Supporting information for

Diterpenoids from the Root Bark of *Pinus massoniana* and Evaluation of Their Phosphodiesterase Type 4D Inhibitory Activity

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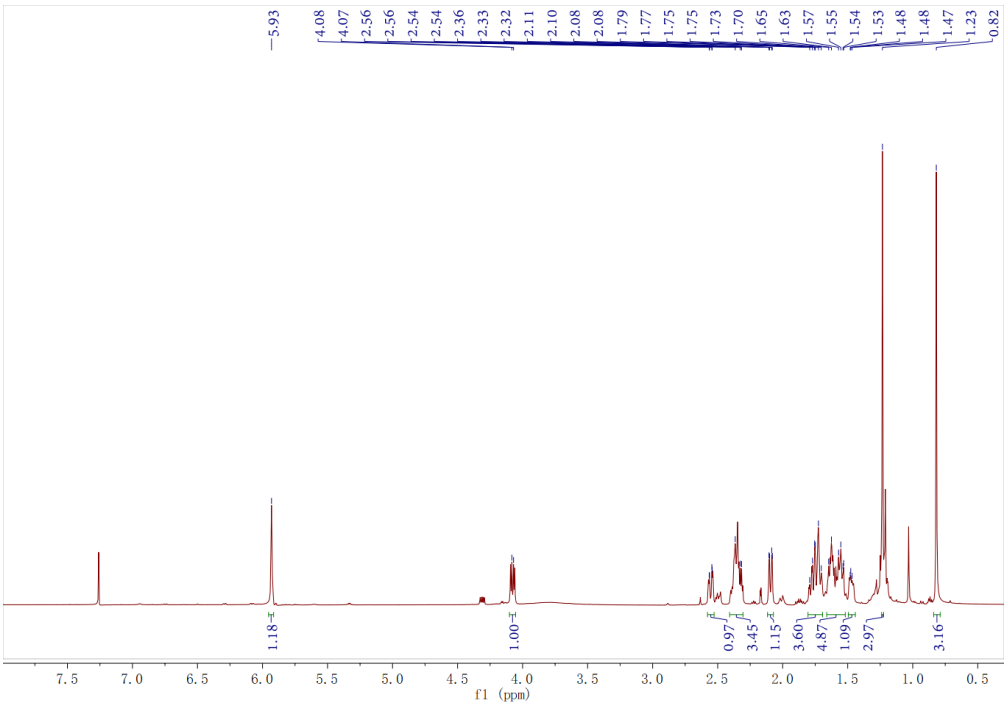
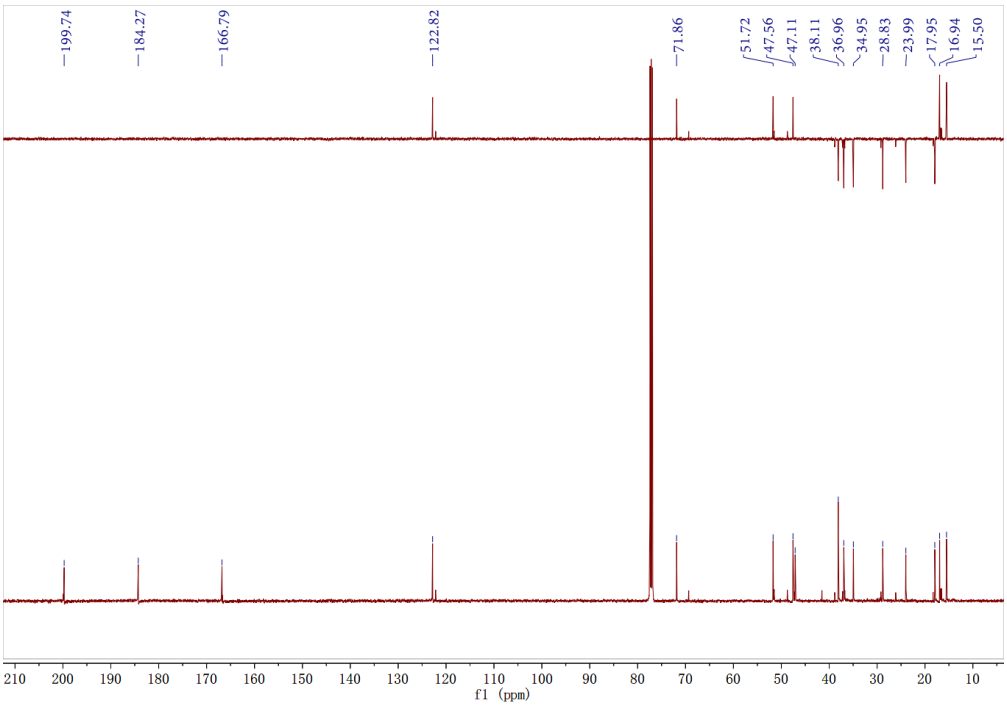
Contents

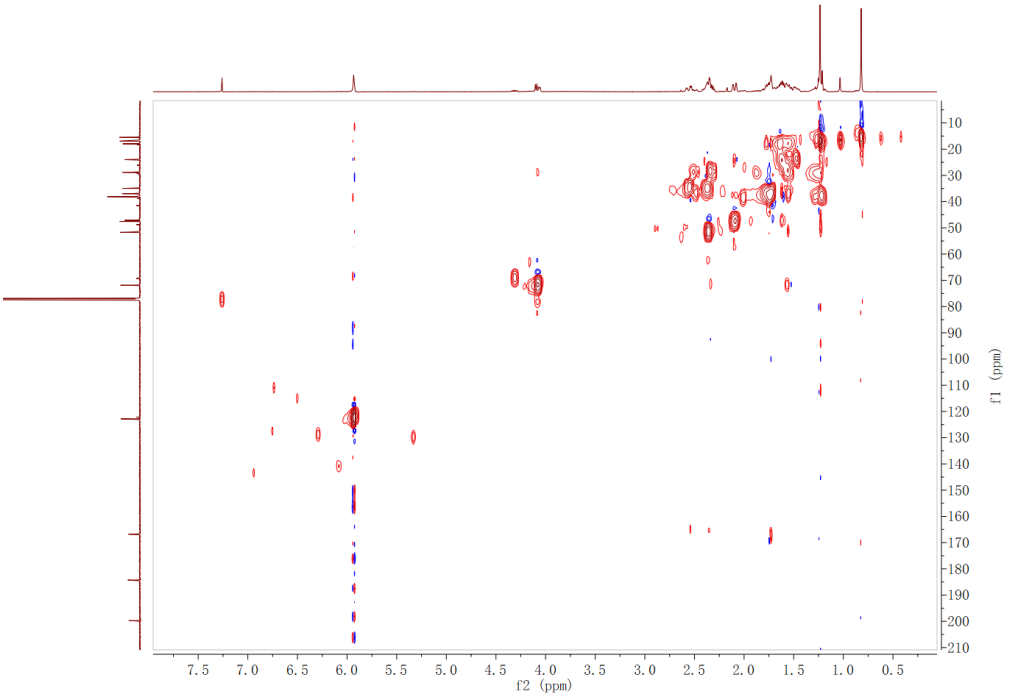
S1. ^{1}H NMR spectrum of Compound 1 in $CDCl_3$ (500 MHz)



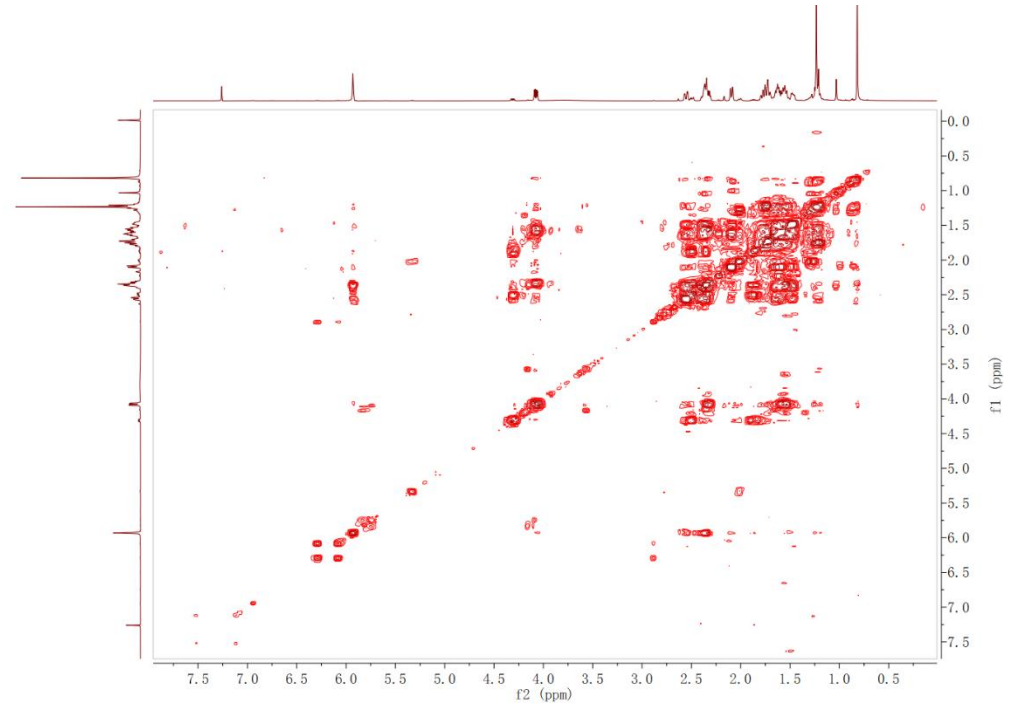
S2. ^{13}C NMR spectrum of Compound 1 in $CDCl_3$ (125 MHz)



