

SUPPORTING INFORMATION

Bifurcatriol, a New Antiprotozoal Acyclic Diterpene from the Brown Alga *Bifurcaria bifurcata*

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Figure S1. Key HMBC (solid line arrows), COSY (bold line) and NOESY (dashed line arrows) correlations observed in **1**.

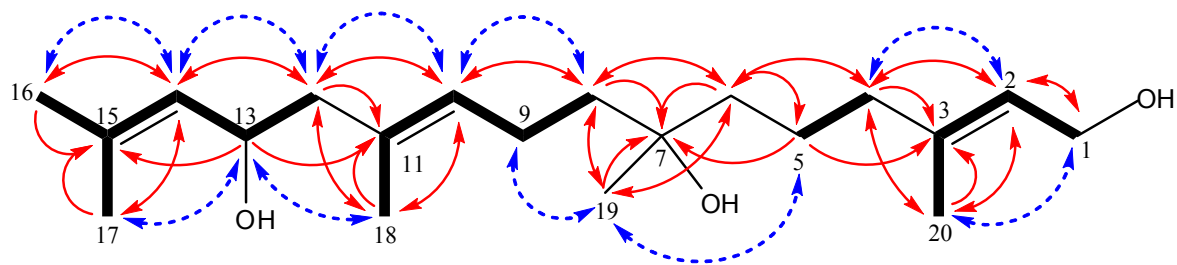


Figure S2. ¹H NMR spectrum (500 MHz, CDCl₃) of compound 1.

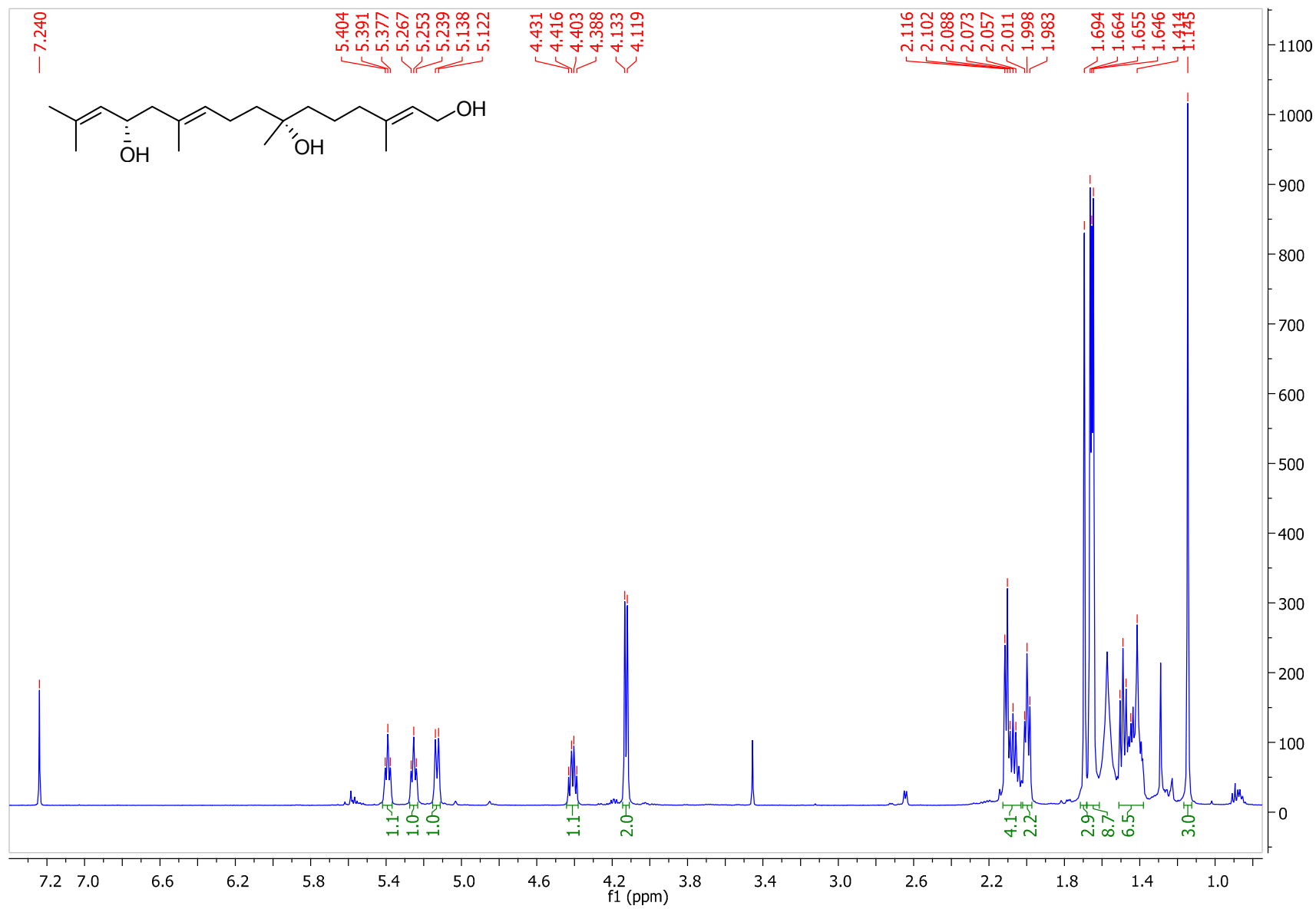


Figure S3. ^{13}C NMR spectrum (125 MHz, CDCl_3) of compound 1.

