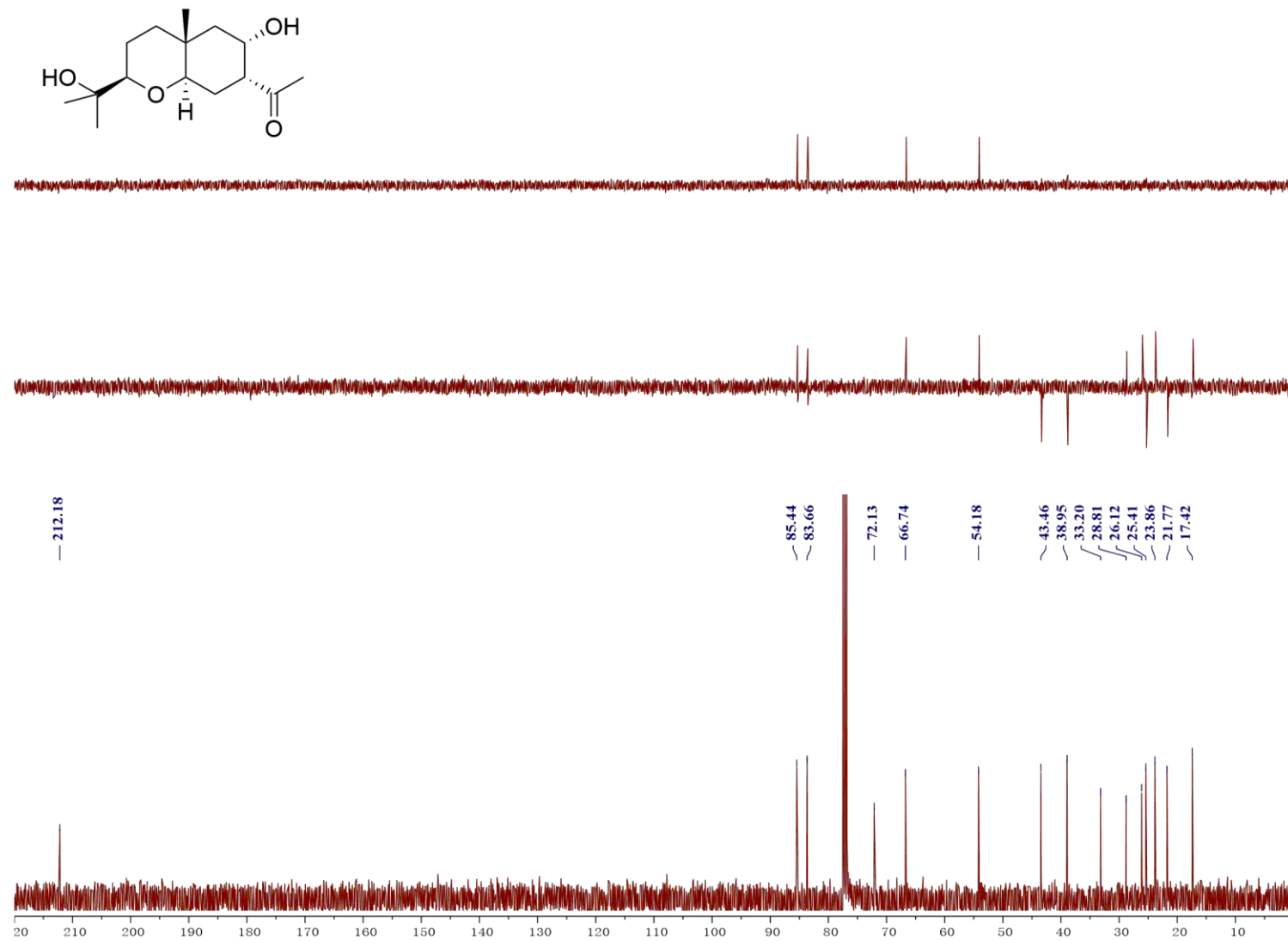


Fig. S23. ^{13}C and DEPT spectra (CDCl_3 , 100 MHz) of 4

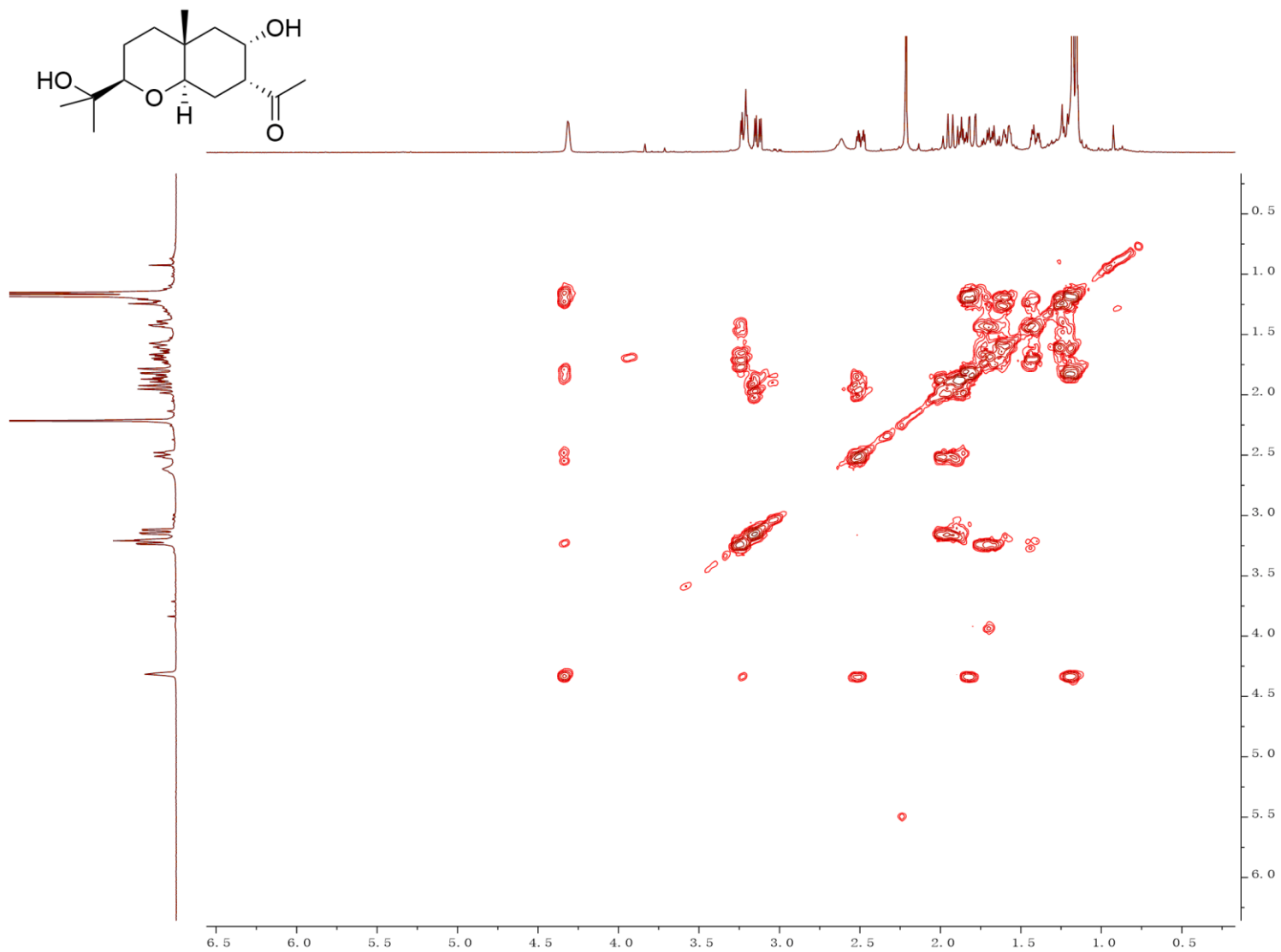


Fig. S24. ^1H - ^1H COSY spectrum (CDCl_3 , 400 MHz) of **4**

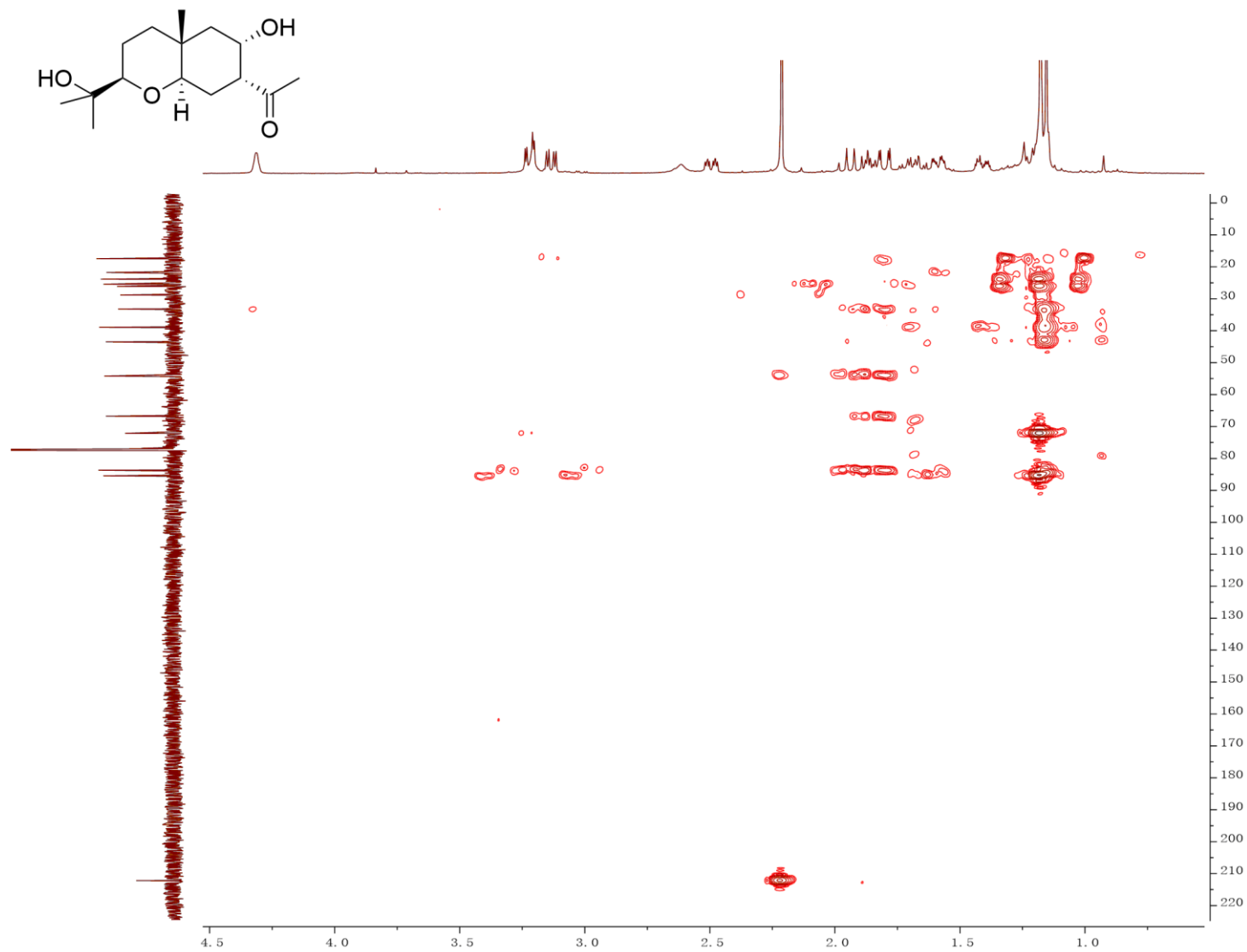


Fig. S25. HMBC spectrum (CDCl₃, 400 MHz) of **4**

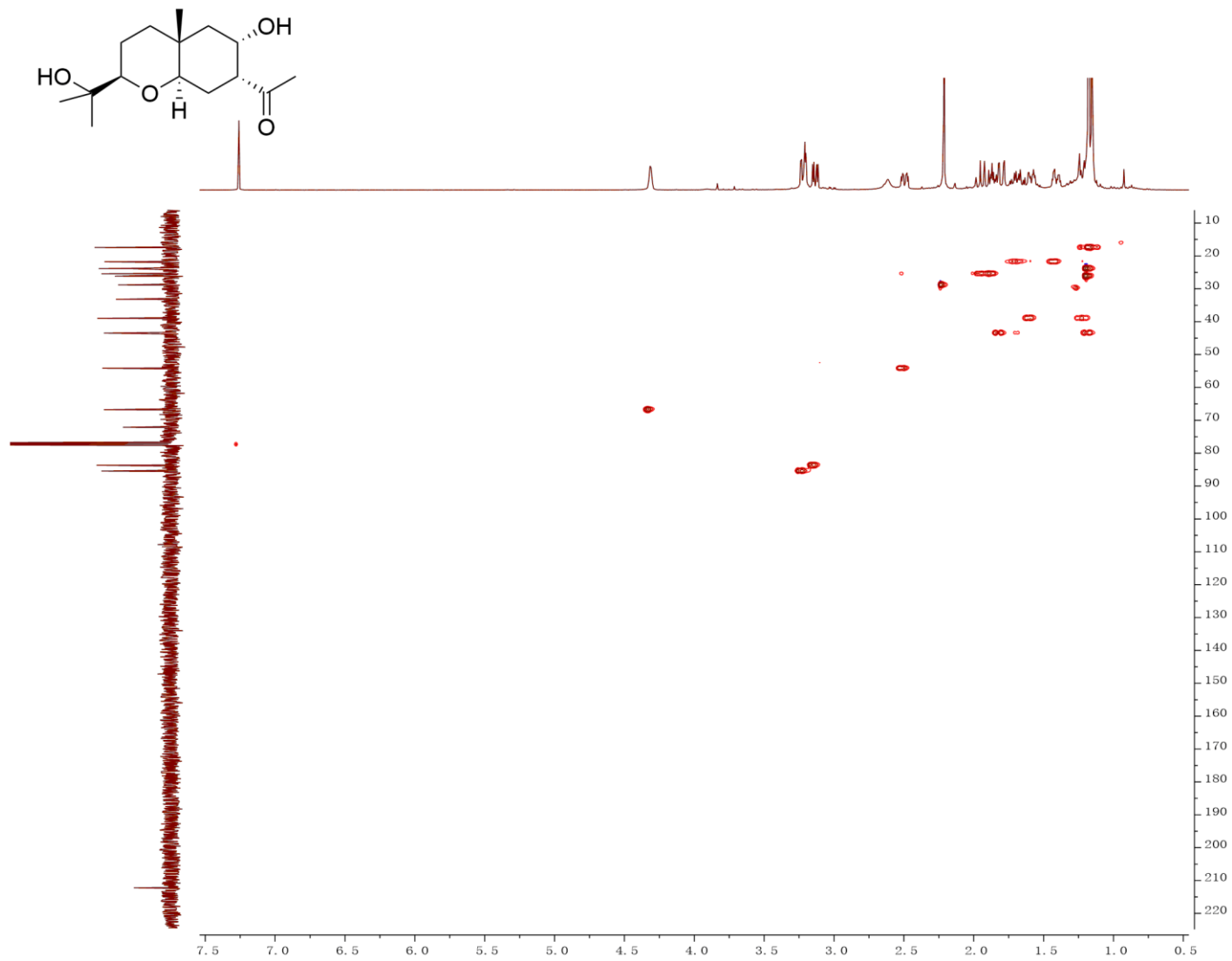


Fig. S26. HSQC spectrum (CDCl₃, 400 MHz) of **4**

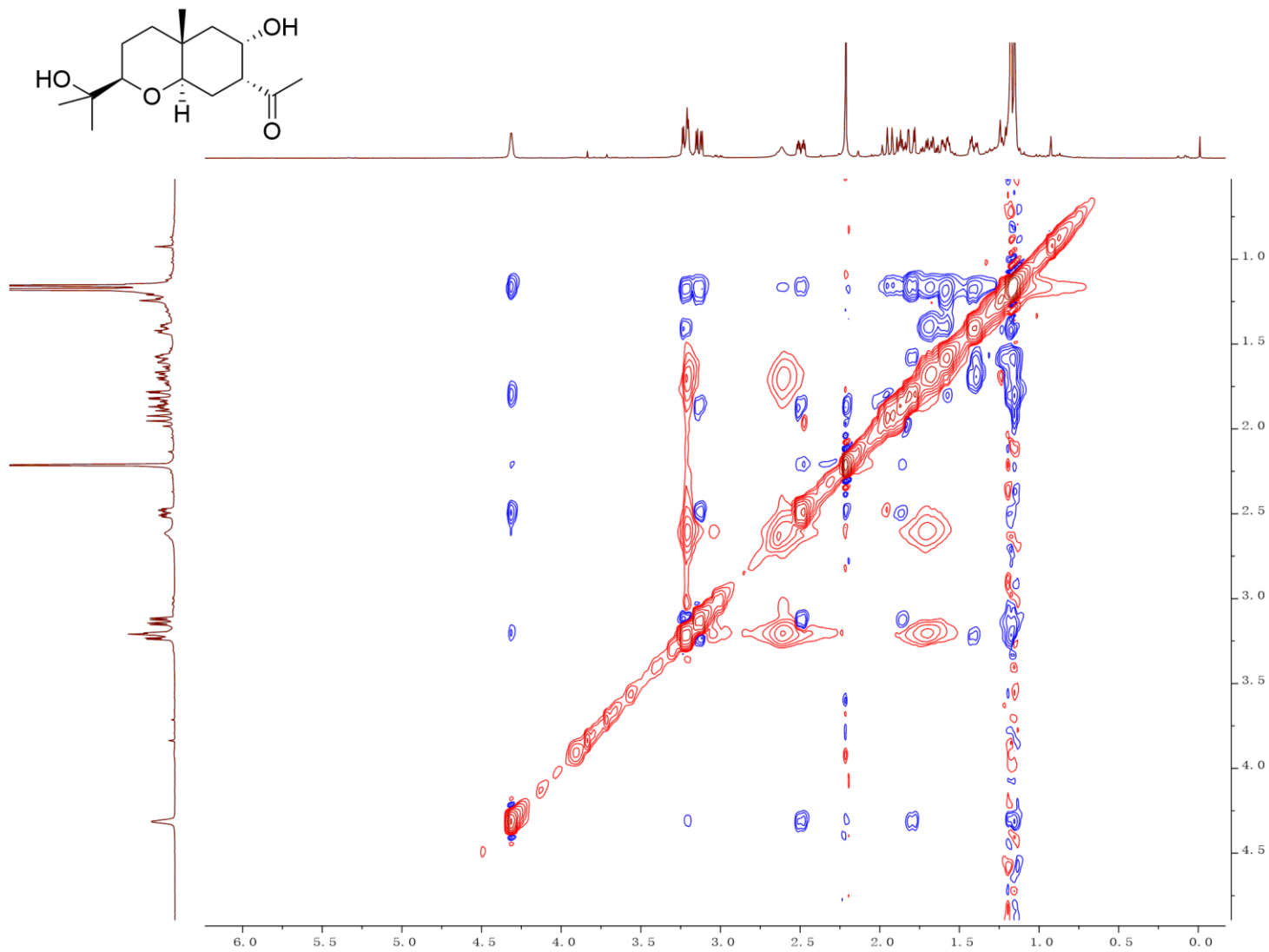


Fig. S27. NOESY spectrum (CDCl₃, 400 MHz) of **4**

210A #47 RT: 0.93 AV: 1 NL: 5.50E7
T: FTMS + c ESI Full ms [50.00-500.00]