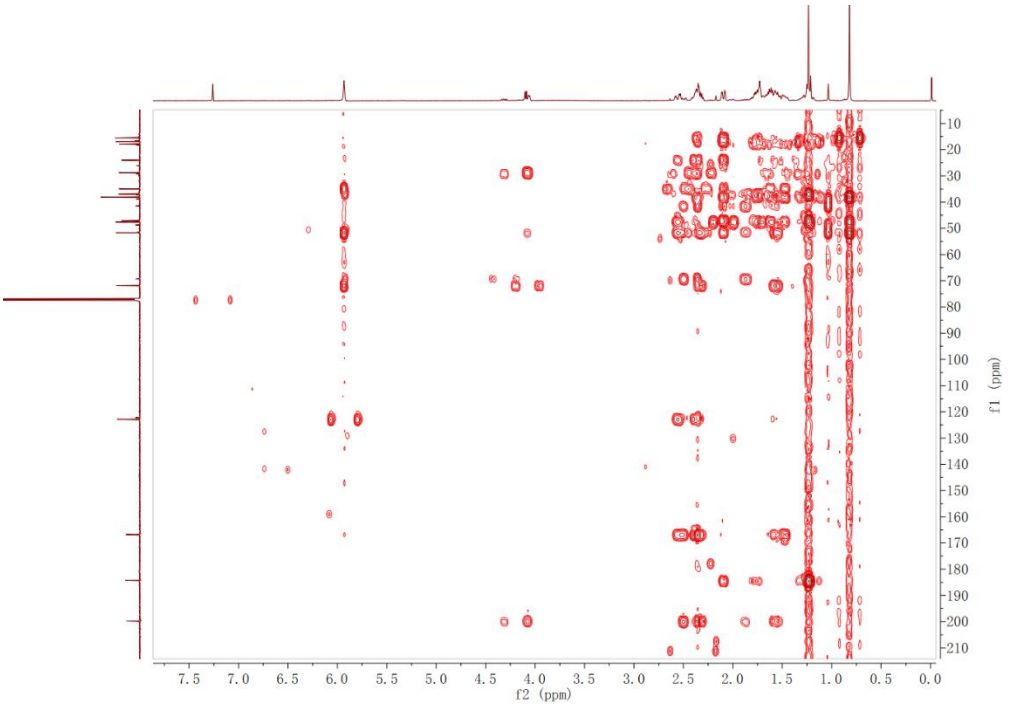
S3. HSQC spectrum of Compound 1 in $CDCl_3$



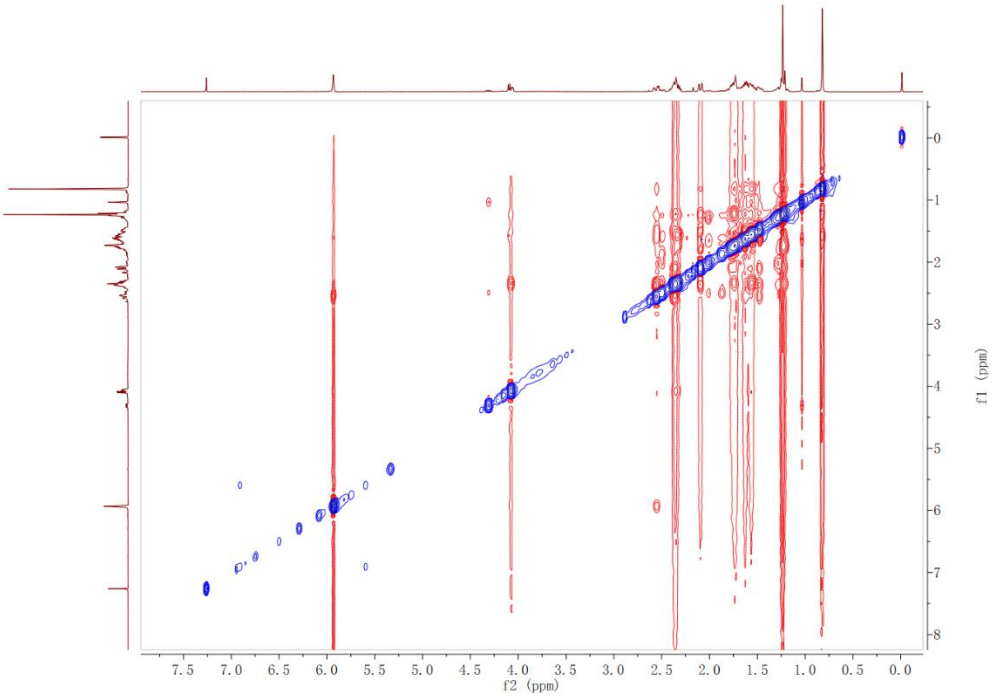
S4. ^{1}H-^{1}H COSY spectrum of Compound 1 in $CDCl_3$



S5. HMBC spectrum of Compound 1 in $CDCl_3$



S6. NOESY spectrum of Compound 1 in $CDCl_3$



S7. HR-ESIMS of Compound 1

Data Filename	ESIH_20191029_ZWM_FYF_01.d	**Sample Name**	D7-MWD62-3-1
Sample Type	Sample	**Position**	P1-A1
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160324_MS_ESIH_NEG_1min.m
Acquired Time	10/29/2019 16:07:50	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by ZZY

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
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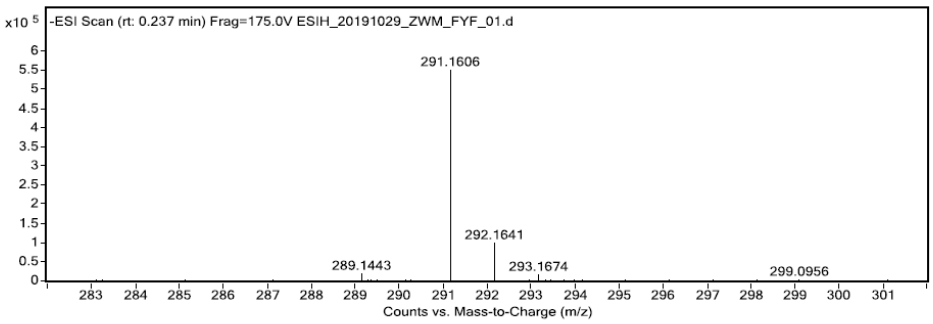

Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
291.1606	291.1602	-0.43	-1.48	C17 H23 O4	(M-H)-