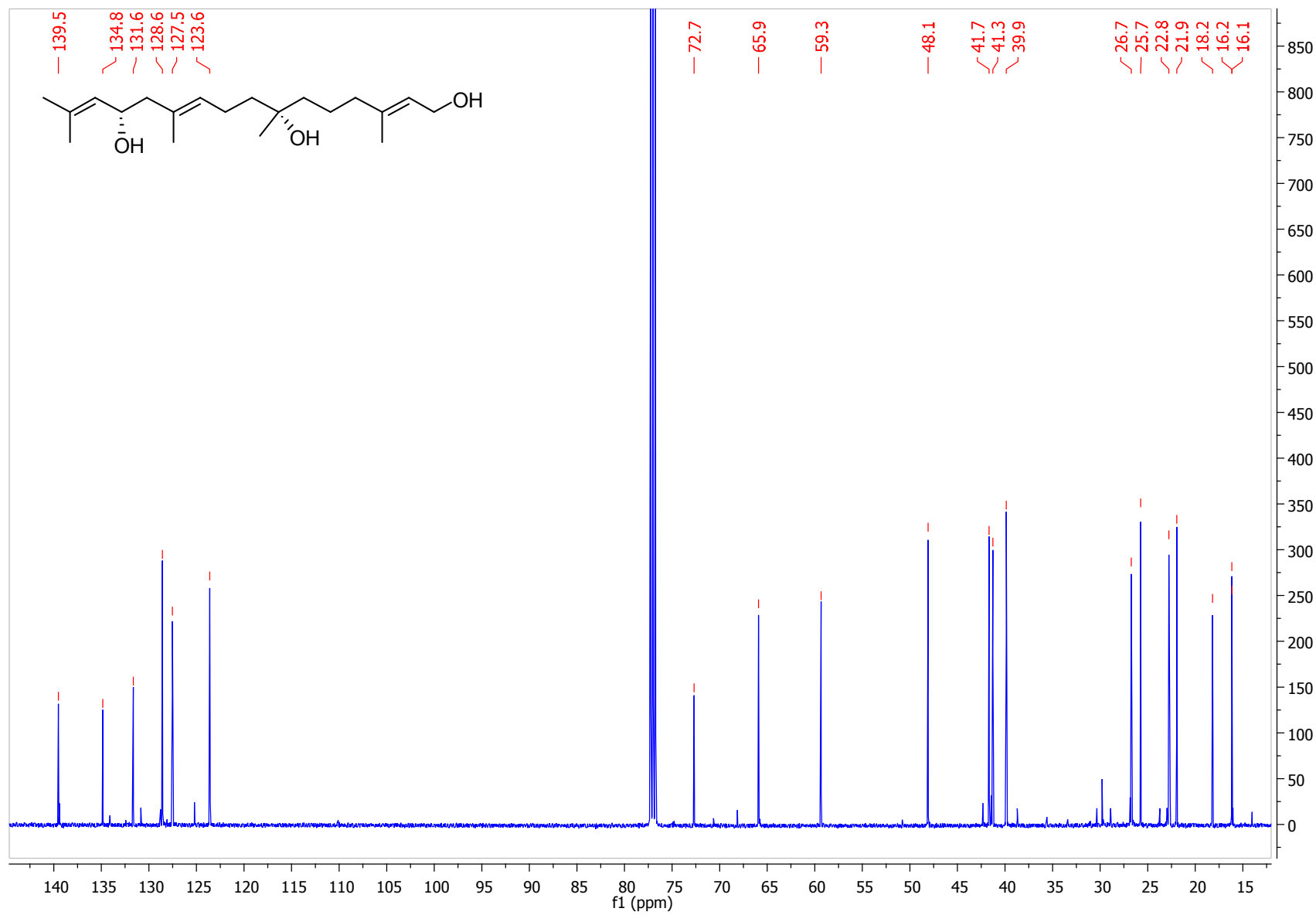


Figure S4. gCOSY spectrum (500 MHz, CDCl₃) of compound 1.

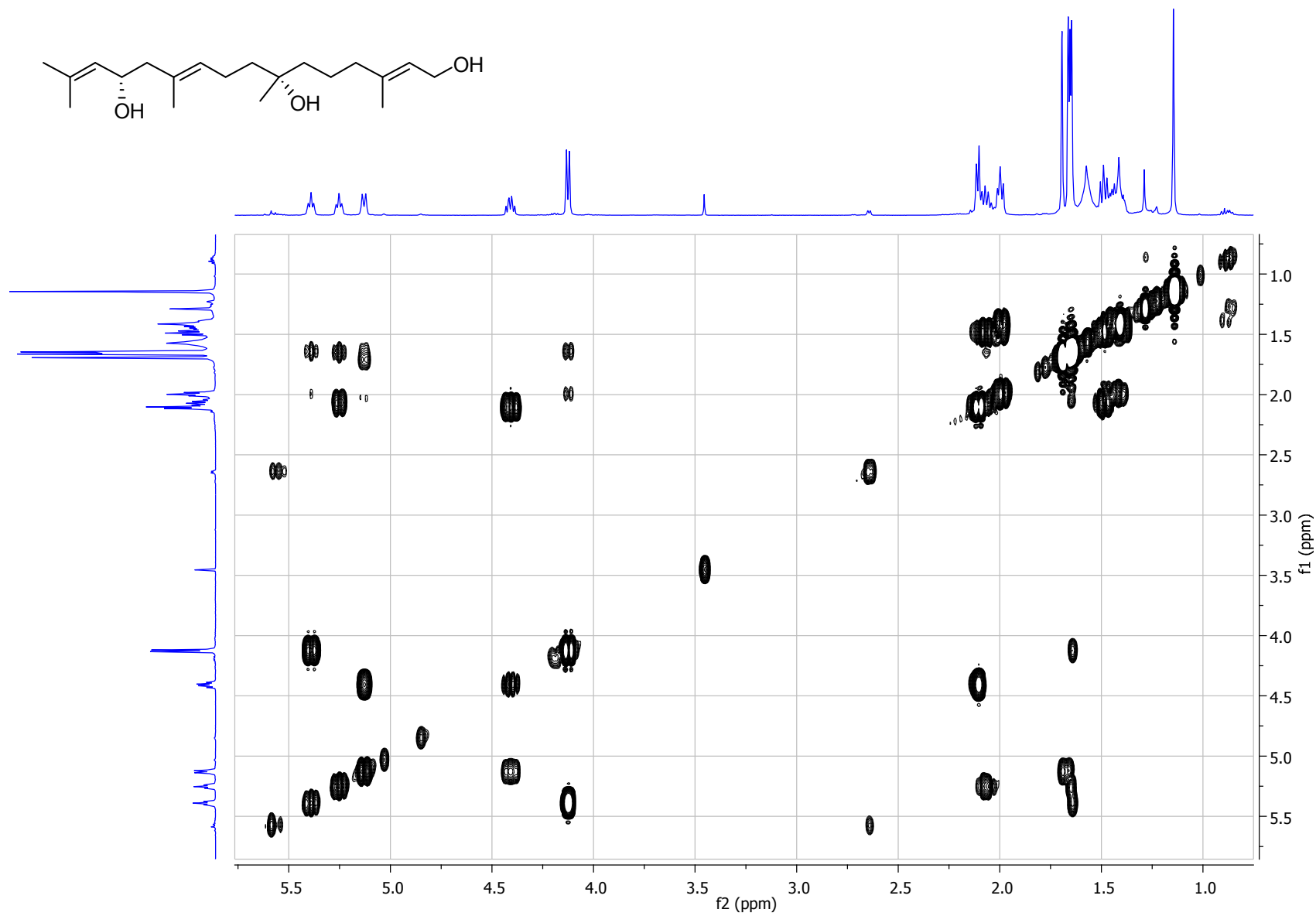


Figure S5. gHSQC spectrum (500/125 MHz, CDCl₃) of compound 1.

