Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Genome Mining Reveals a New Cyclopentane-forming Sesterterpene Synthase with Unprecedented Stereo-control

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Figure S1. Phylogenetic tree of TC domains of BFTSs. (A) 115 (putative) BFTSs found in public database. (B) 15 representative BFTSs belongs to different clades.

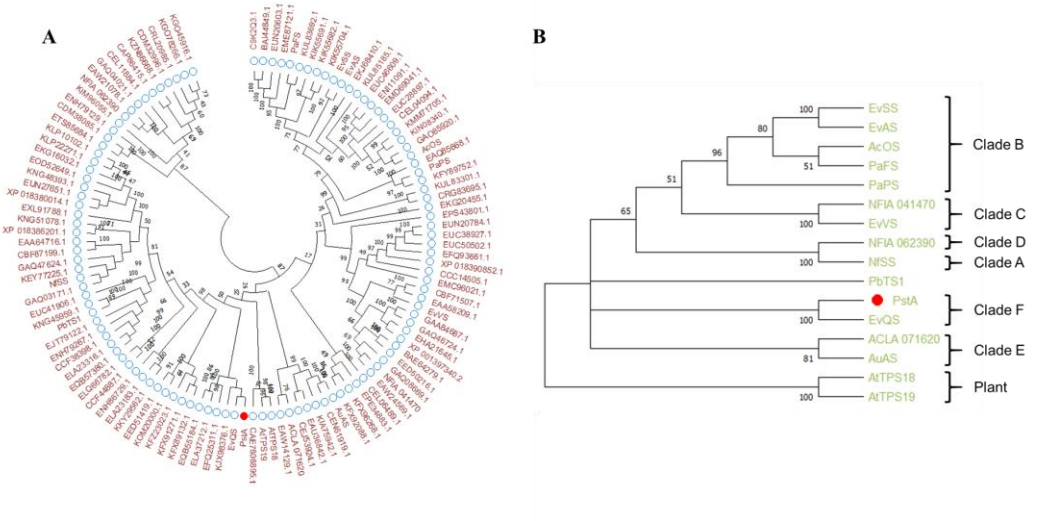


Figure S2. Representative sesterterpenoids with 5/15 *trans*-fused bicyclic ring system.

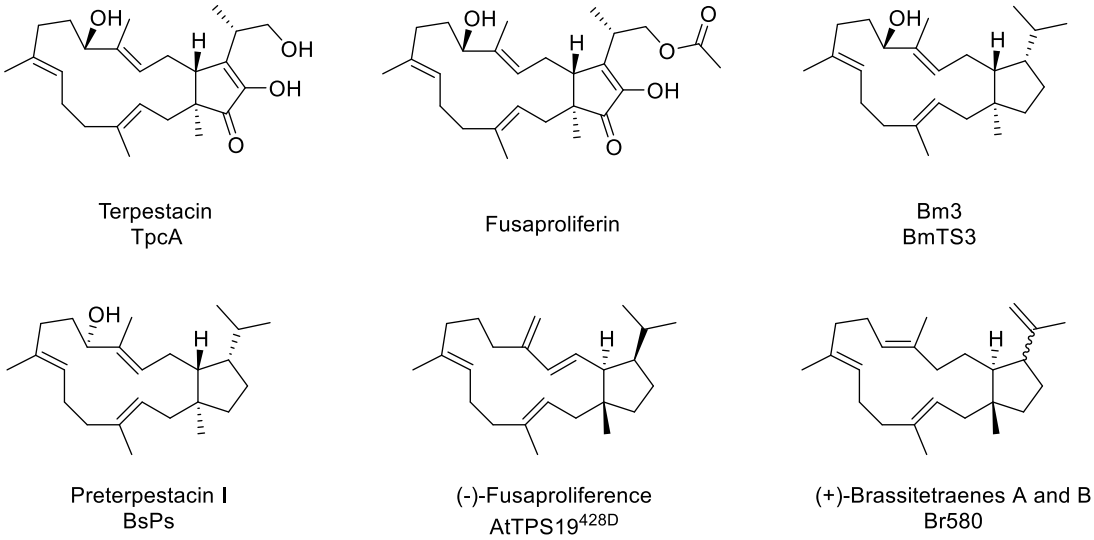


Figure S3. GC-MS analysis for the extract of metabolites of AO-PstA.

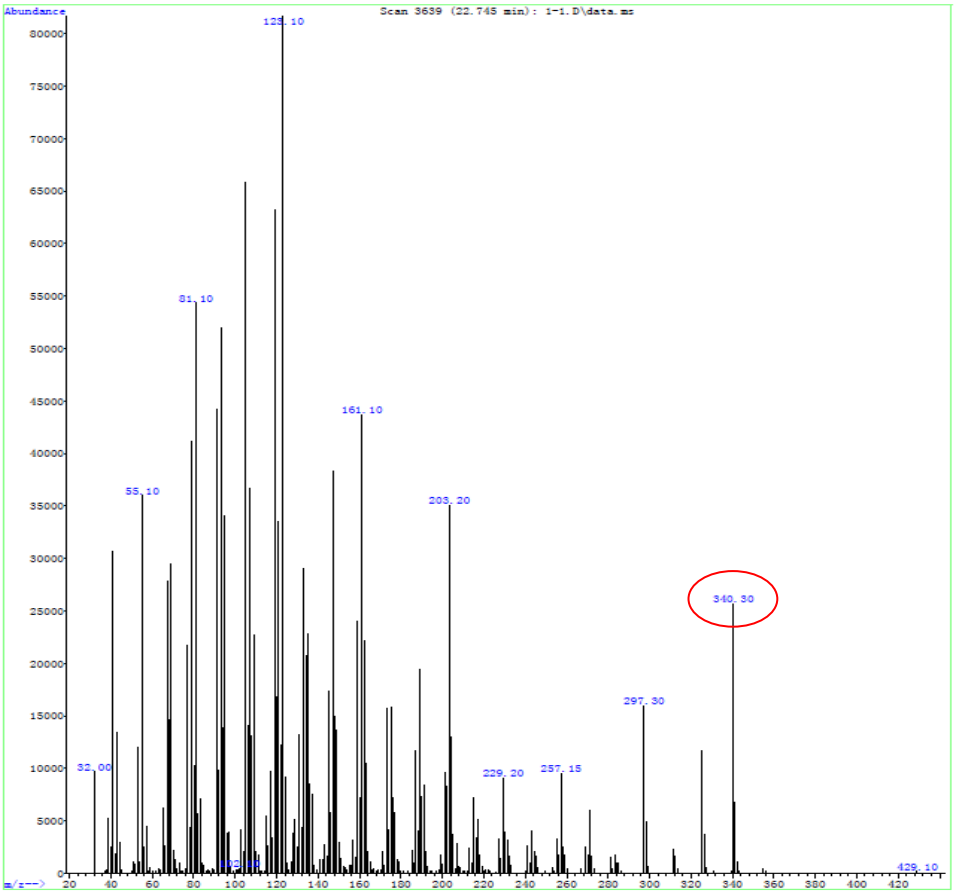


Figure S4. Chemdraw 3D models at C12/13 double bond of 1.

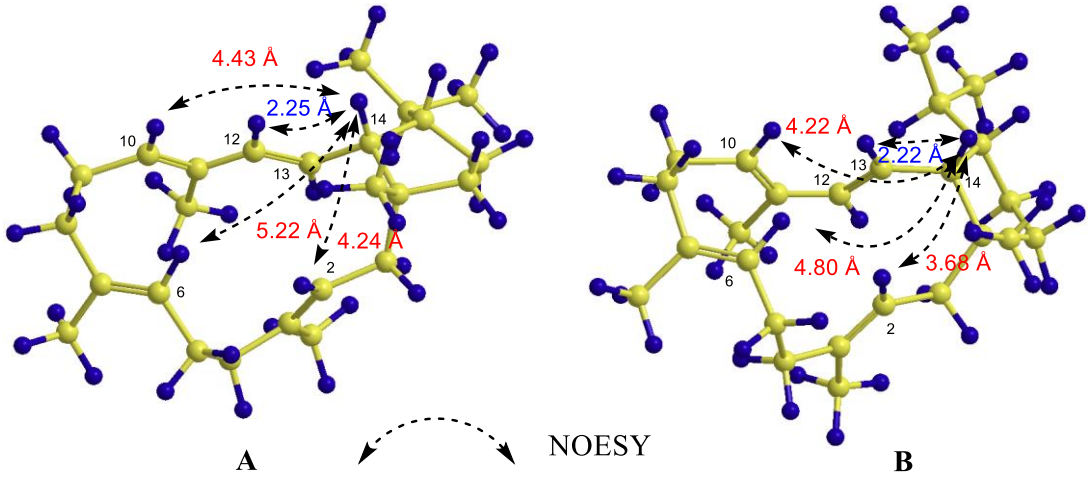


Figure S5. Two most possible C-18 isomers of 1.

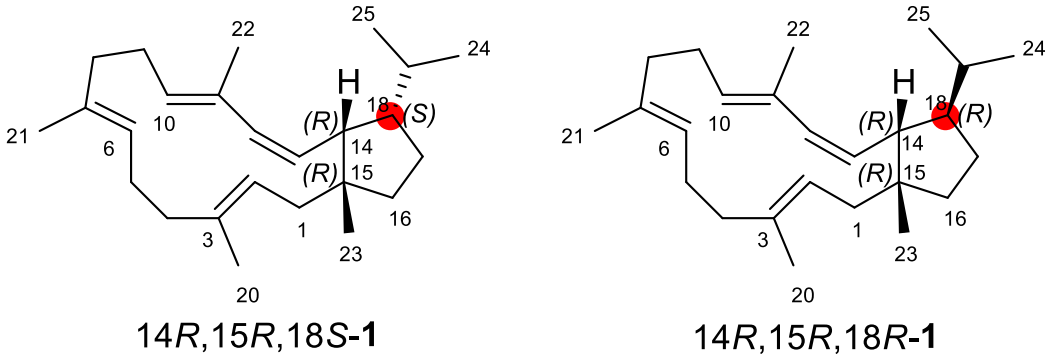


Figure S6. ^{13}C NMR calculation results of two possible isomers of 1.

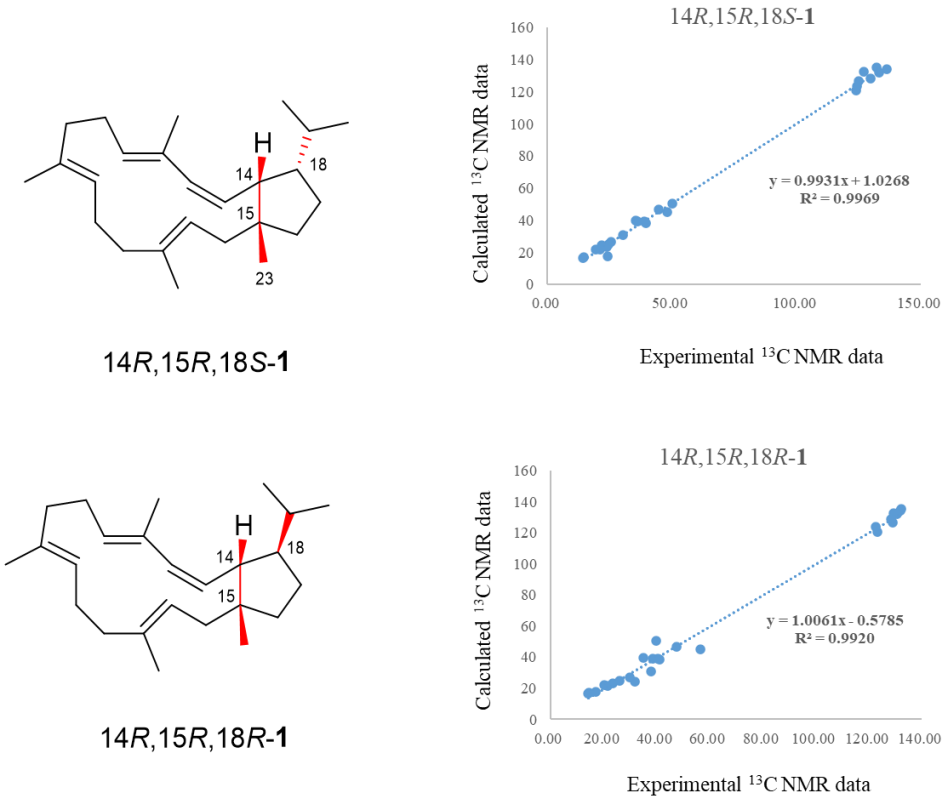


Figure S7. Chemical transformation of 1.

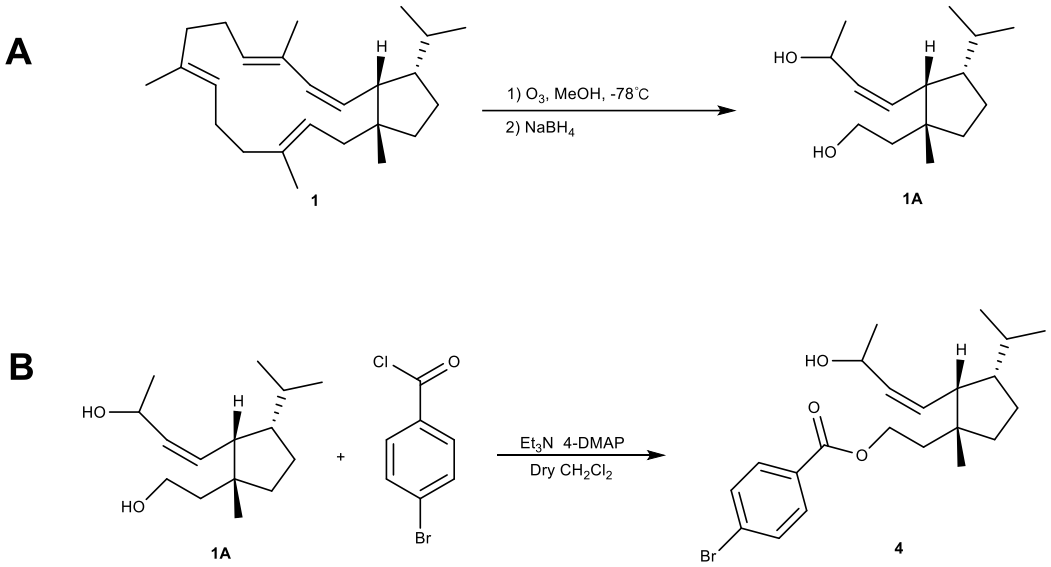


Figure S8. The key NOESY correlations of 4.

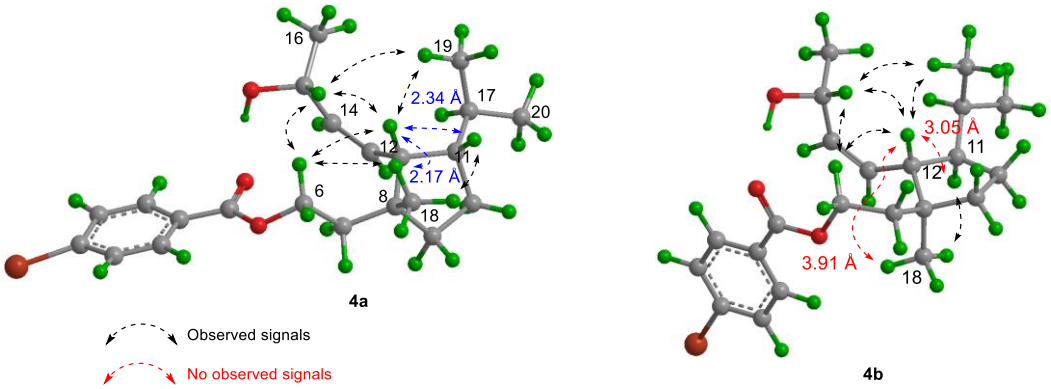
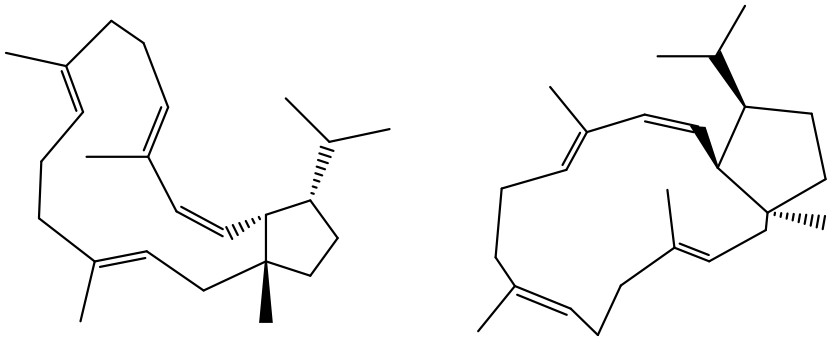


Figure S9. The absolute configuration of 1 and its enantiomer (*ent*-1).



1 *ent*-**1**

Figure S10. ^{1}H NMR spectrum (dark color) of Penisentene (1) produced by *E. coli* BL21 (compare to stand, light colour).

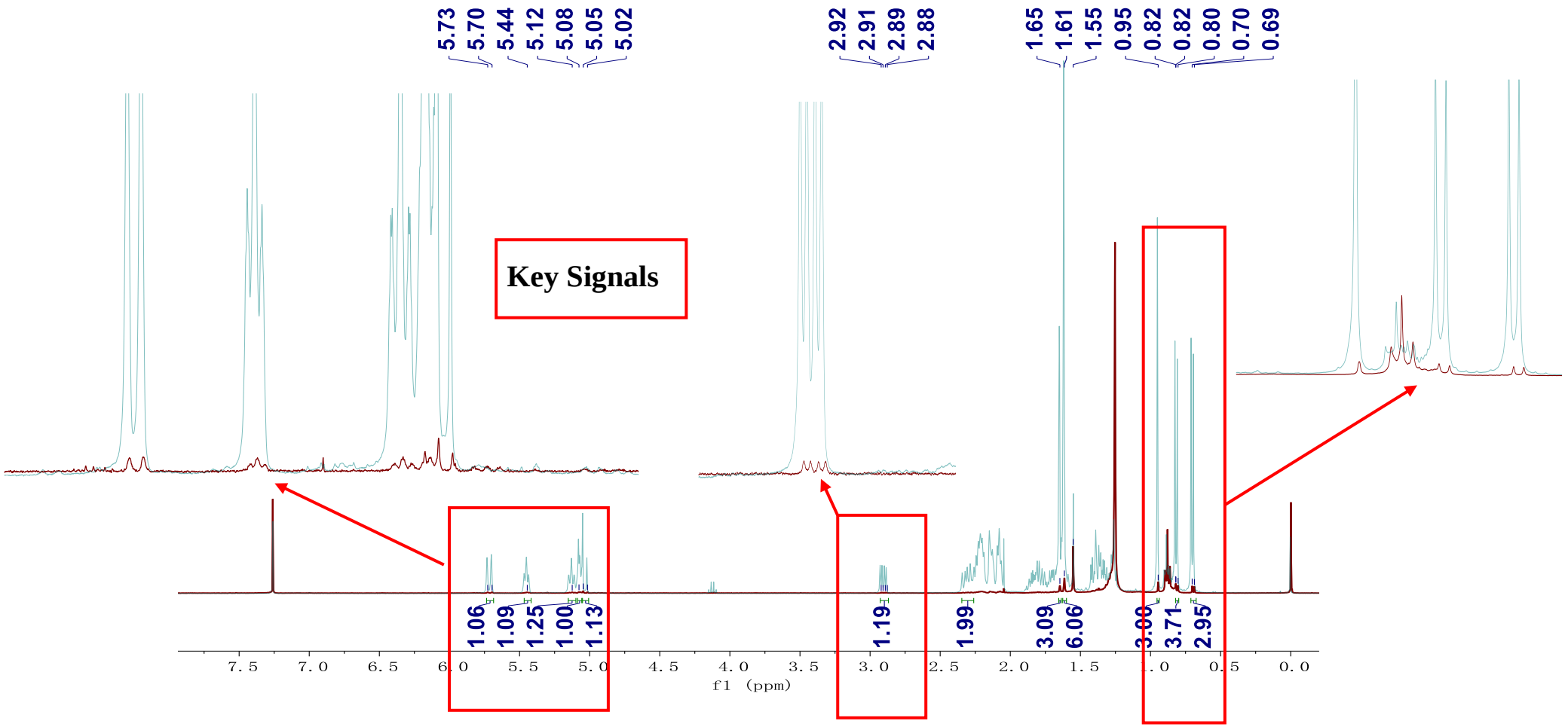
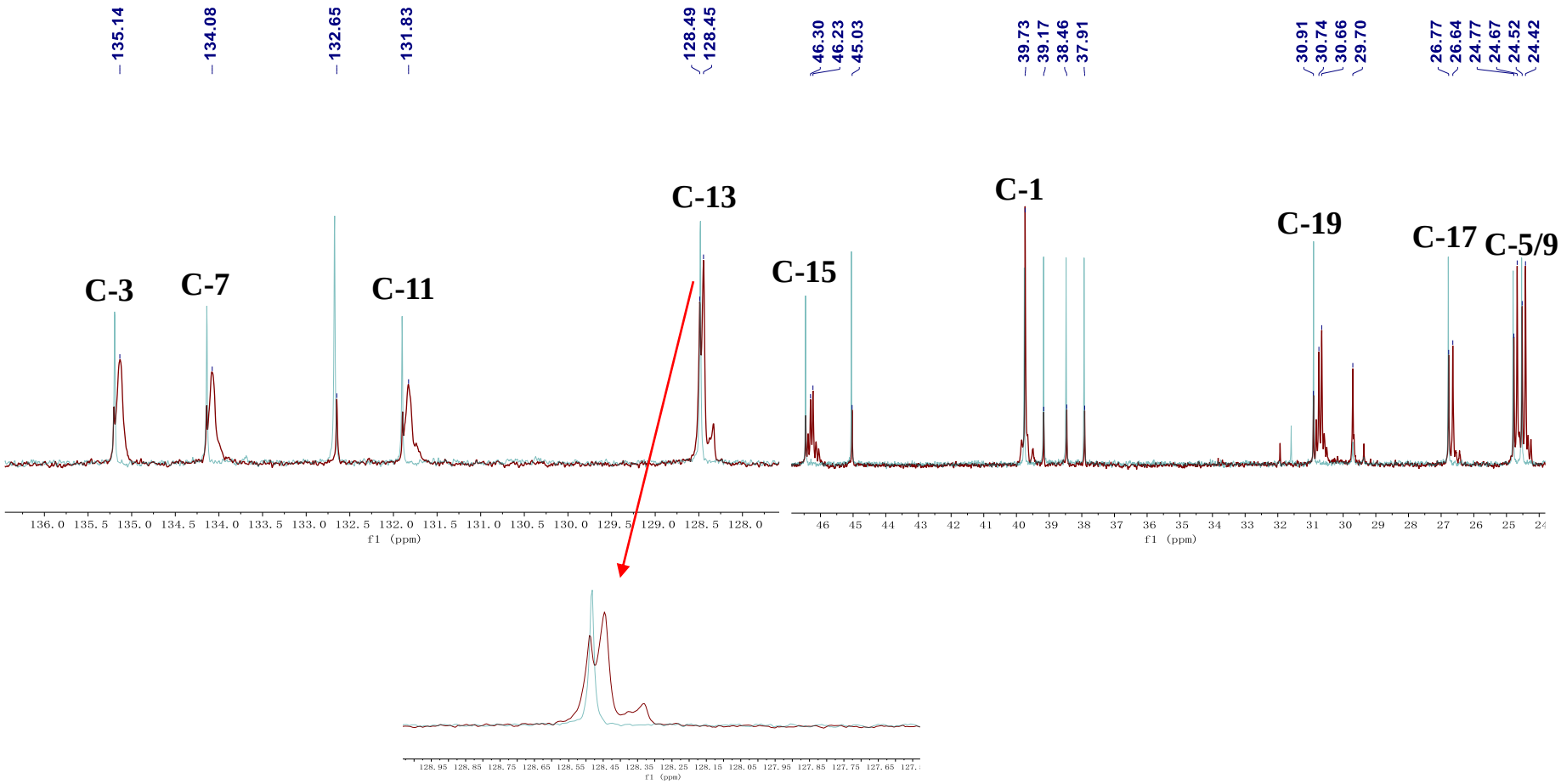


Figure S11. ^{13}C NMR spectrum of 1 prepared by feeding experiment with [1-^{13}C, $^{2}H_3$]acetate (compare to stand, light colour; and the shifted signals marked on the top of peaks).



Scheme S1. Two possible pathways.

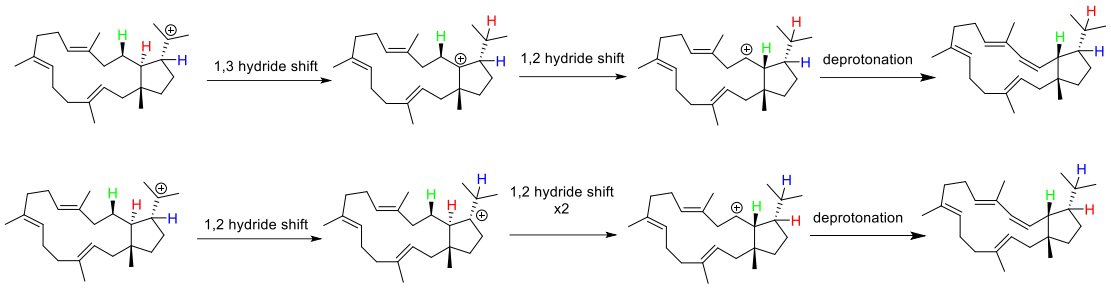
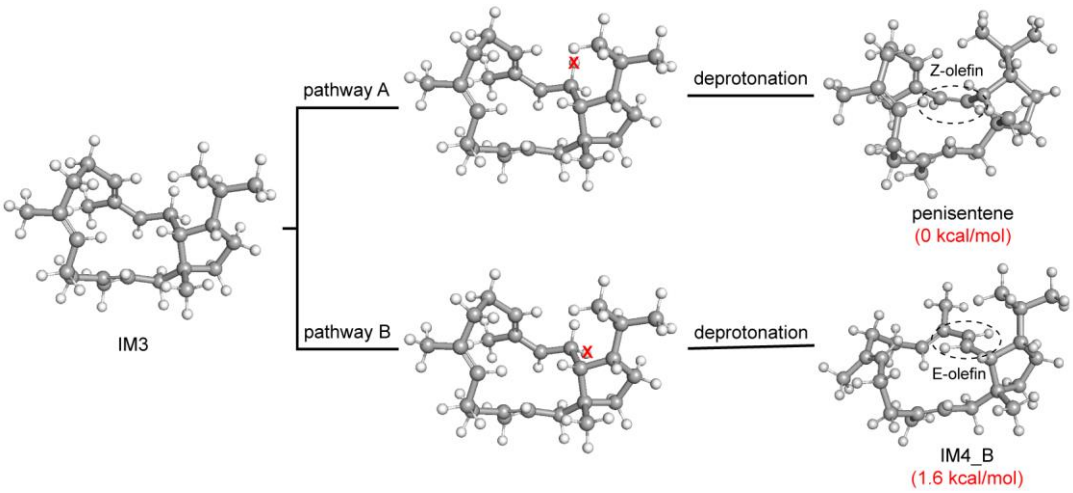


Figure S12. Deprotonation pathways from IM3 to product penisentene in the gas phase. Relative free energies (kcal/mol) are labeled with red numbers in parentheses. Structures are optimized at the M06–2X/6–31 G(d,p) level in the gas phase.



There are two dehydrogenation pathways from **IM3**, one to abstract the proton out of the plane (pathway A) and the other to abstract hydrogen receding away from the plane (pathway B). The abstracted proton is marked with a red fork. According to the DFT calculation result, two pathways produce two products with different structures, and the product penisentene with *Z*-olefin of pathway A has lower energy.

Figure S13. Cell free assay of *E. coli-pstA*.

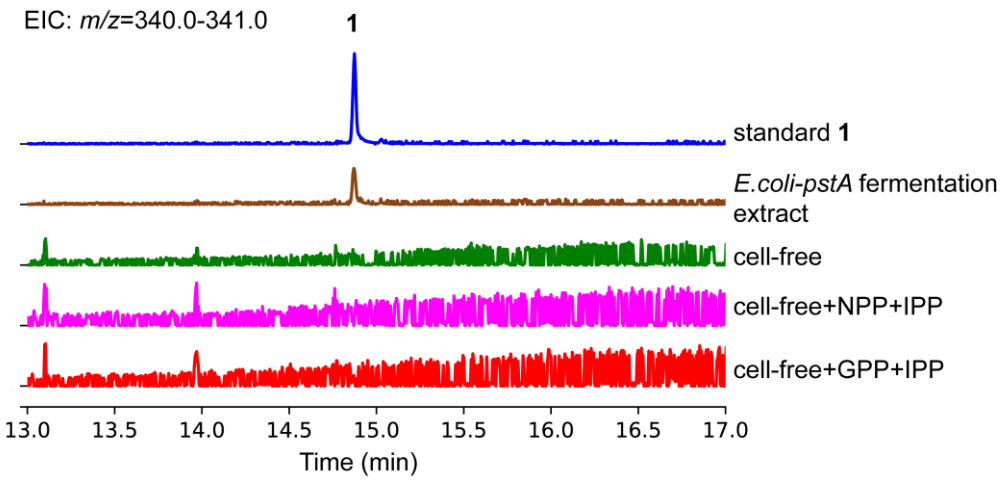


Figure S14. GC-MS analysis for the extract of metabolites of AO-PstAB.

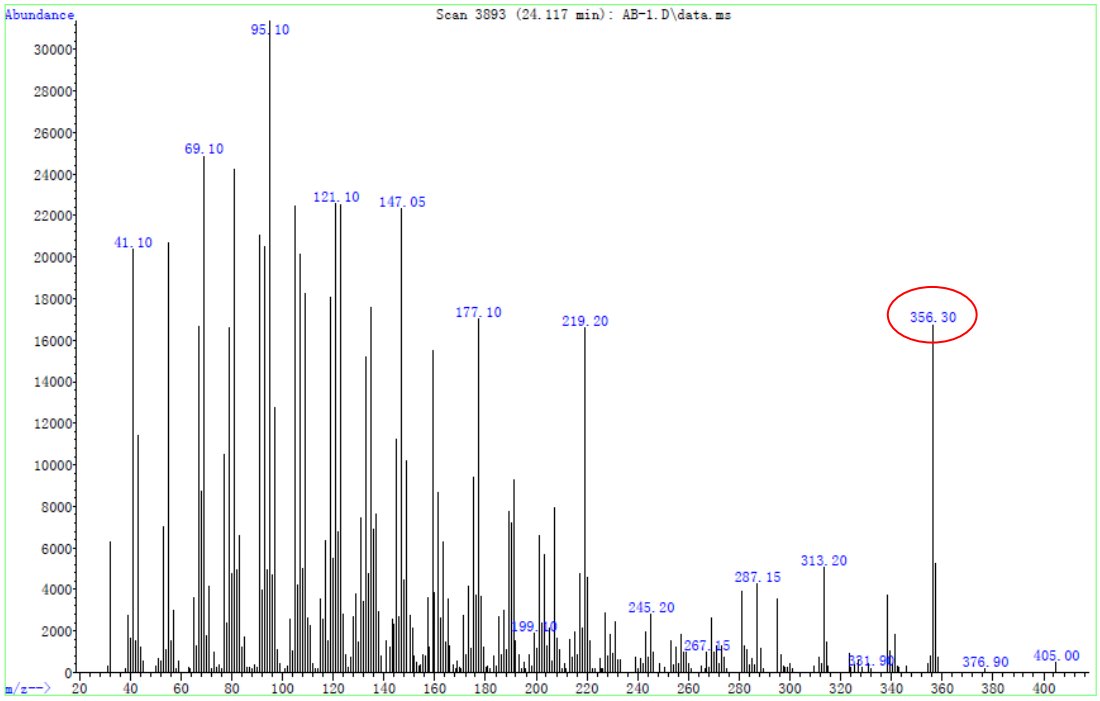


Figure S15. IR spectrum of 2.

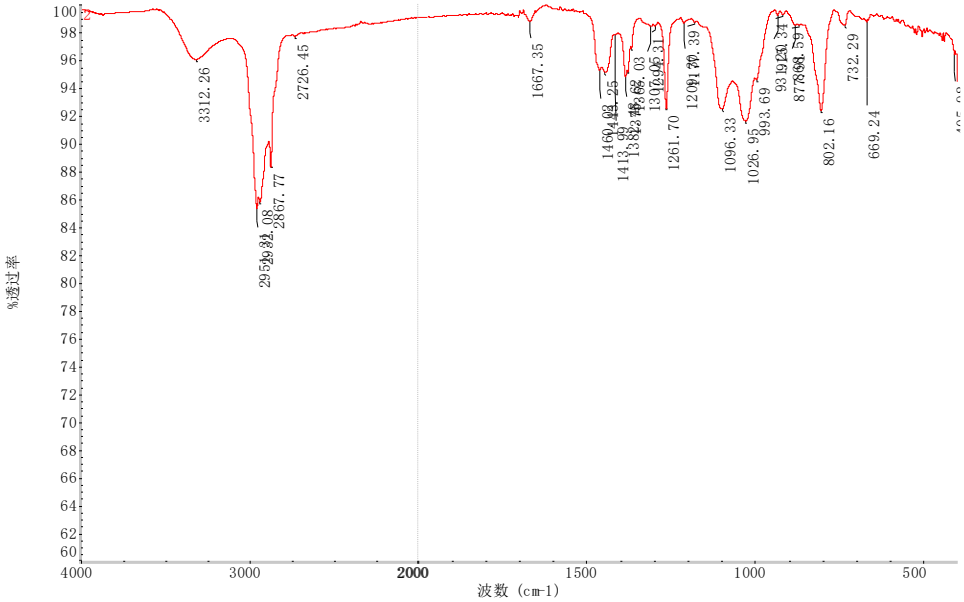


Figure S16. HRESIMS spectrum of Penisentone (3).

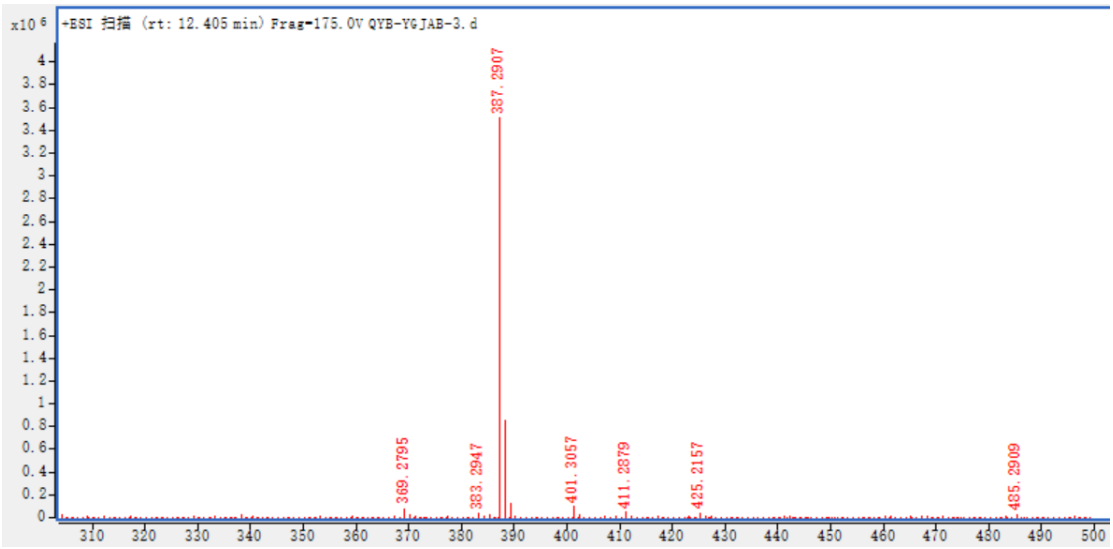


Figure S17. IR spectrum of 3.