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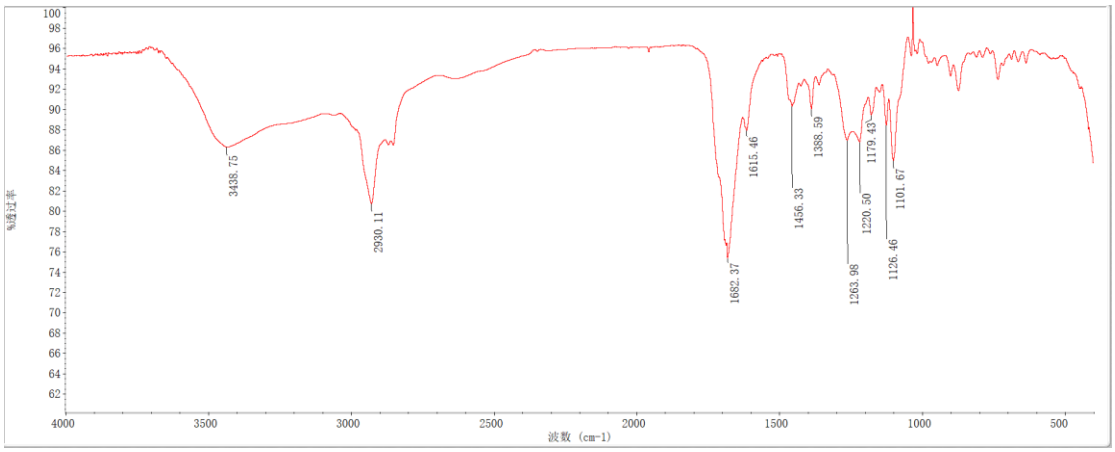
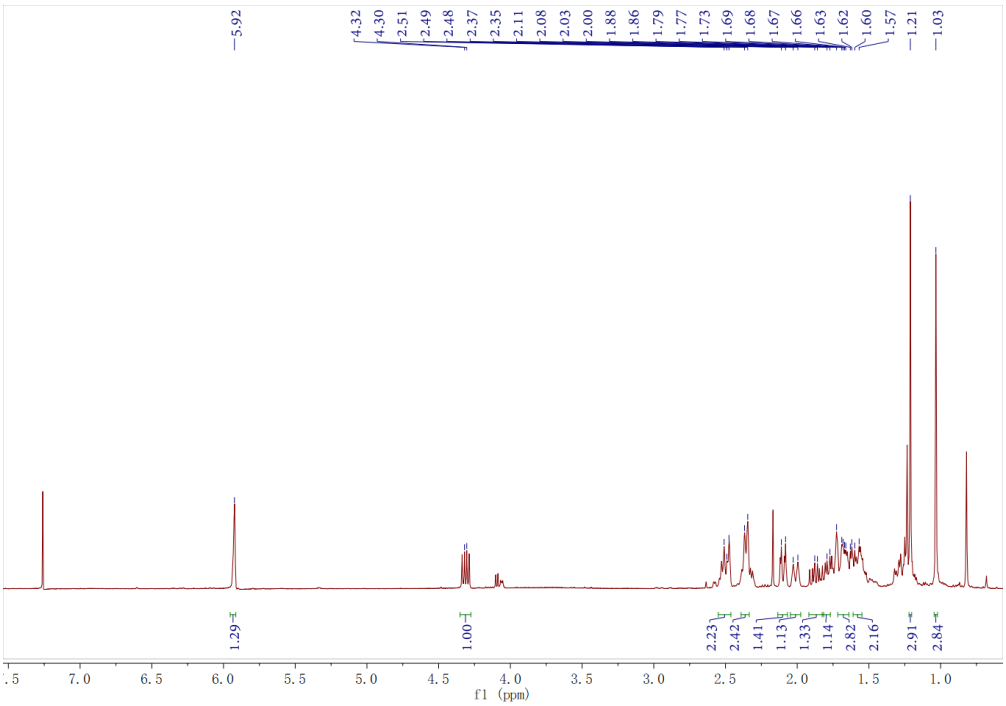
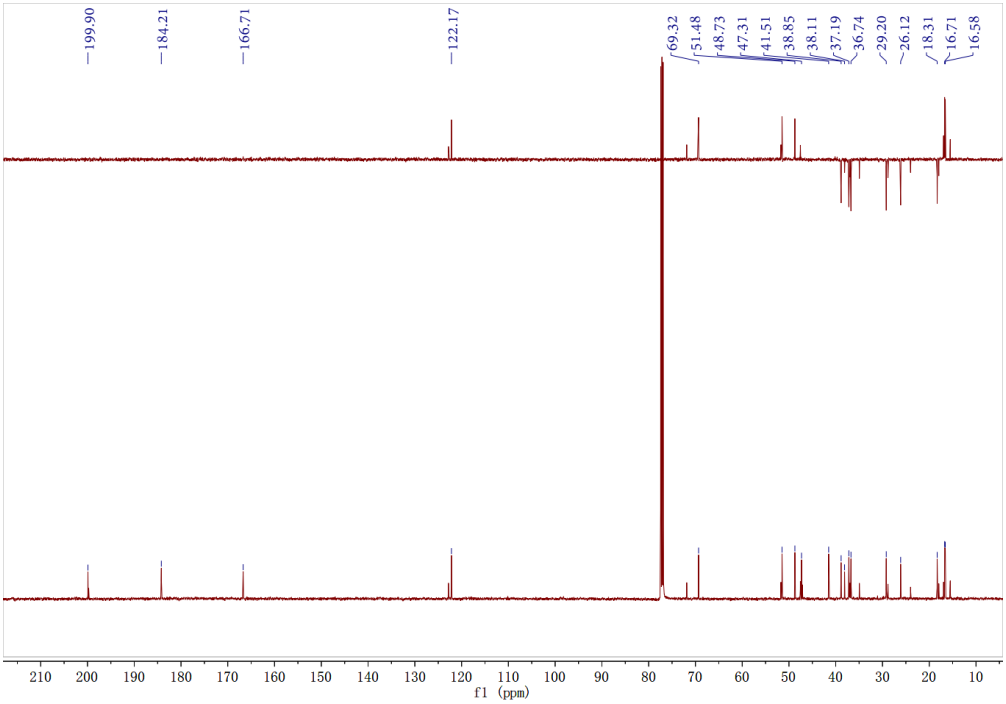
S8. IR spectrum of Compound 1



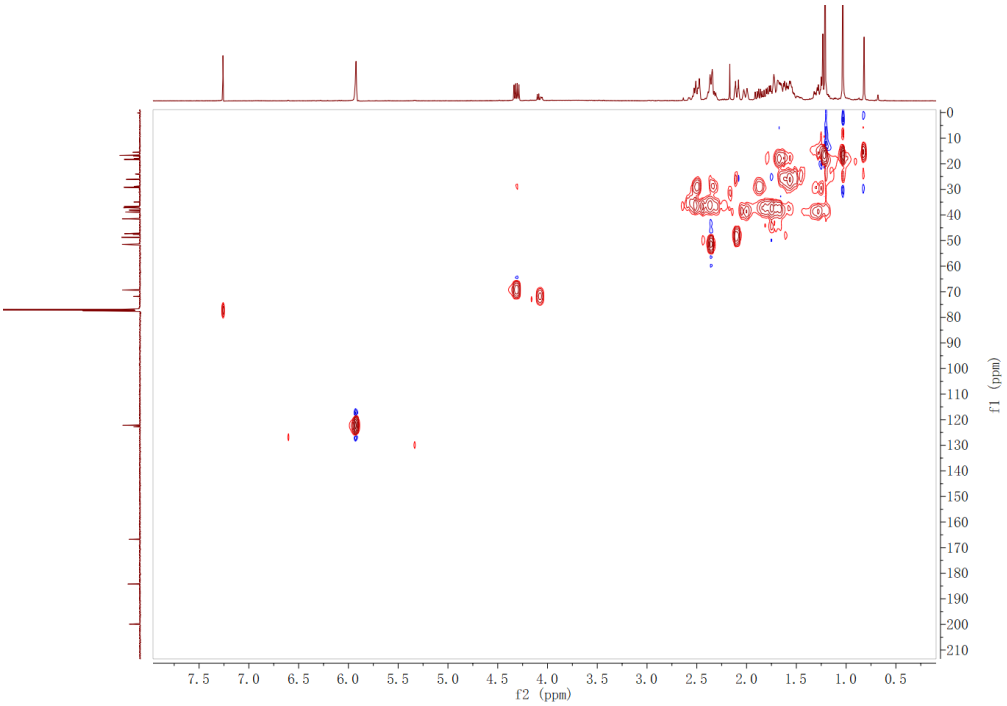
S9. ^{1}H NMR spectrum of Compound 2 in $CDCl_3$ (500 MHz)



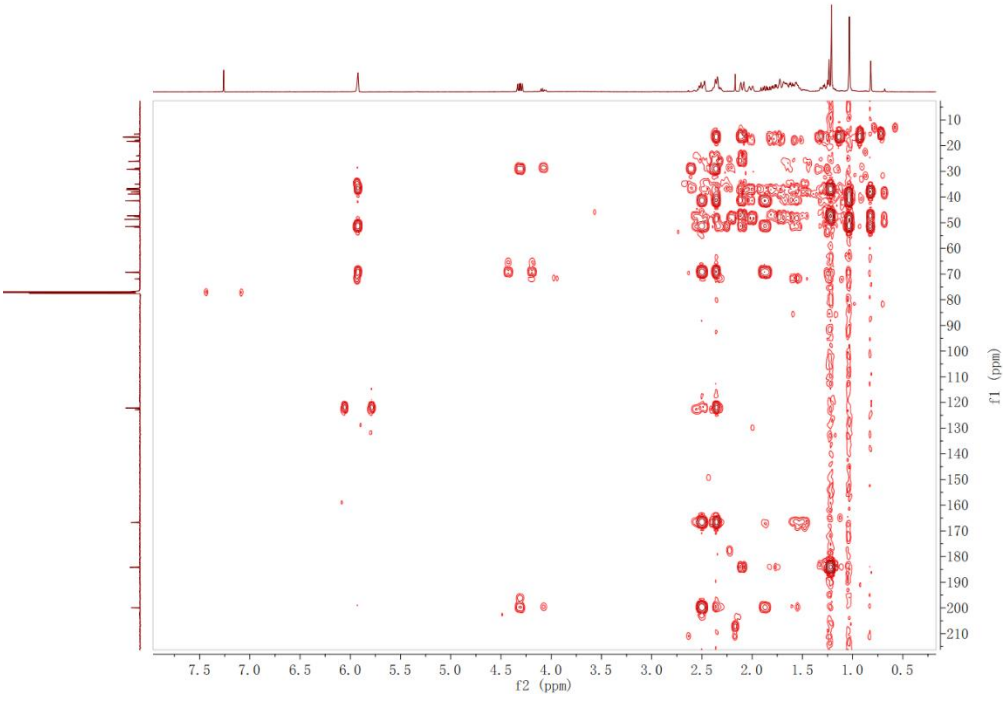
S10. ^{13}C NMR spectrum of Compound 2 in $CDCl_3$ (125 MHz)