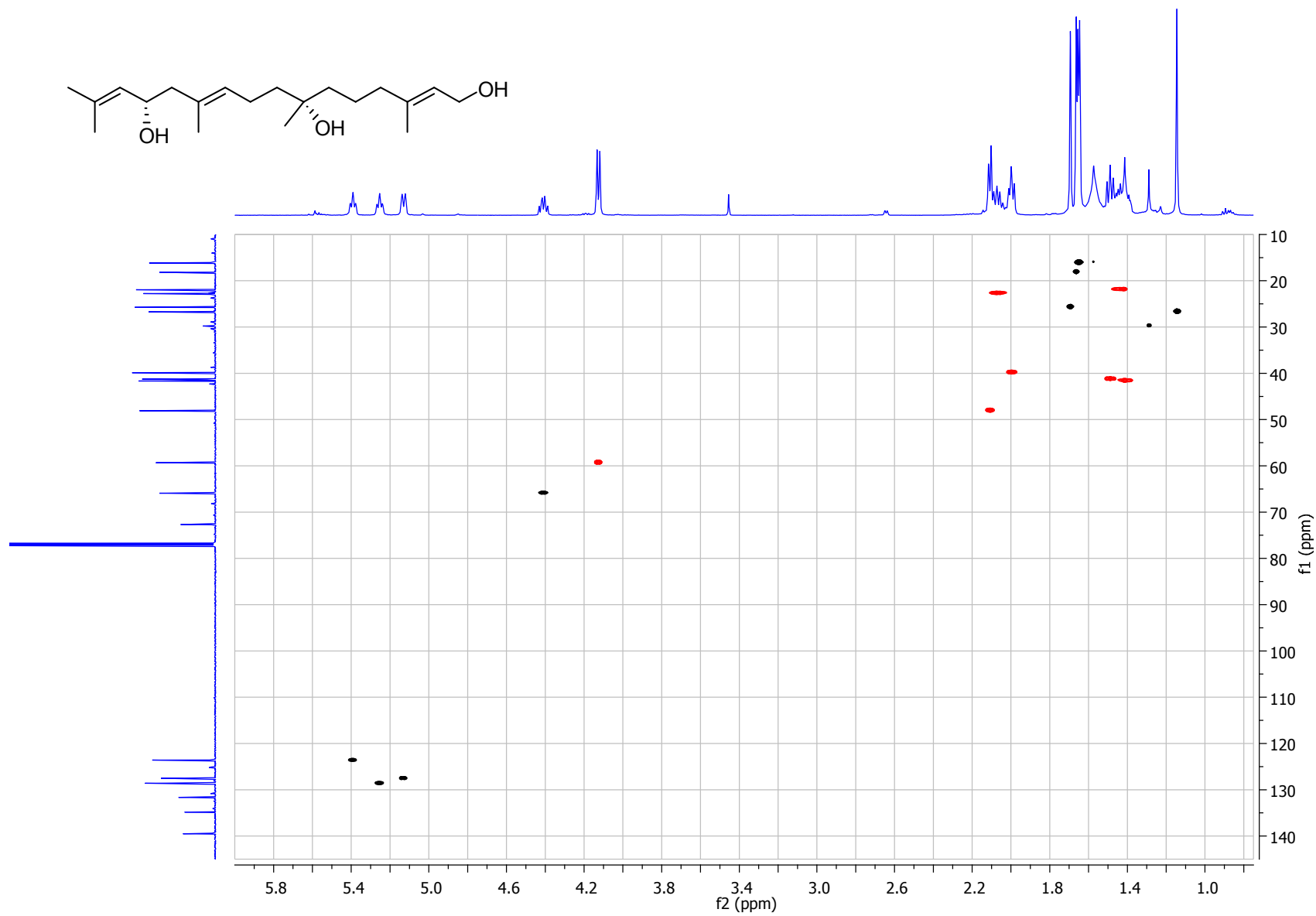


Figure S6. gHMBC spectrum (500/125 MHz, CDCl₃) of compound 1.