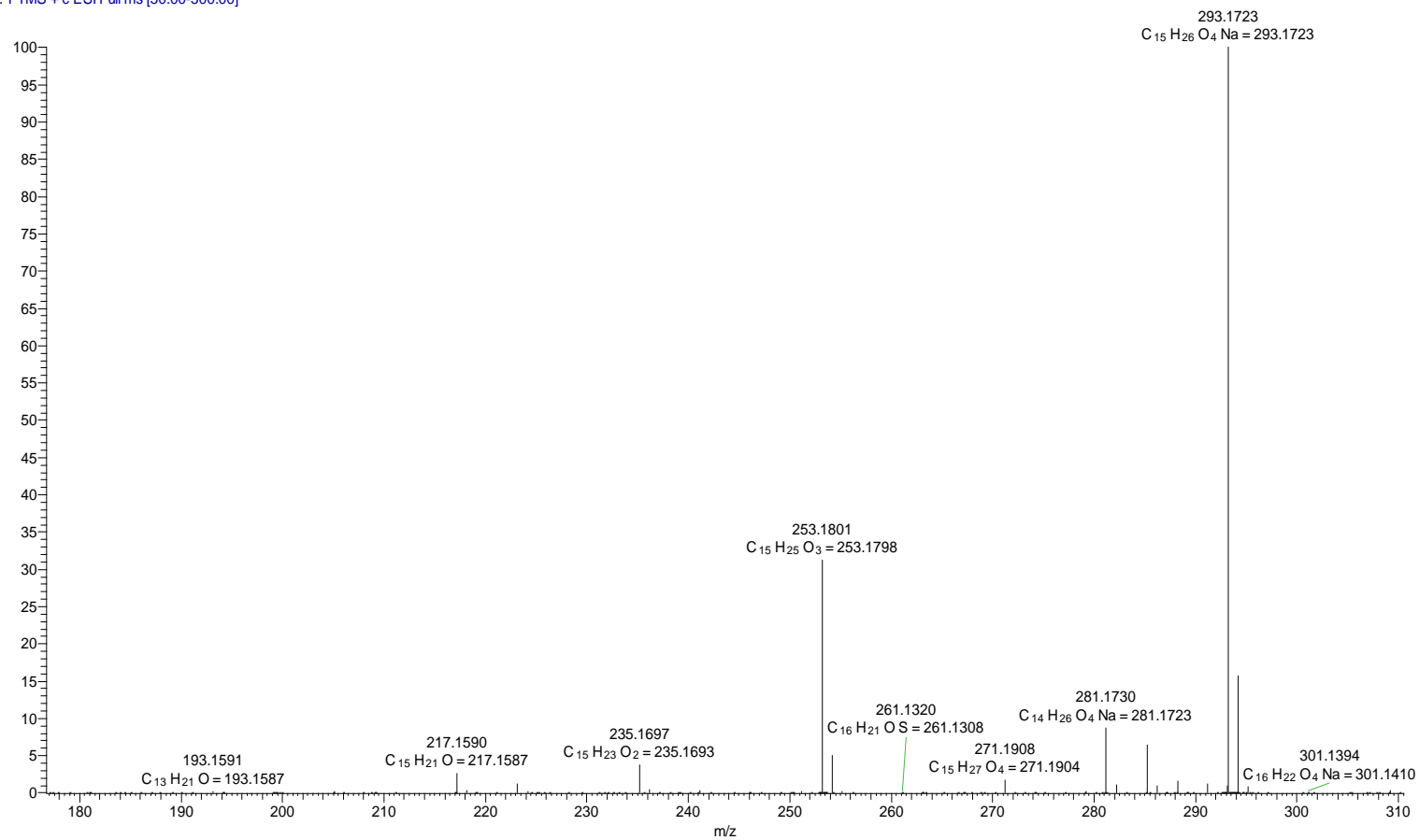


Fig. S28. (+)-HR-ESI-MS (positive mode) of **4**

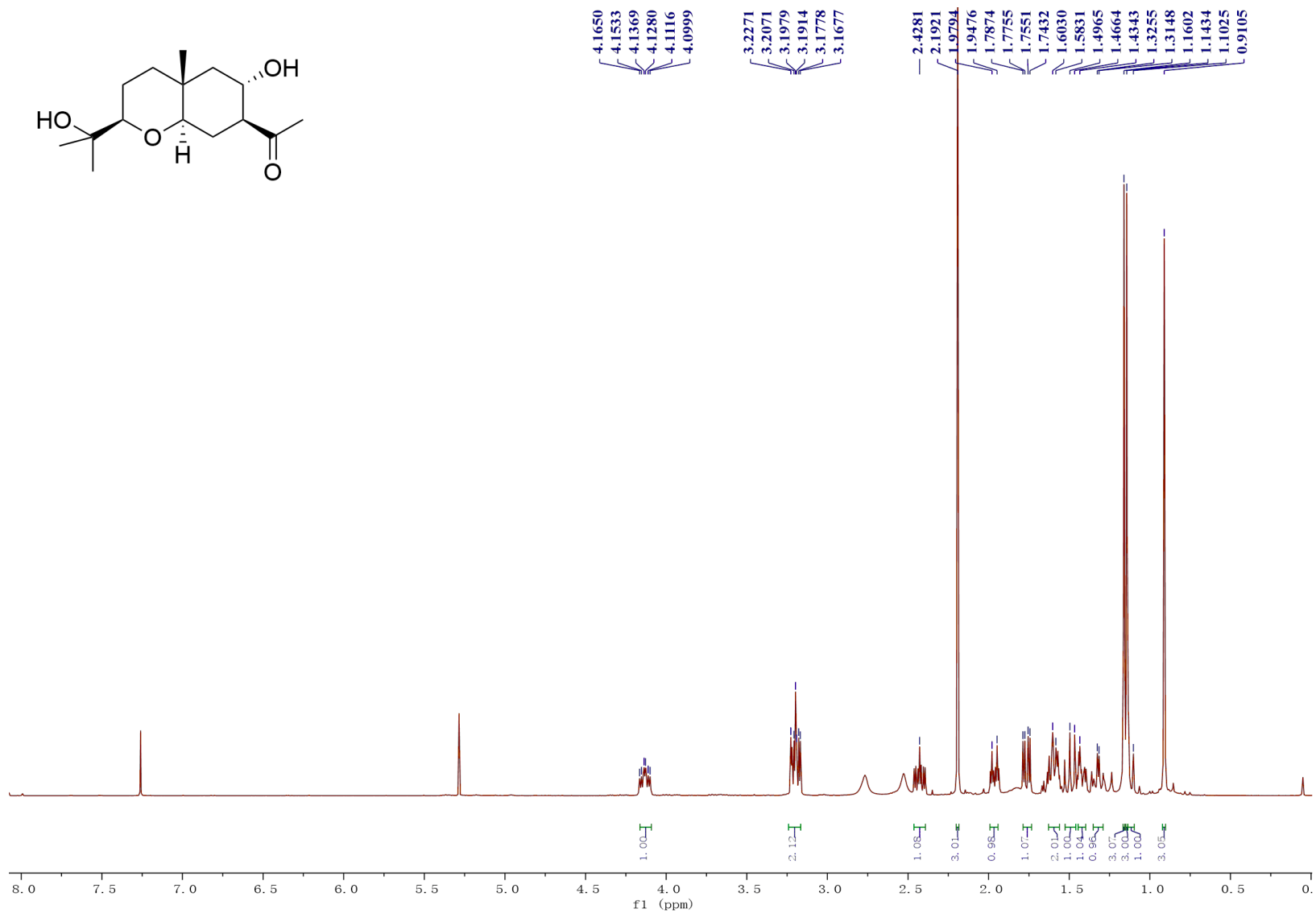


Fig. S29. ¹H NMR spectrum (CDCl₃, 400 MHz) of **5**

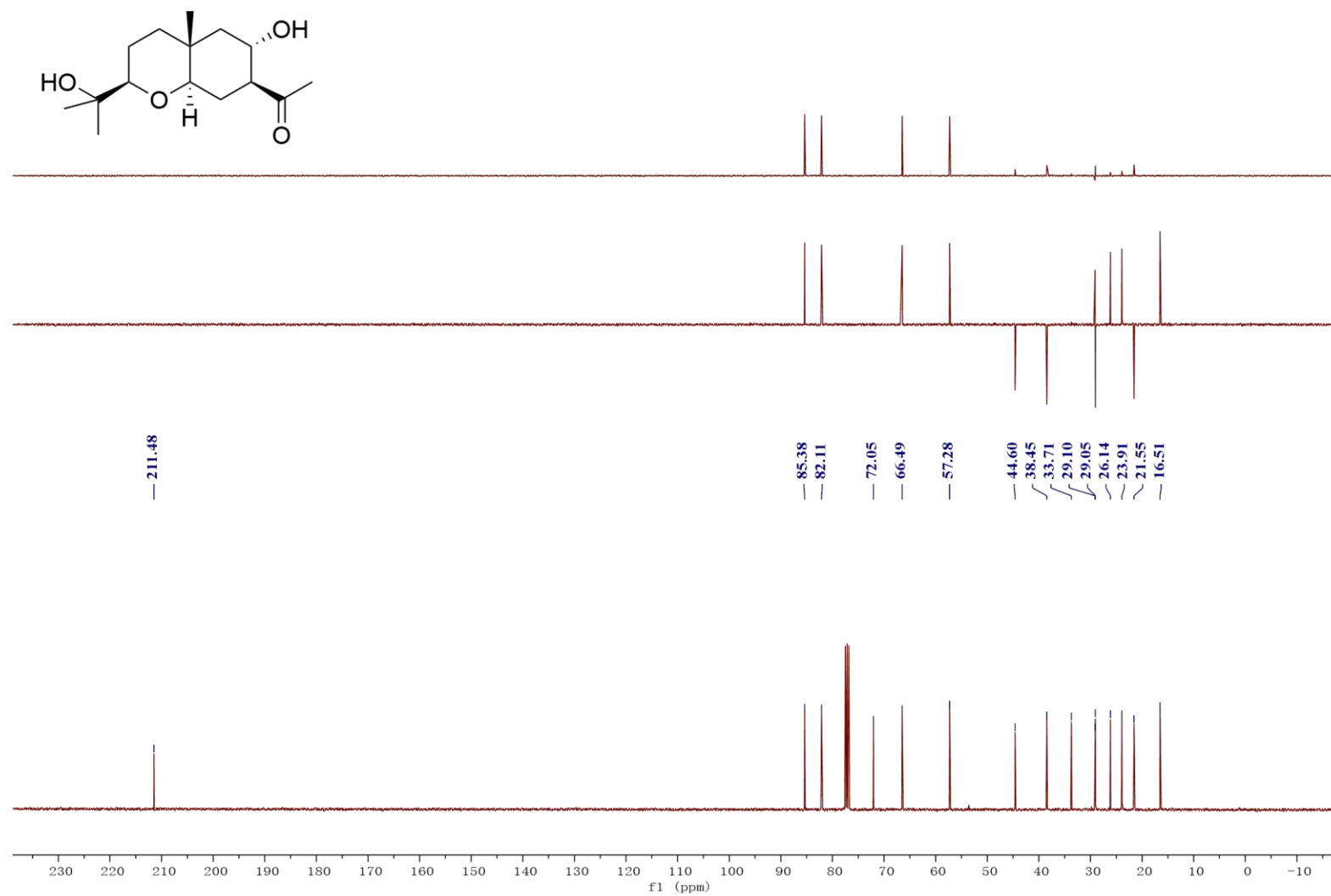


Fig. S30. ^{13}C and DEPT spectra (CDCl_3 , 100 MHz) of **5**

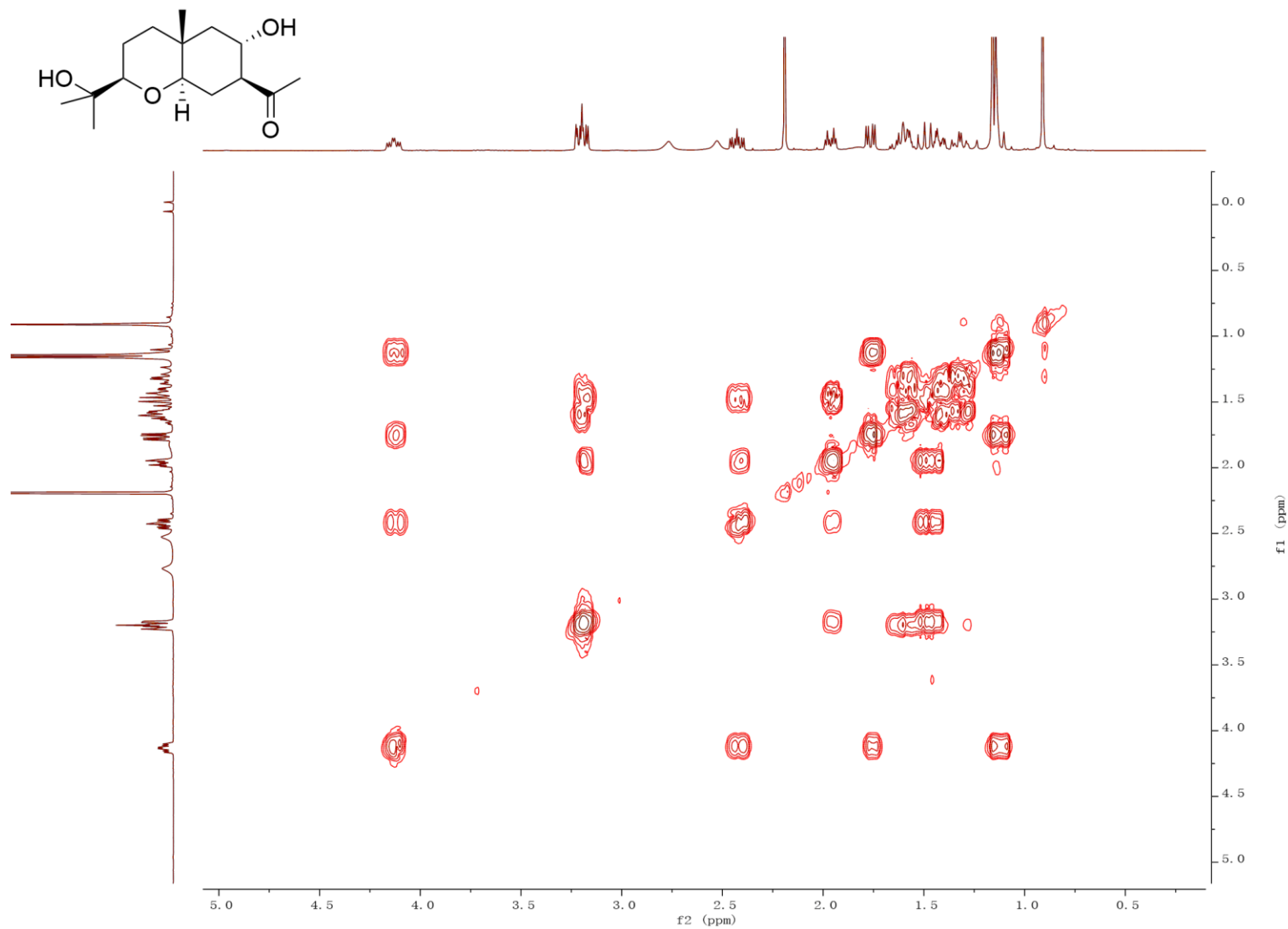


Fig. S31. ^1H - ^1H COSY spectrum (CDCl_3 , 400 MHz) of **5**

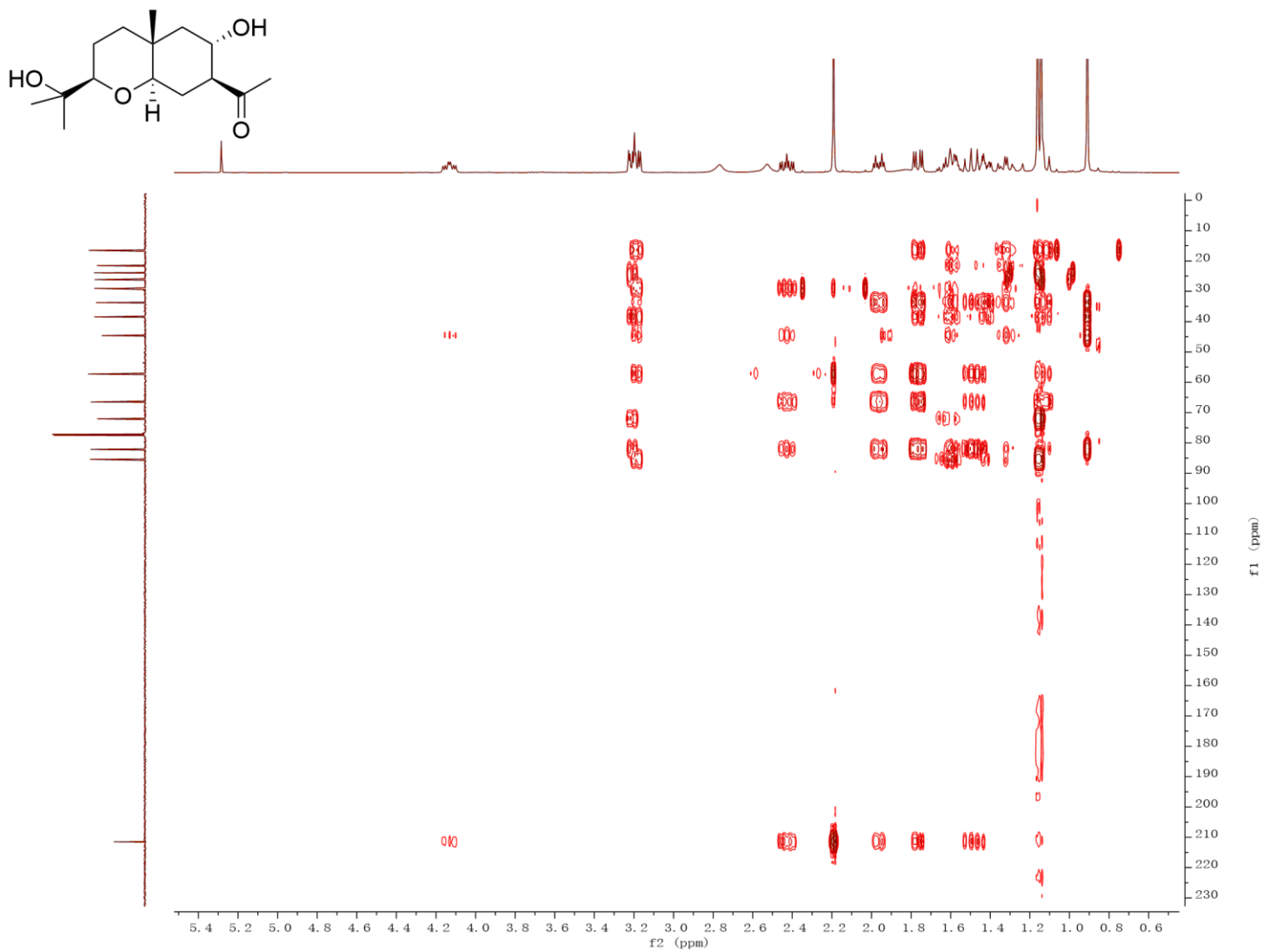


Fig. S32. HMBC spectrum (CDCl₃, 400 MHz) of **5**

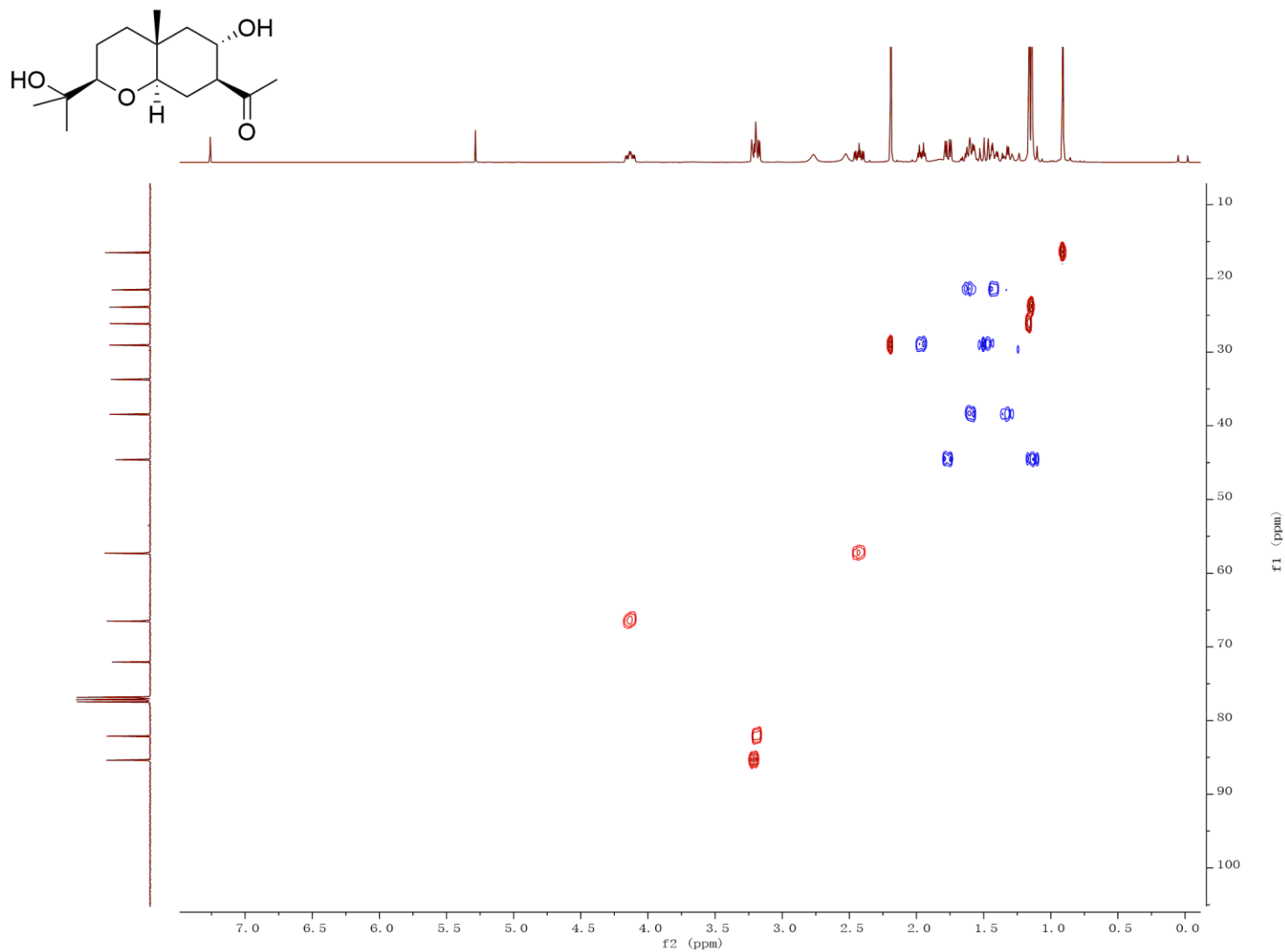


Fig. S33. HSQC spectrum (CDCl₃, 400 MHz) of **5**

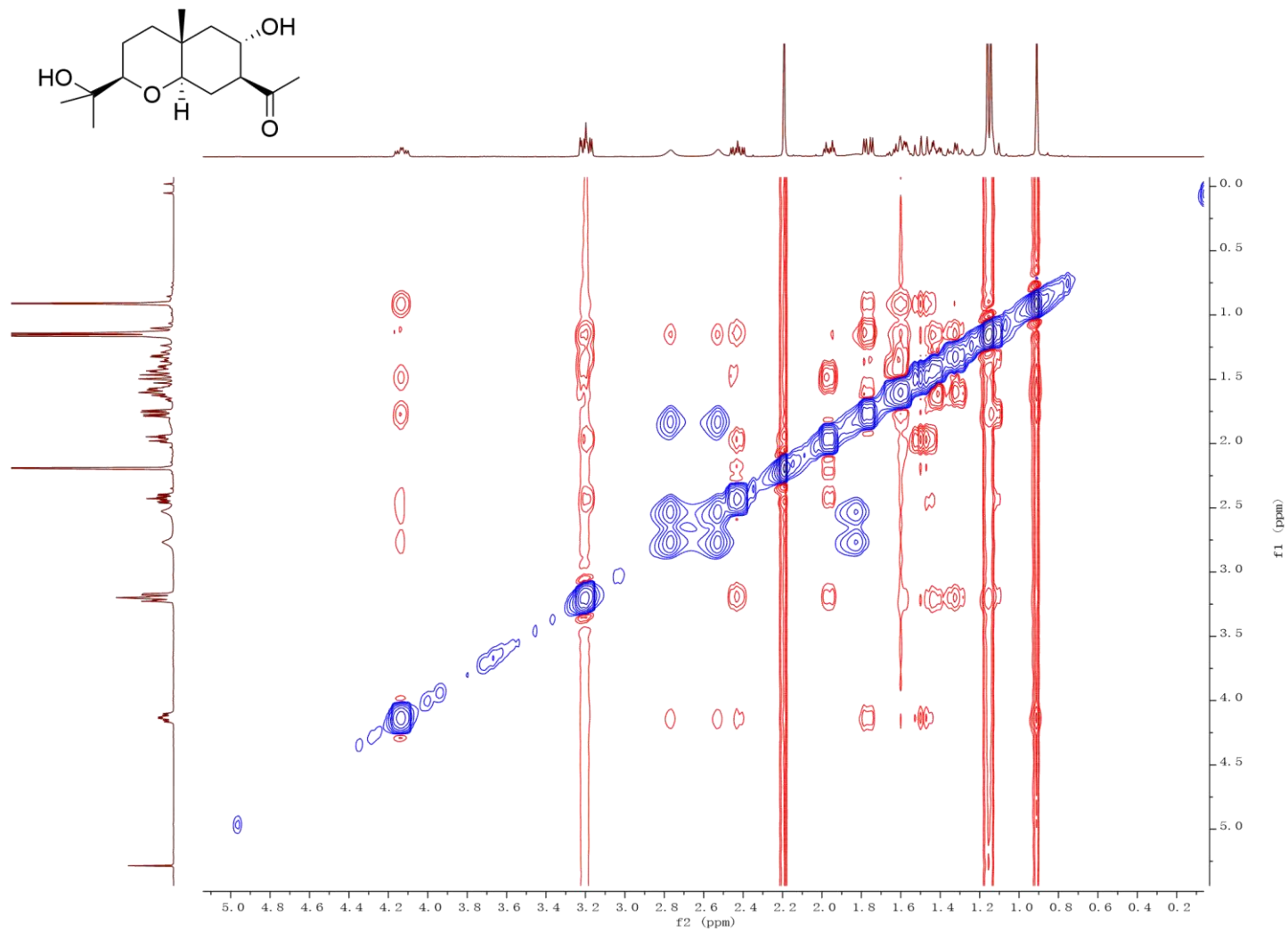


Fig. S34. NOESY spectrum (CDCl₃, 400 MHz) of **5**

DJ1-III7221-IA111 #44 RT: 0.89 AV: 1 NL: 1.73E7
T: FTMS + c ESI Full ms [100.00-850.00]