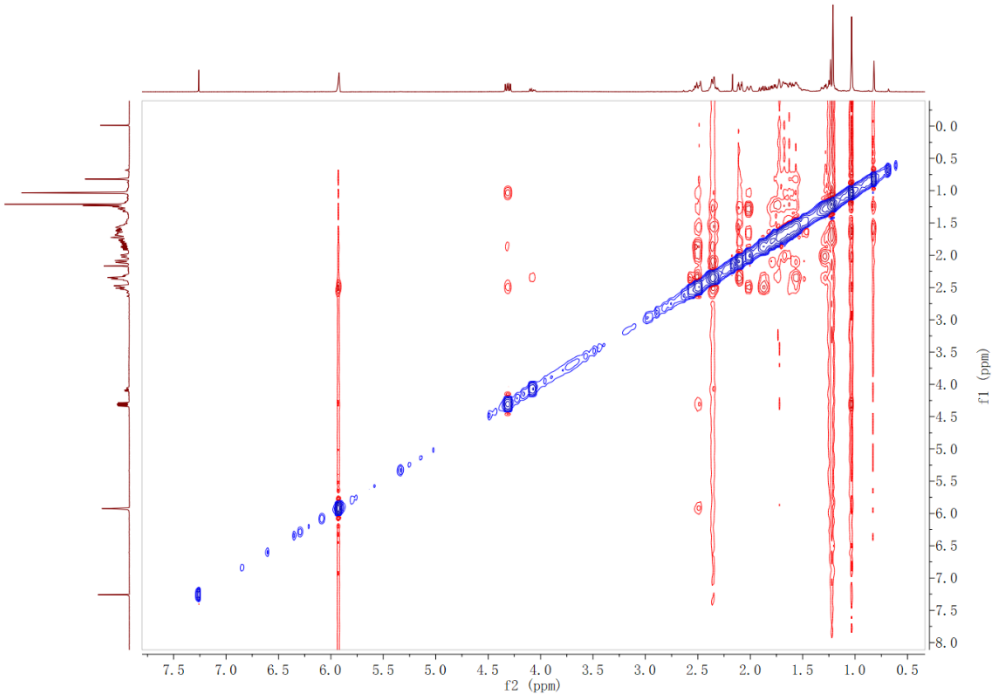
S11. HSQC spectrum of Compound 2 in $CDCl_3$



S12. HMBC spectrum of Compound 2 in $CDCl_3$



S13. NOESY spectrum of Compound 2 in $CDCl_3$

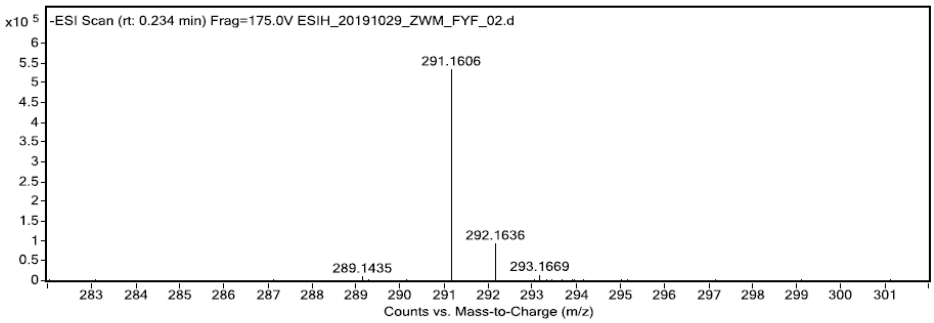


S14. HR-ESIMS of Compound 2

Data Filename	ESIH_20191029_ZWM_FYF_02.d	**Sample Name**	D7-MWD62-4-1
Sample Type	Sample	**Position**	P1-A2
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160324_MS_ESIH_NEG_1min.m
Acquired Time	10/29/2019 16:09:18	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by ZZY

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
175	0	ESI



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
291.1606	291.1602	-0.39	-1.34	C17 H23 O4	(M-H)-

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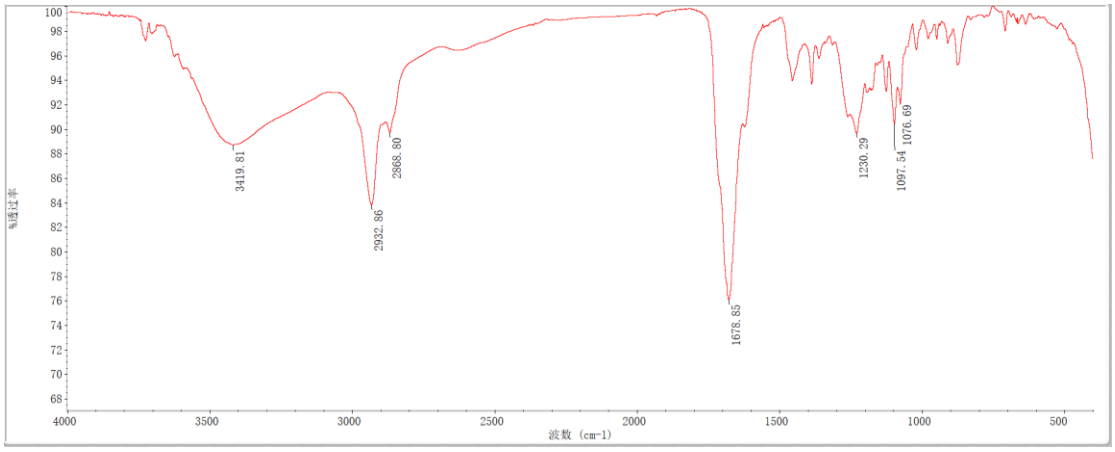
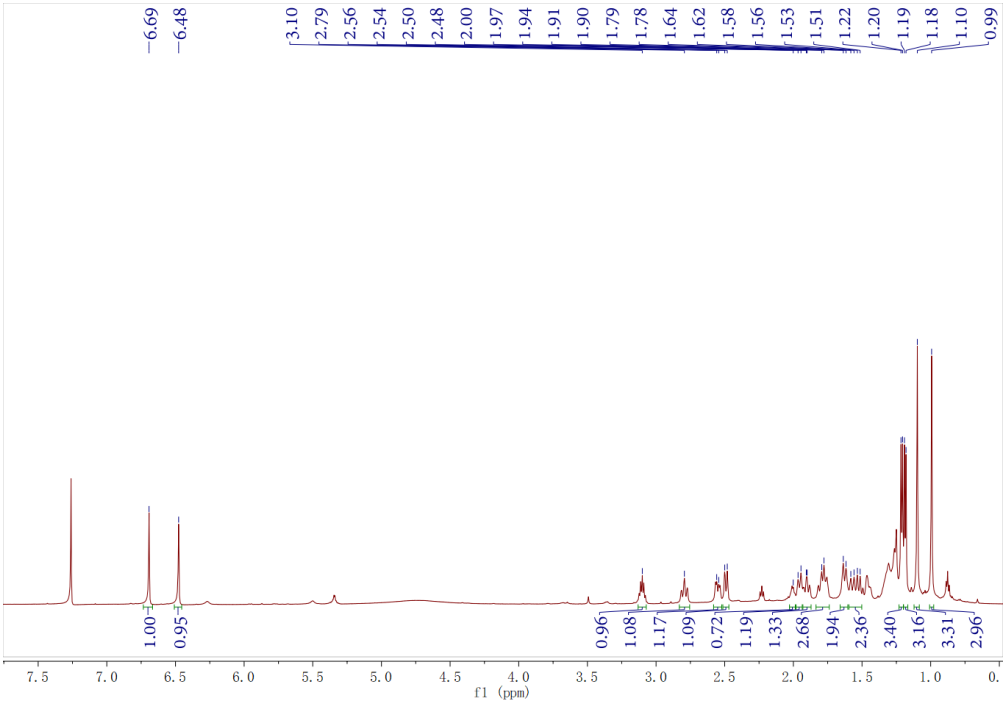
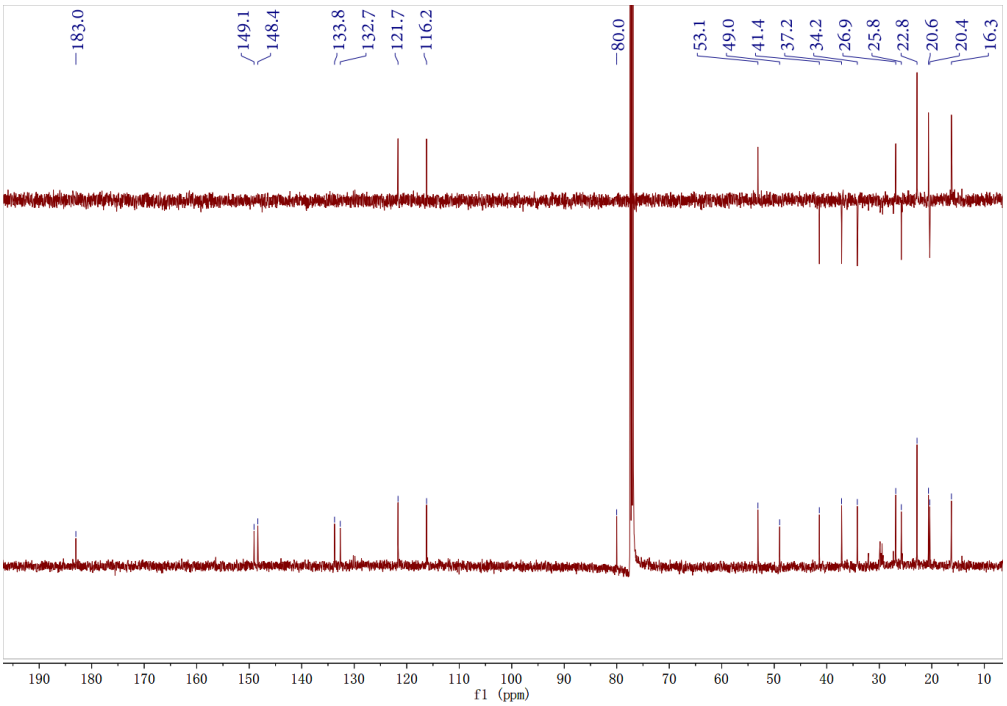
S15. IR spectrum of Compound 2