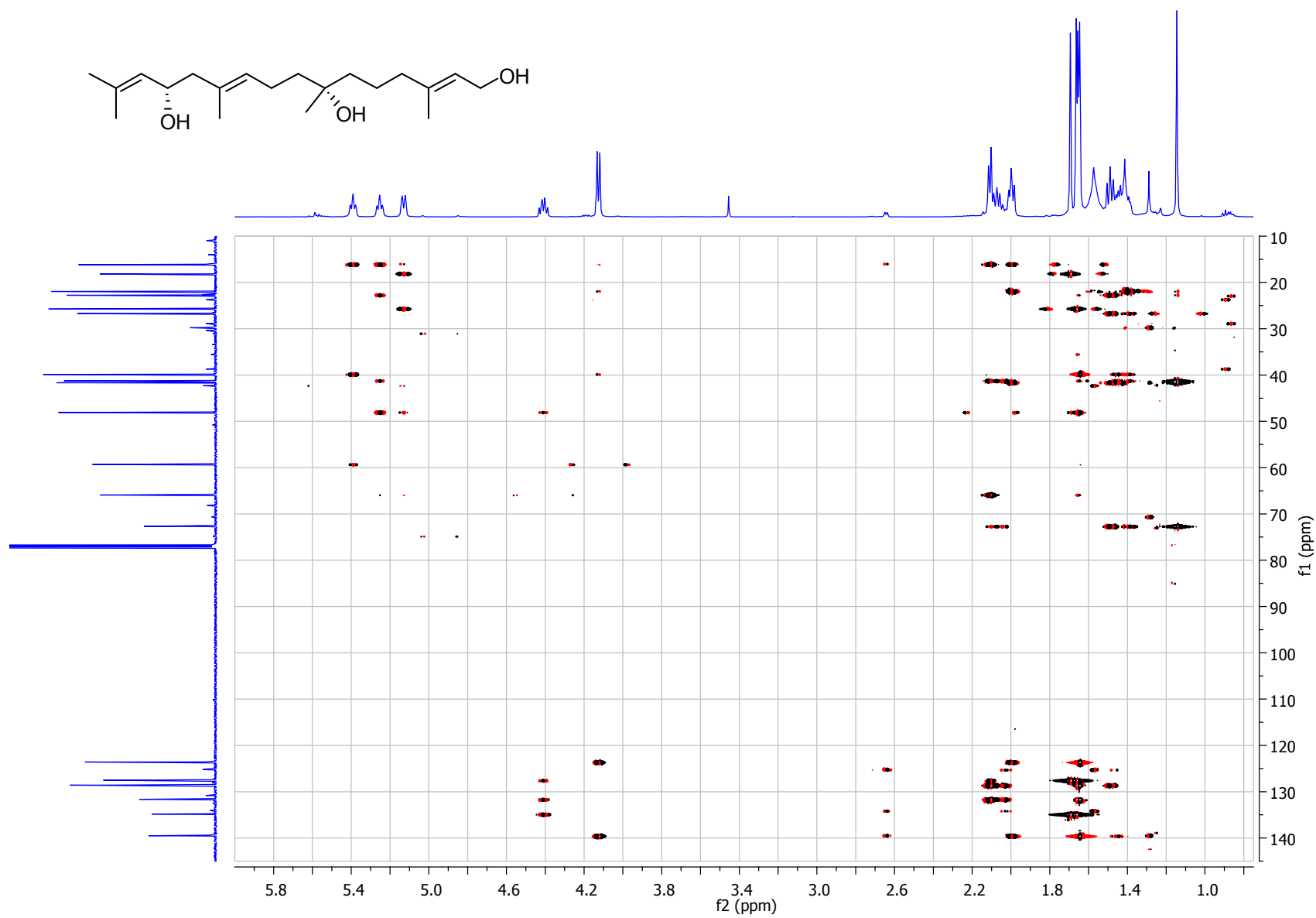


Figure S7. NOESY spectrum (500 MHz, CDCl₃) of compound 1.

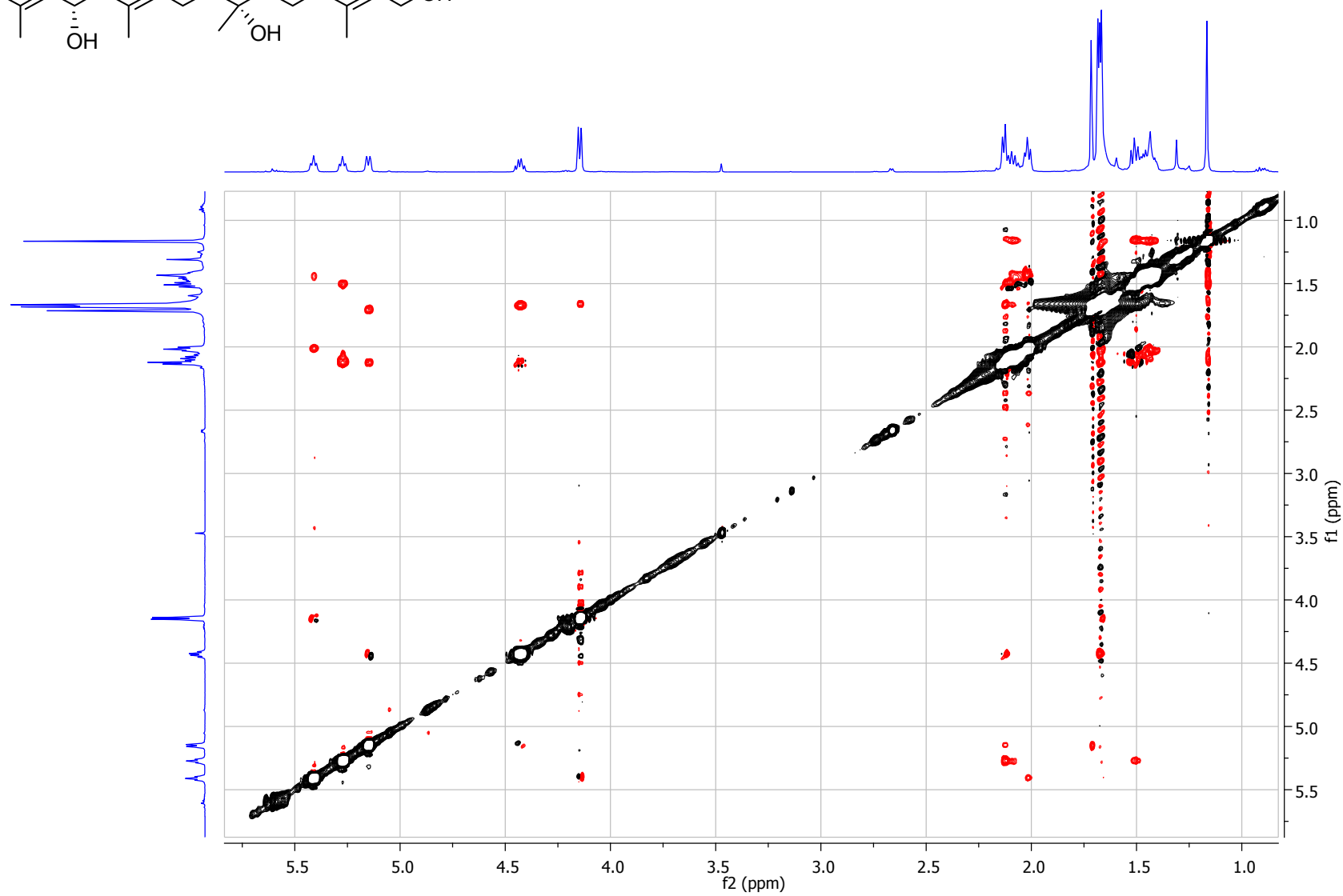
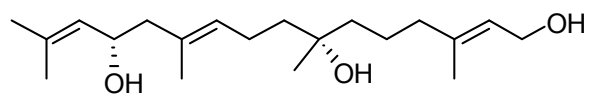
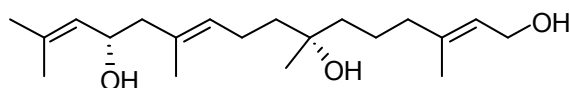


Figure S8. ESI HR-MS report for compound 1.

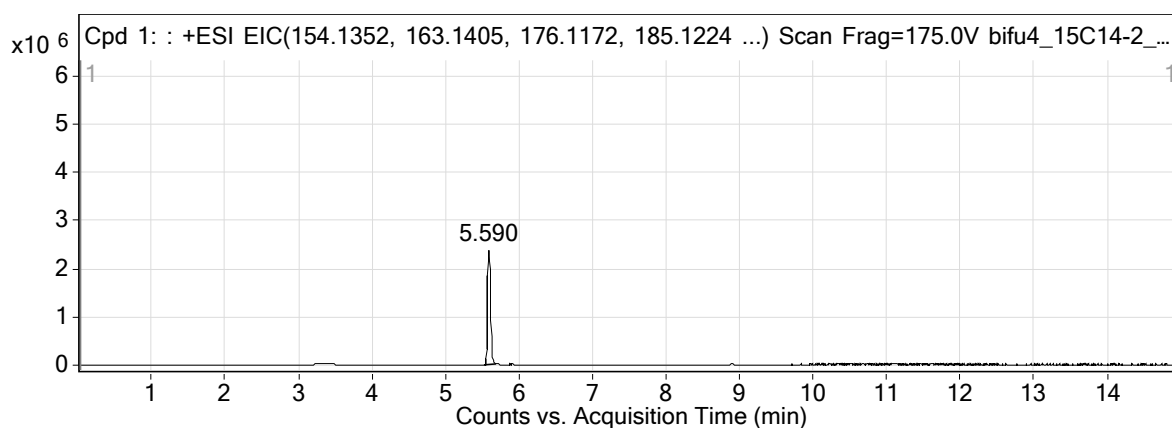
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SampleType	Sample	Position	P1-A3
InstrumentName	Instrument 1	UserName	
AcqMethod	VsmyPosFragile_BDV15.m	AcquiredTime	30-Jul-14 21:23:54
IRM	Success	DA Method	Default.m
CalibrationStatus			
Comment			