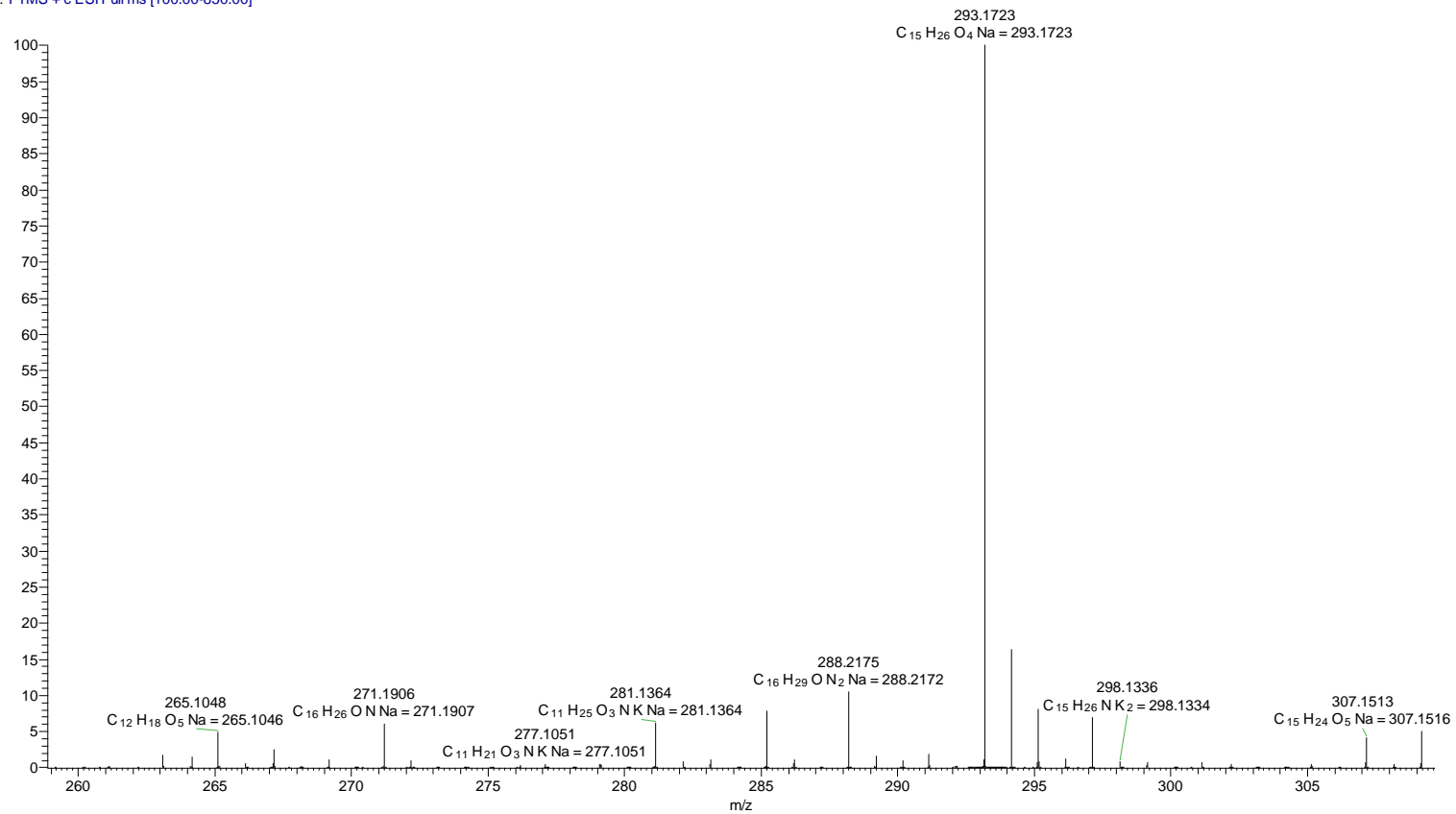


Fig. S35. (+)-HR-ESI-MS (positive mode) of **5**

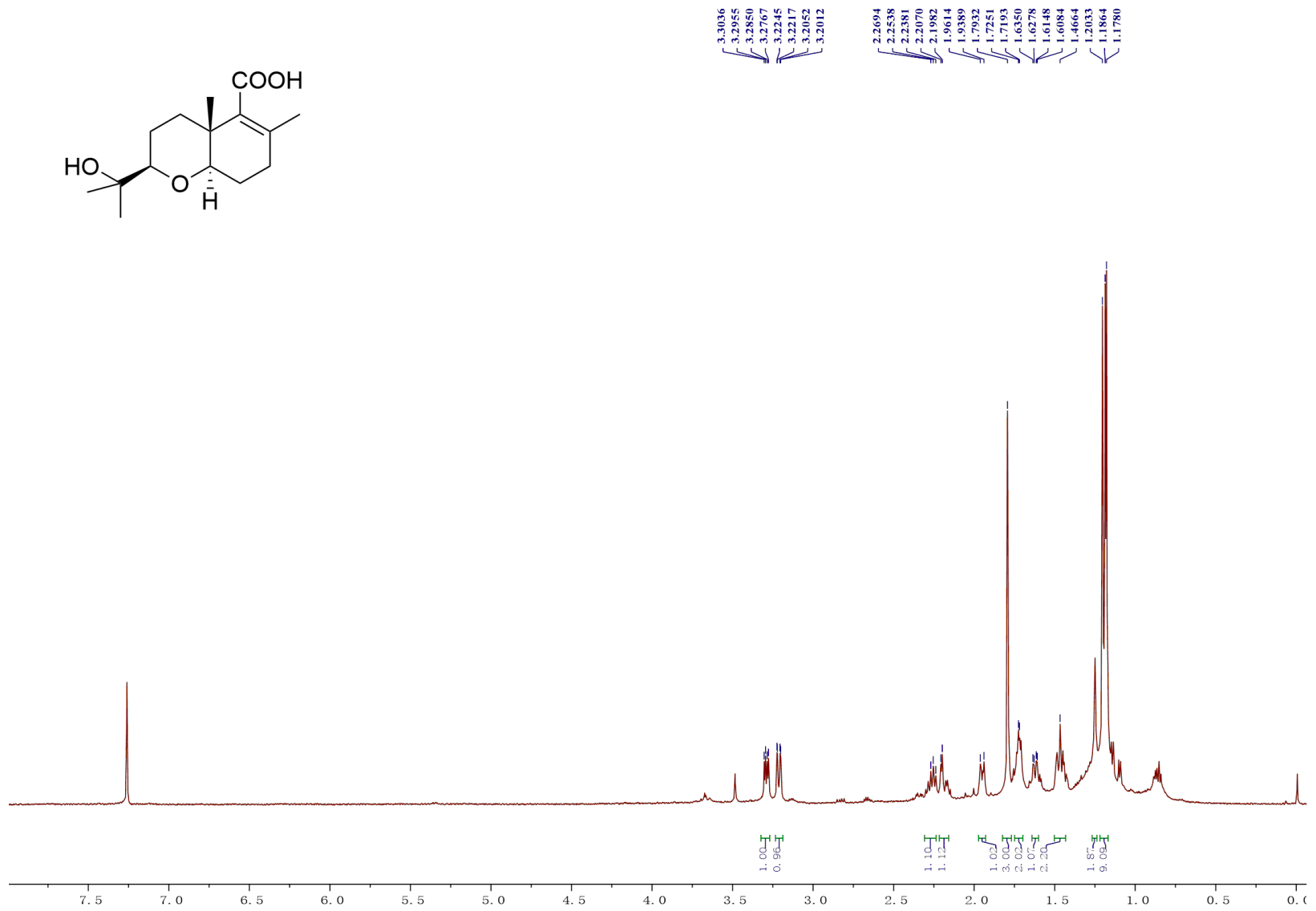


Fig. S36. ¹H NMR spectrum (CDCl₃, 400 MHz) of **6**

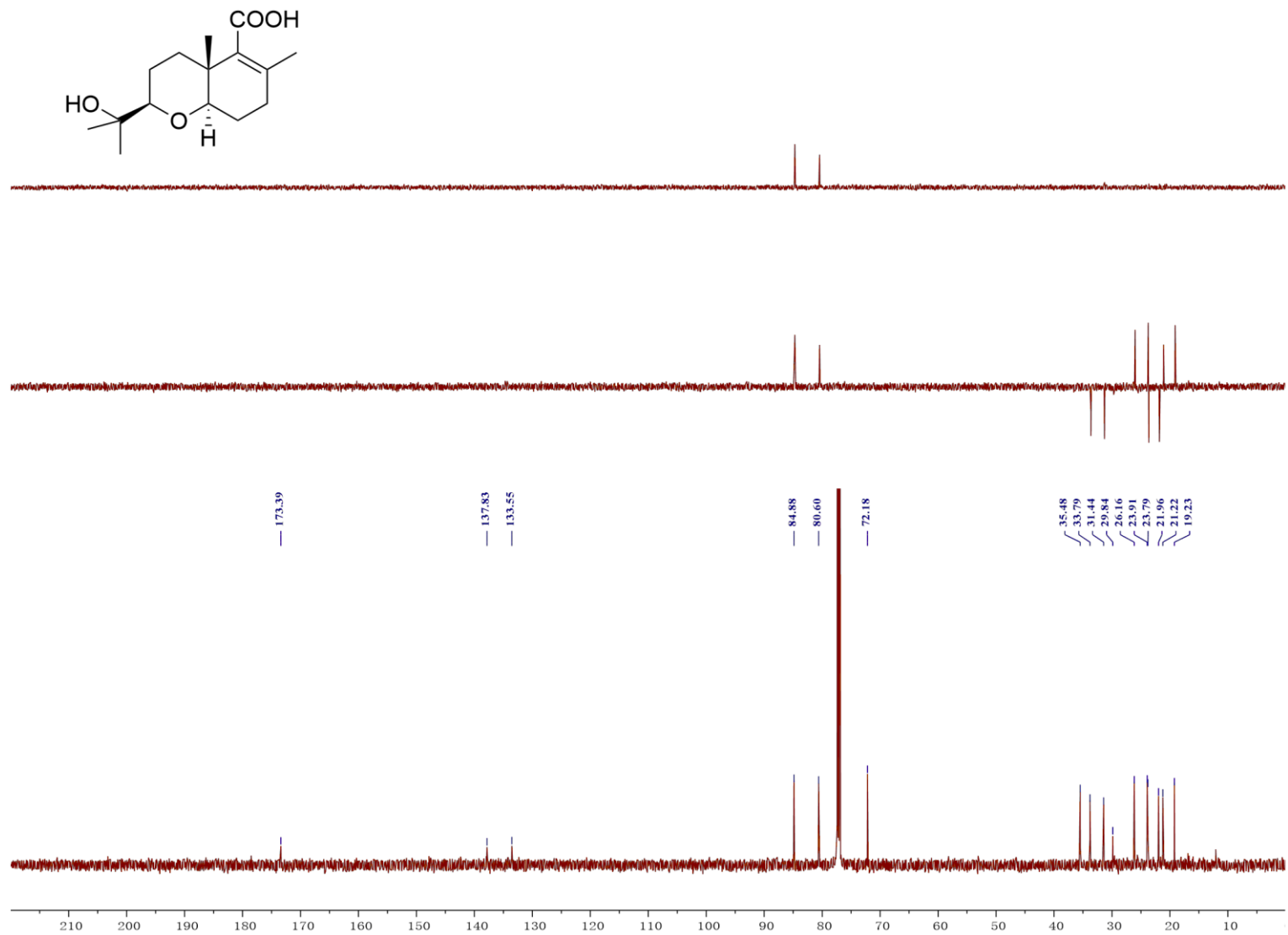


Fig. S37. ^{13}C and DEPT spectra (CDCl_3 , 100 MHz) of 6

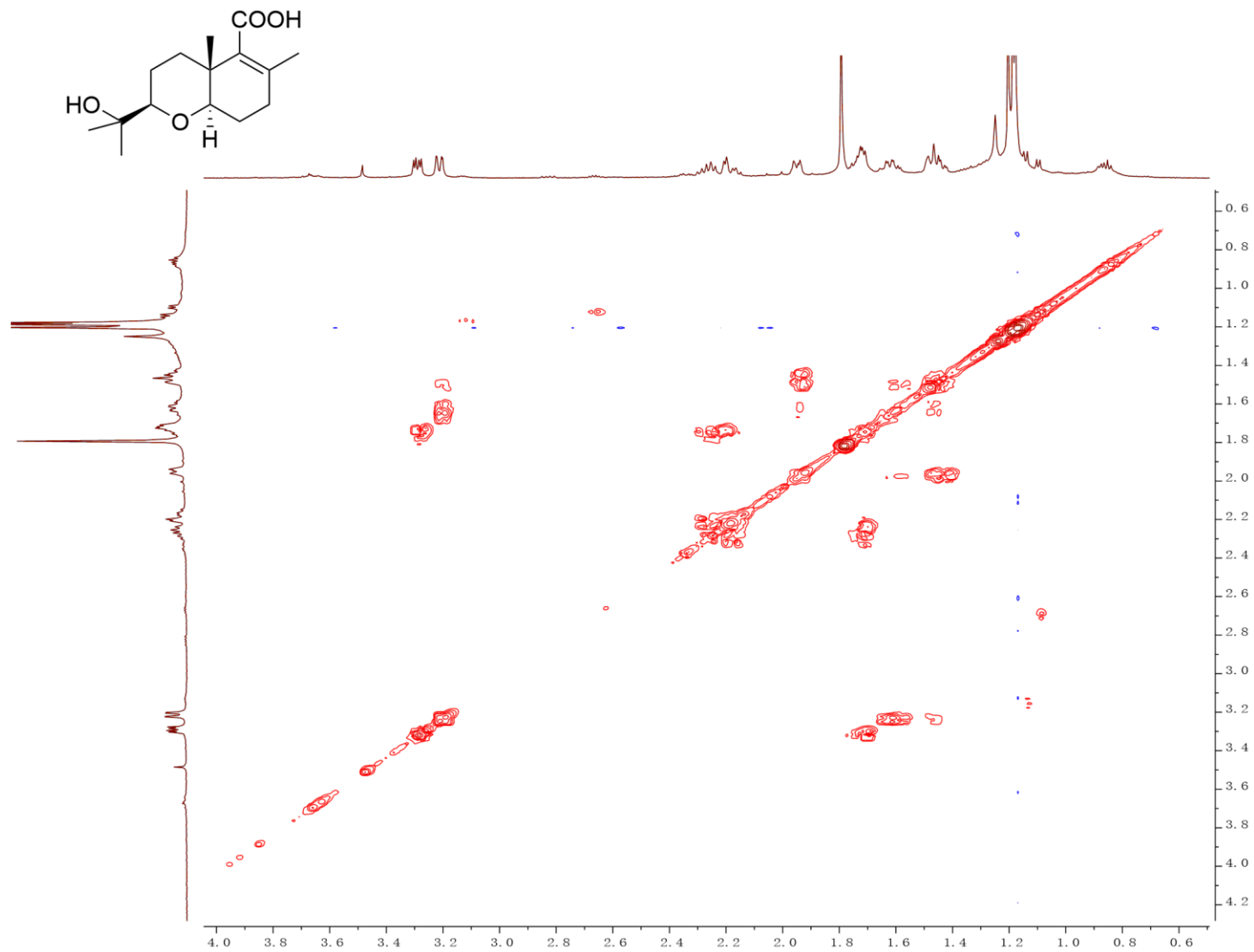


Fig. S38. ^1H - ^1H COSY spectrum (CDCl_3 , 400 MHz) of **6**

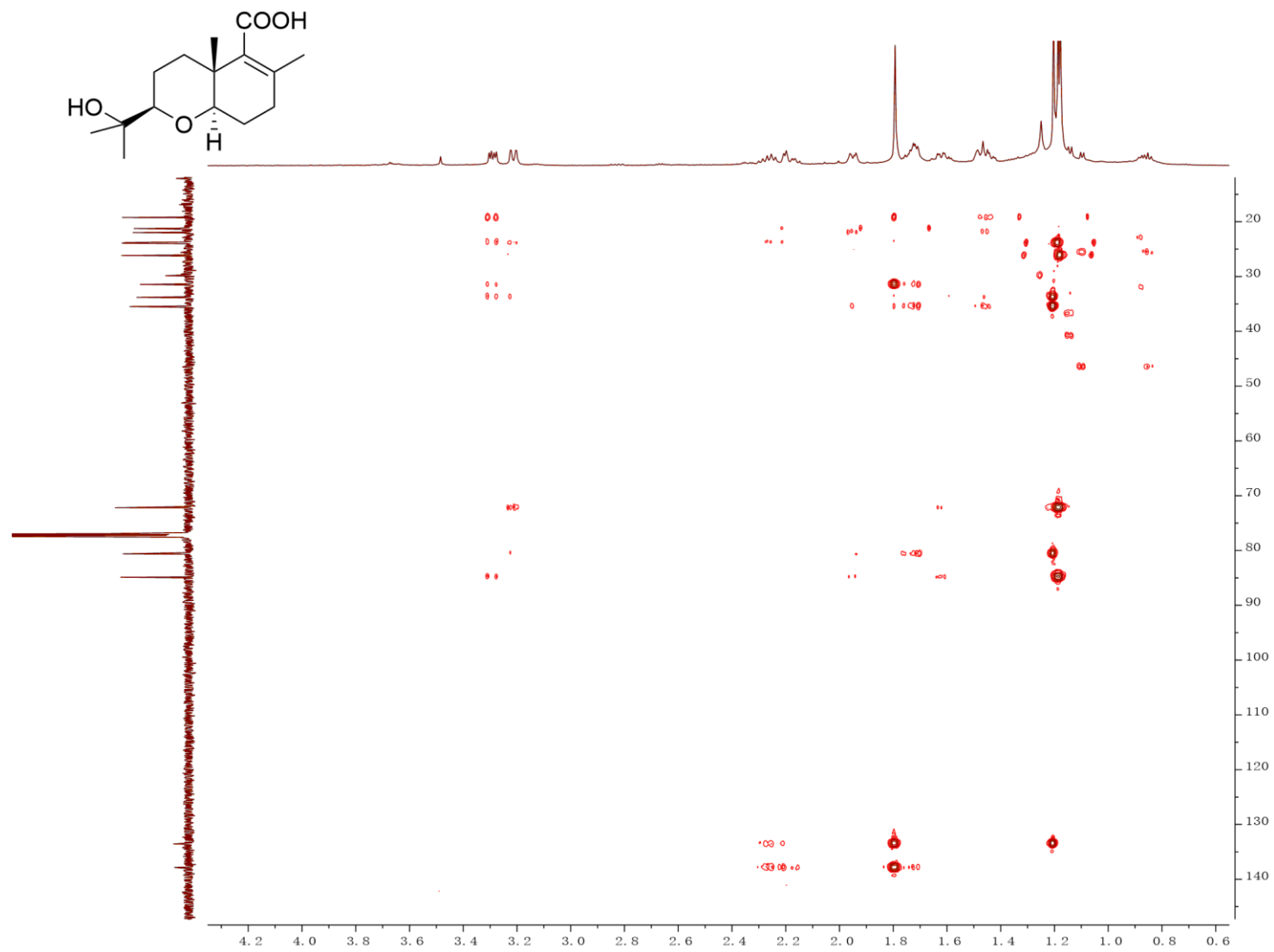


Fig. S39. HMBC spectrum (CDCl₃, 400 MHz) of **6**

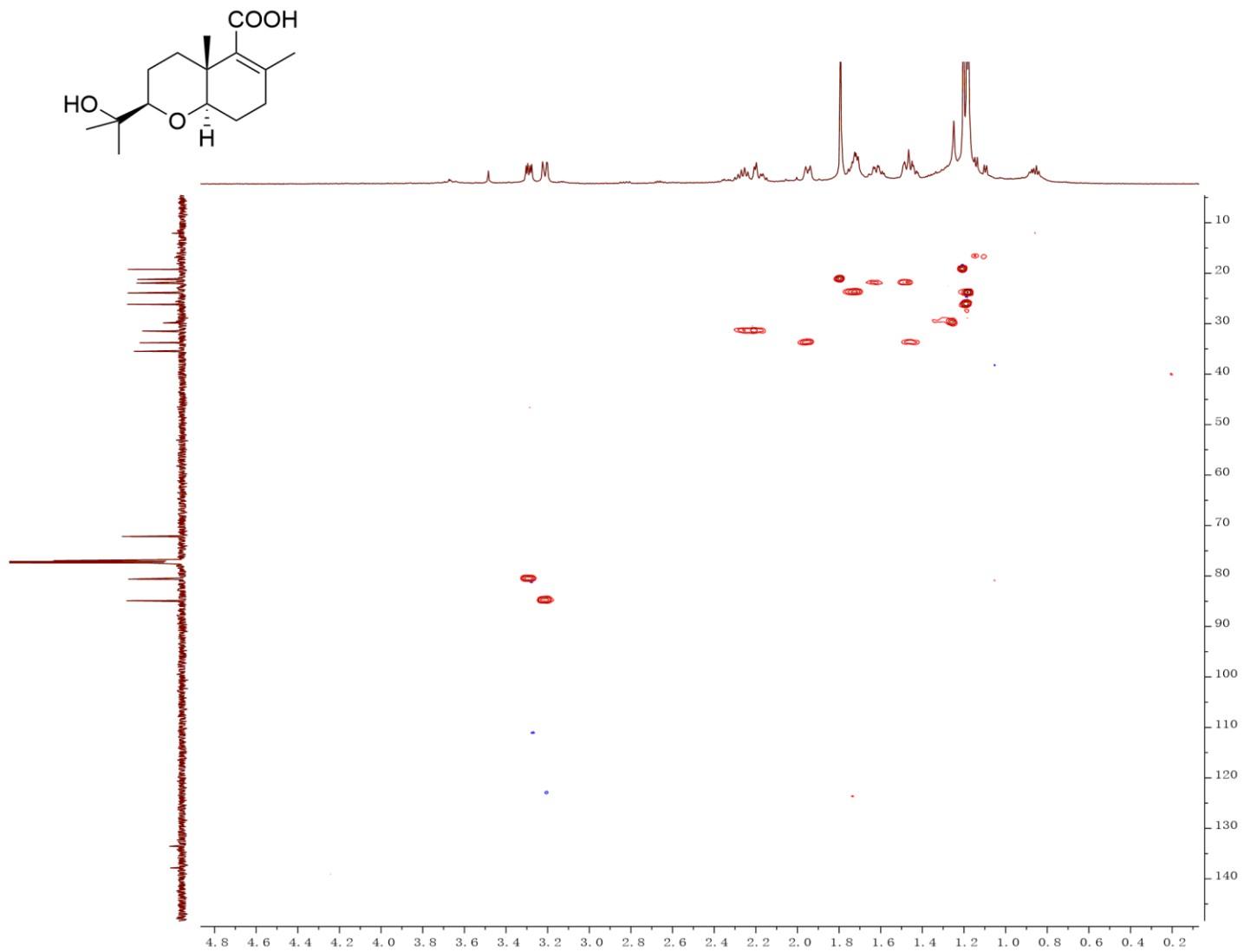


Fig. S40. HSQC spectrum (CDCl₃, 400 MHz) of **6**

