Supporting Information

DFT Calculations and ROESY NMR Data for the Diastereochemical Characterization of Cytotoxic Tetraterpenoids from the Oleoresin of *Abies balsamea*

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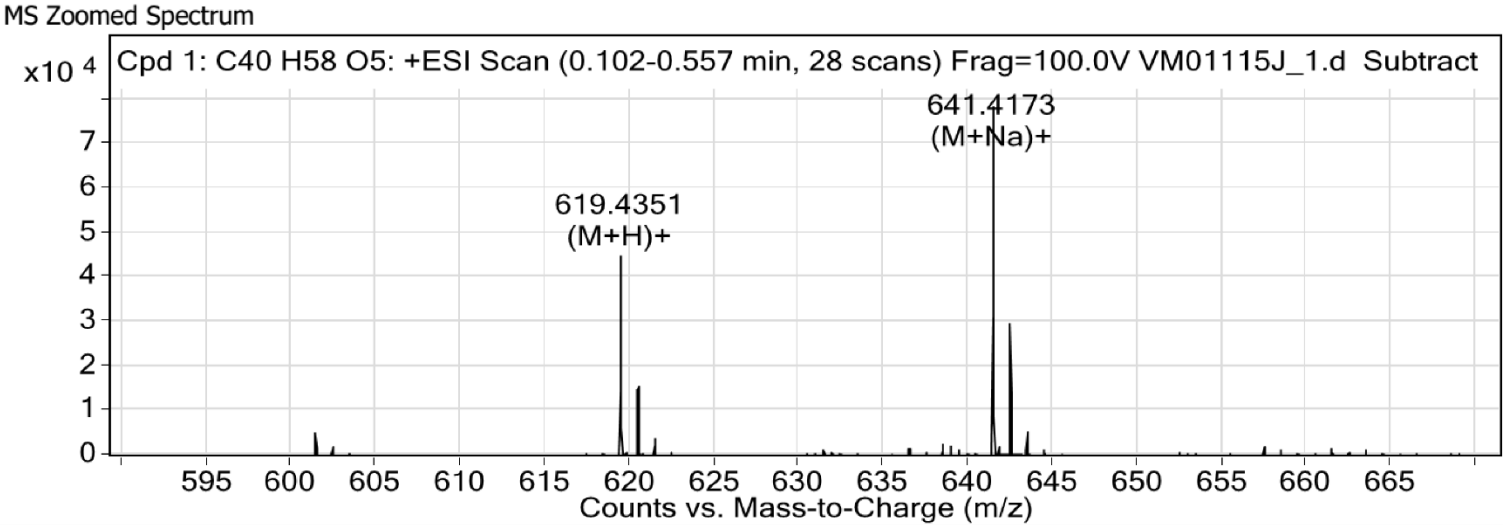


MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
619.4351	619.4357	-0.97	1	45526	C40 H59 O5	(M+H)+
620.4388	620.4391	-0.47	1	16708	C40 H59 O5	(M+H)+
621.4428	621.4423	0.88	1	3787	C40 H59 O5	(M+H)+

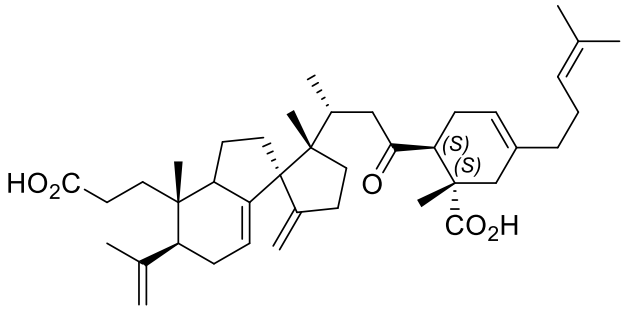


Figure S2. ^{1}H NMR Spectrum of Abibalsamin C (**3**) in $CDCl_3$, 400 MHz

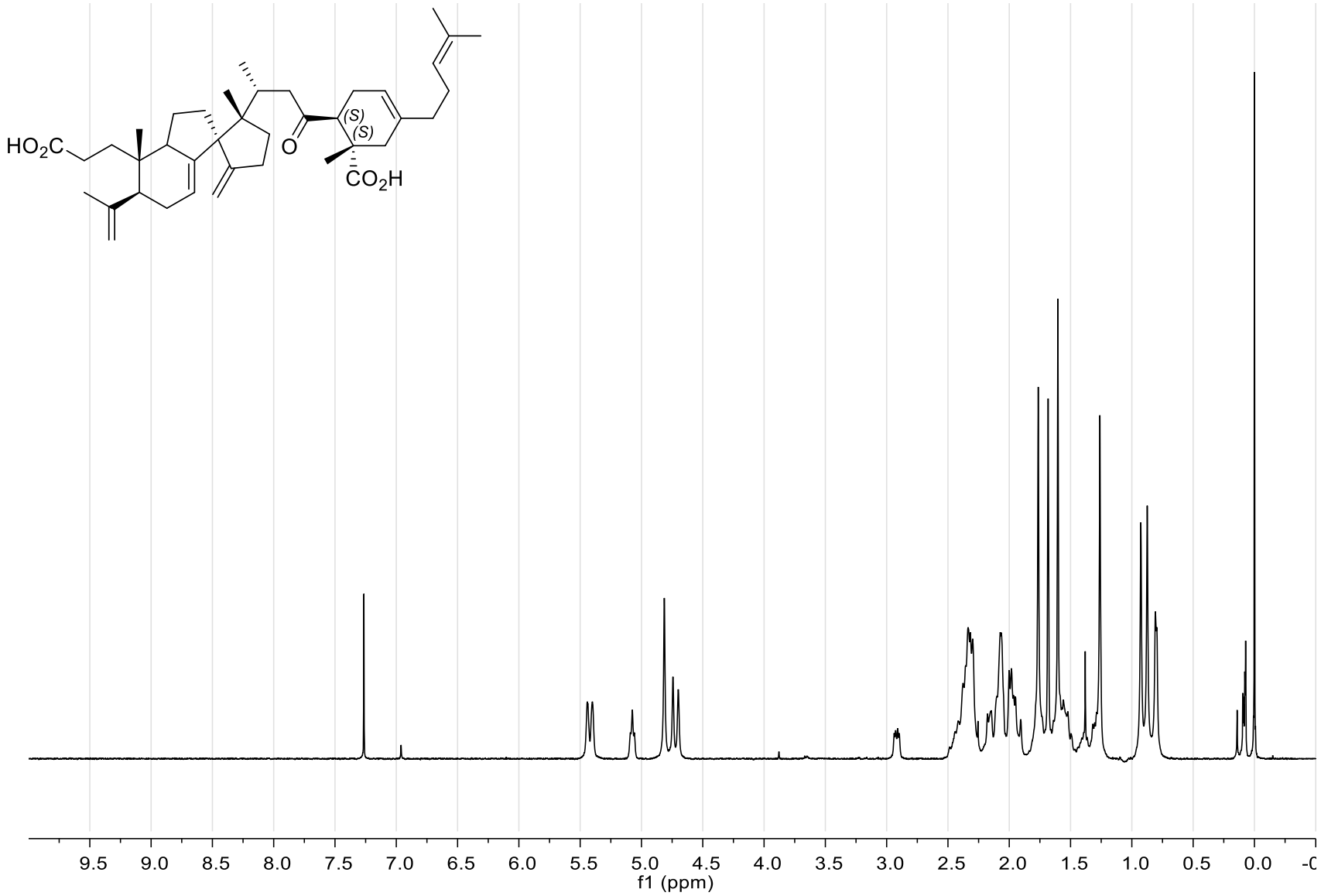


Figure S3. ^{13}C and DEPT NMR Spectra of Abibalsamin C (**3**) in $CDCl_3$, 100 MHz

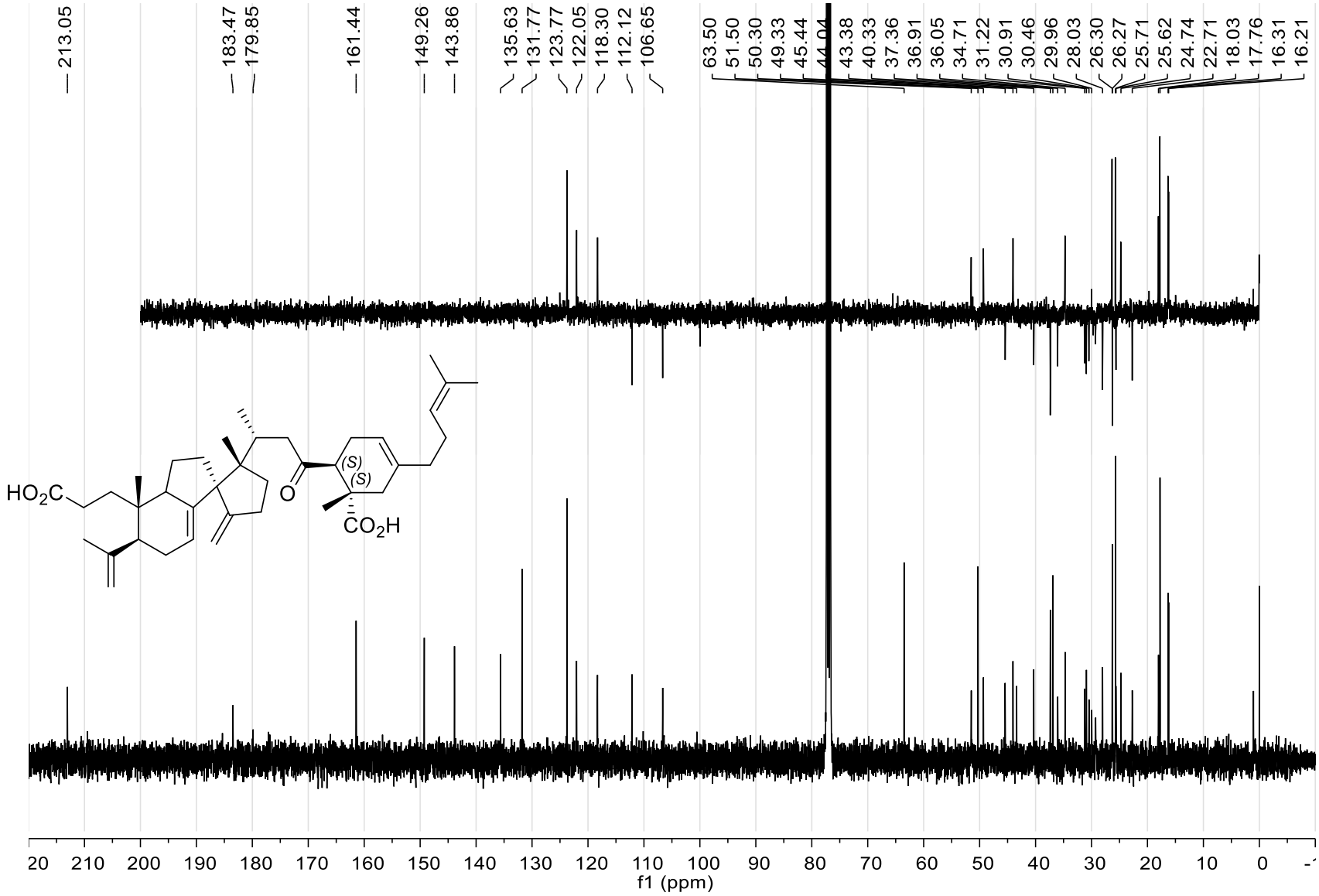


Figure S4. ^{1}H-^{1}H COSY Spectrum of Abibalsamin C (**3**) in $CDCl_3$, 400 MHz

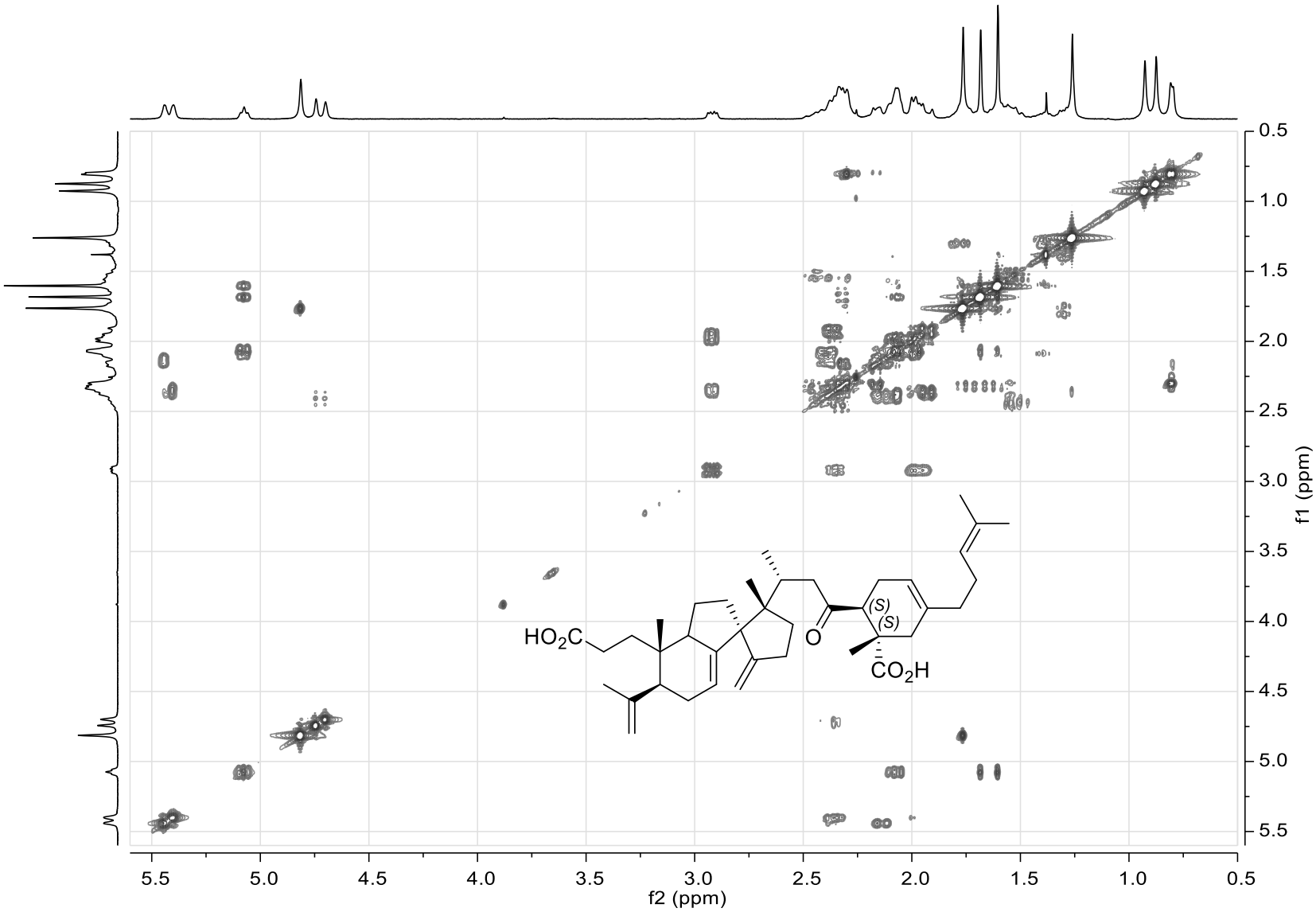


Figure S5. HSQC Spectrum of Abibalsamin C (**3**) in $CDCl_3$, 400 MHz

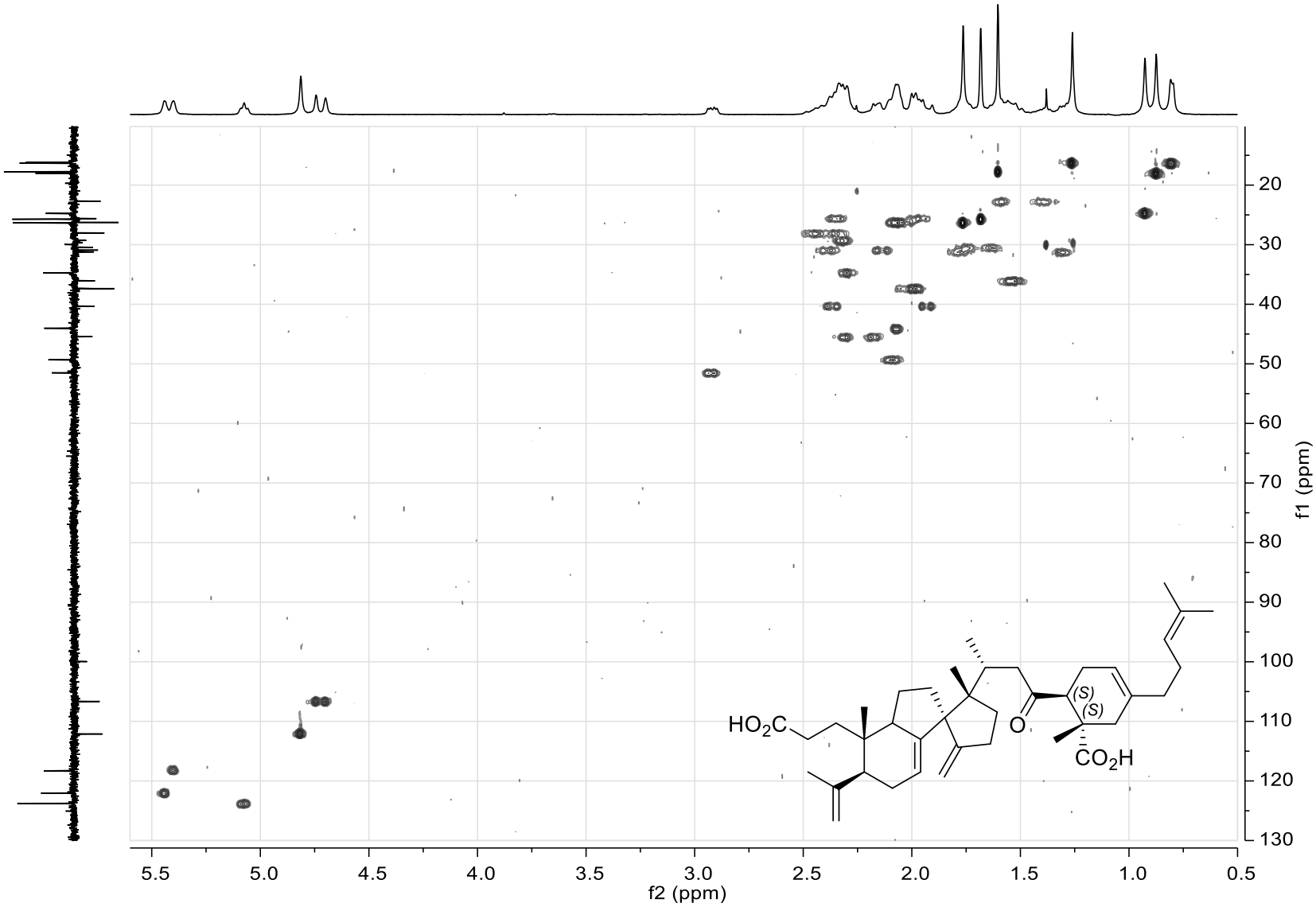


Figure S6. HMBC Spectrum of Abibalsamin C (**3**) in $CDCl_3$, 400 MHz

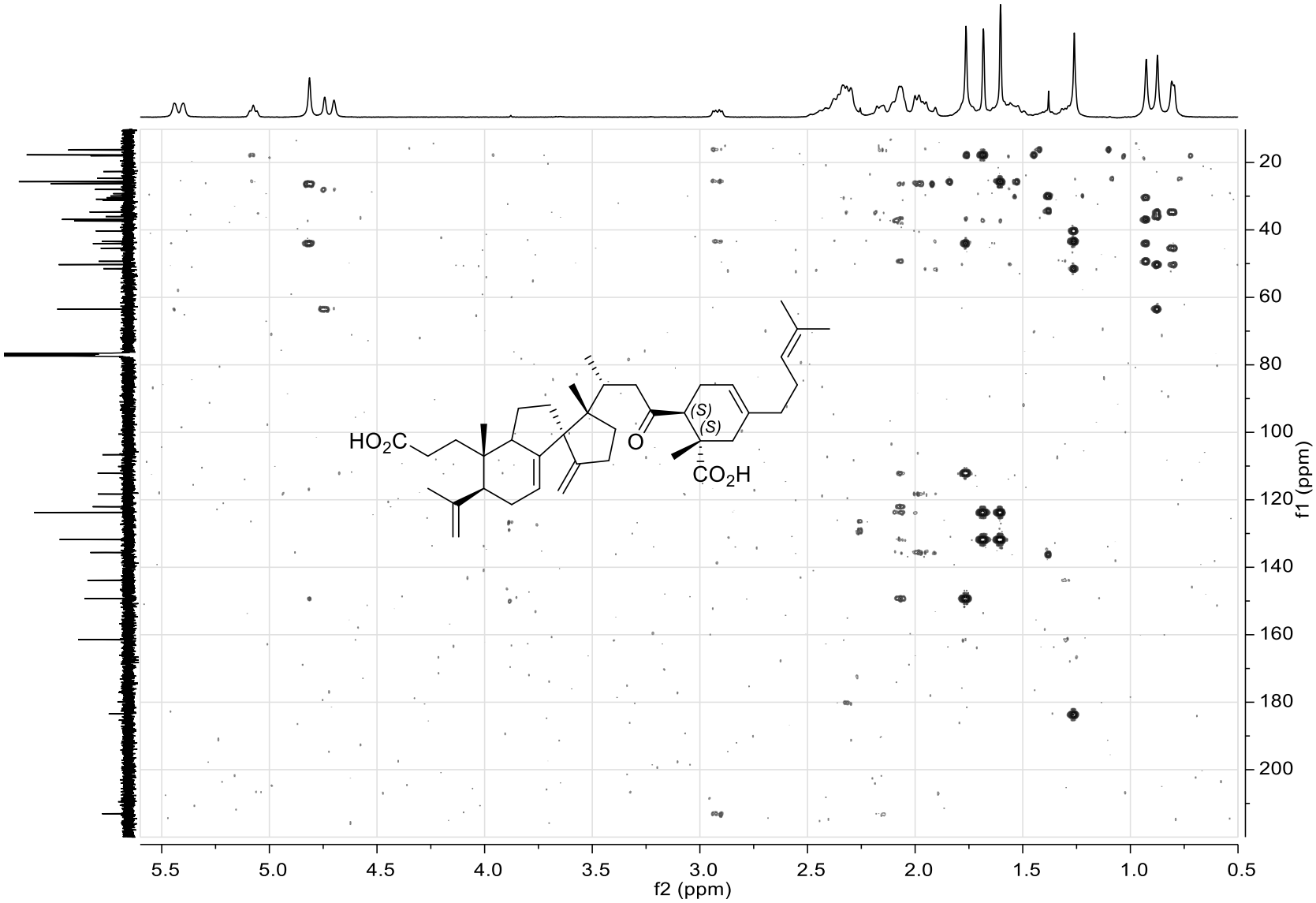
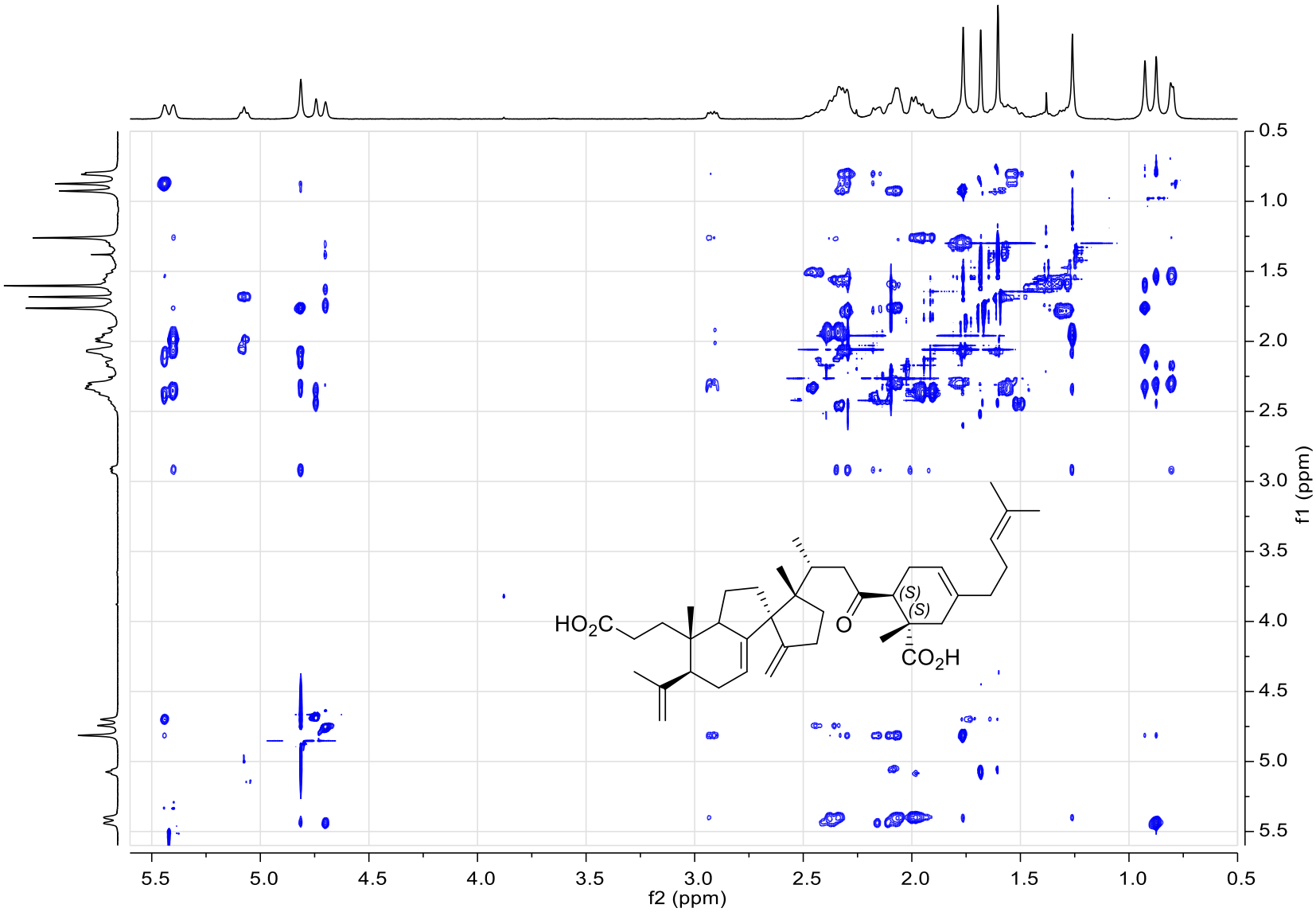


Figure S7. ROESY Spectrum of Abibalsamin C (**3**) in $CDCl_3$, 400 MHz



ABIBALSAMIN D (4)

Figure S8. HRESIMS of Abibalsamin D (**4**)

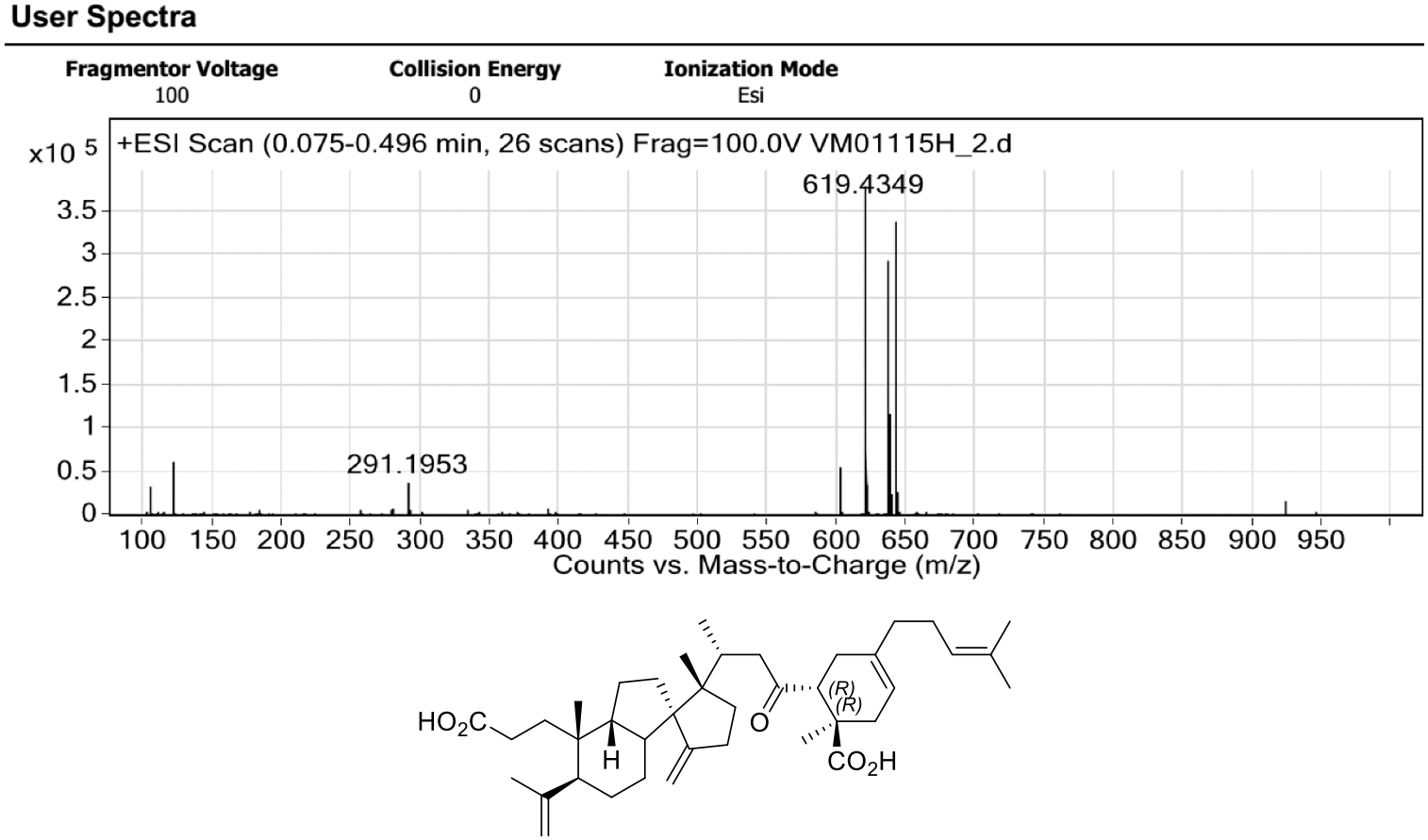


Figure S9. ^{1}H NMR Spectrum of Abibalsamin D (**4**) in $CDCl_3$, 400 MHz

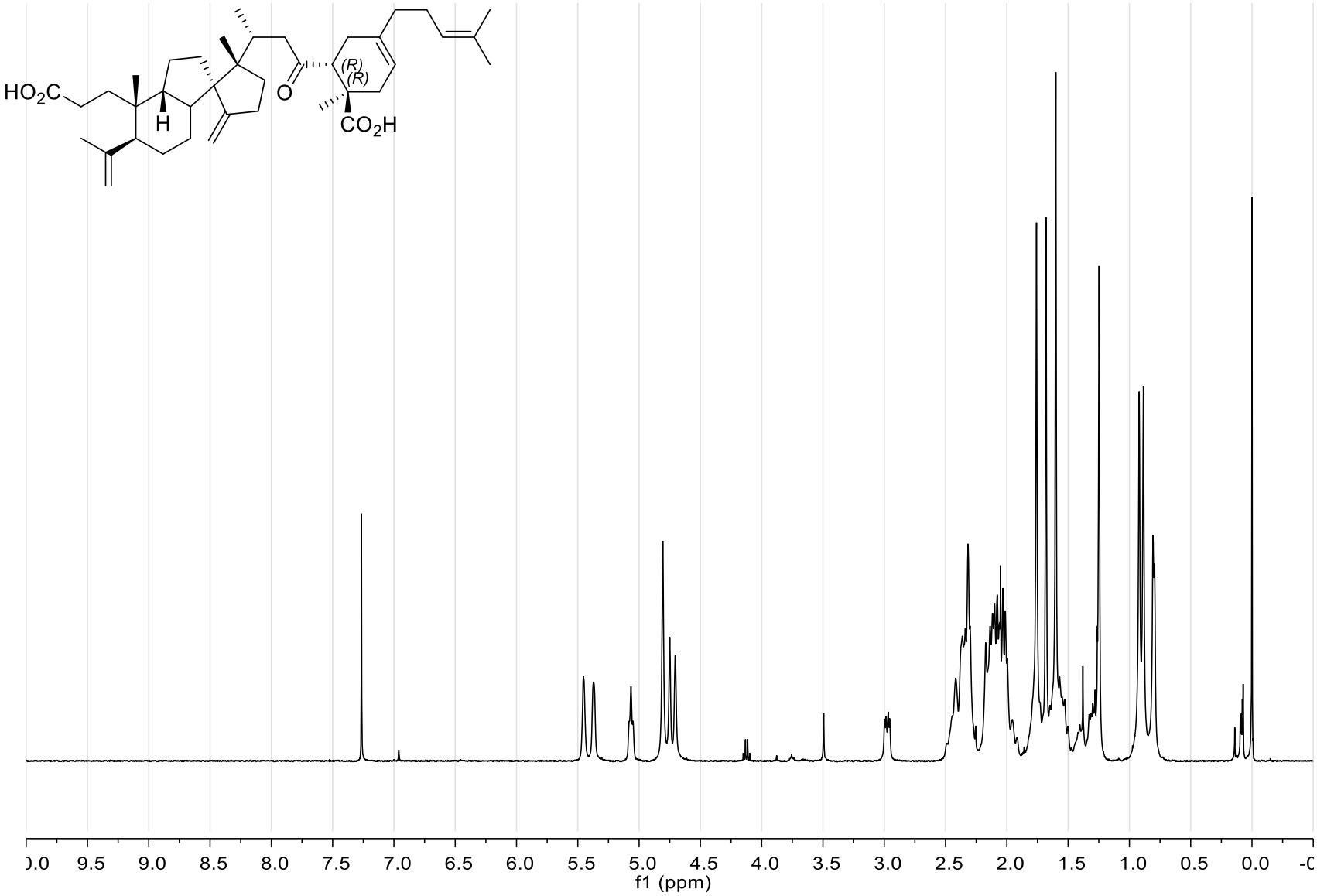


Figure S10. ^{13}C and DEPT NMR Spectra of Abibalsamin D (**4**) in $CDCl_3$, 100 MHz