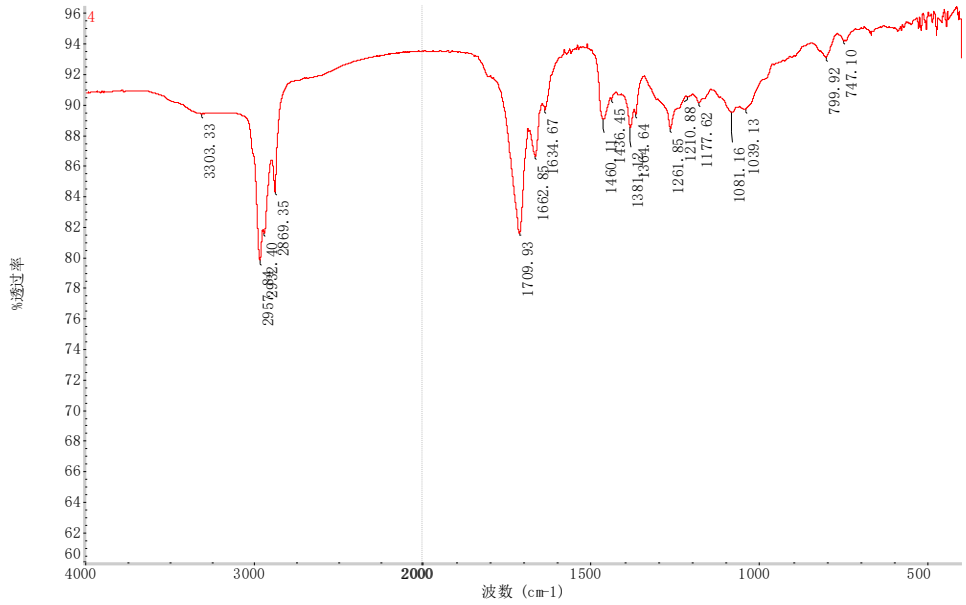


Figure S18. Possible oxidative transformations of 3 and chaetoglobosins.

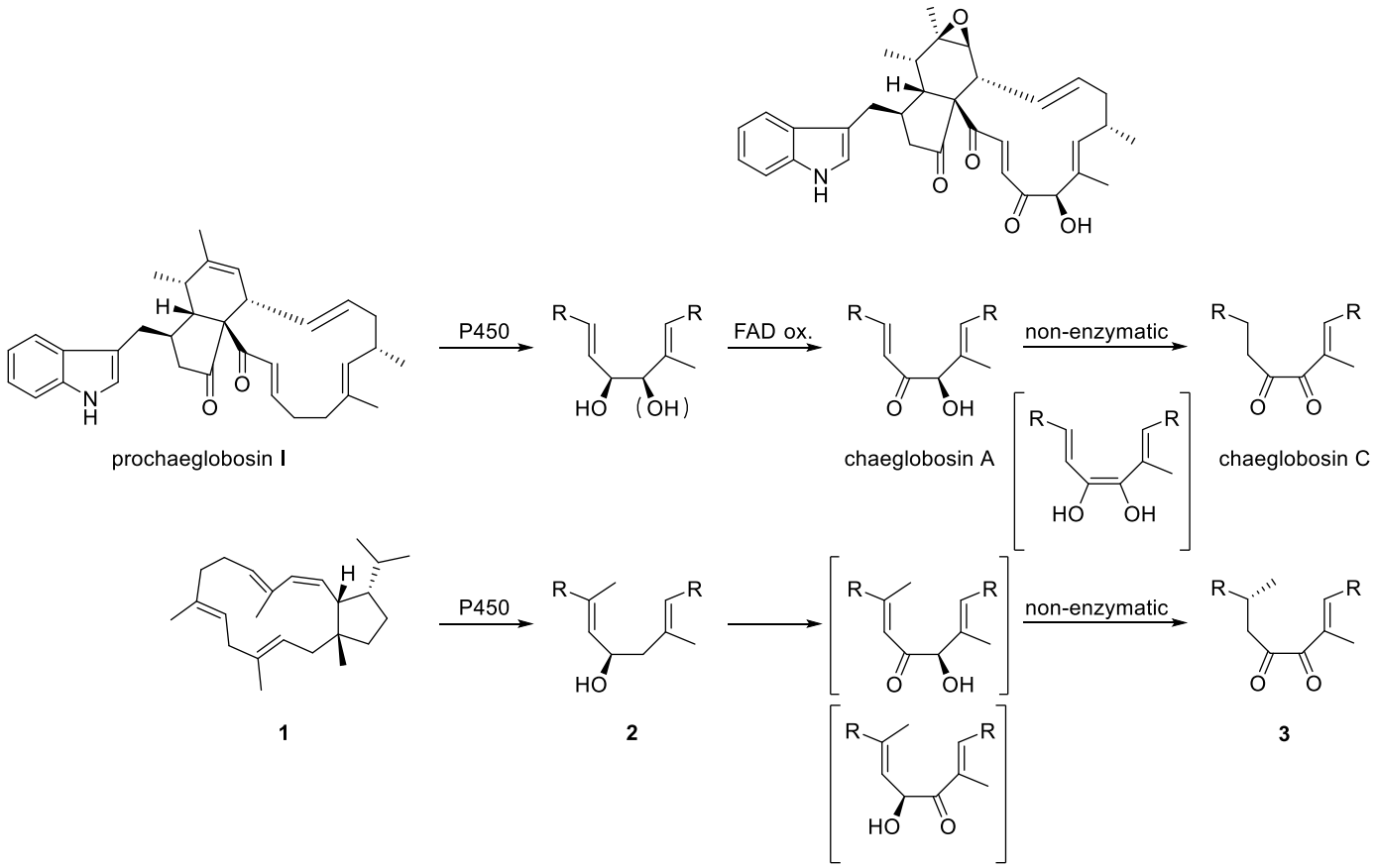


Table S1. ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) data for compound 1–3 in $CDCl_3$ (δ in ppm and J in Hz).

No.	**1**		**2**		**3**	
	δ_H	δ_C, type	δ_H	δ_C, type	δ_H	δ_C, type
1a	1.77, m	39.8, CH_2	1.70, m	39.4, CH_2	1.78, m	40.6, CH_2
1b	2.30, dd (14.5, 8.4)		2.23, m		2.40, dd (14.7, 10.2)	
2	5.13, tq (7.8,1.4)	120.7, CH	4.99, tq (7.6, 2.7)	120.8, CH	5.53, ddt (10.2, 4.6, 1.5)	121.5, CH
3		135.1, C		135.0, C		136.8, C
4a	1.36, m	38.5, CH_2	2.07, m	38.6, CH_2	4.39, br s	73.3, CH
4b	1.61, m		2.07, m			
5a	2.07, m	24.8, CH_2	2.15, m	24.6, CH_2	2.70, m	33.8, CH_2
5b	2.19, m		2.18, m		2.90, ddd (15.9, 9.3, 2.3)	
6	5.07, m	123.6, CH	5.06, tq (6.0, 2.7)	126.3, CH	6.57, ddd (9.3, 4.7, 1.3)	146.2, CH
7		134.1, C		131.2, C		135.9, C
8a	2.08, m	39.2, CH_2	2.28, m	46.9, CH_2		197.6, C
8b	2.15, m		2.28, m			
9	2.07, 2H, m	24.5, CH_2	4.53, m	67.0, CH		203.8, C
10a	5.45, tq (6.6,1.4)	126.6, CH	5.37, dq (8.6, 2.2)	129.3, CH	2.29, dd (12.1, 11.2)	46.2, CH_2
10b					2.80, dd (12.1, 0.9)	
11		131.9, C		136.1, C	2.75, m	26.9, CH
12	5.72, d (12.2)	132.7, CH	5.79, d (11.9)	132.6, CH	5.34, t (10.5)	134.5, CH
13	5.04, t (12.2)	128.5, CH	5.19, t (11.9)	129.8, CH	5.12, t (11.2)	126.8, CH
14	2.91, dd (11.9, 5.4)	45.1, CH	2.75, dd (11.7, 6.3)	45.3, CH	2.46, dd, (11.4, 6.2)	45.3, CH
15		46.5, C		46.3, C		45.3, C
16	2.12, 2H, m	37.9, CH_2	1.42, 2H, m	37.9, CH_2	1.48, 2H, m	39.4, CH_2
17a	1.35, m	26.8, CH_2	1.43, m	26.9, CH_2	1.44, m	27.8, CH_2
17b	1.81, m		1.78, m		1.82, m	
18	1.69, dd (10.1, 5.5)	50.5, CH	1.73, m	50.2, CH	1.61, m	51.0, CH
19	1.32, m	30.9, CH	1.44, m	30.4, CH	1.36, m	29.6, CH
20	1.62, s	16.7, CH_3	1.57, s	16.7, CH_3	1.60, s	14.0, CH_3
21	1.62, s	17.1, CH_3	1.65, s	17.7, CH_3	1.85, s	10.6, CH_3
22	1.65, s	17.7, CH_3	1.71, dd (0.9, 0.6)	18.0, CH_3	1.10, d (6.5)	20.2, CH_3
23	0.95, s	23.4, CH_3	0.88, s	23.8, CH_3	0.91, s	24.8, CH_3
24	0.82, d (6.6)	22.0, CH_3	0.83, d (6.5)	22.7, CH_3	0.83, d (6.5)	22.0, CH_3
25	0.70, d (6.4)	21.8, CH_3	0.82, d (6.5)	21.9, CH_3	0.63, d (6.4)	22.0, CH_3

Table S2. Comparison of the experimental and computed ^{13}C NMR chemical shifts for 1, 14*R*,15*R*,18*S*-1 and 14*R*,15*R*,18*R*-1).

No.	**1**	14*R*,15*R*,18*S*-**1**			14*R*,15*R*,18*R*-**1**		
	Exptl.	Calcd.	$\Delta\delta$	$\lvert\Delta\delta\rvert$	Calcd.	$\Delta\delta$	$\lvert\Delta\delta\rvert$
1	39.8	35.27	-4.53	4.53	35.00	-4.80	4.80
2	120.7	124.03	3.33	3.33	123.30	2.60	2.60
3	135.1	131.96	-3.14	3.14	132.33	-2.77	2.77
4	38.5	39.50	1.00	1.00	41.07	2.57	2.57
5	24.8	24.29	-0.51	0.51	26.06	1.26	1.26
6	123.6	124.27	0.67	0.67	122.68	-0.92	0.92
7	134.1	136.05	1.95	1.95	132.04	-2.06	2.06
8	39.2	38.73	-0.47	0.47	38.51	-0.69	0.69
9	24.5	21.67	-2.83	2.83	31.75	7.25	7.25
10	126.6	124.84	-1.76	1.76	129.06	2.46	2.46
11	131.9	133.29	1.39	1.39	130.66	-1.24	1.24
12	132.7	126.98	-5.72	5.72	129.42	-3.28	3.28
13	128.5	129.79	1.29	1.29	128.35	-0.15	0.15
14	45.1	48.00	2.90	2.90	56.41	11.31	11.31
15	46.5	44.73	-1.77	1.77	47.61	1.11	1.11
16	37.9	36.14	-3.06	3.06	40.32	1.12	1.12
17	26.8	25.38	-1.42	1.42	29.74	2.94	2.94
18	50.5	50.21	-0.29	0.29	39.69	-10.81	10.81
19	30.9	30.40	-0.50	0.50	37.86	6.96	6.96
20	16.7	14.19	-2.51	2.51	14.24	-2.46	2.46
21	17.1	14.64	-2.46	2.46	14.47	-2.63	2.63
22	17.7	24.22	6.52	6.52	16.97	-0.73	0.73
23	23.4	23.76	0.36	0.36	23.47	0.07	0.07
24	22.0	21.04	-0.96	-0.96	20.25	-1.75	1.75
25	21.8	19.26	-2.54	2.54	21.42	-0.38	0.38
AveDev: average absolute deviations				2.08			2.97
MaxDev: maximum absolute deviations				6.52			11.31
R^2: coefficients				0.9969			0.9920

Table S3. ^{1}H NMR (600 MHz) and ^{13}C NMR (150 MHz) data for compound 4 in $CDCl_3$ (δ in ppm and *J* in Hz).

No.	**4**	
	δ_H	δ_C, type
1		129.3, C
2	7.58, dt (8.7, 2.4)	131.7, CH
2	7.58, dt (8.7, 2.4)	131.7, CH
3	7.90, dt (8.7, 2.4)	131.1, CH
3	7.90, dt (8.7, 2.4)	131.1, CH
4		128.0, C
5		165.9, C
6	4.38, 2H, m	62.8, CH_2
7	1.88, m 1.81, m	40.2, CH_2
8		44.4, C
9	1.59, m 1.51, m	37.1, CH_2
10	1.88, m 1.51, m	37.9, CH_2 27.7, CH_2
11	1.81, m	50.4, CH
12	2.69, dd (11.8, 6.0)	48.6, C
13	5.24, td (11.8, 0.7)	129.0, CH
14	5.51, dd (11.2, 9.4)	134.3, CH
15	4.64, m	63.9, CH
16	1.24, d (6.3)	23.8, CH_3
17	1.43, m	30.1, CH
18	0.91, s	23.9, CH_3
19	0.84, d (6.4)	21.9, CH_3
20	0.85, d (6.6)	22.0, CH_3

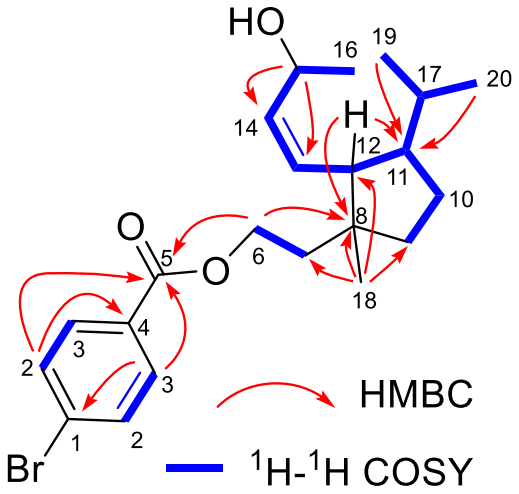


Table S4. Oligonucleotides used in the study

Name	Sequence (5'to3')
pAdeA2-pstA-F	AAGCTCCGAATTCGAATCGATTTGAGCTAGCATGGACACCAATCTGAGATTC
pAdeA2-pstA-R	TACCCGGGTCACTAGTGCGGCCGCTAGCTCATATCCATAGGCGCCTCA
pTAex3-pstB-F	CACAGCAAGCTCCGAATTCCTCGAGATGCCTACCAGTAATGGATTC
pTAex3-pstB-R	ACTACAGATCCCCGGGTACCCTCGAGTCAGGCAGTGACTTCAACCC
pet28a-pstA-F	GGACAGCAAATGGGTCGCGGATCCGAATTCATGGACACCAATCTGAGATTC
pet28a-pstA-R	ATCTCAGTGGTGGTGGTGGTGCTCGAGTCATATCCATAGGCGCCTCAA
petM41-pstA-F	CTTTATTTTCAGGGCGCCATGGTGGACACCAATCTGAGATTCAC
petM41-pstA-R	TCGACGGAGCTCGAATTCGGATCCGGTACCTCATATCCATAGGCGCCTCAAC
pstA-PT-F	AAATGGGTCGCGGATCCGAATTCGTCACAAATGGCGGGAAAGA
pstA-PT-R	GGTGGTGGTGGTGGTGCTCGAGTCATATCCATAGGCGCCTCAA
pstA-TC-R	GGTGGTGGTGGTGGTGCTCGAGTCATTCCCCAAGATTCTCTGC

Table S5. Gibbs free energies[a] and equilibrium populations[b] of low-energy conformers of 14*R*,15*R*,18*S*-1.

Conformers	ΔG(a.u.)	P(%)/100	G(a.u.)
14R,15R,18S-1000001	0.00541	0.32	-976.027102
14R,15R,18S-1000004	0.0	98.85	-976.032517
14R,15R,18S-1000005	0.00698	0.06	-976.025533
14R,15R,18S-1000006	0.00808	0.02	-976.024436
14R,15R,18S-1000007	0.00808	0.02	-976.024441
14R,15R,18S-1000009	0.00607	0.16	-976.02645
14R,15R,18S-1000010	0.005	0.49	-976.027513
14R,15R,18S-1000011	0.00754	0.03	-976.024975
14R,15R,18S-1000012	0.00725	0.05	-976.025265

[a]wB97M-V/def2-TZVP, in a.u.

[b]From ΔG values at 298.15K.

Table S6. Cartesian coordinates for the low-energy reoptimized random research conformers of 14*R*,15*R*,18*S*-1 at B3LYP-D3(BJ)/6-31G* level of theory in methanol.

14R,15R,18S-1000001_en_		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-7.136974	2.298575	-0.883273
1	6	0	-8.726217	0.063817	-1.58812
2	6	0	-7.158241	-1.81185	-3.207246
3	6	0	-5.119642	-3.240331	-1.794253
4	6	0	-2.660411	-2.8264	-2.276758
5	6	0	2.185447	2.857571	-2.620845
6	6	0	2.180425	5.065899	-0.89749
7	6	0	0.527703	5.437766	0.997159
8	6	0	-1.621921	3.732455	1.679465
9	6	0	-4.249314	5.020224	1.520757
10	6	0	-6.274555	3.005058	1.388896
11	6	0	-0.441708	-4.313805	-1.283982
12	6	0	1.098063	-3.285187	1.009554
13	6	0	2.665309	-0.769318	0.506045
14	6	0	3.153664	-5.306234	1.648345
15	6	0	5.599568	-4.328682	0.467799
16	6	0	5.477282	-1.513157	1.124274
17	6	0	7.59322	0.211018	0.096745
18	6	0	9.909524	0.101913	1.844193
19	6	0	8.400733	-0.378148	-2.626332
20	6	0	-0.689804	-2.926212	3.261419
21	6	0	4.157664	7.032864	-1.52522
22	6	0	-6.091805	-5.154277	0.082205
23	6	0	-6.965898	1.764002	3.855591
24	1	0	2.106381	0.652619	1.887151
25	6	0	2.366445	0.386377	-2.067224
26	1	0	-6.443879	3.363235	-2.510094
27	1	0	-10.355065	0.677402	-2.721624
28	1	0	-9.495893	-0.900478	0.072
29	1	0	-8.463395	-3.19385	-4.049312
30	1	0	-6.309353	-0.764408	-4.781439

31	1	0	-2.211505	-1.340122	-3.625276
32	1	0	2.190425	3.363524	-4.622506
33	1	0	0.698711	7.176611	2.092523
34	1	0	-1.651271	2.120398	0.393794
35	1	0	-1.356307	2.968469	3.592516
36	1	0	-4.309692	6.182991	-0.191357
37	1	0	-4.526569	6.292462	3.137841
38	1	0	0.870873	-4.649747	-2.856832
39	1	0	-1.100308	-6.192069	-0.714711
40	1	0	3.396663	-5.431017	3.704606
41	1	0	2.611918	-7.192176	0.988519
42	1	0	5.575432	-4.600374	-1.587968
43	1	0	7.292781	-5.270789	1.198358
44	1	0	5.597262	-1.404324	3.197417
45	1	0	6.868866	2.15524	0.136214
46	1	0	10.674081	-1.82309	1.944487
47	1	0	11.422704	1.338895	1.156958
48	1	0	9.429883	0.691221	3.771441
49	1	0	9.798071	1.008101	-3.273332
50	1	0	6.809637	-0.324329	-3.940272
51	1	0	9.279536	-2.250341	-2.753443
52	1	0	-2.242374	-1.647679	2.791164
53	1	0	-1.513145	-4.73787	3.842267
54	1	0	0.327536	-2.148645	4.890701
55	1	0	6.073445	6.259379	-1.337803
56	1	0	3.970435	7.66868	-3.493028
57	1	0	4.000645	8.689142	-0.296542
58	1	0	-6.853926	-4.21109	1.766039
59	1	0	-7.642271	-6.265926	-0.732204
60	1	0	-4.633949	-6.461993	0.731625
61	1	0	-5.30018	0.921274	4.760876
62	1	0	-7.716752	3.166097	5.189496
63	1	0	-8.38067	0.276027	3.637555
64	1	0	2.439867	-0.905082	-3.66603

14R,15R,18S-1000004_en_		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-7.312619	1.835658	-0.908867
1	6	0	-9.167043	-0.201875	-0.198438
2	6	0	-7.825563	-2.383289	1.236961
3	6	0	-5.720243	-3.610449	-0.260853
4	6	0	-3.306138	-2.933643	0.109522

5	6	0	2.695184	2.443861	-3.203925
6	6	0	2.505692	4.80816	-1.723111
7	6	0	0.626249	5.397079	-0.121379
8	6	0	-1.664434	3.843222	0.448747
9	6	0	-4.163016	5.213388	-0.218601
10	6	0	-6.402112	3.641588	0.613498
11	6	0	-1.01614	-3.938902	-1.260947
12	6	0	1.502682	-3.76035	0.208823
13	6	0	2.805327	-1.092604	0.176032
14	6	0	3.542976	-5.451019	-1.06132
15	6	0	6.134454	-4.206306	-0.500029
16	6	0	5.557784	-1.771741	1.016465
17	6	0	7.555262	0.324342	0.817642
18	6	0	6.957931	2.506365	2.633033
19	6	0	10.213758	-0.703329	1.363539
20	6	0	1.078978	-4.677511	2.941553
21	6	0	4.600463	6.673941	-2.273266
22	6	0	-6.560417	-5.506557	-2.214347
23	6	0	-7.289898	4.087325	3.282795
24	1	0	1.92364	0.205417	1.518572
25	6	0	2.813325	0.025993	-2.445479
26	1	0	-6.466152	1.662443	-2.778033
27	1	0	-10.086057	-0.947478	-1.899684
28	1	0	-10.683811	0.536384	1.00494
29	1	0	-7.061716	-1.609059	2.999022
30	1	0	-9.241283	-3.811388	1.759499
31	1	0	-2.948499	-1.491642	1.529561
32	1	0	2.948665	2.769416	-5.227748
33	1	0	0.704718	7.239421	0.802495
34	1	0	-1.609698	2.068006	-0.599859
35	1	0	-1.697187	3.343796	2.468521
36	1	0	-4.206072	5.526292	-2.265636
37	1	0	-4.196369	7.083821	0.681992
38	1	0	-0.794052	-2.969554	-3.084414
39	1	0	-1.316225	-5.938996	-1.722177
40	1	0	3.420245	-7.392974	-0.354267
41	1	0	3.212336	-5.55603	-3.104045
42	1	0	7.102576	-3.723267	-2.267314
43	1	0	7.402987	-5.464455	0.539806
44	1	0	5.449508	-2.273103	3.026163
45	1	0	7.532254	1.056485	-1.124569
46	1	0	6.999618	1.841983	4.598614
47	1	0	8.362487	4.019617	2.459335

48	1	0	5.095469	3.32406	2.276055
49	1	0	11.618509	0.816747	1.274746
50	1	0	10.777265	-2.162771	0.010038
51	1	0	10.30867	-1.531051	3.264058
52	1	0	-0.007721	-6.441118	2.931416
53	1	0	2.85745	-5.055431	3.924367
54	1	0	0.018608	-3.299407	4.062387
55	1	0	4.669736	7.129203	-4.297783
56	1	0	4.342415	8.437765	-1.224825
57	1	0	6.451916	5.885141	-1.777018
58	1	0	-7.657146	-7.035649	-1.337201
59	1	0	-7.811418	-4.618655	-3.613887
60	1	0	-4.98597	-6.353215	-3.246156
61	1	0	-7.928647	6.047873	3.522124
62	1	0	-8.837687	2.839822	3.839767
63	1	0	-5.739297	3.808382	4.635328
64	1	0	3.101287	-1.346907	-3.95247

14R,15R,18S-1000005_en_		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-4.403809	-0.956041	-2.935709
1	6	0	-6.616618	0.818252	-3.028677
2	6	0	-6.815815	2.403673	-0.559919
3	6	0	-4.530364	4.068599	-0.068982
4	6	0	-2.58408	3.13775	1.261165
5	6	0	1.508314	-1.692434	4.482045
6	6	0	-1.222093	-2.287893	4.303821
7	6	0	-2.398773	-3.842693	2.680996
8	6	0	-1.322624	-5.56023	0.695635
9	6	0	-1.849143	-4.747955	-2.088144
10	6	0	-4.367972	-3.443	-2.450633
11	6	0	-0.062038	4.311905	1.845252
12	6	0	2.097711	3.408113	0.091859
13	6	0	2.709443	0.49828	0.241711
14	6	0	4.666693	4.588125	0.820994
15	6	0	6.698339	2.79179	-0.282973
16	6	0	5.286254	0.378361	-1.19775
17	6	0	6.857188	-2.059118	-0.983759
18	6	0	5.402949	-4.349606	-1.989329
19	6	0	9.374452	-1.786878	-2.402081
20	6	0	1.442516	4.17756	-2.641032
21	6	0	-2.730089	-1.001285	6.376839

22	6	0	-4.612819	6.653063	-1.258718
23	6	0	-6.678888	-5.073895	-2.12714
24	1	0	1.229026	-0.581841	-0.702626
25	6	0	3.06739	-0.456412	2.906151
26	1	0	-2.57722	-0.035252	-3.121726
27	1	0	-8.400158	-0.196813	-3.299325
28	1	0	-6.416685	2.103618	-4.647404
29	1	0	-8.531845	3.567678	-0.66145
30	1	0	-7.067548	1.081492	1.013933
31	1	0	-2.787137	1.209036	1.922094
32	1	0	2.282517	-2.080355	6.35783
33	1	0	-4.44315	-3.971034	2.892557
34	1	0	0.715245	-5.776401	0.963368
35	1	0	-2.150569	-7.440691	0.998723
36	1	0	-1.715522	-6.438735	-3.287862
37	1	0	-0.347245	-3.470772	-2.706813
38	1	0	0.454584	3.854745	3.80048
39	1	0	-0.147159	6.379397	1.722515
40	1	0	4.842176	6.526317	0.114211
41	1	0	4.827699	4.685866	2.884103
42	1	0	8.100607	2.30151	1.161274
43	1	0	7.747886	3.666831	-1.834794
44	1	0	4.860326	0.591941	-3.214223
45	1	0	7.287468	-2.39884	1.019416
46	1	0	3.676381	-4.673703	-0.909983
47	1	0	4.871624	-4.072191	-3.975482
48	1	0	6.552064	-6.069757	-1.880334
49	1	0	9.042506	-1.393941	-4.412223
50	1	0	10.478802	-3.535006	-2.279926
51	1	0	10.535252	-0.252308	-1.642767
52	1	0	-0.206463	3.152553	-3.345692
53	1	0	0.992157	6.197762	-2.702272
54	1	0	3.006675	3.864778	-3.952202
55	1	0	-4.737933	-1.484325	6.265476
56	1	0	-2.032113	-1.573081	8.246648
57	1	0	-2.553172	1.060779	6.276304
58	1	0	-6.290248	7.701904	-0.63018
59	1	0	-2.945538	7.78912	-0.822918
60	1	0	-4.747583	6.511498	-3.32666
61	1	0	-8.441258	-4.028901	-2.381412
62	1	0	-6.660535	-6.637231	-3.493284
63	1	0	-6.73111	-5.946128	-0.245023
64	1	0	4.930451	-0.057701	3.687899

14R,15R,18S-1000006_en_		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-4.9448	-2.588578	-2.464622
1	6	0	-6.673106	-0.355774	-2.770002
2	6	0	-7.33969	0.91565	-0.199922
3	6	0	-5.459808	2.937154	0.561775
4	6	0	-3.370832	2.326036	1.858456
5	6	0	1.350315	-1.966023	4.404243
6	6	0	-0.878377	-3.567066	3.878846
7	6	0	-1.290112	-5.04444	1.856699
8	6	0	0.296765	-5.465893	-0.452332
9	6	0	-1.331264	-5.532887	-2.886721
10	6	0	-2.687853	-3.078341	-3.50949
11	6	0	-1.15552	3.990509	2.51266
12	6	0	1.044541	3.674289	0.60902
13	6	0	2.038392	0.877856	0.471927
14	6	0	3.466892	5.135846	1.346006
15	6	0	5.676914	3.710223	0.034941
16	6	0	4.528218	1.23122	-1.054465
17	6	0	6.369389	-1.014062	-1.388666
18	6	0	8.33879	-0.343852	-3.418023
19	6	0	7.717799	-1.974506	0.994044
20	6	0	0.138275	4.60474	-1.997452
21	6	0	-2.754115	-3.579078	6.044763
22	6	0	-6.088135	5.552947	-0.375215
23	6	0	-1.343697	-1.38439	-5.361007
24	1	0	0.671509	-0.298169	-0.524094
25	6	0	2.527228	-0.155217	3.07255
26	1	0	-5.710566	-4.029668	-1.203385
27	1	0	-8.439289	-1.027937	-3.637109
28	1	0	-5.893706	1.056848	-4.066214
29	1	0	-9.232459	1.751366	-0.340873
30	1	0	-7.446155	-0.55628	1.254933
31	1	0	-3.142235	0.347792	2.360842
32	1	0	2.054088	-2.231727	6.327883
33	1	0	-3.01444	-6.174745	1.894241
34	1	0	1.801275	-4.065094	-0.603346
35	1	0	1.23839	-7.315286	-0.293433
36	1	0	-2.725528	-7.052633	-2.669054
37	1	0	-0.114824	-6.079678	-4.475038
38	1	0	-0.472146	3.503644	4.406482

39	1	0	-1.694524	5.990174	2.566815
40	1	0	3.355852	7.122037	0.773909
41	1	0	3.708864	5.122881	3.402874
42	1	0	7.185109	3.300788	1.390422
43	1	0	6.537577	4.841709	-1.466533
44	1	0	3.911517	1.647408	-2.98621
45	1	0	5.241214	-2.592863	-2.134451
46	1	0	9.528927	-1.978721	-3.86551
47	1	0	7.435655	0.288412	-5.172759
48	1	0	9.588599	1.17718	-2.769267
49	1	0	8.811664	-0.472095	1.910346
50	1	0	9.051135	-3.476365	0.484006
51	1	0	6.395991	-2.740835	2.378201
52	1	0	-1.396583	3.430997	-2.719949
53	1	0	-0.572951	6.542371	-1.82808
54	1	0	1.649445	4.639008	-3.4047
55	1	0	-1.841521	-4.148741	7.820043
56	1	0	-3.533092	-1.682062	6.358234
57	1	0	-4.327832	-4.87221	5.6871
58	1	0	-4.711734	6.975056	0.206383
59	1	0	-6.188414	5.591022	-2.449608
60	1	0	-7.955021	6.144221	0.313241
61	1	0	0.603567	-1.010995	-4.754061
62	1	0	-1.213966	-2.308047	-7.216589
63	1	0	-2.280298	0.434716	-5.623064
64	1	0	4.079638	0.768351	4.059308

14R,15R,18S-1000007_en_		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-4.945081	-2.587945	-2.464638
1	6	0	-6.673302	-0.355066	-2.769851
2	6	0	-7.339672	0.916401	-0.199737
3	6	0	-5.459396	2.937544	0.562006
4	6	0	-3.370808	2.326031	1.859161
5	6	0	1.350288	-1.96653	4.404083
6	6	0	-0.878654	-3.567273	3.878691
7	6	0	-1.290492	-5.044462	1.856399
8	6	0	0.29626	-5.465824	-0.452747
9	6	0	-1.331855	-5.532633	-2.88711
10	6	0	-2.688289	-3.077946	-3.50977
11	6	0	-1.15514	3.990053	2.513339
12	6	0	1.044699	3.674067	0.609451

13	6	0	2.038497	0.877632	0.471919
14	6	0	3.467143	5.135436	1.346622
15	6	0	5.677125	3.709919	0.035352
16	6	0	4.528315	1.231207	-1.054437
17	6	0	6.36935	-1.01414	-1.389189
18	6	0	8.339167	-0.343185	-3.417848
19	6	0	7.717341	-1.975664	0.993343
20	6	0	0.138425	4.604815	-1.996939
21	6	0	-2.754242	-3.579464	6.044685
22	6	0	-6.086875	5.55335	-0.375584
23	6	0	-1.344249	-1.38408	-5.361435
24	1	0	0.67161	-0.298209	-0.52431
25	6	0	2.527383	-0.155848	3.072387
26	1	0	-5.710812	-4.028969	-1.203299
27	1	0	-8.439574	-1.027191	-3.636858
28	1	0	-5.894015	1.057522	-4.066184
29	1	0	-9.232314	1.752409	-0.340643
30	1	0	-7.446353	-0.555591	1.255063
31	1	0	-3.143001	0.347843	2.362096
32	1	0	2.054241	-2.232516	6.32762
33	1	0	-3.014921	-6.174622	1.893873
34	1	0	1.800817	-4.065077	-0.603768
35	1	0	1.237856	-7.315241	-0.29394
36	1	0	-2.726215	-7.052292	-2.669487
37	1	0	-0.115459	-6.079419	-4.475463
38	1	0	-0.471516	3.502634	4.406929
39	1	0	-1.693901	5.98978	2.568087
40	1	0	3.356207	7.121725	0.774852
41	1	0	3.709078	5.122079	3.403492
42	1	0	7.185319	3.300199	1.390767
43	1	0	6.537835	4.841632	-1.465933
44	1	0	3.911629	1.647708	-2.986129
45	1	0	5.241141	-2.59251	-2.135896
46	1	0	9.529705	-1.97774	-3.865441
47	1	0	7.436433	0.289358	-5.172703
48	1	0	9.588594	1.177897	-2.768444
49	1	0	9.050507	-3.477527	0.482866
50	1	0	6.395331	-2.742388	2.377076
51	1	0	8.811342	-0.473727	1.910276
52	1	0	1.649723	4.639545	-3.404051
53	1	0	-1.396141	3.430904	-2.719792
54	1	0	-0.573136	6.542283	-1.827293
55	1	0	-1.841663	-4.150215	7.819644

56	1	0	-3.532571	-1.682348	6.359086
57	1	0	-4.328413	-4.871945	5.68664
58	1	0	-6.184182	5.591863	-2.45011
59	1	0	-7.954828	6.144098	0.310369
60	1	0	-4.711577	6.975652	0.208206
61	1	0	0.603047	-1.010563	-4.754667
62	1	0	-1.214585	-2.307812	-7.216981
63	1	0	-2.280925	0.434994	-5.623509
64	1	0	4.080059	0.767409	4.059032

14R,15R,18S-1000009_en_		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-4.900689	-0.880049	-2.002065
1	6	0	-6.45918	1.458573	-2.413305
2	6	0	-6.379843	3.202628	-0.046181
3	6	0	-3.891582	4.598774	0.208939
4	6	0	-1.967815	3.567019	1.499376
5	6	0	1.673161	-1.624369	4.42391
6	6	0	-1.049626	-2.269775	4.362567
7	6	0	-2.387944	-3.568353	2.635809
8	6	0	-1.601097	-4.803043	0.193778
9	6	0	-3.891266	-5.472282	-1.460037
10	6	0	-5.612379	-3.302138	-2.212141
11	6	0	0.702034	4.512354	1.739301
12	6	0	2.571082	3.309155	-0.166891
13	6	0	2.91955	0.372361	0.112501
14	6	0	5.286946	4.291629	0.243095
15	6	0	7.050038	2.26712	-0.914166
16	6	0	5.391362	-0.10746	-1.437996
17	6	0	6.806239	-2.612681	-1.001824
18	6	0	5.103853	-4.921351	-1.387168
19	6	0	9.121177	-2.778481	-2.744856
20	6	0	1.707913	3.931287	-2.876147
21	6	0	-2.38248	-1.366453	6.739555
22	6	0	-3.769577	7.077975	-1.188594
23	6	0	-8.157544	-4.158811	-3.169041
24	1	0	1.304176	-0.582427	-0.739217
25	6	0	3.258432	-0.484671	2.798699
26	1	0	-3.005785	-0.489041	-1.319148
27	1	0	-8.427708	0.984287	-2.832715
28	1	0	-5.749816	2.529466	-4.048594
29	1	0	-7.936366	4.568314	-0.178555

30	1	0	-6.733351	2.037878	1.62921
31	1	0	-2.319089	1.75422	2.396451
32	1	0	2.47415	-1.954531	6.29893
33	1	0	-4.382191	-3.830883	3.079678
34	1	0	-0.287409	-3.625318	-0.875508
35	1	0	-0.564248	-6.557874	0.595361
36	1	0	-5.047647	-6.866879	-0.436396
37	1	0	-3.240437	-6.464685	-3.167805
38	1	0	1.386317	4.119367	3.655186
39	1	0	0.793914	6.567811	1.486747
40	1	0	5.554517	6.165098	-0.59743
41	1	0	5.650444	4.491698	2.273227
42	1	0	8.585834	1.802557	0.396211
43	1	0	7.952234	2.933268	-2.65155
44	1	0	4.846007	-0.10364	-3.437847
45	1	0	7.48708	-2.64596	0.960519
46	1	0	4.219932	-4.887966	-3.26431
47	1	0	6.197402	-6.675234	-1.241976
48	1	0	3.607225	-4.991186	0.029834
49	1	0	10.157179	-4.54362	-2.426567
50	1	0	10.437648	-1.210646	-2.444706
51	1	0	8.539676	-2.74291	-4.736392
52	1	0	1.458011	5.975316	-3.089441
53	1	0	3.087512	3.334804	-4.293704
54	1	0	-0.098315	3.025245	-3.31334
55	1	0	-1.478405	-2.137108	8.441755
56	1	0	-2.29032	0.700127	6.899173
57	1	0	-4.372769	-1.925244	6.758659
58	1	0	-4.074981	6.798637	-3.223412
59	1	0	-5.274019	8.351511	-0.537957
60	1	0	-1.96477	8.050652	-0.959549
61	1	0	-7.928097	-5.52292	-4.717698
62	1	0	-9.21675	-5.141655	-1.677207
63	1	0	-9.328444	-2.611368	-3.870658
64	1	0	5.137078	-0.112912	3.55803