SampleGroup Info.
Fragmentor NozzleVoltage

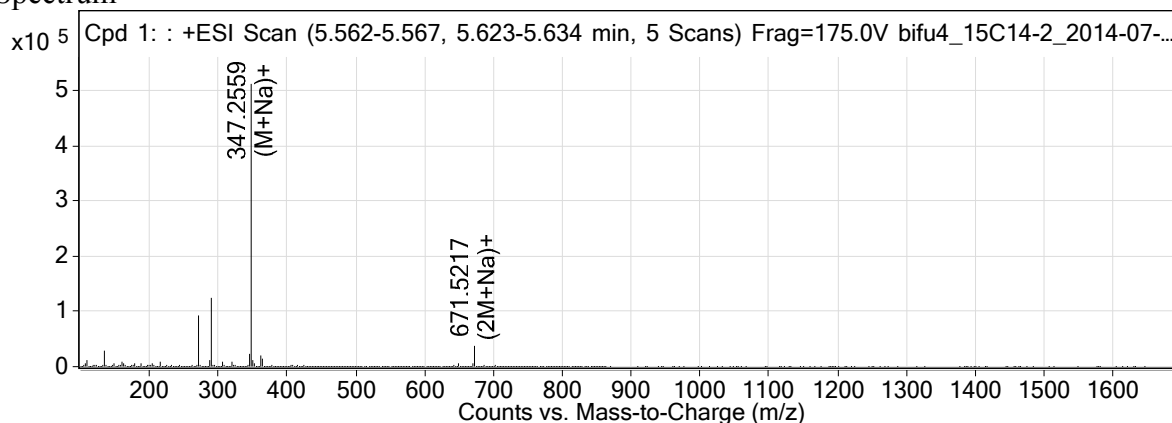


Compound Table

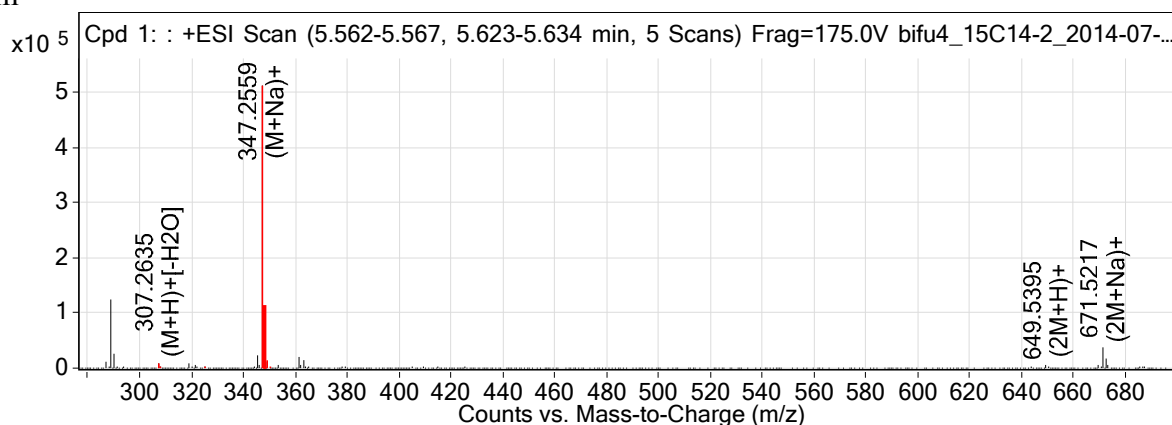
Compound Label	RT	Mass	Abund	Formula	TgtMass	Diff (ppm)	MFG Formula
Cpd 1:	5,59	324,2667	510741	C20H36O3	324,2664	0,83	C20H36O3



MS Spectrum



MS
ZoomedSpectru
m



MS SpectrumPeakList

<i>m/z</i>	<i>Calc m/z</i>	Diff (ppm)	<i>z</i>	Abund	Formula	Ion
307,2635	307,2632	-1,07	1	8316,4	C20H35O2	(M+H) ⁺ - H ₂ O
325,2739	325,2737	-0,42	1	1742,8	C20H37O3	(M+H) ⁺
347,2559	347,2557	-0,77	1	510740,9	C20H36NaO3	(M+Na) ⁺
348,2594	348,2591	-0,78	1	105320,6	C20H36NaO3	(M+Na) ⁺
349,2618	349,262	0,37	1	12928,4	C20H36NaO3	(M+Na) ⁺
631,528	631,5296	2,54	1	1036,3	C40H71O5	(2M+H) ⁺ - H ₂ O
649,5395	649,5402	1,1	1	4832,7	C40H73O6	(2M+H) ⁺
671,5217	671,5221	0,65	1	36792,7	C40H72NaO6	(2M+Na) ⁺
672,5252	672,5255	0,41	1	15971,7	C40H72NaO6	(2M+Na) ⁺

Figure S9. FT-IR (ATR) spectrum of compound **1**.