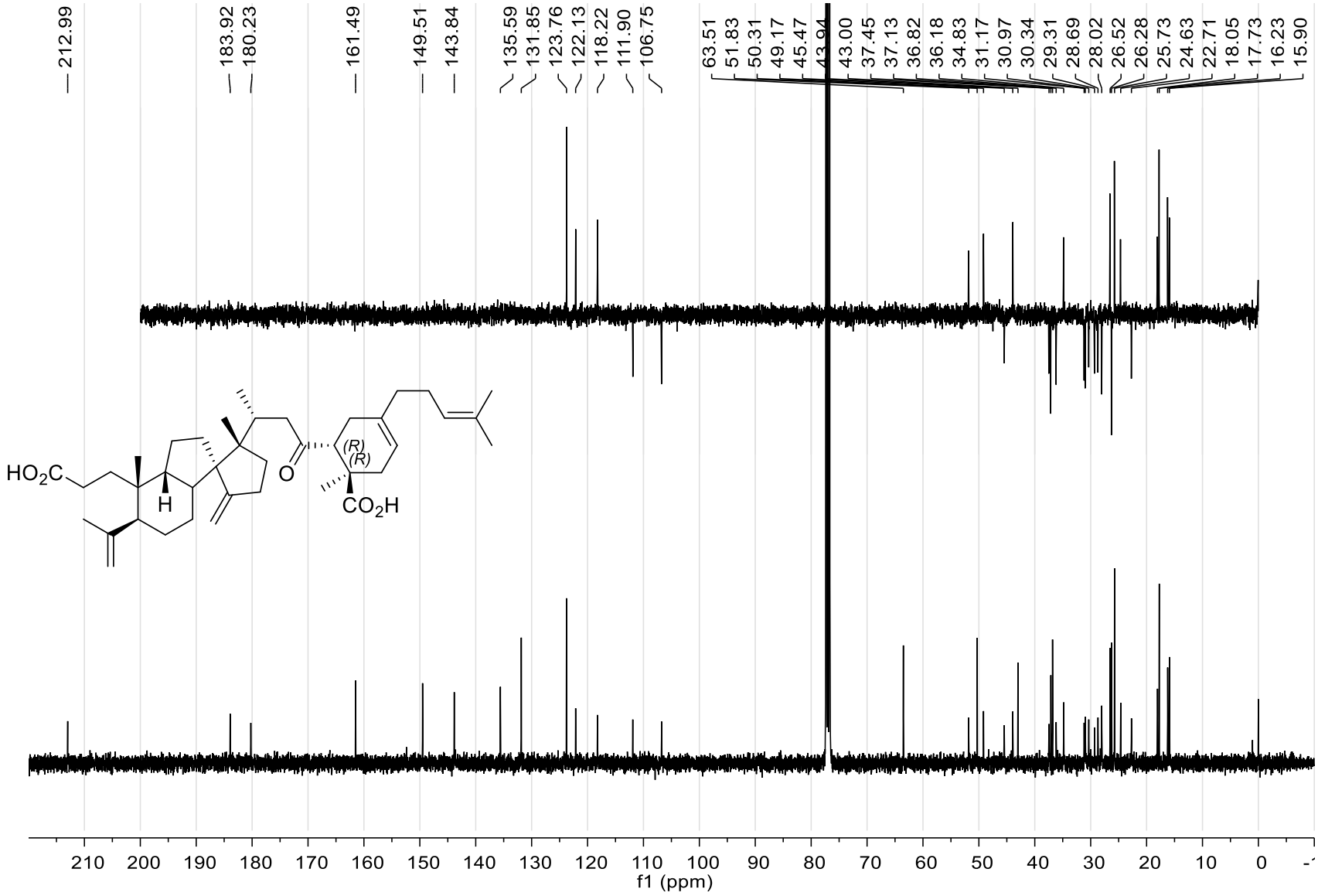


Figure S11. ^{1}H-^{1}H COSY Spectrum of Abibalsamin D (**4**) in $CDCl_3$, 400 MHz

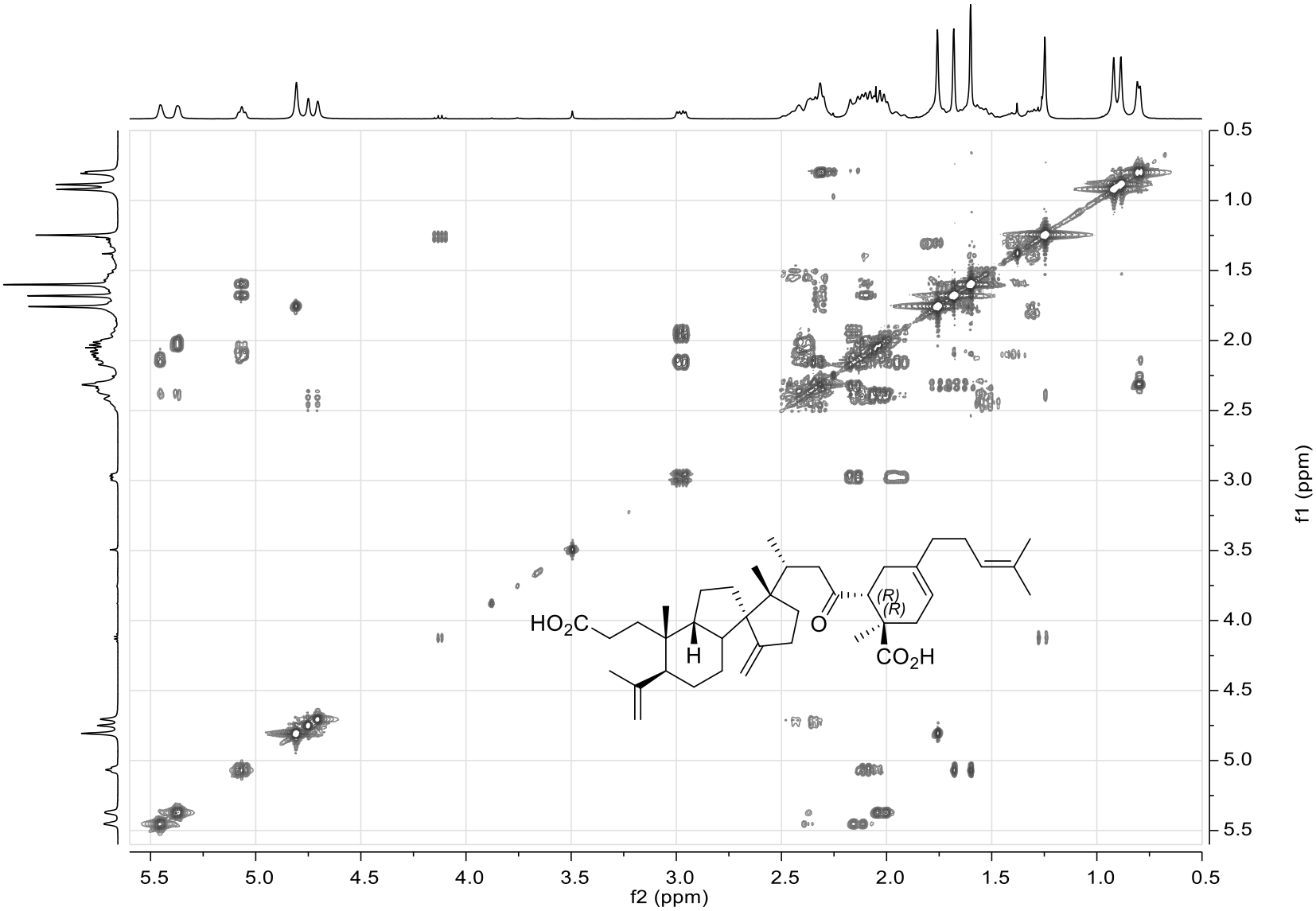


Figure S12. HSQC Spectrum of Abibalsamin D (**4**) in $CDCl_3$, 400 MHz

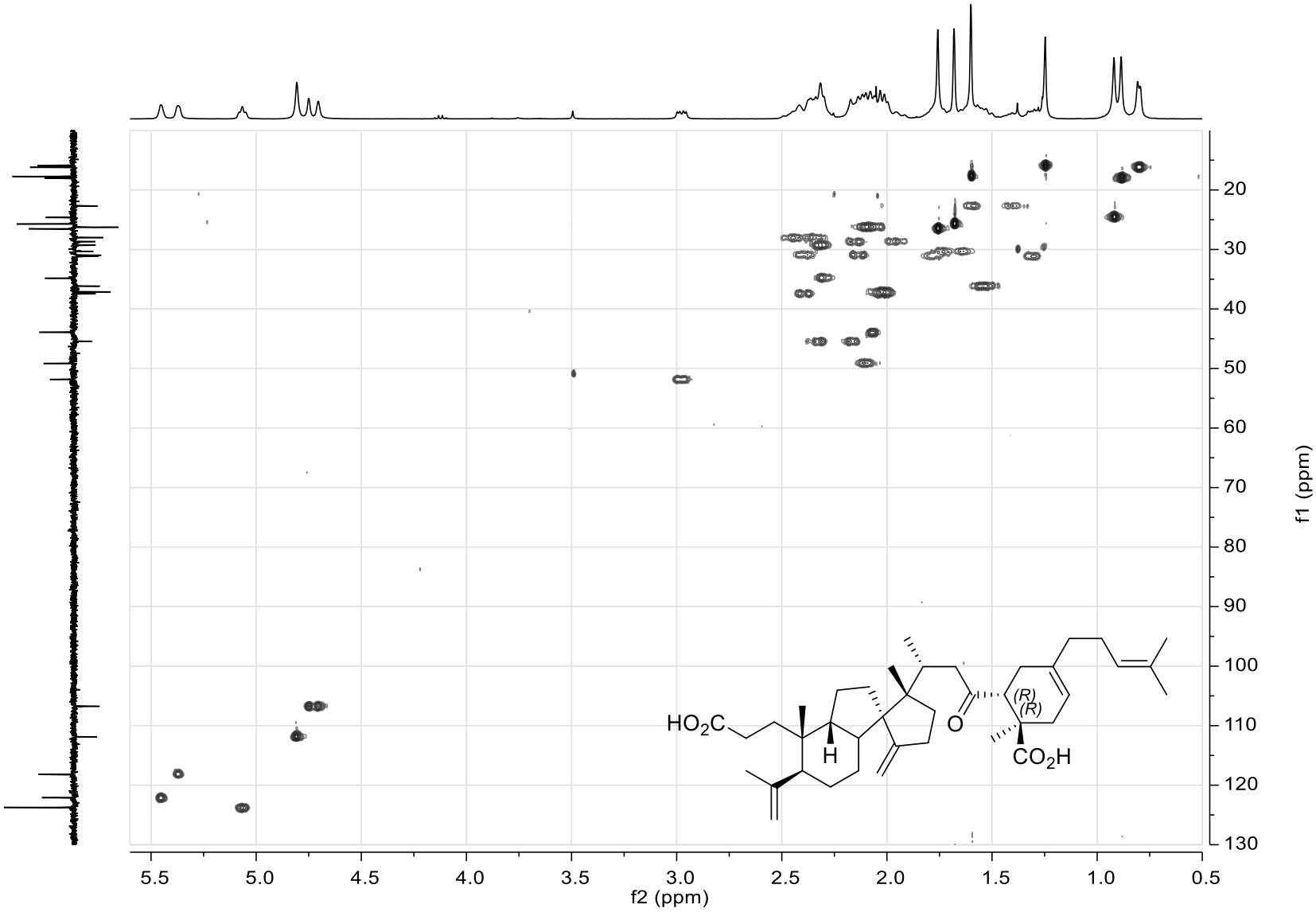


Figure S13. HMBC Spectrum of Abibalsamin D (**4**) in $CDCl_3$, 400 MHz

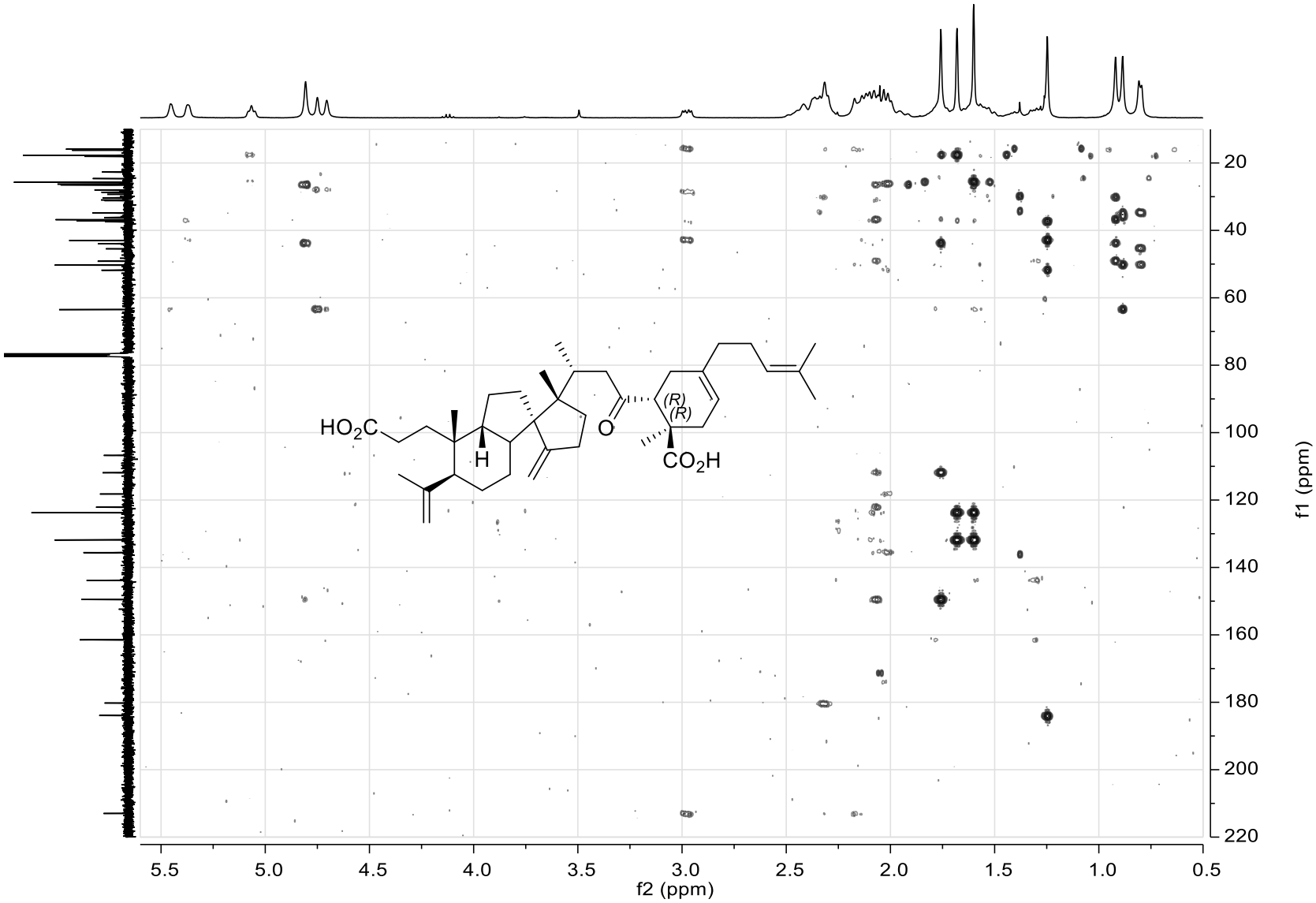
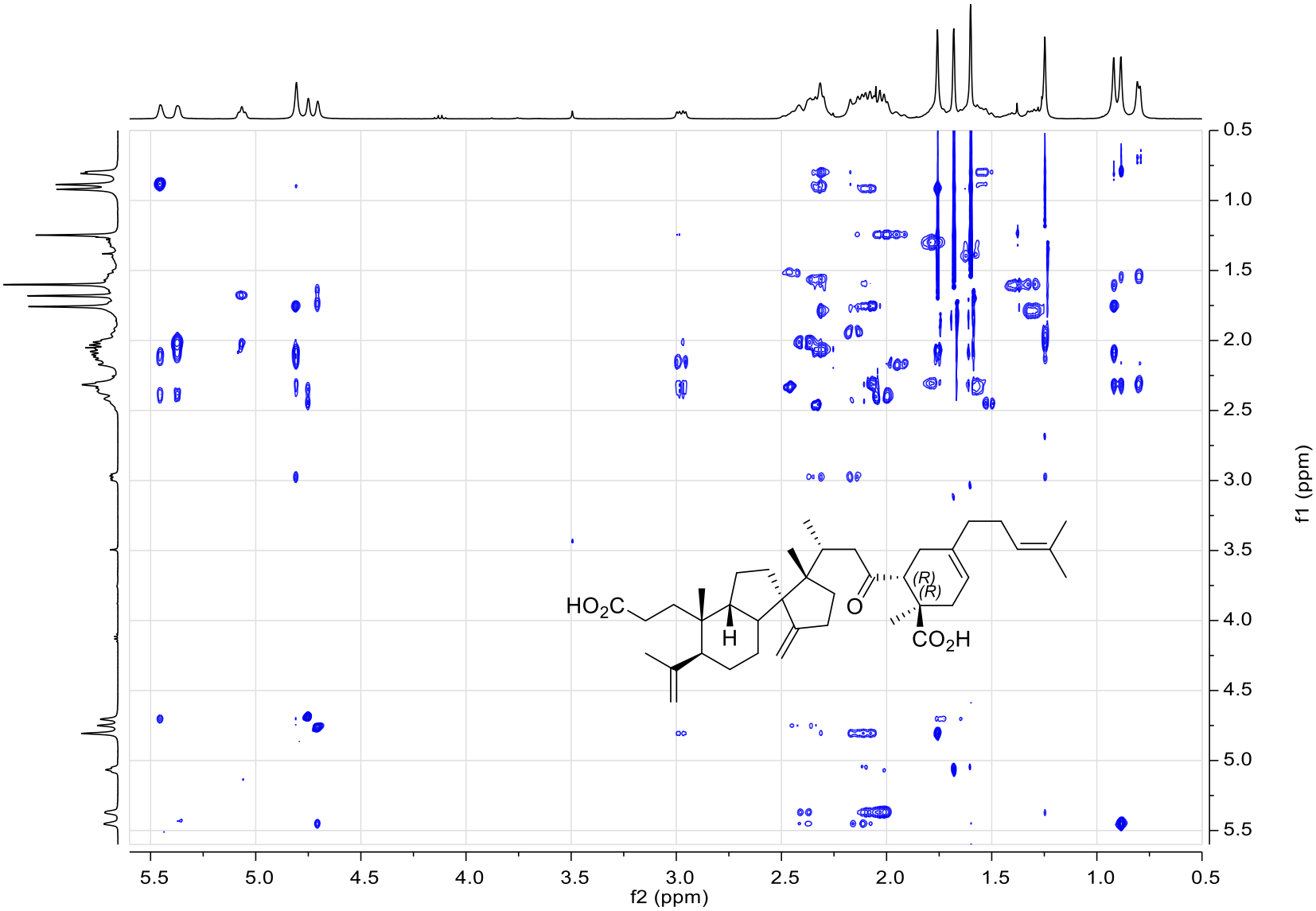
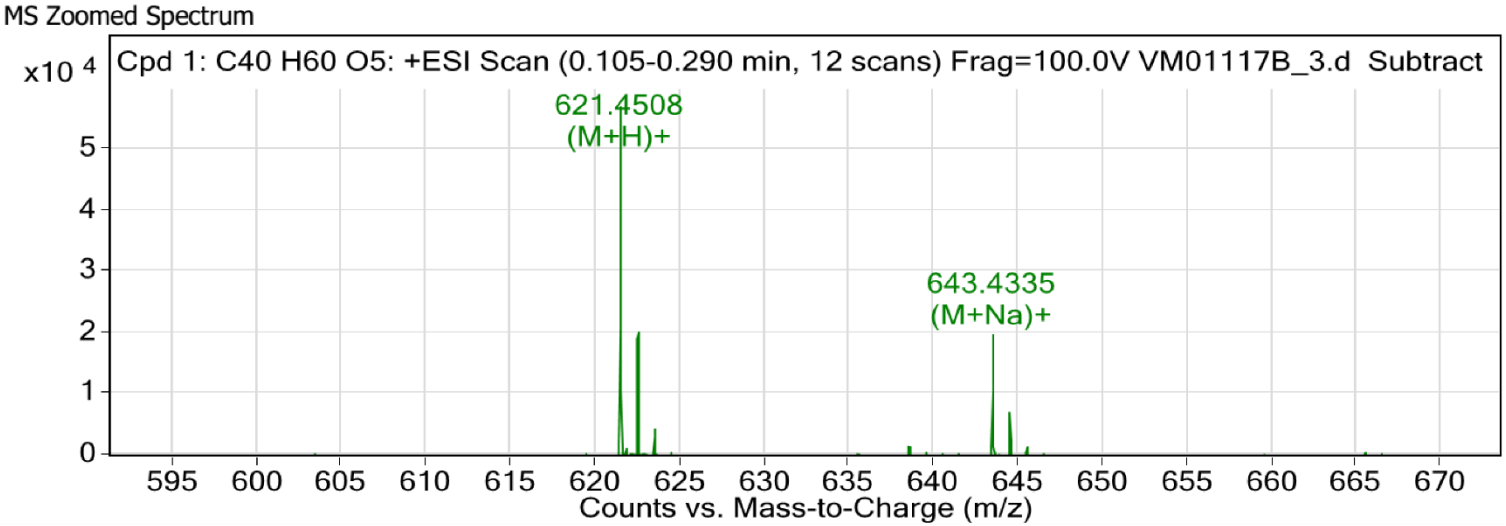


Figure S14. ROESY Spectrum of Abibalsamin D (**4**) in $CDCl_3$, 400 MHz



ABIBALSAMIN E (5)

Figure S15. HRESIMS of Abibalsamin E (**5**)



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
619.4355				315		
621.4508	621.4514	-0.9		58359	C40 H61 O5	(M+H)+

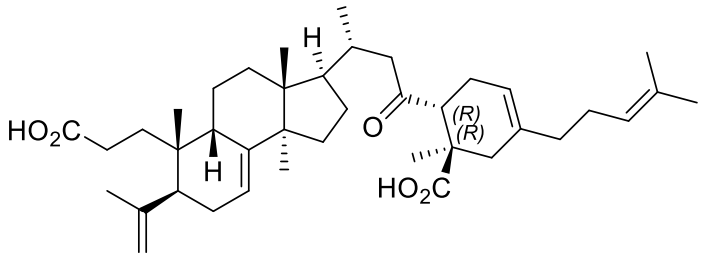


Figure S16. ^{1}H NMR Spectrum of Abibalsamin E (**5**) in $CDCl_3$, 400 MHz

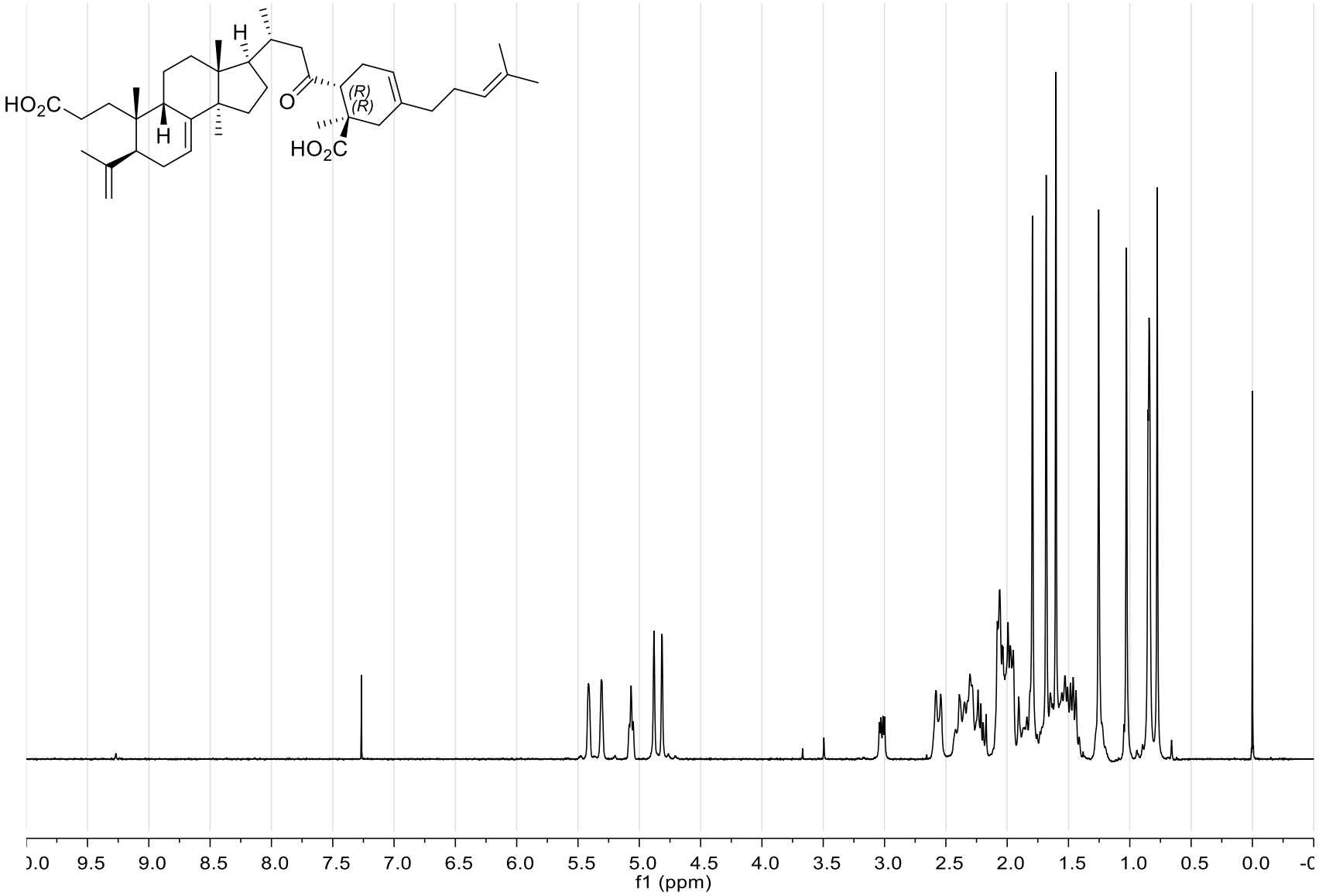


Figure S17. ^{13}C and DEPT NMR Spectra of Abibalsamin E (**5**) in $CDCl_3$, 100 MHz

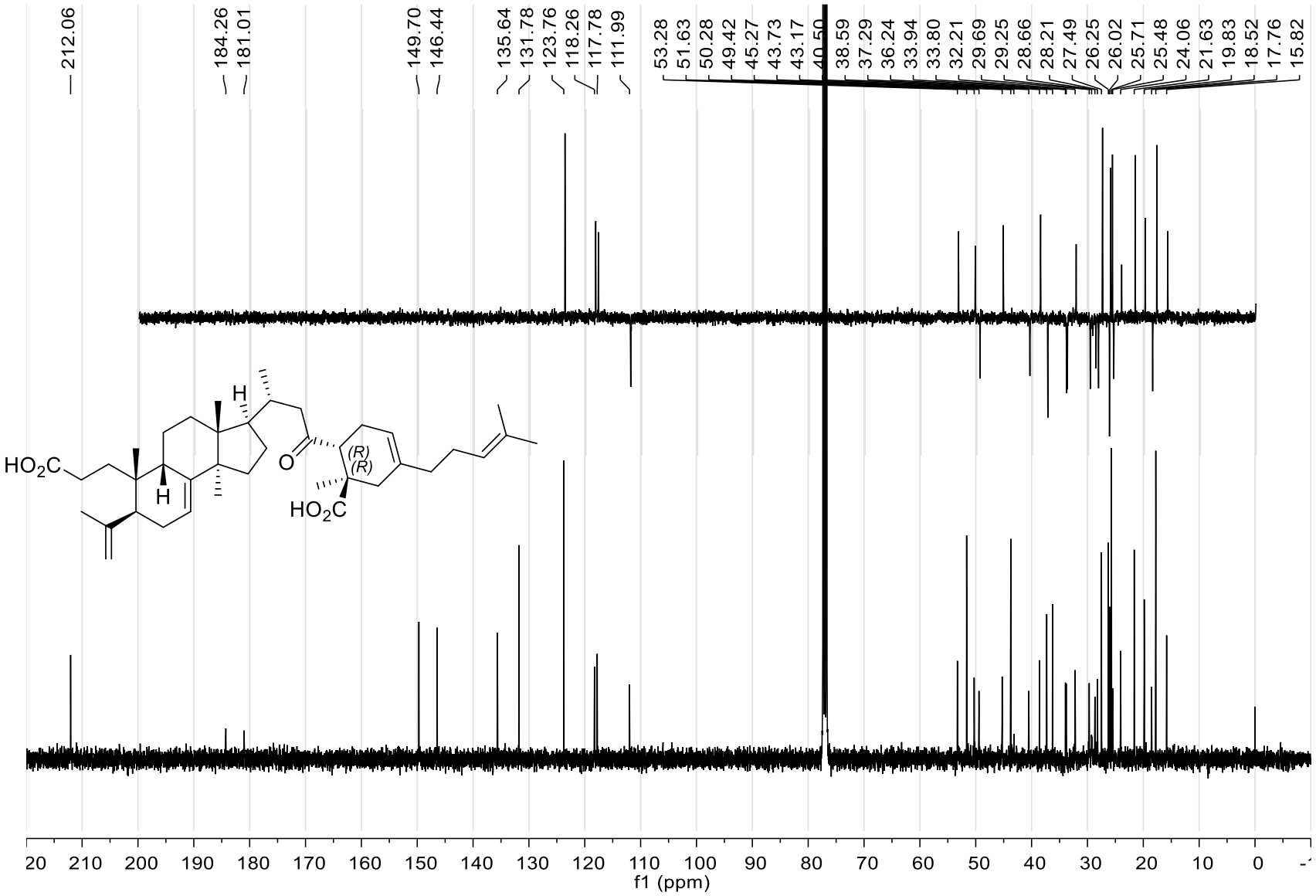


Figure S18. ^{1}H-^{1}H COSY Spectrum of Abibalsamin E (**5**) in $CDCl_3$, 400 MHz