14R,15R,18S-1000010_en_		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-5.605037	-2.396271	-2.24287
1	6	0	-7.01095	0.01969	-2.733173
2	6	0	-7.419754	1.575138	-0.271904
3	6	0	-5.237269	3.328402	0.342214

4	6	0	-3.194122	2.471426	1.573527
5	6	0	1.593324	-1.908343	4.466029
6	6	0	-0.930017	-3.085321	4.166528
7	6	0	-1.780363	-4.581029	2.300071
8	6	0	-0.488411	-5.505671	-0.048835
9	6	0	-2.340014	-5.738809	-2.299841
10	6	0	-3.404974	-3.228966	-3.182738
11	6	0	-0.823204	3.902539	2.229888
12	6	0	1.410944	3.459279	0.396597
13	6	0	2.498563	0.691518	0.40799
14	6	0	3.756584	5.01765	1.143425
15	6	0	6.005977	3.705708	-0.180566
16	6	0	5.064844	1.038956	-1.019606
17	6	0	7.117911	-1.00649	-0.725337
18	6	0	6.150452	-3.670985	-1.307666
19	6	0	9.390852	-0.380968	-2.420261
20	6	0	0.580728	4.21213	-2.289293
21	6	0	-2.621277	-2.559031	6.421247
22	6	0	-5.558666	5.987737	-0.628513
23	6	0	-1.832151	-1.852758	-5.115293
24	1	0	1.204278	-0.54809	-0.610864
25	6	0	2.953401	-0.321489	3.025946
26	1	0	-6.559105	-3.628247	-0.890273
27	1	0	-8.875313	-0.459657	-3.517676
28	1	0	-6.064261	1.193658	-4.150015
29	1	0	-9.155759	2.691577	-0.470196
30	1	0	-7.745481	0.254536	1.29204
31	1	0	-3.184536	0.486946	2.097311
32	1	0	2.370419	-2.24892	6.349519
33	1	0	-3.693996	-5.31098	2.535934
34	1	0	1.09951	-4.300317	-0.559422
35	1	0	0.314608	-7.392019	0.310713
36	1	0	-3.890792	-6.995025	-1.737226
37	1	0	-1.356187	-6.67704	-3.867248
38	1	0	-0.216722	3.362352	4.136205
39	1	0	-1.186455	5.942089	2.284399
40	1	0	3.557067	7.007787	0.607703
41	1	0	3.996484	4.970435	3.201218
42	1	0	7.619424	3.532845	1.106841
43	1	0	6.674648	4.794519	-1.806761
44	1	0	4.612397	1.09892	-3.042158
45	1	0	7.777793	-0.9904	1.244461
46	1	0	5.22649	-3.742616	-3.164526

47	1	0	7.712419	-5.031953	-1.336189
48	1	0	4.797902	-4.299417	0.117253
49	1	0	8.833369	-0.385477	-4.418996
50	1	0	10.893704	-1.78668	-2.185325
51	1	0	10.191235	1.478492	-1.994731
52	1	0	-0.97285	3.024359	-2.946273
53	1	0	-0.083975	6.173443	-2.288995
54	1	0	2.120328	4.090554	-3.661299
55	1	0	-3.008641	-0.528286	6.59338
56	1	0	-4.43058	-3.548126	6.265773
57	1	0	-1.712096	-3.147587	8.191817
58	1	0	-5.773221	5.989815	-2.694967
59	1	0	-7.285626	6.845315	0.140596
60	1	0	-3.971311	7.221945	-0.168691
61	1	0	-2.569059	0.019313	-5.572316
62	1	0	0.122718	-1.618656	-4.464629
63	1	0	-1.737894	-2.948379	-6.87701
64	1	0	4.68484	0.364717	3.905226

14R,15R,18S-1000011_en_		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-6.833866	2.503405	0.074714
1	6	0	-8.536264	0.38192	0.914206
2	6	0	-8.565773	-1.816961	-0.976961
3	6	0	-6.123229	-3.228201	-1.486048
4	6	0	-3.872357	-2.663487	-0.461421
5	6	0	2.756424	1.899397	-3.473109
6	6	0	2.899004	4.442301	-2.315947
7	6	0	1.24548	5.429231	-0.657432
8	6	0	-1.058198	4.151421	0.357191
9	6	0	-3.503789	5.744318	0.356257
10	6	0	-5.5653	4.140547	1.527298
11	6	0	-1.4532	-4.10233	-0.990283
12	6	0	0.833267	-3.621945	0.763471
13	6	0	2.344075	-1.104446	0.332589
14	6	0	2.877835	-5.652872	0.232935
15	6	0	5.433171	-4.543942	1.115172
16	6	0	4.947936	-1.695852	1.614464
17	6	0	7.14409	0.149878	1.044855
18	6	0	8.970756	0.263131	3.299482
19	6	0	8.641786	-0.412895	-1.377013
20	6	0	-0.029453	-3.81415	3.537395
21	6	0	5.10283	5.997691	-3.269248
22	6	0	-6.481229	-5.378918	-3.330992
23	6	0	-5.798181	4.286333	4.360564
24	1	0	1.474616	0.447009	1.366925
25	6	0	2.560382	-0.401305	-2.412683
26	1	0	-6.500316	2.592256	-1.958805
27	1	0	-10.495298	1.045796	1.126136
28	1	0	-7.962396	-0.319043	2.778536
29	1	0	-9.986283	-3.204348	-0.357689
30	1	0	-9.284457	-1.104799	-2.797998
31	1	0	-3.747123	-1.056104	0.806244
32	1	0	3.07189	1.923944	-5.513622
33	1	0	1.590167	7.348118	0.013554
34	1	0	-1.431535	2.431971	-0.723007
35	1	0	-0.708071	3.544979	2.318227
36	1	0	-3.980939	6.259203	-1.592428
37	1	0	-3.216663	7.509658	1.409551
38	1	0	-0.867384	-3.775496	-2.95318

39	1	0	-1.84655	-6.137414	-0.871643
40	1	0	2.408282	-7.444868	1.159222
41	1	0	2.940611	-6.045957	-1.80246
42	1	0	6.875106	-4.828382	-0.335664
43	1	0	6.130137	-5.480059	2.823627
44	1	0	4.572489	-1.487465	3.64098
45	1	0	6.289937	2.029601	0.836041
46	1	0	9.811485	-1.597782	3.663479
47	1	0	10.522521	1.588643	2.940847
48	1	0	8.003468	0.868137	5.028869
49	1	0	9.910925	1.167922	-1.807256
50	1	0	7.412843	-0.695637	-3.010376
51	1	0	9.825651	-2.098589	-1.1547
52	1	0	1.568108	-3.888558	4.848234
53	1	0	-1.214851	-2.207063	4.080276
54	1	0	-1.144343	-5.537781	3.818417
55	1	0	5.088581	7.905431	-2.47117
56	1	0	6.911475	5.103404	-2.789368
57	1	0	5.054598	6.162863	-5.338197
58	1	0	-4.741018	-6.413307	-3.725028
59	1	0	-7.886709	-6.734446	-2.623644
60	1	0	-7.213935	-4.669225	-5.139904
61	1	0	-6.519528	6.147882	4.93122
62	1	0	-7.071669	2.857416	5.135568
63	1	0	-3.950863	4.066899	5.282067
64	1	0	2.689855	-1.988424	-3.718632

14R,15R,18S-1000012_en_		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-6.894072	1.073344	-0.936647
1	6	0	-7.964478	-1.532885	-1.295646
2	6	0	-6.388622	-3.078713	-3.185536
3	6	0	-3.722497	-3.839156	-2.450444
4	6	0	-2.752989	-3.491105	-0.133968
5	6	0	1.020998	2.407028	-2.556243
6	6	0	1.097804	4.976915	-1.433469
7	6	0	-0.315458	5.742413	0.534569
8	6	0	-2.232	4.156951	1.88738
9	6	0	-5.007904	4.783472	1.11743
10	6	0	-6.56379	2.387516	1.200687
11	6	0	-0.25861	-4.446356	0.852038
12	6	0	1.361352	-2.670948	2.543952

13	6	0	2.520643	-0.280827	1.139091
14	6	0	3.720216	-4.221831	3.390719
15	6	0	5.801635	-3.531527	1.514428
16	6	0	5.472316	-0.662989	1.302048
17	6	0	7.133779	0.740889	-0.638525
18	6	0	9.770478	1.240431	0.469354
19	6	0	7.389878	-0.60507	-3.194998
20	6	0	-0.167565	-1.857746	4.870187
21	6	0	2.797211	6.809376	-2.819566
22	6	0	-2.326684	-5.085537	-4.603749
23	6	0	-7.373944	1.517929	3.786661
24	1	0	2.083992	1.410325	2.237216
25	6	0	1.583245	0.169547	-1.501574
26	1	0	-6.191204	1.931684	-2.675998
27	1	0	-9.894632	-1.413898	-2.060164
28	1	0	-8.120817	-2.550158	0.500284
29	1	0	-7.430442	-4.815782	-3.663301
30	1	0	-6.291695	-2.013715	-4.971718
31	1	0	-3.931676	-2.550237	1.257725
32	1	0	0.553093	2.39369	-4.567397
33	1	0	-0.164319	7.713425	1.119655
34	1	0	-1.915154	2.18165	1.40747
35	1	0	-2.006181	4.335334	3.941664
36	1	0	-5.000612	5.530833	-0.811746
37	1	0	-5.789455	6.261991	2.345511
38	1	0	0.924382	-5.160901	-0.685816
39	1	0	-0.670754	-6.106746	2.038138
40	1	0	4.301911	-3.634687	5.293749
41	1	0	3.316391	-6.250542	3.479483
42	1	0	5.466645	-4.451493	-0.313554
43	1	0	7.691122	-4.091657	2.149846
44	1	0	5.988712	0.103897	3.163755
45	1	0	6.240278	2.581021	-0.982916
46	1	0	10.741439	-0.537367	0.912756
47	1	0	10.957952	2.280022	-0.872829
48	1	0	9.659132	2.350751	2.214788
49	1	0	8.464561	0.573146	-4.517812
50	1	0	5.554779	-0.997957	-4.055059
51	1	0	8.407188	-2.399112	-2.996485
52	1	0	-1.853488	-0.77969	4.361833
53	1	0	-0.777593	-3.511885	5.962863
54	1	0	0.983455	-0.667421	6.115337
55	1	0	4.777522	6.195259	-2.756312

56	1	0	2.281858	6.918929	-4.828152
57	1	0	2.678631	8.713485	-2.020041
58	1	0	-3.384333	-6.722254	-5.319826
59	1	0	-2.13722	-3.768093	-6.198303
60	1	0	-0.437483	-5.73955	-4.096765
61	1	0	-8.663982	2.89918	4.645615
62	1	0	-8.337031	-0.308399	3.758749
63	1	0	-5.74678	1.362735	5.06643
64	1	0	1.466155	-1.472542	-2.727766

Table S7. Gibbs free energies[a] and equilibrium populations[b] of low-energy conformers of 14*R*,15*R*,18*R*-1.

Conformers	ΔG(a.u.)	P(%)/100	G(a.u.)
14R,15R,18R-1000001	0.00266	4.22	-976.022152
14R,15R,18R-1000002	0.0	70.64	-976.024812
14R,15R,18R-1000003	0.00133	17.2	-976.023478
14R,15R,18R-1000004	0.00206	7.94	-976.022748

[a]wB97M-V/def2-TZVP, in a.u.

[b]From ΔG values at 298.15K.

Table S8. Cartesian coordinates for the low-energy reoptimized random research conformers of 14*R*,15*R*,18*R*-1 at B3LYP-D3(BJ)/6-31G* level of theory in methanol.

14R,15R,18R-1000001_en_		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	7.11833	-0.621942	-1.541312
1	6	0	8.339731	1.539405	-0.131792
2	6	0	6.470057	3.121028	1.484101
3	6	0	4.221926	4.081228	0.009352
4	6	0	1.867336	3.419416	0.67528
5	6	0	-1.071774	-2.227796	3.26425
6	6	0	-0.19328	-3.792653	1.127578
7	6	0	0.963895	-2.732	-0.869474
8	6	0	2.35448	-4.046941	-2.974803
9	6	0	5.069044	-4.828559	-2.170008
10	6	0	6.421596	-2.852725	-0.570972
11	6	0	-0.508356	3.990981	-0.786593
12	6	0	-3.036914	4.017389	0.684741
13	6	0	-4.047853	1.345907	1.505286
14	6	0	-5.135975	4.739064	-1.204577
15	6	0	-5.594501	2.326389	-2.762601
16	6	0	-5.02451	0.06589	-0.950478
17	6	0	-7.401505	-1.595394	-0.58164
18	6	0	-7.222125	-3.507207	1.586194
19	6	0	-8.037515	-2.994542	-3.04399
20	6	0	-2.867599	5.857372	2.907779
21	6	0	-0.354591	-6.614221	1.534965
22	6	0	4.84259	5.683105	-2.265854
23	6	0	6.791141	-3.558119	2.162329
24	1	0	-5.767137	1.824671	2.583792
25	6	0	-2.479037	-0.115892	3.386169
26	1	0	6.706568	-0.275806	-3.531479
27	1	0	9.273645	2.789894	-1.493907
28	1	0	9.837743	0.845753	1.122644
29	1	0	5.802726	1.965599	3.066589
30	1	0	7.527904	4.719549	2.29437

31	1	0	1.644375	2.224345	2.330681
32	1	0	-0.393419	-2.930806	5.085902
33	1	0	1.15823	-0.697822	-0.86362
34	1	0	1.346542	-5.726729	-3.651623
35	1	0	2.481499	-2.748187	-4.583594
36	1	0	6.171046	-5.267772	-3.871467
37	1	0	4.941803	-6.586482	-1.08207
38	1	0	-0.668154	2.633499	-2.349586
39	1	0	-0.336056	5.8448	-1.700729
40	1	0	-6.851801	5.244275	-0.153098
41	1	0	-4.630043	6.375357	-2.369441
42	1	0	-4.354147	2.277344	-4.418117
43	1	0	-7.531832	2.257944	-3.484484
44	1	0	-3.539619	-1.125147	-1.754421
45	1	0	-8.976491	-0.30441	-0.144604
46	1	0	-8.982788	-4.591858	1.725757
47	1	0	-6.884896	-2.601046	3.411135
48	1	0	-5.678365	-4.846263	1.26341
49	1	0	-9.80011	-4.066889	-2.858072
50	1	0	-8.248809	-1.703502	-4.647126
51	1	0	-6.528753	-4.338449	-3.513039
52	1	0	-2.397241	7.764352	2.245951
53	1	0	-4.67131	5.963448	3.923681
54	1	0	-1.401087	5.292706	4.254532
55	1	0	0.733327	-7.168274	3.214847
56	1	0	-2.30821	-7.217559	1.873778
57	1	0	0.379134	-7.684618	-0.071066
58	1	0	3.214903	6.745235	-2.963878
59	1	0	6.349878	7.037428	-1.822042
60	1	0	5.536519	4.517899	-3.838329
61	1	0	7.895892	-2.167952	3.215876
62	1	0	4.946915	-3.747388	3.095031
63	1	0	7.739547	-5.396512	2.33059
64	1	0	-2.64548	0.674283	5.283634

14R,15R,18R-1000002_en_		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-6.64336	-0.498405	1.674144
1	6	0	-8.213427	1.062865	-0.107952
2	6	0	-6.535258	2.682396	-1.905964
3	6	0	-4.46274	4.053286	-0.491615
4	6	0	-2.089648	3.177267	-0.645064

5	6	0	1.21762	-1.816711	-3.68013
6	6	0	0.415536	-3.807686	-1.899509
7	6	0	-0.573155	-3.297354	0.388756
8	6	0	-1.732865	-5.127536	2.227657
9	6	0	-4.187541	-4.061833	3.417644
10	6	0	-5.992681	-2.939965	1.500964
11	6	0	0.138689	3.886511	0.964165
12	6	0	2.739014	4.187479	-0.355037
13	6	0	3.941064	1.651552	-1.341082
14	6	0	4.698123	4.862611	1.691407
15	6	0	5.261476	2.351208	3.049884
16	6	0	4.849806	0.21607	1.04968
17	6	0	7.280792	-1.360637	0.674917
18	6	0	7.207732	-3.156503	-1.596087
19	6	0	7.871763	-2.879195	3.077104
20	6	0	2.553241	6.198234	-2.422089
21	6	0	0.585428	-6.438976	-3.006123
22	6	0	-5.321584	6.167642	1.212796
23	6	0	-6.862646	-4.696845	-0.563652
24	1	0	5.68963	2.304696	-2.272181
25	6	0	2.520477	0.351703	-3.439377
26	1	0	-5.829076	0.567097	3.236883
27	1	0	-9.435658	2.326537	0.994487
28	1	0	-9.471763	-0.10887	-1.259739
29	1	0	-5.682523	1.416777	-3.305016
30	1	0	-7.757412	4.015776	-2.929056
31	1	0	-1.765986	1.625858	-1.943415
32	1	0	0.59581	-2.222712	-5.607889
33	1	0	-0.700945	-1.330264	0.952537
34	1	0	-2.137232	-6.937047	1.312279
35	1	0	-0.403601	-5.554395	3.769134
36	1	0	-3.688973	-2.604001	4.803018
37	1	0	-5.111459	-5.597831	4.471027
38	1	0	0.323485	2.445192	2.450929
39	1	0	-0.236721	5.657131	1.973074
40	1	0	6.415832	5.579033	0.774918
41	1	0	4.028537	6.344673	2.974279
42	1	0	3.998871	2.095659	4.668956
43	1	0	7.187714	2.32638	3.803248
44	1	0	3.372786	-1.072352	1.699741
45	1	0	8.836531	-0.011369	0.362315
46	1	0	5.679245	-4.536637	-1.389539
47	1	0	8.991868	-4.201694	-1.73688

48	1	0	6.909207	-2.158919	-3.379282
49	1	0	9.658632	-3.909209	2.884709
50	1	0	8.014109	-1.674849	4.753481
51	1	0	6.376581	-4.273747	3.428263
52	1	0	1.976067	8.018792	-1.616646
53	1	0	4.378186	6.470024	-3.367068
54	1	0	1.147655	5.684644	-3.851124
55	1	0	-0.372405	-6.517965	-4.845334
56	1	0	2.563952	-6.956411	-3.351753
57	1	0	-0.238545	-7.888236	-1.791475
58	1	0	-3.751249	7.256114	1.995774
59	1	0	-6.555436	7.479187	0.182058
60	1	0	-6.436187	5.445244	2.810091
61	1	0	-8.334915	-3.86317	-1.747129
62	1	0	-5.278631	-5.209181	-1.801272
63	1	0	-7.603718	-6.46544	0.231181
64	1	0	2.652595	1.432409	-5.190214

14R,15R,18R-1000003_en_		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	6.562535	-0.157067	-1.2106
1	6	0	7.884367	2.122832	-0.149816
2	6	0	6.080957	3.760207	1.491757
3	6	0	3.745745	4.581023	0.065179
4	6	0	1.462568	3.680498	0.701736
5	6	0	-0.988106	-2.145962	3.359833
6	6	0	0.051603	-3.712683	1.297567
7	6	0	1.141441	-2.657845	-0.740649
8	6	0	2.68365	-3.988269	-2.735704
9	6	0	5.349322	-4.705776	-1.783775
10	6	0	6.972587	-2.601313	-0.696708
11	6	0	-0.937569	4.01752	-0.79161
12	6	0	-3.480869	3.839601	0.64321
13	6	0	-4.260062	1.099468	1.484068
14	6	0	-5.606344	4.350474	-1.283637
15	6	0	-5.828953	1.886375	-2.814524
16	6	0	-5.071923	-0.29298	-0.968899
17	6	0	-7.283813	-2.170037	-0.612904
18	6	0	-6.93433	-4.049639	1.562736
19	6	0	-7.7675	-3.632946	-3.072825
20	6	0	-3.50805	5.71705	2.840736
21	6	0	0.123846	-6.515021	1.850136

22	6	0	4.223747	6.260445	-2.190771
23	6	0	9.045646	-3.558397	1.010606
24	1	0	-6.03426	1.43155	2.528405
25	6	0	-2.588682	-0.174409	3.410882
26	1	0	5.009887	0.305067	-2.474217
27	1	0	8.610261	3.292644	-1.705442
28	1	0	9.522664	1.598613	0.996673
29	1	0	5.529199	2.665015	3.160283
30	1	0	7.141012	5.421259	2.15557
31	1	0	1.347365	2.441527	2.334911
32	1	0	-0.261556	-2.719294	5.208269
33	1	0	1.116815	-0.617425	-0.853853
34	1	0	1.75316	-5.726223	-3.376095
35	1	0	2.837693	-2.77254	-4.405998
36	1	0	6.391271	-5.656934	-3.314733
37	1	0	5.124582	-6.145423	-0.304797
38	1	0	-0.951824	2.625598	-2.333346
39	1	0	-0.916116	5.862493	-1.738398
40	1	0	-7.374703	4.715886	-0.261918
41	1	0	-5.228381	6.010321	-2.463279
42	1	0	-4.574305	1.931177	-4.459385
43	1	0	-7.745549	1.633898	-3.55014
44	1	0	-3.468682	-1.346863	-1.737117
45	1	0	-8.977271	-1.032962	-0.190764
46	1	0	-8.587475	-5.291579	1.704065
47	1	0	-6.68213	-3.109034	3.383921
48	1	0	-5.273117	-5.240527	1.242354
49	1	0	-6.133685	-4.827209	-3.527877
50	1	0	-9.419461	-4.869699	-2.891815
51	1	0	-8.093105	-2.37506	-4.683
52	1	0	-3.200157	7.649226	2.1569
53	1	0	-5.328661	5.673992	3.830635
54	1	0	-2.016399	5.304929	4.214532
55	1	0	1.308785	-6.902333	3.511029
56	1	0	-1.76736	-7.235624	2.295641
57	1	0	0.871816	-7.614681	0.271016
58	1	0	2.51964	7.230831	-2.83861
59	1	0	5.650586	7.698194	-1.745984
60	1	0	4.960368	5.175448	-3.801781
61	1	0	10.149713	-5.036376	0.057919
62	1	0	10.35748	-2.083627	1.612062
63	1	0	8.241703	-4.433038	2.713967
64	1	0	-2.840674	0.649886	5.284249

14R,15R,18R-1000004_en_		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-6.810511	-0.011095	1.478076
1	6	0	-8.160791	1.588521	-0.444424
2	6	0	-6.269784	2.992206	-2.212613
3	6	0	-4.171221	4.266581	-0.744809
4	6	0	-1.89195	3.161605	-0.670061
5	6	0	1.172622	-2.162471	-3.393241
6	6	0	0.126194	-4.005	-1.579841
7	6	0	-0.909422	-3.324669	0.64304
8	6	0	-2.31166	-4.975733	2.481813
9	6	0	-4.734927	-3.672695	3.487632
10	6	0	-6.346319	-2.500528	1.433531
11	6	0	0.302802	3.768737	1.023332
12	6	0	2.96681	3.846843	-0.196939
13	6	0	4.031196	1.208874	-1.070386
14	6	0	4.900638	4.459897	1.897323
15	6	0	5.267897	1.959532	3.337791
16	6	0	4.778754	-0.20318	1.389534
17	6	0	7.070195	-2.0184	1.181301
18	6	0	9.446948	-0.782419	0.066563
19	6	0	6.460974	-4.473623	-0.231908
20	6	0	2.992492	5.798451	-2.329173
21	6	0	0.12219	-6.682471	-2.581832
22	6	0	-4.932069	6.56937	0.74693
23	6	0	-7.241519	-4.270642	-0.608491
24	1	0	5.828513	1.744735	-1.966484
25	6	0	2.620513	-0.083604	-3.179221
26	1	0	-5.992203	1.054475	3.038496
27	1	0	-9.332955	2.988793	0.54148
28	1	0	-9.448951	0.469257	-1.615555
29	1	0	-5.447769	1.602253	-3.508314
30	1	0	-7.327611	4.365639	-3.35809
31	1	0	-1.645537	1.498098	-1.840233
32	1	0	0.617147	-2.608831	-5.332235
33	1	0	-0.876141	-1.336408	1.139741
34	1	0	-2.808721	-6.786003	1.615937
35	1	0	-1.108363	-5.437403	4.114095
36	1	0	-4.197168	-2.197643	4.839812
37	1	0	-5.829329	-5.086668	4.548778
38	1	0	0.324822	2.36536	2.556899

39	1	0	0.01001	5.593014	1.960838
40	1	0	6.685845	5.046568	1.018344
41	1	0	4.279932	6.016219	3.115338
42	1	0	3.928142	1.821331	4.909477
43	1	0	7.155748	1.827585	4.173983
44	1	0	3.18785	-1.345163	2.041671
45	1	0	7.519734	-2.543533	3.143266
46	1	0	9.24441	-0.449089	-1.967729
47	1	0	11.088752	-2.018927	0.32137
48	1	0	9.884383	1.031807	0.964912
49	1	0	8.072308	-5.775164	-0.159289
50	1	0	4.824494	-5.425887	0.601378
51	1	0	6.02707	-4.103612	-2.219678
52	1	0	1.611193	5.331321	-3.797319
53	1	0	2.507685	7.678484	-1.60324
54	1	0	4.86611	5.920735	-3.207504
55	1	0	-0.882481	-8.008404	-1.362073
56	1	0	-0.744913	-6.756116	-4.465542
57	1	0	2.065519	-7.373695	-2.7968
58	1	0	-5.870139	7.955213	-0.480331
59	1	0	-6.299117	6.083653	2.233474
60	1	0	-3.332314	7.50655	1.655627
61	1	0	-5.639696	-4.946255	-1.740047
62	1	0	-8.153181	-5.947109	0.208386
63	1	0	-8.584965	-3.379764	-1.898879
64	1	0	2.911564	0.900063	-4.967522

Table S9. Gibbs free energies[a] and equilibrium populations[b] of low-energy conformers of 1.

Conformers	ΔG	P(%)/100	Single point energy(a.u.)
CMD1000002_tddft_	0.0	64.99	-976.573385327
CMD1000004_tddft_	0.00312	2.38	-976.5702657806
CMD1000006_tddft_	0.00201	7.68	-976.5713705845
CMD1000010_tddft_	0.00244	4.87	-976.5709405518
CMD1000011_tddft_	0.00135	15.5	-976.5720327869
CMD1000012_tddft_	0.0025	4.58	-976.5708816196

[a]wB97M-V/def2-TZVP, in kcal/mol.

[b]From ΔG values at 298.15K.

Table S10. Cartesian coordinates for the low-energy reoptimized random research conformers of 1 at PBE0-D3(BJ)/def2-SVP level of theory in methanol.

CMD1000002_en_		Standard Orientation (Ångstroms)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-17.80222	-2.969839	1.600162
1	6	0	-18.963713	-5.119775	0.194394
2	6	0	-18.664977	-4.810013	-2.685614
3	6	0	-15.982932	-4.907253	-3.610819
4	6	0	-14.886444	-2.866411	-4.616228
5	6	0	-14.286255	4.210451	-4.924006
6	6	0	-15.625369	4.828347	-2.580353
7	6	0	-16.096738	3.141194	-0.753574
8	6	0	-17.304451	3.66476	1.751
9	6	0	-17.44272	1.303799	3.423636
10	6	0	-18.926146	-0.80513	2.244462
11	6	0	-12.30366	-2.666424	-5.727048
12	6	0	-10.227753	-1.438342	-4.086897
13	6	0	-10.704424	1.386351	-3.364072
14	6	0	-12.223023	2.790909	-5.2733
15	6	0	-7.713692	-1.379353	-5.608802
16	6	0	-6.625638	1.290497	-5.394823
17	6	0	-7.991407	2.478631	-3.152977
18	6	0	-7.794241	5.346201	-2.928891
19	6	0	-9.132659	6.30136	-0.56689
20	6	0	-5.050619	6.220476	-2.938602
21	6	0	-9.903385	-2.979473	-1.673871
22	6	0	-16.412313	7.547294	-2.382532
23	6	0	-14.707011	-7.415978	-3.312472
24	6	0	-21.652991	-0.238714	1.743017
25	1	0	-11.637416	1.490017	-1.543918
26	1	0	-15.797339	-3.146512	1.998459
27	1	0	-20.972451	-5.284098	0.618058
28	1	0	-18.108672	-6.899484	0.788502
29	1	0	-19.742181	-6.316164	-3.609512
30	1	0	-19.527579	-3.024813	-3.240651
31	1	0	-15.99708	-1.146331	-4.707114
32	1	0	-14.994017	5.199865	-6.581178

33	1	0	-15.586949	1.190495	-1.083654
34	1	0	-19.204828	4.437274	1.503263
35	1	0	-16.255029	5.12778	2.764441
36	1	0	-18.293114	1.833956	5.231787
37	1	0	-15.528175	0.658308	3.832663
38	1	0	-12.440539	-1.59807	-7.486415
39	1	0	-11.603632	-4.531052	-6.256984
40	1	0	-11.495721	2.73087	-7.190966
41	1	0	-6.40409	-2.774096	-4.84588
42	1	0	-8.028796	-1.901018	-7.575523
43	1	0	-7.018836	2.38256	-7.101064
44	1	0	-4.582572	1.286462	-5.161507
45	1	0	-7.170729	1.688863	-1.424918
46	1	0	-8.733532	6.172831	-4.574571
47	1	0	-9.028413	8.354803	-0.436094
48	1	0	-11.114202	5.764617	-0.536966
49	1	0	-8.248201	5.528309	1.129934
50	1	0	-4.928846	8.262614	-2.697493
51	1	0	-4.088732	5.74652	-4.693481
52	1	0	-3.9967	5.351799	-1.391646
53	1	0	-11.656003	-3.0425	-0.598994
54	1	0	-9.372076	-4.920151	-2.117663
55	1	0	-8.434575	-2.199554	-0.46251
56	1	0	-17.37924	8.152872	-4.100544
57	1	0	-17.663172	7.898709	-0.794129
58	1	0	-14.766476	8.775266	-2.176121
59	1	0	-15.954265	-8.949293	-3.901421
60	1	0	-12.967198	-7.561417	-4.388719
61	1	0	-14.226633	-7.777242	-1.338155
62	1	0	-22.521308	0.696054	3.363311
63	1	0	-21.859388	1.046921	0.142351
64	1	0	-22.753321	-1.916969	1.314755

CMD1000002_tddft_		Standard Orientation (Ångstroms)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-17.80222	-2.969839	1.600162
1	6	0	-18.963713	-5.119775	0.194394
2	6	0	-18.664977	-4.810013	-2.685614
3	6	0	-15.982932	-4.907253	-3.610819
4	6	0	-14.886444	-2.866411	-4.616228
5	6	0	-14.286255	4.210451	-4.924006
6	6	0	-15.625369	4.828347	-2.580353

7	6	0	-16.096738	3.141194	-0.753574
8	6	0	-17.304451	3.66476	1.751
9	6	0	-17.44272	1.303799	3.423636
10	6	0	-18.926146	-0.80513	2.244462
11	6	0	-12.30366	-2.666424	-5.727048
12	6	0	-10.227753	-1.438342	-4.086897
13	6	0	-10.704424	1.386351	-3.364072
14	6	0	-12.223023	2.790909	-5.2733
15	6	0	-7.713692	-1.379353	-5.608802
16	6	0	-6.625638	1.290497	-5.394823
17	6	0	-7.991407	2.478631	-3.152977
18	6	0	-7.794241	5.346201	-2.928891
19	6	0	-9.132659	6.30136	-0.56689
20	6	0	-5.050619	6.220476	-2.938602
21	6	0	-9.903385	-2.979473	-1.673871
22	6	0	-16.412313	7.547294	-2.382532
23	6	0	-14.707011	-7.415978	-3.312472
24	6	0	-21.652991	-0.238714	1.743017
25	1	0	-11.637416	1.490017	-1.543918
26	1	0	-15.797339	-3.146512	1.998459
27	1	0	-20.972451	-5.284098	0.618058
28	1	0	-18.108672	-6.899484	0.788502
29	1	0	-19.742181	-6.316164	-3.609512
30	1	0	-19.527579	-3.024813	-3.240651
31	1	0	-15.99708	-1.146331	-4.707114
32	1	0	-14.994017	5.199865	-6.581178
33	1	0	-15.586949	1.190495	-1.083654
34	1	0	-19.204828	4.437274	1.503263
35	1	0	-16.255029	5.12778	2.764441
36	1	0	-18.293114	1.833956	5.231787
37	1	0	-15.528175	0.658308	3.832663
38	1	0	-12.440539	-1.59807	-7.486415
39	1	0	-11.603632	-4.531052	-6.256984
40	1	0	-11.495721	2.73087	-7.190966
41	1	0	-6.40409	-2.774096	-4.84588
42	1	0	-8.028796	-1.901018	-7.575523
43	1	0	-7.018836	2.38256	-7.101064
44	1	0	-4.582572	1.286462	-5.161507
45	1	0	-7.170729	1.688863	-1.424918
46	1	0	-8.733532	6.172831	-4.574571
47	1	0	-9.028413	8.354803	-0.436094
48	1	0	-11.114202	5.764617	-0.536966
49	1	0	-8.248201	5.528309	1.129934

50	1	0	-4.928846	8.262614	-2.697493
51	1	0	-4.088732	5.74652	-4.693481
52	1	0	-3.9967	5.351799	-1.391646
53	1	0	-11.656003	-3.0425	-0.598994
54	1	0	-9.372076	-4.920151	-2.117663
55	1	0	-8.434575	-2.199554	-0.46251
56	1	0	-17.37924	8.152872	-4.100544
57	1	0	-17.663172	7.898709	-0.794129
58	1	0	-14.766476	8.775266	-2.176121
59	1	0	-15.954265	-8.949293	-3.901421
60	1	0	-12.967198	-7.561417	-4.388719
61	1	0	-14.226633	-7.777242	-1.338155
62	1	0	-22.521308	0.696054	3.363311
63	1	0	-21.859388	1.046921	0.142351
64	1	0	-22.753321	-1.916969	1.314755

CMD1000004_en_		Standard Orientation (Ångstroms)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-20.448012	-2.03594	-1.075455
1	6	0	-20.287289	-4.561091	-2.302809
2	6	0	-18.748115	-4.471143	-4.770622
3	6	0	-15.922978	-4.554665	-4.475416
4	6	0	-14.491779	-2.555936	-5.061701
5	6	0	-14.021951	4.294135	-4.492462
6	6	0	-15.544712	4.745122	-2.221679
7	6	0	-16.094995	2.875512	-0.604949
8	6	0	-17.435951	3.020979	1.862614
9	6	0	-19.880153	1.447092	1.926882
10	6	0	-19.530933	-1.258445	1.138445
11	6	0	-11.676074	-2.468733	-5.270278
12	6	0	-10.087526	-1.300132	-3.116531
13	6	0	-10.489462	1.611885	-2.661891
14	6	0	-11.887726	2.954606	-4.701821
15	6	0	-7.250375	-1.541843	-3.854936
16	6	0	-6.278084	1.125153	-4.289023
17	6	0	-7.764723	2.661233	-2.367837
18	6	0	-7.492657	5.528893	-2.484501
19	6	0	-8.930276	6.791311	-0.335384
20	6	0	-4.729835	6.339647	-2.442791
21	6	0	-10.618565	-2.708753	-0.665925
22	6	0	-16.401382	7.432695	-1.920155
23	6	0	-14.900848	-7.049568	-3.615389

24	6	0	-18.080482	-2.886573	2.93584
25	1	0	-11.509025	1.872066	-0.904779
26	1	0	-21.434234	-0.633439	-2.209225
27	1	0	-22.201951	-5.182404	-2.773354
28	1	0	-19.523562	-5.991973	-1.038492
29	1	0	-19.306474	-6.085229	-5.937443
30	1	0	-19.288321	-2.784977	-5.825001
31	1	0	-15.463535	-0.839516	-5.612289
32	1	0	-14.645718	5.305524	-6.169856
33	1	0	-15.530388	0.986271	-1.146006
34	1	0	-17.887989	4.959349	2.380971
35	1	0	-16.156796	2.334408	3.336246
36	1	0	-21.26002	2.344072	0.688712
37	1	0	-20.651002	1.525192	3.844203
38	1	0	-11.209889	-1.470726	-7.016227
39	1	0	-10.95553	-4.381015	-5.5316
40	1	0	-11.00633	2.937135	-6.554059
41	1	0	-6.203051	-2.403646	-2.301443
42	1	0	-6.986563	-2.765632	-5.489559
43	1	0	-6.708601	1.774072	-6.202444
44	1	0	-4.240232	1.267333	-4.048405
45	1	0	-7.11337	2.068838	-0.49044
46	1	0	-8.316846	6.17381	-4.266796
47	1	0	-10.91722	6.273898	-0.332001
48	1	0	-8.135947	6.243578	1.488522
49	1	0	-8.810508	8.843712	-0.468341
50	1	0	-3.779193	5.624643	-0.756798
51	1	0	-4.568124	8.393021	-2.419281
52	1	0	-3.695609	5.655002	-4.082964
53	1	0	-9.559592	-1.887895	0.899066
54	1	0	-12.619585	-2.646911	-0.193304
55	1	0	-10.071354	-4.689953	-0.814602
56	1	0	-17.711703	7.69077	-0.36277
57	1	0	-14.799961	8.697567	-1.623741
58	1	0	-17.339418	8.077093	-3.640996
59	1	0	-15.465615	-7.445577	-1.67053
60	1	0	-15.650171	-8.59111	-4.764396
61	1	0	-12.854295	-7.147138	-3.673495
62	1	0	-17.850692	-4.811247	2.264771
63	1	0	-16.19463	-2.124052	3.278045
64	1	0	-19.016106	-2.960681	4.774544