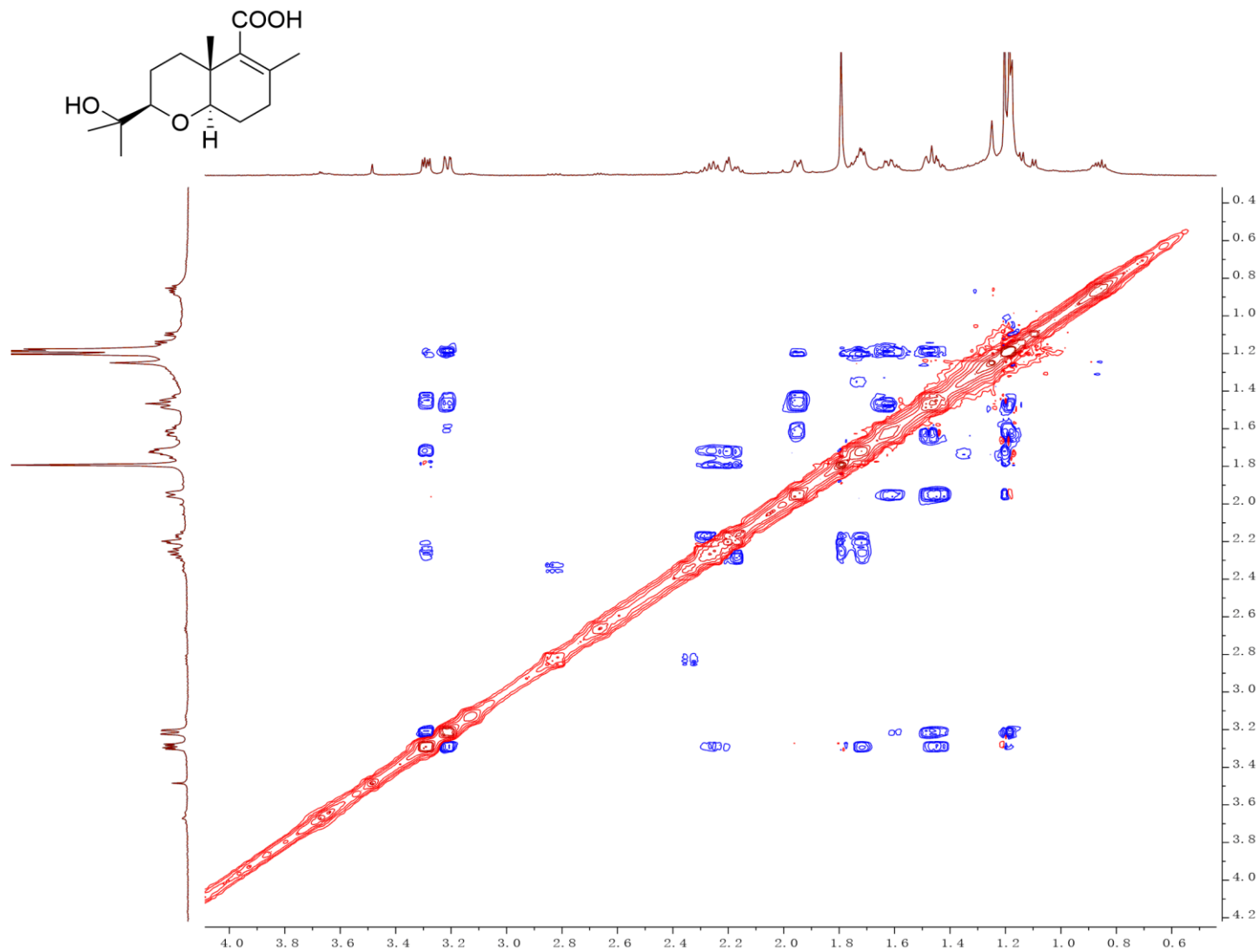


Fig. S41. NOESY spectrum (CDCl₃, 400 MHz) of **6**

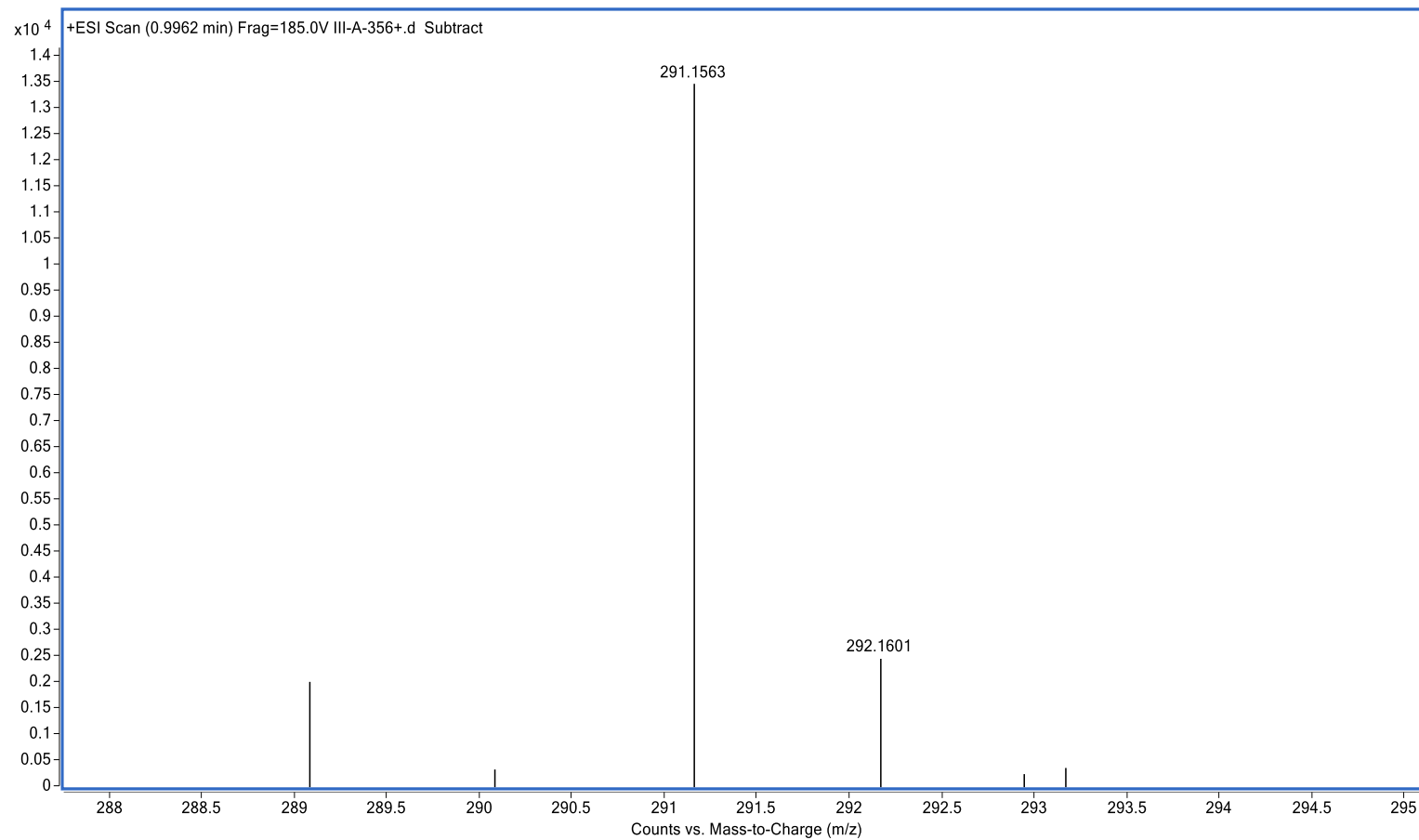


Fig. S42. (+)-HR-ESI-MS (positive mode) of **6**

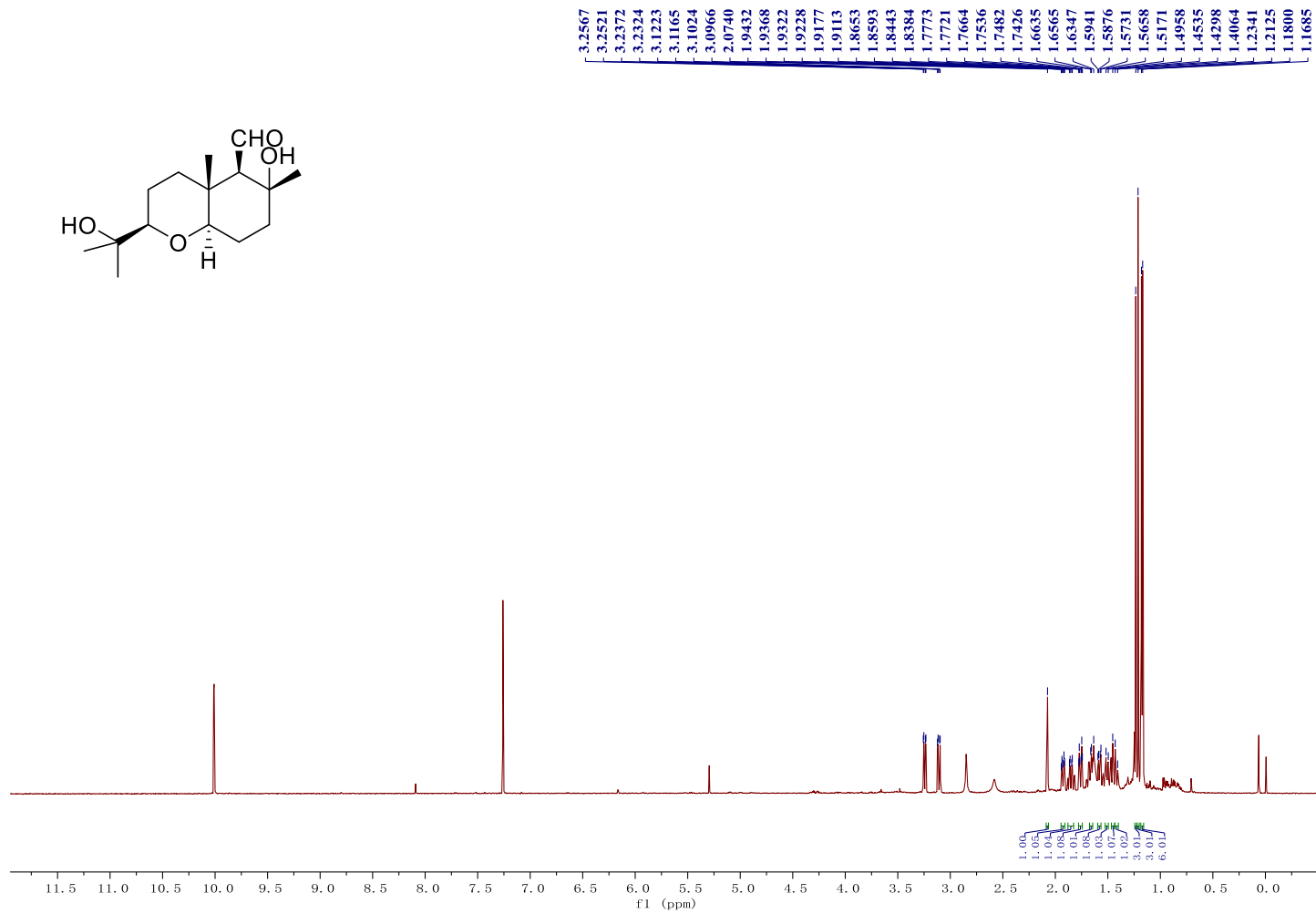


Fig. S43. ^1H NMR spectrum (CDCl_3 , 600 MHz) of **7**

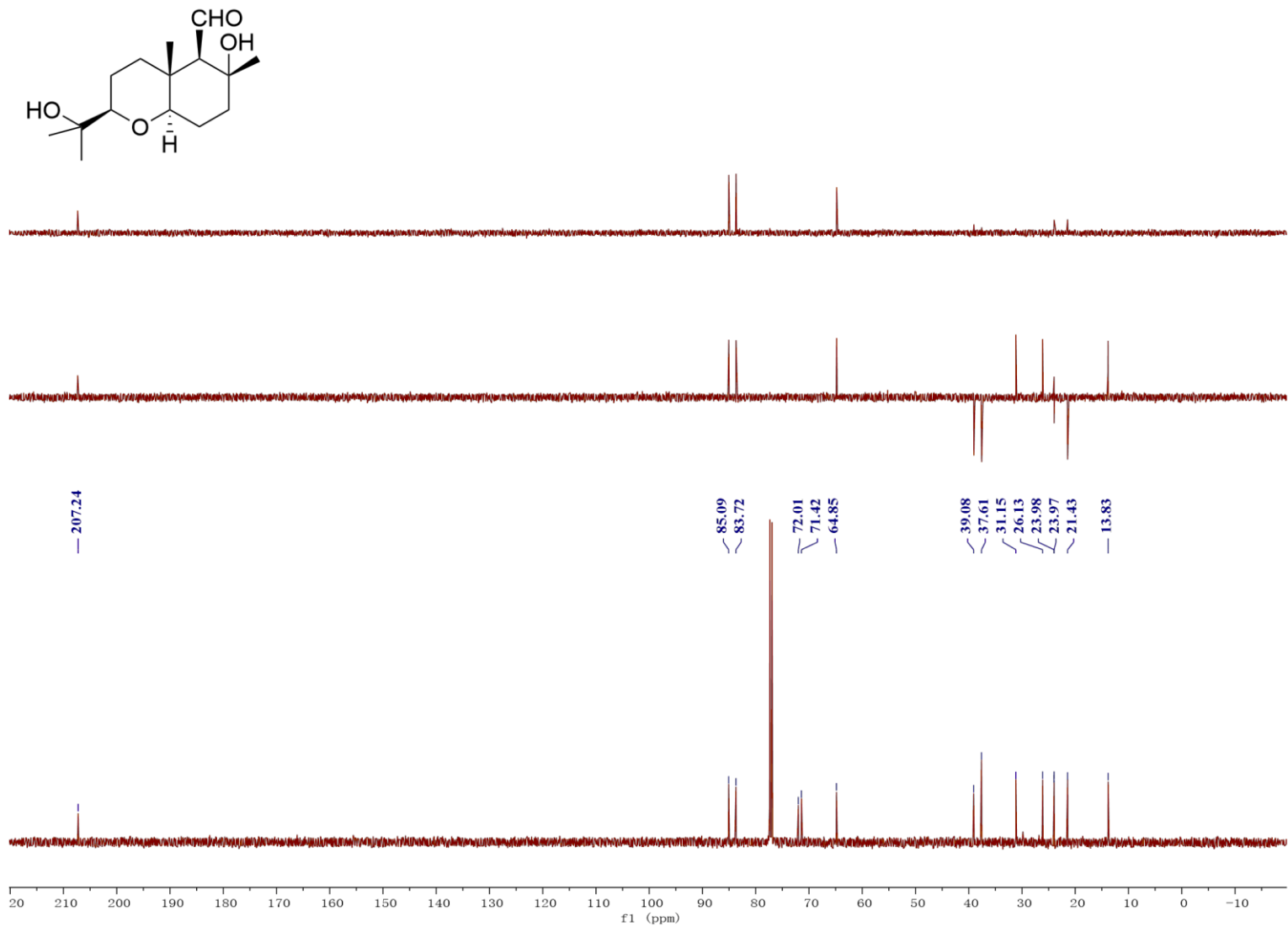
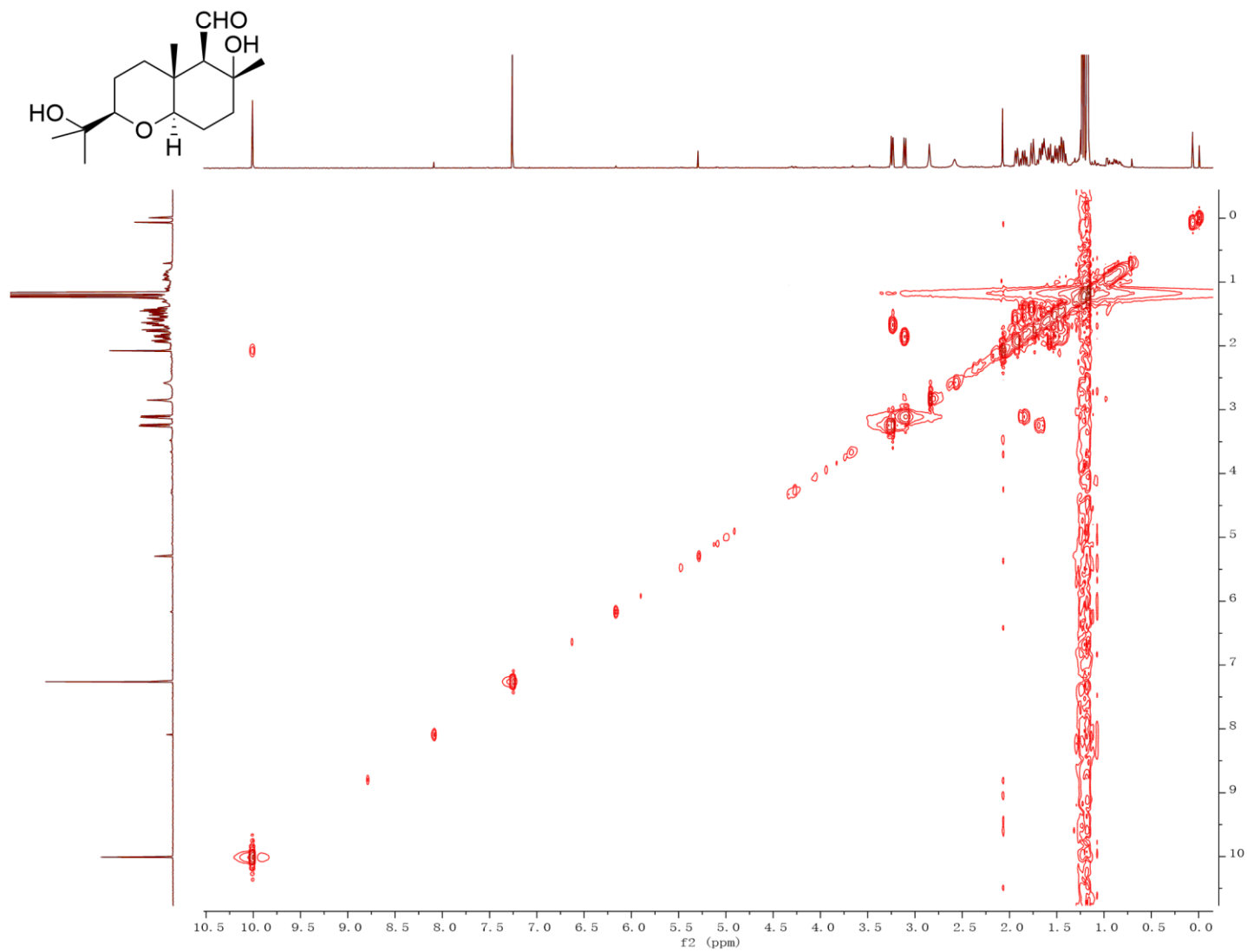


Fig. S44. ^{13}C and DEPT spectra (CDCl_3 , 150 MHz) of 7



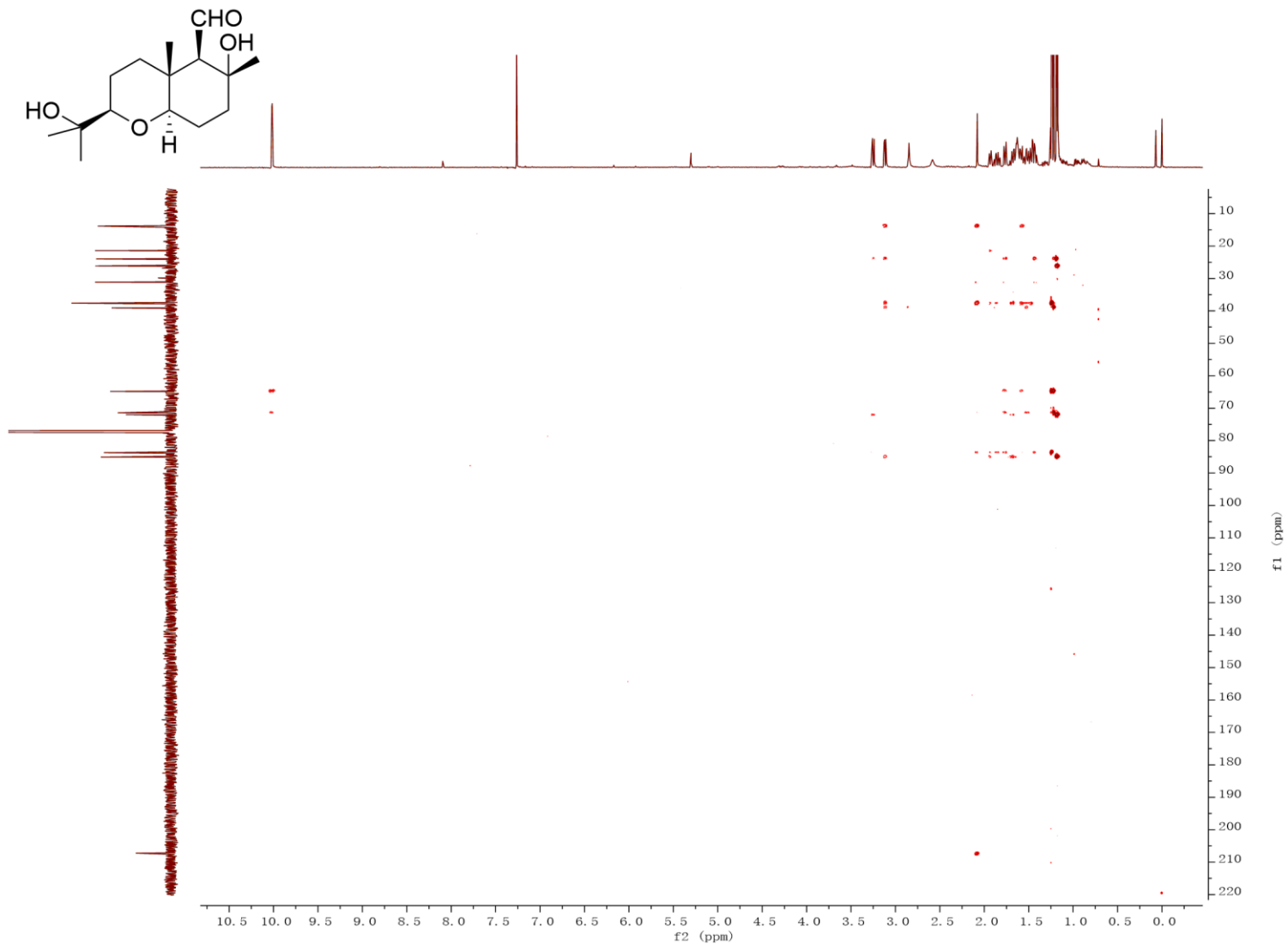


Fig. S46. HMBC spectrum (CDCl₃, 600 MHz) of **7**

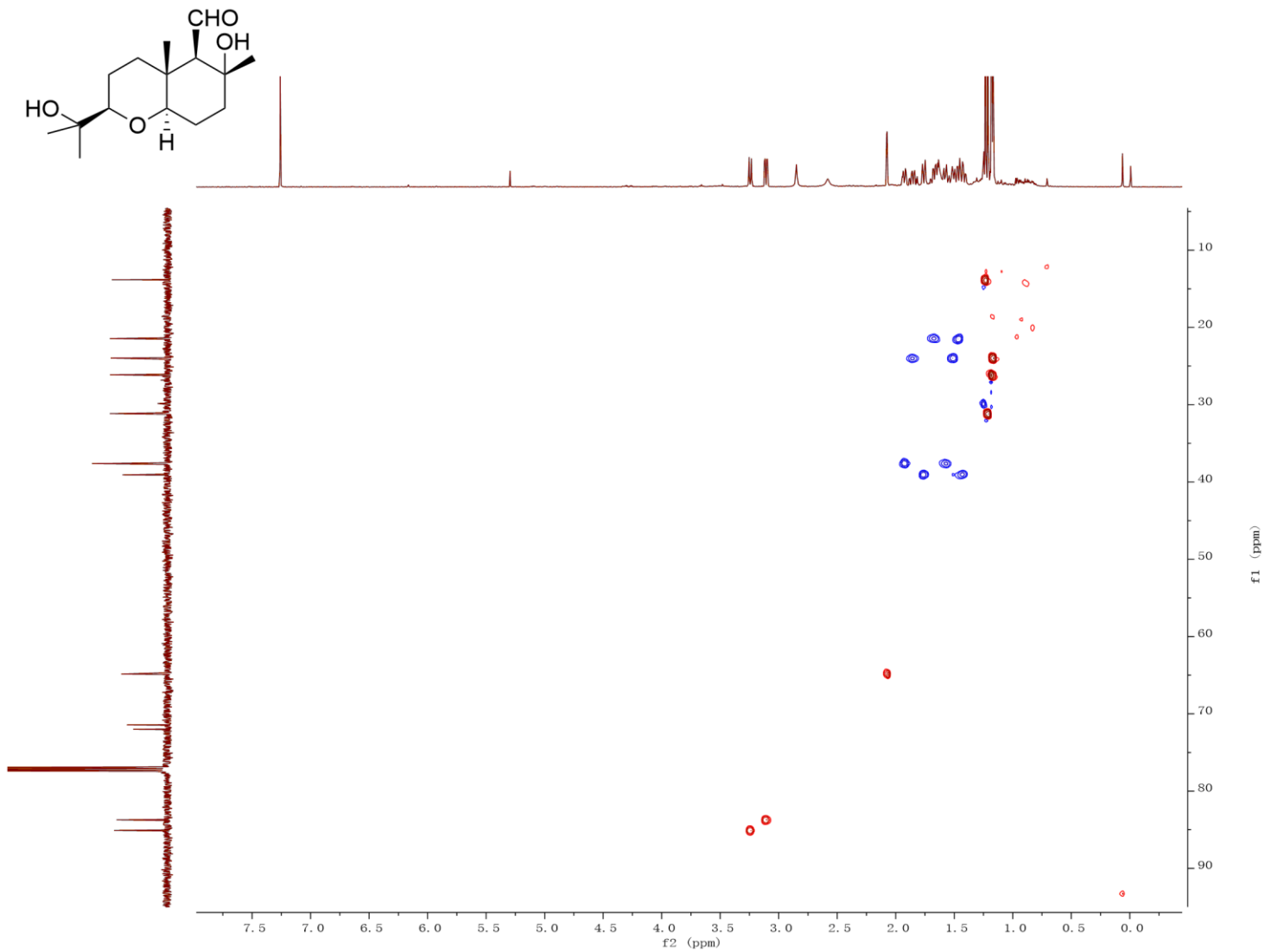
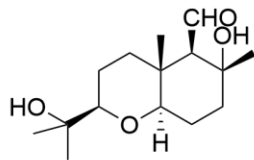