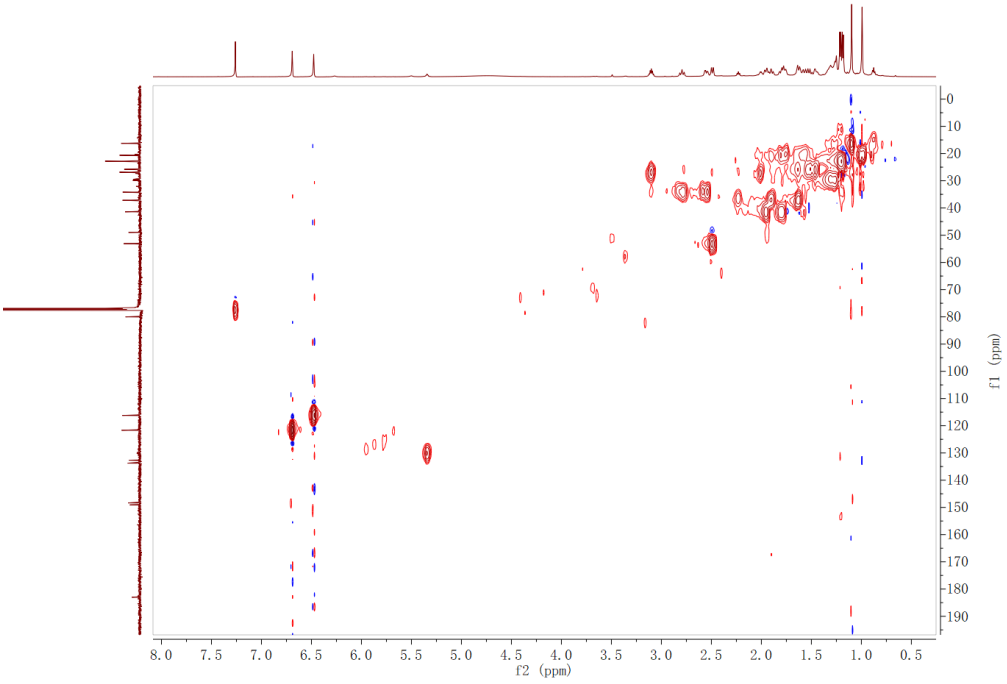
S16. ^{1}H NMR spectrum of Compound 3 in $CDCl_3$ (500 MHz)



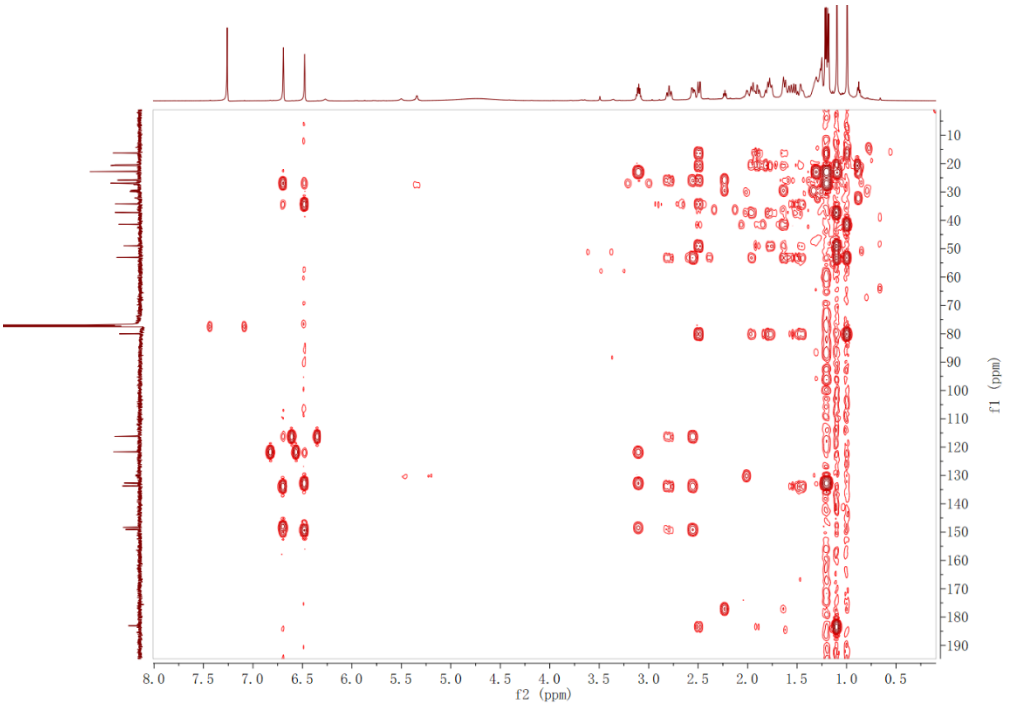
S17. ^{13}C NMR spectrum of Compound 3 in $CDCl_3$ (125 MHz)



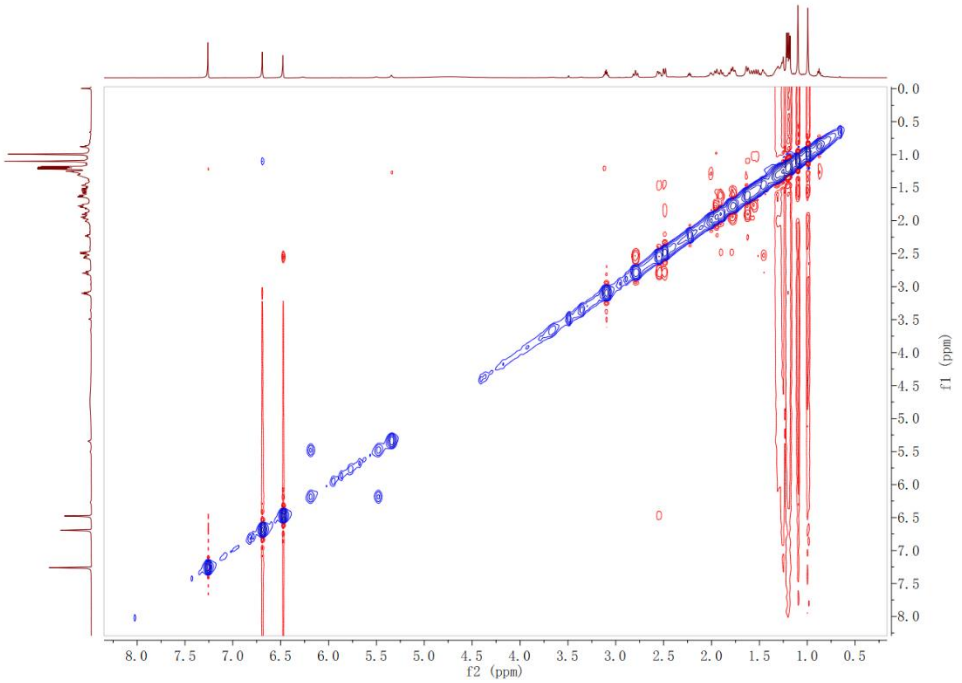
S18. HSQC spectrum of Compound 3 in $CDCl_3$



S19. HMBC spectrum of Compound 3 in $CDCl_3$



S20. NOESY spectrum of Compound 3 in $CDCl_3$



S21. HR-ESIMS of Compound 3

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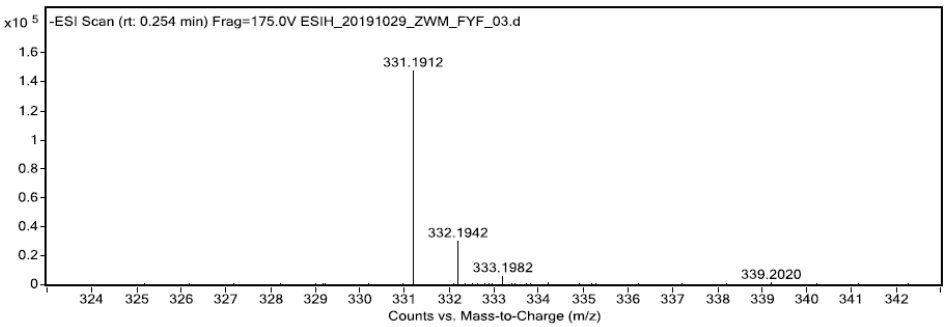
Sample Type	Sample	**Position**	P1-A3
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160324_MS_ESIH_NEG_1min.m
Acquired Time	10/29/2019 16:10:45	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by ZZY

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
175	0	ESI



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
331.1912	331.1915	0.31	0.94	C20 H27 O4	(M-H)-