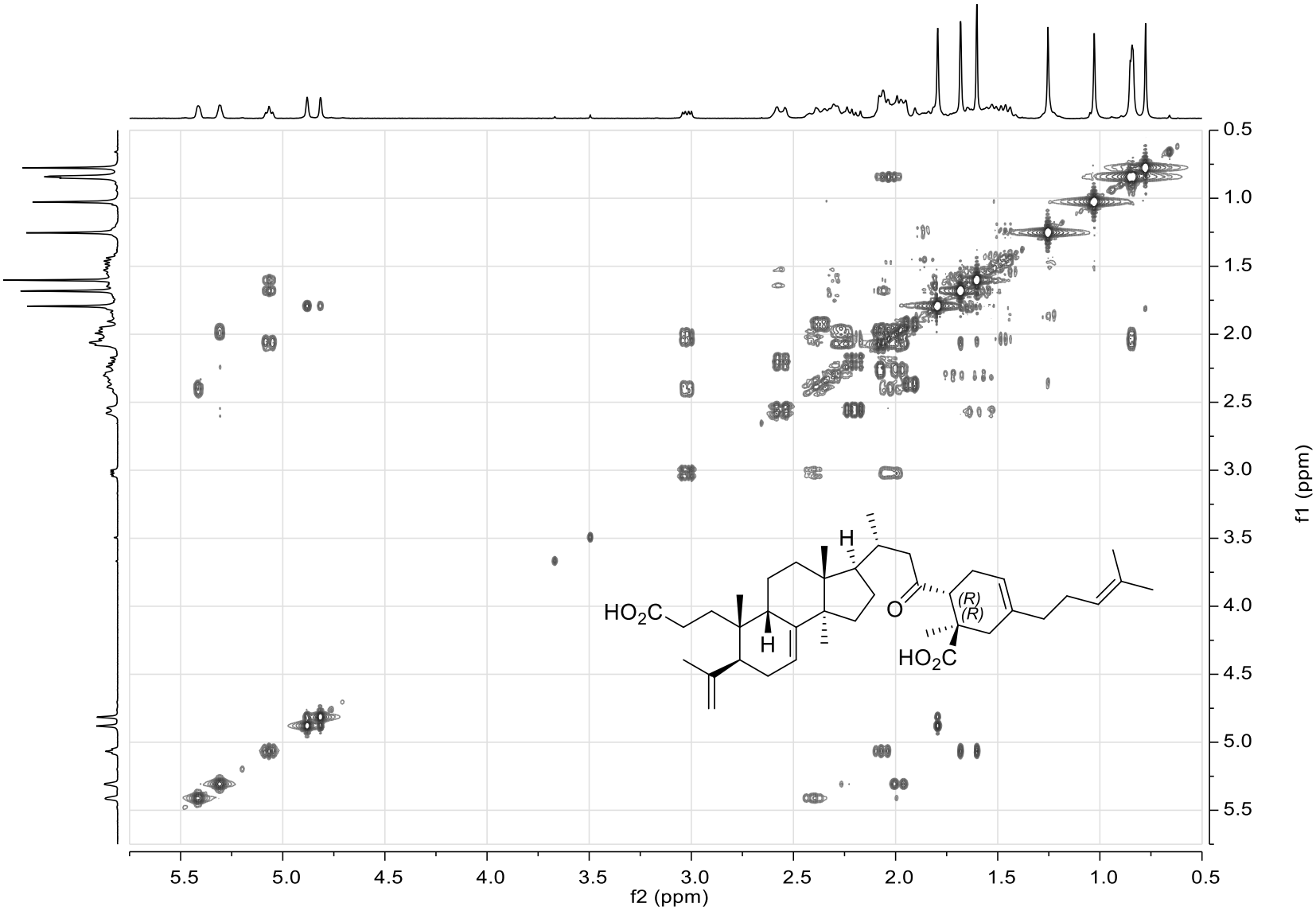


Figure S19. HSQC Spectrum of Abibalsamin E (**5**) in $CDCl_3$, 400 MHz

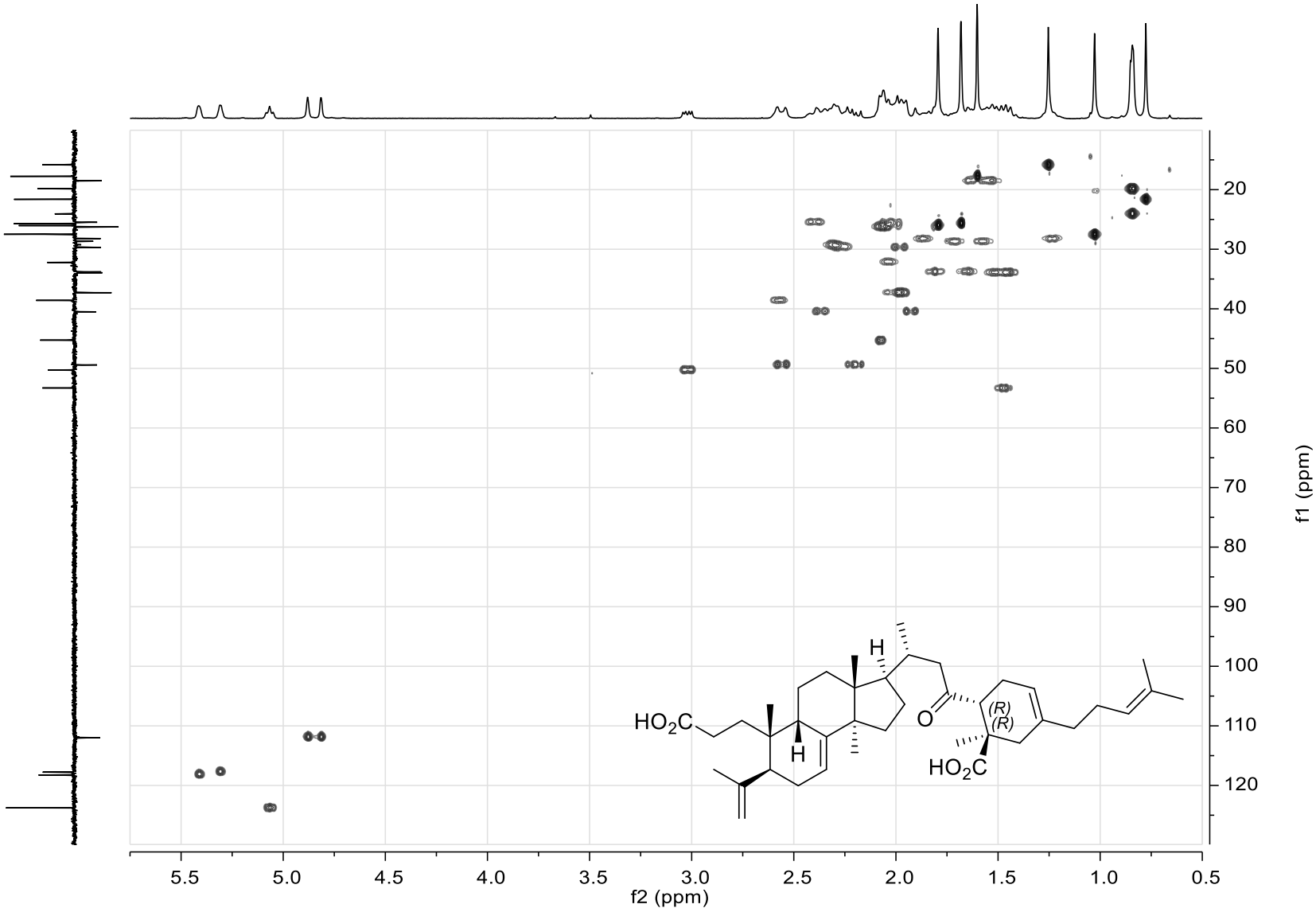


Figure S20. HMBC Spectrum of Abibalsamin E (**5**) in $CDCl_3$, 400 MHz

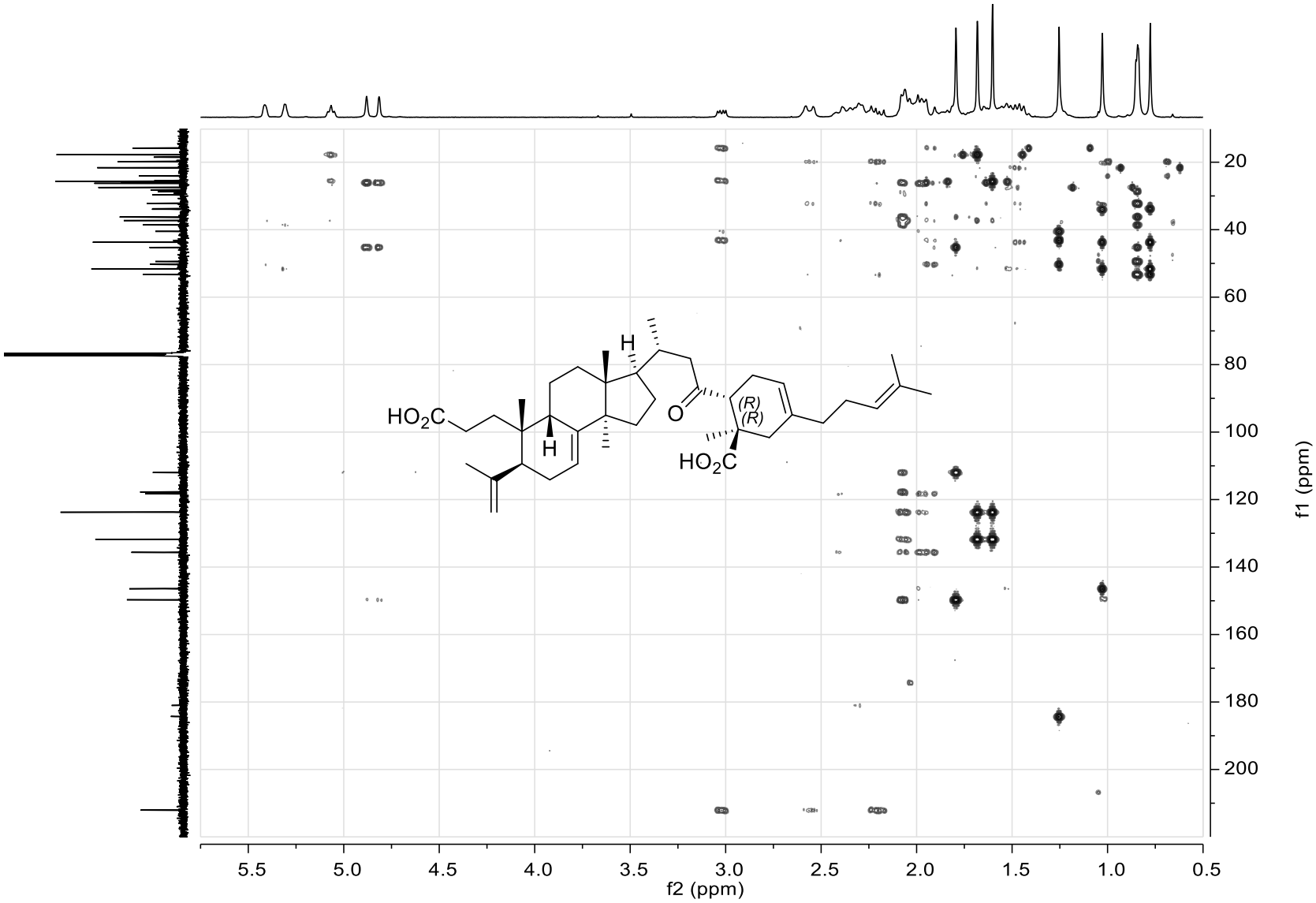
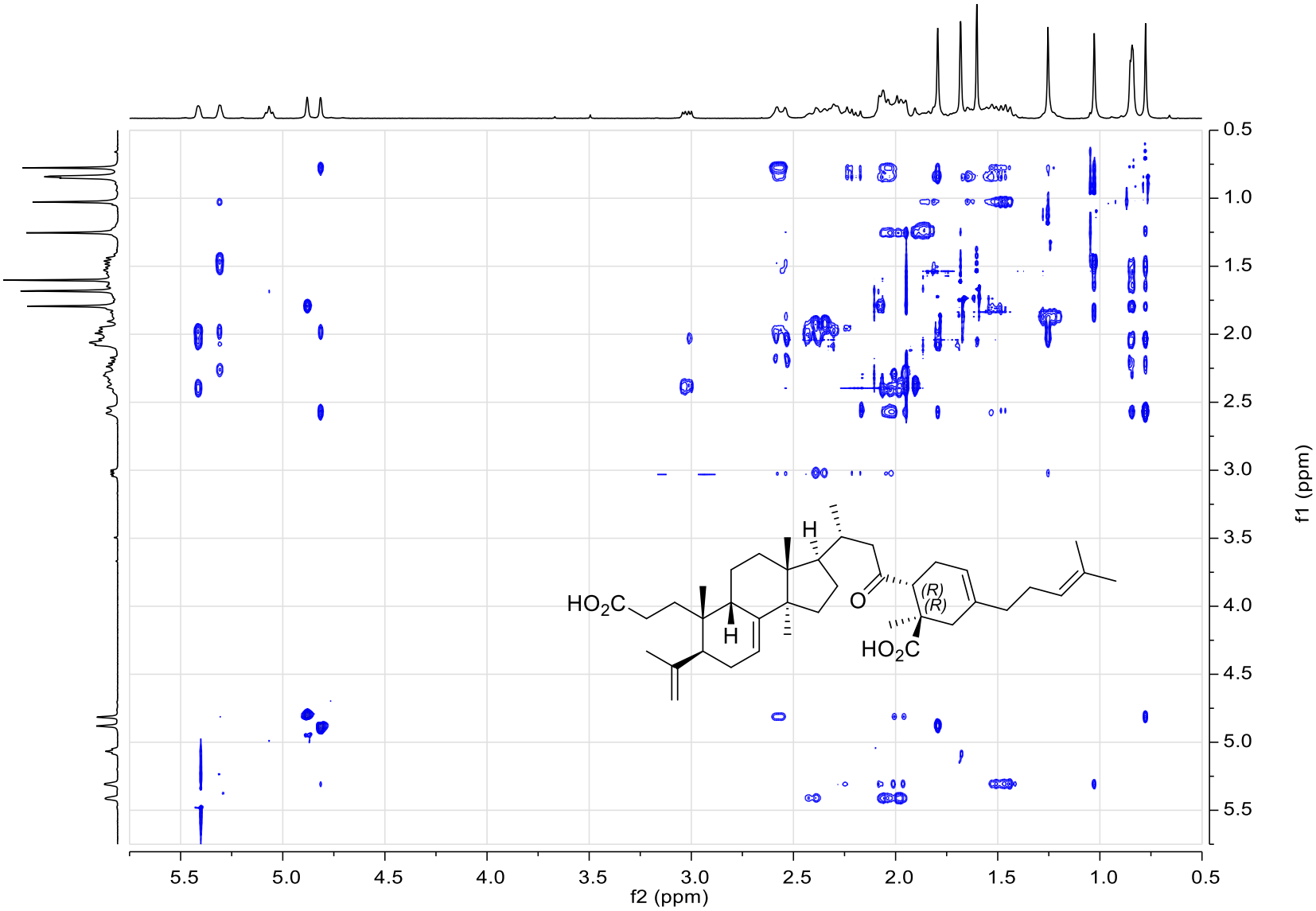
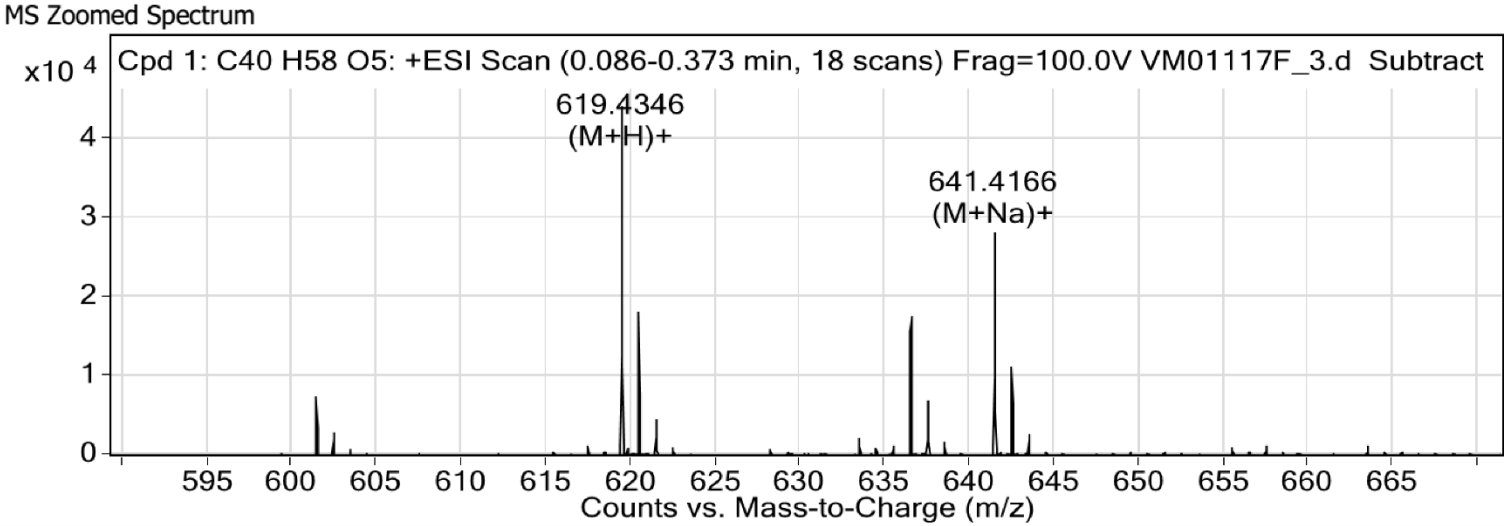


Figure S21. ROESY Spectrum of Abibalsamin E (**5**) in $CDCl_3$, 400 MHz



ABIBALSAMIN F (6)

Figure S22. HRESIMS of Abibalsamin F (**6**)



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
617.4192				1229		
618.4226				582		
619.4346	619.4357	-1.86		46962	C40 H59 O5	(M+H)+

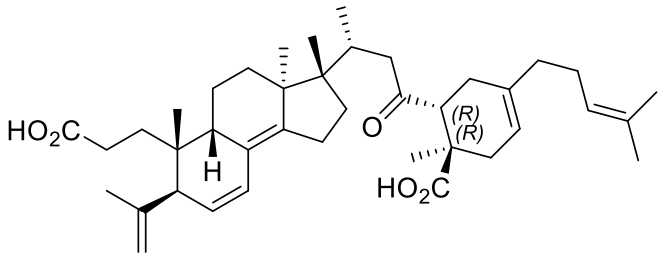


Figure S23. ^{1}H NMR Spectrum of Abibalsamin F (**6**) in $CDCl_3$, 400 MHz

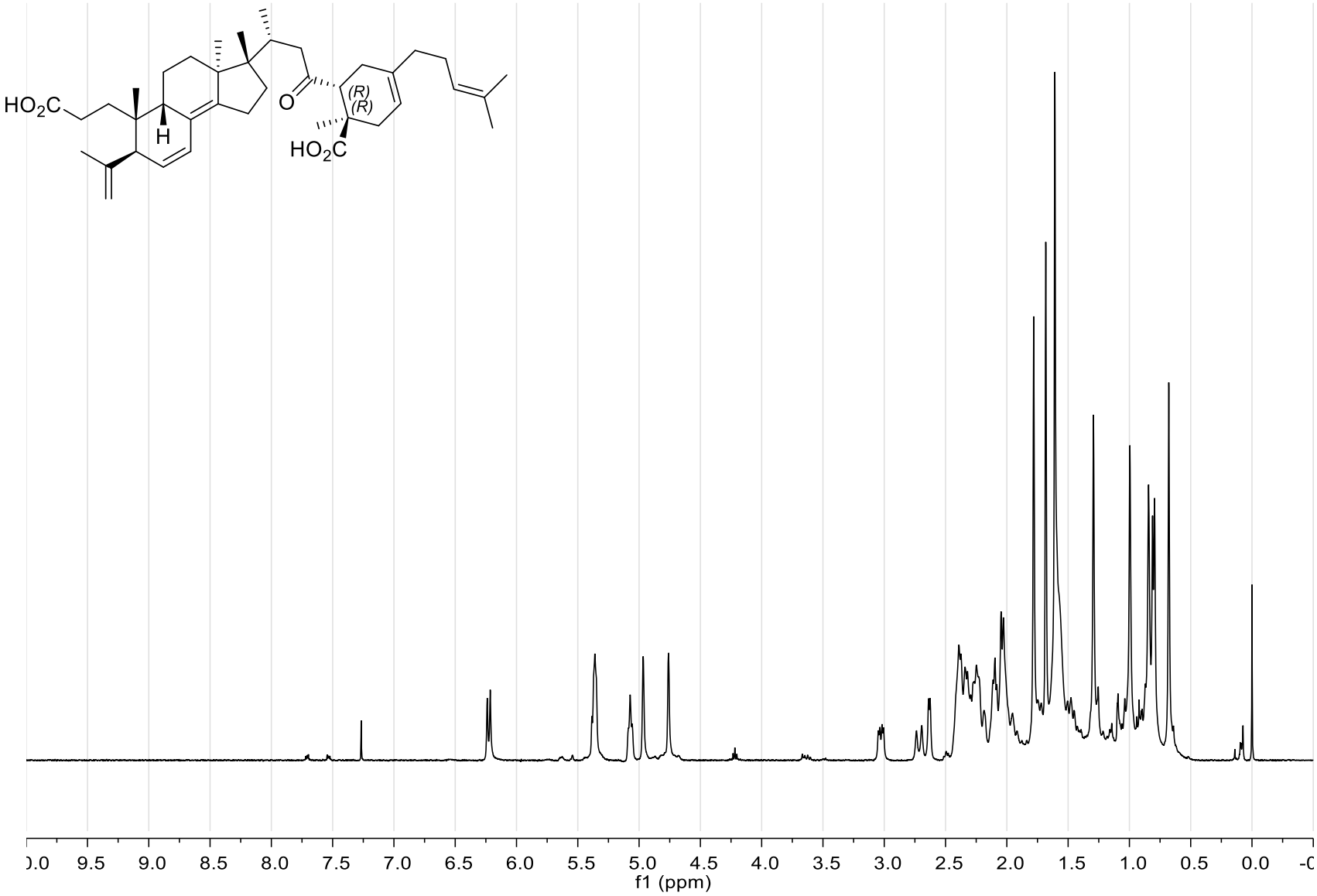


Figure S24. ^{13}C and DEPT NMR Spectra of Abibalsamin F (**6**) in $CDCl_3$, 100 MHz

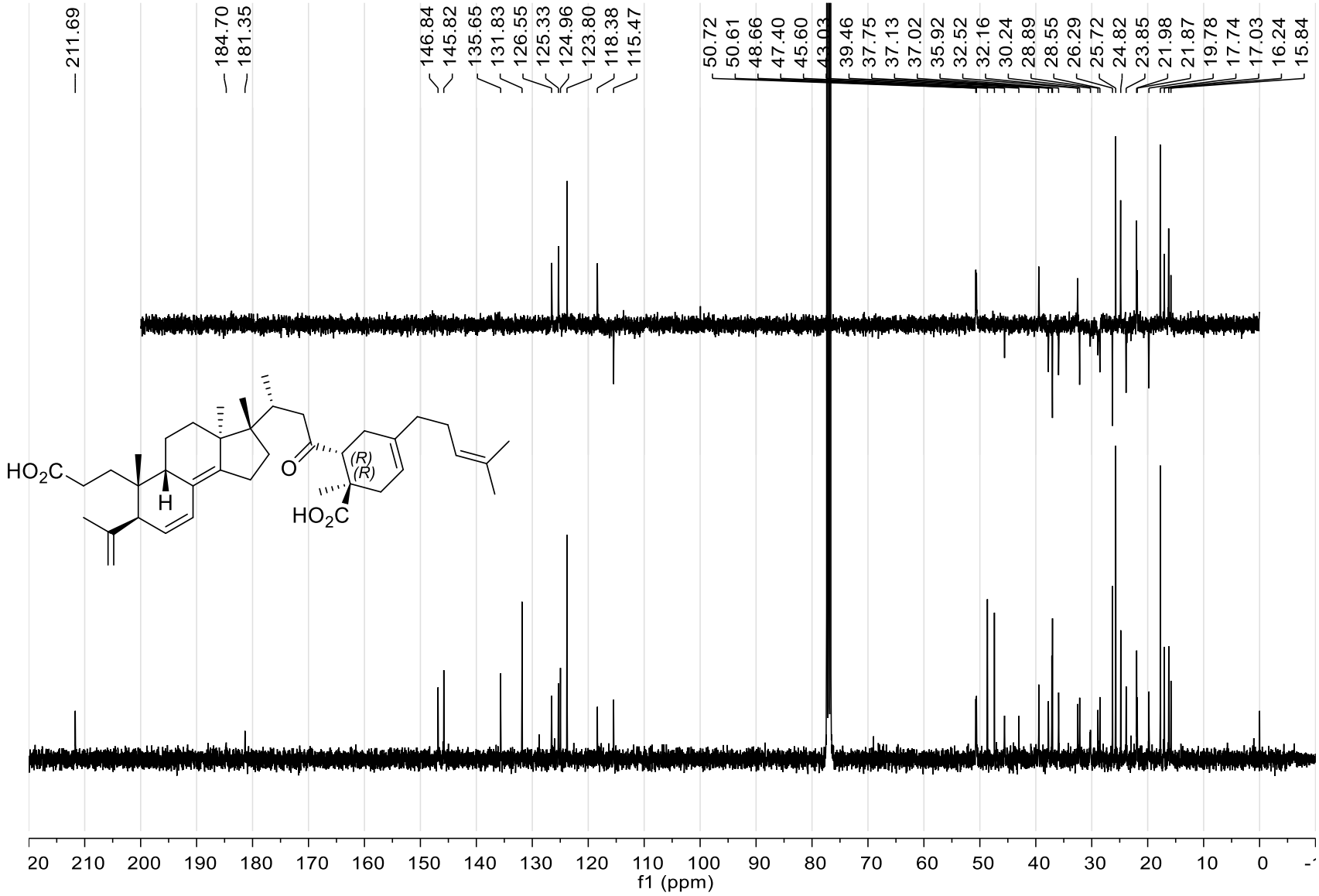


Figure S25. ^{1}H-^{1}H COSY Spectrum of Abibalsamin F (**6**) in $CDCl_3$, 400 MHz