CMD1000004_tddft_	Standard Orientation (Ångstroms)

Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-20.448012	-2.03594	-1.075455
1	6	0	-20.287289	-4.561091	-2.302809
2	6	0	-18.748115	-4.471143	-4.770622
3	6	0	-15.922978	-4.554665	-4.475416
4	6	0	-14.491779	-2.555936	-5.061701
5	6	0	-14.021951	4.294135	-4.492462
6	6	0	-15.544712	4.745122	-2.221679
7	6	0	-16.094995	2.875512	-0.604949
8	6	0	-17.435951	3.020979	1.862614
9	6	0	-19.880153	1.447092	1.926882
10	6	0	-19.530933	-1.258445	1.138445
11	6	0	-11.676074	-2.468733	-5.270278
12	6	0	-10.087526	-1.300132	-3.116531
13	6	0	-10.489462	1.611885	-2.661891
14	6	0	-11.887726	2.954606	-4.701821
15	6	0	-7.250375	-1.541843	-3.854936
16	6	0	-6.278084	1.125153	-4.289023
17	6	0	-7.764723	2.661233	-2.367837
18	6	0	-7.492657	5.528893	-2.484501
19	6	0	-8.930276	6.791311	-0.335384
20	6	0	-4.729835	6.339647	-2.442791
21	6	0	-10.618565	-2.708753	-0.665925
22	6	0	-16.401382	7.432695	-1.920155
23	6	0	-14.900848	-7.049568	-3.615389
24	6	0	-18.080482	-2.886573	2.93584
25	1	0	-11.509025	1.872066	-0.904779
26	1	0	-21.434234	-0.633439	-2.209225
27	1	0	-22.201951	-5.182404	-2.773354
28	1	0	-19.523562	-5.991973	-1.038492
29	1	0	-19.306474	-6.085229	-5.937443
30	1	0	-19.288321	-2.784977	-5.825001
31	1	0	-15.463535	-0.839516	-5.612289
32	1	0	-14.645718	5.305524	-6.169856
33	1	0	-15.530388	0.986271	-1.146006
34	1	0	-17.887989	4.959349	2.380971
35	1	0	-16.156796	2.334408	3.336246
36	1	0	-21.26002	2.344072	0.688712
37	1	0	-20.651002	1.525192	3.844203
38	1	0	-11.209889	-1.470726	-7.016227
39	1	0	-10.95553	-4.381015	-5.5316
40	1	0	-11.00633	2.937135	-6.554059

41	1	0	-6.203051	-2.403646	-2.301443
42	1	0	-6.986563	-2.765632	-5.489559
43	1	0	-6.708601	1.774072	-6.202444
44	1	0	-4.240232	1.267333	-4.048405
45	1	0	-7.11337	2.068838	-0.49044
46	1	0	-8.316846	6.17381	-4.266796
47	1	0	-10.91722	6.273898	-0.332001
48	1	0	-8.135947	6.243578	1.488522
49	1	0	-8.810508	8.843712	-0.468341
50	1	0	-3.779193	5.624643	-0.756798
51	1	0	-4.568124	8.393021	-2.419281
52	1	0	-3.695609	5.655002	-4.082964
53	1	0	-9.559592	-1.887895	0.899066
54	1	0	-12.619585	-2.646911	-0.193304
55	1	0	-10.071354	-4.689953	-0.814602
56	1	0	-17.711703	7.69077	-0.36277
57	1	0	-14.799961	8.697567	-1.623741
58	1	0	-17.339418	8.077093	-3.640996
59	1	0	-15.465615	-7.445577	-1.67053
60	1	0	-15.650171	-8.59111	-4.764396
61	1	0	-12.854295	-7.147138	-3.673495
62	1	0	-17.850692	-4.811247	2.264771
63	1	0	-16.19463	-2.124052	3.278045
64	1	0	-19.016106	-2.960681	4.774544

CMD1000006_en_		Standard Orientation (Ångstroms)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-17.163383	-2.719151	1.90079
1	6	0	-17.98572	-5.118678	0.653348
2	6	0	-18.562949	-4.716708	-2.151839
3	6	0	-16.449127	-3.793859	-3.825763
4	6	0	-14.017807	-4.075208	-3.222366
5	6	0	-14.160286	3.454481	-5.250168
6	6	0	-15.648072	4.356032	-3.094827
7	6	0	-16.249715	2.887624	-1.124845
8	6	0	-17.644326	3.678411	1.207132
9	6	0	-17.503819	1.692381	3.323143
10	6	0	-18.643894	-0.780579	2.538639
11	6	0	-11.755146	-3.433286	-4.771802
12	6	0	-9.739973	-1.746363	-3.528922
13	6	0	-10.548979	1.054701	-3.118753
14	6	0	-12.03816	2.083616	-5.277848

15	6	0	-7.433185	-1.507092	-5.305805
16	6	0	-6.329778	1.150014	-4.919587
17	6	0	-7.962467	2.419895	-2.888768
18	6	0	-8.015913	5.30192	-2.970854
19	6	0	-9.561929	6.382273	-0.797924
20	6	0	-5.353101	6.397744	-2.935712
21	6	0	-8.908167	-2.899544	-1.015801
22	6	0	-16.471183	7.062559	-3.315156
23	6	0	-17.381587	-2.600359	-6.213468
24	6	0	-21.463466	-0.818142	2.321929
25	1	0	-11.612283	1.246998	-1.37822
26	1	0	-15.14237	-2.462496	2.122401
27	1	0	-19.684917	-5.873648	1.546252
28	1	0	-16.546773	-6.574489	0.887152
29	1	0	-19.308414	-6.473703	-2.959605
30	1	0	-20.117955	-3.365252	-2.291812
31	1	0	-13.5941	-4.982682	-1.437044
32	1	0	-14.805822	4.15852	-7.071533
33	1	0	-15.723406	0.914411	-1.216496
34	1	0	-19.630879	4.053566	0.771909
35	1	0	-16.900405	5.461497	1.933405
36	1	0	-18.47016	2.439885	4.988676
37	1	0	-15.528891	1.417021	3.844853
38	1	0	-12.305547	-2.586873	-6.559831
39	1	0	-10.798172	-5.205528	-5.262369
40	1	0	-11.202533	1.777564	-7.12761
41	1	0	-6.064947	-2.996042	-4.915268
42	1	0	-8.021761	-1.768896	-7.262597
43	1	0	-6.43073	2.230317	-6.672397
44	1	0	-4.346141	1.108456	-4.38002
45	1	0	-7.201827	1.908263	-1.03749
46	1	0	-8.917508	5.868096	-4.742813
47	1	0	-11.497454	5.699375	-0.817647
48	1	0	-8.729621	5.858471	1.016459
49	1	0	-9.614842	8.440424	-0.879791
50	1	0	-4.245475	5.798724	-4.561973
51	1	0	-4.337671	5.813401	-1.236743
52	1	0	-5.406734	8.456811	-2.943808
53	1	0	-7.213847	-1.999216	-0.279679
54	1	0	-10.370113	-2.73361	0.423218
55	1	0	-8.47702	-4.901873	-1.247519
56	1	0	-17.643202	7.666466	-1.743137
57	1	0	-14.845334	8.326331	-3.430387

58	1	0	-17.55242	7.346488	-5.050055
59	1	0	-18.357968	-0.834494	-5.780549
60	1	0	-15.892852	-2.165252	-7.552815
61	1	0	-18.753289	-3.823967	-7.153225
62	1	0	-22.333994	-0.091918	4.045739
63	1	0	-22.1193	0.390664	0.783604
64	1	0	-22.20982	-2.699284	1.981213

CMD1000006_tddft_		Standard Orientation (Ångstroms)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-17.163383	-2.719151	1.90079
1	6	0	-17.98572	-5.118678	0.653348
2	6	0	-18.562949	-4.716708	-2.151839
3	6	0	-16.449127	-3.793859	-3.825763
4	6	0	-14.017807	-4.075208	-3.222366
5	6	0	-14.160286	3.454481	-5.250168
6	6	0	-15.648072	4.356032	-3.094827
7	6	0	-16.249715	2.887624	-1.124845
8	6	0	-17.644326	3.678411	1.207132
9	6	0	-17.503819	1.692381	3.323143
10	6	0	-18.643894	-0.780579	2.538639
11	6	0	-11.755146	-3.433286	-4.771802
12	6	0	-9.739973	-1.746363	-3.528922
13	6	0	-10.548979	1.054701	-3.118753
14	6	0	-12.03816	2.083616	-5.277848
15	6	0	-7.433185	-1.507092	-5.305805
16	6	0	-6.329778	1.150014	-4.919587
17	6	0	-7.962467	2.419895	-2.888768
18	6	0	-8.015913	5.30192	-2.970854
19	6	0	-9.561929	6.382273	-0.797924
20	6	0	-5.353101	6.397744	-2.935712
21	6	0	-8.908167	-2.899544	-1.015801
22	6	0	-16.471183	7.062559	-3.315156
23	6	0	-17.381587	-2.600359	-6.213468
24	6	0	-21.463466	-0.818142	2.321929
25	1	0	-11.612283	1.246998	-1.37822
26	1	0	-15.14237	-2.462496	2.122401
27	1	0	-19.684917	-5.873648	1.546252
28	1	0	-16.546773	-6.574489	0.887152
29	1	0	-19.308414	-6.473703	-2.959605
30	1	0	-20.117955	-3.365252	-2.291812
31	1	0	-13.5941	-4.982682	-1.437044

32	1	0	-14.805822	4.15852	-7.071533
33	1	0	-15.723406	0.914411	-1.216496
34	1	0	-19.630879	4.053566	0.771909
35	1	0	-16.900405	5.461497	1.933405
36	1	0	-18.47016	2.439885	4.988676
37	1	0	-15.528891	1.417021	3.844853
38	1	0	-12.305547	-2.586873	-6.559831
39	1	0	-10.798172	-5.205528	-5.262369
40	1	0	-11.202533	1.777564	-7.12761
41	1	0	-6.064947	-2.996042	-4.915268
42	1	0	-8.021761	-1.768896	-7.262597
43	1	0	-6.43073	2.230317	-6.672397
44	1	0	-4.346141	1.108456	-4.38002
45	1	0	-7.201827	1.908263	-1.03749
46	1	0	-8.917508	5.868096	-4.742813
47	1	0	-11.497454	5.699375	-0.817647
48	1	0	-8.729621	5.858471	1.016459
49	1	0	-9.614842	8.440424	-0.879791
50	1	0	-4.245475	5.798724	-4.561973
51	1	0	-4.337671	5.813401	-1.236743
52	1	0	-5.406734	8.456811	-2.943808
53	1	0	-7.213847	-1.999216	-0.279679
54	1	0	-10.370113	-2.73361	0.423218
55	1	0	-8.47702	-4.901873	-1.247519
56	1	0	-17.643202	7.666466	-1.743137
57	1	0	-14.845334	8.326331	-3.430387
58	1	0	-17.55242	7.346488	-5.050055
59	1	0	-18.357968	-0.834494	-5.780549
60	1	0	-15.892852	-2.165252	-7.552815
61	1	0	-18.753289	-3.823967	-7.153225
62	1	0	-22.333994	-0.091918	4.045739
63	1	0	-22.1193	0.390664	0.783604
64	1	0	-22.20982	-2.699284	1.981213

CMD1000010_en_		Standard Orientation (Ångstroms)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-18.711286	-2.217303	0.464901
1	6	0	-18.408567	-5.016011	0.230479
2	6	0	-18.403867	-5.925124	-2.503921
3	6	0	-16.191231	-5.213167	-4.141106
4	6	0	-14.34359	-3.676366	-3.382794
5	6	0	-13.915084	4.010752	-5.659762

6	6	0	-15.898153	4.704561	-3.852002
7	6	0	-17.007982	2.952663	-2.405244
8	6	0	-18.953337	3.305307	-0.398511
9	6	0	-18.126641	2.149271	2.119611
10	6	0	-17.716141	-0.669753	2.184126
11	6	0	-12.026126	-2.972696	-4.856104
12	6	0	-10.085085	-1.417306	-3.381814
13	6	0	-10.877825	1.38276	-2.94411
14	6	0	-11.854354	2.597092	-5.298003
15	6	0	-7.605914	-1.11563	-4.87591
16	6	0	-6.409606	1.380589	-3.976707
17	6	0	-8.33314	2.609763	-2.171662
18	6	0	-8.282207	5.488408	-2.068846
19	6	0	-10.231263	6.493014	-0.205191
20	6	0	-5.658736	6.464363	-1.39243
21	6	0	-9.498026	-2.721036	-0.86572
22	6	0	-16.578767	7.456888	-3.891221
23	6	0	-16.234076	-6.414124	-6.704432
24	6	0	-16.101921	-1.536665	4.339202
25	1	0	-12.262251	1.520655	-1.43399
26	1	0	-19.862877	-1.393218	-1.017055
27	1	0	-19.976399	-5.962867	1.194221
28	1	0	-16.695549	-5.671356	1.167107
29	1	0	-18.551423	-7.98939	-2.507586
30	1	0	-20.144794	-5.279552	-3.425938
31	1	0	-14.4998	-2.859256	-1.520324
32	1	0	-14.105853	4.884212	-7.512312
33	1	0	-16.415976	1.018894	-2.700701
34	1	0	-20.743873	2.454438	-0.985099
35	1	0	-19.35959	5.297129	-0.086647
36	1	0	-19.503275	2.653446	3.582554
37	1	0	-16.369411	3.071471	2.699682
38	1	0	-12.546348	-1.928514	-6.560451
39	1	0	-11.07919	-4.687585	-5.51864
40	1	0	-10.617914	2.41596	-6.92436
41	1	0	-6.374456	-2.740937	-4.587277
42	1	0	-8.004859	-1.043962	-6.896036
43	1	0	-6.049042	2.623003	-5.579619
44	1	0	-4.596092	1.086625	-3.053302
45	1	0	-7.935429	1.957638	-0.253628
46	1	0	-8.768318	6.20111	-3.948171
47	1	0	-12.134228	5.880605	-0.679127
48	1	0	-9.817614	5.830529	1.704991

49	1	0	-10.22192	8.552435	-0.159507
50	1	0	-5.640847	8.522022	-1.296589
51	1	0	-4.240345	5.895271	-2.768746
52	1	0	-5.061974	5.75442	0.450956
53	1	0	-7.779783	-1.995989	-0.003867
54	1	0	-11.017343	-2.501621	0.503851
55	1	0	-9.222498	-4.740756	-1.164653
56	1	0	-14.9393	8.630128	-3.461421
57	1	0	-17.209343	8.006076	-5.778534
58	1	0	-18.074161	7.939715	-2.573265
59	1	0	-16.210189	-8.473915	-6.559697
60	1	0	-17.96882	-5.925174	-7.711851
61	1	0	-14.650298	-5.846378	-7.878833
62	1	0	-14.201854	-0.739592	4.20235
63	1	0	-16.874745	-0.871708	6.13458
64	1	0	-15.928634	-3.577215	4.458081

CMD1000010_tddft_		Standard Orientation (Ångstroms)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-18.711286	-2.217303	0.464901
1	6	0	-18.408567	-5.016011	0.230479
2	6	0	-18.403867	-5.925124	-2.503921
3	6	0	-16.191231	-5.213167	-4.141106
4	6	0	-14.34359	-3.676366	-3.382794
5	6	0	-13.915084	4.010752	-5.659762
6	6	0	-15.898153	4.704561	-3.852002
7	6	0	-17.007982	2.952663	-2.405244
8	6	0	-18.953337	3.305307	-0.398511
9	6	0	-18.126641	2.149271	2.119611
10	6	0	-17.716141	-0.669753	2.184126
11	6	0	-12.026126	-2.972696	-4.856104
12	6	0	-10.085085	-1.417306	-3.381814
13	6	0	-10.877825	1.38276	-2.94411
14	6	0	-11.854354	2.597092	-5.298003
15	6	0	-7.605914	-1.11563	-4.87591
16	6	0	-6.409606	1.380589	-3.976707
17	6	0	-8.33314	2.609763	-2.171662
18	6	0	-8.282207	5.488408	-2.068846
19	6	0	-10.231263	6.493014	-0.205191
20	6	0	-5.658736	6.464363	-1.39243
21	6	0	-9.498026	-2.721036	-0.86572
22	6	0	-16.578767	7.456888	-3.891221

23	6	0	-16.234076	-6.414124	-6.704432
24	6	0	-16.101921	-1.536665	4.339202
25	1	0	-12.262251	1.520655	-1.43399
26	1	0	-19.862877	-1.393218	-1.017055
27	1	0	-19.976399	-5.962867	1.194221
28	1	0	-16.695549	-5.671356	1.167107
29	1	0	-18.551423	-7.98939	-2.507586
30	1	0	-20.144794	-5.279552	-3.425938
31	1	0	-14.4998	-2.859256	-1.520324
32	1	0	-14.105853	4.884212	-7.512312
33	1	0	-16.415976	1.018894	-2.700701
34	1	0	-20.743873	2.454438	-0.985099
35	1	0	-19.35959	5.297129	-0.086647
36	1	0	-19.503275	2.653446	3.582554
37	1	0	-16.369411	3.071471	2.699682
38	1	0	-12.546348	-1.928514	-6.560451
39	1	0	-11.07919	-4.687585	-5.51864
40	1	0	-10.617914	2.41596	-6.92436
41	1	0	-6.374456	-2.740937	-4.587277
42	1	0	-8.004859	-1.043962	-6.896036
43	1	0	-6.049042	2.623003	-5.579619
44	1	0	-4.596092	1.086625	-3.053302
45	1	0	-7.935429	1.957638	-0.253628
46	1	0	-8.768318	6.20111	-3.948171
47	1	0	-12.134228	5.880605	-0.679127
48	1	0	-9.817614	5.830529	1.704991
49	1	0	-10.22192	8.552435	-0.159507
50	1	0	-5.640847	8.522022	-1.296589
51	1	0	-4.240345	5.895271	-2.768746
52	1	0	-5.061974	5.75442	0.450956
53	1	0	-7.779783	-1.995989	-0.003867
54	1	0	-11.017343	-2.501621	0.503851
55	1	0	-9.222498	-4.740756	-1.164653
56	1	0	-14.9393	8.630128	-3.461421
57	1	0	-17.209343	8.006076	-5.778534
58	1	0	-18.074161	7.939715	-2.573265
59	1	0	-16.210189	-8.473915	-6.559697
60	1	0	-17.96882	-5.925174	-7.711851
61	1	0	-14.650298	-5.846378	-7.878833
62	1	0	-14.201854	-0.739592	4.20235
63	1	0	-16.874745	-0.871708	6.13458
64	1	0	-15.928634	-3.577215	4.458081

CMD1000011_en_		Standard Orientation (Ångstroms)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-19.233764	-1.896275	0.193732
1	6	0	-19.591714	-4.570838	-0.599671
2	6	0	-18.783589	-4.966319	-3.369599
3	6	0	-15.976244	-5.000602	-3.807516
4	6	0	-14.807432	-3.036655	-4.882441
5	6	0	-14.062918	4.222429	-5.597124
6	6	0	-15.861902	4.911605	-3.601762
7	6	0	-16.770452	3.199668	-1.97767
8	6	0	-18.396312	3.606518	0.291891
9	6	0	-17.599518	1.877402	2.46516
10	6	0	-17.800682	-0.93427	2.027269
11	6	0	-12.090858	-2.797746	-5.611326
12	6	0	-10.300275	-1.419857	-3.768828
13	6	0	-10.991619	1.382974	-3.194504
14	6	0	-12.013888	2.748912	-5.437461
15	6	0	-7.638347	-1.226103	-4.965278
16	6	0	-6.513288	1.327926	-4.170114
17	6	0	-8.420908	2.507639	-2.341752
18	6	0	-8.298856	5.377119	-2.095667
19	6	0	-10.177597	6.342141	-0.140726
20	6	0	-5.638019	6.260576	-1.43545
21	6	0	-10.194734	-2.890971	-1.292213
22	6	0	-16.567579	7.658235	-3.577513
23	6	0	-14.674481	-7.377298	-2.998261
24	6	0	-16.264202	-2.478483	3.830439
25	1	0	-12.3407	1.46193	-1.655805
26	1	0	-20.260517	-0.576615	-0.992385
27	1	0	-21.598614	-5.050513	-0.458337
28	1	0	-18.604832	-5.893437	0.626925
29	1	0	-19.577211	-6.758184	-4.026117
30	1	0	-19.646897	-3.488934	-4.519179
31	1	0	-15.966851	-1.423678	-5.387278
32	1	0	-14.362904	5.180655	-7.391063
33	1	0	-16.241846	1.25281	-2.281752
34	1	0	-20.389198	3.279394	-0.154283
35	1	0	-18.289633	5.556517	0.942416
36	1	0	-18.683573	2.365739	4.159638
37	1	0	-15.634786	2.308795	2.94625
38	1	0	-12.016687	-1.812953	-7.422037
39	1	0	-11.269285	-4.659151	-5.955696

40	1	0	-10.874311	2.605872	-7.138448
41	1	0	-6.466838	-2.815154	-4.378654
42	1	0	-7.778841	-1.343487	-7.016907
43	1	0	-6.276581	2.551352	-5.812199
44	1	0	-4.653599	1.136009	-3.314777
45	1	0	-8.050964	1.743272	-0.457253
46	1	0	-8.807509	6.188814	-3.928334
47	1	0	-12.108116	5.810222	-0.594624
48	1	0	-9.737425	5.57788	1.725495
49	1	0	-10.106837	8.395992	0.002797
50	1	0	-5.57988	8.306536	-1.203292
51	1	0	-4.271841	5.762799	-2.889546
52	1	0	-5.001643	5.417691	0.337364
53	1	0	-8.912266	-2.029482	0.063549
54	1	0	-12.059797	-2.999102	-0.433847
55	1	0	-9.536848	-4.815344	-1.61669
56	1	0	-17.96102	8.113046	-2.141604
57	1	0	-14.910885	8.848254	-3.271934
58	1	0	-17.353303	8.209753	-5.404268
59	1	0	-14.69446	-7.577751	-0.944749
60	1	0	-15.641811	-9.035163	-3.755755
61	1	0	-12.71359	-7.456574	-3.590745
62	1	0	-16.48372	-4.500126	3.558923
63	1	0	-14.258244	-2.029284	3.647643
64	1	0	-16.778471	-2.046975	5.782818

CMD1000011_tddft_		Standard Orientation (Ångstroms)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-19.233764	-1.896275	0.193732
1	6	0	-19.591714	-4.570838	-0.599671
2	6	0	-18.783589	-4.966319	-3.369599
3	6	0	-15.976244	-5.000602	-3.807516
4	6	0	-14.807432	-3.036655	-4.882441
5	6	0	-14.062918	4.222429	-5.597124
6	6	0	-15.861902	4.911605	-3.601762
7	6	0	-16.770452	3.199668	-1.97767
8	6	0	-18.396312	3.606518	0.291891
9	6	0	-17.599518	1.877402	2.46516
10	6	0	-17.800682	-0.93427	2.027269
11	6	0	-12.090858	-2.797746	-5.611326
12	6	0	-10.300275	-1.419857	-3.768828
13	6	0	-10.991619	1.382974	-3.194504

14	6	0	-12.013888	2.748912	-5.437461
15	6	0	-7.638347	-1.226103	-4.965278
16	6	0	-6.513288	1.327926	-4.170114
17	6	0	-8.420908	2.507639	-2.341752
18	6	0	-8.298856	5.377119	-2.095667
19	6	0	-10.177597	6.342141	-0.140726
20	6	0	-5.638019	6.260576	-1.43545
21	6	0	-10.194734	-2.890971	-1.292213
22	6	0	-16.567579	7.658235	-3.577513
23	6	0	-14.674481	-7.377298	-2.998261
24	6	0	-16.264202	-2.478483	3.830439
25	1	0	-12.3407	1.46193	-1.655805
26	1	0	-20.260517	-0.576615	-0.992385
27	1	0	-21.598614	-5.050513	-0.458337
28	1	0	-18.604832	-5.893437	0.626925
29	1	0	-19.577211	-6.758184	-4.026117
30	1	0	-19.646897	-3.488934	-4.519179
31	1	0	-15.966851	-1.423678	-5.387278
32	1	0	-14.362904	5.180655	-7.391063
33	1	0	-16.241846	1.25281	-2.281752
34	1	0	-20.389198	3.279394	-0.154283
35	1	0	-18.289633	5.556517	0.942416
36	1	0	-18.683573	2.365739	4.159638
37	1	0	-15.634786	2.308795	2.94625
38	1	0	-12.016687	-1.812953	-7.422037
39	1	0	-11.269285	-4.659151	-5.955696
40	1	0	-10.874311	2.605872	-7.138448
41	1	0	-6.466838	-2.815154	-4.378654
42	1	0	-7.778841	-1.343487	-7.016907
43	1	0	-6.276581	2.551352	-5.812199
44	1	0	-4.653599	1.136009	-3.314777
45	1	0	-8.050964	1.743272	-0.457253
46	1	0	-8.807509	6.188814	-3.928334
47	1	0	-12.108116	5.810222	-0.594624
48	1	0	-9.737425	5.57788	1.725495
49	1	0	-10.106837	8.395992	0.002797
50	1	0	-5.57988	8.306536	-1.203292
51	1	0	-4.271841	5.762799	-2.889546
52	1	0	-5.001643	5.417691	0.337364
53	1	0	-8.912266	-2.029482	0.063549
54	1	0	-12.059797	-2.999102	-0.433847
55	1	0	-9.536848	-4.815344	-1.61669
56	1	0	-17.96102	8.113046	-2.141604

57	1	0	-14.910885	8.848254	-3.271934
58	1	0	-17.353303	8.209753	-5.404268
59	1	0	-14.69446	-7.577751	-0.944749
60	1	0	-15.641811	-9.035163	-3.755755
61	1	0	-12.71359	-7.456574	-3.590745
62	1	0	-16.48372	-4.500126	3.558923
63	1	0	-14.258244	-2.029284	3.647643
64	1	0	-16.778471	-2.046975	5.782818

CMD1000012_en_		Standard Orientation (Ångstroms)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-18.799717	-2.119399	0.479031
1	6	0	-18.513483	-4.921864	0.264671
2	6	0	-18.52407	-5.85621	-2.46172
3	6	0	-16.30369	-5.187609	-4.107232
4	6	0	-14.466475	-3.620961	-3.386266
5	6	0	-13.904431	4.066854	-5.631324
6	6	0	-15.886526	4.780804	-3.829671
7	6	0	-17.041936	3.034804	-2.411466
8	6	0	-18.998684	3.403636	-0.418463
9	6	0	-18.192655	2.254361	2.109823
10	6	0	-17.796741	-0.566446	2.188886
11	6	0	-12.140357	-2.953635	-4.862043
12	6	0	-10.17329	-1.441413	-3.377741
13	6	0	-10.920852	1.368549	-2.922083
14	6	0	-11.869812	2.615527	-5.270898
15	6	0	-7.687396	-1.171237	-4.866038
16	6	0	-6.45092	1.298017	-3.946082
17	6	0	-8.35712	2.546798	-2.135784
18	6	0	-8.256696	5.423469	-2.011307
19	6	0	-10.190882	6.445718	-0.141722
20	6	0	-5.617749	6.347365	-1.321801
21	6	0	-9.610725	-2.772448	-0.870643
22	6	0	-16.512323	7.546277	-3.844493
23	6	0	-16.324438	-6.471979	-6.630166
24	6	0	-16.187076	-1.429163	4.349294
25	1	0	-12.307678	1.519732	-1.415233
26	1	0	-19.94791	-1.298902	-1.007764
27	1	0	-20.083532	-5.850908	1.242111
28	1	0	-16.800643	-5.579545	1.199741
29	1	0	-18.696783	-7.918311	-2.445432
30	1	0	-20.258349	-5.198815	-3.387818

31	1	0	-14.638823	-2.742239	-1.553377
32	1	0	-14.073033	4.95574	-7.478757
33	1	0	-16.482918	1.093622	-2.721371
34	1	0	-20.787296	2.555583	-1.014194
35	1	0	-19.400023	5.397944	-0.117513
36	1	0	-19.574722	2.772635	3.562596
37	1	0	-16.433589	3.169149	2.695585
38	1	0	-12.644962	-1.888321	-6.558779
39	1	0	-11.225409	-4.679989	-5.53744
40	1	0	-10.62996	2.425255	-6.893562
41	1	0	-6.48484	-2.819559	-4.586673
42	1	0	-8.080883	-1.079359	-6.886394
43	1	0	-6.063618	2.545508	-5.538882
44	1	0	-4.645009	0.965826	-3.020523
45	1	0	-7.973328	1.874534	-0.222176
46	1	0	-8.727588	6.159025	-3.885369
47	1	0	-12.102207	5.863034	-0.619297
48	1	0	-9.787303	5.766507	1.764815
49	1	0	-10.152711	8.504508	-0.084144
50	1	0	-5.562588	8.403537	-1.20904
51	1	0	-4.20683	5.763851	-2.6998
52	1	0	-5.037975	5.611465	0.516836
53	1	0	-7.890145	-2.070852	0.005394
54	1	0	-11.135674	-2.5514	0.492232
55	1	0	-9.353215	-4.791823	-1.187269
56	1	0	-18.024647	8.040746	-2.550378
57	1	0	-14.859447	8.680301	-3.363786
58	1	0	-17.092081	8.134643	-5.735973
59	1	0	-14.795378	-5.857185	-7.85246
60	1	0	-16.183526	-8.521962	-6.419776
61	1	0	-18.101043	-6.114692	-7.619148
62	1	0	-16.950008	-0.740446	6.139896
63	1	0	-16.032991	-3.470159	4.486194
64	1	0	-14.279727	-0.651469	4.202185

CMD1000012_tddft_		Standard Orientation (Ångstroms)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-18.799717	-2.119399	0.479031
1	6	0	-18.513483	-4.921864	0.264671
2	6	0	-18.52407	-5.85621	-2.46172
3	6	0	-16.30369	-5.187609	-4.107232
4	6	0	-14.466475	-3.620961	-3.386266

5	6	0	-13.904431	4.066854	-5.631324
6	6	0	-15.886526	4.780804	-3.829671
7	6	0	-17.041936	3.034804	-2.411466
8	6	0	-18.998684	3.403636	-0.418463
9	6	0	-18.192655	2.254361	2.109823
10	6	0	-17.796741	-0.566446	2.188886
11	6	0	-12.140357	-2.953635	-4.862043
12	6	0	-10.17329	-1.441413	-3.377741
13	6	0	-10.920852	1.368549	-2.922083
14	6	0	-11.869812	2.615527	-5.270898
15	6	0	-7.687396	-1.171237	-4.866038
16	6	0	-6.45092	1.298017	-3.946082
17	6	0	-8.35712	2.546798	-2.135784
18	6	0	-8.256696	5.423469	-2.011307
19	6	0	-10.190882	6.445718	-0.141722
20	6	0	-5.617749	6.347365	-1.321801
21	6	0	-9.610725	-2.772448	-0.870643
22	6	0	-16.512323	7.546277	-3.844493
23	6	0	-16.324438	-6.471979	-6.630166
24	6	0	-16.187076	-1.429163	4.349294
25	1	0	-12.307678	1.519732	-1.415233
26	1	0	-19.94791	-1.298902	-1.007764
27	1	0	-20.083532	-5.850908	1.242111
28	1	0	-16.800643	-5.579545	1.199741
29	1	0	-18.696783	-7.918311	-2.445432
30	1	0	-20.258349	-5.198815	-3.387818
31	1	0	-14.638823	-2.742239	-1.553377
32	1	0	-14.073033	4.95574	-7.478757
33	1	0	-16.482918	1.093622	-2.721371
34	1	0	-20.787296	2.555583	-1.014194
35	1	0	-19.400023	5.397944	-0.117513
36	1	0	-19.574722	2.772635	3.562596
37	1	0	-16.433589	3.169149	2.695585
38	1	0	-12.644962	-1.888321	-6.558779
39	1	0	-11.225409	-4.679989	-5.53744
40	1	0	-10.62996	2.425255	-6.893562
41	1	0	-6.48484	-2.819559	-4.586673
42	1	0	-8.080883	-1.079359	-6.886394
43	1	0	-6.063618	2.545508	-5.538882
44	1	0	-4.645009	0.965826	-3.020523
45	1	0	-7.973328	1.874534	-0.222176
46	1	0	-8.727588	6.159025	-3.885369
47	1	0	-12.102207	5.863034	-0.619297

48	1	0	-9.787303	5.766507	1.764815
49	1	0	-10.152711	8.504508	-0.084144
50	1	0	-5.562588	8.403537	-1.20904
51	1	0	-4.20683	5.763851	-2.6998
52	1	0	-5.037975	5.611465	0.516836
53	1	0	-7.890145	-2.070852	0.005394
54	1	0	-11.135674	-2.5514	0.492232
55	1	0	-9.353215	-4.791823	-1.187269
56	1	0	-18.024647	8.040746	-2.550378
57	1	0	-14.859447	8.680301	-3.363786
58	1	0	-17.092081	8.134643	-5.735973
59	1	0	-14.795378	-5.857185	-7.85246
60	1	0	-16.183526	-8.521962	-6.419776
61	1	0	-18.101043	-6.114692	-7.619148
62	1	0	-16.950008	-0.740446	6.139896
63	1	0	-16.032991	-3.470159	4.486194
64	1	0	-14.279727	-0.651469	4.202185

Table S11. Gibbs free energies[a] and equilibrium populations[b] of low-energy conformers of *ent*-1.

Conformers	ΔG	P(%)/100	Single point energy(a.u.)
ENT-1000002_tddft_	9e-05	43.4	-976.5736758555
ENT-1000006_tddft_	0.00299	2.01	-976.570779013
ENT-1000007_tddft_	0.00327	1.5	-976.5705021681
ENT-1000008_tddft_	0.0	47.87	-976.5737684017
ENT-1000013_tddft_	0.00209	5.21	-976.5716757577

[a]wB97M-V/def2-TZVP, in kcal/mol.

[b]From ΔG values at 298.15K.

Table S12. Cartesian coordinates for the low-energy reoptimized random research conformers of *ent*-1 at PBE0-D3(BJ)/def2-SVP level of theory in methanol.