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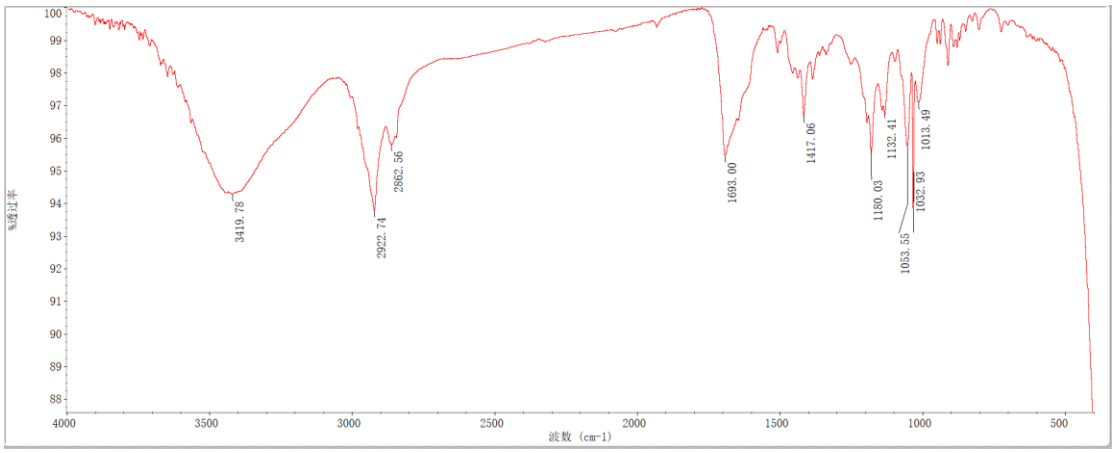
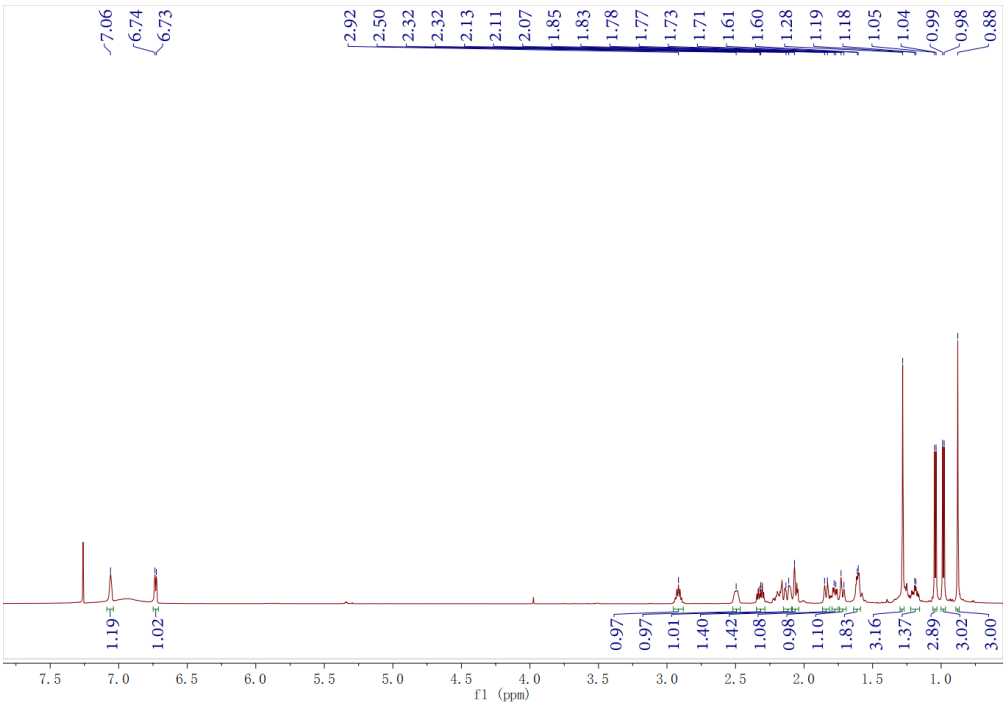
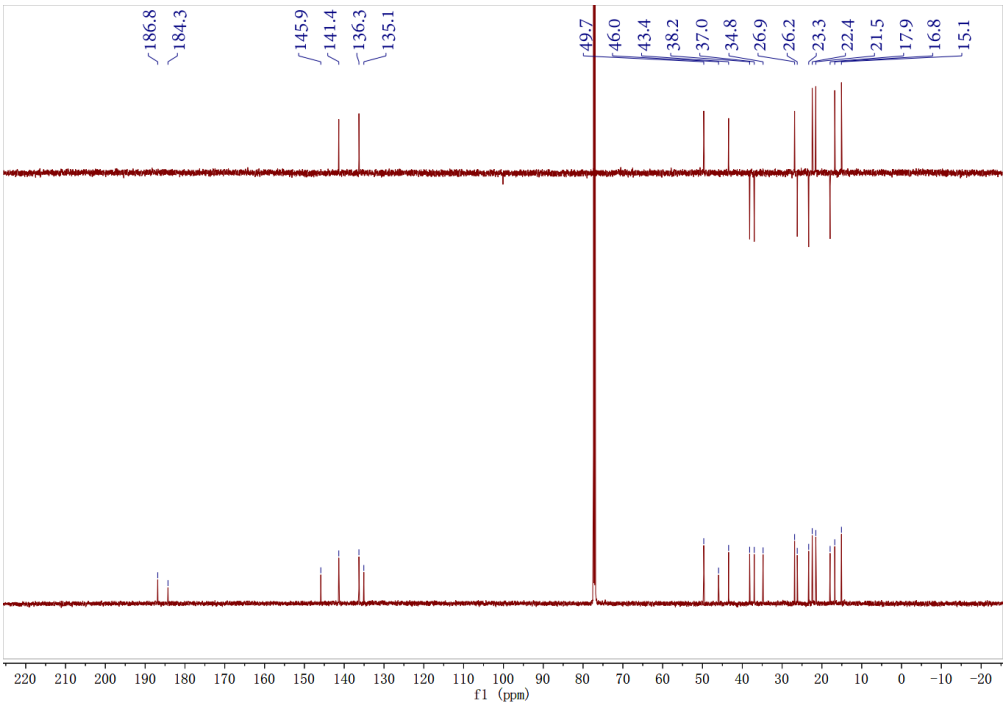
S22. IR spectrum of Compound 3



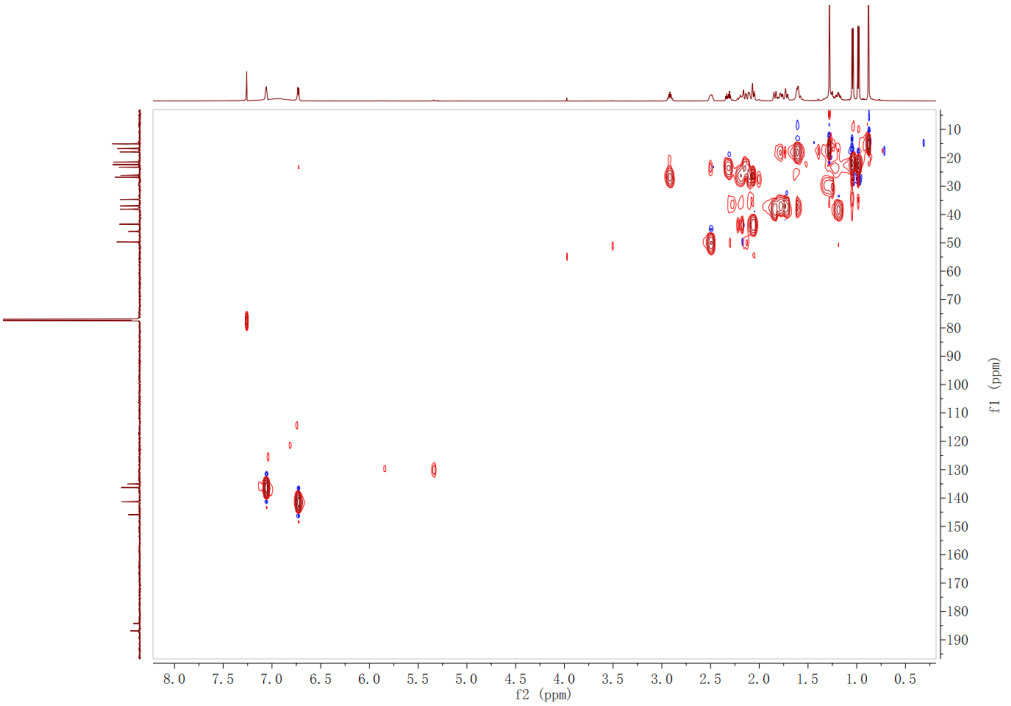
S23. ^{1}H NMR spectrum of Compound 4 in $CDCl_3$ (500 MHz)



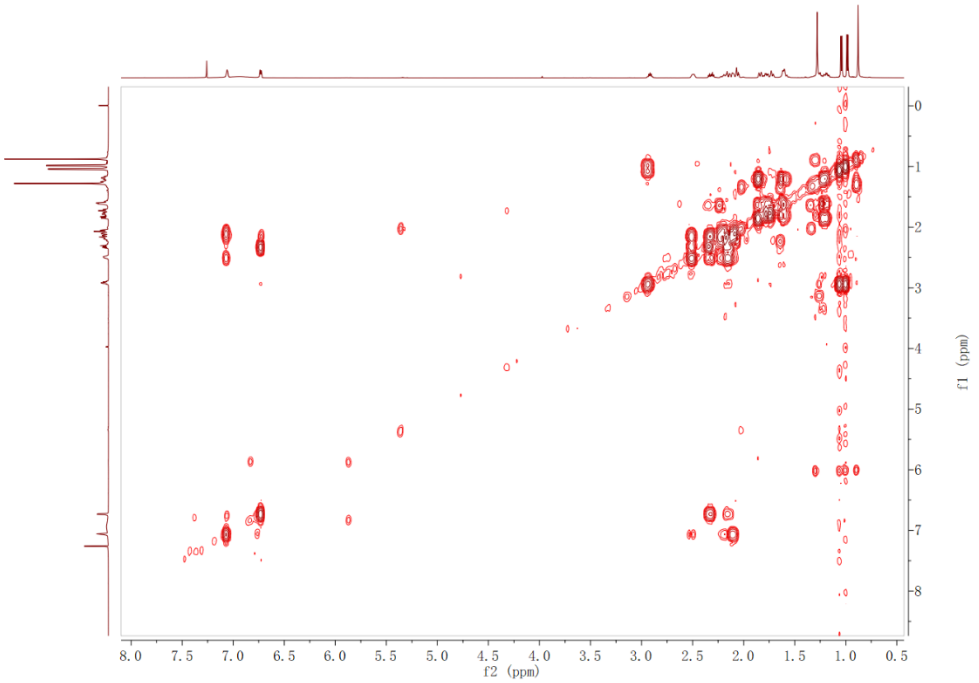
S24. ^{13}C NMR spectrum of Compound 4 in $CDCl_3$ (125 MHz)