Fig. S47. HSQC spectrum (CDCl₃, 600 MHz) of **7**



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ROESY CDCl₃

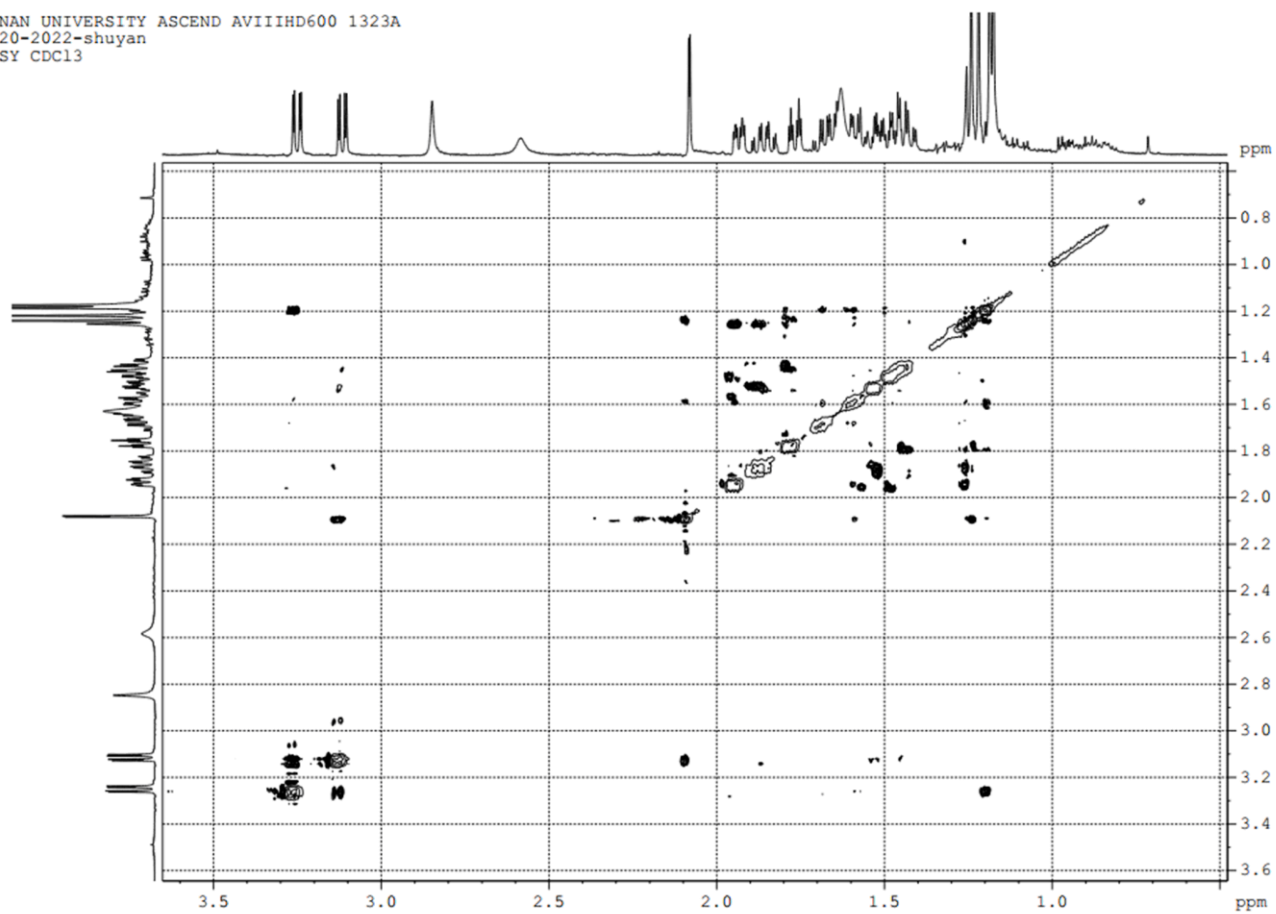


Fig. S48. ROESY spectrum (CDCl₃, 600 MHz) of **7**

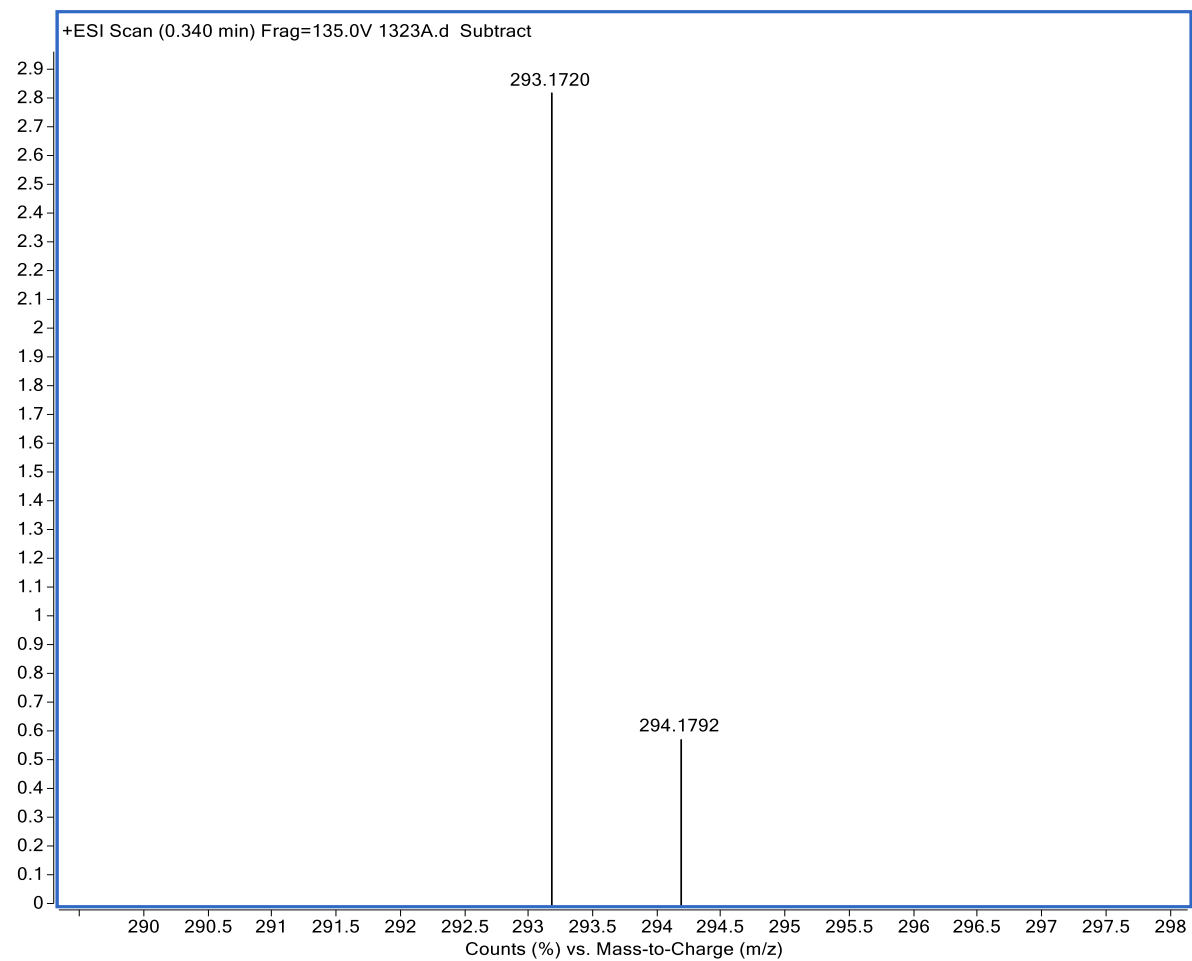


Fig. S49. (+)-HR-ESI-MS (positive mode) of **7**

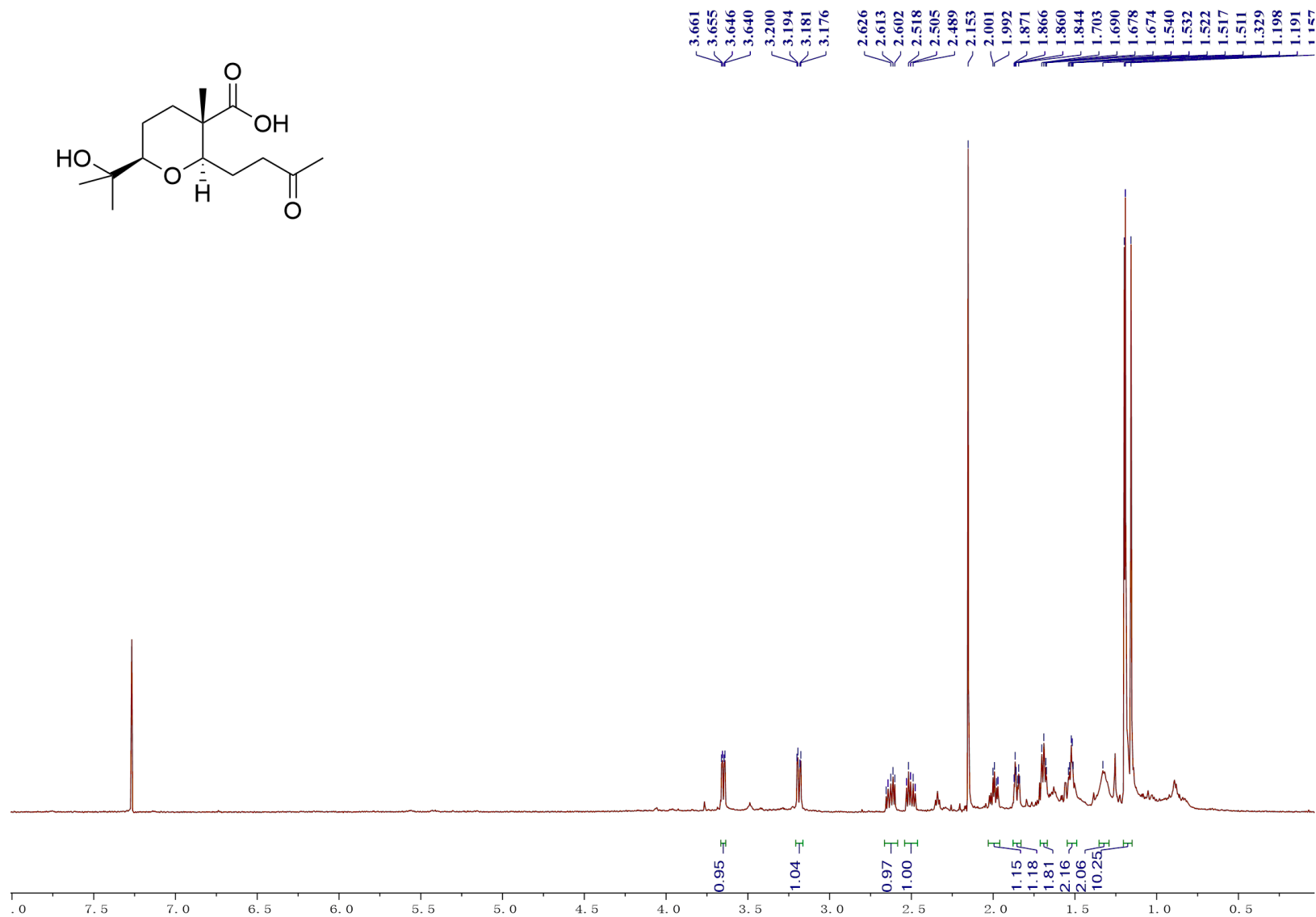


Fig. S50. ^1H NMR spectrum (CDCl₃, 600 MHz) of **8**

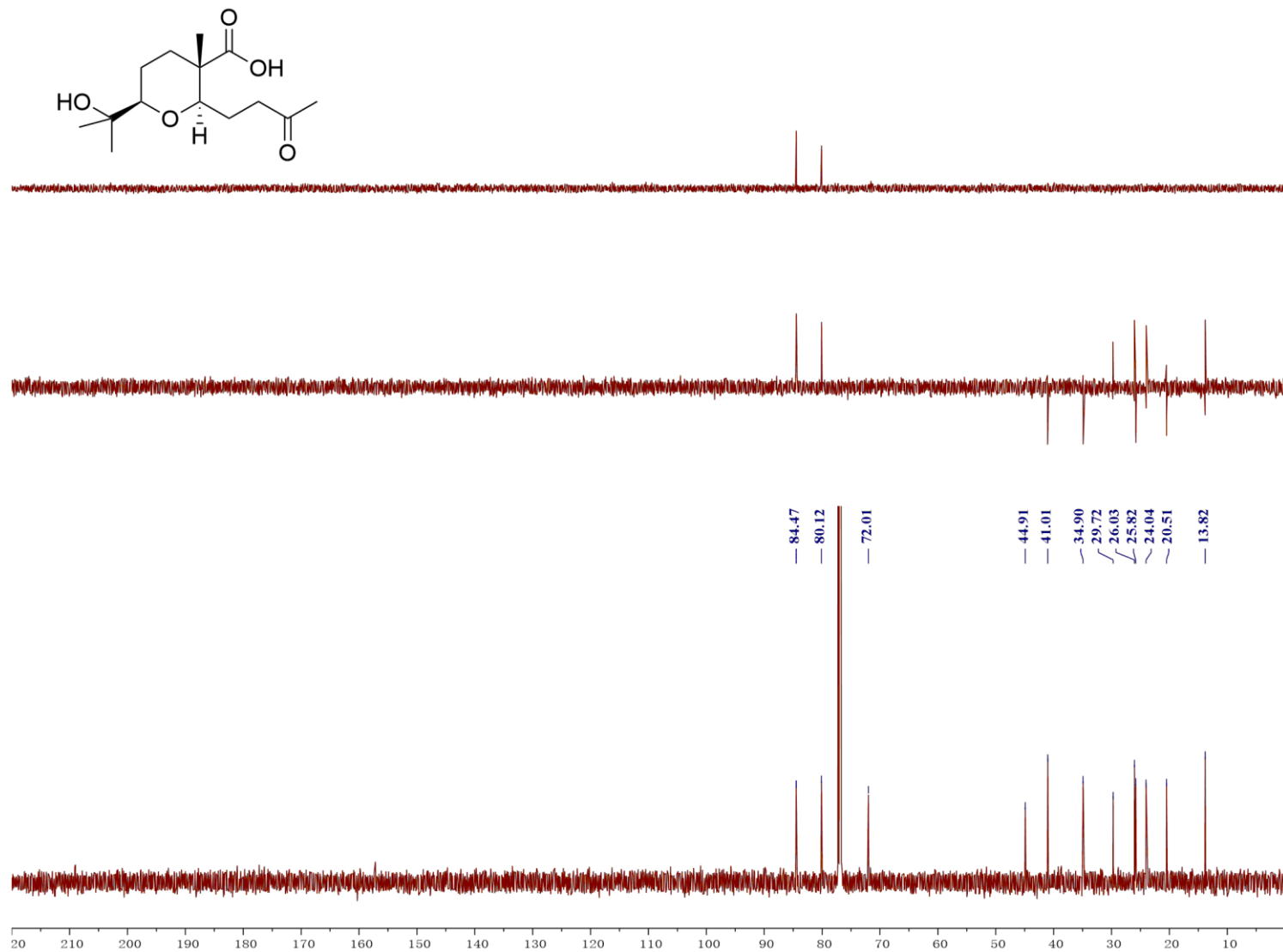


Fig. S51. ^{13}C and DEPT spectra (CDCl_3 , 150 MHz) of **8**

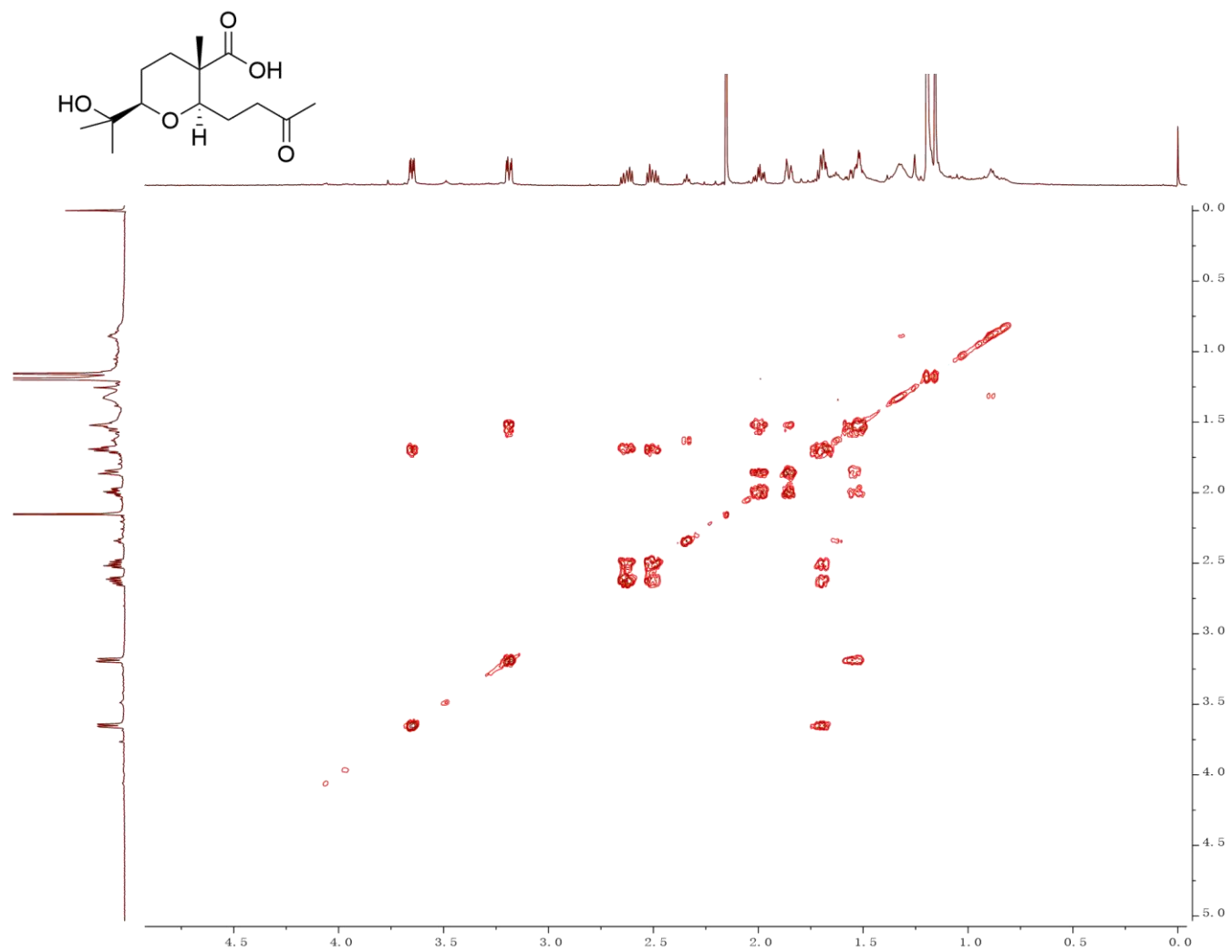


Fig. S52. ^1H - ^1H COSY spectrum (CDCl_3 , 600 MHz) of **8**

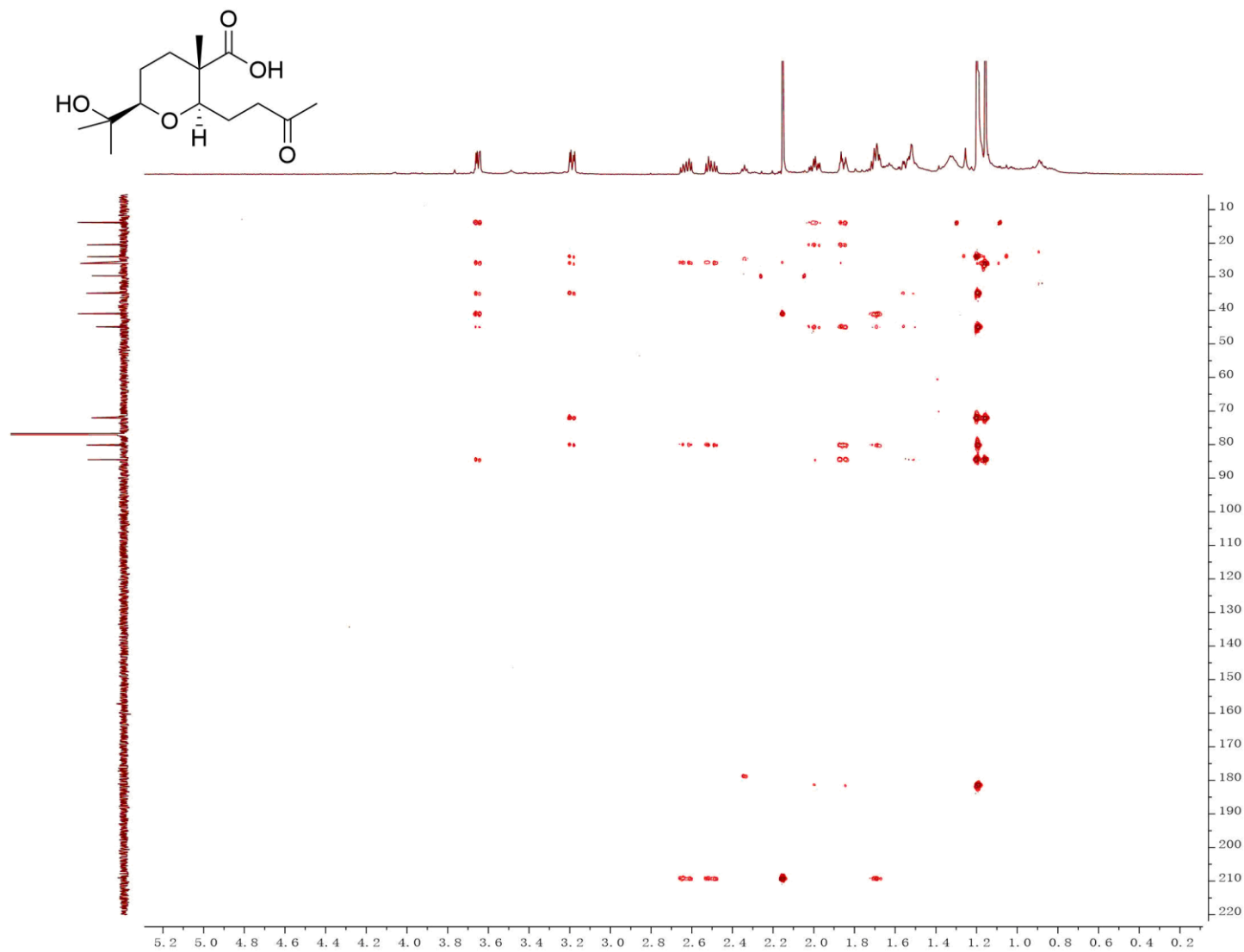


Fig. S53. HMBC spectrum (CDCl₃, 600 MHz) of **8**

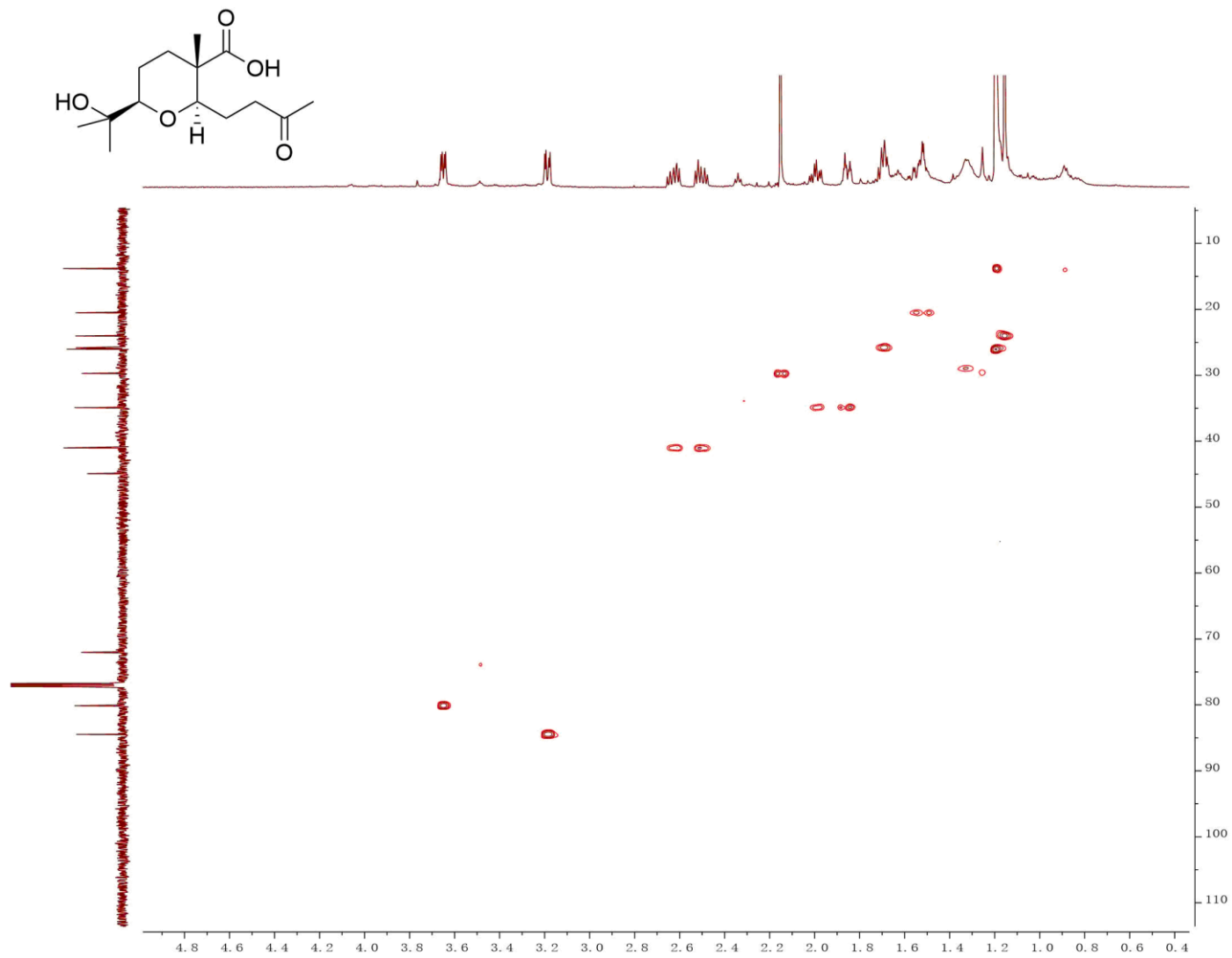


Fig. S54. HSQC spectrum (CDCl₃, 600 MHz) of **8**

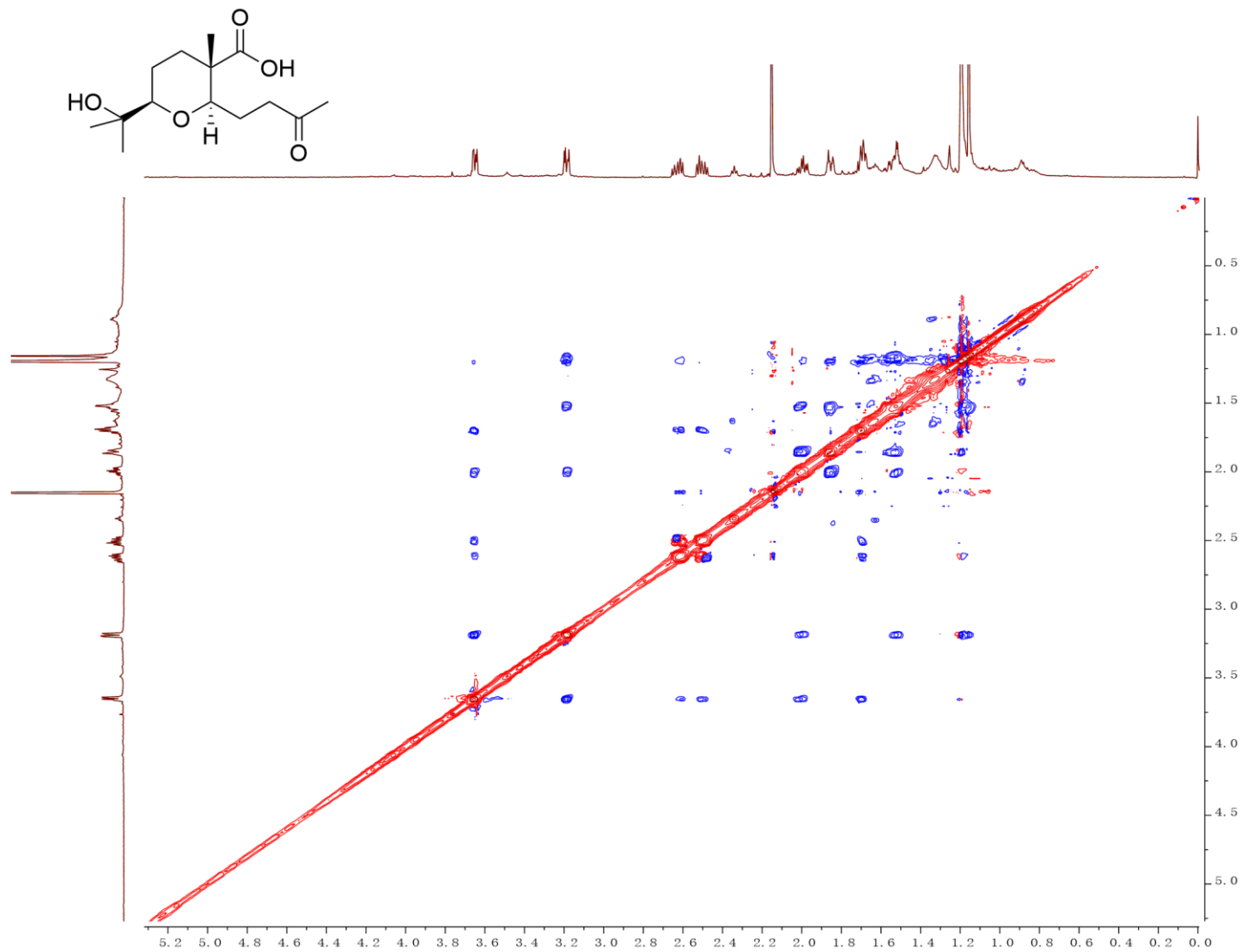


Fig. S55. NOESY spectrum (CDCl₃, 600 MHz) of **8**

DJ1-4-2 #42 RT: 0.91 AV: 1 NL: 4.21E7
T: FTMS + c ESI Full ms [100.00-850.00]