ENT-1000002_en_		Standard Orientation (Ångstroms)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-22.015612	1.191386	-0.728154
1	6	0	-23.407946	-0.698554	-2.292649
2	6	0	-22.361658	-3.39411	-1.94203
3	6	0	-19.724957	-3.773447	-2.923934
4	6	0	-17.787119	-4.066436	-1.331758
5	6	0	-14.322762	-2.778991	5.029269
6	6	0	-16.053939	-0.839885	5.987236
7	6	0	-17.819574	0.279955	4.563078
8	6	0	-19.52921	2.392563	5.343305
9	6	0	-20.846838	3.627673	3.075614
10	6	0	-22.535492	1.849467	1.651383
11	6	0	-15.081353	-4.540711	-1.961295
12	6	0	-13.275951	-2.253418	-1.887533
13	6	0	-12.967195	-0.985849	0.753384
14	6	0	-13.015529	-2.846102	2.865882
15	6	0	-10.563493	-3.139651	-2.540754
16	6	0	-8.730474	-1.636507	-0.869506
17	6	0	-10.345515	0.309584	0.531839
18	6	0	-9.216261	1.330447	2.979784
19	6	0	-10.908822	3.342392	4.148584
20	6	0	-6.568428	2.380624	2.555131
21	6	0	-14.175672	-0.284525	-3.79148
22	6	0	-15.672657	-0.212313	8.728587
23	6	0	-19.488408	-3.786717	-5.742925
24	6	0	-24.722041	0.817564	3.121055
25	1	0	-14.422108	0.429531	1.035155
26	1	0	-20.342831	2.007196	-1.591071
27	1	0	-23.312754	-0.171401	-4.283488
28	1	0	-25.410411	-0.723518	-1.809192
29	1	0	-23.633313	-4.710317	-2.906022
30	1	0	-22.429725	-3.855227	0.064014

31	1	0	-18.209485	-4.010352	0.673289
32	1	0	-13.922947	-4.284686	6.370894
33	1	0	-18.075088	-0.380169	2.646061
34	1	0	-18.469774	3.843829	6.358003
35	1	0	-20.960977	1.725576	6.677527
36	1	0	-19.414975	4.392401	1.805087
37	1	0	-21.952616	5.23315	3.763697
38	1	0	-14.913882	-5.371011	-3.841169
39	1	0	-14.361546	-5.962803	-0.652698
40	1	0	-11.727685	-4.429979	2.654106
41	1	0	-10.187222	-2.867873	-4.547151
42	1	0	-10.374574	-5.160497	-2.190419
43	1	0	-7.805265	-2.882163	0.489551
44	1	0	-7.229025	-0.745352	-1.955039
45	1	0	-10.609014	1.935693	-0.716366
46	1	0	-9.075303	-0.244598	4.311854
47	1	0	-11.11749	4.947313	2.867818
48	1	0	-10.106643	4.056433	5.906784
49	1	0	-12.786991	2.623275	4.559599
50	1	0	-5.806387	3.179025	4.294244
51	1	0	-5.254884	0.935958	1.908751
52	1	0	-6.591063	3.883788	1.141938
53	1	0	-14.248351	-1.091397	-5.684557
54	1	0	-16.06496	0.380586	-3.323203
55	1	0	-12.924378	1.345627	-3.872543
56	1	0	-15.631761	-1.935356	9.861821
57	1	0	-17.147967	0.999049	9.480681
58	1	0	-13.85865	0.723505	9.02878
59	1	0	-20.903901	-5.025659	-6.589736
60	1	0	-19.816271	-1.90622	-6.525546
61	1	0	-17.640485	-4.395058	-6.391986
62	1	0	-25.656352	2.307433	4.19838
63	1	0	-26.131744	-0.080862	1.930531
64	1	0	-24.096597	-0.593574	4.490847

ENT-1000002_tddft_		Standard Orientation (Ångstroms)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-22.015612	1.191386	-0.728154
1	6	0	-23.407946	-0.698554	-2.292649
2	6	0	-22.361658	-3.39411	-1.94203
3	6	0	-19.724957	-3.773447	-2.923934
4	6	0	-17.787119	-4.066436	-1.331758

5	6	0	-14.322762	-2.778991	5.029269
6	6	0	-16.053939	-0.839885	5.987236
7	6	0	-17.819574	0.279955	4.563078
8	6	0	-19.52921	2.392563	5.343305
9	6	0	-20.846838	3.627673	3.075614
10	6	0	-22.535492	1.849467	1.651383
11	6	0	-15.081353	-4.540711	-1.961295
12	6	0	-13.275951	-2.253418	-1.887533
13	6	0	-12.967195	-0.985849	0.753384
14	6	0	-13.015529	-2.846102	2.865882
15	6	0	-10.563493	-3.139651	-2.540754
16	6	0	-8.730474	-1.636507	-0.869506
17	6	0	-10.345515	0.309584	0.531839
18	6	0	-9.216261	1.330447	2.979784
19	6	0	-10.908822	3.342392	4.148584
20	6	0	-6.568428	2.380624	2.555131
21	6	0	-14.175672	-0.284525	-3.79148
22	6	0	-15.672657	-0.212313	8.728587
23	6	0	-19.488408	-3.786717	-5.742925
24	6	0	-24.722041	0.817564	3.121055
25	1	0	-14.422108	0.429531	1.035155
26	1	0	-20.342831	2.007196	-1.591071
27	1	0	-23.312754	-0.171401	-4.283488
28	1	0	-25.410411	-0.723518	-1.809192
29	1	0	-23.633313	-4.710317	-2.906022
30	1	0	-22.429725	-3.855227	0.064014
31	1	0	-18.209485	-4.010352	0.673289
32	1	0	-13.922947	-4.284686	6.370894
33	1	0	-18.075088	-0.380169	2.646061
34	1	0	-18.469774	3.843829	6.358003
35	1	0	-20.960977	1.725576	6.677527
36	1	0	-19.414975	4.392401	1.805087
37	1	0	-21.952616	5.23315	3.763697
38	1	0	-14.913882	-5.371011	-3.841169
39	1	0	-14.361546	-5.962803	-0.652698
40	1	0	-11.727685	-4.429979	2.654106
41	1	0	-10.187222	-2.867873	-4.547151
42	1	0	-10.374574	-5.160497	-2.190419
43	1	0	-7.805265	-2.882163	0.489551
44	1	0	-7.229025	-0.745352	-1.955039
45	1	0	-10.609014	1.935693	-0.716366
46	1	0	-9.075303	-0.244598	4.311854
47	1	0	-11.11749	4.947313	2.867818

48	1	0	-10.106643	4.056433	5.906784
49	1	0	-12.786991	2.623275	4.559599
50	1	0	-5.806387	3.179025	4.294244
51	1	0	-5.254884	0.935958	1.908751
52	1	0	-6.591063	3.883788	1.141938
53	1	0	-14.248351	-1.091397	-5.684557
54	1	0	-16.06496	0.380586	-3.323203
55	1	0	-12.924378	1.345627	-3.872543
56	1	0	-15.631761	-1.935356	9.861821
57	1	0	-17.147967	0.999049	9.480681
58	1	0	-13.85865	0.723505	9.02878
59	1	0	-20.903901	-5.025659	-6.589736
60	1	0	-19.816271	-1.90622	-6.525546
61	1	0	-17.640485	-4.395058	-6.391986
62	1	0	-25.656352	2.307433	4.19838
63	1	0	-26.131744	-0.080862	1.930531
64	1	0	-24.096597	-0.593574	4.490847

ENT-1000006_en_		Standard Orientation (Ångstroms)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-22.541216	-0.064117	0.601795
1	6	0	-23.380557	-1.181096	-1.851308
2	6	0	-22.776994	-3.993962	-2.02323
3	6	0	-20.044125	-4.775939	-2.075778
4	6	0	-18.131257	-3.135491	-2.15499
5	6	0	-14.08273	-3.175007	4.74333
6	6	0	-16.030196	-1.62072	5.957011
7	6	0	-18.043356	-0.808087	4.65969
8	6	0	-20.122012	0.883457	5.53568
9	6	0	-20.668385	2.995999	3.64028
10	6	0	-21.567065	2.212727	1.052002
11	6	0	-15.380993	-3.789354	-2.372822
12	6	0	-13.509328	-1.604656	-2.059488
13	6	0	-13.157655	-0.66853	0.708298
14	6	0	-12.906084	-2.799875	2.540099
15	6	0	-10.81602	-2.476006	-2.745977
16	6	0	-8.99309	-0.786513	-1.240008
17	6	0	-10.643953	0.827061	0.529081
18	6	0	-9.420264	1.582982	3.026492
19	6	0	-11.188263	3.232978	4.585203
20	6	0	-6.920098	2.944798	2.5917
21	6	0	-14.251199	0.594138	-3.784605

22	6	0	-15.581577	-1.143904	8.716025
23	6	0	-19.675495	-7.582895	-2.102529
24	6	0	-21.230841	4.206467	-0.92582
25	1	0	-14.695744	0.569074	1.265112
26	1	0	-22.707163	-1.359168	2.180553
27	1	0	-22.563352	-0.188907	-3.460076
28	1	0	-25.430427	-0.976788	-2.04904
29	1	0	-23.692283	-4.771149	-3.709961
30	1	0	-23.701115	-4.963329	-0.442247
31	1	0	-18.594345	-1.148937	-2.126927
32	1	0	-13.43116	-4.769222	5.867349
33	1	0	-18.20702	-1.443134	2.723007
34	1	0	-19.664651	1.745319	7.34686
35	1	0	-21.849076	-0.207117	5.858612
36	1	0	-18.943626	4.11309	3.40585
37	1	0	-22.045711	4.30627	4.460893
38	1	0	-15.034314	-4.610907	-4.242451
39	1	0	-14.88582	-5.265864	-1.023075
40	1	0	-11.459697	-4.173247	2.056831
41	1	0	-10.508508	-2.380598	-4.780334
42	1	0	-10.569152	-4.451761	-2.214162
43	1	0	-7.683123	-1.939294	-0.14431
44	1	0	-7.834709	0.393776	-2.462268
45	1	0	-11.094607	2.593652	-0.440714
46	1	0	-9.034939	-0.142176	4.09856
47	1	0	-11.625591	4.978727	3.574048
48	1	0	-10.324615	3.759837	6.379985
49	1	0	-12.965291	2.288591	4.993821
50	1	0	-6.072401	3.51838	4.379329
51	1	0	-5.552976	1.765622	1.605981
52	1	0	-7.202113	4.65042	1.464967
53	1	0	-15.85901	1.645778	-3.051123
54	1	0	-12.711166	1.928825	-4.042769
55	1	0	-14.765787	-0.109207	-5.651364
56	1	0	-15.495266	-2.93318	9.741861
57	1	0	-17.049338	-0.003198	9.584977
58	1	0	-13.770903	-0.208507	9.024202
59	1	0	-17.700387	-8.1337	-2.141936
60	1	0	-20.540894	-8.450835	-0.441142
61	1	0	-20.596917	-8.4311	-3.744716
62	1	0	-22.03588	3.69555	-2.742372
63	1	0	-22.115863	5.974058	-0.331059
64	1	0	-19.229833	4.634028	-1.208875

ENT-1000006_tddft_		Standard Orientation (Ångstroms)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-22.541216	-0.064117	0.601795
1	6	0	-23.380557	-1.181096	-1.851308
2	6	0	-22.776994	-3.993962	-2.02323
3	6	0	-20.044125	-4.775939	-2.075778
4	6	0	-18.131257	-3.135491	-2.15499
5	6	0	-14.08273	-3.175007	4.74333
6	6	0	-16.030196	-1.62072	5.957011
7	6	0	-18.043356	-0.808087	4.65969
8	6	0	-20.122012	0.883457	5.53568
9	6	0	-20.668385	2.995999	3.64028
10	6	0	-21.567065	2.212727	1.052002
11	6	0	-15.380993	-3.789354	-2.372822
12	6	0	-13.509328	-1.604656	-2.059488
13	6	0	-13.157655	-0.66853	0.708298
14	6	0	-12.906084	-2.799875	2.540099
15	6	0	-10.81602	-2.476006	-2.745977
16	6	0	-8.99309	-0.786513	-1.240008
17	6	0	-10.643953	0.827061	0.529081
18	6	0	-9.420264	1.582982	3.026492
19	6	0	-11.188263	3.232978	4.585203
20	6	0	-6.920098	2.944798	2.5917
21	6	0	-14.251199	0.594138	-3.784605
22	6	0	-15.581577	-1.143904	8.716025
23	6	0	-19.675495	-7.582895	-2.102529
24	6	0	-21.230841	4.206467	-0.92582
25	1	0	-14.695744	0.569074	1.265112
26	1	0	-22.707163	-1.359168	2.180553
27	1	0	-22.563352	-0.188907	-3.460076
28	1	0	-25.430427	-0.976788	-2.04904
29	1	0	-23.692283	-4.771149	-3.709961
30	1	0	-23.701115	-4.963329	-0.442247
31	1	0	-18.594345	-1.148937	-2.126927
32	1	0	-13.43116	-4.769222	5.867349
33	1	0	-18.20702	-1.443134	2.723007
34	1	0	-19.664651	1.745319	7.34686
35	1	0	-21.849076	-0.207117	5.858612
36	1	0	-18.943626	4.11309	3.40585
37	1	0	-22.045711	4.30627	4.460893
38	1	0	-15.034314	-4.610907	-4.242451

39	1	0	-14.88582	-5.265864	-1.023075
40	1	0	-11.459697	-4.173247	2.056831
41	1	0	-10.508508	-2.380598	-4.780334
42	1	0	-10.569152	-4.451761	-2.214162
43	1	0	-7.683123	-1.939294	-0.14431
44	1	0	-7.834709	0.393776	-2.462268
45	1	0	-11.094607	2.593652	-0.440714
46	1	0	-9.034939	-0.142176	4.09856
47	1	0	-11.625591	4.978727	3.574048
48	1	0	-10.324615	3.759837	6.379985
49	1	0	-12.965291	2.288591	4.993821
50	1	0	-6.072401	3.51838	4.379329
51	1	0	-5.552976	1.765622	1.605981
52	1	0	-7.202113	4.65042	1.464967
53	1	0	-15.85901	1.645778	-3.051123
54	1	0	-12.711166	1.928825	-4.042769
55	1	0	-14.765787	-0.109207	-5.651364
56	1	0	-15.495266	-2.93318	9.741861
57	1	0	-17.049338	-0.003198	9.584977
58	1	0	-13.770903	-0.208507	9.024202
59	1	0	-17.700387	-8.1337	-2.141936
60	1	0	-20.540894	-8.450835	-0.441142
61	1	0	-20.596917	-8.4311	-3.744716
62	1	0	-22.03588	3.69555	-2.742372
63	1	0	-22.115863	5.974058	-0.331059
64	1	0	-19.229833	4.634028	-1.208875

ENT-1000007_en_		Standard Orientation (Ångstroms)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-21.205721	0.931473	-0.624653
1	6	0	-22.61003	-0.939205	-2.208114
2	6	0	-22.017874	-3.709186	-1.529199
3	6	0	-19.422082	-4.545626	-2.336083
4	6	0	-17.4698	-4.319283	-0.756957
5	6	0	-14.651774	-2.491124	5.144901
6	6	0	-17.047664	-1.132997	5.47546
7	6	0	-17.193213	1.370937	5.160051
8	6	0	-19.415493	3.073893	5.418609
9	6	0	-20.445202	3.974752	2.841536
10	6	0	-22.040407	2.074185	1.464262
11	6	0	-14.765401	-4.965362	-1.190648
12	6	0	-13.013758	-2.663882	-1.477437

13	6	0	-12.995584	-0.881638	0.874451
14	6	0	-12.955994	-2.364826	3.276357
15	6	0	-10.221529	-3.486881	-1.702019
16	6	0	-8.633936	-1.487691	-0.313837
17	6	0	-10.490681	0.589422	0.490036
18	6	0	-9.660696	2.307236	2.662822
19	6	0	-11.201044	4.741159	2.667642
20	6	0	-6.858471	2.962973	2.547776
21	6	0	-13.801751	-1.185883	-3.82764
22	6	0	-19.205322	-2.761542	6.329344
23	6	0	-19.259796	-5.536307	-4.978888
24	6	0	-24.602317	1.638697	2.585757
25	1	0	-14.633939	0.356133	0.832819
26	1	0	-19.301634	1.371908	-1.242217
27	1	0	-22.155445	-0.623482	-4.196654
28	1	0	-24.640991	-0.645358	-2.042651
29	1	0	-23.434237	-4.917653	-2.423673
30	1	0	-22.241092	-3.935763	0.505216
31	1	0	-17.865161	-3.513367	1.082033
32	1	0	-14.272362	-3.879861	6.614274
33	1	0	-15.45687	2.327416	4.662869
34	1	0	-18.830213	4.747077	6.478168
35	1	0	-20.925799	2.210686	6.516341
36	1	0	-18.857947	4.550255	1.658973
37	1	0	-21.57844	5.673884	3.166097
38	1	0	-14.530948	-6.154141	-2.856583
39	1	0	-14.098067	-6.084615	0.410442
40	1	0	-11.336369	-3.607099	3.48005
41	1	0	-9.679883	-3.675202	-3.679718
42	1	0	-9.953834	-5.344233	-0.852783
43	1	0	-7.727647	-2.315883	1.340158
44	1	0	-7.118399	-0.731219	-1.47949
45	1	0	-10.768798	1.820857	-1.1429
46	1	0	-10.007358	1.305087	4.43759
47	1	0	-10.678603	5.92076	1.057658
48	1	0	-10.871023	5.841325	4.377216
49	1	0	-13.220111	4.391131	2.526063
50	1	0	-6.359109	4.281349	4.049494
51	1	0	-5.659491	1.305817	2.754392
52	1	0	-6.381814	3.863189	0.753979
53	1	0	-15.711427	-0.446996	-3.63817
54	1	0	-12.537573	0.385452	-4.218335
55	1	0	-13.775205	-2.416808	-5.47955

56	1	0	-20.922481	-1.695343	6.67206
57	1	0	-18.713958	-3.757581	8.068701
58	1	0	-19.632711	-4.211414	4.928848
59	1	0	-19.989696	-4.154455	-6.327501
60	1	0	-17.348104	-6.007785	-5.553009
61	1	0	-20.425141	-7.226654	-5.195932
62	1	0	-25.708295	3.382377	2.579722
63	1	0	-25.684519	0.198756	1.606064
64	1	0	-24.462621	1.056362	4.558285

ENT-1000007_tddft_		Standard Orientation (Ångstroms)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-21.205721	0.931473	-0.624653
1	6	0	-22.61003	-0.939205	-2.208114
2	6	0	-22.017874	-3.709186	-1.529199
3	6	0	-19.422082	-4.545626	-2.336083
4	6	0	-17.4698	-4.319283	-0.756957
5	6	0	-14.651774	-2.491124	5.144901
6	6	0	-17.047664	-1.132997	5.47546
7	6	0	-17.193213	1.370937	5.160051
8	6	0	-19.415493	3.073893	5.418609
9	6	0	-20.445202	3.974752	2.841536
10	6	0	-22.040407	2.074185	1.464262
11	6	0	-14.765401	-4.965362	-1.190648
12	6	0	-13.013758	-2.663882	-1.477437
13	6	0	-12.995584	-0.881638	0.874451
14	6	0	-12.955994	-2.364826	3.276357
15	6	0	-10.221529	-3.486881	-1.702019
16	6	0	-8.633936	-1.487691	-0.313837
17	6	0	-10.490681	0.589422	0.490036
18	6	0	-9.660696	2.307236	2.662822
19	6	0	-11.201044	4.741159	2.667642
20	6	0	-6.858471	2.962973	2.547776
21	6	0	-13.801751	-1.185883	-3.82764
22	6	0	-19.205322	-2.761542	6.329344
23	6	0	-19.259796	-5.536307	-4.978888
24	6	0	-24.602317	1.638697	2.585757
25	1	0	-14.633939	0.356133	0.832819
26	1	0	-19.301634	1.371908	-1.242217
27	1	0	-22.155445	-0.623482	-4.196654
28	1	0	-24.640991	-0.645358	-2.042651
29	1	0	-23.434237	-4.917653	-2.423673

30	1	0	-22.241092	-3.935763	0.505216
31	1	0	-17.865161	-3.513367	1.082033
32	1	0	-14.272362	-3.879861	6.614274
33	1	0	-15.45687	2.327416	4.662869
34	1	0	-18.830213	4.747077	6.478168
35	1	0	-20.925799	2.210686	6.516341
36	1	0	-18.857947	4.550255	1.658973
37	1	0	-21.57844	5.673884	3.166097
38	1	0	-14.530948	-6.154141	-2.856583
39	1	0	-14.098067	-6.084615	0.410442
40	1	0	-11.336369	-3.607099	3.48005
41	1	0	-9.679883	-3.675202	-3.679718
42	1	0	-9.953834	-5.344233	-0.852783
43	1	0	-7.727647	-2.315883	1.340158
44	1	0	-7.118399	-0.731219	-1.47949
45	1	0	-10.768798	1.820857	-1.1429
46	1	0	-10.007358	1.305087	4.43759
47	1	0	-10.678603	5.92076	1.057658
48	1	0	-10.871023	5.841325	4.377216
49	1	0	-13.220111	4.391131	2.526063
50	1	0	-6.359109	4.281349	4.049494
51	1	0	-5.659491	1.305817	2.754392
52	1	0	-6.381814	3.863189	0.753979
53	1	0	-15.711427	-0.446996	-3.63817
54	1	0	-12.537573	0.385452	-4.218335
55	1	0	-13.775205	-2.416808	-5.47955
56	1	0	-20.922481	-1.695343	6.67206
57	1	0	-18.713958	-3.757581	8.068701
58	1	0	-19.632711	-4.211414	4.928848
59	1	0	-19.989696	-4.154455	-6.327501
60	1	0	-17.348104	-6.007785	-5.553009
61	1	0	-20.425141	-7.226654	-5.195932
62	1	0	-25.708295	3.382377	2.579722
63	1	0	-25.684519	0.198756	1.606064
64	1	0	-24.462621	1.056362	4.558285

ENT-1000008_en_		Standard Orientation (Ångstroms)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-22.012561	0.6369	-1.137144
1	6	0	-23.239174	-1.40499	-2.647708
2	6	0	-22.099252	-4.025128	-2.082072
3	6	0	-19.402165	-4.341083	-2.908348

4	6	0	-17.538936	-4.432797	-1.207114
5	6	0	-14.472881	-2.562114	5.238872
6	6	0	-16.322482	-0.639565	5.986412
7	6	0	-18.083727	0.275449	4.417762
8	6	0	-19.926944	2.349525	4.958998
9	6	0	-21.159747	3.373834	2.544067
10	6	0	-22.696322	1.436027	1.156209
11	6	0	-14.785323	-4.818562	-1.66702
12	6	0	-13.092897	-2.446819	-1.649541
13	6	0	-13.007841	-0.992446	0.911351
14	6	0	-13.073414	-2.71329	3.138976
15	6	0	-10.307677	-3.235298	-2.075396
16	6	0	-8.655517	-1.520066	-0.418745
17	6	0	-10.447633	0.429391	0.745779
18	6	0	-9.517764	1.682545	3.16934
19	6	0	-11.36123	3.696122	4.079254
20	6	0	-6.895987	2.821283	2.817805
21	6	0	-13.966352	-0.654524	-3.732351
22	6	0	-16.070846	0.213303	8.681133
23	6	0	-19.01789	-4.537555	-5.704067
24	6	0	-24.925586	0.419748	2.573551
25	1	0	-14.552248	0.349282	1.009767
26	1	0	-20.318017	1.453584	-1.955769
27	1	0	-23.059416	-0.993038	-4.659965
28	1	0	-25.261302	-1.491726	-2.26578
29	1	0	-23.263379	-5.452312	-3.023567
30	1	0	-22.24966	-4.368088	-0.056958
31	1	0	-18.070232	-4.265516	0.765766
32	1	0	-14.068115	-3.955037	6.696135
33	1	0	-18.228976	-0.547722	2.552363
34	1	0	-18.996109	3.911546	5.933759
35	1	0	-21.40399	1.698874	6.251308
36	1	0	-19.687266	4.112326	1.305494
37	1	0	-22.365453	4.972025	3.059294
38	1	0	-14.481816	-5.758899	-3.477076
39	1	0	-14.076498	-6.119845	-0.232475
40	1	0	-11.709333	-4.246025	3.086196
41	1	0	-9.819391	-3.094544	-4.071298
42	1	0	-10.046635	-5.212201	-1.558456
43	1	0	-7.751946	-2.615432	1.077043
44	1	0	-7.139683	-0.627267	-1.482828
45	1	0	-10.71655	1.948451	-0.629172
46	1	0	-9.393749	0.222789	4.627593

47	1	0	-11.554069	5.19653	2.674578
48	1	0	-10.698315	4.569985	5.823199
49	1	0	-13.232019	2.927541	4.432476
50	1	0	-6.271431	3.77486	4.533433
51	1	0	-5.487837	1.396206	2.352709
52	1	0	-6.899435	4.217568	1.298913
53	1	0	-15.907899	-0.053319	-3.414037
54	1	0	-12.787986	1.026316	-3.852263
55	1	0	-13.892339	-1.583786	-5.56838
56	1	0	-16.103915	-1.40828	9.956247
57	1	0	-17.571563	1.490229	9.252865
58	1	0	-14.266075	1.162826	8.991172
59	1	0	-17.107007	-5.082245	-6.212461
60	1	0	-20.315346	-5.915427	-6.525396
61	1	0	-19.404514	-2.740968	-6.641946
62	1	0	-25.957009	1.936503	3.515834
63	1	0	-26.246897	-0.590268	1.37113
64	1	0	-24.327826	-0.891054	4.051319

ENT-1000008_tddft_		Standard Orientation (Ångstroms)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-22.012561	0.6369	-1.137144
1	6	0	-23.239174	-1.40499	-2.647708
2	6	0	-22.099252	-4.025128	-2.082072
3	6	0	-19.402165	-4.341083	-2.908348
4	6	0	-17.538936	-4.432797	-1.207114
5	6	0	-14.472881	-2.562114	5.238872
6	6	0	-16.322482	-0.639565	5.986412
7	6	0	-18.083727	0.275449	4.417762
8	6	0	-19.926944	2.349525	4.958998
9	6	0	-21.159747	3.373834	2.544067
10	6	0	-22.696322	1.436027	1.156209
11	6	0	-14.785323	-4.818562	-1.66702
12	6	0	-13.092897	-2.446819	-1.649541
13	6	0	-13.007841	-0.992446	0.911351
14	6	0	-13.073414	-2.71329	3.138976
15	6	0	-10.307677	-3.235298	-2.075396
16	6	0	-8.655517	-1.520066	-0.418745
17	6	0	-10.447633	0.429391	0.745779
18	6	0	-9.517764	1.682545	3.16934
19	6	0	-11.36123	3.696122	4.079254
20	6	0	-6.895987	2.821283	2.817805

21	6	0	-13.966352	-0.654524	-3.732351
22	6	0	-16.070846	0.213303	8.681133
23	6	0	-19.01789	-4.537555	-5.704067
24	6	0	-24.925586	0.419748	2.573551
25	1	0	-14.552248	0.349282	1.009767
26	1	0	-20.318017	1.453584	-1.955769
27	1	0	-23.059416	-0.993038	-4.659965
28	1	0	-25.261302	-1.491726	-2.26578
29	1	0	-23.263379	-5.452312	-3.023567
30	1	0	-22.24966	-4.368088	-0.056958
31	1	0	-18.070232	-4.265516	0.765766
32	1	0	-14.068115	-3.955037	6.696135
33	1	0	-18.228976	-0.547722	2.552363
34	1	0	-18.996109	3.911546	5.933759
35	1	0	-21.40399	1.698874	6.251308
36	1	0	-19.687266	4.112326	1.305494
37	1	0	-22.365453	4.972025	3.059294
38	1	0	-14.481816	-5.758899	-3.477076
39	1	0	-14.076498	-6.119845	-0.232475
40	1	0	-11.709333	-4.246025	3.086196
41	1	0	-9.819391	-3.094544	-4.071298
42	1	0	-10.046635	-5.212201	-1.558456
43	1	0	-7.751946	-2.615432	1.077043
44	1	0	-7.139683	-0.627267	-1.482828
45	1	0	-10.71655	1.948451	-0.629172
46	1	0	-9.393749	0.222789	4.627593
47	1	0	-11.554069	5.19653	2.674578
48	1	0	-10.698315	4.569985	5.823199
49	1	0	-13.232019	2.927541	4.432476
50	1	0	-6.271431	3.77486	4.533433
51	1	0	-5.487837	1.396206	2.352709
52	1	0	-6.899435	4.217568	1.298913
53	1	0	-15.907899	-0.053319	-3.414037
54	1	0	-12.787986	1.026316	-3.852263
55	1	0	-13.892339	-1.583786	-5.56838
56	1	0	-16.103915	-1.40828	9.956247
57	1	0	-17.571563	1.490229	9.252865
58	1	0	-14.266075	1.162826	8.991172
59	1	0	-17.107007	-5.082245	-6.212461
60	1	0	-20.315346	-5.915427	-6.525396
61	1	0	-19.404514	-2.740968	-6.641946
62	1	0	-25.957009	1.936503	3.515834
63	1	0	-26.246897	-0.590268	1.37113

64	1	0	-24.327826	-0.891054	4.051319

ENT-1000013_en_		Standard Orientation (Ångstroms)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-22.79806	-0.754459	0.839208
1	6	0	-23.759595	-2.662982	-0.988578
2	6	0	-22.082177	-5.041782	-0.984352
3	6	0	-19.530786	-4.710632	-2.189668
4	6	0	-17.427946	-4.660376	-0.791177
5	6	0	-14.2262	-2.525549	5.211212
6	6	0	-16.24383	-0.80806	6.026254
7	6	0	-18.066426	-0.032057	4.452441
8	6	0	-20.125562	1.839389	4.94783
9	6	0	-20.914611	3.201126	2.530569
10	6	0	-21.986275	1.594272	0.43386
11	6	0	-14.753293	-4.568232	-1.687806
12	6	0	-13.376173	-1.997147	-1.714178
13	6	0	-13.064962	-0.693738	0.916304
14	6	0	-12.881101	-2.497849	3.069173
15	6	0	-10.618218	-2.405143	-2.643062
16	6	0	-8.867769	-0.969969	-0.840398
17	6	0	-10.588577	0.839877	0.598486
18	6	0	-9.49057	1.986704	3.004697
19	6	0	-11.341407	3.829237	4.212582
20	6	0	-6.971595	3.285612	2.498449
21	6	0	-14.776648	-0.19194	-3.469634
22	6	0	-16.091408	-0.041459	8.752946
23	6	0	-19.573945	-4.495144	-5.009397
24	6	0	-22.032449	2.885963	-2.081309
25	1	0	-14.634847	0.579958	1.24172
26	1	0	-22.666417	-1.486447	2.748763
27	1	0	-23.922575	-1.913219	-2.895975
28	1	0	-25.666718	-3.238742	-0.433364
29	1	0	-23.091947	-6.548632	-1.976818
30	1	0	-21.854237	-5.678425	0.962877
31	1	0	-17.649261	-4.809604	1.241004
32	1	0	-13.664044	-3.908645	6.624311
33	1	0	-18.093315	-0.833912	2.575805
34	1	0	-19.521649	3.250846	6.320715
35	1	0	-21.774817	0.921207	5.795507
36	1	0	-19.263073	4.198964	1.783489
37	1	0	-22.274781	4.690759	2.993049

38	1	0	-14.628252	-5.318588	-3.604948
39	1	0	-13.654541	-5.860056	-0.513451
40	1	0	-11.393975	-3.904103	2.923577
41	1	0	-10.419524	-1.719124	-4.575195
42	1	0	-10.150618	-4.410065	-2.693218
43	1	0	-7.96397	-2.266094	0.487228
44	1	0	-7.351721	0.003719	-1.831224
45	1	0	-11.034934	2.420592	-0.661141
46	1	0	-9.157533	0.44639	4.343344
47	1	0	-13.118363	2.923455	4.701365
48	1	0	-11.761503	5.38338	2.921642
49	1	0	-10.55755	4.649829	5.931999
50	1	0	-6.242672	4.168422	4.210967
51	1	0	-5.542759	1.968924	1.824779
52	1	0	-7.178757	4.76873	1.078857
53	1	0	-13.860871	1.648723	-3.548715
54	1	0	-14.833073	-0.931093	-5.391769
55	1	0	-16.715458	0.078999	-2.840338
56	1	0	-17.717866	1.047159	9.367949
57	1	0	-14.393555	1.070867	9.120555
58	1	0	-15.963803	-1.710572	9.959019
59	1	0	-20.455774	-2.726664	-5.603085
60	1	0	-17.704497	-4.5458	-5.849358
61	1	0	-20.695088	-6.013361	-5.843656
62	1	0	-22.91217	1.759502	-3.553004
63	1	0	-23.058141	4.673788	-1.964509
64	1	0	-20.120197	3.355451	-2.700286

ENT-1000013_tddft_		Standard Orientation (Ångstroms)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-22.79806	-0.754459	0.839208
1	6	0	-23.759595	-2.662982	-0.988578
2	6	0	-22.082177	-5.041782	-0.984352
3	6	0	-19.530786	-4.710632	-2.189668
4	6	0	-17.427946	-4.660376	-0.791177
5	6	0	-14.2262	-2.525549	5.211212
6	6	0	-16.24383	-0.80806	6.026254
7	6	0	-18.066426	-0.032057	4.452441
8	6	0	-20.125562	1.839389	4.94783
9	6	0	-20.914611	3.201126	2.530569
10	6	0	-21.986275	1.594272	0.43386
11	6	0	-14.753293	-4.568232	-1.687806

12	6	0	-13.376173	-1.997147	-1.714178
13	6	0	-13.064962	-0.693738	0.916304
14	6	0	-12.881101	-2.497849	3.069173
15	6	0	-10.618218	-2.405143	-2.643062
16	6	0	-8.867769	-0.969969	-0.840398
17	6	0	-10.588577	0.839877	0.598486
18	6	0	-9.49057	1.986704	3.004697
19	6	0	-11.341407	3.829237	4.212582
20	6	0	-6.971595	3.285612	2.498449
21	6	0	-14.776648	-0.19194	-3.469634
22	6	0	-16.091408	-0.041459	8.752946
23	6	0	-19.573945	-4.495144	-5.009397
24	6	0	-22.032449	2.885963	-2.081309
25	1	0	-14.634847	0.579958	1.24172
26	1	0	-22.666417	-1.486447	2.748763
27	1	0	-23.922575	-1.913219	-2.895975
28	1	0	-25.666718	-3.238742	-0.433364
29	1	0	-23.091947	-6.548632	-1.976818
30	1	0	-21.854237	-5.678425	0.962877
31	1	0	-17.649261	-4.809604	1.241004
32	1	0	-13.664044	-3.908645	6.624311
33	1	0	-18.093315	-0.833912	2.575805
34	1	0	-19.521649	3.250846	6.320715
35	1	0	-21.774817	0.921207	5.795507
36	1	0	-19.263073	4.198964	1.783489
37	1	0	-22.274781	4.690759	2.993049
38	1	0	-14.628252	-5.318588	-3.604948
39	1	0	-13.654541	-5.860056	-0.513451
40	1	0	-11.393975	-3.904103	2.923577
41	1	0	-10.419524	-1.719124	-4.575195
42	1	0	-10.150618	-4.410065	-2.693218
43	1	0	-7.96397	-2.266094	0.487228
44	1	0	-7.351721	0.003719	-1.831224
45	1	0	-11.034934	2.420592	-0.661141
46	1	0	-9.157533	0.44639	4.343344
47	1	0	-13.118363	2.923455	4.701365
48	1	0	-11.761503	5.38338	2.921642
49	1	0	-10.55755	4.649829	5.931999
50	1	0	-6.242672	4.168422	4.210967
51	1	0	-5.542759	1.968924	1.824779
52	1	0	-7.178757	4.76873	1.078857
53	1	0	-13.860871	1.648723	-3.548715
54	1	0	-14.833073	-0.931093	-5.391769

55	1	0	-16.715458	0.078999	-2.840338
56	1	0	-17.717866	1.047159	9.367949
57	1	0	-14.393555	1.070867	9.120555
58	1	0	-15.963803	-1.710572	9.959019
59	1	0	-20.455774	-2.726664	-5.603085
60	1	0	-17.704497	-4.5458	-5.849358
61	1	0	-20.695088	-6.013361	-5.843656
62	1	0	-22.91217	1.759502	-3.553004
63	1	0	-23.058141	4.673788	-1.964509
64	1	0	-20.120197	3.355451	-2.700286

Table S13. Energy profiles (a.u.) of the reaction forming the carbocation precursor to IM3 at the M06–2X/6–31 G(d,p) level.

Key states	Gibbs free energy (a.u.)	Relative free energy (kcal/mol)
IM1	-976.047012	0
TS_1-2	-976.037173	6.2
IM2	-976.067279	-12.7
TS_2-3	-976.045699	0.8
IM3	-976.077659	-19.2

Table S14. Gibbs free energy (a.u.) and relative free energy (kcal/mol) of deprotonation product at the M06–2X/6–31 G(d,p) level.