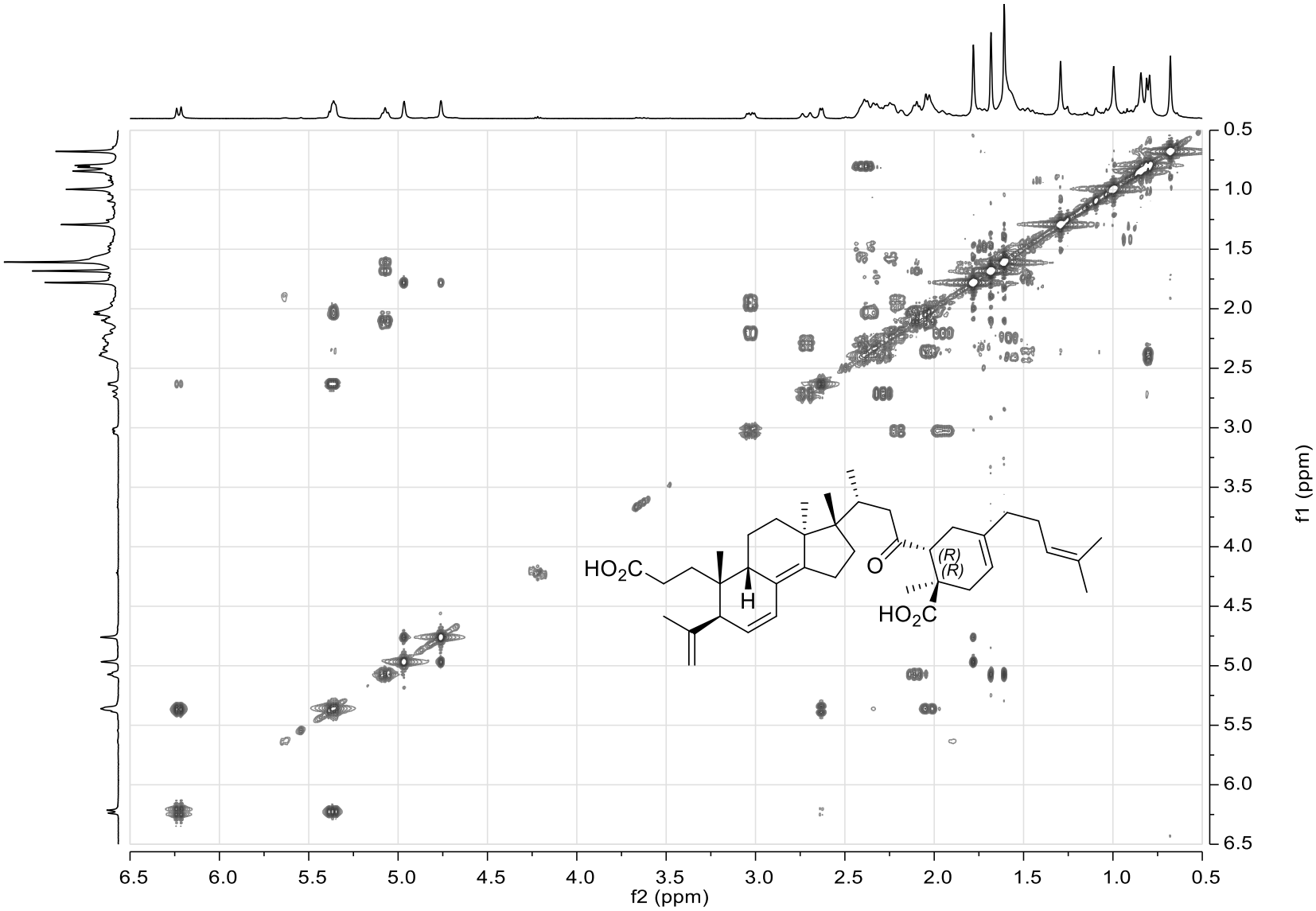


Figure S26. HSQC Spectrum of Abibalsamin F (**6**) in $CDCl_3$, 400 MHz

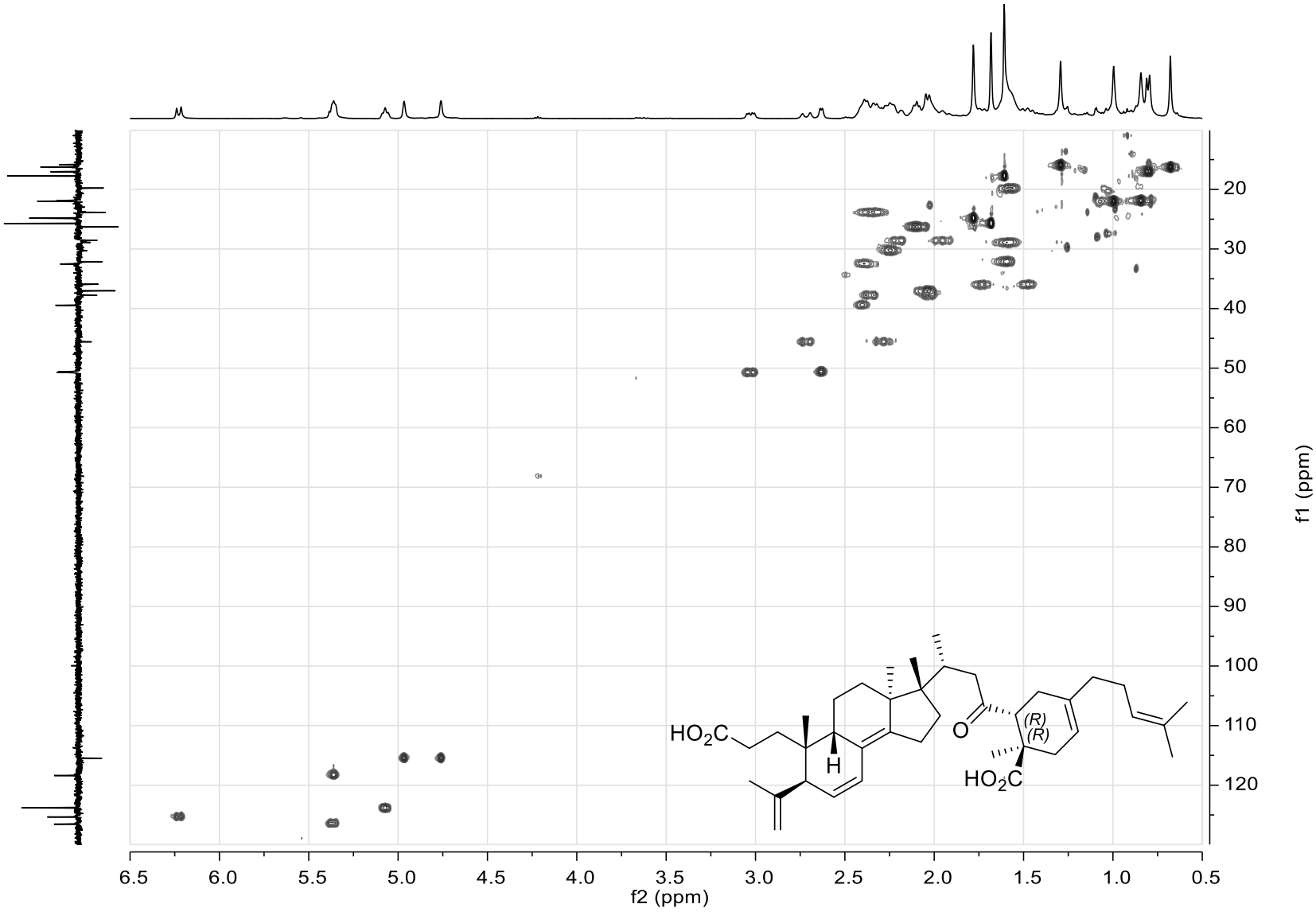


Figure S27. HMBC Spectrum of Abibalsamin F (**6**) in $CDCl_3$, 400 MHz

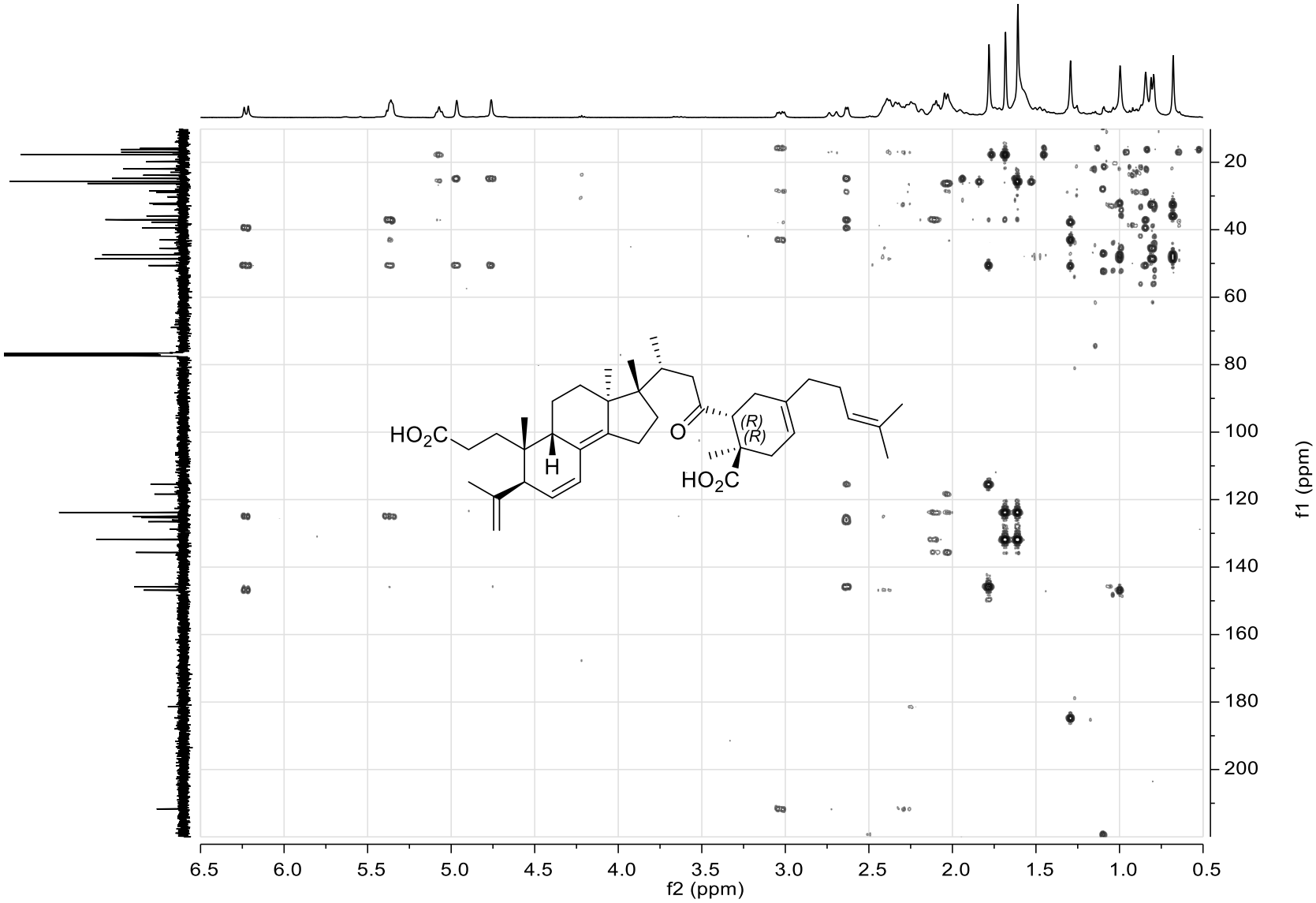
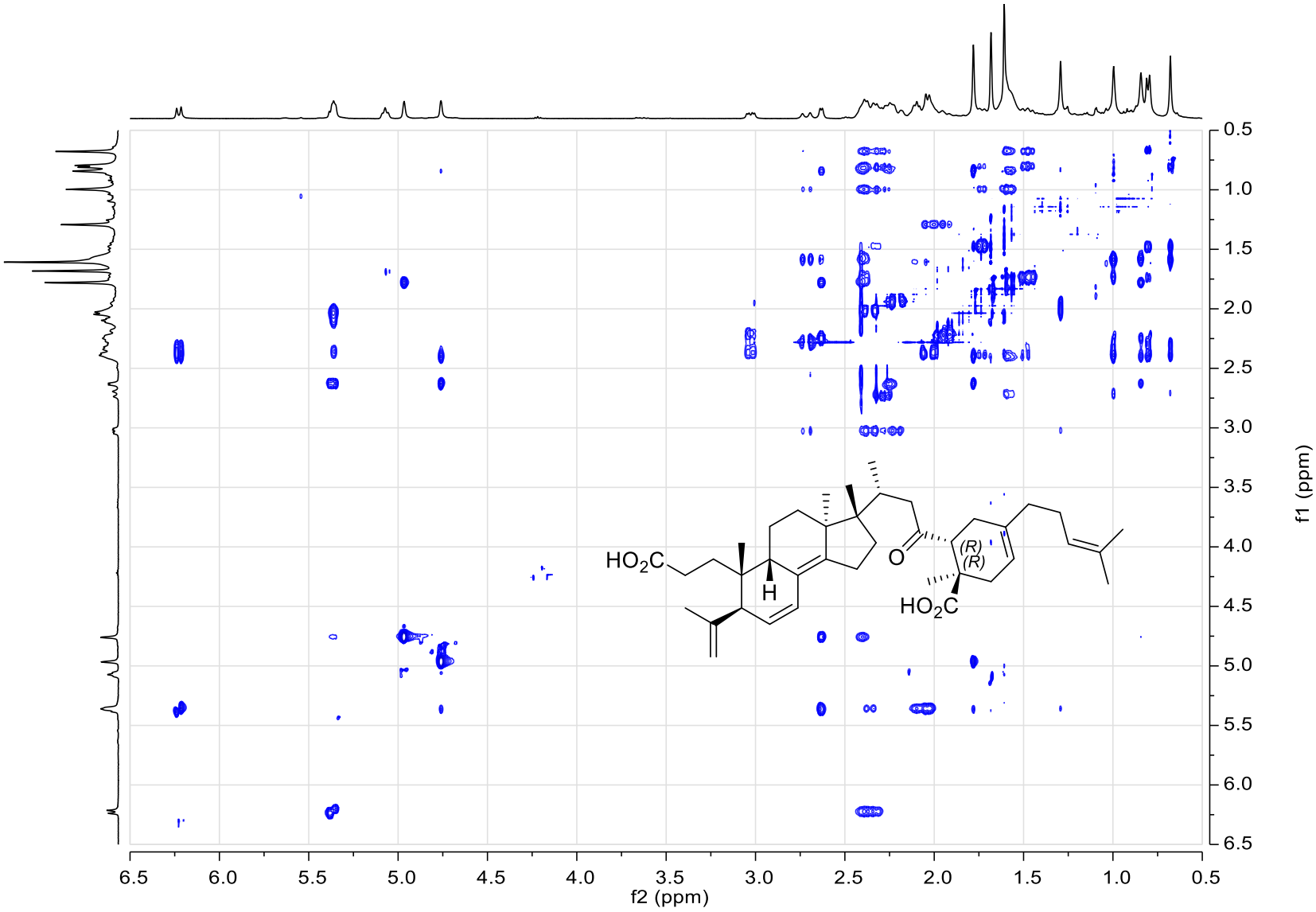
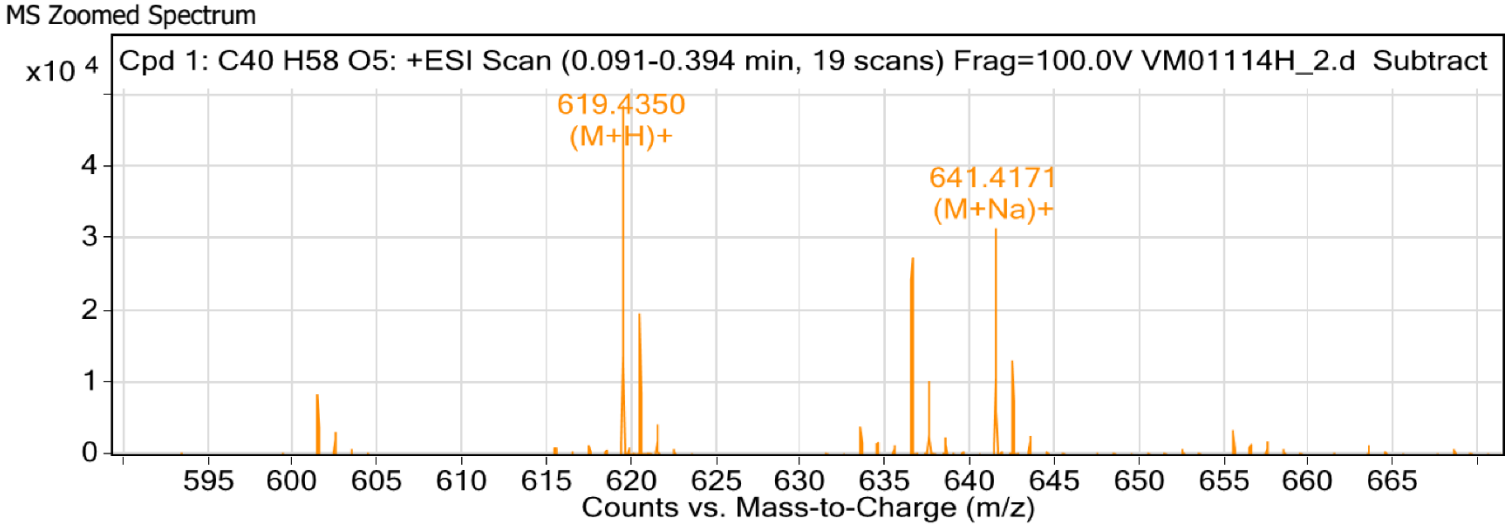


Figure S28. ROESY Spectrum of Abibalsamin F (**6**) in $CDCl_3$, 400 MHz



ABIBALSAMIN G (7)

Figure S29. HRESIMS of Abibalsamin G (7)



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
615.4349				1000		
617.4207				1548		
618.4275				794		
619.435	619.4357	-1.18		51495	C40 H59 O5	(M+H)+

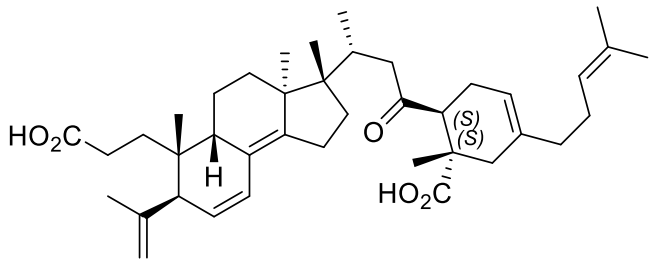


Figure S30. ^{1}H NMR Spectrum of Abibalsamin G (**7**) in $CDCl_3$, 400 MHz

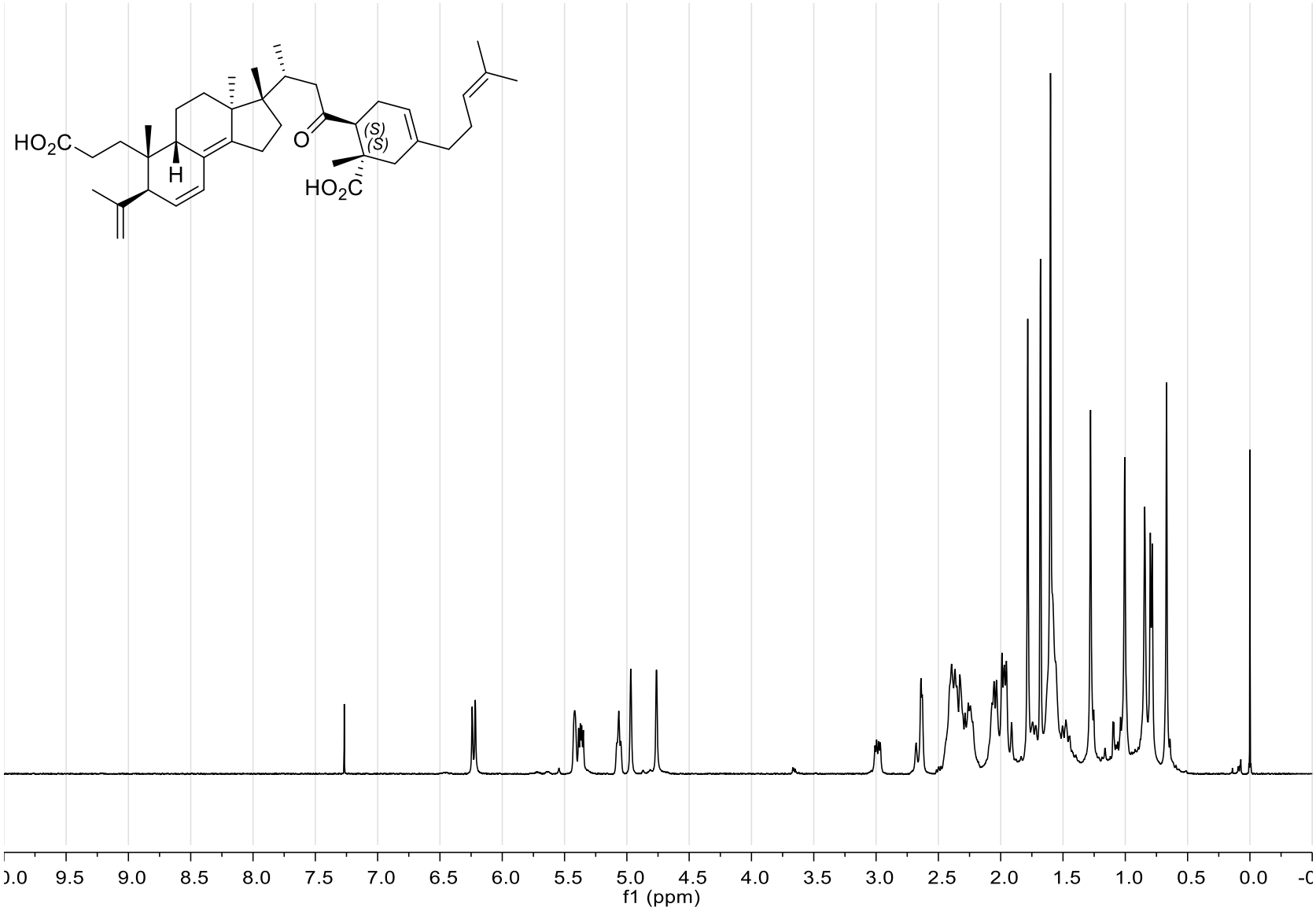


Figure S31. ^{13}C and DEPT NMR Spectra of Abibalsamin G (**7**) in $CDCl_3$, 100 MHz

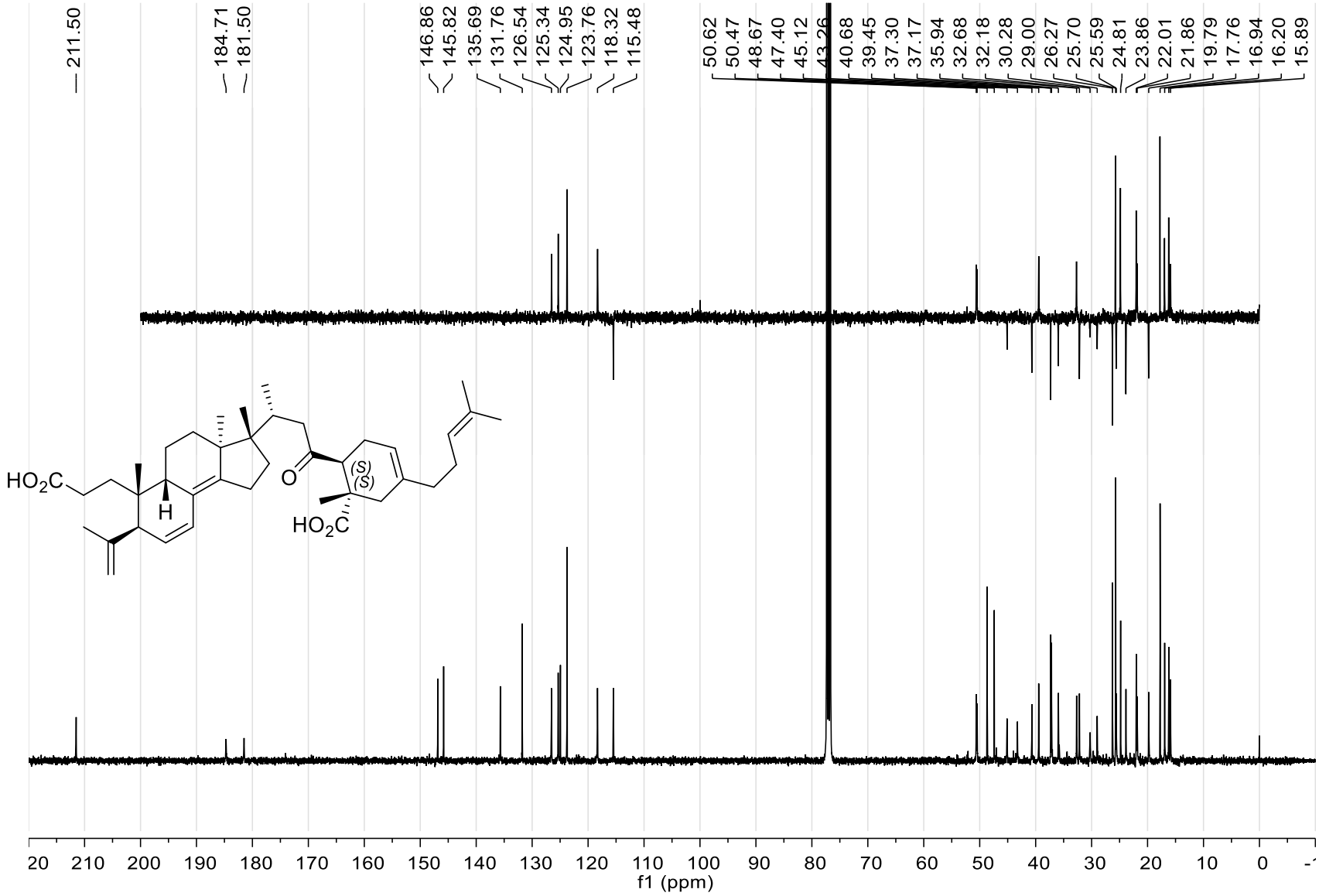


Figure S32. ^{1}H-^{1}H COSY Spectrum of Abibalsamin G (**7**) in $CDCl_3$, 400 MHz