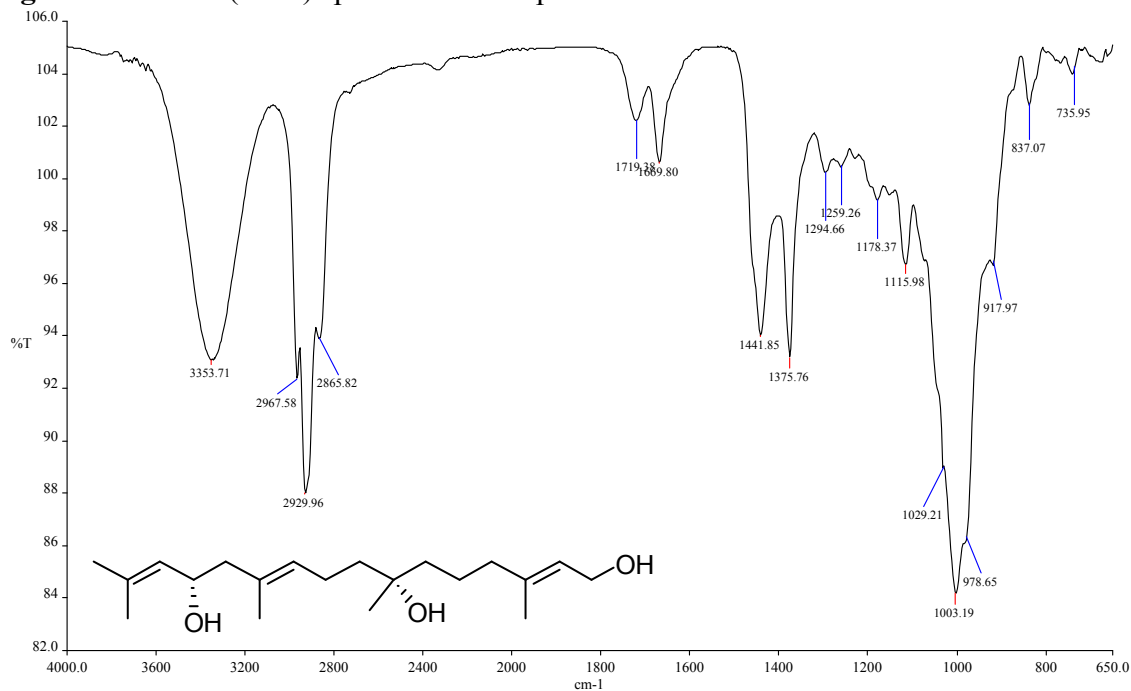


Figure S10. Comparison of the calculated VCD spectra of some key conformers of both possible stereoisomers. The green shaded area used to distinguish the isomers is found to be almost unaffected by conformational changes.

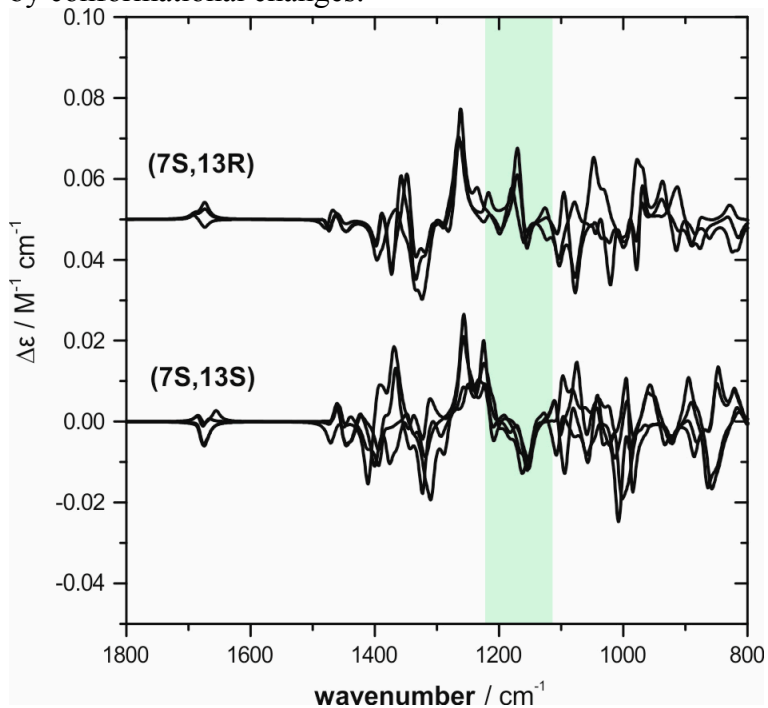


Figure S11. Correlation of experimental and predicted ^{13}C -NMR chemical shifts of (7*S*,13*S*)-**1** and (7*R*,13*S*)-**1**.

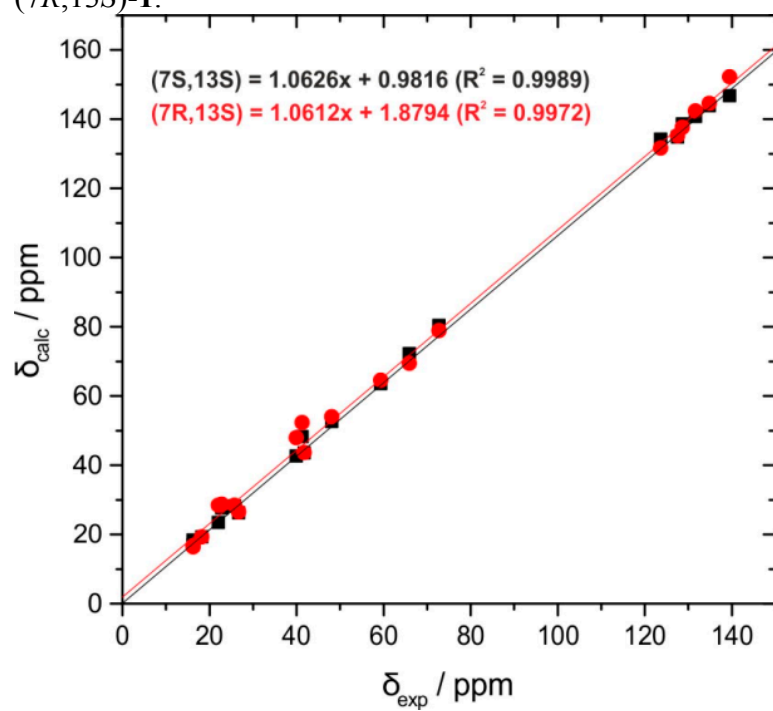


Table S1. Comparison of experimental and calculated ^{13}C chemical shifts (CDCl_3).

Carbon	$\delta_{\text{C exp}}$	$\delta_{\text{C calc (7S,13S)}}$	$\delta_{\text{C calc (7R,13S)}}$
1	59.3	64.2	64.9
2	123.6	132.8	131.3
3	139.5	147.9	153.4
4	39.9	42.1	48.1
5	22.0	23.5	28.7
6	41.7	43.2	43.7
7	72.7	81.2	79.4
8	41.3	48.9	52.2
9	22.8	27.7	28.8
10	128.6	138.8	138.2
11	131.6	141.4	142.5
12	48.1	53.0	53.9
13	65.9	72.0	69.7
14	127.5	134.4	134.8
15	134.8	145.3	145.9
16	25.7	28.4	28.5
17	18.2	19.4	19.4
18	16.1	17.0	16.5
19	26.7	26.2	26.6
20	16.2	18.9	16.8
MAD ^(a)		3.0	3.2
R ² ^(b)		0.9987	0.9971
DP4 ^(c)		100%	0%

^(a) mean average deviation (in ppm), ^(b) square of the correlation factor, ^(c) DP4 probability [25].