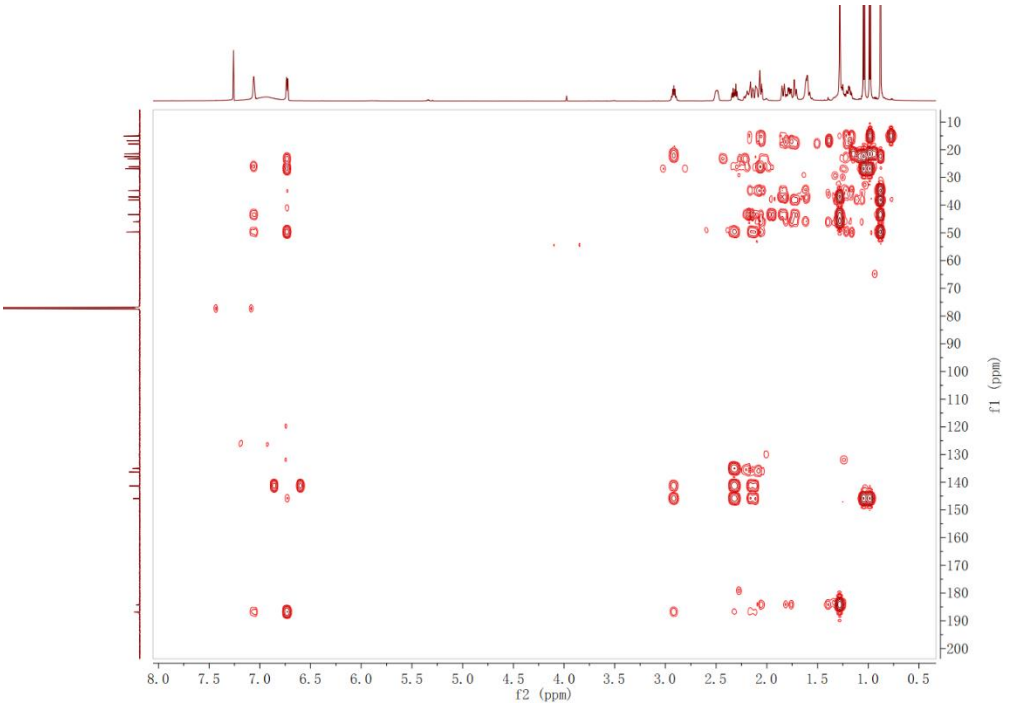
S25. HSQC spectrum of Compound 4 in $CDCl_3$



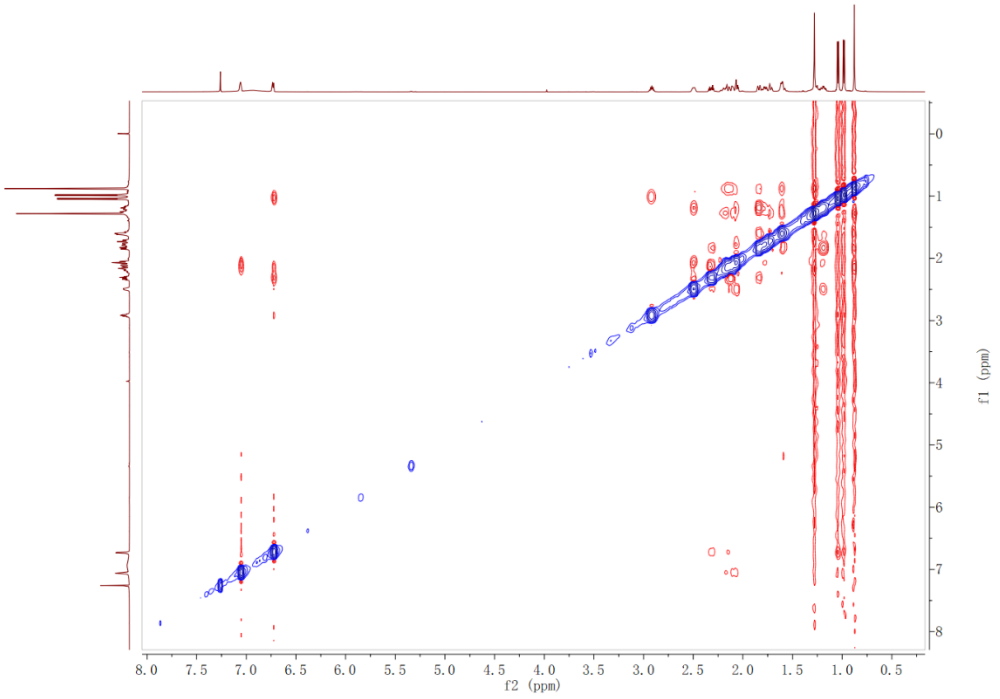
S26. COSY spectrum of Compound 4 in $CDCl_3$



S27. HMBC spectrum of Compound 4 in $CDCl_3$



S28. NOESY spectrum of Compound 4 in $CDCl_3$

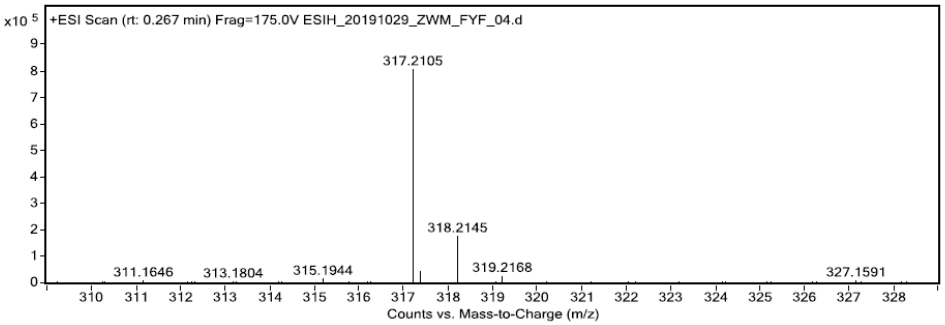


S29. HR-ESIMS of Compound 4

Data Filename	ESIH_20191029_ZWM_FYF_04.d	**Sample Name**	D7-MWD43-6-1-2
Sample Type	Sample	**Position**	P1-A4
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	10/29/2019 16:12:13	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by ZZY

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
175	0	ESI



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
317.2105	317.2111	0.6	1.89	C20 H29 O3	(M+H)+