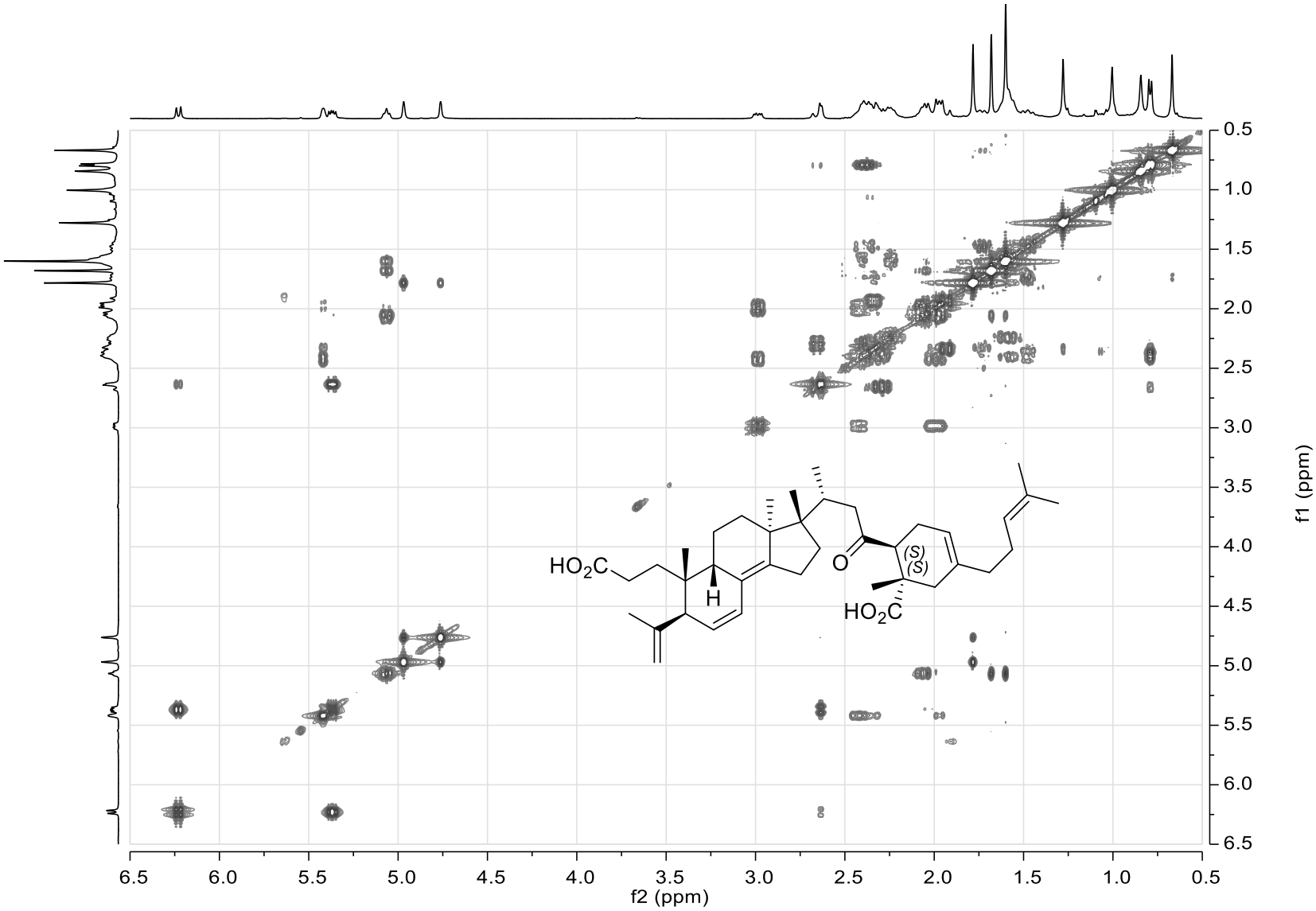


Figure S33. HSQC Spectrum of Abibalsamin G (**7**) in $CDCl_3$, 400 MHz

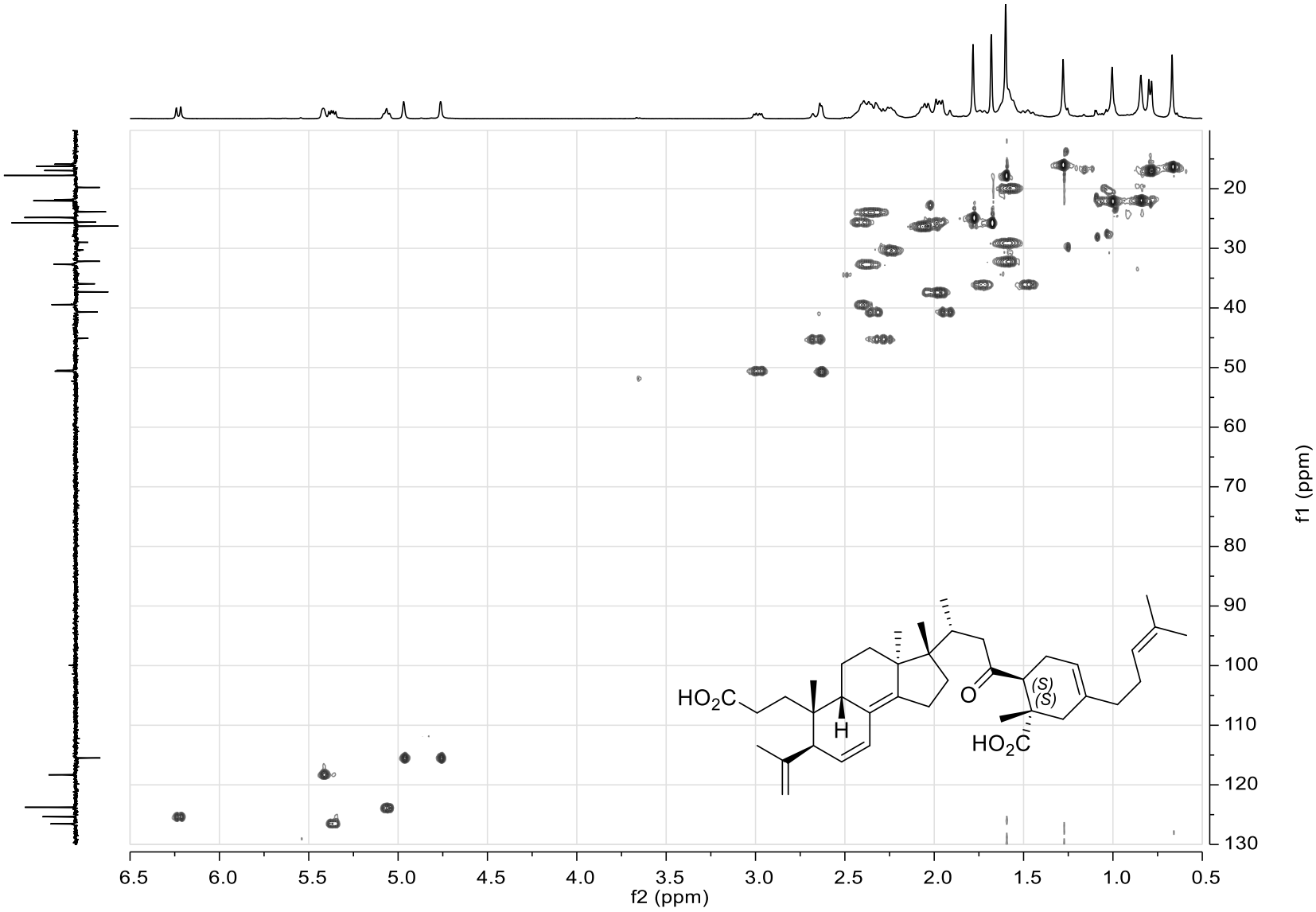


Figure S34. HMBC Spectrum of Abibalsamin G (**7**) in $CDCl_3$, 400 MHz

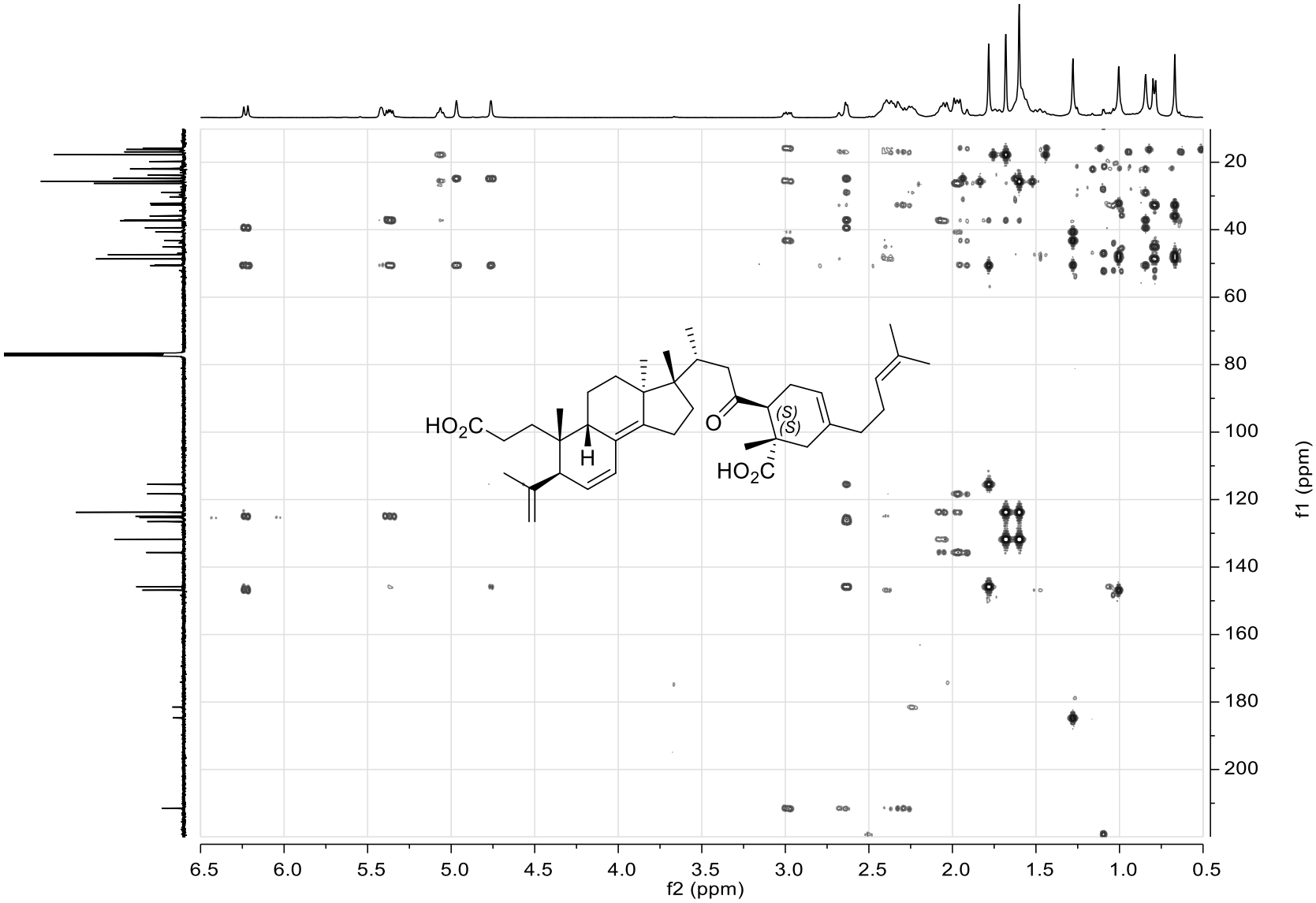
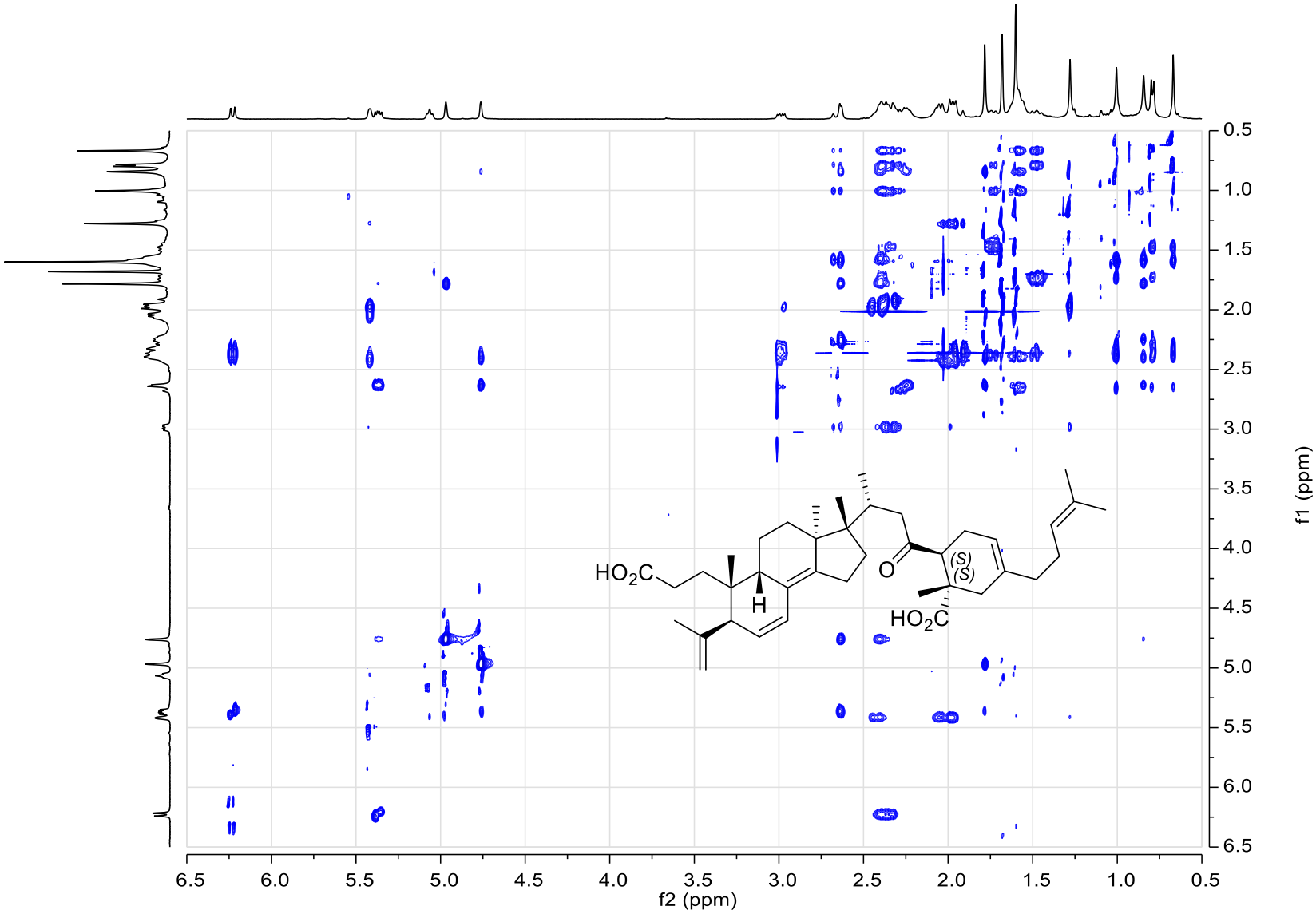
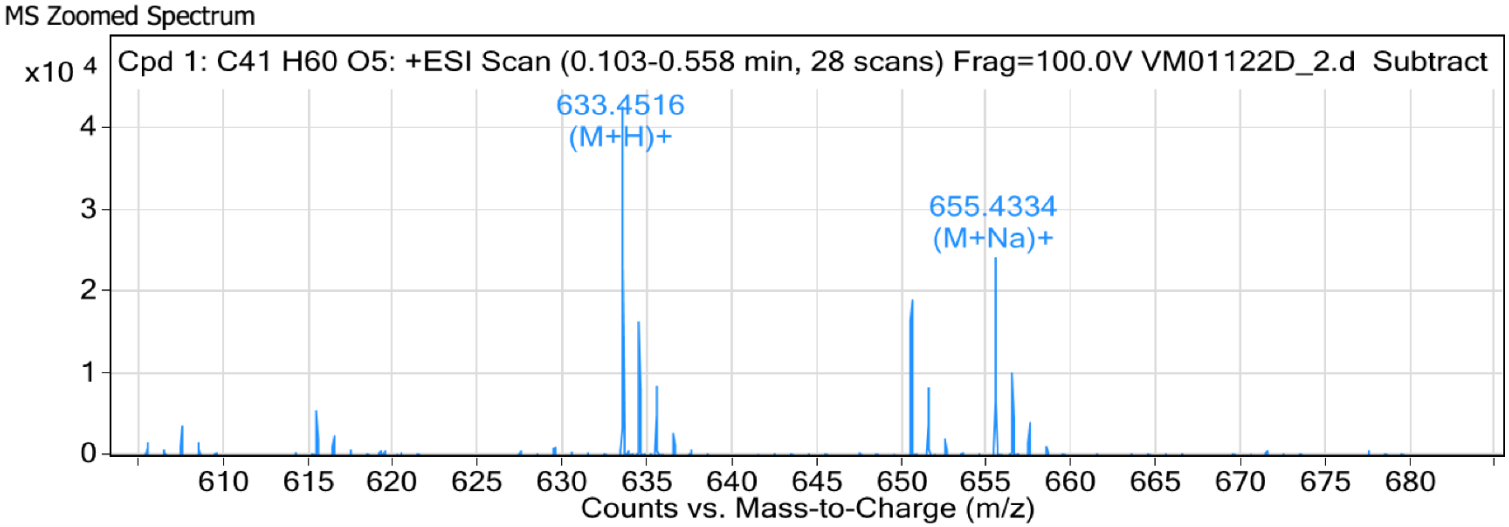


Figure S35. ROESY Spectrum of Abibalsamin G (**7**) in $CDCl_3$, 400 MHz



ABIBALSAMIN H (8)

Figure S36. HRESIMS of Abibalsamin H (**8**)



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
279.0931				47273		
279.2973				1875		
280.0972				7555		
633.4516	633.4514	0.32	1	42568	C41 H61 O5	(M+H)+

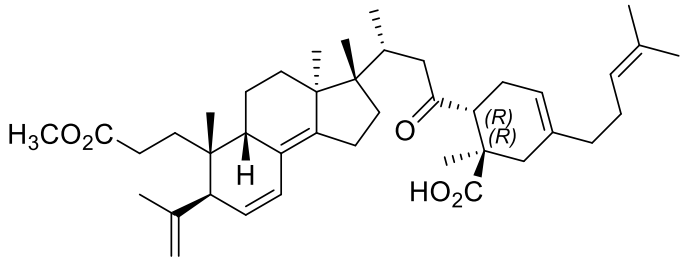


Figure S37. ^{1}H NMR Spectrum of Abibalsamin H (**8**) in $CDCl_3$, 400 MHz

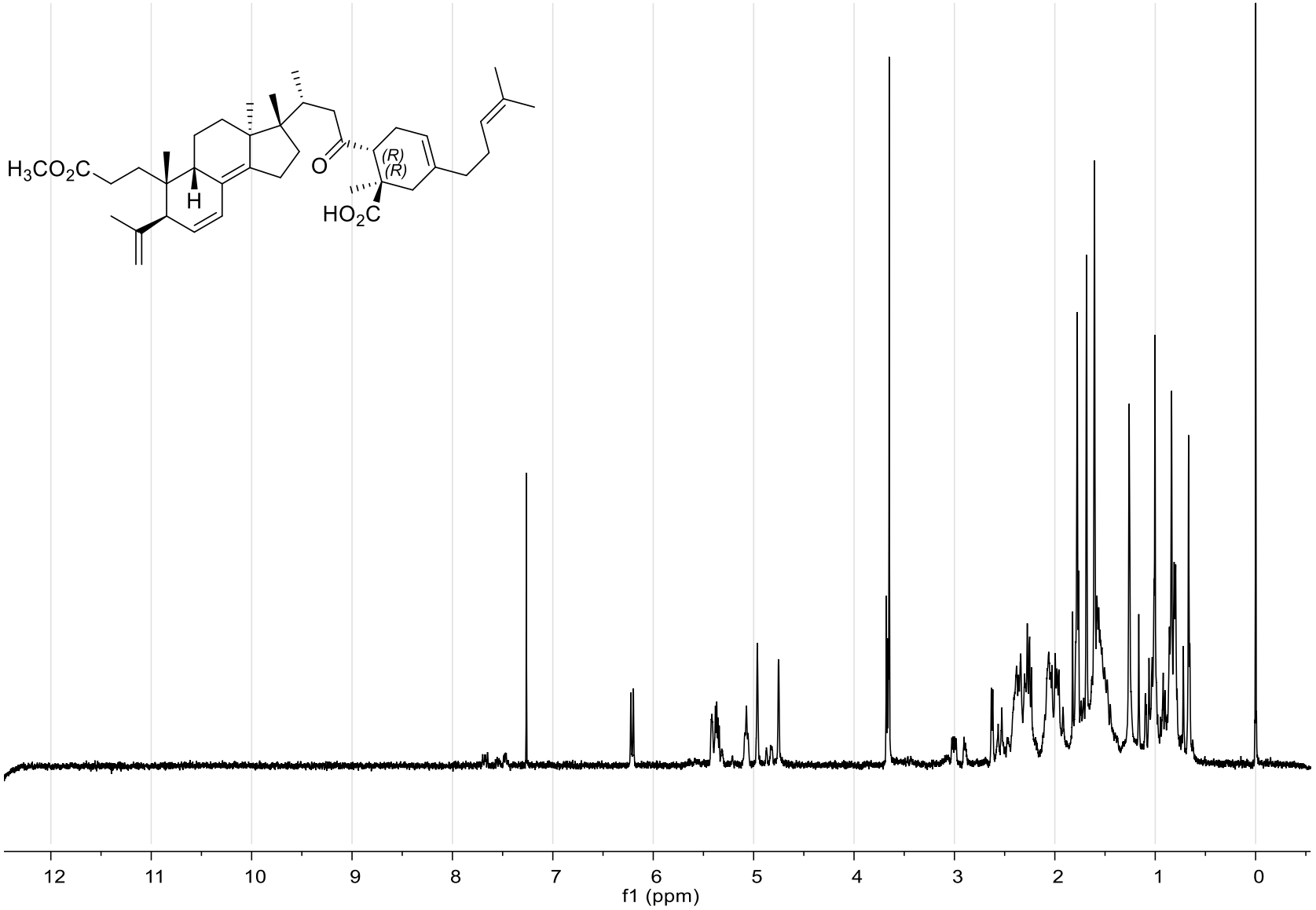


Figure S38. ^{13}C and DEPT NMR Spectra of Abibalsamin H (**8**) in $CDCl_3$, 100 MHz

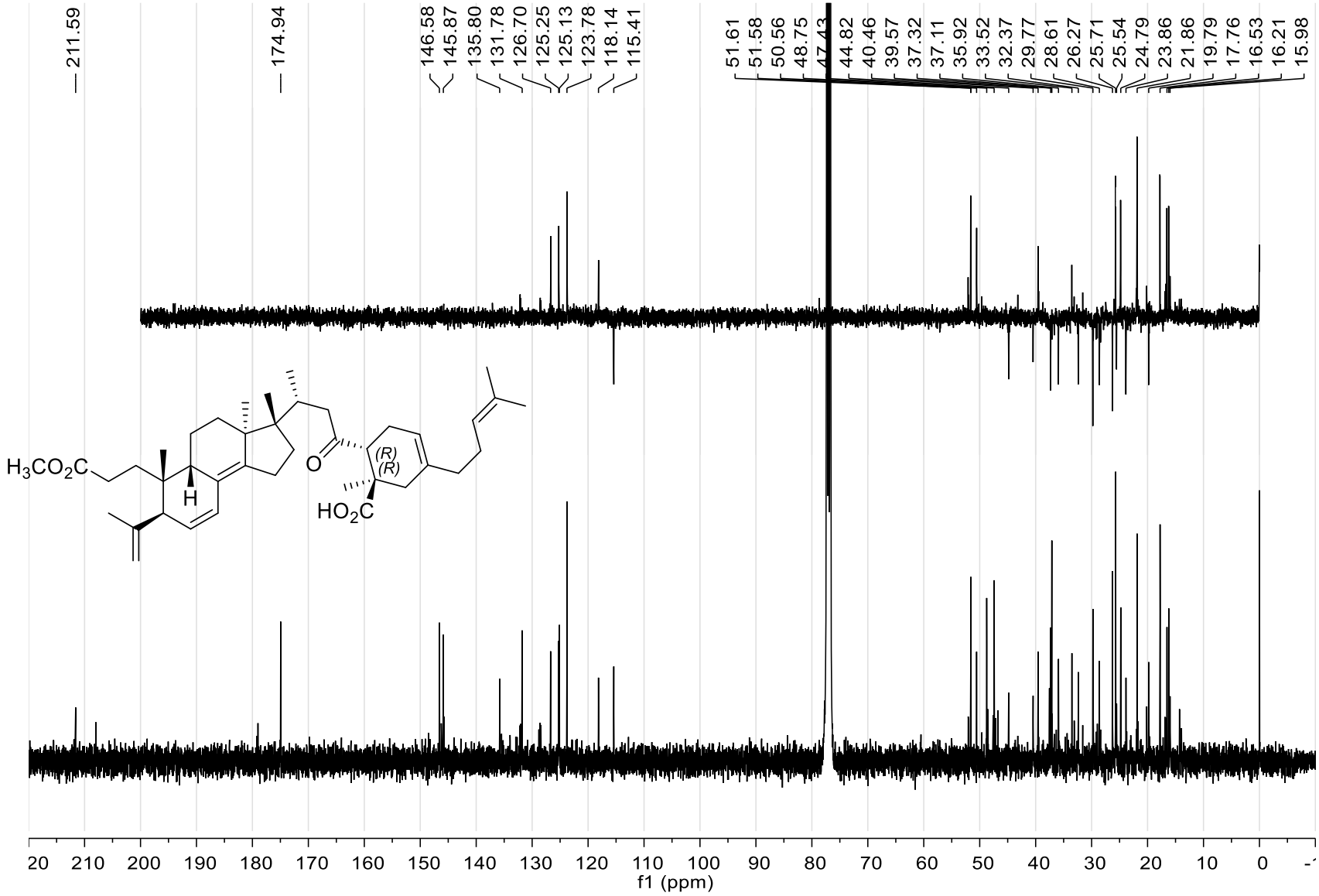


Figure S39. ^{1}H-^{1}H COSY Spectrum of Abibalsamin H (**8**) in $CDCl_3$, 400 MHz

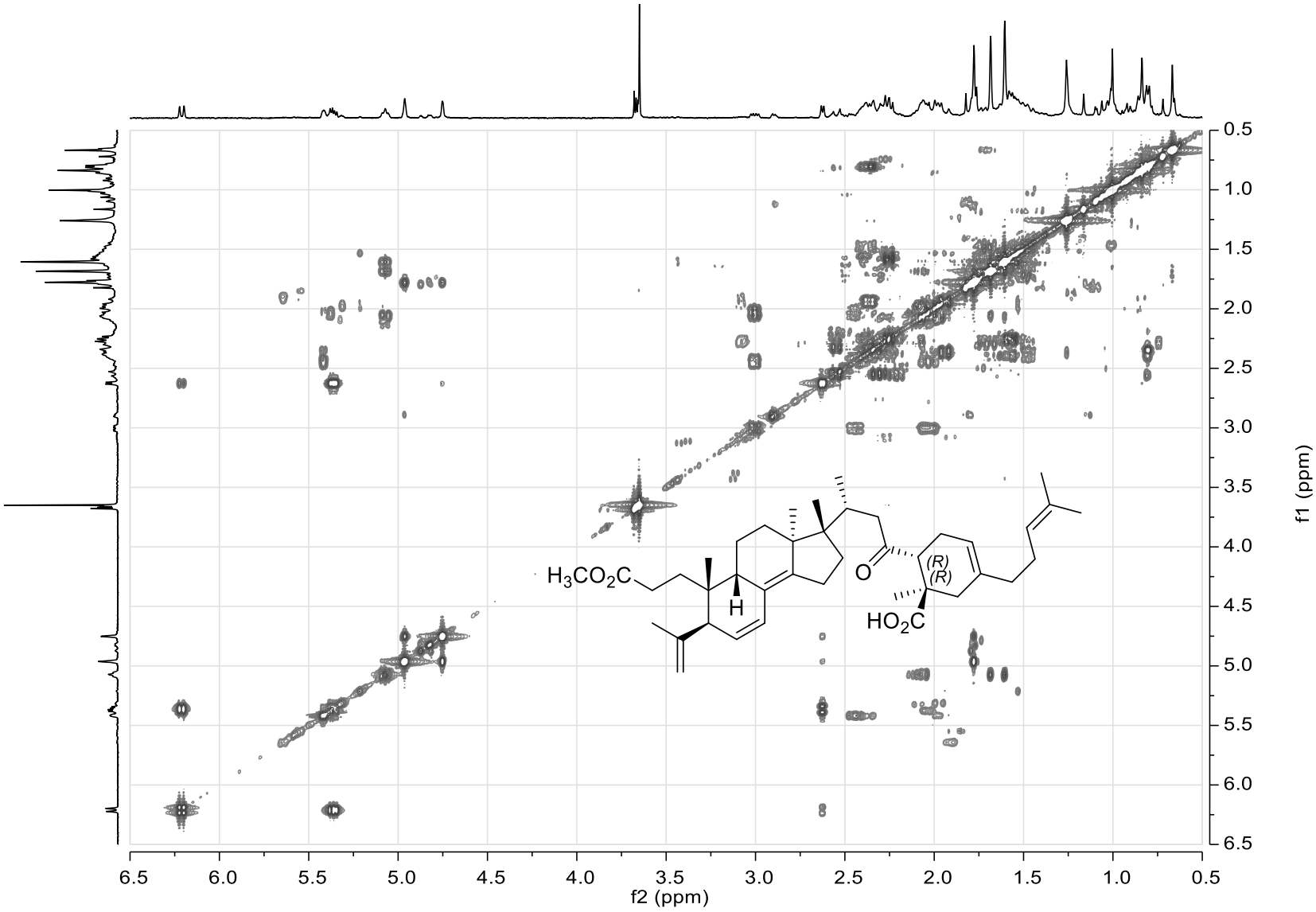


Figure S40. HSQC Spectrum of Abibalsamin H (**8**) in $CDCl_3$, 400 MHz

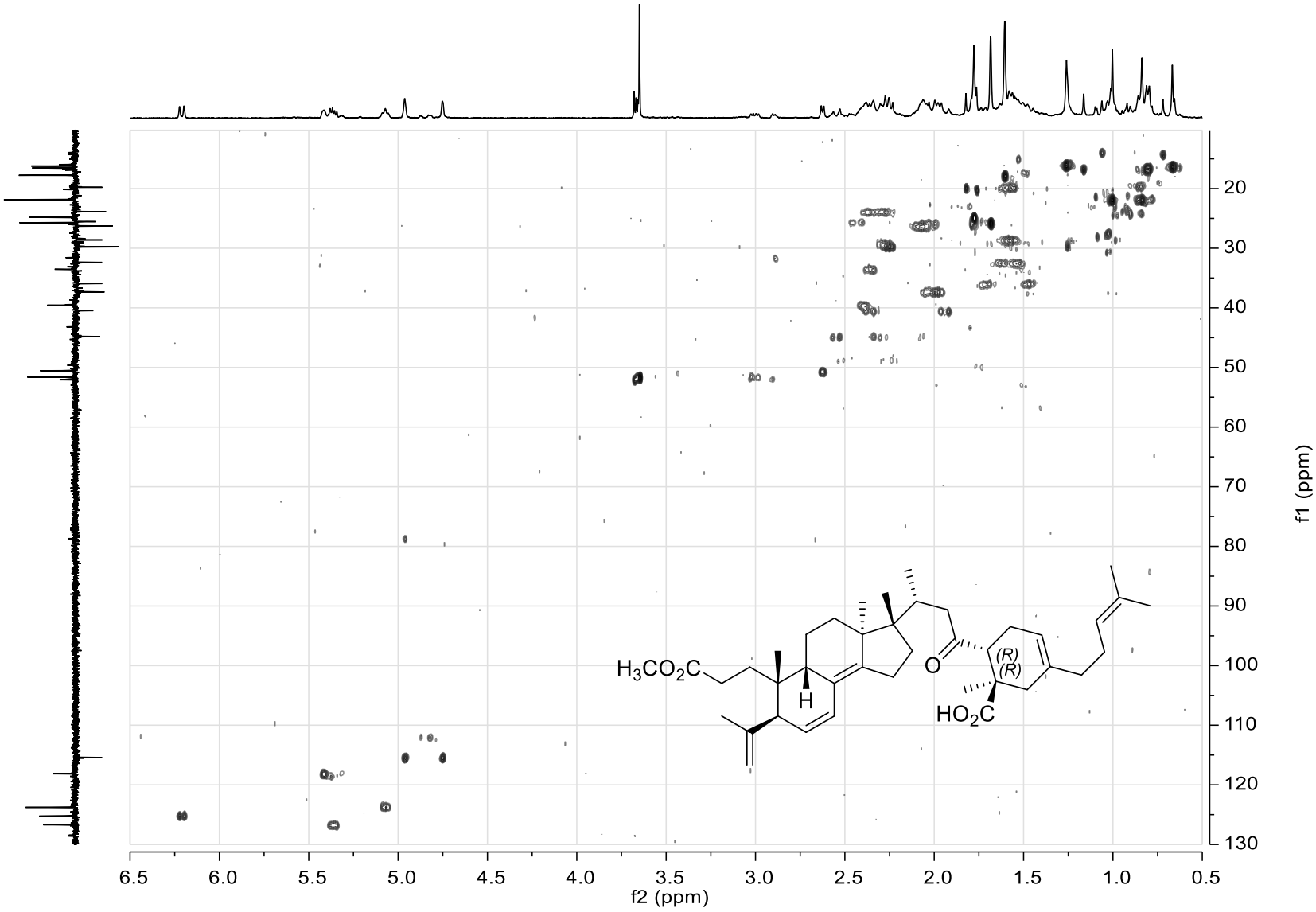


Figure S41. HMBC Spectrum of Abibalsamin H (**8**) in $CDCl_3$, 400 MHz

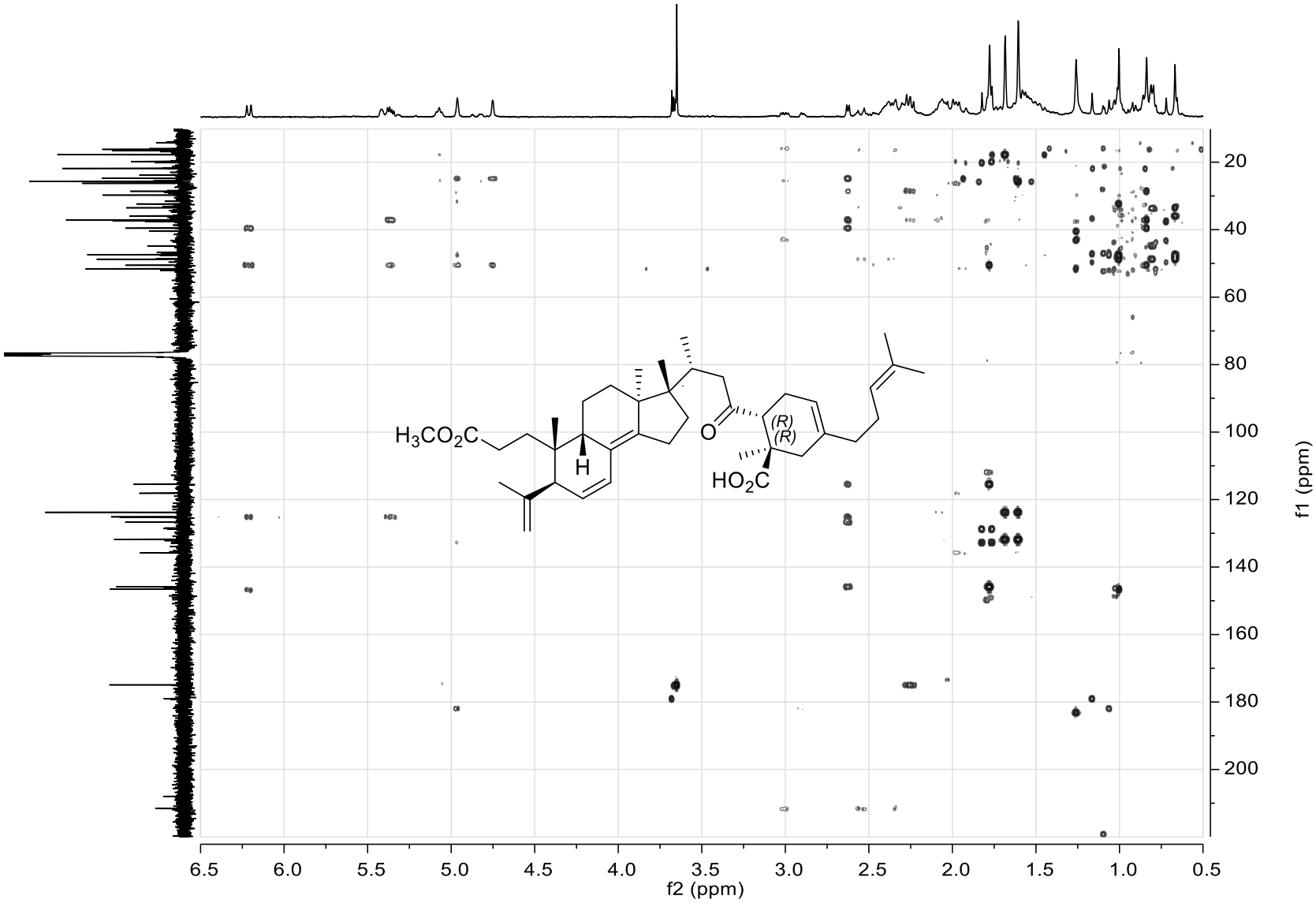
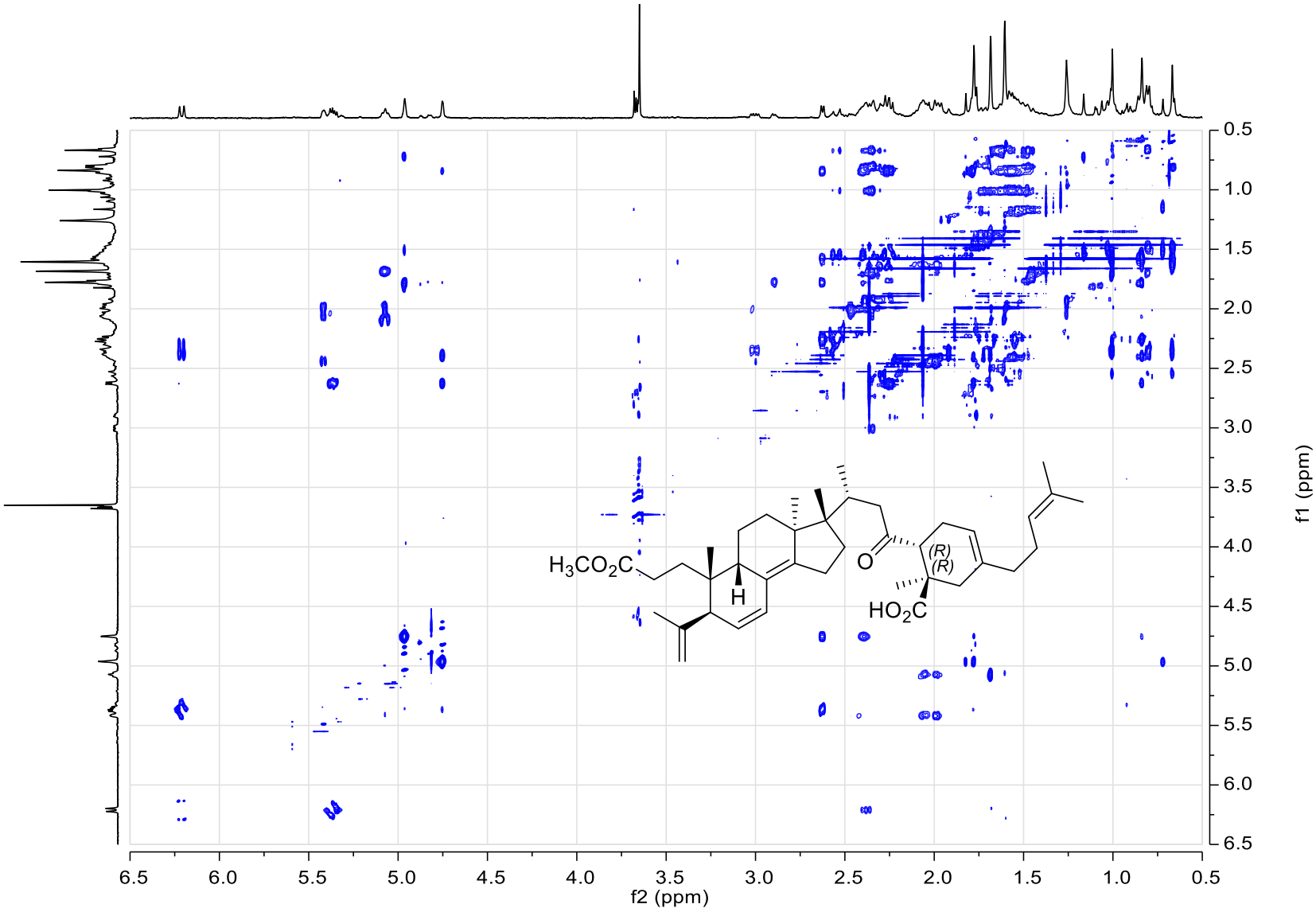
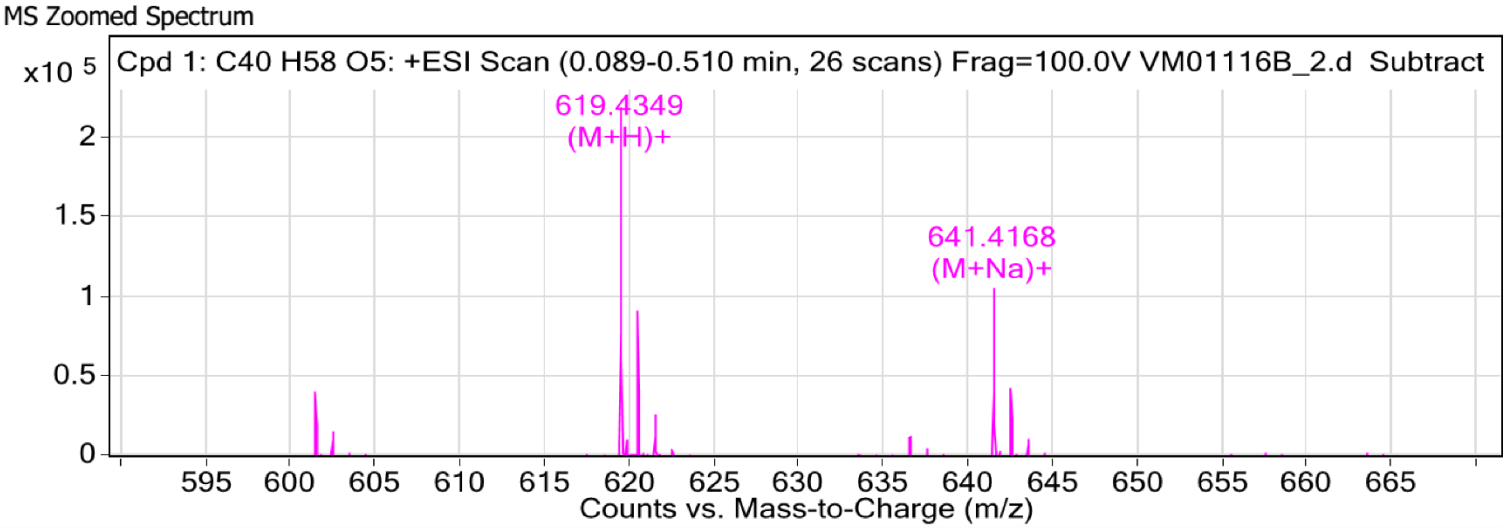