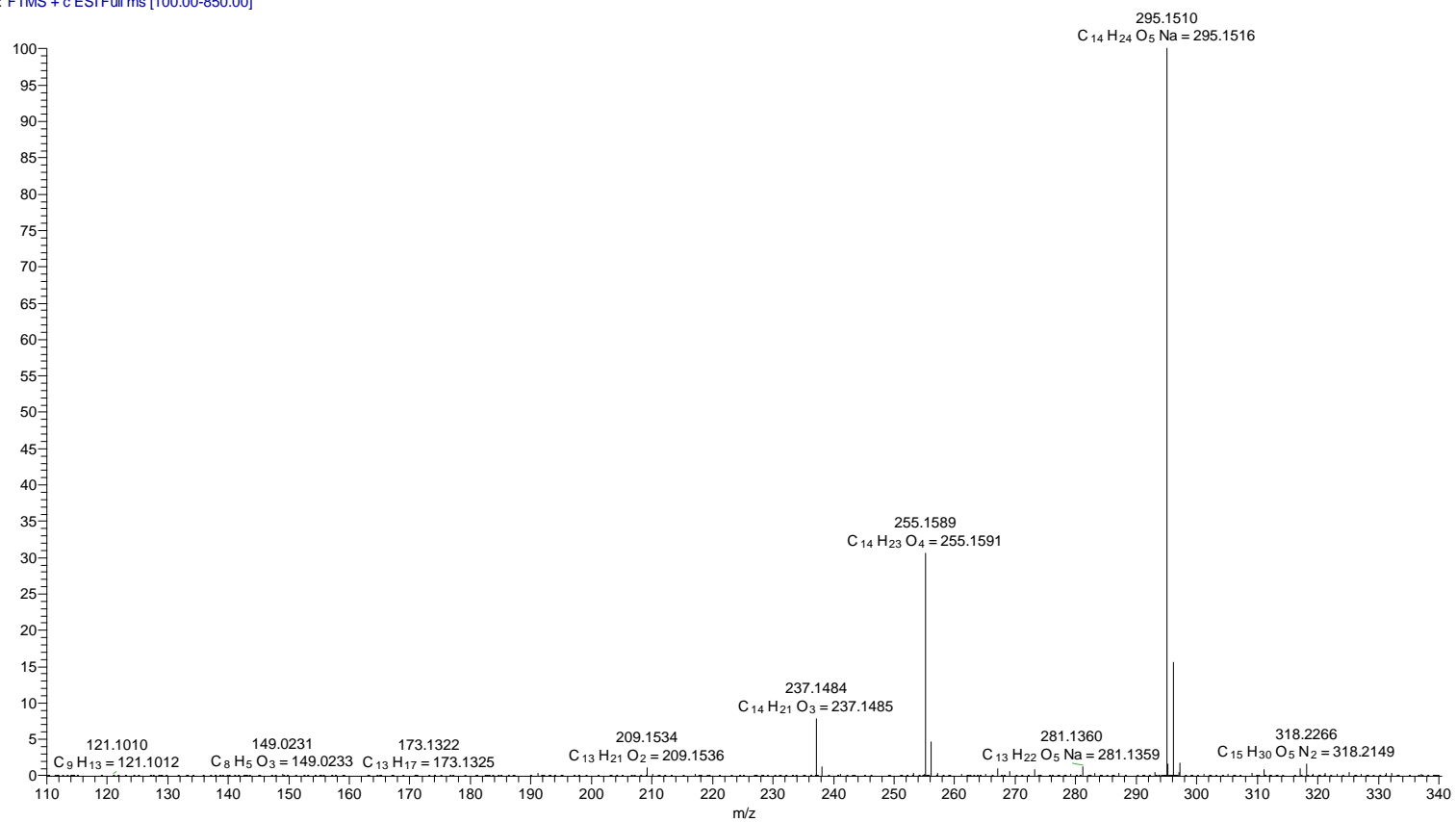


Fig. S56. (+)-HR-ESI-MS (positive mode) of **8**

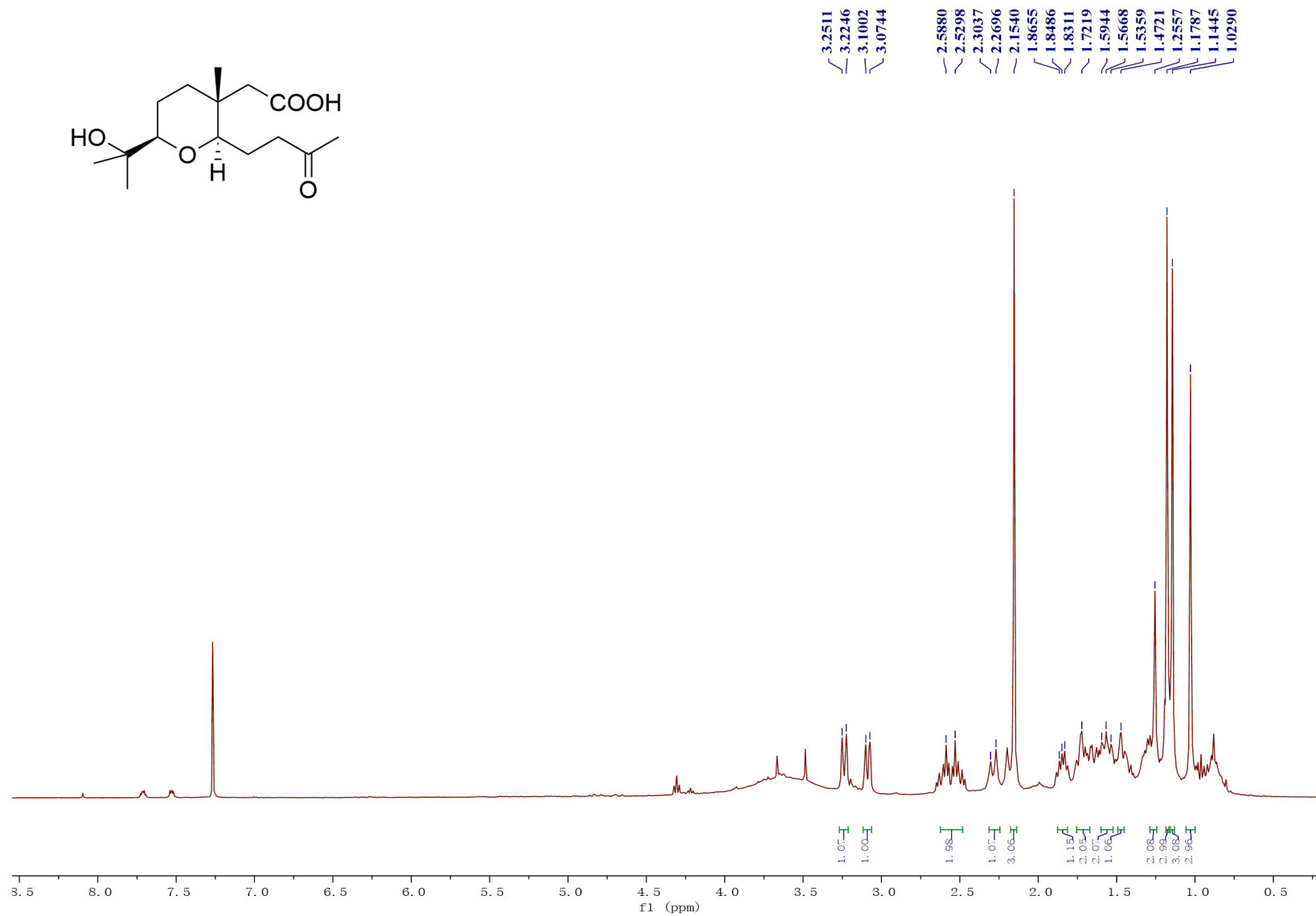


Fig. S57. ¹H NMR spectrum (CDCl₃, 600 MHz) of **9**

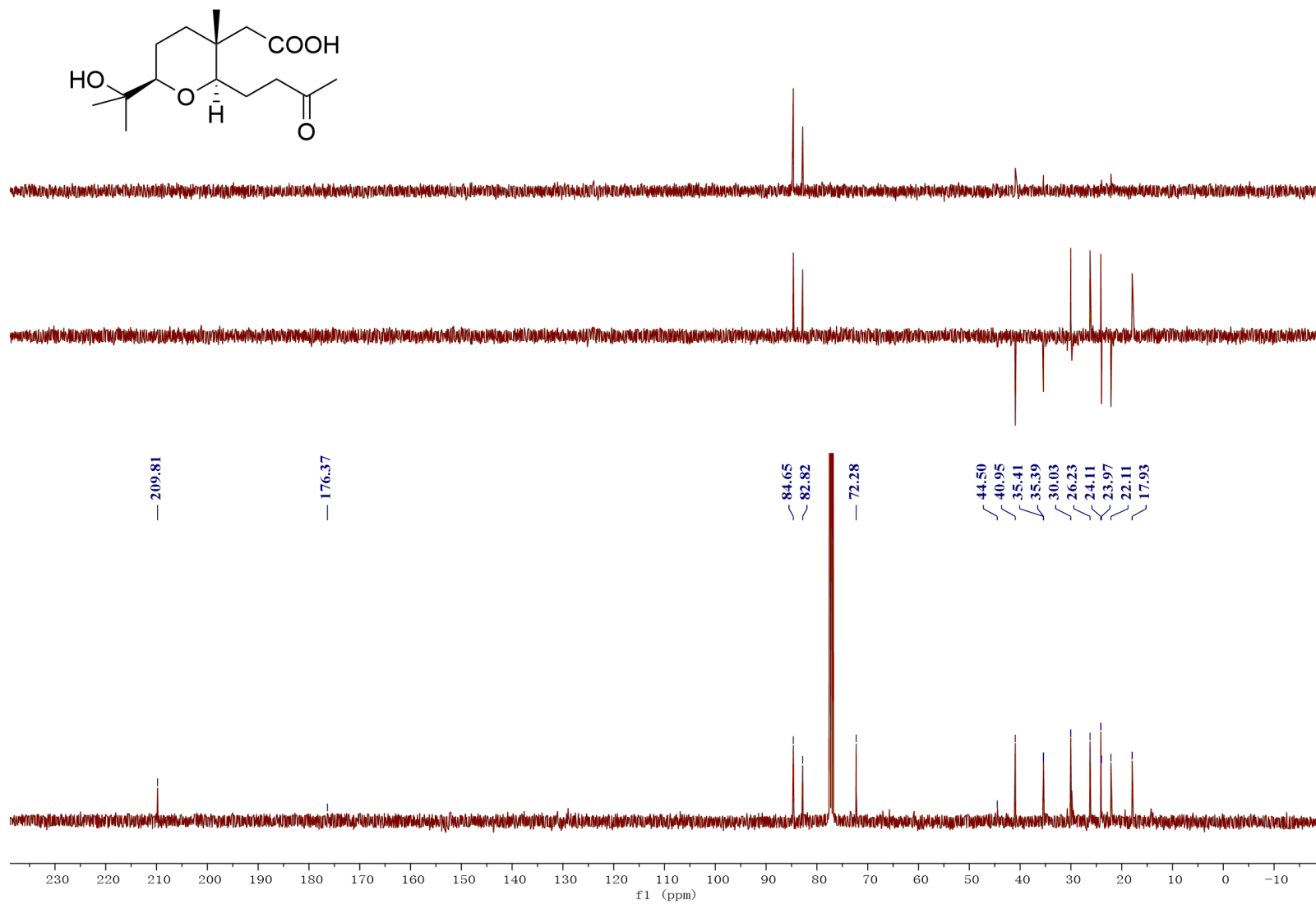


Fig. S58. ^{13}C and DEPT spectra (CDCl_3 , 150 MHz) of **9**

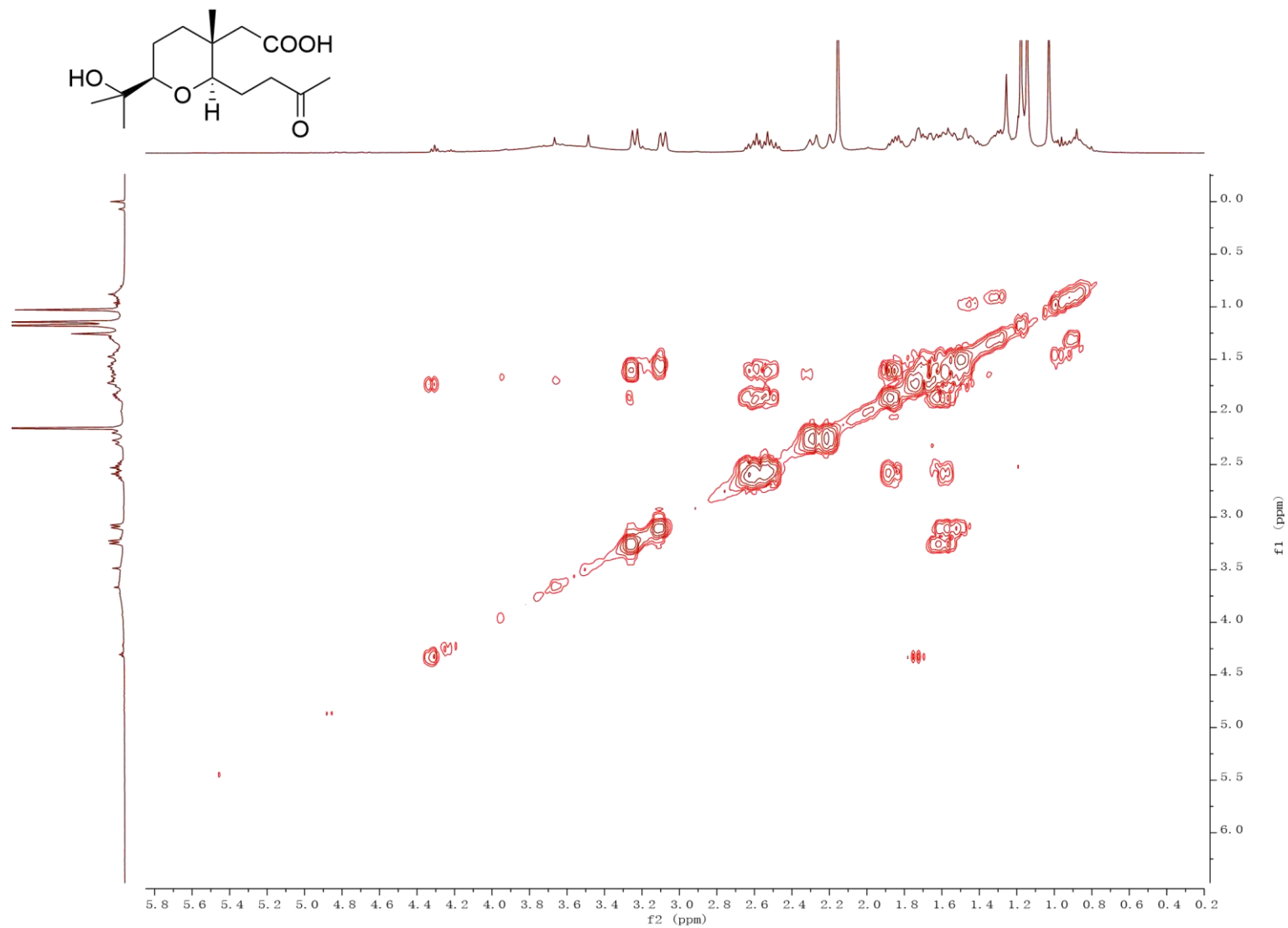


Fig. S59. ^1H - ^1H COSY spectrum (CDCl_3 , 600 MHz) of **9**

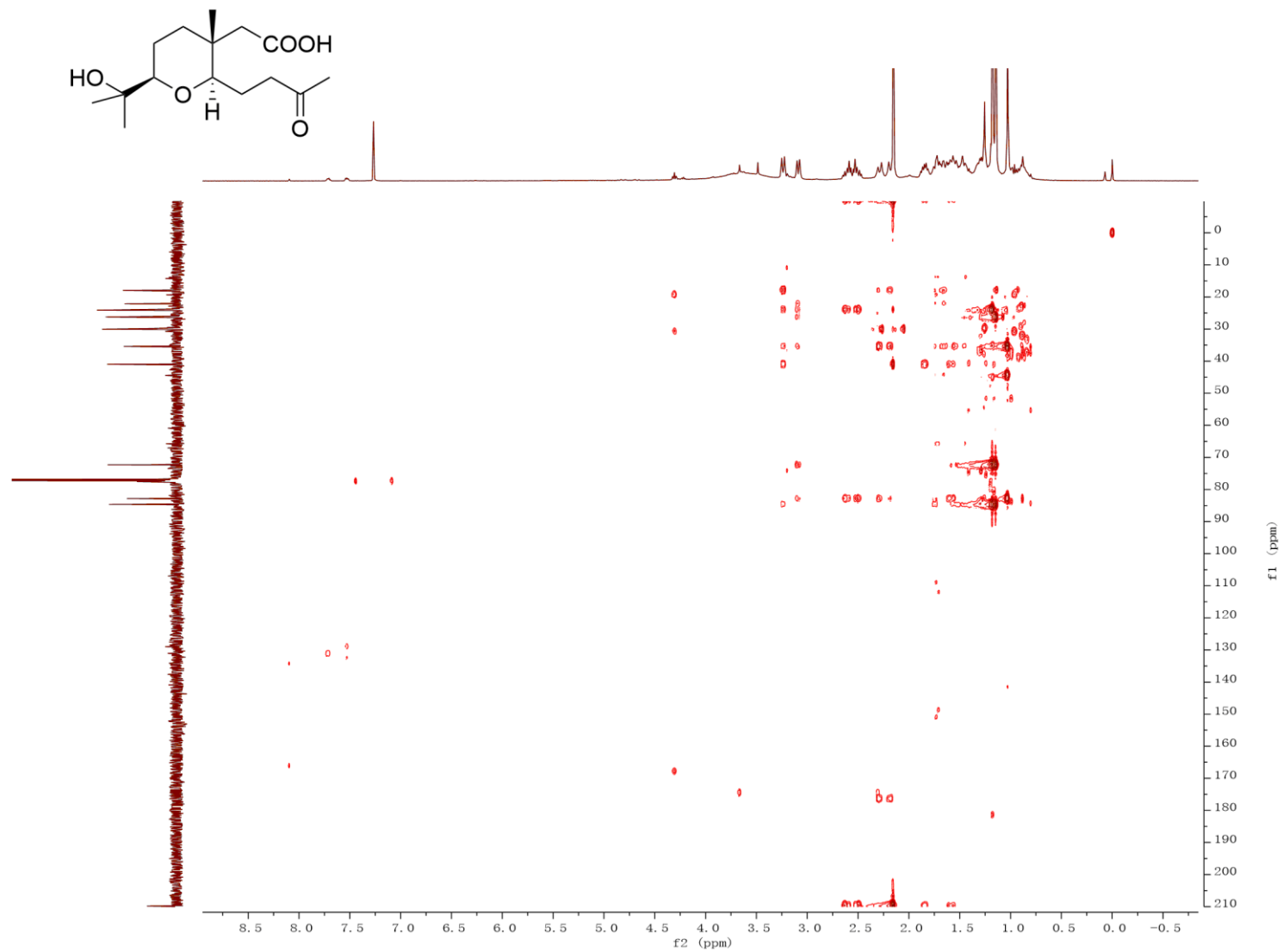


Fig. S60. HMBC spectrum (CDCl₃, 600 MHz) of **9**

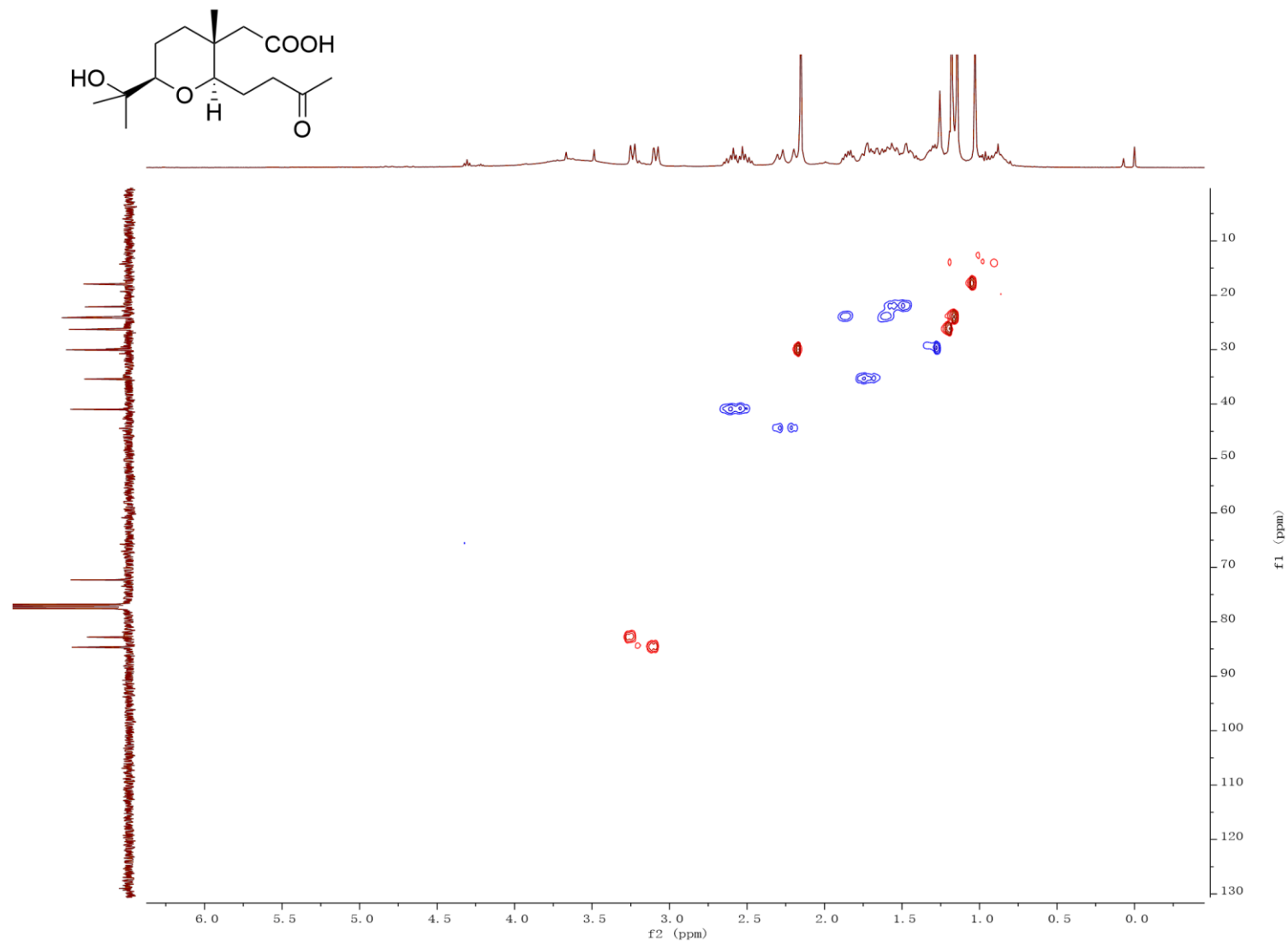


Fig. S61. HSQC spectrum (CDCl₃, 600 MHz) of **9**

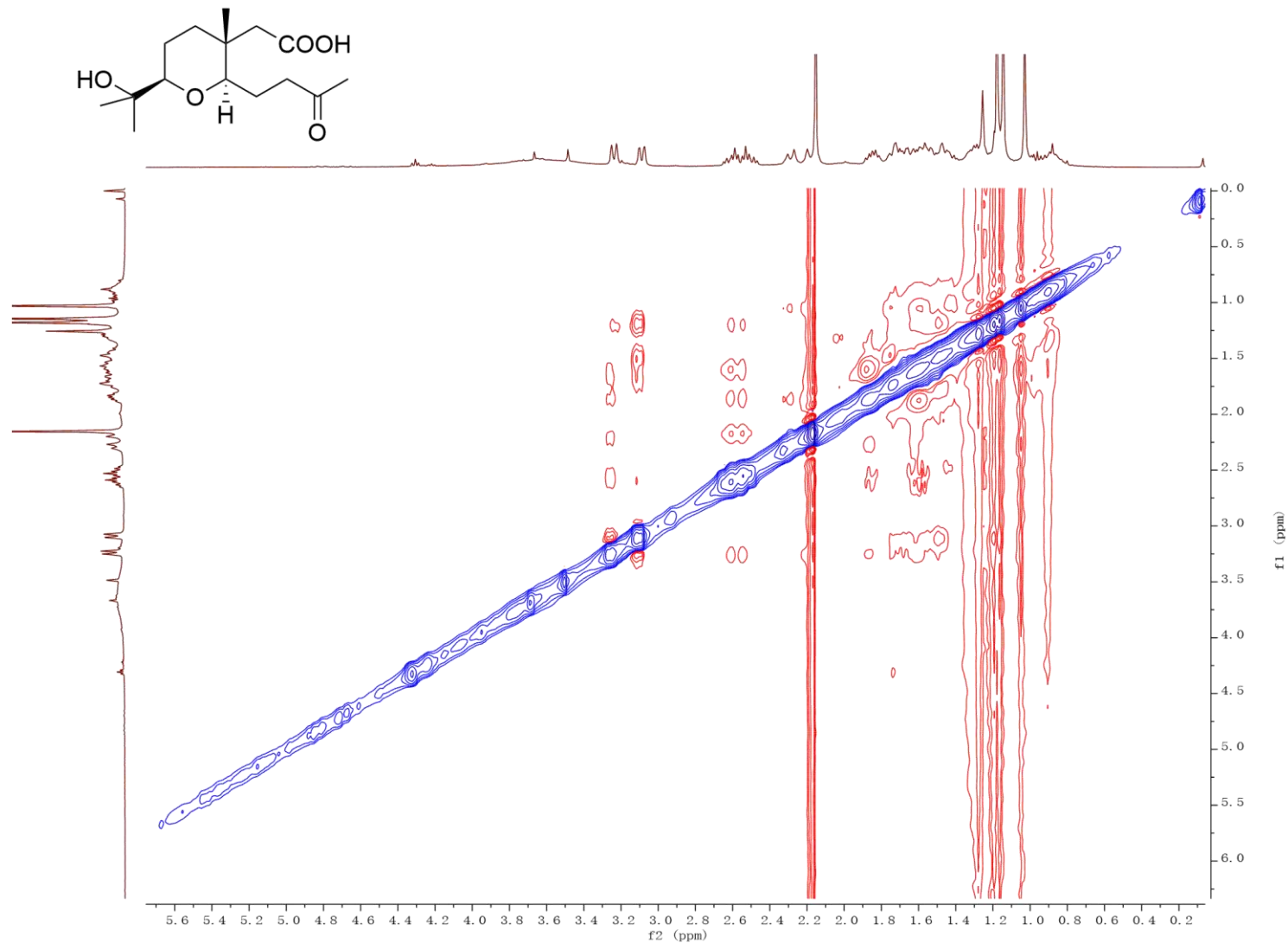


Fig. S62. NOESY spectrum (CDCl₃, 600 MHz) of **9**

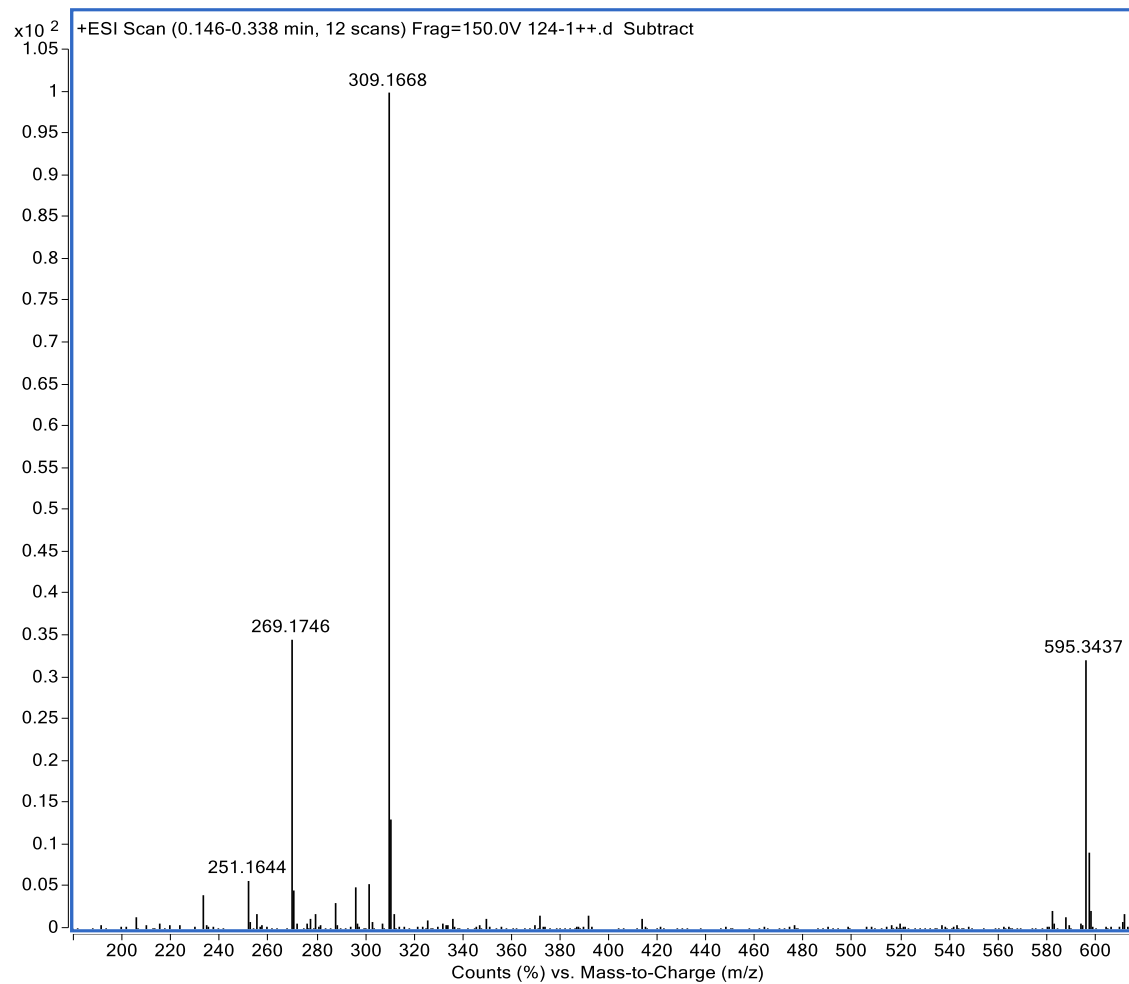


Fig. S63. (+)-HR-ESI-MS (positive mode) of **9**

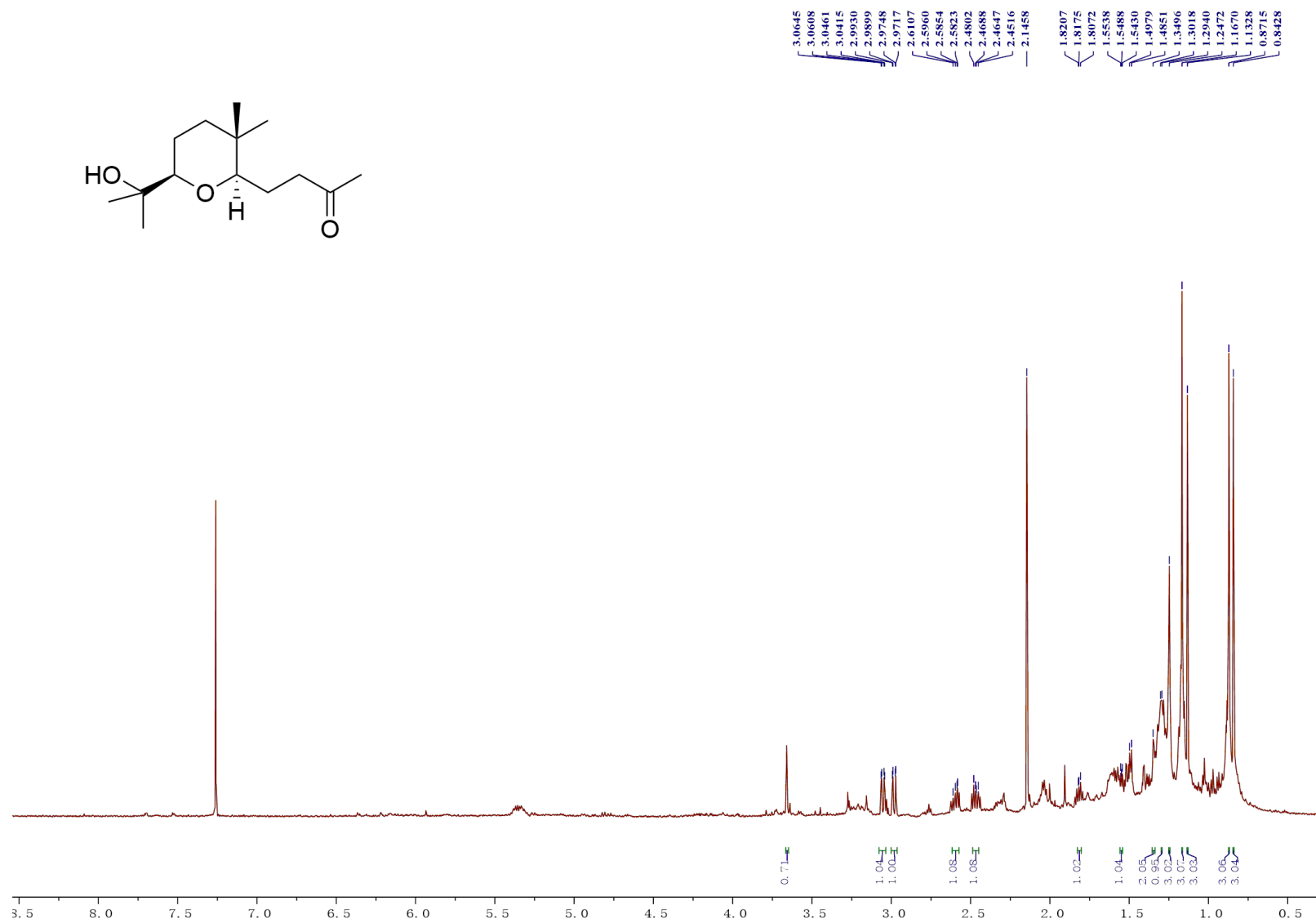


Fig. S64. ¹H NMR spectrum (CDCl₃, 600 MHz) of **10**

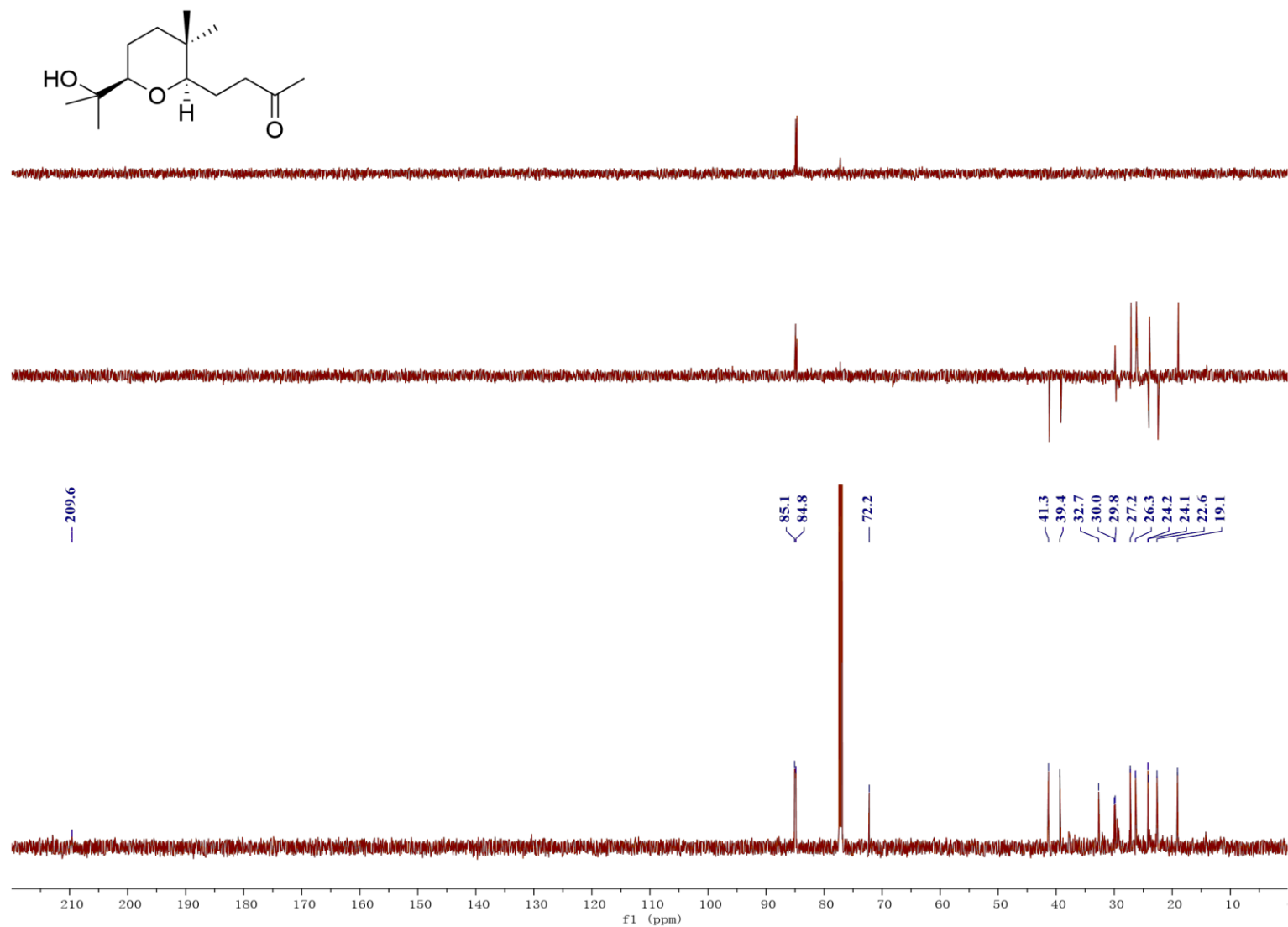


Fig. S65. ^{13}C and DEPT spectra (CDCl_3 , 150 MHz) of **10**

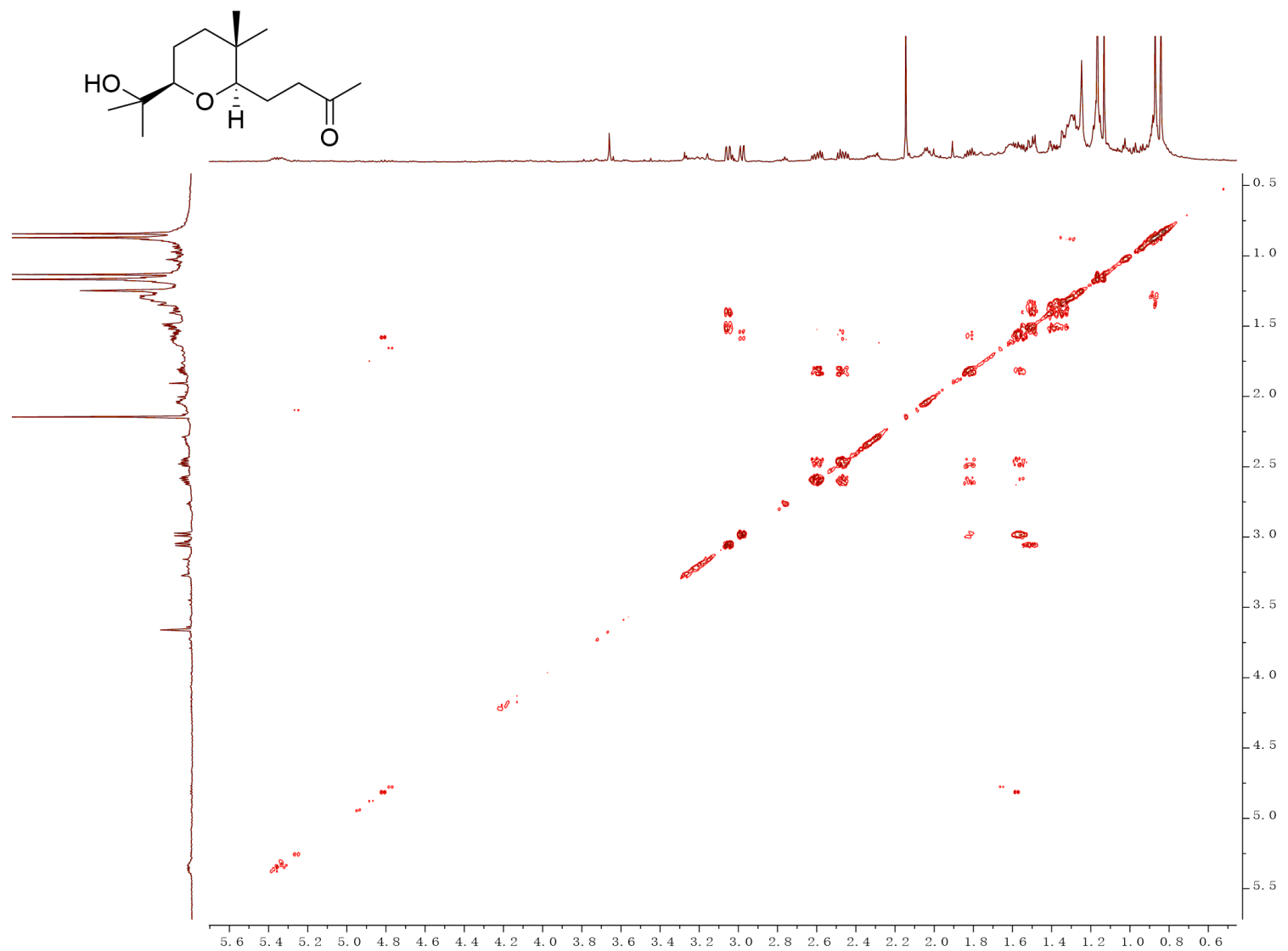


Fig. S66. ^1H - ^1H COSY spectrum (CDCl_3 , 600 MHz) of **10**

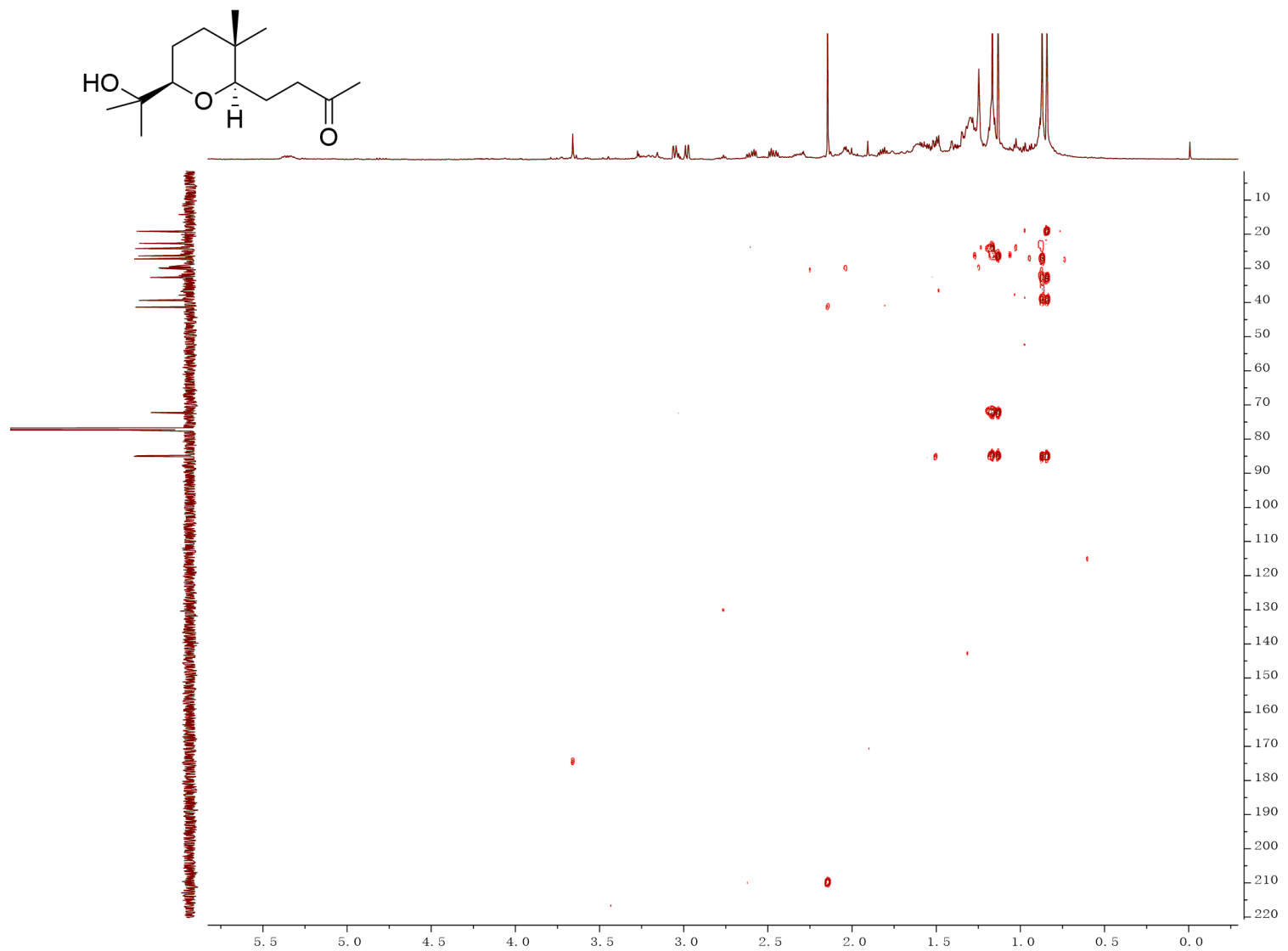