Table S2. Calculated ^{13}C -chemical shifts for (7*S*,13*S*)-**1** and (7*R*,13*S*)-**1** (b3lyp/6-311++G(2d,p)/IEFPCM/CHCl₃).

Calculated ^{13}C -chemical shifts for (7 <i>S</i> ,13 <i>S</i>)-isomer (b3lyp/6-311++G(2d,p)/IEFPCM/CHCl ₃)																								
ΔE	ΔG	pop- ΔE	pop- ΔG	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	
bifu4_isomer1_c1	0.00	0.00	34.86	19.86	62.79	136.54	151.34	47.38	23.81	47.67	80.14	48.22	28.41	141.93	137.81	53.41	72.61	134.44	145.16	28.44	19.41	16.98	23.88	16.48
bifu4_isomer1_c2	0.45	0.19	16.31	14.35	63.61	136.45	146.92	42.66	23.61	43.42	82.03	46.01	27.07	142.08	138.64	53.57	71.95	134.67	144.20	28.34	19.41	16.58	26.28	16.30
bifu4_isomer1_c3	4.05	0.30	0.04	11.92	65.22	127.37	150.03	41.58	21.63	44.61	81.49	52.41	27.72	140.28	141.33	53.75	69.70	134.64	146.16	28.53	19.42	16.12	22.92	19.75
bifu4_isomer1_c4	4.04	0.43	0.04	9.58	65.19	127.43	149.99	41.63	21.61	44.24	81.55	51.49	27.57	140.26	141.03	53.70	69.55	134.61	146.19	28.53	19.41	16.15	22.82	19.73
bifu4_isomer1_c5	1.05	0.67	5.93	6.41	64.31	129.34	145.89	39.73	21.67	41.20	79.61	48.30	27.36	134.24	147.01	50.31	73.48	134.39	147.30	28.54	19.13	17.76	28.38	19.66
bifu4_isomer1_c6	1.19	0.72	4.70	5.94	65.25	133.92	140.73	39.27	22.32	38.10	82.37	49.07	27.34	135.65	143.13	53.28	73.14	134.17	145.14	28.40	19.44	17.42	29.99	19.80
bifu4_isomer1_c7	0.82	0.77	8.75	5.41	64.06	129.95	144.84	39.58	21.99	38.53	82.42	49.30	27.20	135.65	143.23	52.30	73.27	134.43	144.23	28.36	19.38	17.68	30.03	19.55
bifu4_isomer1_c8	2.19	0.83	0.87	4.87	64.25	129.07	147.23	42.22	22.01	44.38	80.39	53.72	29.54	137.52	144.48	53.10	72.20	132.95	147.47	28.49	19.42	16.63	25.67	19.87
bifu4_isomer1_c9	1.14	0.84	5.08	4.80	64.50	136.85	147.61	38.33	30.69	39.34	81.26	45.98	27.31	134.42	144.41	53.51	72.87	134.56	144.19	28.37	19.43	17.66	29.96	22.89
bifu4_isomer1_c10	0.87	0.88	7.96	4.47	64.13	129.76	144.29	39.19	21.62	40.47	82.19	46.51	27.17	135.03	144.00	52.33	73.18	134.42	144.31	28.38	19.40	17.82	30.36	19.64
bifu4_isomer1_c11	1.54	1.06	2.57	3.30	64.60	136.75	147.62	38.75	30.71	37.61	81.60	48.84	27.27	134.61	143.81	53.46	72.92	134.74	143.71	28.35	19.40	17.73	29.75	22.73
bifu4_isomer1_c12	1.42	1.25	3.16	2.40	64.54	136.39	147.12	38.25	29.14	43.77	81.74	46.24	27.14	141.86	138.93	53.68	71.39	134.20	144.96	28.38	19.49	16.61	25.86	22.82
bifu4_isomer1_c13	1.77	1.32	1.76	2.15	65.64	132.84	141.99	39.53	21.83	40.31	79.58	47.79	27.50	133.77	147.87	51.60	73.37	134.46	146.92	28.50	19.11	17.53	28.60	19.98
bifu4_isomer1_c14	1.59	1.48	2.37	1.64	63.97	134.67	148.15	42.40	25.15	37.87	82.18	49.04	28.17	133.88	141.51	46.66	73.73	134.71	142.62	28.24	19.26	21.92	29.89	16.37
bifu4_isomer1_c15	1.79	1.50	1.69	1.57	65.08	134.62	150.31	39.15	30.30	40.16	78.63	48.16	27.59	133.96	146.81	51.07	73.03	134.43	147.00	28.52	19.09	17.72	28.33	22.68
bifu4_isomer1_c16	1.33	1.70	3.67	1.12	63.83	133.56	150.53	43.30	22.01	50.89	80.17	45.89	29.24	139.74	138.55	53.23	71.87	134.88	145.38	28.51	19.35	16.96	23.55	20.90
bifu4_isomer1_c17	3.79	2.87	0.06	0.16	62.95	129.41	150.35	39.47	21.18	41.35	81.97	48.93	27.04	136.40	144.14	52.88	73.53	133.74	145.20	28.38	19.45	16.86	26.93	20.60
bifu4_isomer1_c18	3.60	3.73	0.08	0.04	63.62	139.25	148.16	47.45	23.91	47.94	80.45	48.41	28.73	140.09	139.57	51.99	74.10	131.03	151.08	29.13	21.72	17.31	23.83	16.14
bifu4_isomer1_c19	3.96	4.56	0.04	0.01	63.63	127.88	149.07	38.51	24.39	34.67	83.20	50.80	28.36	133.89	141.29	47.18	73.92	134.70	142.69	28.24	19.30	21.85	29.34	19.42
bifu4_isomer1_c20	3.96	4.73	0.04	0.01	63.95	136.52	146.37	42.70	23.70	43.08	82.53	45.79	27.12	141.67	139.33	51.90	73.25	130.85	151.62	29.07	21.87	16.43	25.33	16.29
bifu4_isomer1_c21	5.43	5.28	0.00	0.00	64.14	129.72	145.70	39.55	21.70	40.88	80.07	48.18	27.12	132.82	149.47	49.48	77.15	133.52	152.15	29.51	21.78	18.62	28.27	19.70
bifu4_isomer1_c22	4.97	5.35	0.01	0.00	64.27	136.60	147.86	37.99	30.73	39.89	81.48	45.89	27.15	133.84	145.49	51.51	74.27	131.54	150.66	29.04	22.20	18.04	29.78	22.84
bifu4_isomer1_c23	5.29	6.23	0.00	0.00	64.42	136.71	147.73	38.43	30.94	37.95	81.87	48.70	27.12	134.23	144.69	51.46	74.24	131.58	150.77	29.03	22.32	18.07	29.62	22.64
Boltzmann average					64.18	132.75	147.89	42.07	23.54	43.17	81.17	48.86	27.71	138.79	141.44	52.99	72.03	134.44	145.33	28.44	19.38	17.03	26.17	18.92