Product	Gibbs free energy (a.u.)	Relative free energy (kcal/mol)
Penisentene (**IM4**_A)	-975.7320246	0
IM4_B	-975.7294146	1.6

IM1

C	2.98367	-0.14610	-1.51496
C	3.70622	-1.42604	-1.15713
C	3.56240	-1.86187	0.30952
C	2.15873	-2.06814	0.83370
C	1.11351	-2.09307	-0.00045
C	-0.13806	0.60445	1.93340
C	0.94658	1.44691	1.29211
C	0.78517	2.13855	0.15867
C	1.82046	2.99695	-0.51546
C	2.52541	2.27579	-1.68758
C	3.37837	1.10555	-1.25754
C	-0.33532	-2.14955	0.35767
C	-1.88958	-1.42550	-0.85773
C	-0.96808	-0.64751	-0.11095
C	-1.34438	0.22158	1.07696
C	-3.19461	-1.89533	-0.31572
C	-4.33754	-1.12138	-1.04298
C	-4.16101	0.37682	-1.00466
C	-4.48189	1.17711	0.01911
C	-4.25562	2.66250	-0.05315
C	-5.07587	0.68982	1.31246
C	-1.57767	-1.75553	-2.27579
C	2.23119	1.44687	2.08280
C	2.07942	-2.26806	2.32288
C	4.67195	1.45096	-0.56863
H	2.04879	-0.25238	-2.06709
H	4.77581	-1.32159	-1.36456
H	3.36067	-2.23370	-1.81189
H	4.13826	-2.78115	0.48002
H	4.03324	-1.10366	0.95117
H	1.30050	-2.01488	-1.06681
H	0.33001	-0.30619	2.32841
H	-0.17292	2.08333	-0.36160
H	2.57075	3.34205	0.20148
H	1.33687	3.89613	-0.91105
H	3.15033	3.00798	-2.21336
H	1.76632	1.93390	-2.40095
H	-0.58089	-2.18796	1.41947
H	-0.81147	-3.02682	-0.10195
H	-0.18099	-0.19454	-0.71584
H	-2.08746	-0.28050	1.70431
H	-3.31163	-2.96695	-0.50997
H	-3.26351	-1.71582	0.75860
H	-5.27050	-1.42939	-0.56442
H	-4.39463	-1.46650	-2.07919
H	-3.74048	0.83783	-1.89836
H	-5.20249	3.19959	0.06460
H	-3.60449	2.99579	0.76372
H	-3.80639	2.96271	-1.00191
H	-6.02457	1.19961	1.50880
H	-4.41250	0.93926	2.14931
H	-5.26141	-0.38573	1.33161
H	-0.51196	-1.67829	-2.49742
H	-1.97090	-2.72807	-2.57796
H	-2.08668	-0.98888	-2.87695
H	2.89155	0.64912	1.72105
H	2.77714	2.38799	2.00251
H	2.03760	1.26495	3.14454
H	2.44290	-1.38182	2.85396
H	1.07735	-2.50321	2.68558
H	2.73419	-3.09713	2.61103
H	4.49889	2.05545	0.32809
H	5.24094	0.56845	-0.27056
H	5.30187	2.05119	-1.23430
H	-0.50510	1.13829	2.81956
H	-1.83361	1.11683	0.67896

TS_1-2

C	2.75014	-0.05807	-1.52970
C	3.41464	-1.40193	-1.33201
C	3.30694	-1.97467	0.08913
C	1.91667	-2.21471	0.63607
C	0.84394	-2.17421	-0.16319
C	-0.08303	0.51960	2.00860
C	1.01170	1.38822	1.42917
C	0.83774	2.23488	0.40847
C	1.90128	3.07755	-0.23778
C	2.47704	2.40282	-1.50543
C	3.25776	1.14098	-1.22114
C	-0.58830	-2.40407	0.21833
C	-1.72565	-1.50748	-0.59857
C	-1.17599	-0.28197	-0.10605
C	-1.38668	0.37054	1.19318
C	-3.11243	-1.90481	-0.09919
C	-4.22276	-1.13298	-0.85112
C	-3.91289	0.33066	-1.03747
C	-4.14960	1.31233	-0.15265
C	-3.79399	2.74015	-0.45969
C	-4.77180	1.09112	1.19742
C	-1.54342	-1.74329	-2.09733
C	2.32788	1.20134	2.13997
C	1.88574	-2.55667	2.10169
C	4.62056	1.34003	-0.61165
H	1.77030	-0.06371	-2.01091
H	4.47859	-1.32821	-1.57653
H	3.00181	-2.12106	-2.04790
H	3.85965	-2.92241	0.14306
H	3.82775	-1.30134	0.78363
H	1.01339	-2.00575	-1.22108
H	0.33160	-0.47489	2.20636
H	-0.14574	2.31666	-0.05889
H	2.71265	3.29427	0.46229
H	1.47333	4.04296	-0.52515
H	3.12739	3.12558	-2.01266
H	1.65275	2.17925	-2.19305
H	-0.77956	-2.32557	1.29060
H	-0.93531	-3.39302	-0.11023
H	-0.35987	0.15017	-0.69468
H	-2.17086	-0.11274	1.77764
H	-3.24368	-2.98213	-0.24445
H	-3.19396	-1.72110	0.97669
H	-5.15900	-1.26863	-0.30327
H	-4.37821	-1.59339	-1.83056
H	-3.48805	0.62119	-1.99899
H	-4.68407	3.37602	-0.40836
H	-3.09438	3.13937	0.28761
H	-3.34878	2.85040	-1.45050
H	-5.72367	1.62863	1.26530
H	-4.13077	1.50630	1.98512
H	-4.95944	0.03983	1.42246
H	-0.55851	-1.43375	-2.45147
H	-1.67708	-2.80408	-2.32533
H	-2.28841	-1.18066	-2.66210
H	2.89414	0.39033	1.66775
H	2.94859	2.09756	2.11592

H	2.17064	0.93363	3.18963
H	2.32104	-1.74736	2.69843
H	0.88728	-2.77402	2.48571
H	2.50386	-3.44272	2.28120
H	4.56309	1.93507	0.30608
H	5.11776	0.40007	-0.36647
H	5.26410	1.89419	-1.30377
H	-0.37452	0.91858	2.98789
H	-1.73892	1.38434	0.94864

IM2

C	-2.66667	0.04893	-1.36129
C	-3.30463	1.40962	-1.19571
C	-3.13829	2.03279	0.19650
C	-1.73845	2.42599	0.61427
C	-0.70629	2.38605	-0.23650
C	0.93154	-1.29110	1.74695
C	-0.47625	-1.65678	1.33031
C	-0.69127	-2.64576	0.45492
C	-2.01100	-3.17288	-0.03637
C	-2.53326	-2.43476	-1.29123
C	-3.21382	-1.11775	-1.00021
C	0.72306	2.75901	0.03785
C	1.73993	1.80186	-0.61921
C	1.55583	0.32361	-0.15901
C	1.37132	0.12439	1.34112
C	3.17692	2.13722	-0.18648
C	3.99773	0.84694	-0.40215
C	2.97808	-0.26730	-0.71978
C	3.22519	-1.60756	-0.25534
C	2.68140	-2.74102	-1.02669
C	4.12161	-1.88756	0.88215
C	1.62903	1.90313	-2.15132
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C	-1.64832	2.89233	2.04454
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H	-3.52909	1.32950	0.94641
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H	-2.76380	-3.12999	0.75691
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H	-3.25373	-3.08907	-1.79794
H	-1.70102	-2.27926	-1.98784
H	0.92247	2.82455	1.11050
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H	0.73357	-0.17231	-0.69004
H	0.58871	0.81882	1.66664
H	3.57765	2.97969	-0.75574
H	3.19575	2.42520	0.86893
H	4.59530	0.61683	0.48237
H	4.69683	0.92983	-1.23839
H	2.77263	-0.33497	-1.79389
H	3.48727	-3.01339	-1.73100
H	2.48671	-3.62160	-0.41290
H	1.81025	-2.46161	-1.62276
H	4.01855	-2.90102	1.26765
H	4.00444	-1.14633	1.67829
H	5.14853	-1.75795	0.50291
H	0.75920	1.36360	-2.53862
H	1.52998	2.95109	-2.44678
H	2.51853	1.52107	-2.66208
H	-2.55183	-1.31265	1.84467
H	-1.38542	-0.76551	3.06630
H	-1.60807	0.14403	1.56185
H	-2.04861	2.13137	2.72415
H	-0.63481	3.13953	2.36331
H	-2.26388	3.78784	2.18263
H	-4.51793	-1.82131	0.57653
H	-5.00244	-0.26512	-0.09474
H	-5.26348	-1.75746	-1.01050
H	1.61924	-2.04984	1.34678
H	2.27879	0.41771	1.88611

TS_2-3

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C	-0.96265	1.21251	1.64176
C	0.41021	1.61624	1.42814
C	0.64662	2.81919	0.84785
C	1.95662	3.27593	0.29234
C	2.27792	2.57479	-1.06781
C	2.99567	1.24626	-0.95820
C	-0.69416	-2.90633	0.17085
C	-1.72456	-1.95467	-0.46272
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C	-2.78526	1.70443	-0.22815
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C	1.90717	-2.95234	1.91865
C	4.39022	1.32358	-0.38981
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H	4.15545	-1.13429	-1.74567
H	2.64511	-1.88216	-2.17770
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H	1.35234	2.45989	-1.64227
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H	-4.88695	1.97778	0.14518
H	-0.87636	-1.61026	-2.47718
H	-1.62194	-3.19763	-2.24403
H	-2.63285	-1.77563	-2.45699
H	2.46886	1.06971	1.71314
H	1.33702	0.26788	2.81279
H	1.45876	-0.24692	1.11577
H	2.27914	-2.15173	2.56939
H	0.95633	-3.31176	2.31456
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H	4.38943	1.61235	0.66853
H	4.92527	0.37648	-0.46269
H	4.97424	2.08521	-0.91769
H	-1.83000	1.83850	0.39850
H	-2.30442	-0.42834	1.91713

IM3

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C	-1.17884	-0.79099	1.61165
C	-1.00357	-2.00498	0.98555
C	-2.07148	-2.97309	0.67880
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C	-3.19235	-1.46127	-1.05362
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C	1.88725	1.68125	-0.44305
C	1.77649	0.16174	-0.14824
C	1.32127	-0.16973	1.31850
C	3.21656	2.07083	0.24292
C	4.10050	0.80254	0.21987
C	3.23096	-0.33015	-0.37244
C	3.61265	-1.73539	0.10521
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C	-2.50880	-0.38041	2.19195
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C	-4.66463	-1.45065	-0.73625
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H	-0.60328	1.41772	-1.29792
H	-0.31187	1.06681	2.10513
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H	-2.94179	-2.84105	1.32553
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H	-3.14019	-3.61883	-1.07495
H	-1.59514	-2.85627	-1.45070
H	0.75875	2.57790	1.17885
H	0.85488	3.55378	-0.25713
H	1.06689	-0.33090	-0.82689
H	1.94706	0.41469	2.00369
H	3.68199	2.91916	-0.26601
H	3.03263	2.39405	1.27389
H	4.42083	0.53642	1.23408
H	5.01294	0.94295	-0.36343
H	3.36571	-0.34223	-1.46222
H	3.48060	-1.79120	1.19616
H	2.92220	-2.80602	-1.64718
H	2.99426	-3.80338	-0.18920
H	1.67815	-2.64221	-0.41328
H	5.35794	-3.02957	0.11687
H	5.74797	-1.32299	0.34860
H	5.29502	-1.91787	-1.25691
H	1.19967	1.43366	-2.52201
H	2.00869	2.97050	-2.18311
H	2.95528	1.49833	-2.35244
H	-2.48625	0.66297	2.51233
H	-3.30837	-0.49572	1.45743
H	-2.75320	-0.99391	3.06415
H	-2.88012	2.93885	1.91646
H	-1.12561	3.22453	1.98679
H	-2.15261	4.24178	0.98948
H	-4.86280	-1.89423	0.24713
H	-5.09156	-0.44661	-0.74151
H	-5.21403	-2.05636	-1.46521
H	1.53646	-1.22596	1.49226

Sequence S1. The protein sequence of PstA

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TISDIPGFGLCHVTSLAMPQCRPERLSLLTVFTETTFLNDDYYDSAGAEKIDSYNQRLKKALS
RDSQGNESDKNPGMYKGKQLQAGYLIQMLQIDHDLASAVMATYSRTLDAVSVSVLEKSGLV
SLEDYCNFRLSNSGMETFQDMCCFGIGLKIDQKTKEKLASIVNAAHKSTALINDYYSWPKEV
KGYFEVDENPNLPVNAVCIMMQYHEFSEREALKRIRDEIVVQQELHLSMIKELEESEGPLPES
WRIYLEAAQYPATGSELWTIYSPRYPTKSDLNQPECIIVGNSMKYKTTYDIPCGLTERGSEVET
RQDIMAGMNSHPVSHLSTPYLAADSEKTADFNSFSTVACAAENLGEVTNGGKENGIQPPGN
GQNKNDISASAHGDCESSSYKEGLCSHQQPRDSNIFLQKATETVTSPSKYIASLPSKNVRDKF
LDALNLWFRIPEEPLSRIKRIVGLLHHSSLMLDDIEDDSTLRRGMPCAHSLYGPAQTINSANYA
FVTAFAETLSLRNSSATDMFIDEVQNMHRGQAMDLHWKYHTHCPTADEYMQMIDNKTGA
MFRLCVRLMQAESNLAGQNISPDPFVLQLGRYFQVRDDYQNLLSDEYSSQKGFCEDLDEGK
ISLPIIYTIMNPSFNGSVIKGIFQHKVPGEMPLPTKKYILEQMKQAGALDMTLSLIRDMQSDLL
DKLSAVEDAFGSKNPLVELVLRRLWI*

Sequence S2. The nucleotide sequence of *pstA* gene

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TGTCGAAGACGCACGCGAACTTAGATACGAGTTCAGTTCTGAGGTCAACATGGATGTGG
ACACCAAGACTATCTCTGATATTCCAGGATTTGGCCTTTGTCATGTCACTTCTTTGGCAAT
GCCTCAGTGTCGCCCAGAAAGGCTATCCCTGCTGACGGTCTTCACTGAGACCACGTTCCT
CAATGATGGTGAGTTGCAATGACTCCATACTTCACAGTCAATAGTCGAAACGTGGGTAAC
ATATAGGTCTAGATTACTATGACAGTGCAGGCGCCGAGAAGGTACGCACAAACTCTTACC
ATGAGATTTCTCCGCCGCGTCTGTTGACAAATGACCCGTGTACCAGATCGATAGTTATAAC
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TGGTATGTACAAAGGGAAGCAGCTCCAAGCGGGCTATCTCATTCAAATGCTCCAAATCGA
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GAAGTATATTCTAGAGCAGATGAAACAGGCAGGGGCACTGGATATGACTCTTTCATTGATT
CGCGATATGCAGAGTGATCTTCTGGACAAACTCAGTGCTGTGGAAGATGCGTTTGGGTCG
AAGAATCCTCTTGTCGAGCTGGTGTTGAGGCGCCTATGGATATGA

Sequence S3. The nucleotide sequence of *pstB* gene

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CAGACTAGCCTCGAACTTCATCAAGAGCTATAGAGATATAAGTGTCAGAAAACAAAGTCA
AATCAATCTGACGATAGTGGAACCAGGATTAACCCACTGAGATAGGAGTTTTGTATAGCAT
CATCTGAGCAAAGTTTTTGCCAAGGCAGATCCGGGATCCATATCCCCAAGCAAGGTTGTA
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TGCGTCCTCCCCATATATTGCCTTATCTCGATGGATAATCCAGGGATTTGCTGCAACCTCGA
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Figure S19. ^{1}H NMR spectrum of Penisentene (1) in $CDCl_3$.

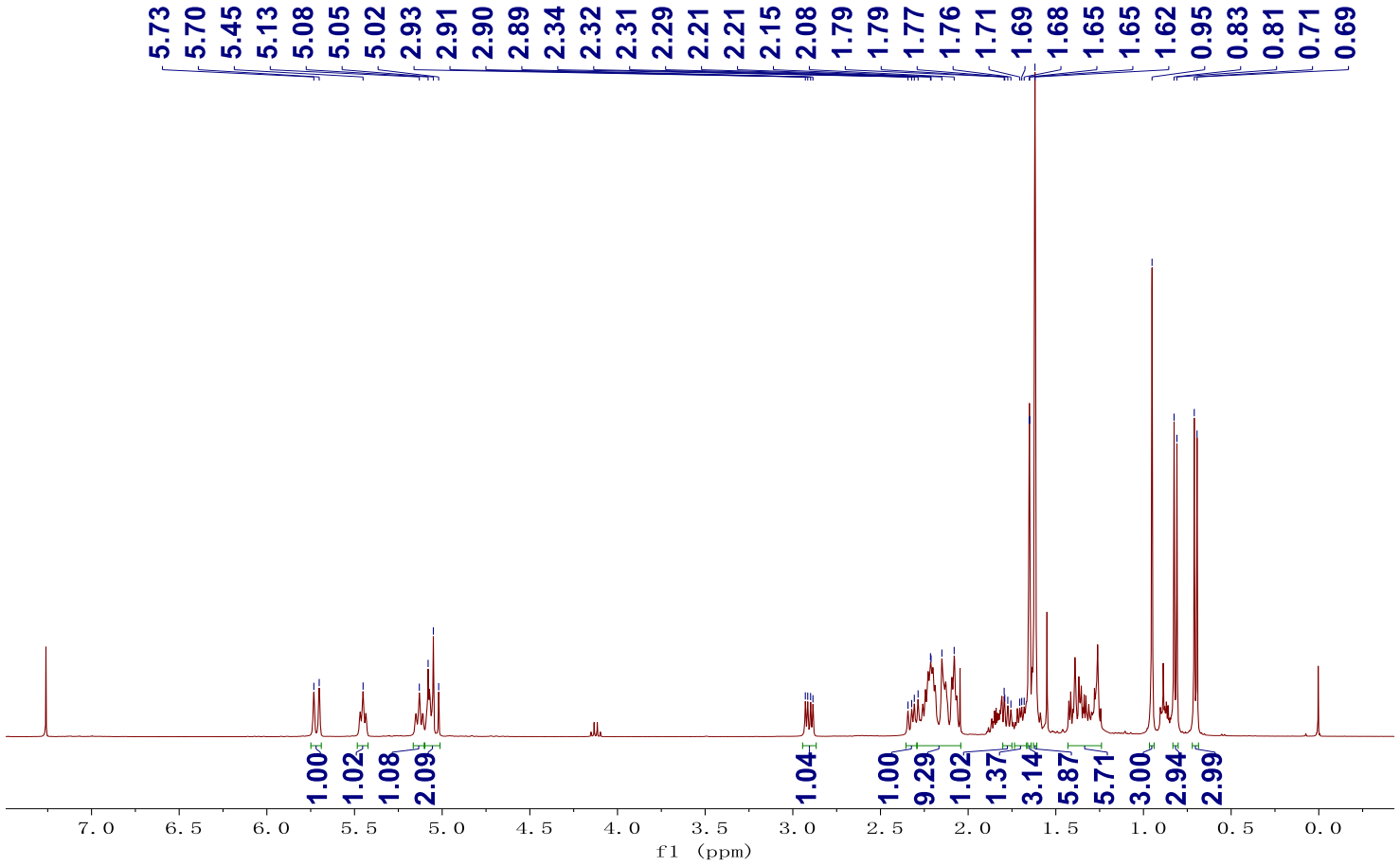

Figure S20. ^{13}C NMR and DEPT spectra of Penisentene (1) in $CDCl_3$.

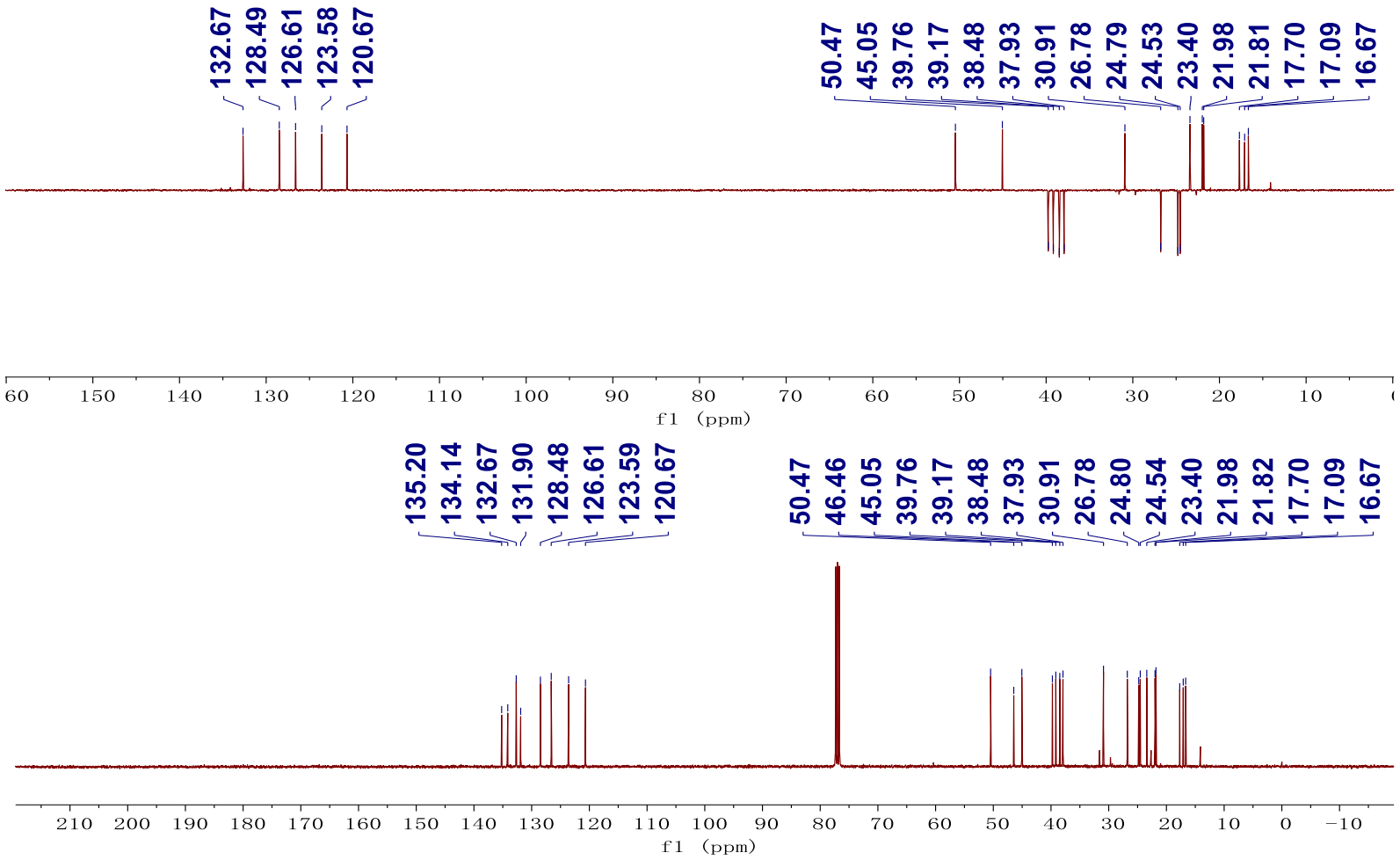

Figure S21. HSQC spectrum of Penisentene (1) in $CDCl_3$.

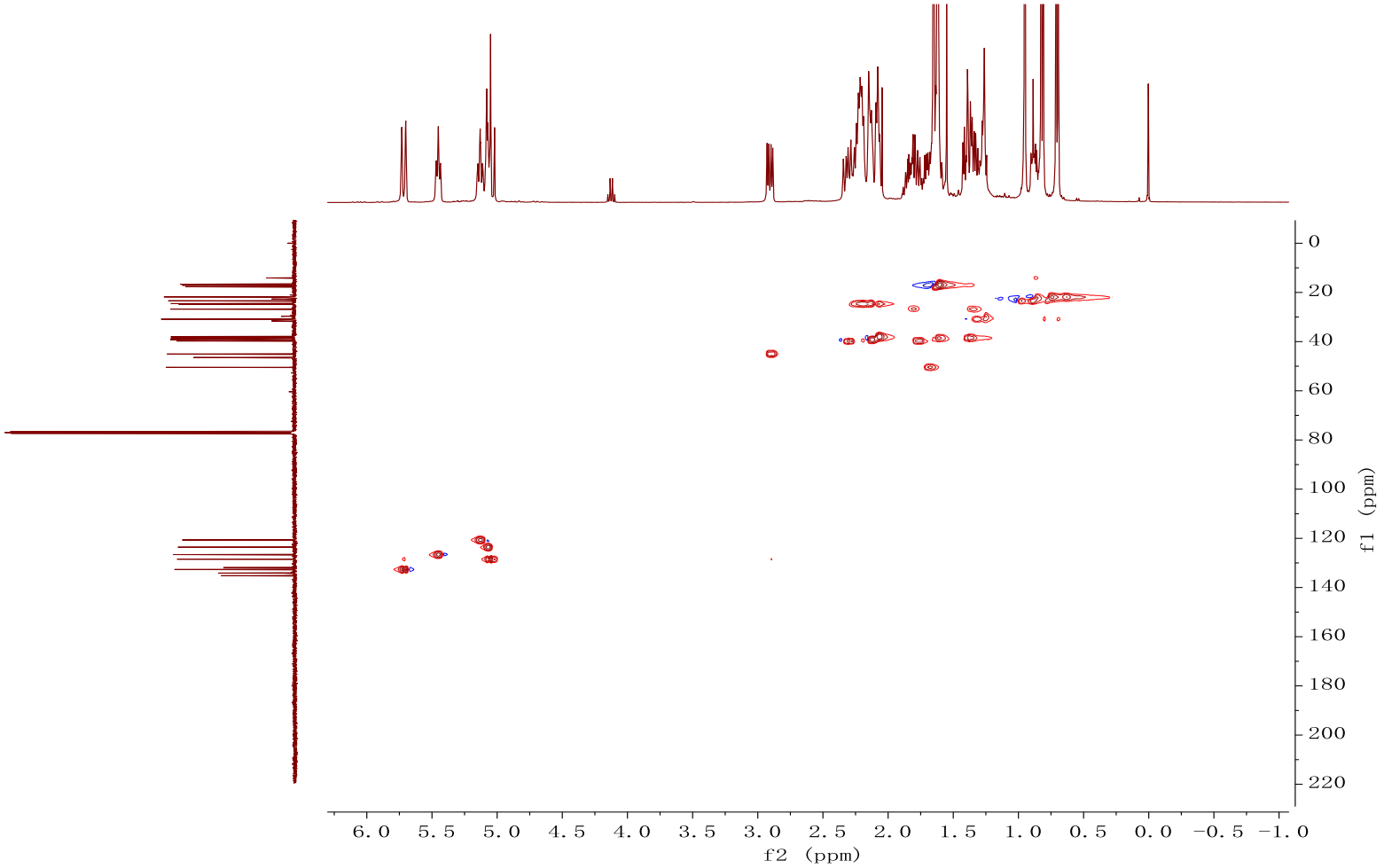

Figure S22. HMBC spectrum of Penisentene (1) in $CDCl_3$.

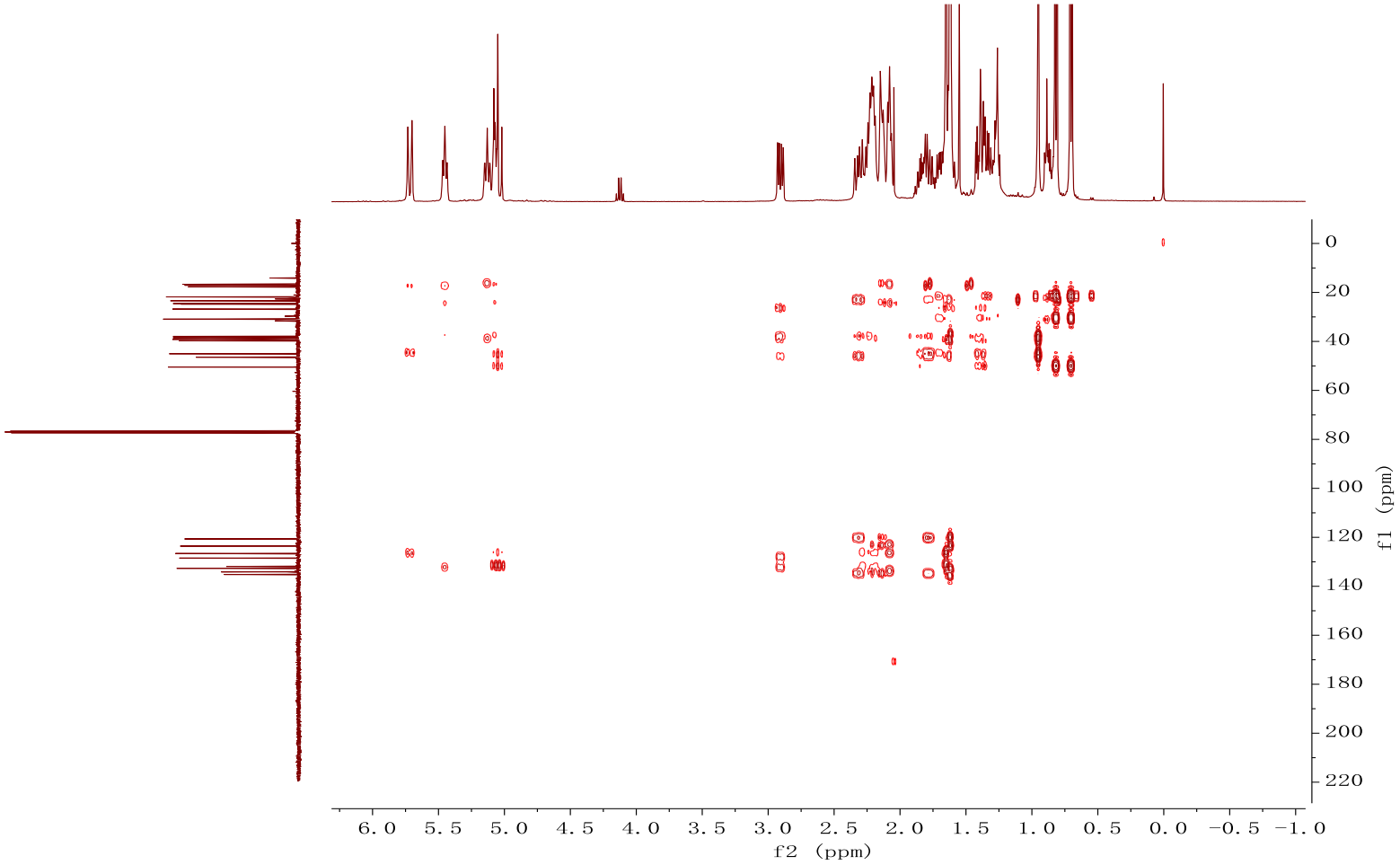

Figure S23. $^{1}H–^{1}H$ COSY spectrum of Penisentene (1) in $CDCl_3$.

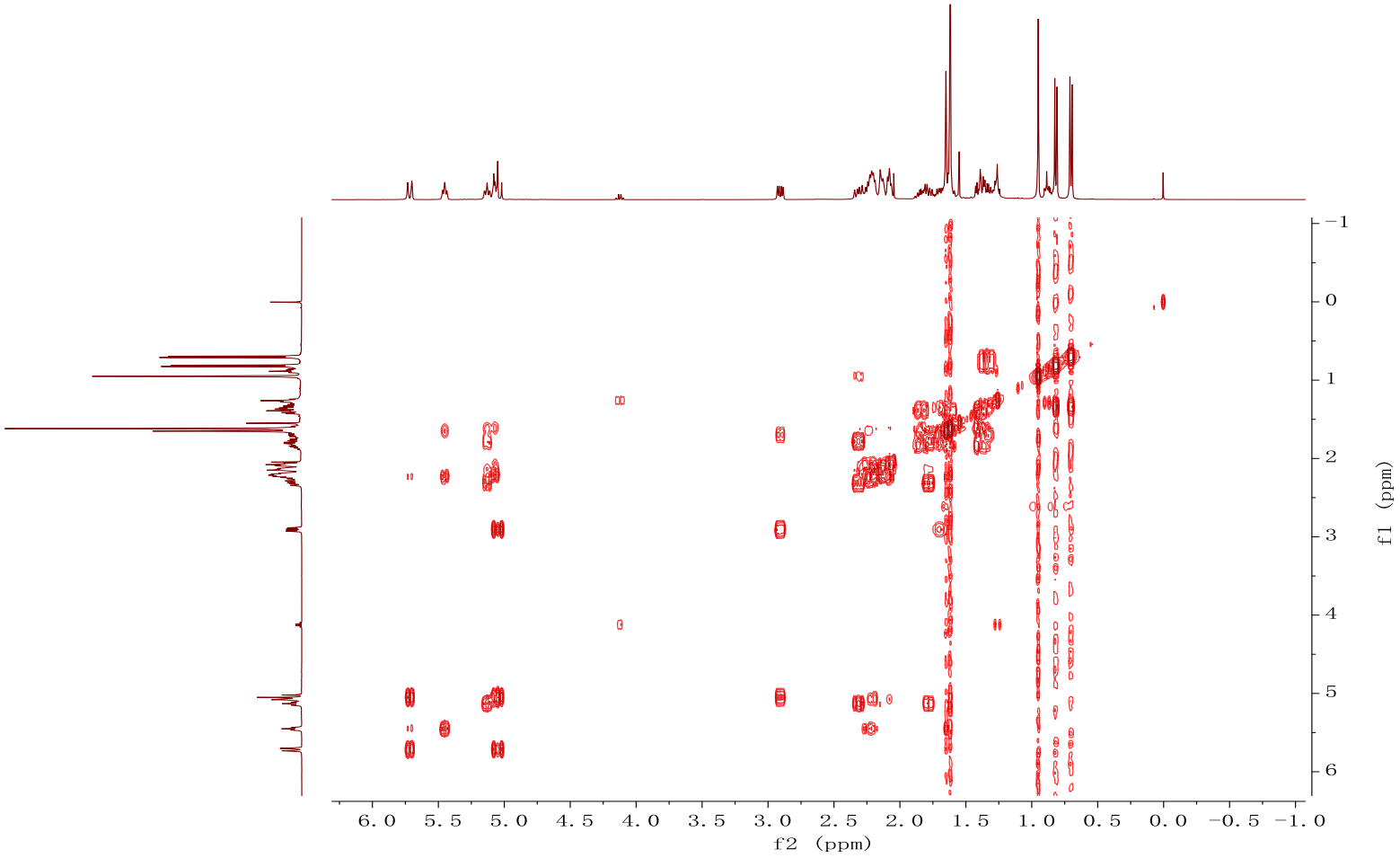

Figure S24. NOESY spectrum of Penisentene (1) in $CDCl_3$.

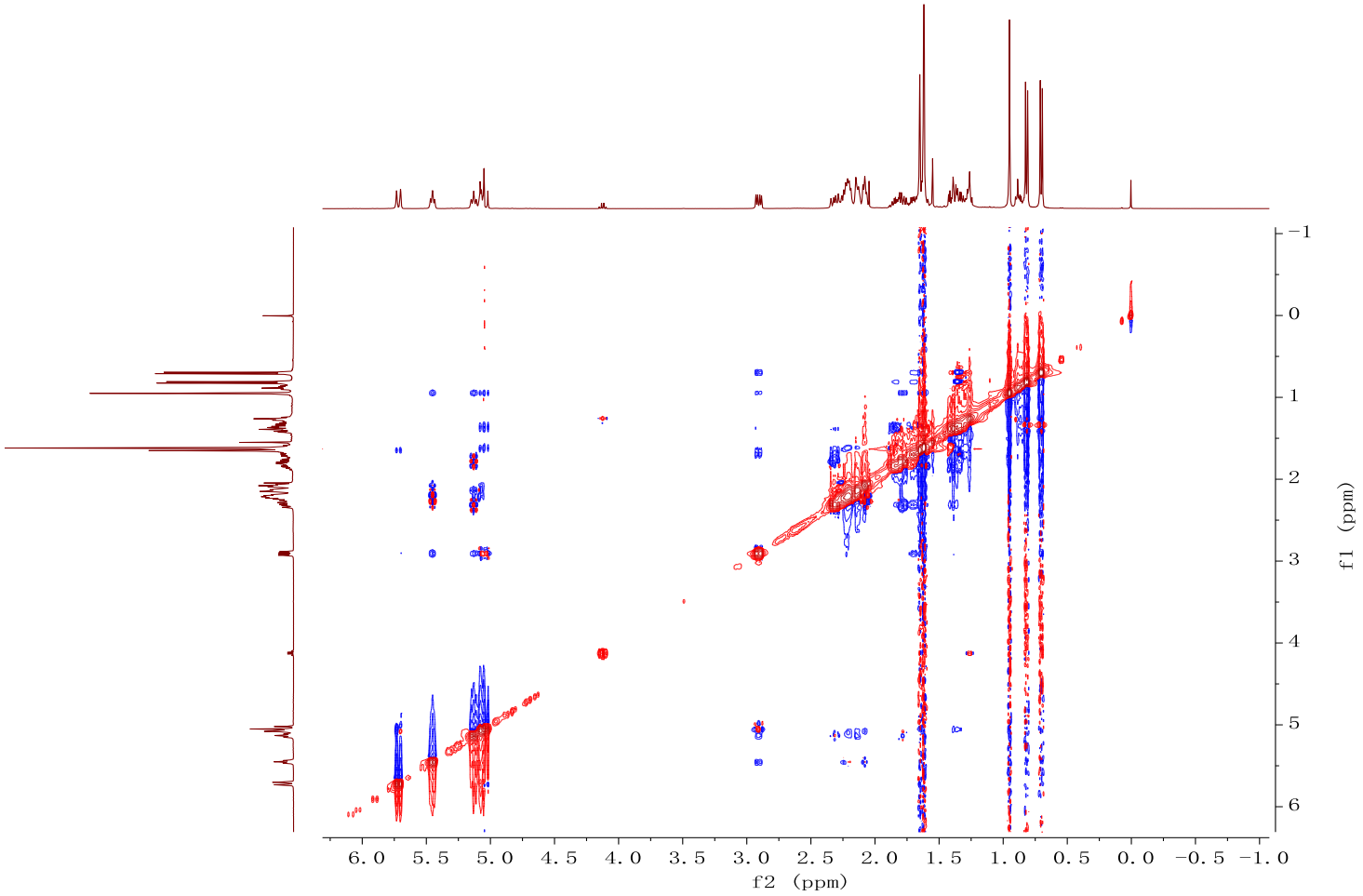

Figure S25. ^{1}H NMR spectrum of Penisentenol (2) in $CDCl_3$.