Fig. S67. HMBC spectrum (CDCl₃, 600 MHz) of **10**

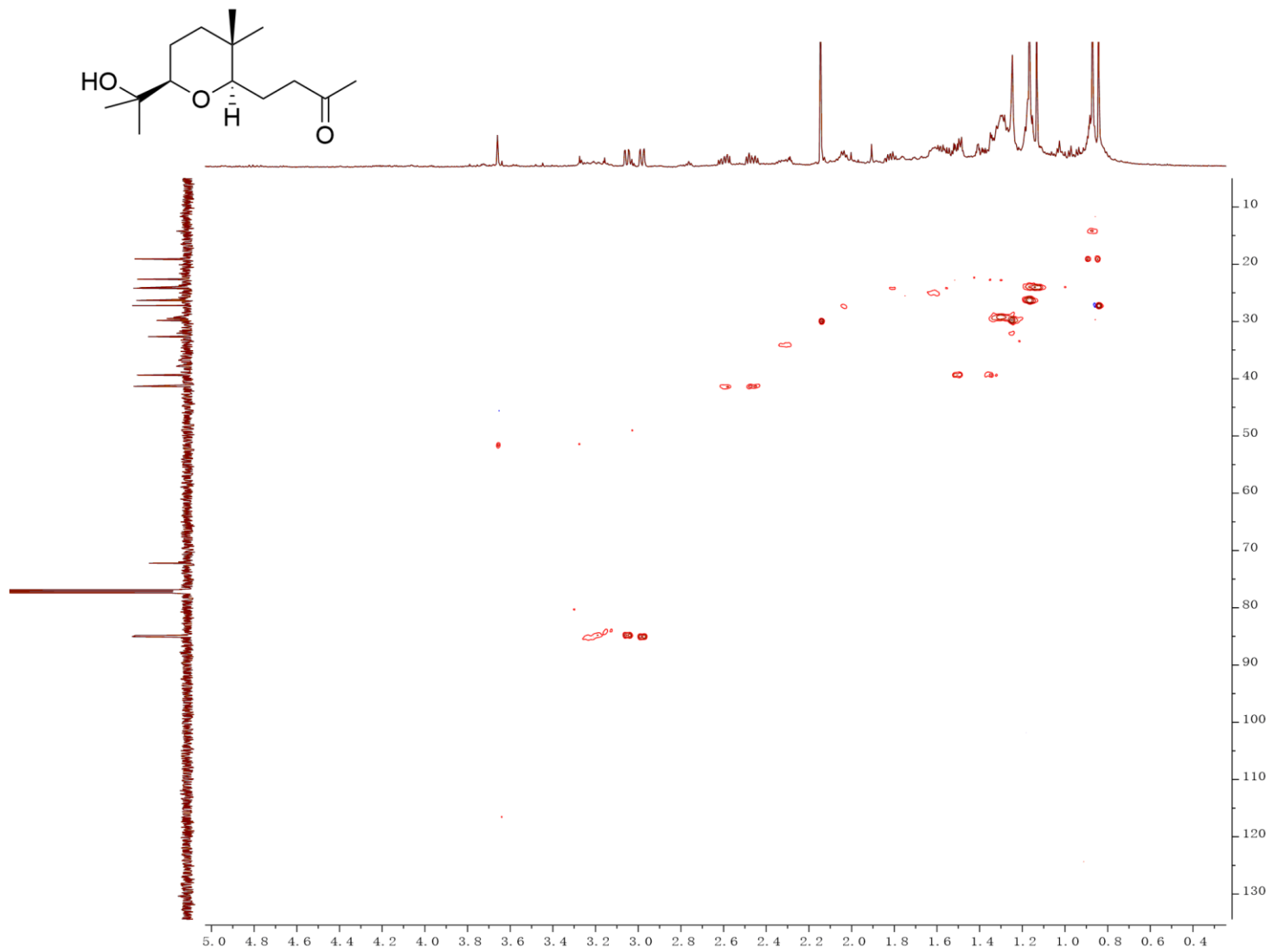


Fig. S68. HSQC spectrum (CDCl₃, 600 MHz) of **10**

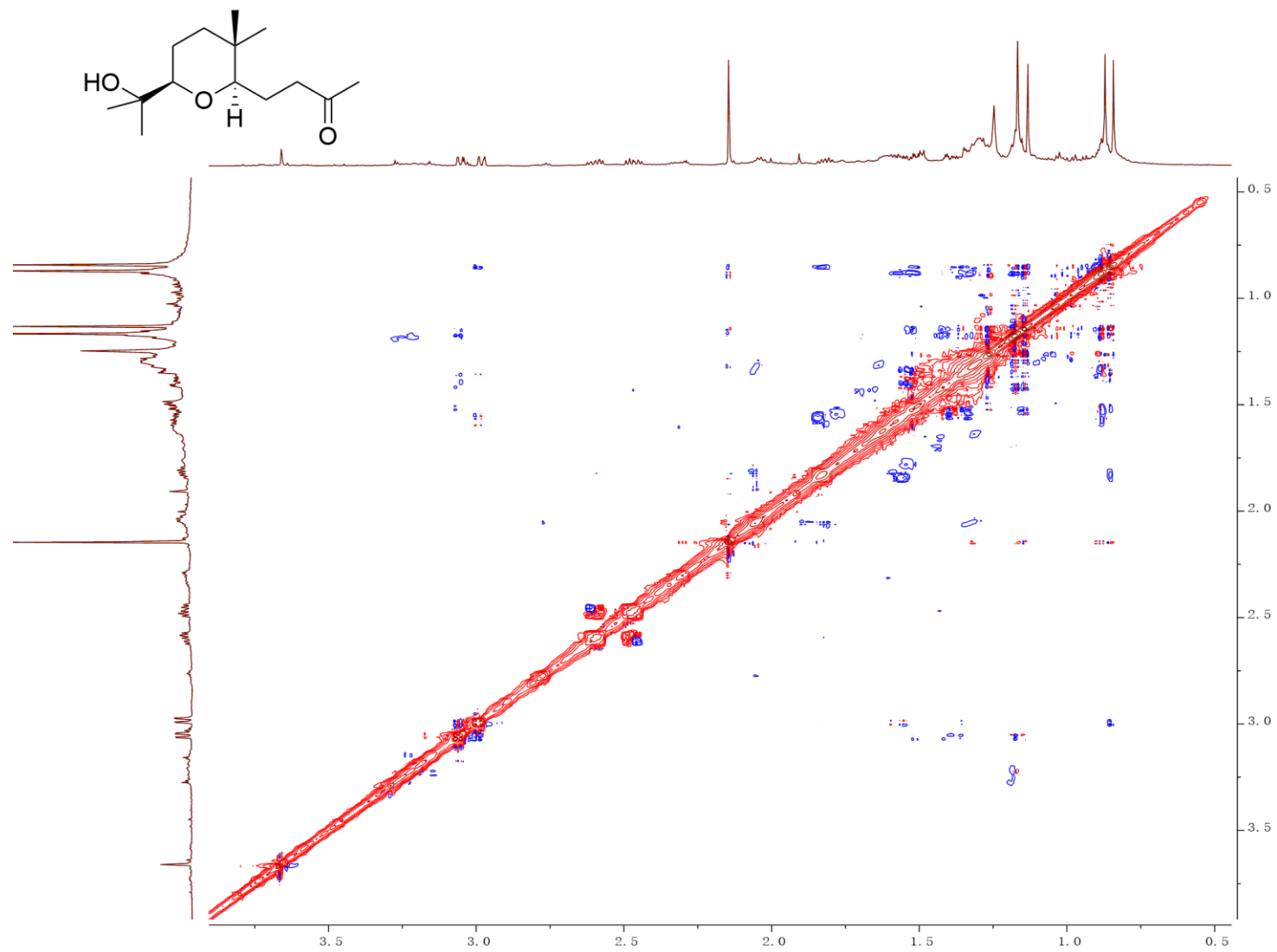


Fig. S69. NOESY spectrum (CDCl₃, 600 MHz) of **10**

DJ1-III311 #58 RT: 1.03 AV: 1 NL: 5.33E7
T: FTMS + c ESI Full ms [100.00-850.00]

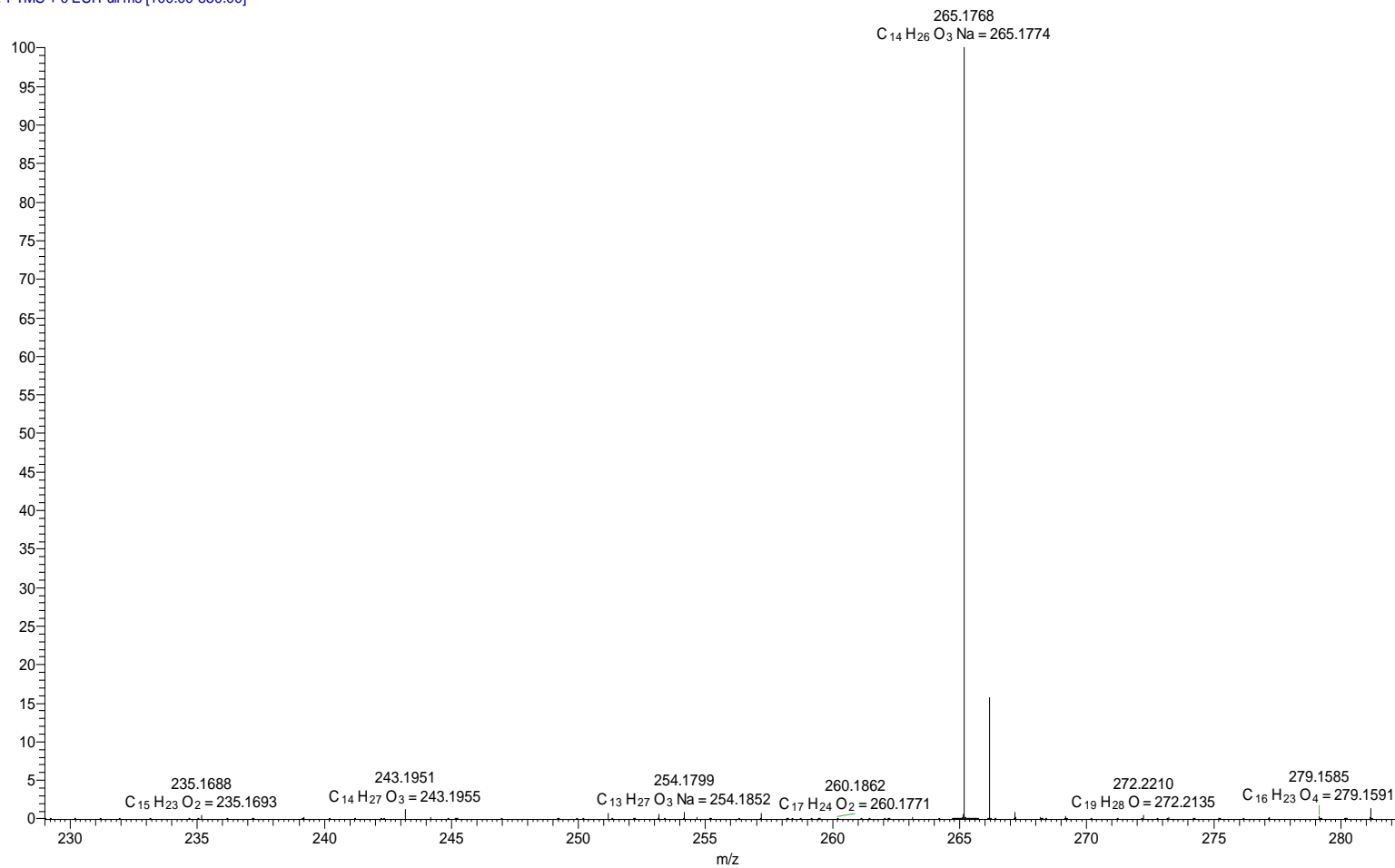


Fig. S70. (+)-HR-ESI-MS (positive mode) of **10**

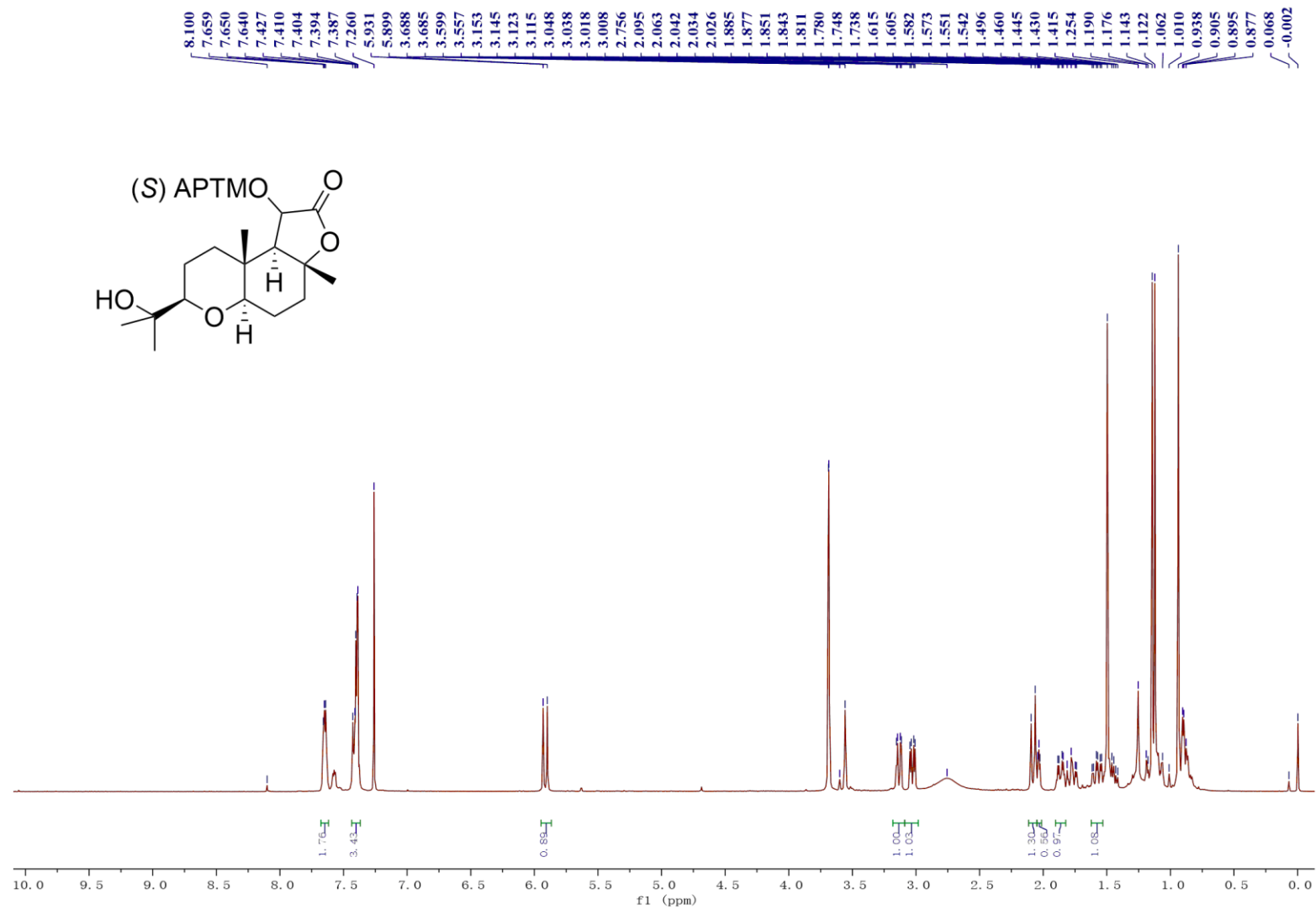


Fig. S71. ^1H NMR spectrum of S-MTPA ester of **1**

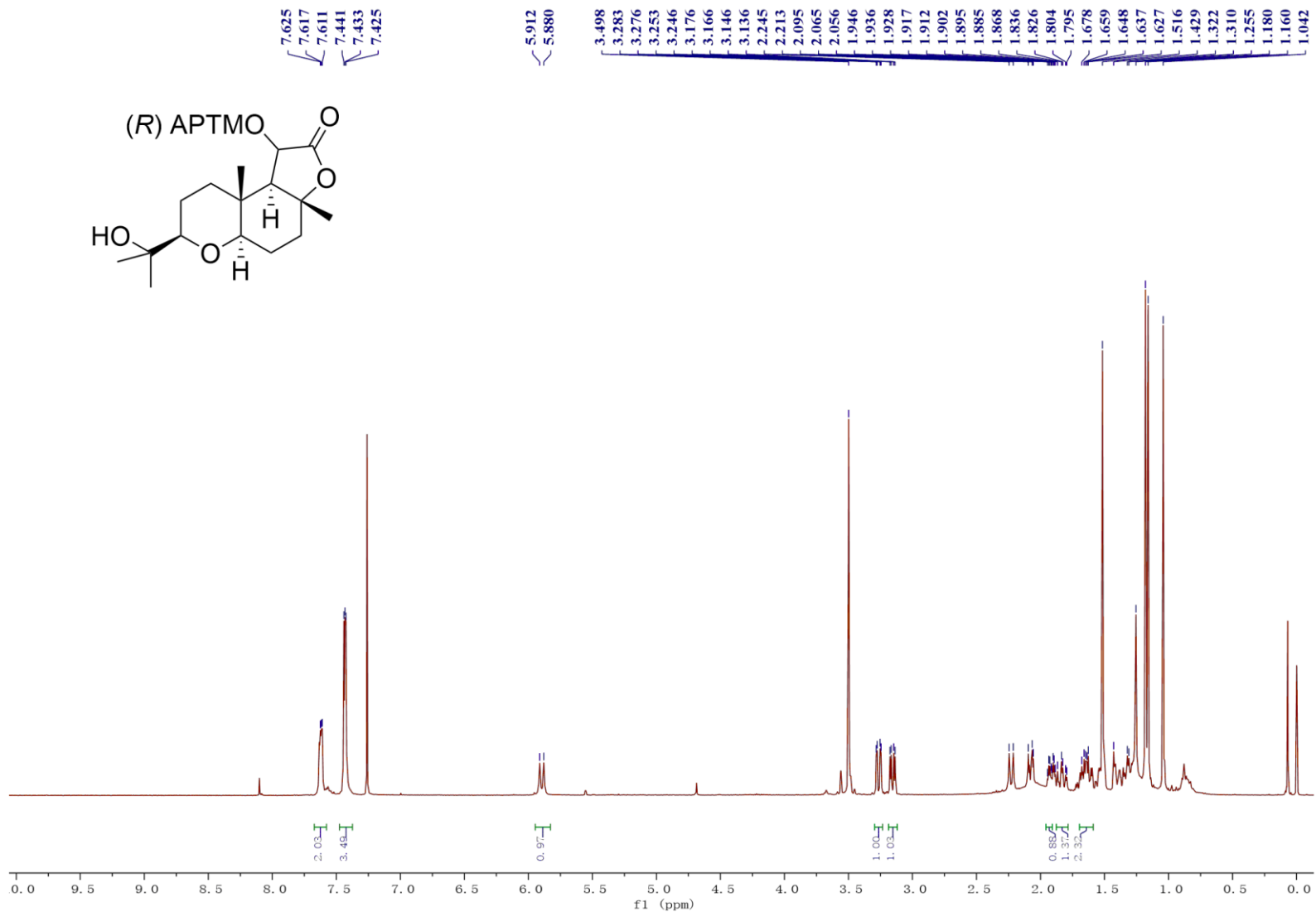


Fig. S72. ¹H NMR spectrum of *R*-MTPA ester of **1**

	A	B	C	D	E	F	G	H
1	Functional		Solvent?		Basis Set		Type of Data	
2	mPW1PW91		PC1		6-31+G(d,p)		Shielding Tensors	
3								
12			DP4+	0.00%	100.00%	-	-	-
14	Nuclei	sp2?	xperimenta	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5
15	C		40.6	43.6	44.5			
16	C	x	138.5	146.7	150.9			
17	C	x	137.8	148.3	143.3			
18	C		198.5	209.9	205.3			
19	C		26.9	51.9	29.9			
20	C		79	82.2	81.6			
21	C		31.6	39.6	34.5			
22	C		37.9	42.3	40.8			
23	C		22.3	25.2	25.5			
24	C		84.6	87.8	87.6			
25	C		72	74.1	74.3			
26	C		26.1	27.12	27.47			
27	C		23.9	24.27	24.45			