Figure S42. ROESY Spectrum of Abibalsamin H (**8**) in $CDCl_3$, 400 MHz



ABIBALSAMIN I (9)

Figure S43. HRESIMS of Abibalsamin I (**9**)



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
619.4349	619.4357	-1.22		231036	C40 H59 O5	(M+H)+
619.7407				10997		
620.4388	620.4391	-0.44		92512	C40 H59 O5	(M+H)+

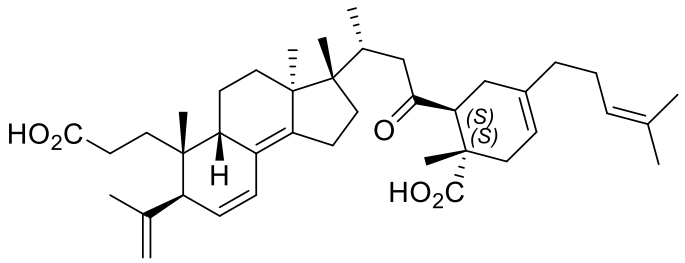


Figure S44. ^{1}H NMR Spectrum of Abibalsamin I (**9**) in $CDCl_3$, 400 MHz

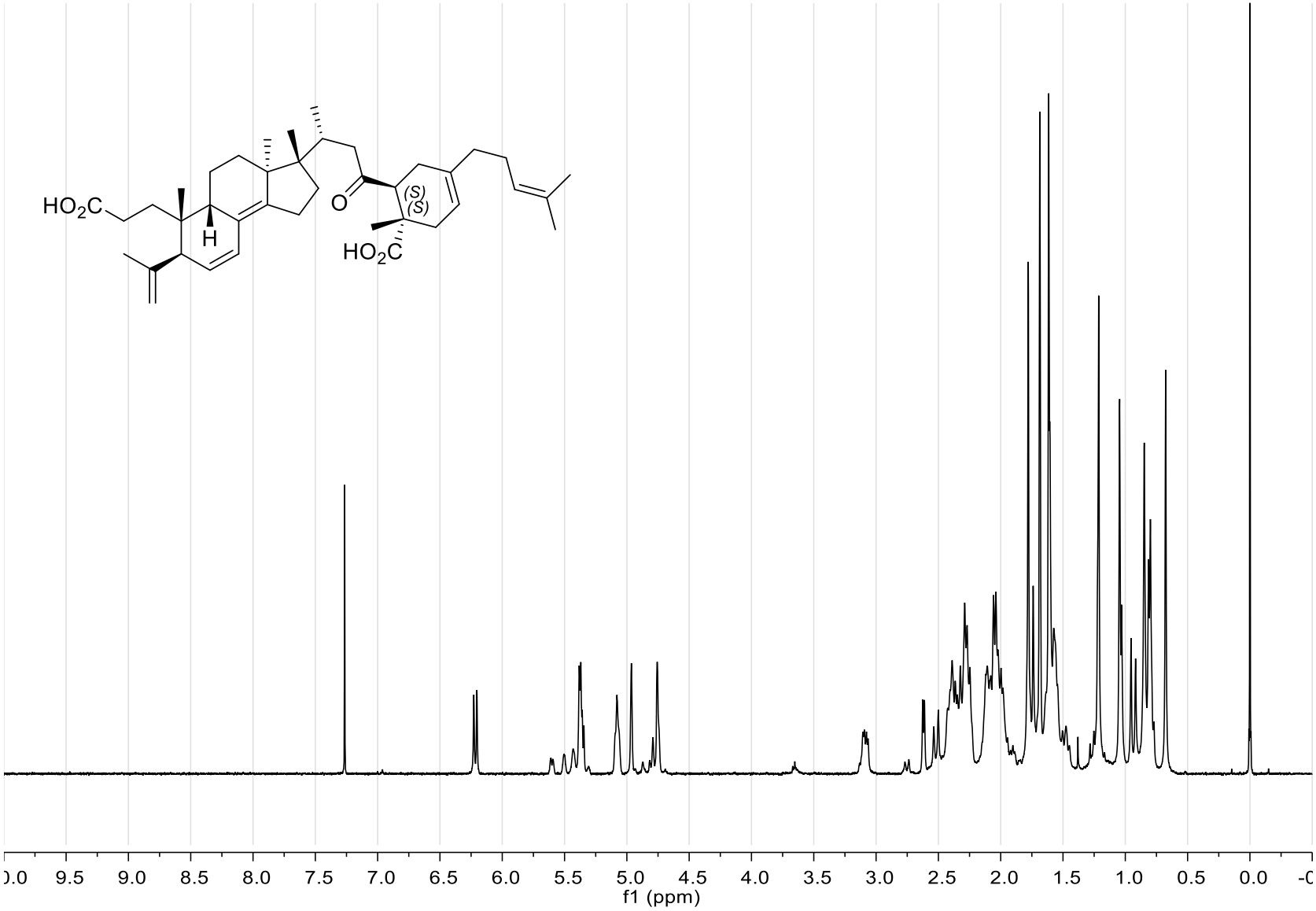


Figure S45. ^{13}C and DEPT NMR Spectra of Abibalsamin I (**9**) in $CDCl_3$, 100 MHz

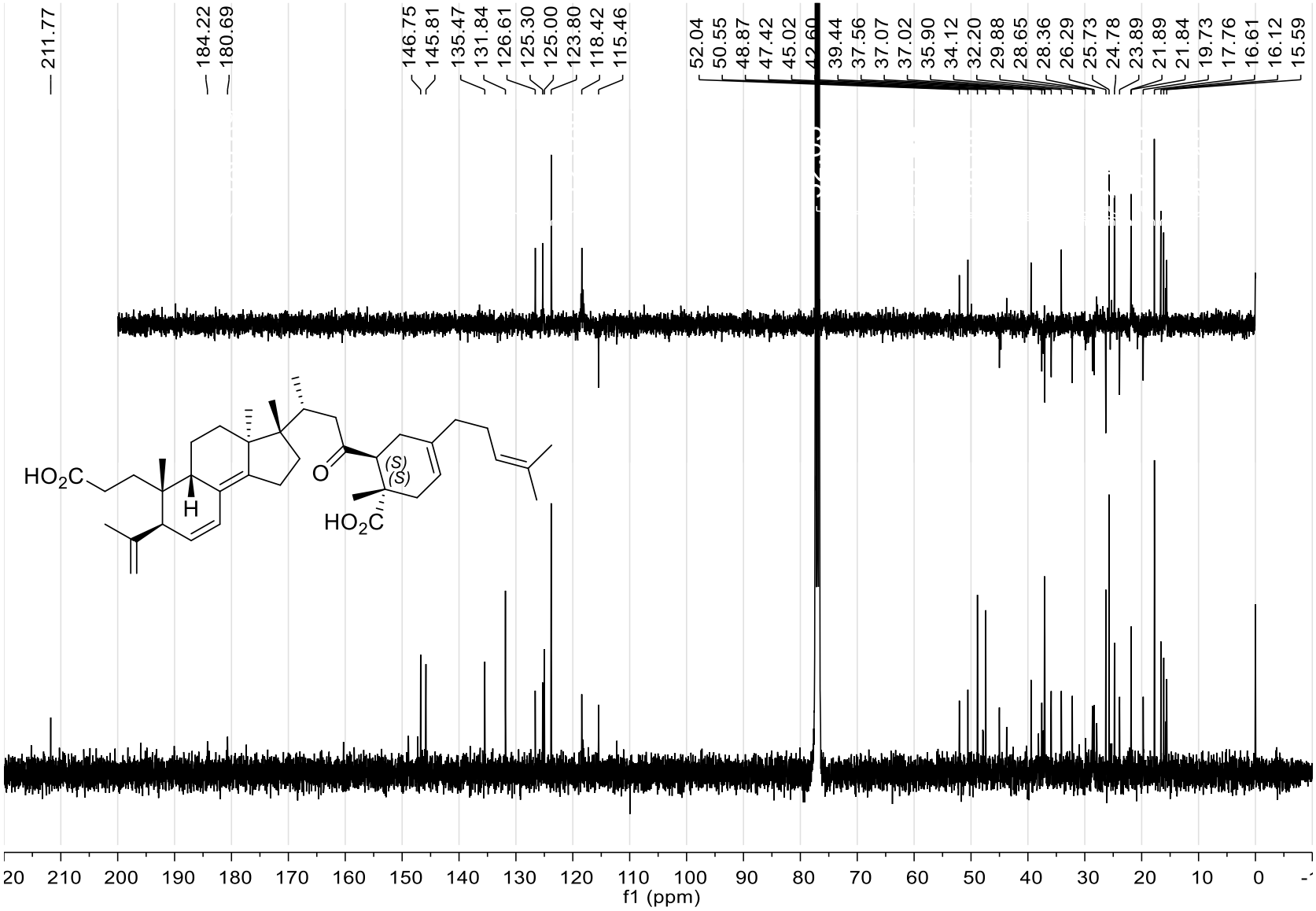


Figure S46. ^{1}H-^{1}H COSY Spectrum of Abibalsamin I (**9**) in $CDCl_3$, 400 MHz

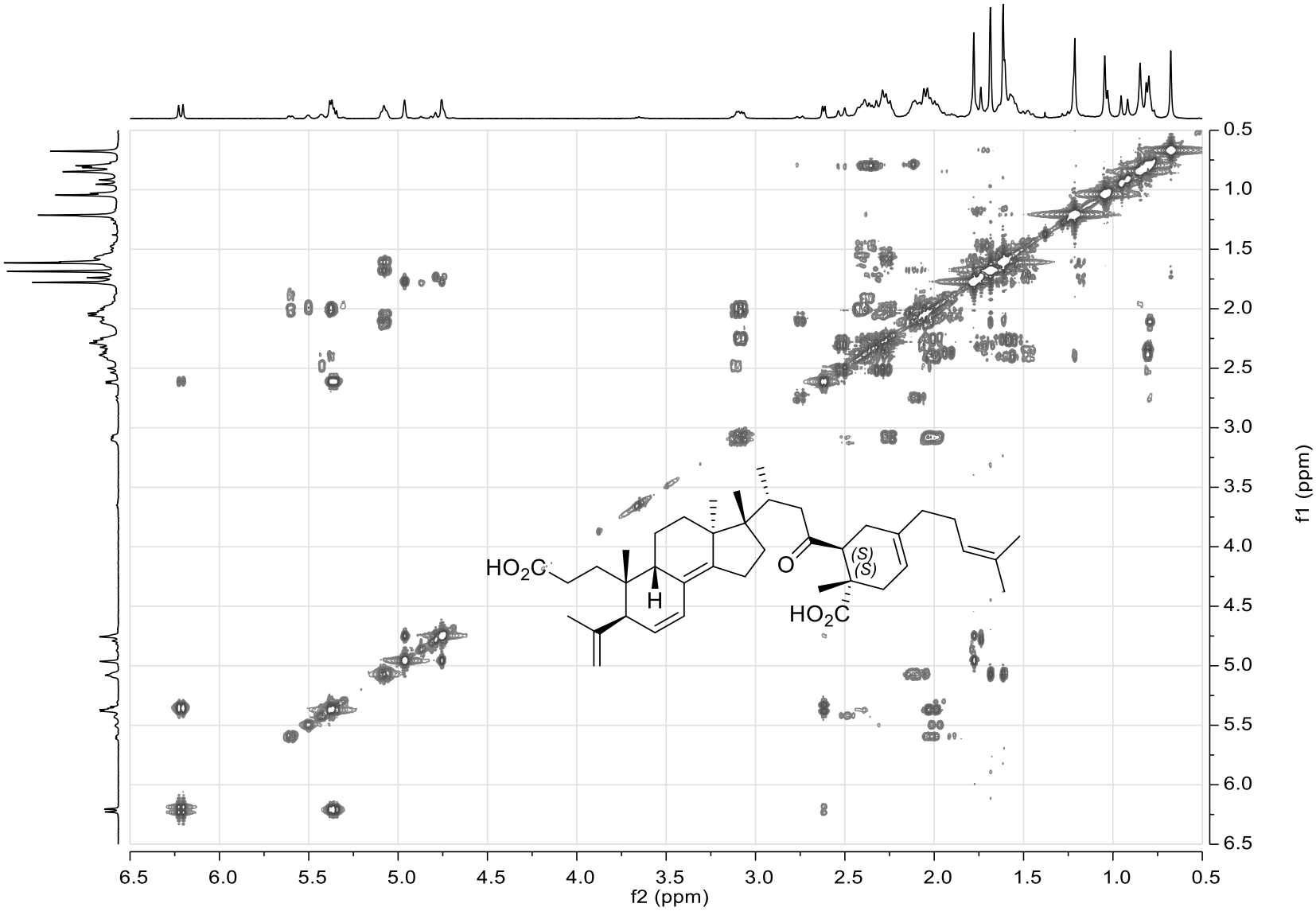


Figure S47. HSQC Spectrum of Abibalsamin I (**9**) in $CDCl_3$, 400 MHz

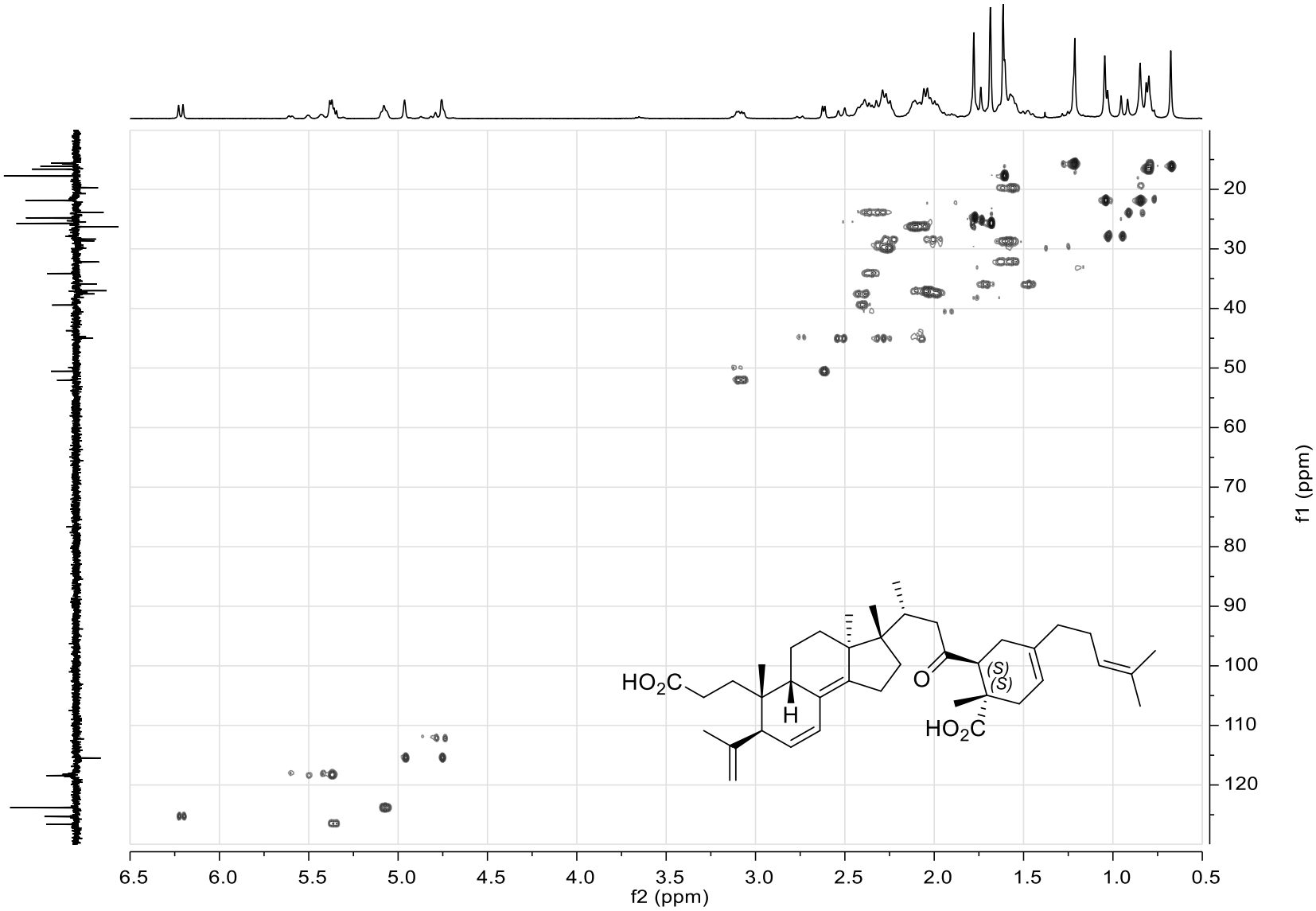


Figure S48. HMBC Spectrum of Abibalsamin I (**9**) in $CDCl_3$, 400 MHz

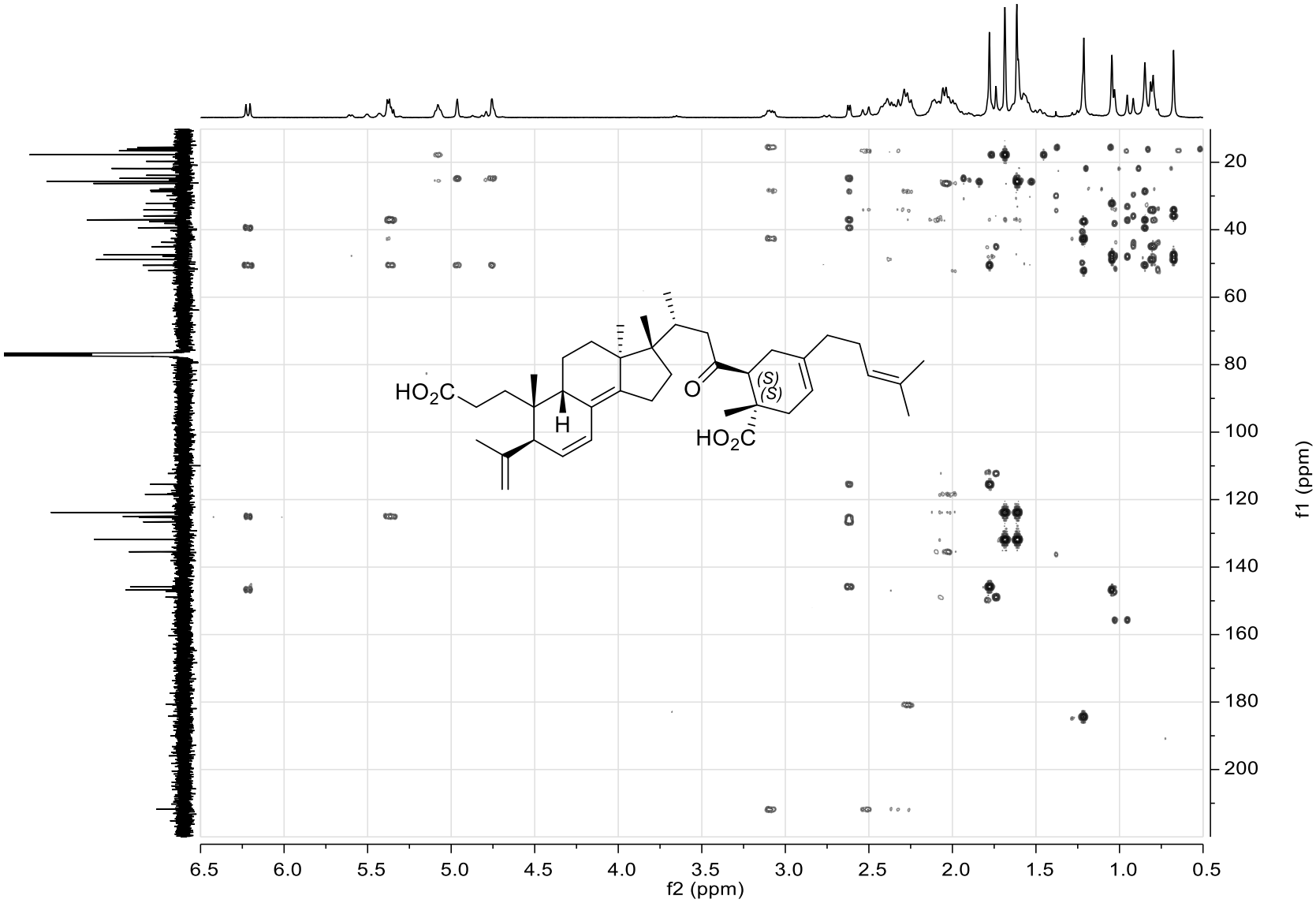
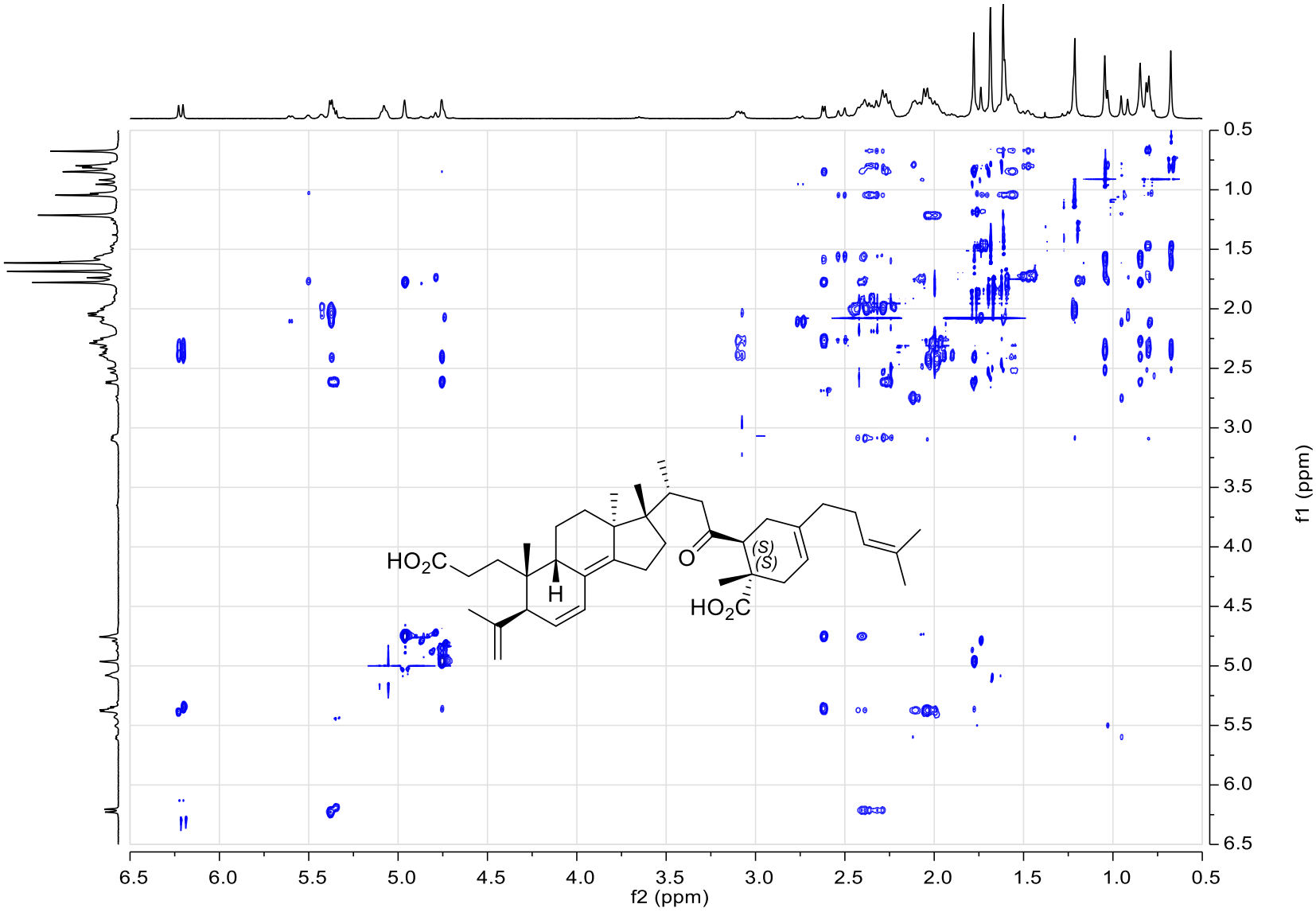
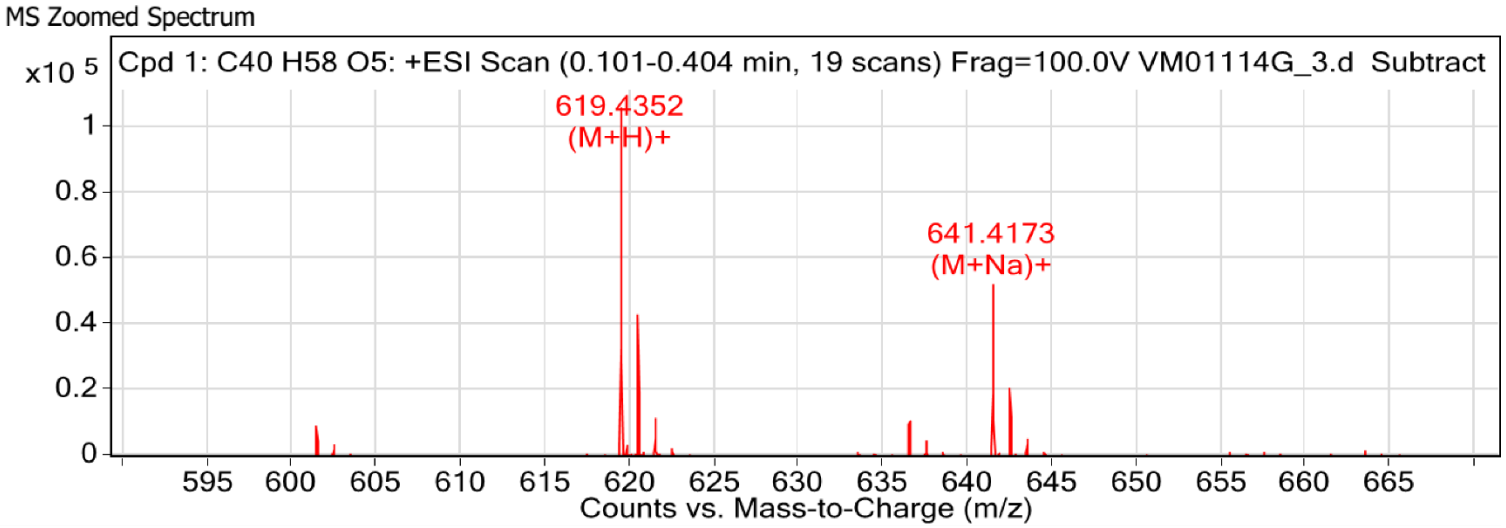


Figure S49. ROESY Spectrum of Abibalsamin I (**9**) in $CDCl_3$, 400 MHz



ABIBALSAMIN J (10)

Figure S50. HRESIMS of Abibalsamin J (**10**)



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
619.4352	619.4357	-0.84		112653	C40 H59 O5	(M+H)+
619.741				3343		
620.4394	620.4391	0.51		43737	C40 H59 O5	(M+H)+

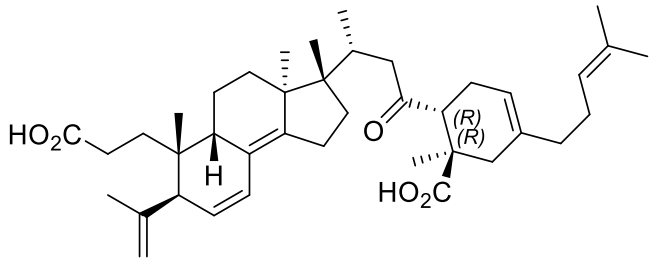


Figure S51. ^{1}H NMR Spectrum of Abibalsamin J (**10**) in $CDCl_3$, 400 MHz

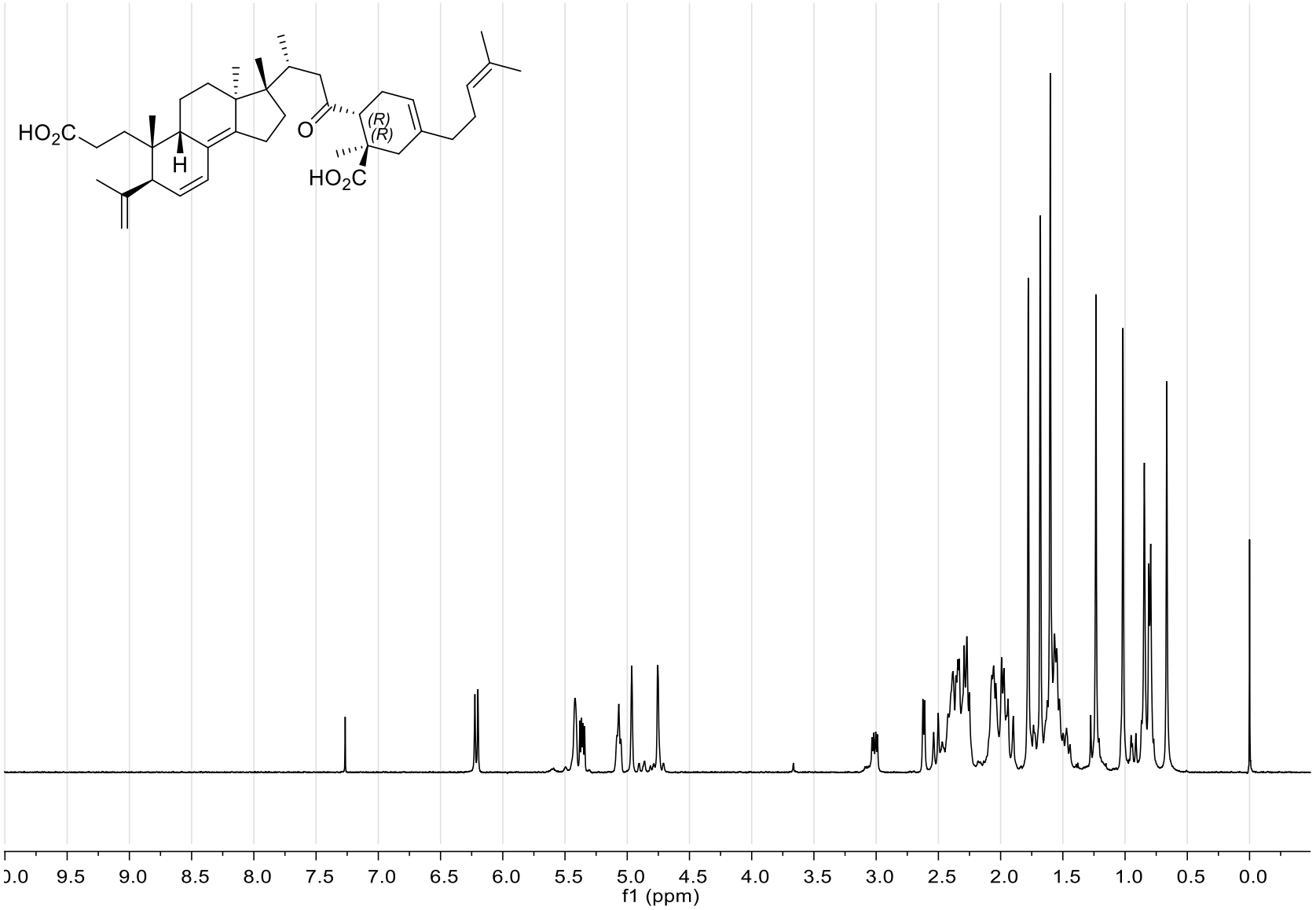


Figure S52. ^{13}C and DEPT NMR Spectra of Abibalsamin J (**10**) in $CDCl_3$, 100 MHz