Calculated ¹³ C-chemical shifts for (7R,13S)-isomer (b3lyp/6-311++G(2d,p)/IEFPCM/CHCl ₃)																								
ΔE	ΔG	pop- ΔE	pop- ΔG	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	
bifu4_isomer2_c1	0.00	0.16	35.05	31.81	64.82	131.26	154.07	47.09	28.76	43.30	79.44	52.97	29.73	138.23	142.47	54.08	69.66	134.79	145.98	28.52	19.40	16.47	26.25	16.36
bifu4_isomer2_c2	0.00	0.00	34.86	41.86	64.97	131.42	153.03	48.62	28.54	43.38	79.36	52.99	29.78	138.16	142.47	54.02	69.72	134.79	145.94	28.52	19.39	16.52	26.30	17.05
bifu4_isomer2_c3	0.17	0.30	26.50	25.38	64.93	131.25	153.06	48.52	28.95	45.00	79.19	50.15	26.07	138.19	142.61	53.67	69.73	134.83	145.80	28.51	19.42	16.43	27.47	17.02
bifu4_isomer2_c4	2.01	4.95	1.19	0.01	64.57	135.86	146.33	45.63	24.01	42.31	80.26	48.47	26.28	133.42	142.03	48.97	70.80	132.28	148.00	28.49	19.48	20.34	27.20	15.21
bifu4_isomer2_c5	2.15	2.42	0.93	0.70	64.87	126.26	153.60	41.74	25.97	39.73	80.71	52.79	26.80	139.29	142.09	53.69	69.52	134.80	146.01	28.53	19.40	16.55	29.80	19.42
bifu4_isomer2_c6	2.78	3.92	0.32	0.06	64.69	132.63	151.65	46.23	23.62	45.11	79.85	47.10	28.10	137.62	146.41	50.56	75.69	133.41	146.35	28.63	19.03	20.60	24.20	16.10
bifu4_isomer2_c7	2.90	4.05	0.26	0.04	65.00	131.46	153.23	47.13	29.87	50.08	82.56	41.77	27.58	136.31	142.56	53.73	72.23	136.06	143.70	28.46	19.50	16.98	30.61	16.45
bifu4_isomer2_c8	2.91	4.70	0.26	0.02	64.84	131.60	152.68	48.42	31.28	46.65	82.26	42.73	27.77	137.05	141.29	50.55	75.43	136.38	140.75	28.32	19.04	20.05	31.89	16.92
bifu4_isomer2_c9	3.04	3.71	0.21	0.08	64.75	133.26	150.15	47.21	27.30	44.32	79.49	42.85	26.82	140.06	140.48	50.87	72.54	136.62	141.55	28.27	19.07	20.62	31.74	16.39
bifu4_isomer2_c10	3.10	4.29	0.19	0.03	64.71	129.90	152.47	48.53	28.22	52.63	81.52	40.66	28.89	139.19	138.75	50.61	74.99	136.71	140.63	28.32	18.96	20.85	29.80	17.47
bifu4_isomer2_c11	3.23	6.04	0.15	0.00	64.07	127.28	157.43	46.98	28.10	44.22	80.12	46.09	29.51	130.64	151.11	50.89	77.78	139.38	141.08	28.29	19.85	19.89	31.42	16.51
bifu4_isomer2_c12	4.18	5.19	0.03	0.01	64.70	132.64	151.61	46.30	23.62	45.15	79.86	47.13	28.17	136.40	145.61	53.06	74.24	135.02	150.79	29.32	20.95	16.39	24.30	16.10
bifu4_isomer2_c13	4.25	5.42	0.03	0.00	64.91	131.29	153.07	48.63	30.73	49.58	79.38	44.07	28.05	133.92	147.67	51.51	75.07	134.29	150.37	29.35	20.85	16.81	26.32	17.02
bifu4_isomer2_c14	4.70	6.67	0.01	0.00	65.21	132.60	154.86	42.73	34.07	47.37	79.62	42.97	29.37	139.30	141.28	49.01	75.02	134.46	145.44	28.54	19.08	20.73	25.21	21.30
bifu4_isomer2_c15	5.20	9.81	0.01	0.00	63.68	128.40	149.10	38.40	24.52	34.85	83.38	51.65	27.40	136.91	141.24	49.29	74.96	133.76	143.17	28.47	19.12	20.38	29.53	19.53
bifu4_isomer2_c16	5.74	8.76	0.00	0.00	63.96	127.42	157.57	47.08	28.01	47.88	80.46	41.32	28.74	130.87	151.16	50.75	81.04	136.80	147.44	29.40	20.59	19.57	31.70	16.47
bifu4_isomer2_c17	5.83	8.99	0.00	0.00	63.91	127.80	157.20	47.01	27.90	46.43	80.11	45.07	29.06	130.82	151.32	50.60	81.18	136.70	147.59	29.39	20.60	19.63	28.24	16.41
bifu4_isomer2_c18	7.04	10.69	0.00	0.00	64.65	132.58	149.99	46.38	29.11	47.65	80.28	41.18	29.16	135.29	146.03	50.31	81.79	130.80	151.06	29.08	21.45	20.77	31.45	16.66
bifu4_isomer2_c19	7.18	11.02	0.00	0.00	66.54	134.93	148.74	41.01	27.23	36.95	81.51	50.53	26.97	125.71	150.24	48.12	72.94	135.94	148.43	29.36	20.82	19.60	28.79	17.14
bifu4_isomer2_c20	7.23	10.94	0.00	0.00	64.94	130.12	151.79	47.01	27.03	47.02	79.88	39.26	28.51	134.16	147.70	49.77	80.90	136.97	146.73	29.61	20.22	20.86	33.58	17.11
bifu4_isomer2_c21	7.35	11.15	0.00	0.00	64.67	133.00	149.42	46.34	28.91	46.27	79.93	44.84	29.50	135.12	146.29	50.27	81.84	130.75	151.12	29.07	21.45	20.78	28.00	16.62
Boltzmann average					64.91	131.29	153.37	48.06	28.69	43.75	79.36	52.24	28.80	138.20	142.50	53.94	69.71	134.80	145.91	28.52	19.40	16.49	26.61	16.84