28	C		16.5	17.85	17.60			
29	C		25.5	24.54	28.12			
30								
31	H		2.14	2.19	2.22			
32	H		2.03	2.09	2.16			
33	H	x	6.74	6.62	7.37			
34	H		1.98	2.65	2.03			
35	H		2.63	2.88	2.70			
36	H		3.32	3.48	3.35			
37	H		1.35	1.40	1.38			
38	H		1.72	1.55	1.72			
39	H		1.49	1.38	1.43			
40	H		1.62	1.62	1.74			
41	H		3.2	3.19	3.22			
42	H		1.18	1.14	1.16			
43	H		1.17	1.11	1.11			
44	H		0.85	1.1	0.91			
45	H		2.3	1.9	2.34			
46								

	A	B	C	D	E	F	G	H
1	Functional		Solvent?		Basis Set		Type of Data	
2	mPW1PW91		PC1		6-31+G(d,p)		Shielding Tensors	
3								
4				Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5
5	sDP4+ (H data)		0.00%	100.00%	-	-	-	-
6	sDP4+ (C data)		0.00%	100.00%	-	-	-	-
7	sDP4+ (all data)		0.00%	100.00%	-	-	-	-
8	uDP4+ (H data)		46.40%	53.60%	-	-	-	-
9	uDP4+ (C data)		75.32%	24.68%	-	-	-	-
10	uDP4+ (all data)		72.54%	27.46%	-	-	-	-
11	DP4+ (H data)		0.00%	100.00%	-	-	-	-
12	DP4+ (C data)		0.00%	100.00%	-	-	-	-
13	DP4+ (all data)		0.00%	100.00%	-	-	-	-

Fig. S73. DP4+ analysis of **3a** (Isomer 1) and **3b** (Isomer 2).

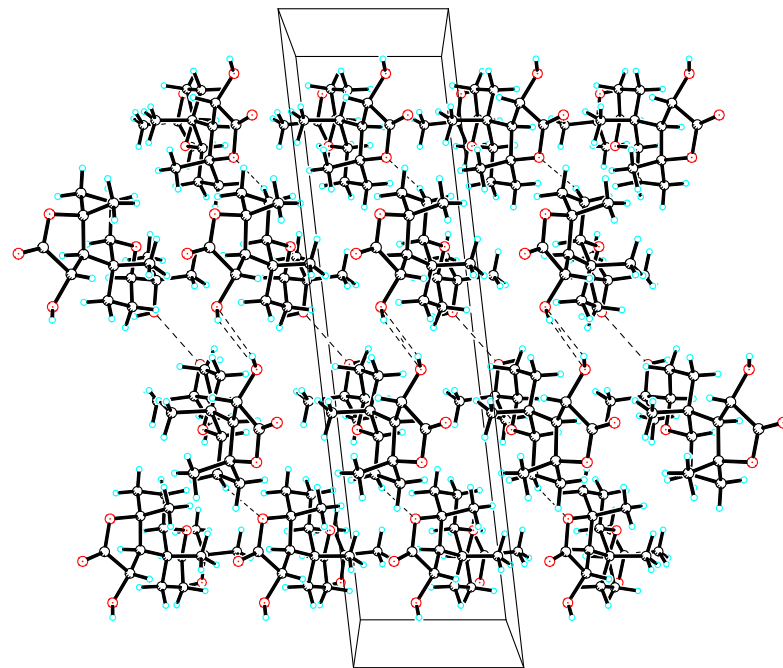


Fig. 74. View of the pack drawing of bipodonine A (**1**).