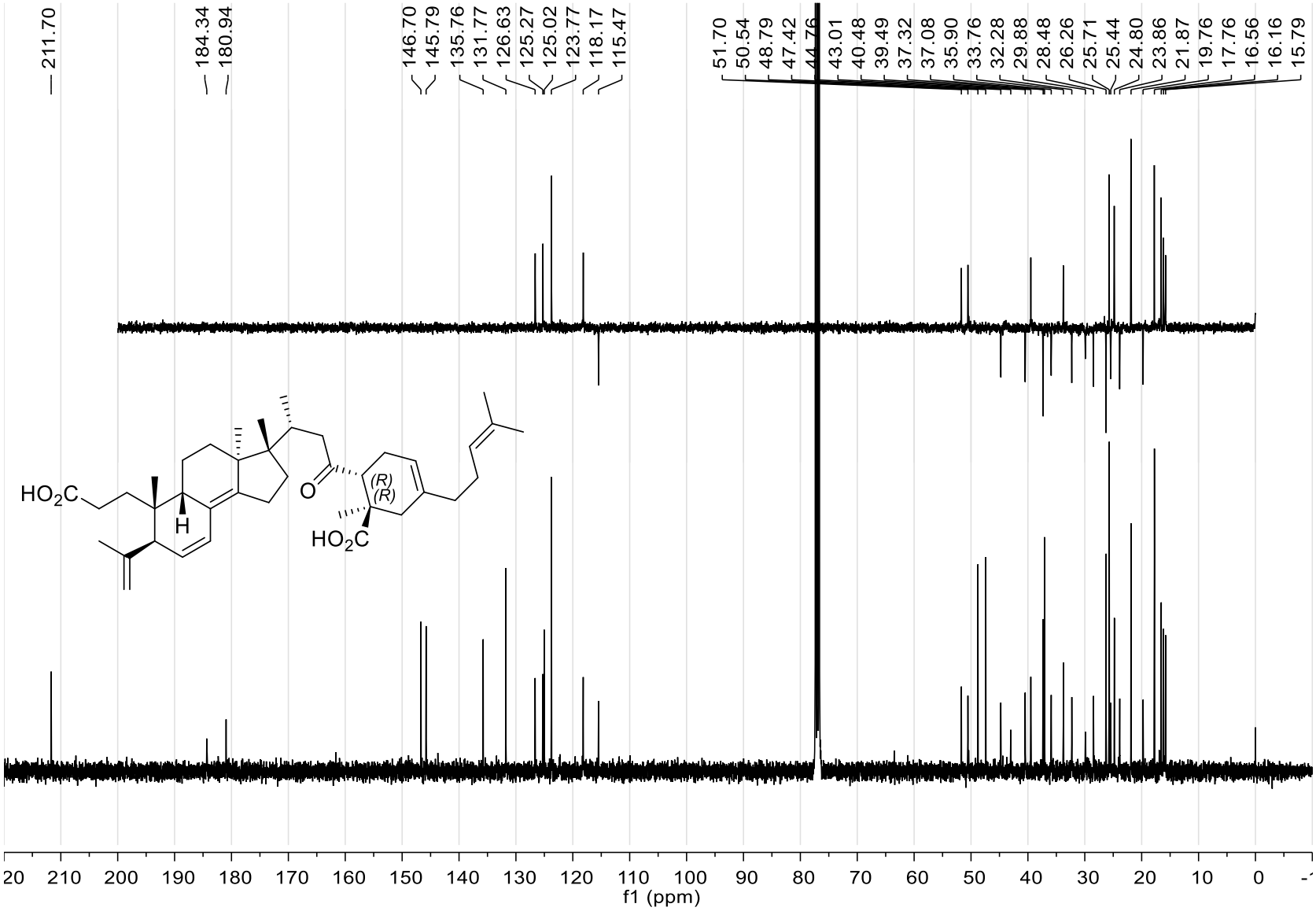


Figure S53. ^{1}H-^{1}H COSY Spectrum of Abibalsamin J (**10**) in $CDCl_3$, 400 MHz

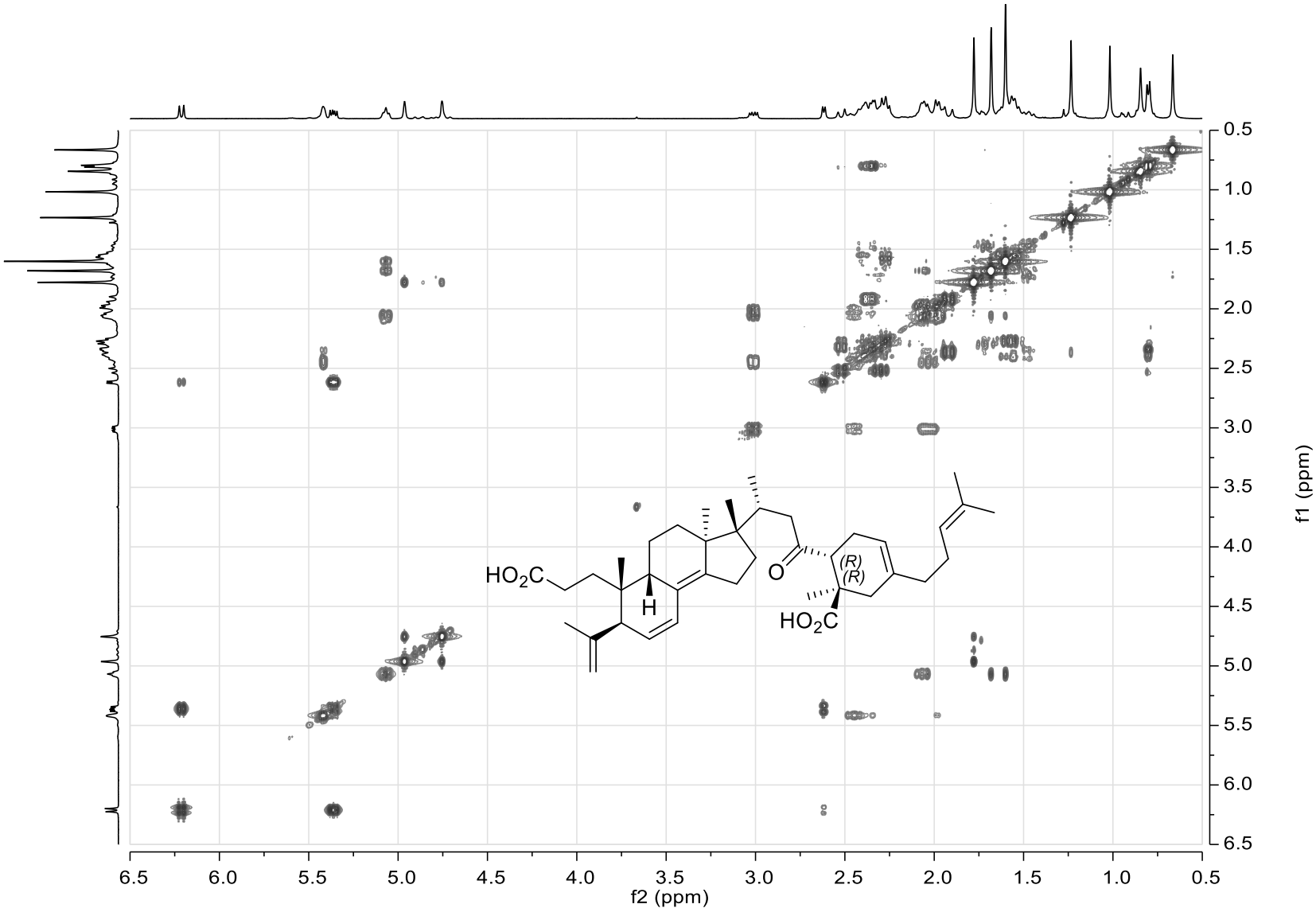


Figure S54. HSQC Spectrum of Abibalsamin J (**10**) in $CDCl_3$, 400 MHz

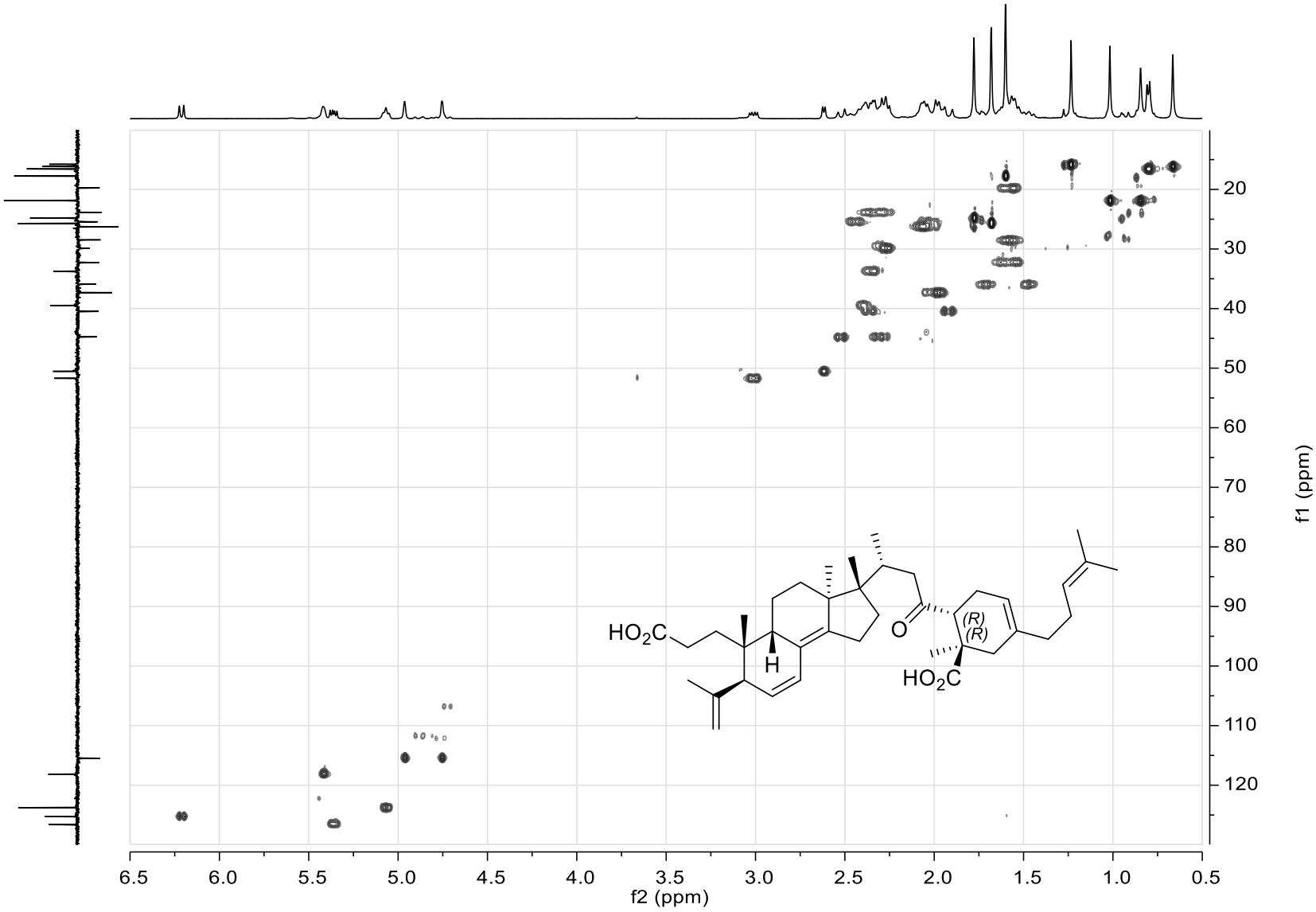


Figure S55. HMBC Spectrum of Abibalsamin J (**10**) in $CDCl_3$, 400 MHz

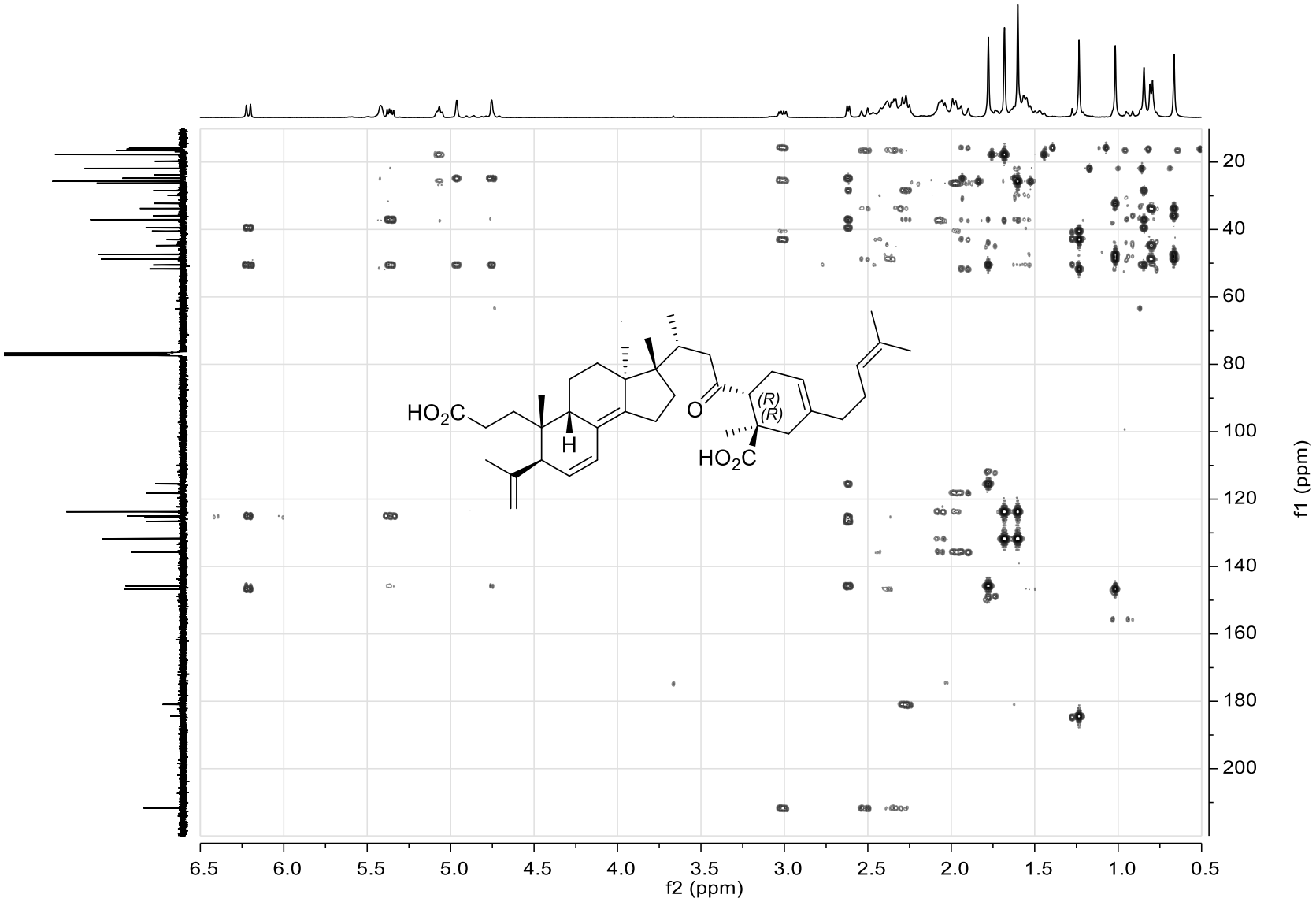
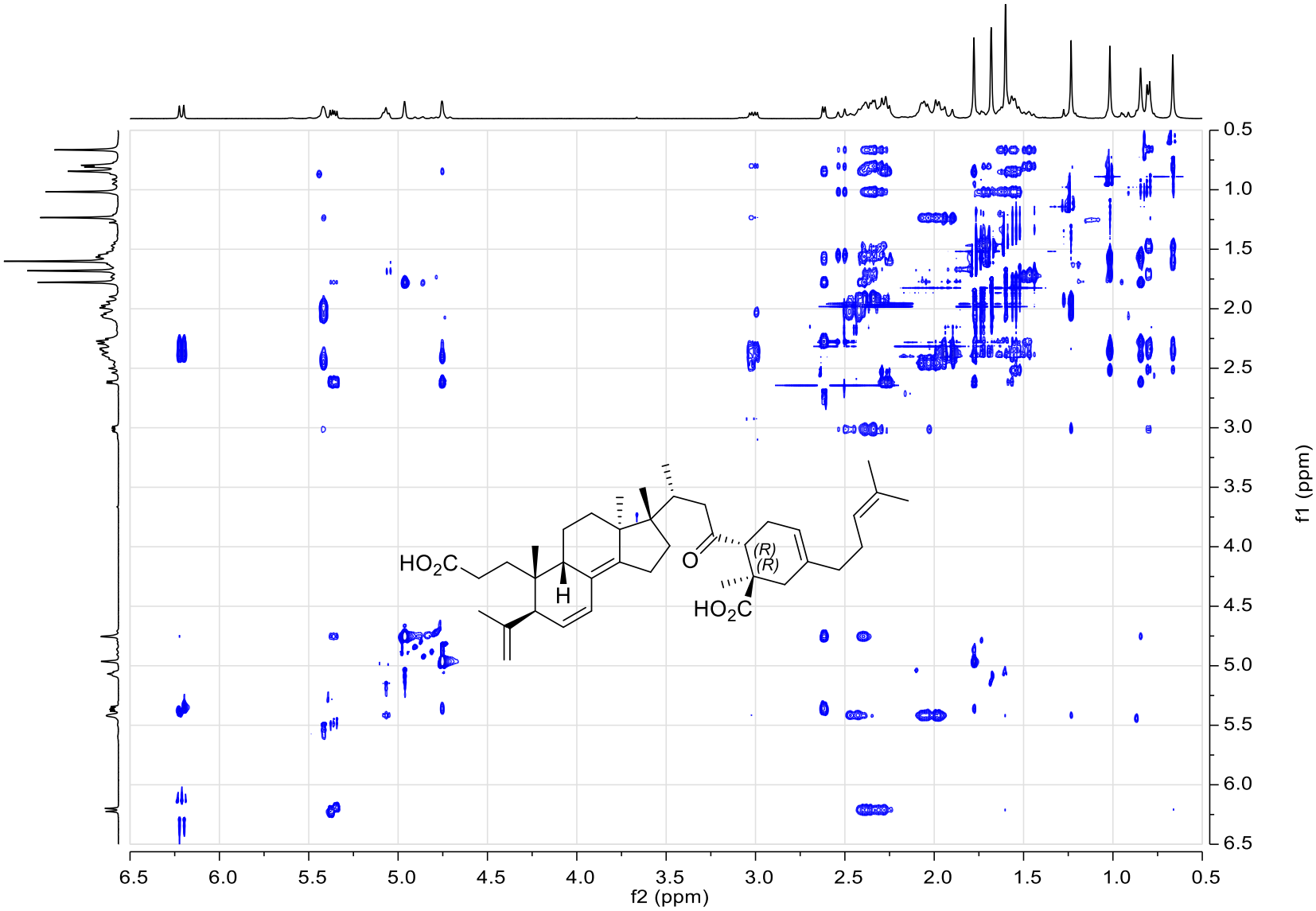


Figure S56. ROESY Spectrum of Abibalsamin J (**10**) in $CDCl_3$, 400 MHz



DATA COMPARISON

Figure S57. ^{1}H NMR Comparison of Compounds **1** and **4**

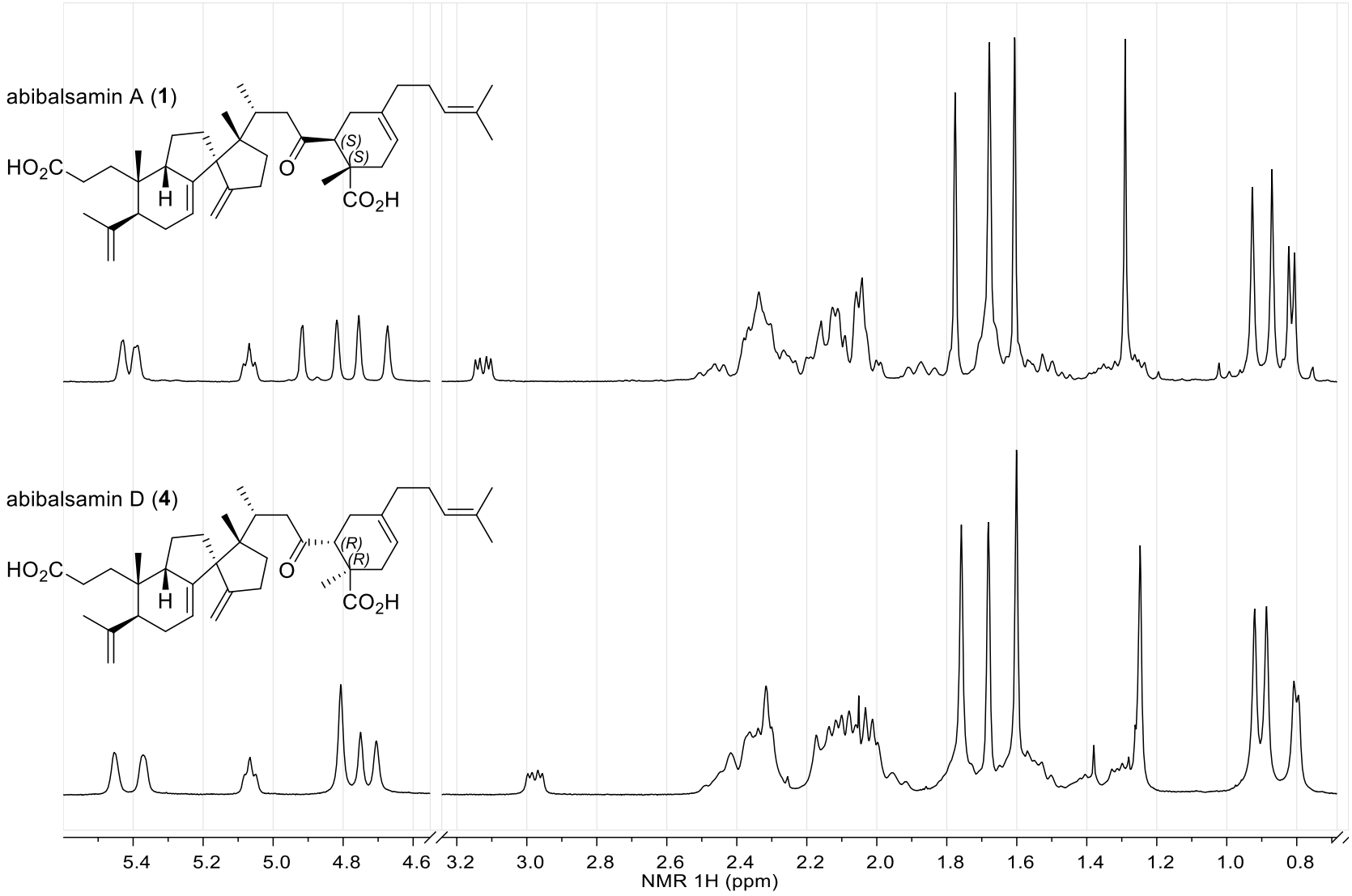


Figure S58. ^{13}C NMR Comparison of Compounds **1** and **4**

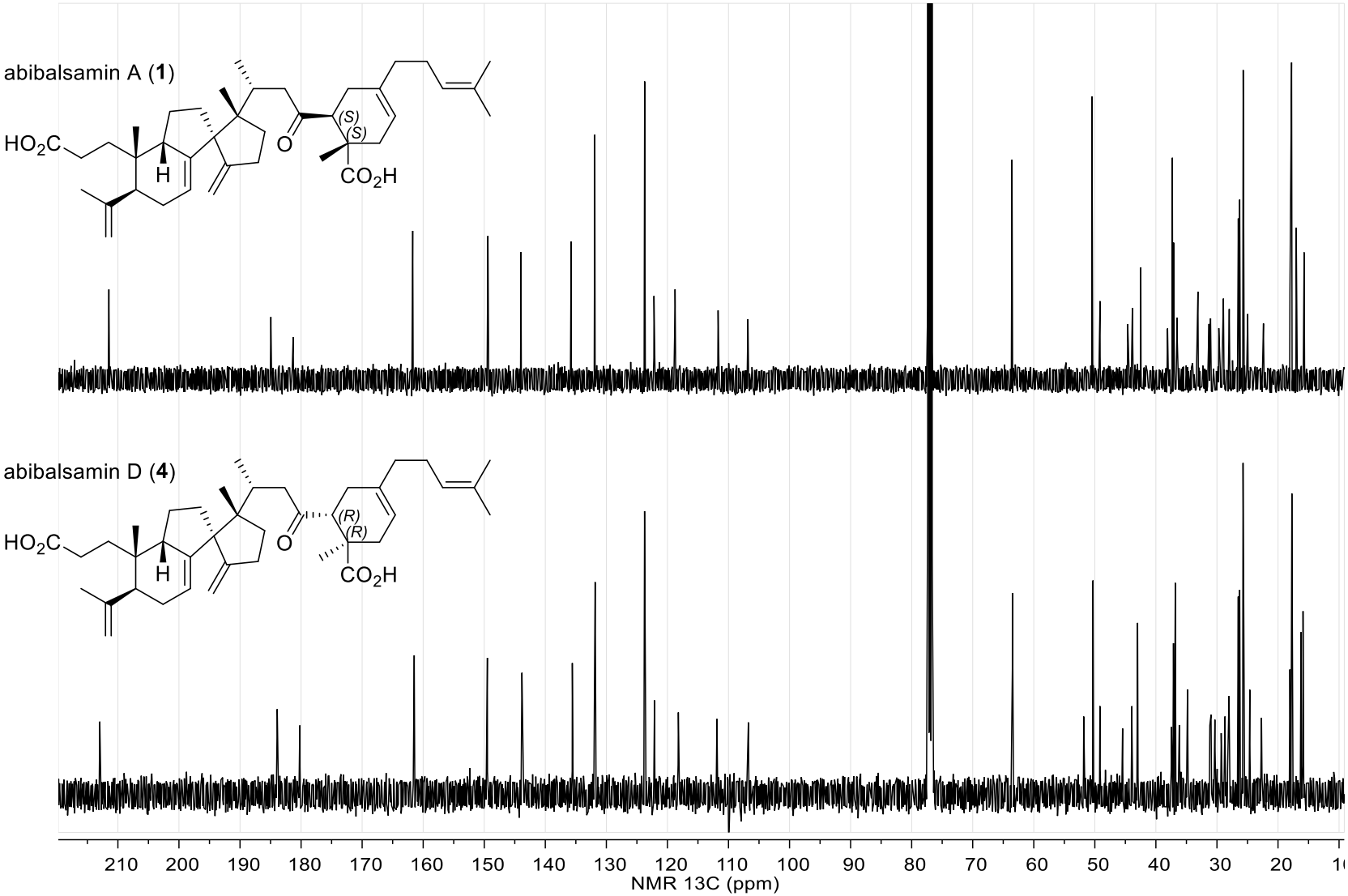


Table S1. ^{1}H and ^{13}C NMR Spectroscopic Data Comparison for Compounds **1** and **4**

position	^{13}C			^{1}H		
	1	**4**	**$\delta_4-\delta_1$**	**1**	**4**	**$\delta_4-\delta_1$**
1	29.7	30.3	+0.6	1.68	1.73; 1.64	+0.01
2	28.7	29.3	+0.6	2.34	2.32	−0.02
3	181.3	180.2	−1.1			
4	149.4	149.5	+0.1			
5	43.9	43.9	0.0	2.05	2.07	+0.02
6	31.1	31.0	−0.1	2.34; 2.14	2.39; 2.14	+0.05; 0.00
7	122.2	122.1	−0.1	5.43	5.45	+0.02
8	144.0	143.8	−0.2			
9	49.2	49.2	0.0	2.15	2.10	−0.05
10	37.3	36.8	−0.5			
11	22.4	22.7	+0.3	1.67; 1.34	1.59; 1.41	−0.08; +0.07
12	31.3	31.2	−0.1	1.66; 1.26	1.78	+0.32
13	63.6	63.5	−0.1			
14	161.7	161.5	−0.2			
15	28.0	28.0	0.0	2.47; 2.35	2.45; 2.35	−0.02; 0.00
16	36.5	36.2	−0.3	1.54	1.53	−0.01
17	50.5	50.3	−0.2			
18	18.0	18.0	0.0	0.87	0.89	+0.02
19	25.0	24.6	−0.4	0.93	0.92	−0.01
20	33.1	34.8	+1.7	2.31	2.31	0.00
21	17.0	16.2	−0.8	0.81	0.80	−0.01
22	44.6	45.5	+0.9	2.36; 2.12	2.33; 2.17	−0.03; +0.05
23	211.5	213.0	+1.5			
24	50.4	51.8	+1.4	3.12	2.98	−0.14
25	42.5	43.0	+0.5			
26	185.0	183.9	−1.1			
27	15.7	15.9	+0.2	1.29	1.25	−0.04
28	111.7	111.9	+0.2	4.92; 4.82	4.81	−0.06
29	26.5	26.5	0.0	1.78	1.76	−0.02
30	106.8	106.8	0.0	4.76; 4.67	4.75; 4.70	−0.01; +0.03
31	38.1	37.5	−0.6	2.28; 2.01	2.39; 2.02	+0.11; +0.01
32	118.8	118.2	−0.6	5.39	5.37	−0.02
33	135.8	135.6	−0.2			
34	29.0	28.7	−0.3	2.22; 1.87	2.16; 1.96	−0.06; +0.09
35	37.1	37.1	0.0	2.06	2.01	−0.05
36	26.3	26.3	0.0	2.10	2.08	−0.02
37	123.7	123.8	+0.1	5.07	5.07	0.00
38	131.9	131.9	0.0			
39	25.7	25.7	0.0	1.68	1.68	0.00
40	17.8	17.7	−0.1	1.61	1.60	−0.01