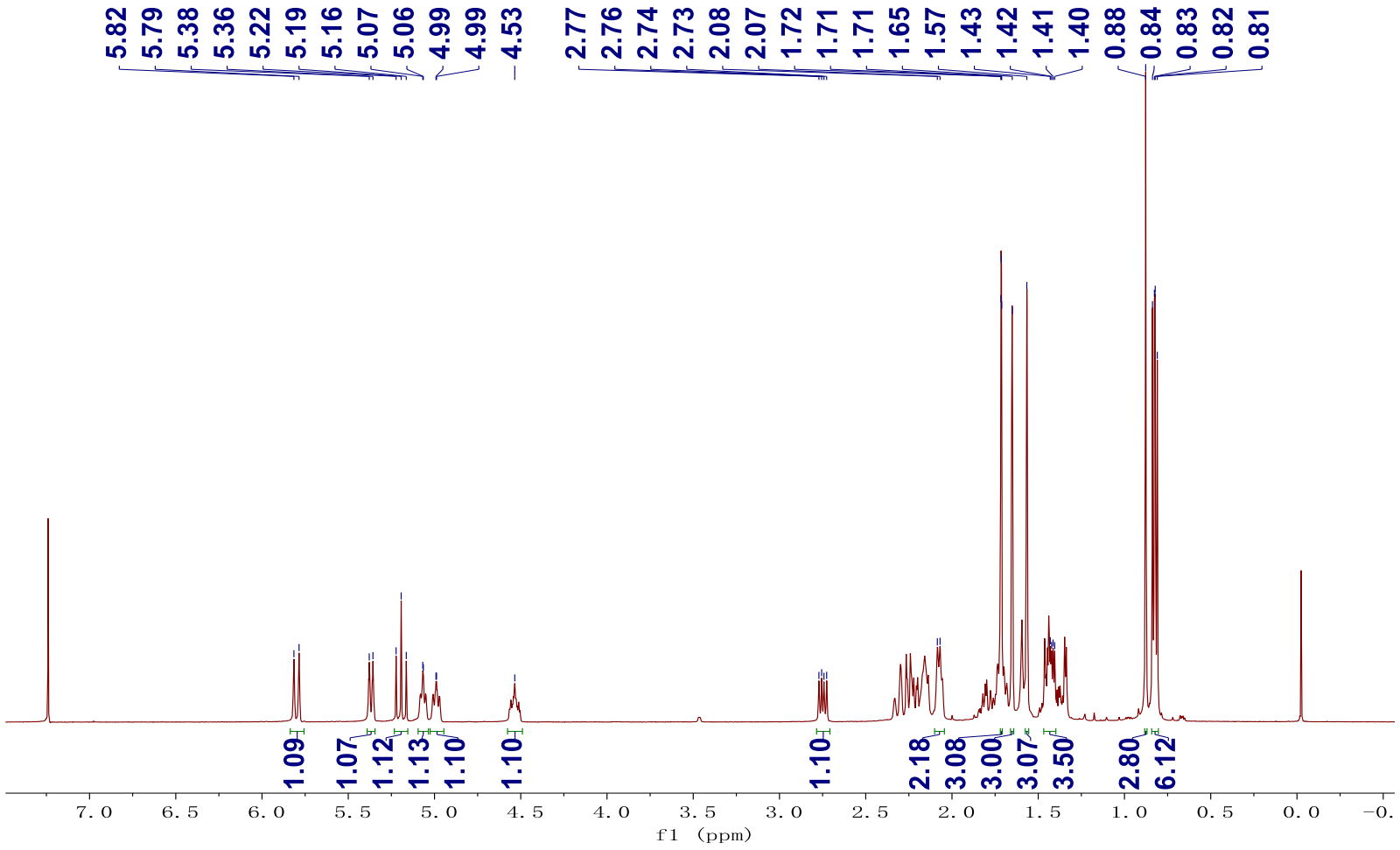

Figure S26. ^{13}C NMR and DEPT spectra of Penisentenol (2) in $CDCl_3$.

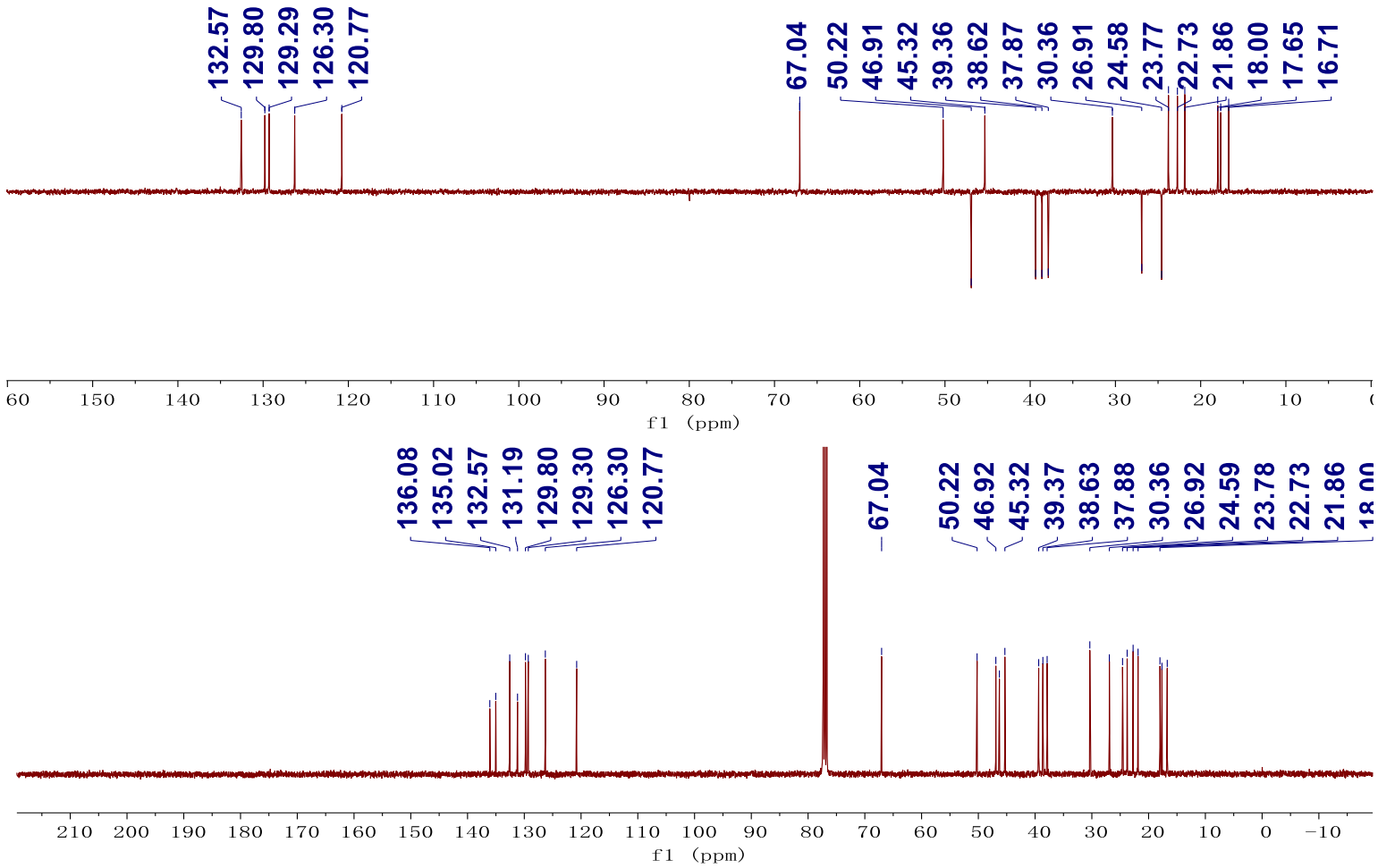

Figure S27. HSQC spectrum of Penisentenol (2) in $CDCl_3$.

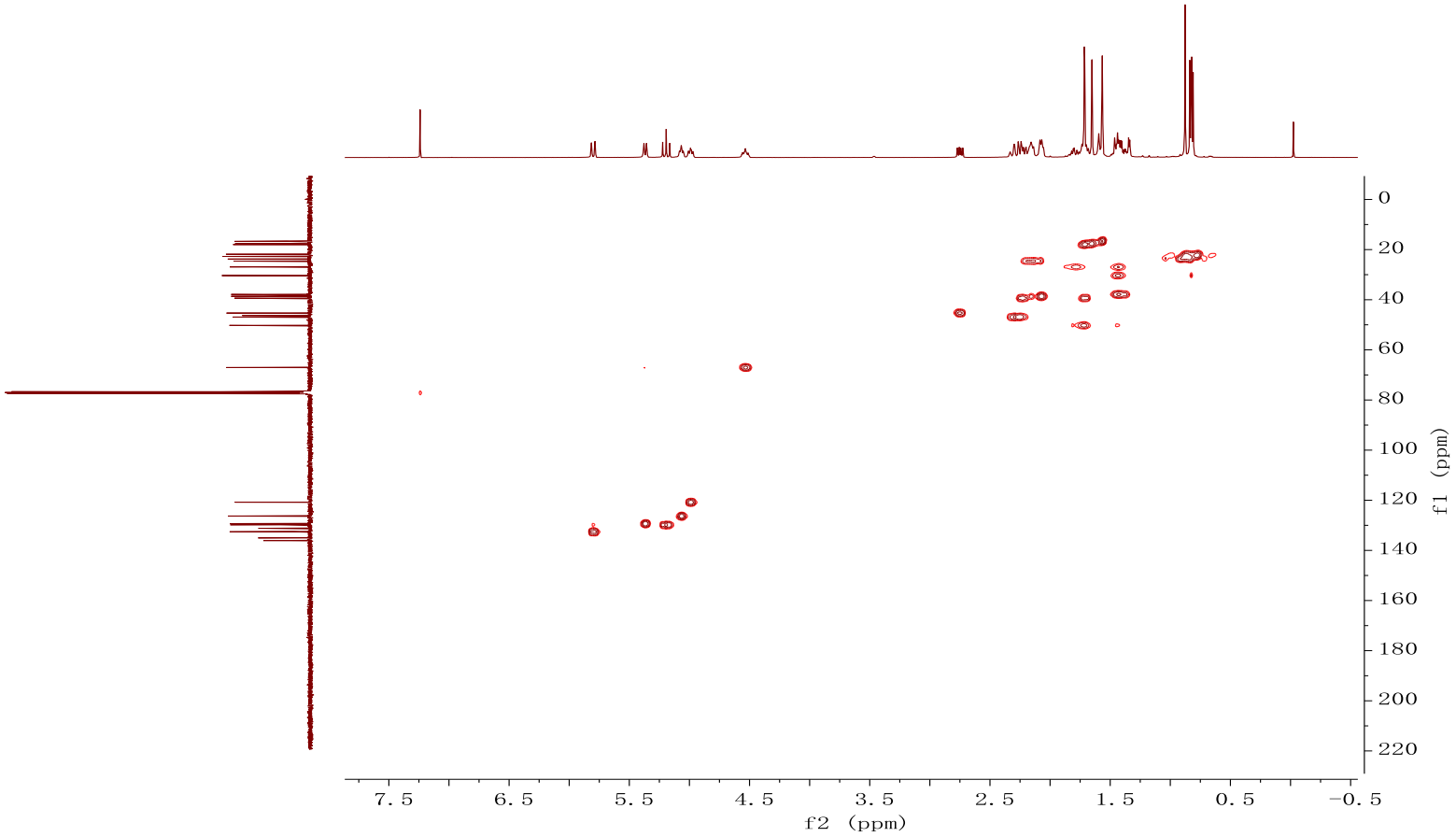

Figure S28. HMBC spectrum of Penisentenol (2) in $CDCl_3$.

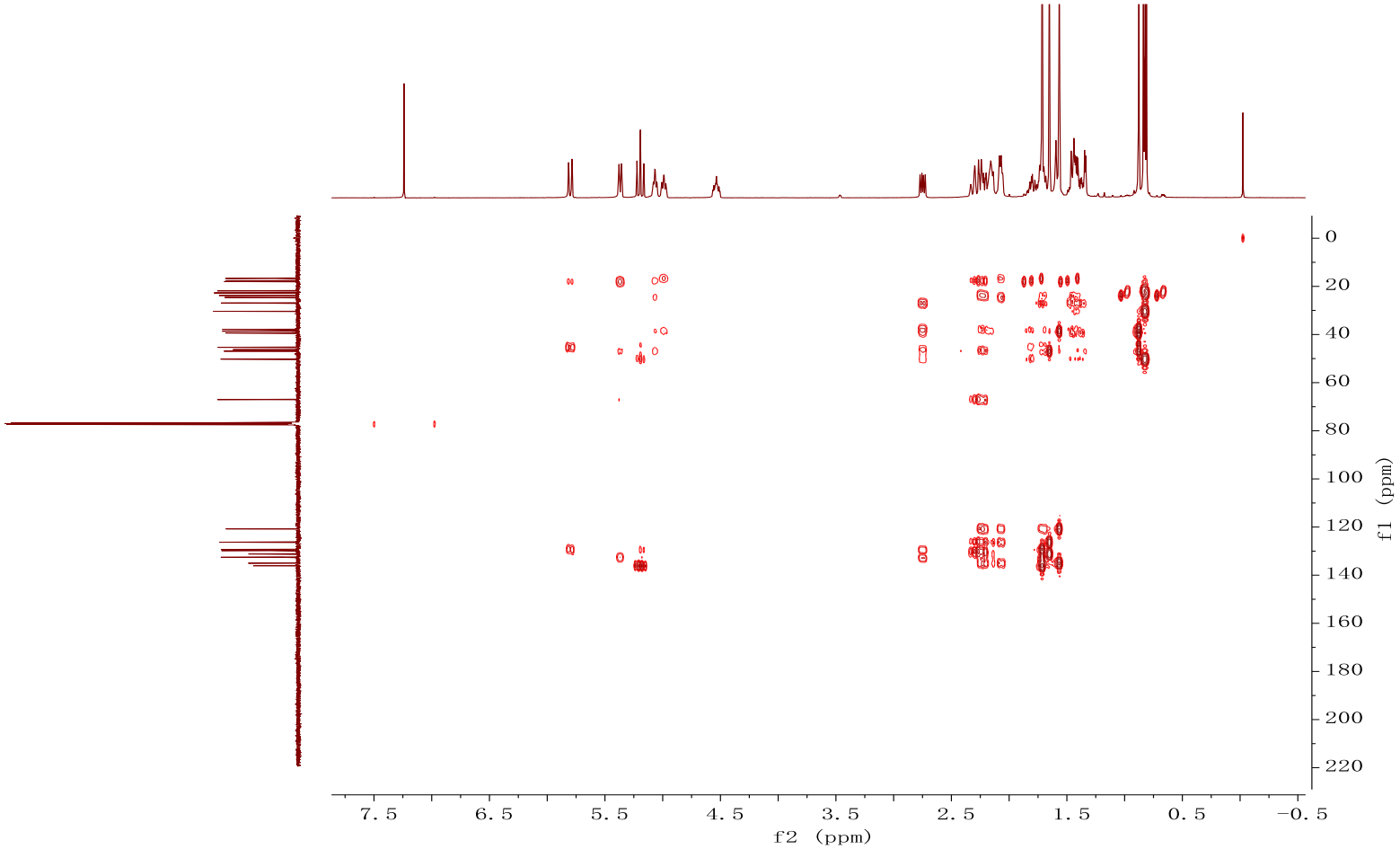

Figure S29. $^{1}H–^{1}H$ COSY spectrum of Penisentenol (2) in $CDCl_3$.

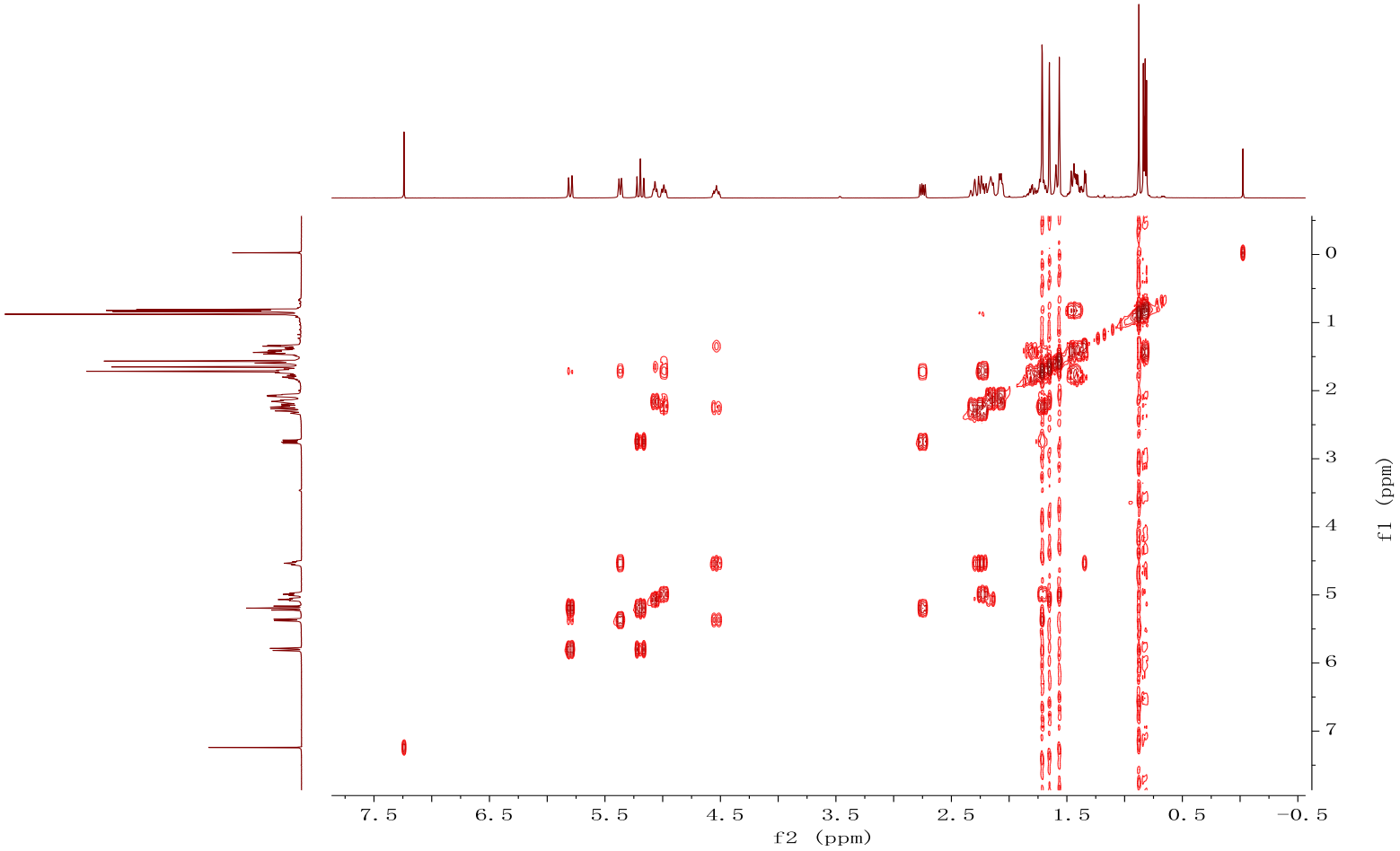

Figure S30. NOESY spectrum of Penisentenol (2) in $CDCl_3$.

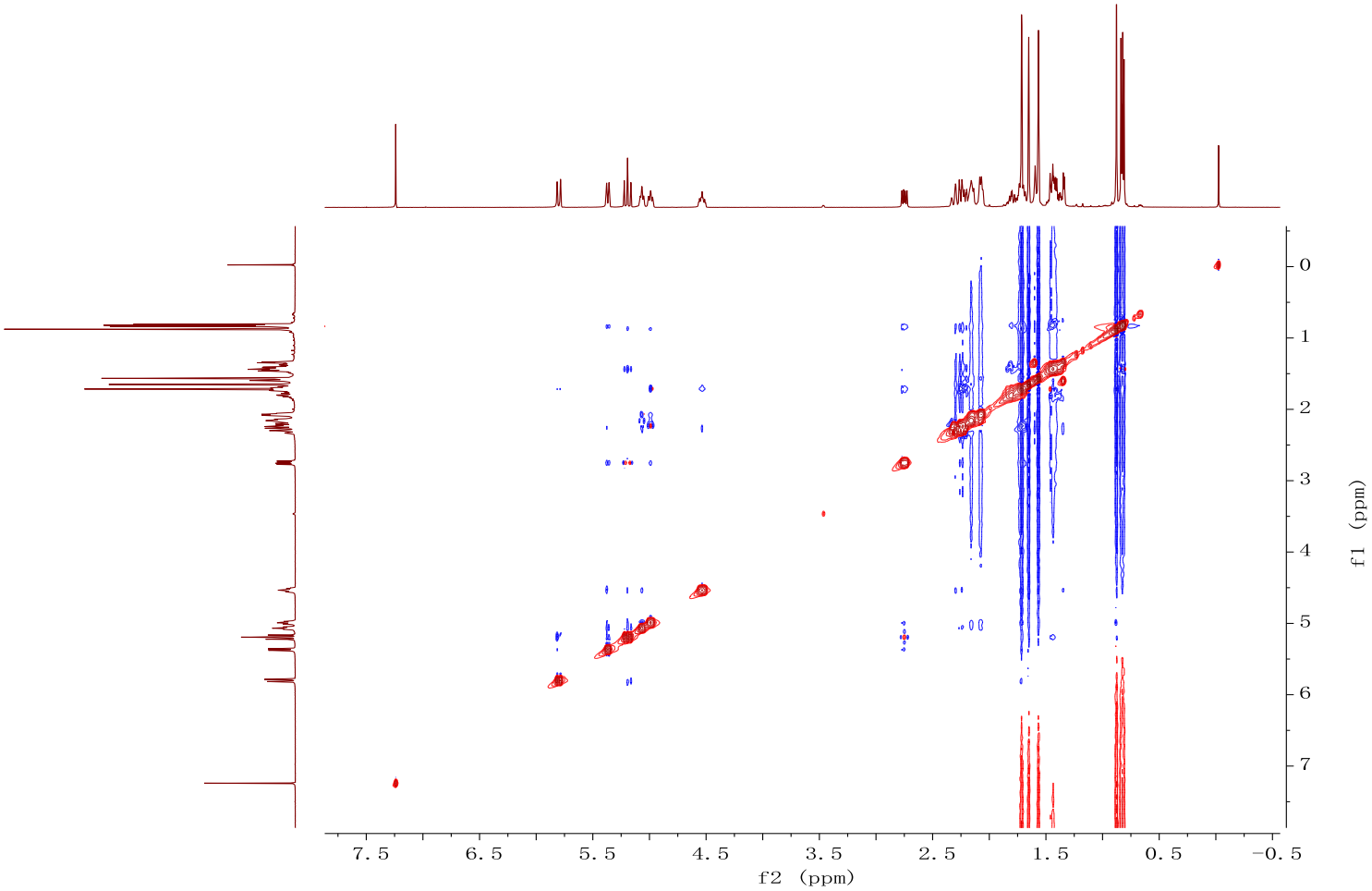

Figure S31. ^{1}H NMR spectrum of Penisentone (3) in $CDCl_3$.

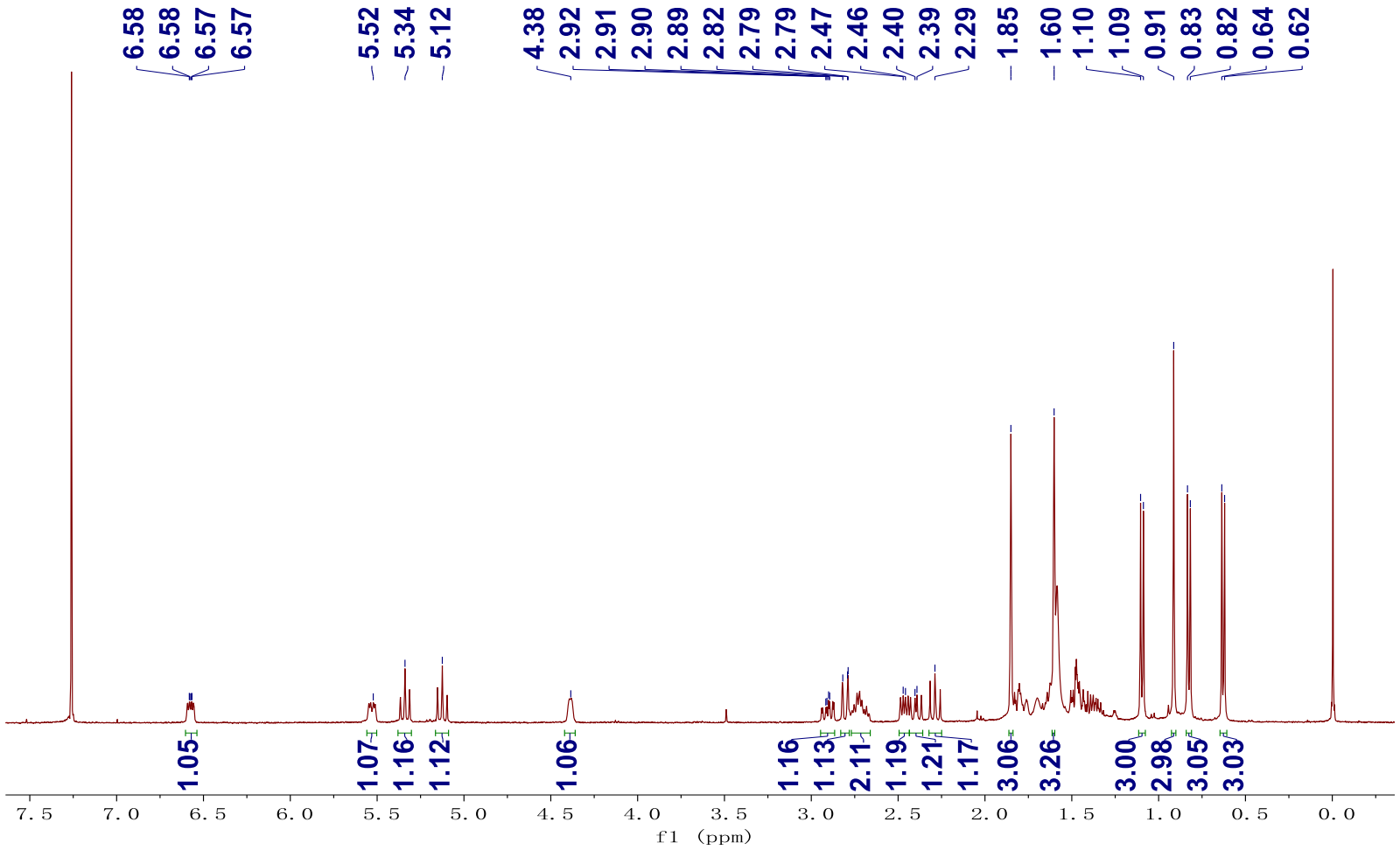

Figure S32. ^{13}C NMR and DEPT spectra of Penisentone (3) in $CDCl_3$.

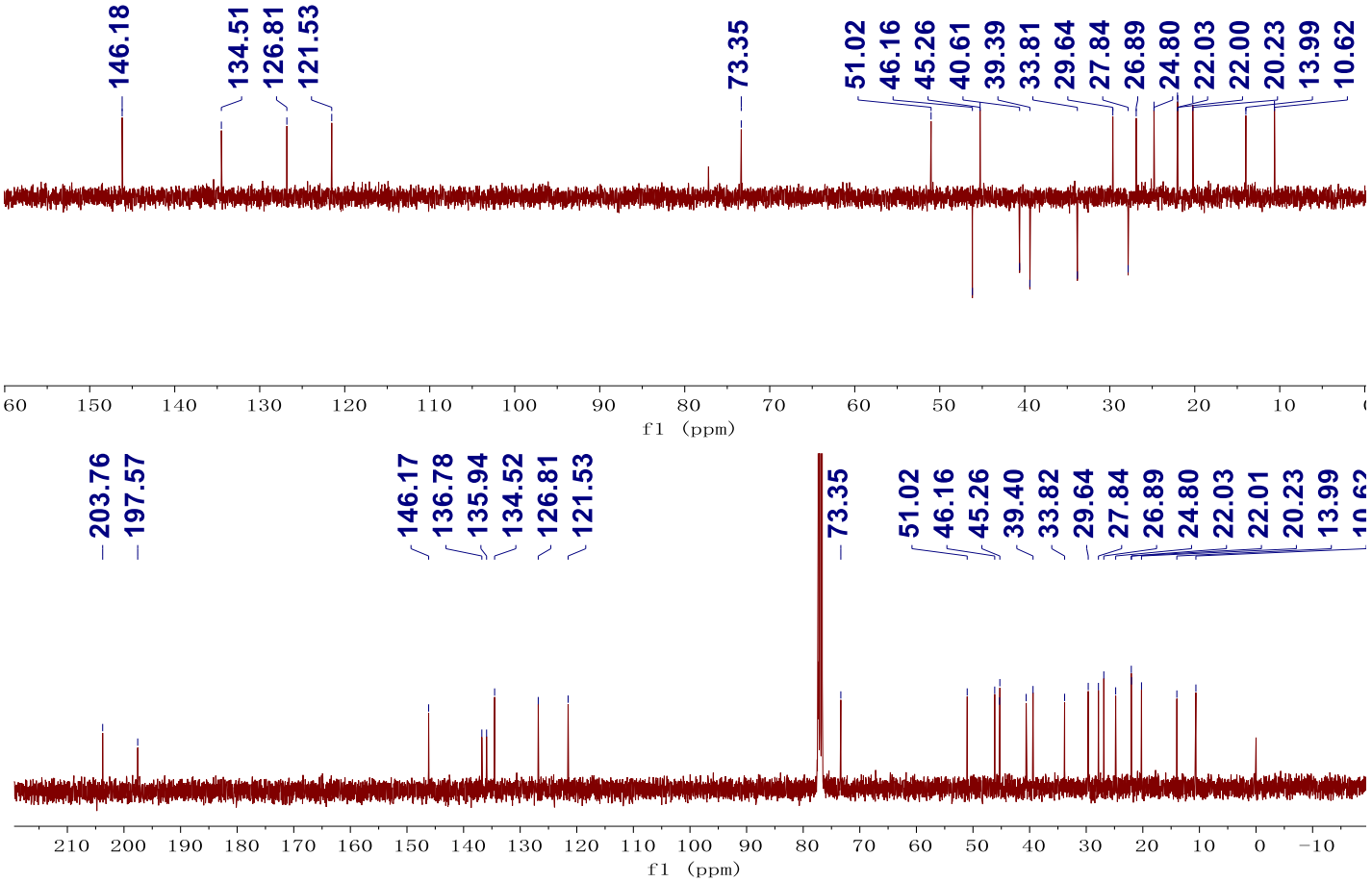

Figure S33. HSQC spectrum of Penisentone (3) in $CDCl_3$.

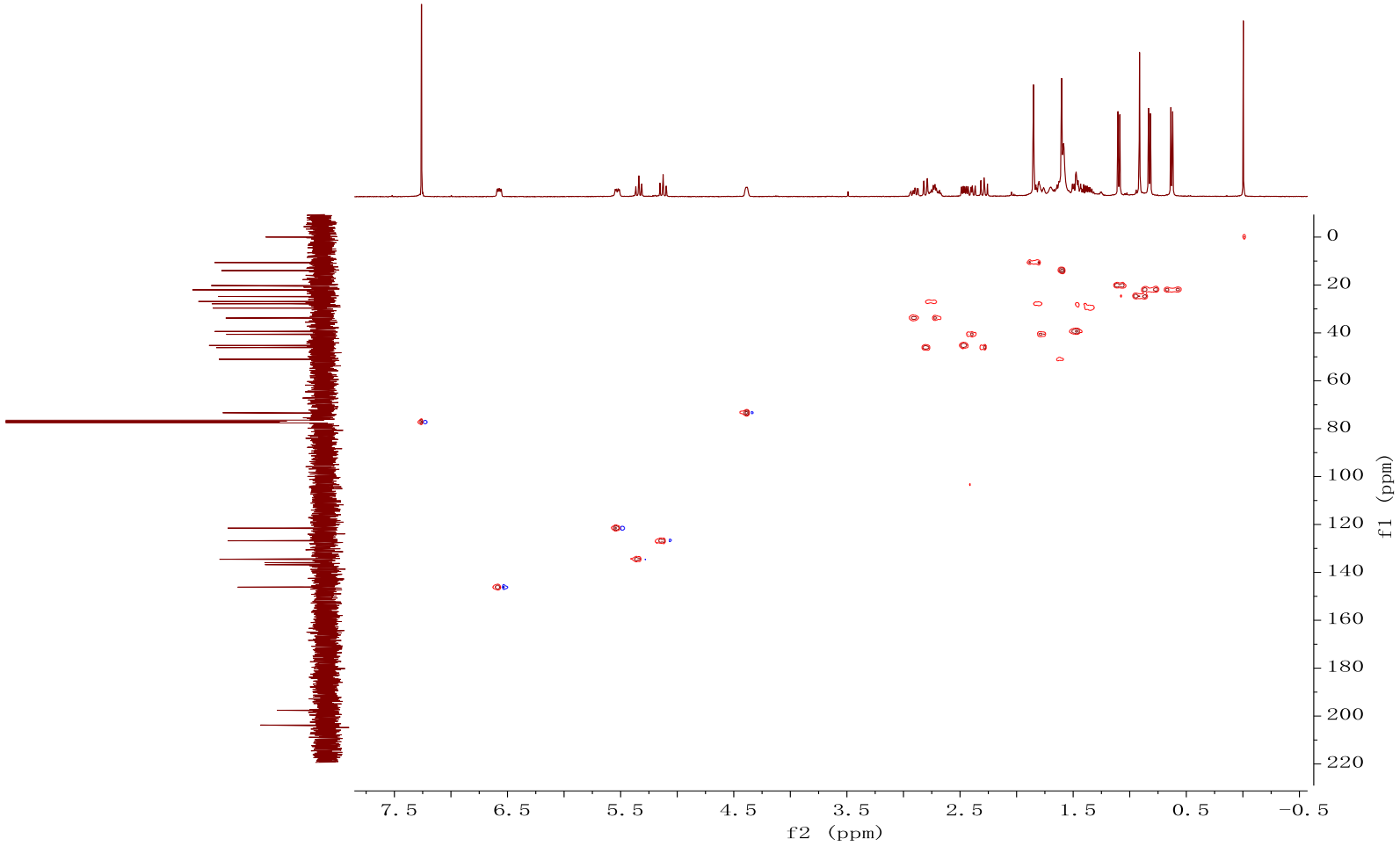

Figure S34. HMBC spectrum of Penisentone (3) in $CDCl_3$.