Figure S59. ^{1}H NMR Comparison of Compounds **6** and **9**

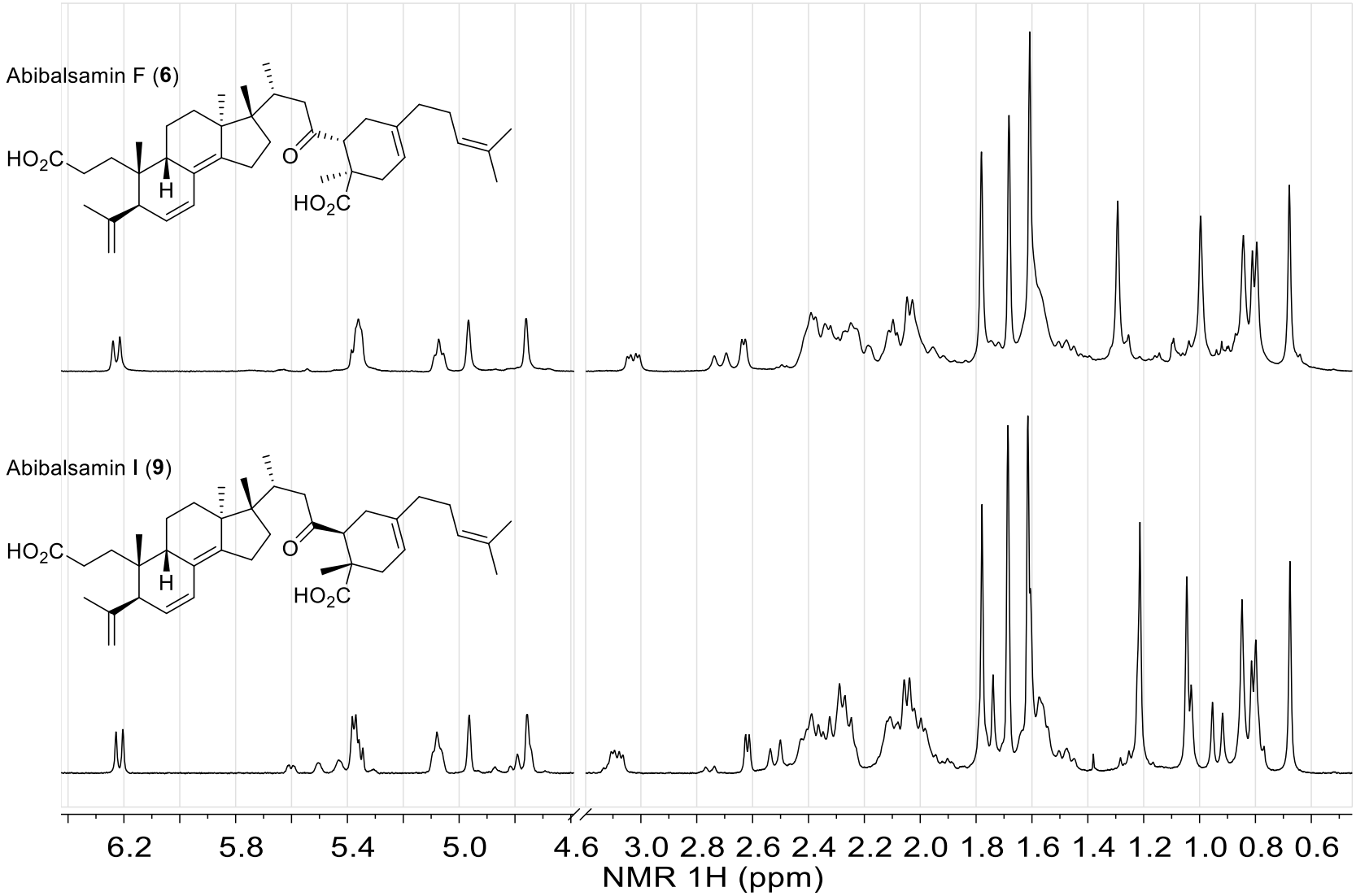


Figure S60. ^{13}C NMR Comparison of Compounds **6** and **9**

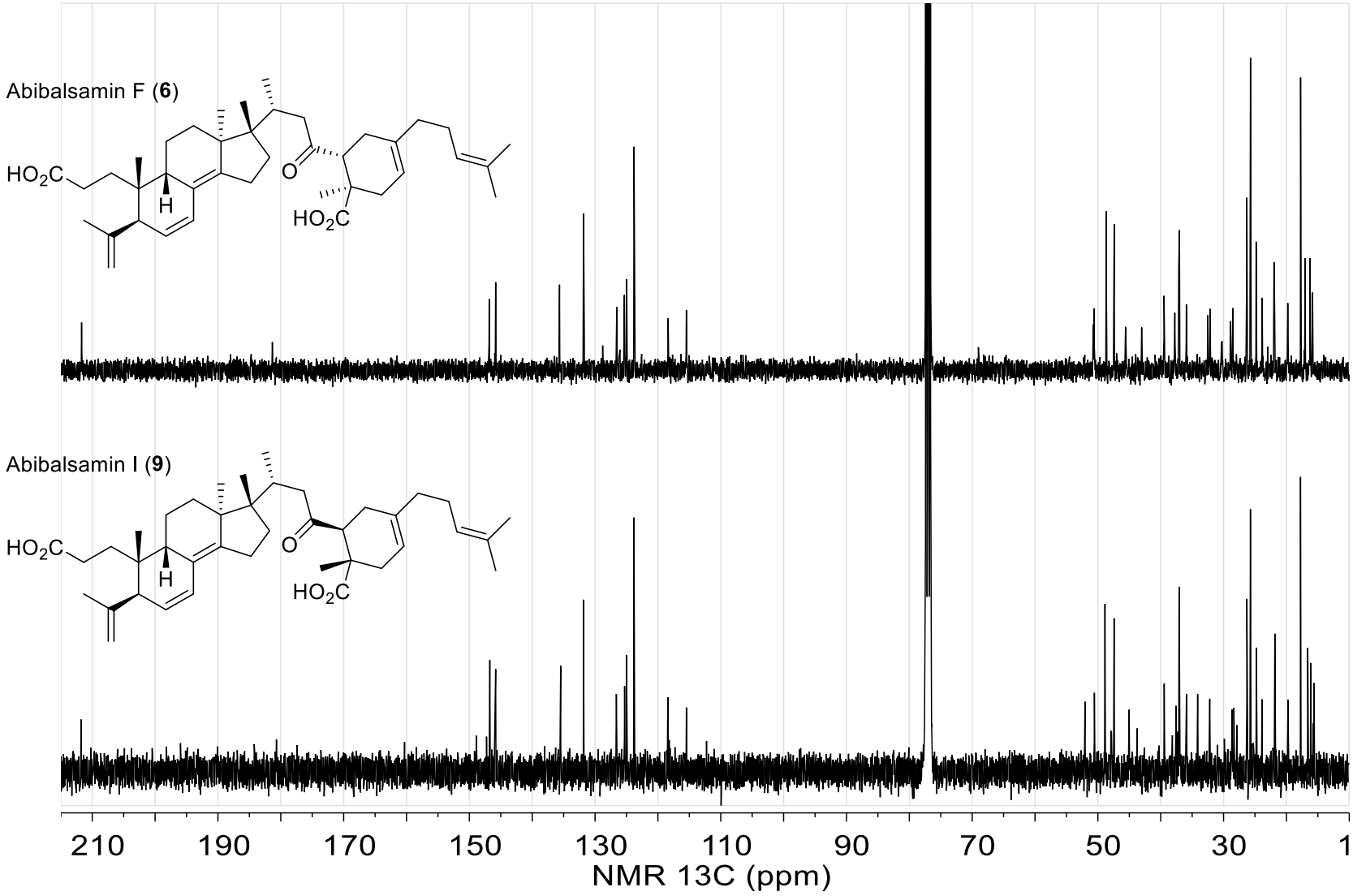


Table S2. ^{1}H and ^{13}C NMR Spectroscopic Data Comparison for Compounds **6** and **9**

position	^{13}C			^{1}H		
	6	**9**	**$\delta_9-\delta_6$**	**6**	**9**	**$\delta_9-\delta_6$**
1	28.9	28.6	−0.3	1.59	1.58	−0.01
2	30.2	29.9	−0.3	2.24	2.27	+0.03
3	181.4	180.7	−0.7			
4	145.8	145.8	0.0			
5	50.6	50.6	0.0	2.63	2.62	−0.01
6	126.5	126.6	+0.1	5.37	5.36	−0.01
7	125.3	125.3	0.0	6.23	6.22	−0.01
8	125.0	125.0	0.0			
9	39.5	39.4	−0.1	2.40	2.40	0.00
10	37.1	37.1	0.0			
11	19.8	19.7	−0.1	1.58	1.59	+0.01
12	32.2	32.2	0.0	1.59	1.63; 1.56	0.00
13	47.4	47.4	0.0			
14	146.8	146.7	−0.1			
15	23.9	23.9	0.0	2.34	2.37; 2.30	0.00
16	35.9	35.9	0.0	1.73; 1.47	1.71; 1.47	−0.02; 0.00
17	48.7	48.9	+0.2			
18	16.2	16.1	−0.1	0.68	0.68	0.00
19	21.9	21.9	0.0	0.84	0.85	+0.01
20	32.5	34.1	+1.6	2.39	2.35	−0.04
21	17.0	16.6	−0.4	0.80	0.81	+0.01
22	45.6	45.0	−0.6	2.72; 2.28	2.52; 2.28	−0.10; 0.00
23	211.7	211.8	+0.1			
24	50.7	52.0	+1.3	3.03	3.09	+0.06
25	43.0	42.6	−0.4			
26	184.7	184.2	−0.5			
27	15.8	15.6	−0.2	1.29	1.21	−0.08
28	115.5	115.5	0.0	4.97; 4.76	4.96; 4.76	−0.01; 0.00
29	24.8	24.8	0.0	1.78	1.78	0.00
30	22.0	21.8	−0.2	1.00	1.05	+0.05
31	37.8	37.6	−0.2	2.36; 2.03	2.41; 2.00	+0.05; −0.03
32	118.4	118.4	0.0	5.36	5.37	+0.01
33	135.7	135.5	−0.2			
34	28.5	28.4	−0.1	2.20; 1.95	2.25; 2.00	+0.05; +0.05
35	37.0	37.0	0.0	2.03	2.10; 2.03	+0.04
36	26.3	26.3	0.0	2.09	2.09	0.00
37	123.8	123.8	0.0	5.07	5.08	+0.01
38	131.8	131.8	0.0			
39	25.7	25.7	0.0	1.68	1.69	+0.01
40	17.7	17.8	+0.1	1.61	1.61	0.00

Figure S61. ^{1}H NMR Comparison of Compounds **7** and **10**

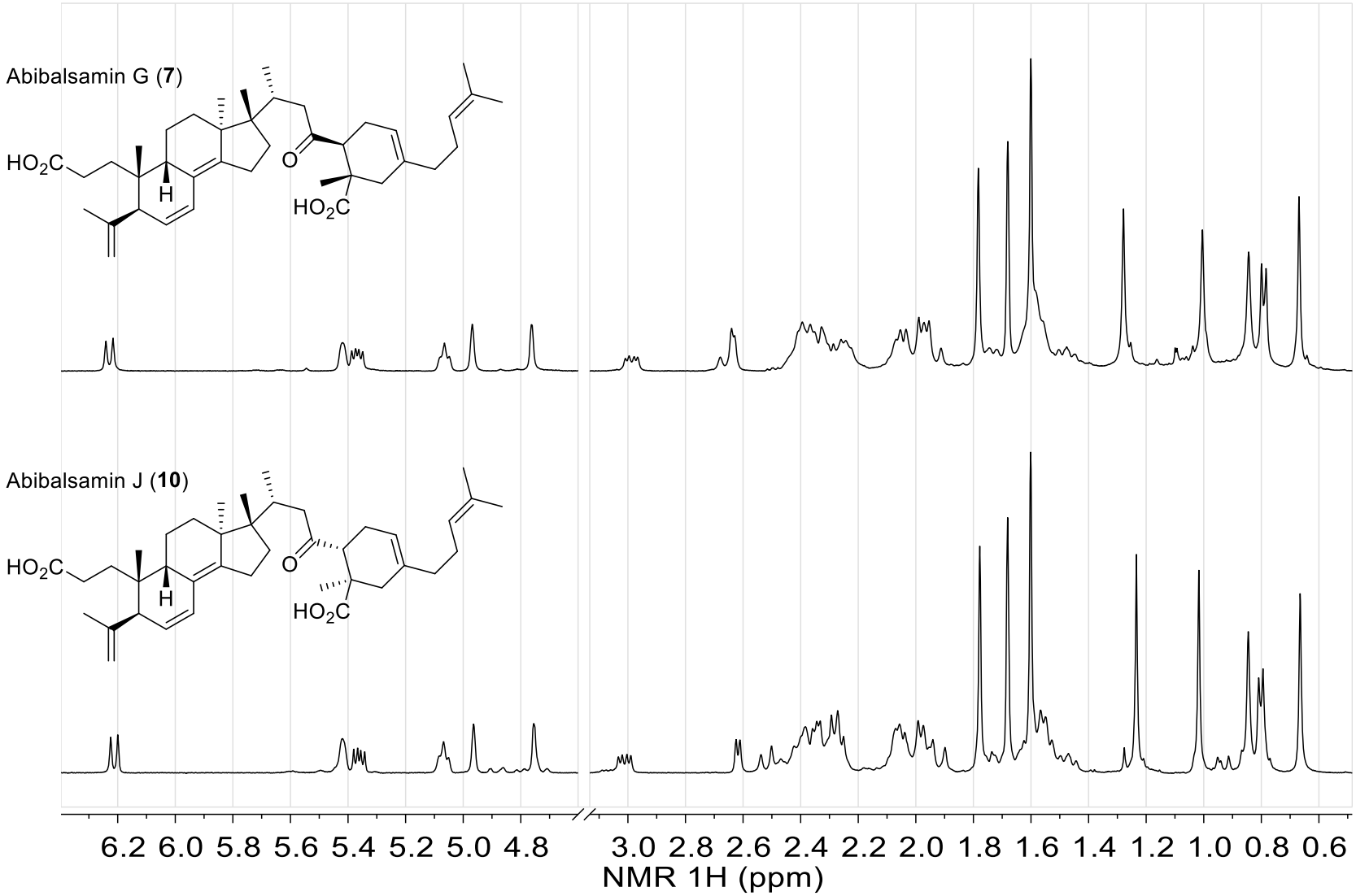


Figure S62. ^{13}C NMR Comparison of Compounds **7** and **10**

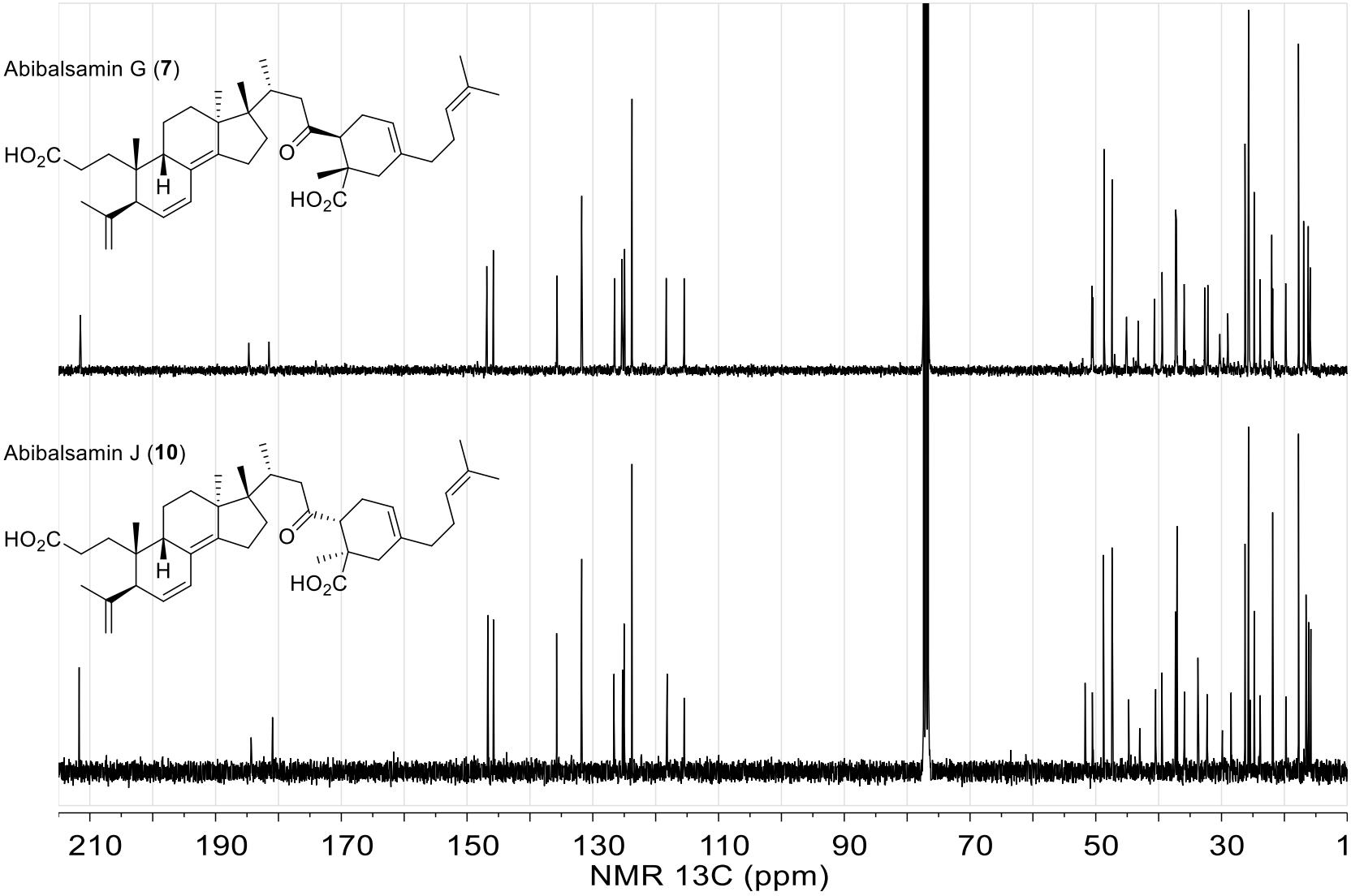


Table S3. ^{1}H and ^{13}C NMR Spectroscopic Data Comparison for Compounds **7** and **10**

position	^{13}C			^{1}H		
	7	**10**	**$\delta_{10}-\delta_7$**	**7**	**10**	**$\delta_{10}-\delta_7$**
1	29.0	28.5	−0.5	1.59	1.58	−0.01
2	30.3	29.9	−0.4	2.24	2.27	+0.03
3	181.5	180.9	−0.6			
4	145.8	145.8	+0.0			
5	50.6	50.5	−0.1	2.63	2.62	−0.01
6	126.5	126.6	+0.1	5.37	5.36	−0.01
7	125.3	125.3	0.0	6.23	6.21	−0.02
8	124.9	125.0	+0.1			
9	39.5	39.5	0.0	2.40	2.39	−0.01
10	37.2	37.1	−0.1			
11	19.8	19.8	0.0	1.57	1.61; 1.56	+0.01
12	32.2	32.3	+0.1	1.58	1.63; 1.54	0.00
13	47.4	47.4	0.0			
14	146.9	146.7	−0.2			
15	23.9	23.9	0.0	2.34	2.37; 2.28	−0.01
16	35.9	35.9	0.0	1.73; 1.47	1.71; 1.47	−0.02; 0.00
17	48.7	48.8	+0.1			
18	16.2	16.2	0.0	0.67	0.67	0.00
19	21.9	21.9	0.0	0.84	0.85	+0.01
20	32.7	33.8	+1.1	2.38	2.35	−0.03
21	16.9	16.6	−0.3	0.79	0.80	+0.01
22	45.1	44.8	−0.3	2.66; 2.28	2.52; 2.29	−0.14; +0.01
23	211.5	211.7	+0.2			
24	50.5	51.7	+1.2	2.99	3.01	+0.02
25	43.3	43.0	−0.3			
26	184.7	184.3	−0.4			
27	15.9	15.8	−0.1	1.28	1.23	−0.05
28	115.5	115.5	0.0	4.97; 4.76	4.96; 4.75	−0.01; −0.01
29	24.8	24.8	0.0	1.78	1.78	0.00
30	22.0	21.9	−0.1	1.00	1.02	+0.02
31	40.7	40.5	−0.2	2.33; 1.93	2.36; 1.92	+0.03; −0.01
32	135.7	135.8	+0.1			
33	118.3	118.2	−0.1	5.42	5.42	0.00
34	25.6	25.4	−0.2	2.41; 1.99	2.44; 2.03	+0.03; +0.04
35	37.3	37.3	0.0	1.97	1.97	0.00
36	26.3	26.3	0.0	2.06	2.06	0.00
37	123.8	123.8	0.0	5.06	5.07	+0.01
38	131.8	131.8	0.0			
39	25.7	25.7	0.0	1.68	1.68	0.00
40	17.8	17.8	0.0	1.60	1.60	0.00

DETAILED MODEL CHARACTERISTICS

Table S4. Characteristics of the *in silico* Models

model ID	dienophile precursor[a]	isohexenyl position	configuration		possible compounds	nbr conformer below cutoff energy (kJ mol^{-1})[b]			unique DFT geometries[c]	
			C-24	C-25		E < 21	E < 8	E < 4	nbr	ΔG_{min} (Hartree)
I	A	C-33	*S*	*S*	**6**, **9**	9325	117	20	32	−1923.89707
II	A	C-33	*R*	*R*	**6**, **9**	14372	610	77	40	−1923.89592
III	A	C-32	*S*	*S*	**7**, **8**, **10**	14218	214	31	19	−1923.91307
IV	A	C-32	*R*	*R*	**7**, **8**, **10**	17116	1178	169	50	−1923.89608
V	B	C-32	*S*	*S*	**3**	5959	362	64	30	−1923.88788
VI	B	C-32	*R*	*R*	**3**	4154	119	5	43	−1923.87910
VII	C	C-32	*S*	*S*	**5**	18043	1234	118	45	−1925.07734
VIII	C	C-32	*R*	*R*	**5**	14625	659	71	23	−1925.07815

[a] dienophile precusors are: A = *trans*-sibiric acid; B = abiesonic acid; C = (24*E*)-23-oxo-3,4-seco-9*βH*-lanosta-4(28),7,24-triene-3,26-dioic acid [b] Number of conformer after molecular mechanic conformational search. [c] Number of unique DFT geometries at the B3LYP/3-21G level of theory and Gibbs free energy of the lowest energy conformer

Table S5. Relative Free Energy and Room Temperature Population for the Optimized Conformers of Model I–IV[a]

# conf.	I		II		III		IV	
	ΔG[b]	%[c]	ΔG[b]	%[c]	ΔG[b]	%[c]	ΔG[b]	%[c]
i	**0.00**	**35.1**	**0.00**	**20.1**	**0.00**	**75.1**	**0.00**	**14.5**
ii	**0.56**	**28.0**	**0.25**	**18.2**	**3.82**	**16.1**	**1.12**	**9.2**
iii	**3.00**	**10.5**	**1.39**	**11.5**	**7.39**	**3.8**	**2.08**	**6.3**
iv	**3.58**	**8.3**	**2.26**	**8.1**	9.54	1.6	**2.12**	**6.2**
v	**5.09**	**4.5**	**3.11**	**5.7**	11.27	0.8	**2.96**	**4.4**
vi	**6.25**	**2.8**	**3.21**	**5.5**	11.40	0.8	**3.03**	**4.3**
vii	7.26	1.9	**3.39**	**5.1**	12.39	0.5	**3.20**	**4.0**
viii	8.01	1.4	**3.89**	**4.2**	13.25	0.4	**3.60**	**3.4**
ix	8.17	1.3	**4.02**	**4.0**	13.64	0.3	**3.62**	**3.4**
x	9.34	0.8	**4.27**	**3.6**	13.80	0.3	**3.99**	**2.9**
xi	9.38	0.8	**5.14**	**2.5**	15.17	0.2	**4.08**	**2.8**
xii	10.02	0.6	6.07	1.7	16.72	0.1	**4.45**	**2.4**
xiii	10.09	0.6	7.48	1.0	18.75	0.0	**4.50**	**2.4**
xiv	10.10	0.6	7.68	0.9	18.82	0.0	**4.90**	**2.0**
xv	10.89	0.4	8.40	0.7	19.04	0.0	**4.93**	**2.0**
xvi	12.03	0.3	8.41	0.7	19.60	0.0	**4.96**	**2.0**
xvii	12.10	0.3	8.51	0.6	19.80	0.0	5.06	1.9
xviii	12.10	0.3	8.77	0.6	20.36	0.0	5.41	1.6
xix	12.15	0.3	8.79	0.6	24.07	0.0	5.53	1.6
xx	12.46	0.2	9.00	0.5			5.57	1.5
xxi	12.76	0.2	9.31	0.5			5.63	1.5
xxii	12.78	0.2	9.47	0.4			5.88	1.4
xxiii	13.47	0.2	9.55	0.4			5.94	1.3
xxiv	14.42	0.1	10.01	0.4			5.94	1.3
xxv	14.77	0.1	10.23	0.3			6.00	1.3
xxvi	14.87	0.1	10.55	0.3			6.44	1.1
xxvii	16.13	0.1	10.58	0.3			6.44	1.1
xxviii	16.14	0.1	10.91	0.2			6.51	1.0
xxix	16.56	0.0	11.07	0.2			6.60	1.0
xxx	17.64	0.0	11.31	0.2			6.61	1.0
xxxi	25.17	0.0	11.88	0.2			6.61	1.0
xxxii	26.05	0.0	12.26	0.1			6.70	1.0
xxxiii			12.70	0.1			6.77	0.9
xxxiv			13.05	0.1			7.26	0.8
xxxv			13.41	0.1			7.71	0.6
xxxvi			14.47	0.1			8.03	0.6
xxxvii			14.54	0.1			8.04	0.6
xxxviii			14.90	0.0			8.20	0.5
xxxix			16.24	0.0			8.46	0.5
xl			17.64	0.0			8.78	0.4
xli							8.86	0.4
xlii							8.93	0.4

# conf.	I		II		III		IV	
	ΔG[b]	%[c]	ΔG[b]	%[c]	ΔG[b]	%[c]	ΔG[b]	%[c]
xliii							9.04	0.4
xliv							9.51	0.3
xlv							9.60	0.3
xlvi							10.57	0.2
xlvii							10.92	0.2
xlviii							11.21	0.2
xlix							11.70	0.1
l							22.92	0.0

[a] Conformers in bold were selected for the computation of the ECD spectra. [b] Relative Free energy in kJ mol^{-1} calculated at the B3LYP/3-21G level of theory. [c] Room temperature population in %.

Figure S63. Calculated ECD Spectra of Theoretical Model I–IV at B3LYP/3-21G and their Corresponding Experimental ECD Spectra

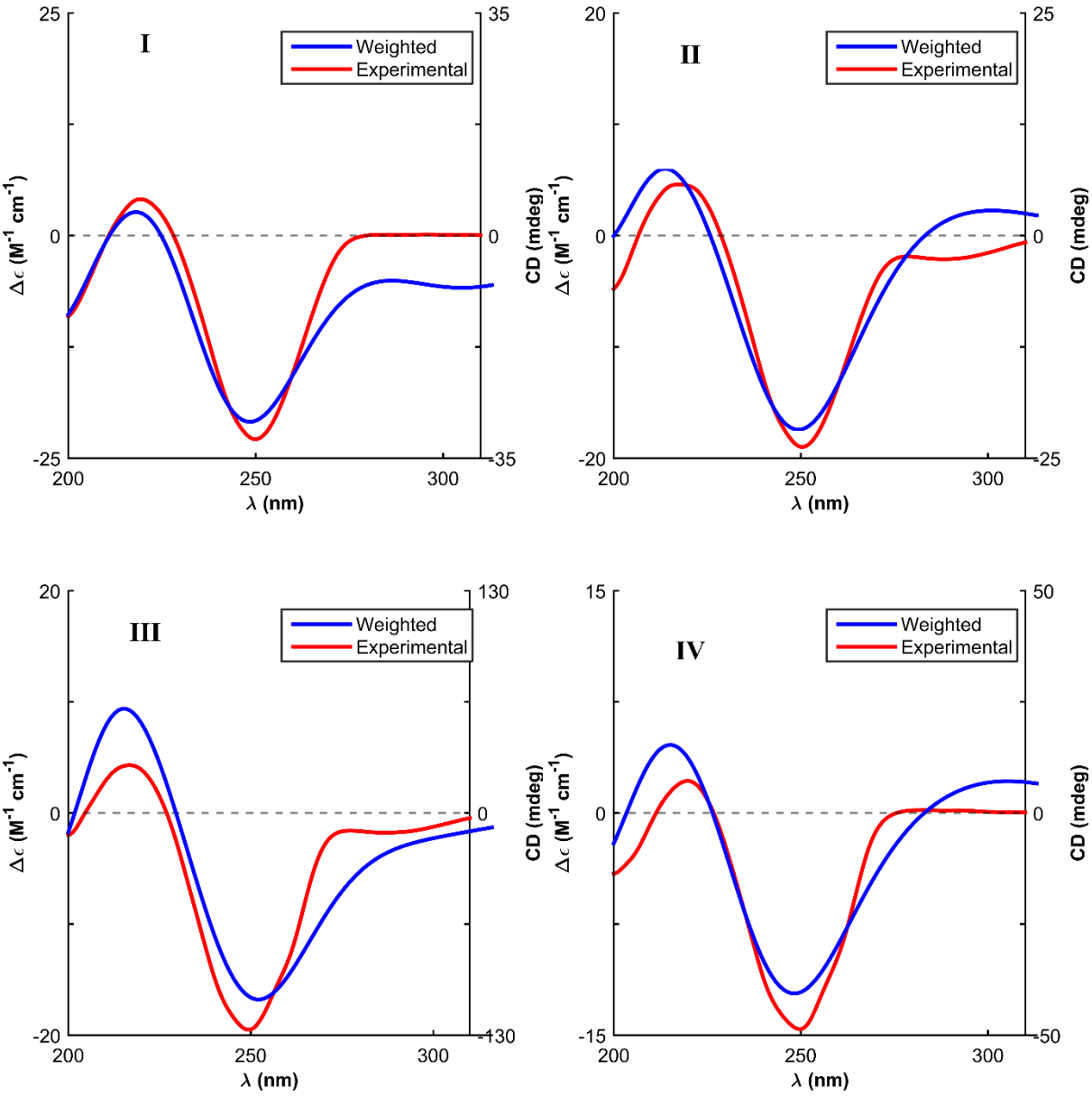


Table S6. Relative Free Energy and Room Temperature Population for the Optimized Conformers of Model V-VIII

# conf.	V		VI		VII		VIII	
	ΔG^a	$\%^b$	ΔG^a	$\%^b$	ΔG^a	$\%^b$	ΔG^a	$\%^b$
i	**0.00**	**28.1**	**0.00**	**27.9**	**0.00**	**12.1**	**0.00**	**29.9**
ii	**1.98**	**12.6**	**2.14**	**11.8**	**0.46**	**10.0**	**1.67**	**15.2**
iii	**2.06**	**12.2**	**3.38**	**7.1**	**0.91**	**8.3**	**1.71**	**15.0**
iv	**2.64**	**9.7**	**3.80**	**6.0**	**1.41**	**6.8**	**2.96**	**9.1**
v	**3.54**	**6.7**	**4.09**	**5.4**	**1.53**	**6.5**	**3.70**	**6.7**
vi	**3.99**	**5.6**	**4.29**	**4.9**	**1.81**	**5.8**	**4.28**	**5.3**
vii	**4.05**	**5.5**	**4.43**	**4.7**	**1.83**	**5.8**	**4.82**	**4.3**
viii	**4.75**	**4.1**	**4.65**	**4.3**	**2.22**	**4.9**	**5.98**	**2.7**
ix	**4.99**	**3.8**	**4.89**	**3.9**	**2.24**	**4.9**	**6.47**	**2.2**
x	**5.52**	**3.0**	**5.48**	**3.1**	**2.46**	**4.5**	**6.59**	**2.1**
xi	6.71	1.9	**6.26**	**2.2**	**2.60**	**4.2**	7.96	1.2
xii	7.61	1.3	**6.27**	**2.2**	**2.97**	**3.6**	8.71	0.9
xiii	8.26	1.0	**6.54**	**2.0**	**3.62**	**2.8**	8.78	0.9
xiv	8.58	0.9	6.74	1.8	4.72	1.8	9.03	0.8
xv	9.39	0.6	7.05	1.6	4.87	1.7	9.14	0.7
xvi	9.60	0.6	7.20	1.5	4.97	1.6	9.23	0.7
xvii	9.80	0.5	8.18	1.0	5.39	1.4	9.36	0.7
xviii	10.10	0.5	8.38	1.0	5.39	1.4	10.48	0.4
xix	10.56	0.4	8.56	0.9	5.89	1.1	10.88	0.4
xx	10.83	0.4	8.92	0.8	6.05	1.0	11.23	0.3
xxi	12.33	0.2	9.07	0.7	6.21	1.0	11.76	0.3
xxii	14.94	0.1	9.15	0.7	6.22	1.0	13.30	0.1
xxiii	15.16	0.1	9.40	0.6	6.44	0.9	13.75	0.1
xxiv	16.54	0.0	10.07	0.5	6.59	0.8		
xxv	17.58	0.0	10.09	0.5	6.94	0.7		
xxvi	18.92	0.0	10.24	0.4	7.28	0.6		
xxvii	19.09	0.0	10.25	0.4	7.81	0.5		
xxviii	19.14	0.0	10.32	0.4	8.07	0.5		
xxix	19.16	0.0	11.11	0.3	8.16	0.4		
xxx	22.72	0.0	11.44	0.3	8.56	0.4		
xxxi			11.82	0.2	8.67	0.4		
xxxii			11.89	0.2	8.86	0.3		
xxxiii			14.37	0.1	8.86	0.3		
xxxiv			15.09	0.1	8.88	0.3		
xxxv			15.09	0.1	9.69	0.2		
xxxvi			15.64	0.1	9.80	0.2		
xxxvii			15.85	0.0	9.93	0.2		
xxxviii			17.54	0.0	10.08	0.2		
xxxix			17.54	0.0	10.71	0.2		
xl			18.02	0.0	11.90	0.1		
xli			18.48	0.0	12.44	0.1		
xlii			22.72	0.0	12.64	0.1		

# conf.	V		VI		VII		VIII	
	ΔG^a	$\%^b$	ΔG^a	$\%^b$	ΔG^a	$\%^b$	ΔG^a	$\%^b$
xliii			25.18	0.0	12.99	0.1		
xliv					13.42	0.1		
xlv					14.24	0.0		

[a]Relative Free energy in kJ mol^{-1} calculated at the B3LYP/3-21G level of theory. [b]Room temperature population in %.