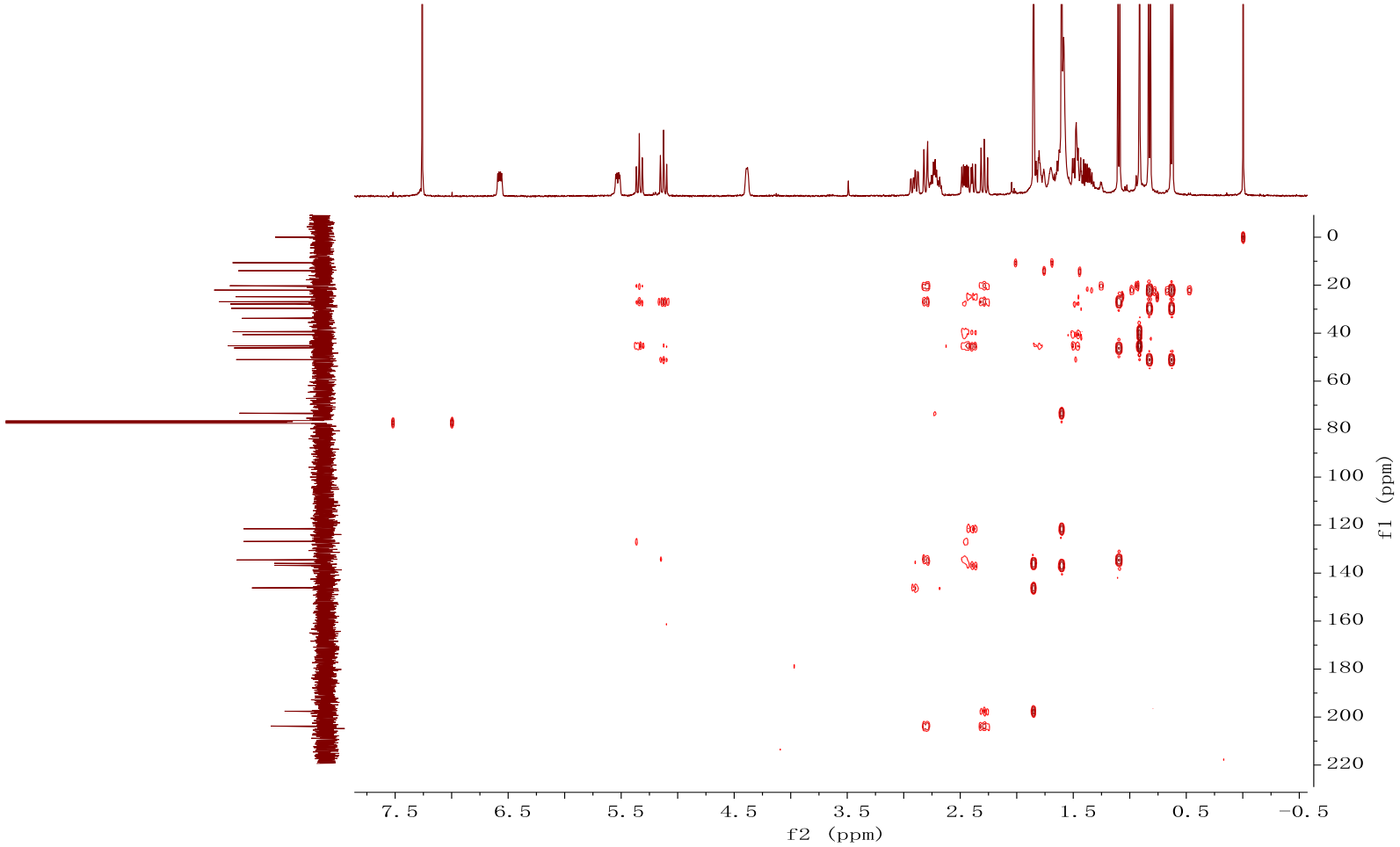

Figure S35. $^{1}H–^{1}H$ COSY spectrum of Penisentone (3) in $CDCl_3$.

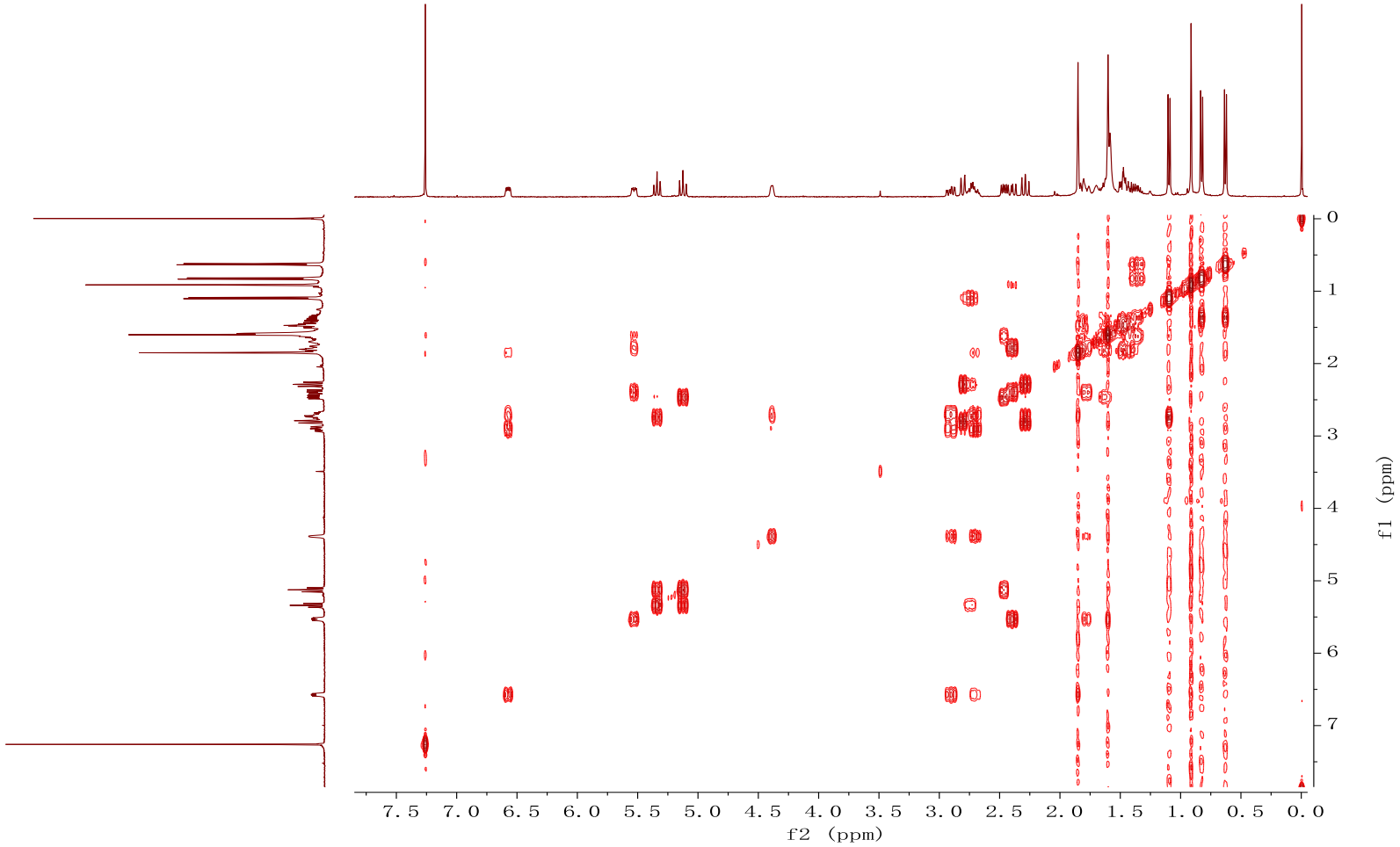

Figure S36. NOESY spectrum of Penisentone (3) in $CDCl_3$.

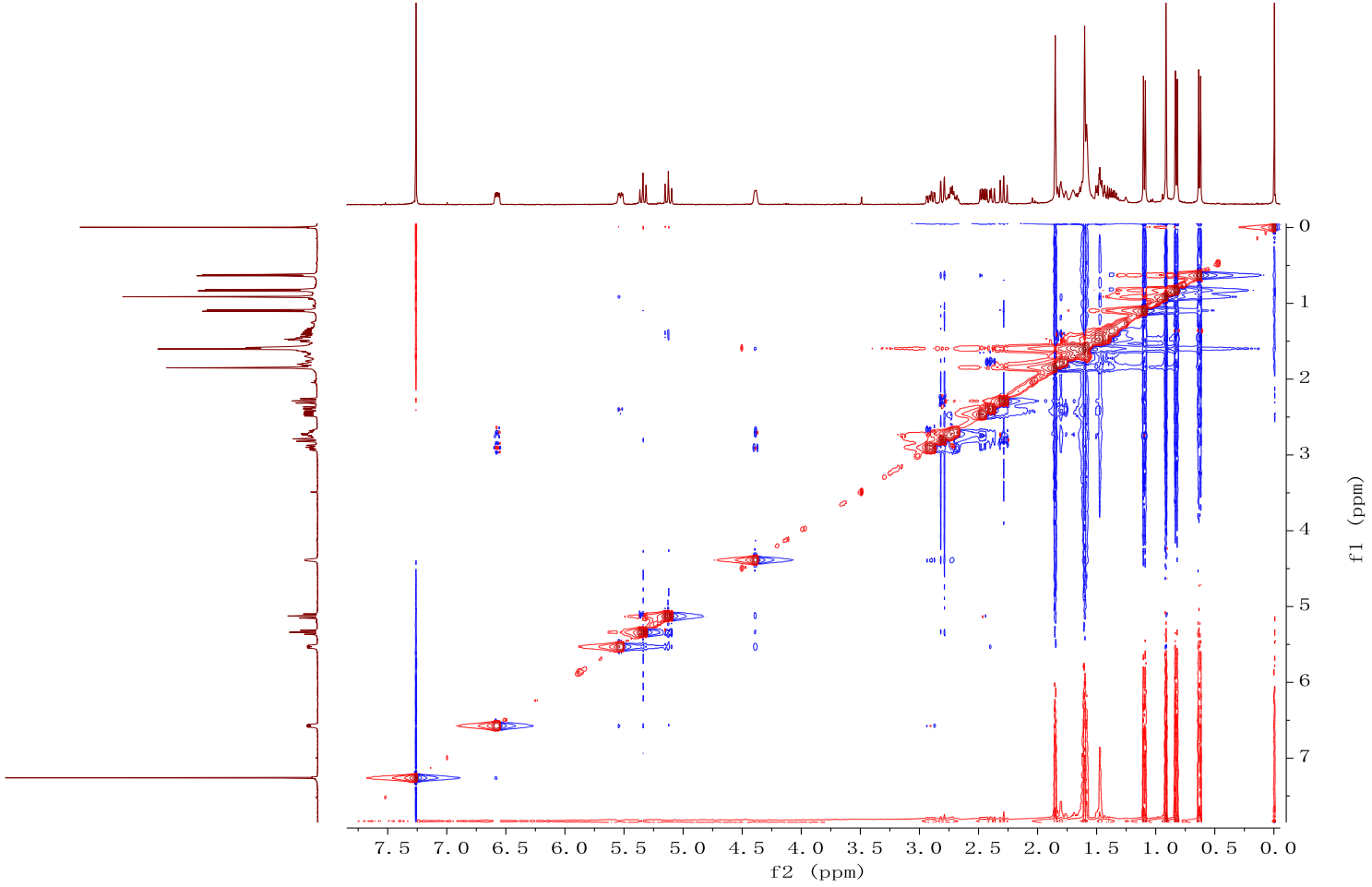

Figure S37. ^{1}H NMR spectrum of Derivepenisentene (4) in $CDCl_3$.

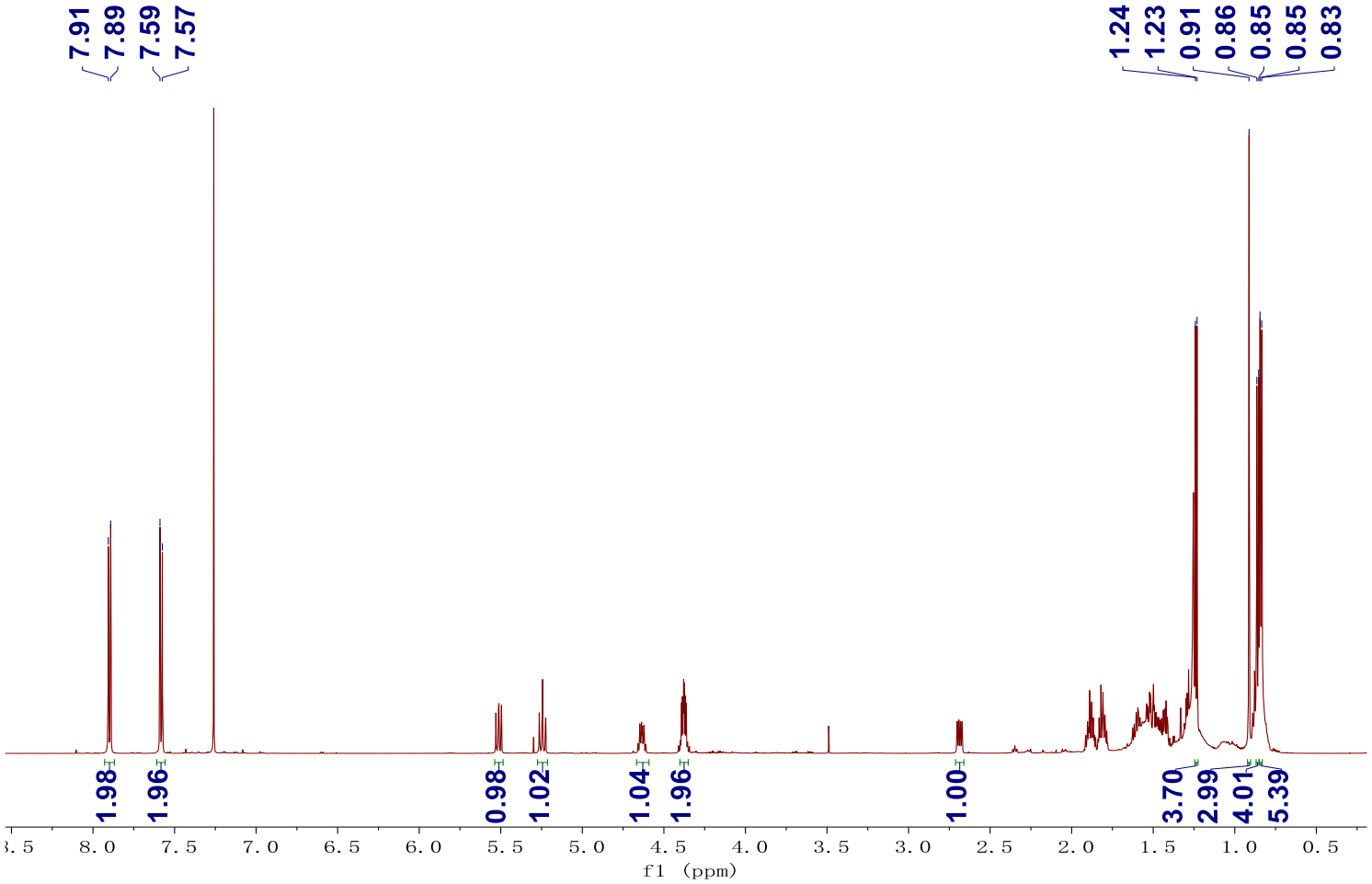

Figure S38. ^{13}C NMR and DEPT spectra of Derivepenisentene (4) in $CDCl_3$.

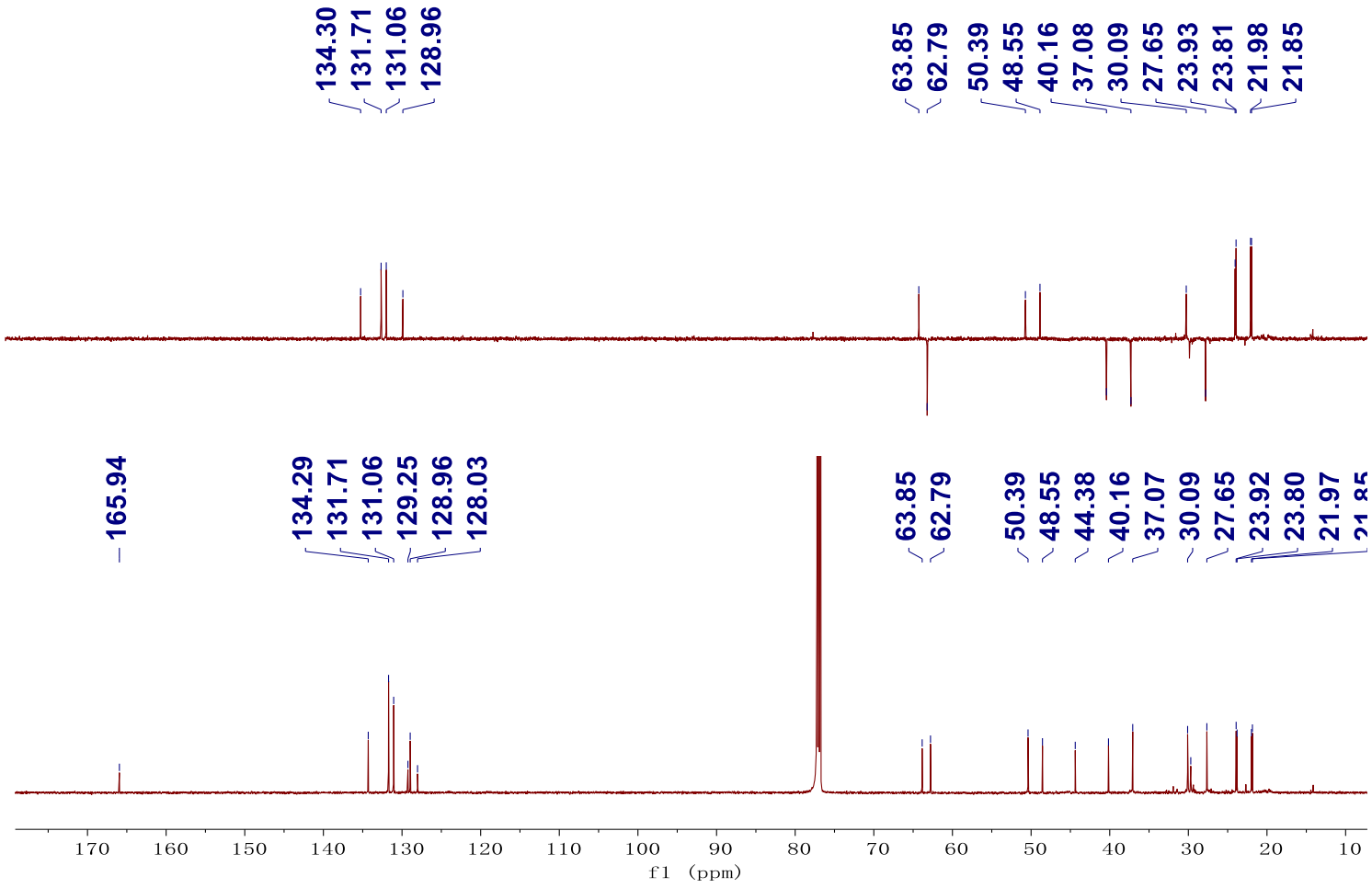

Figure S39. HSQC spectrum of Derivepenisentene (4) in $CDCl_3$.

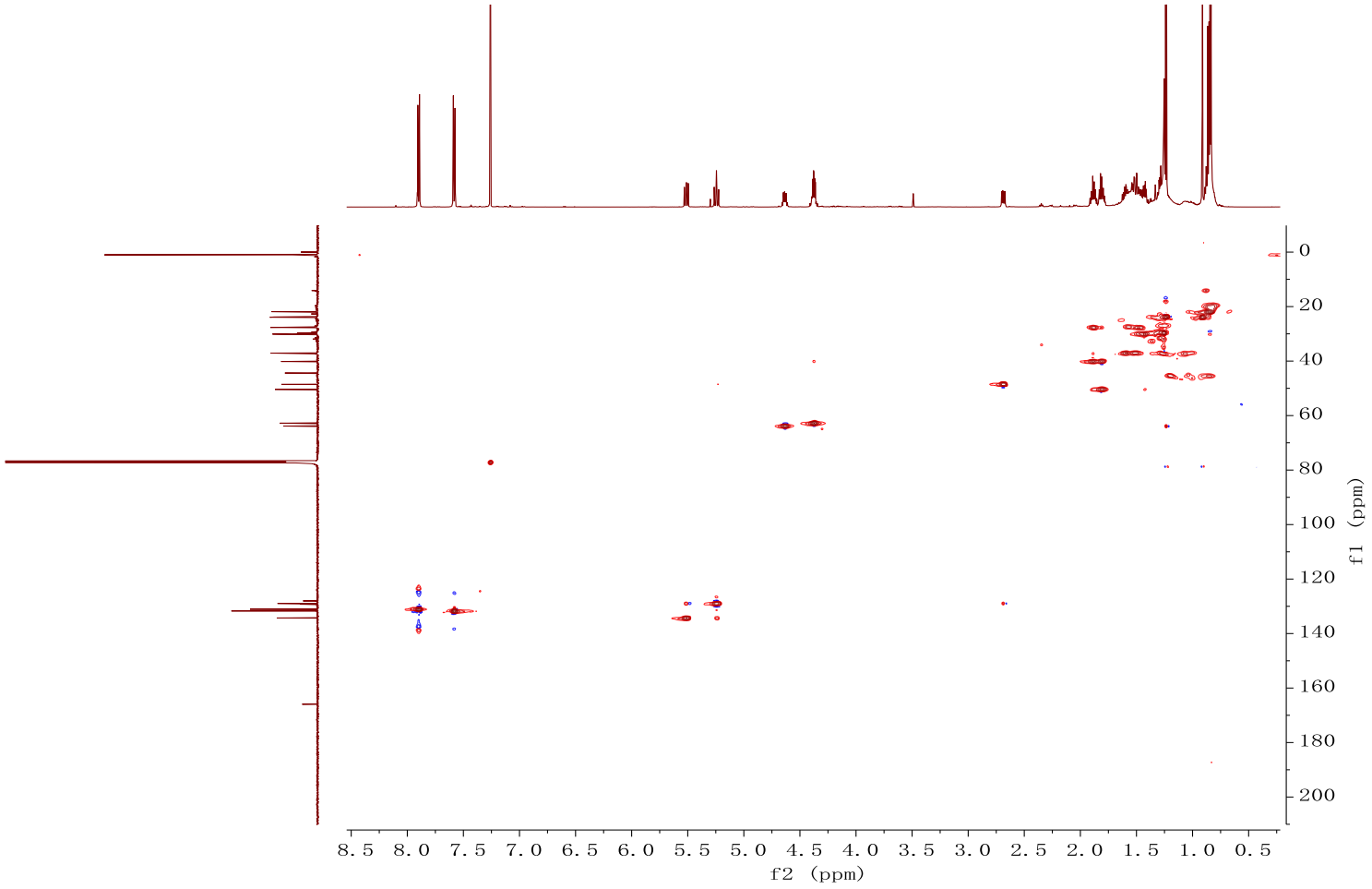

Figure S40. HMBC spectrum of Derivepenisentene (4) in $CDCl_3$.

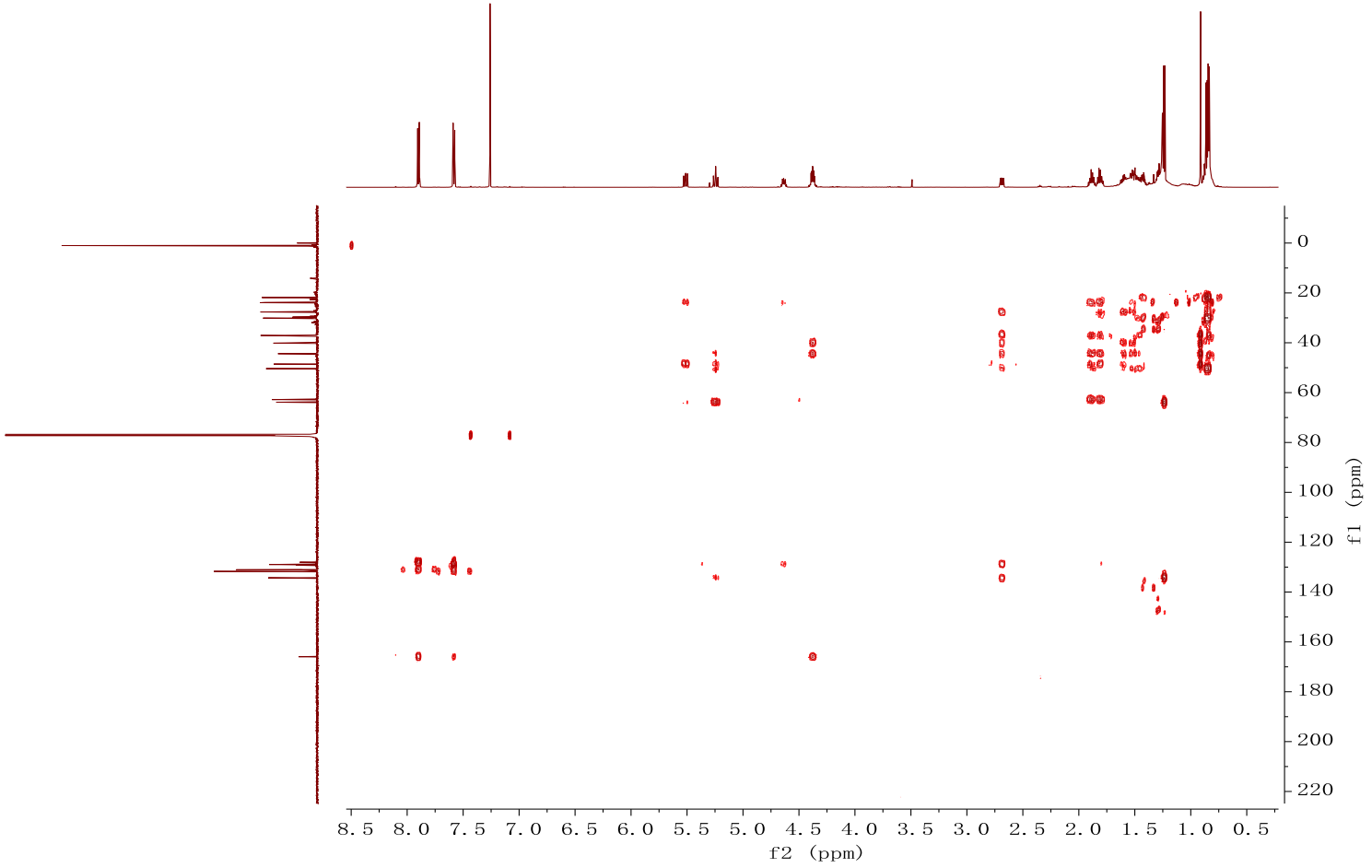

Figure S41. $^{1}H–^{1}H$ COSY spectrum of Derivepenisentene (4) in $CDCl_3$.

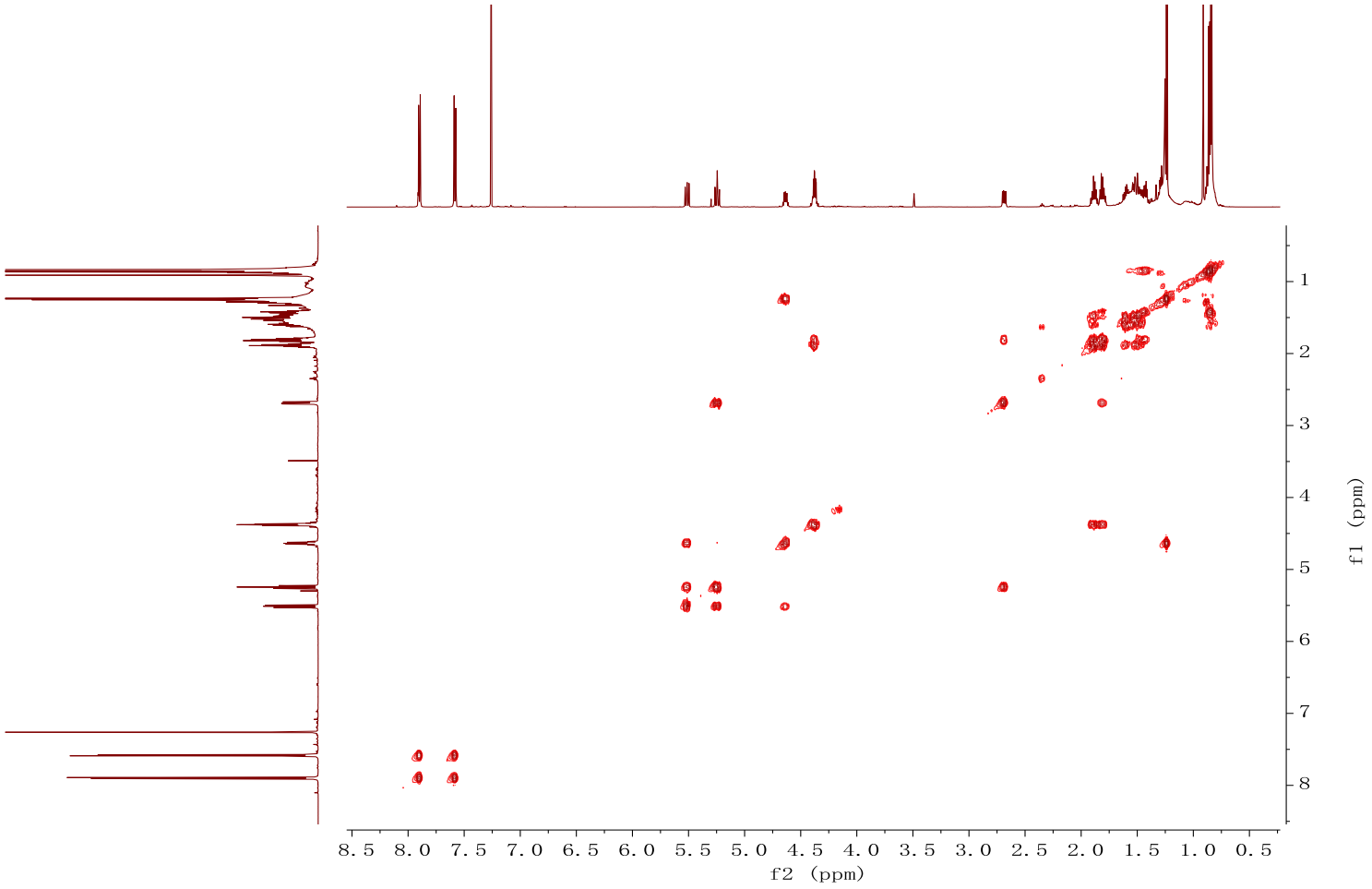

Figure S42. NOESY spectrum of Derivepenisentene (4) in $CDCl_3$.

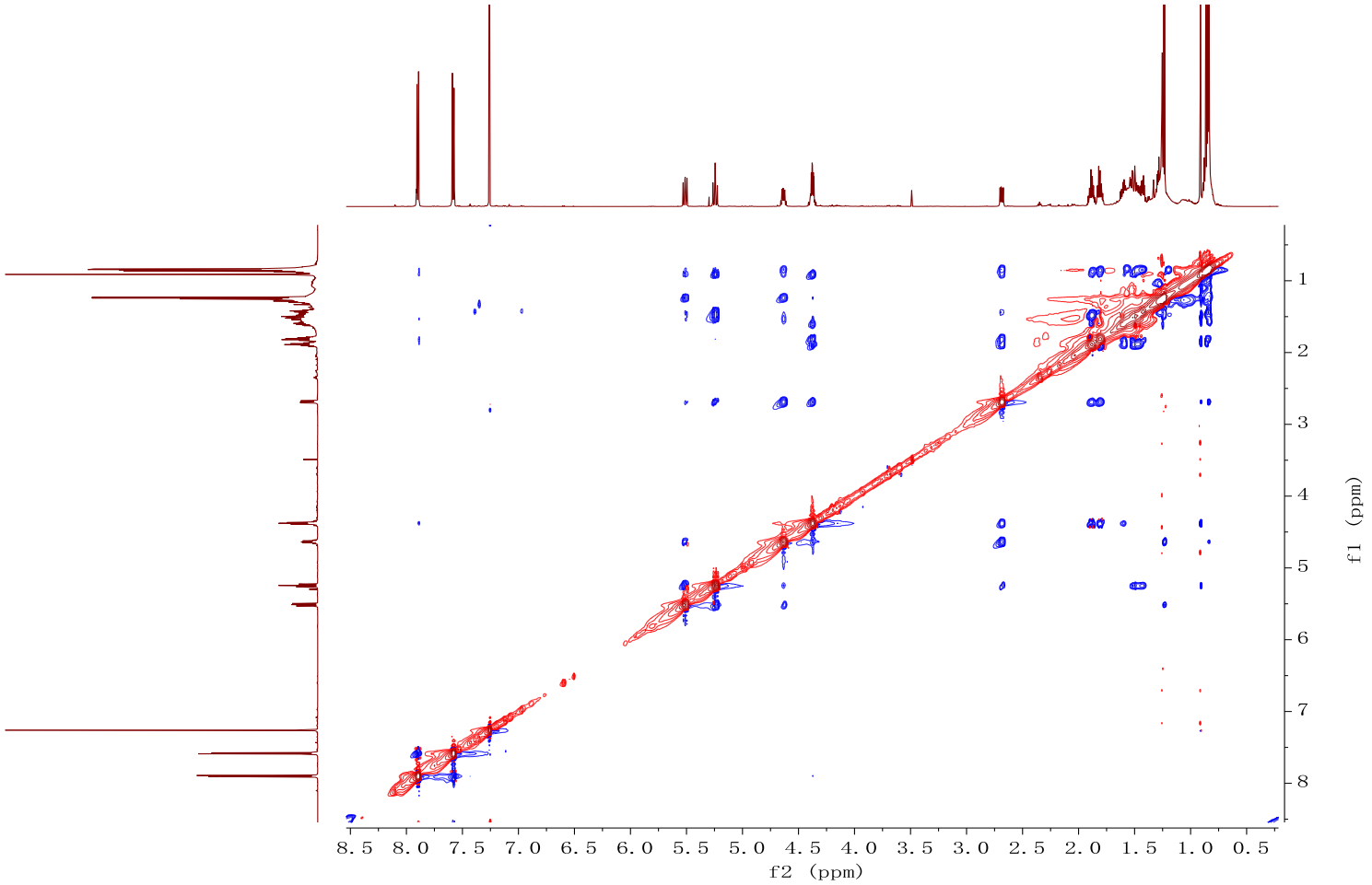

Figure S43. Experimental ECD and UV spectra of 1–3.

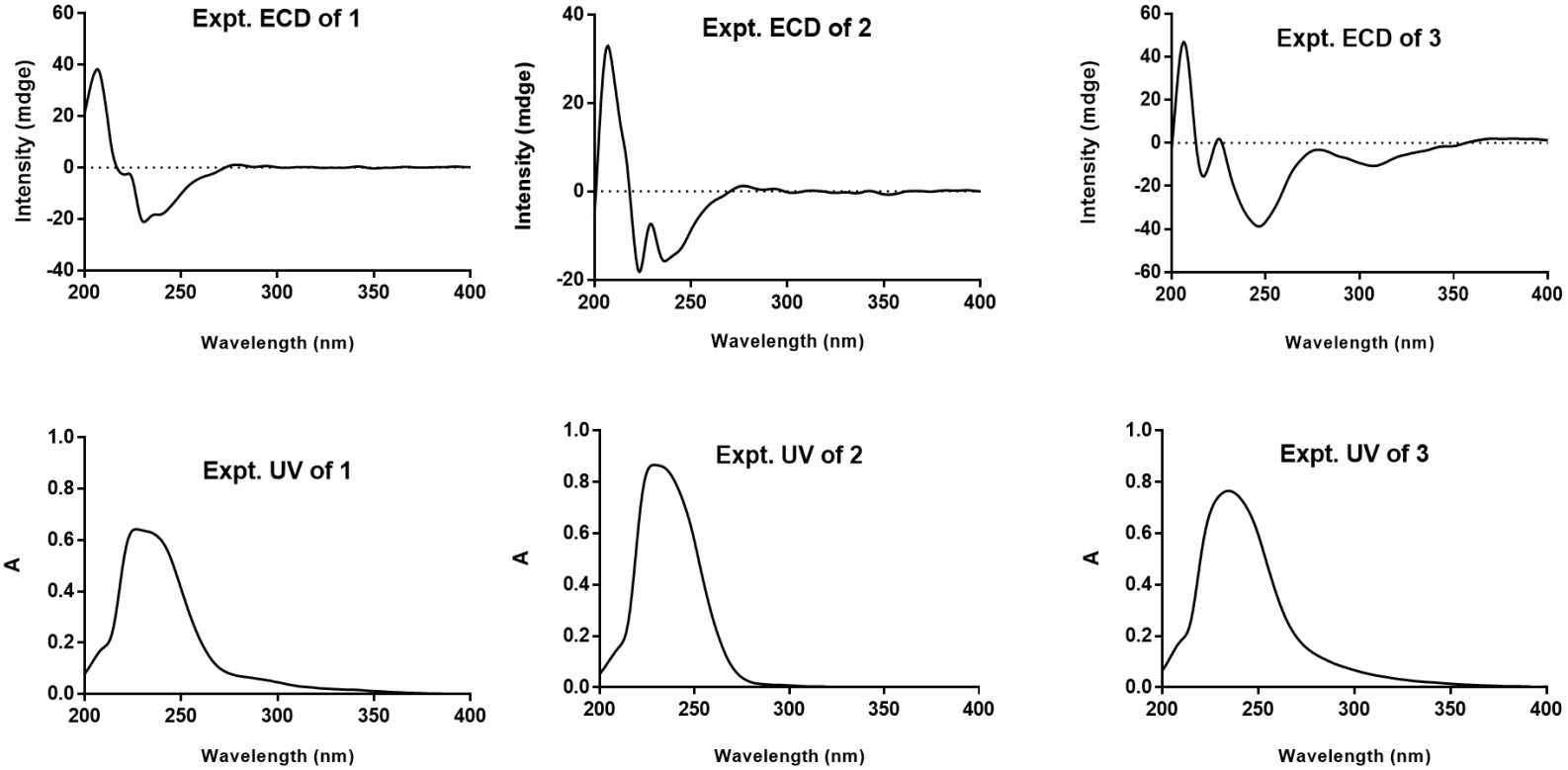

Figure S44. IR spectrum of 1.