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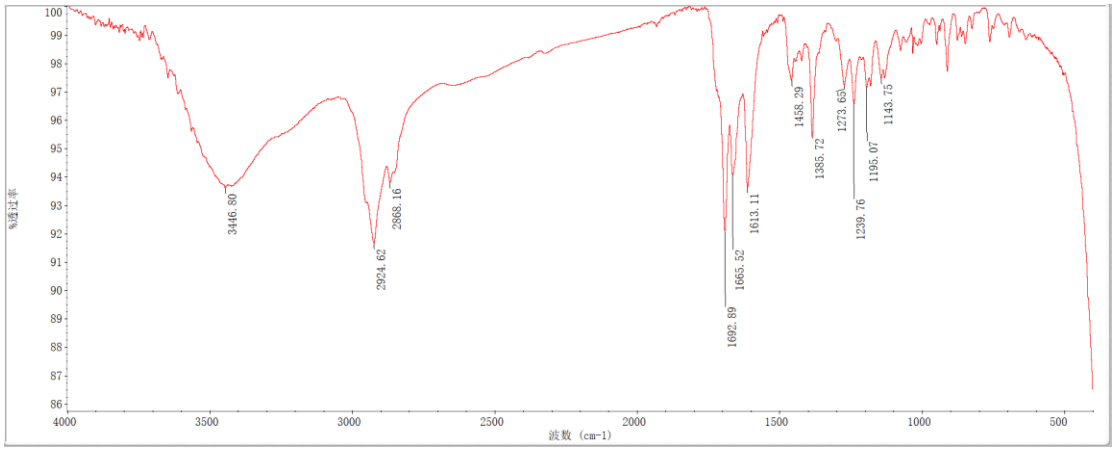
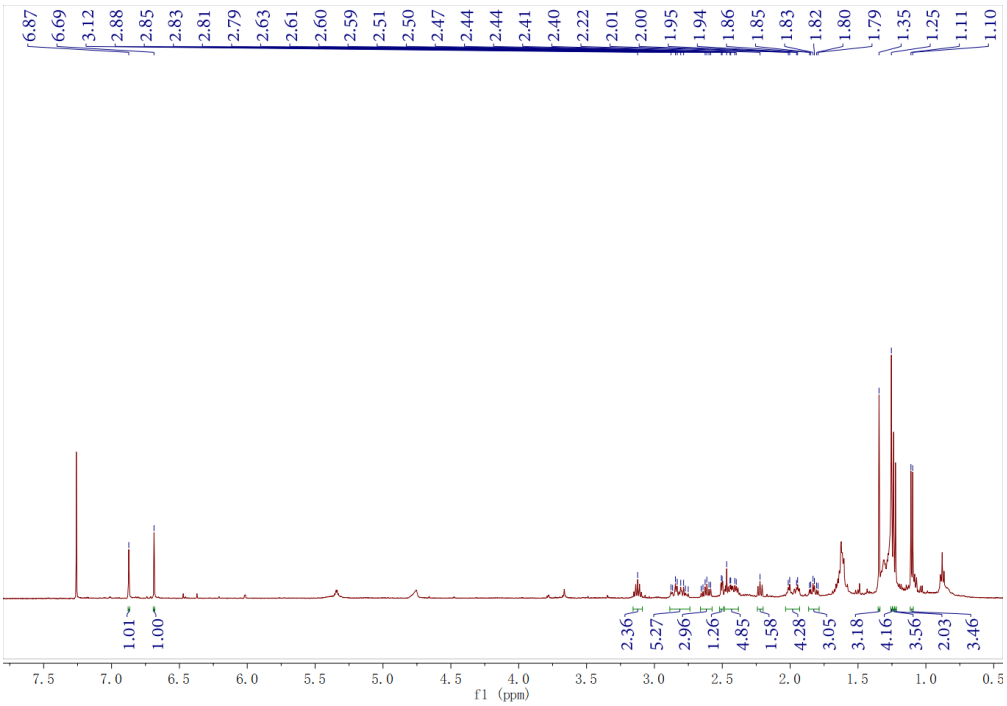
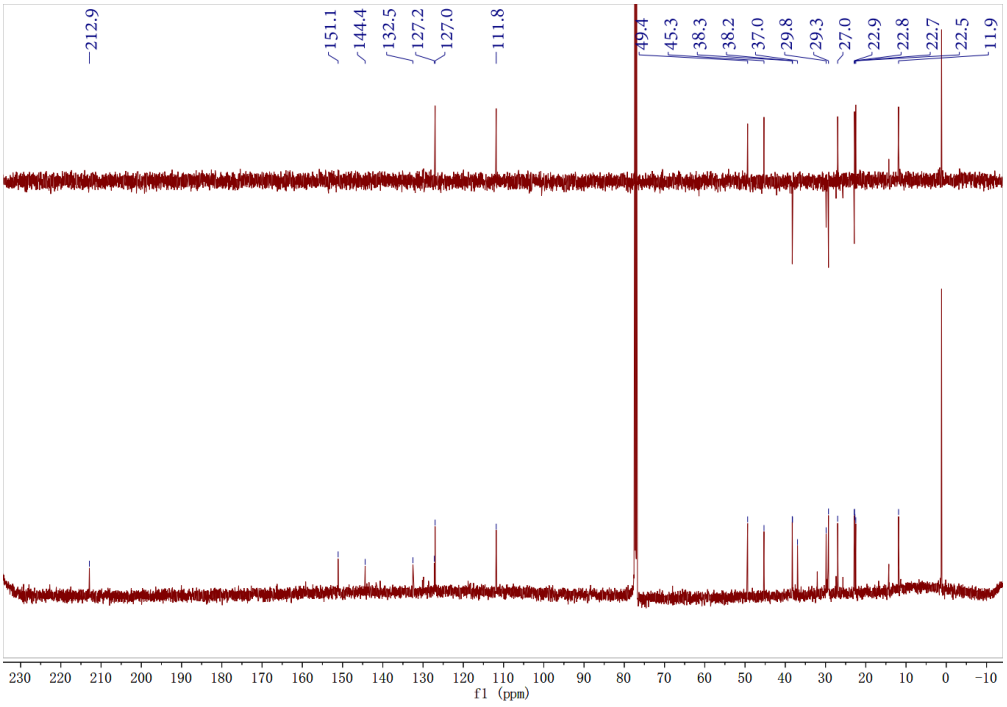
S30. IR spectrum of Compound 4



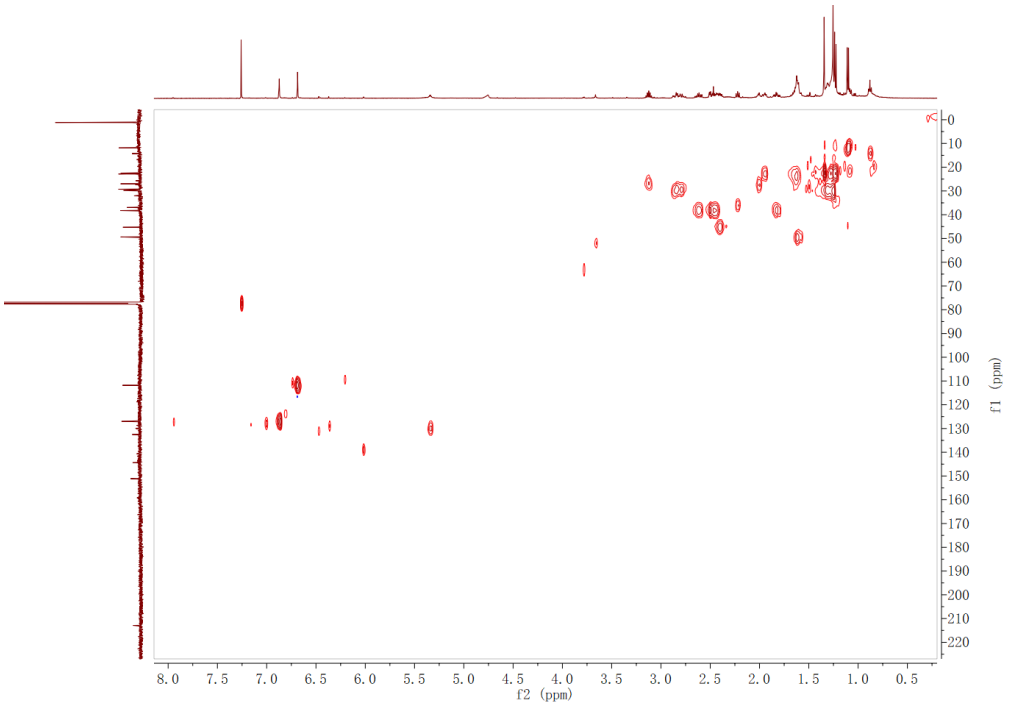
S31. ^{1}H NMR spectrum of Compound 5 in $CDCl_3$ (500 MHz)



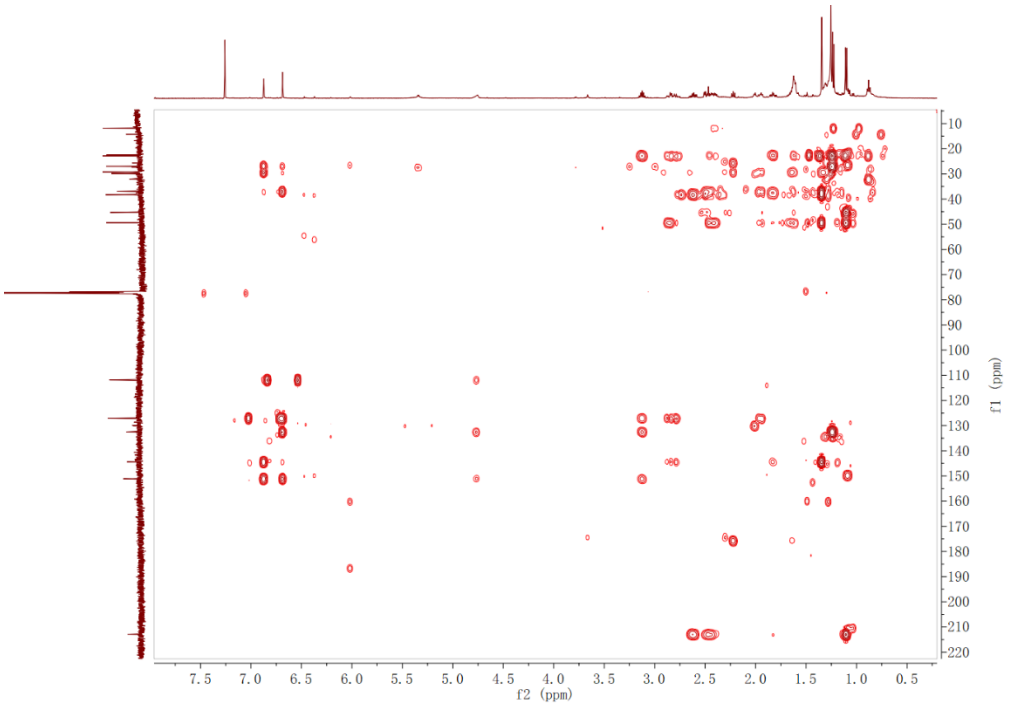
S32. ^{13}C NMR spectrum of Compound 5 in $CDCl_3$ (125 MHz)



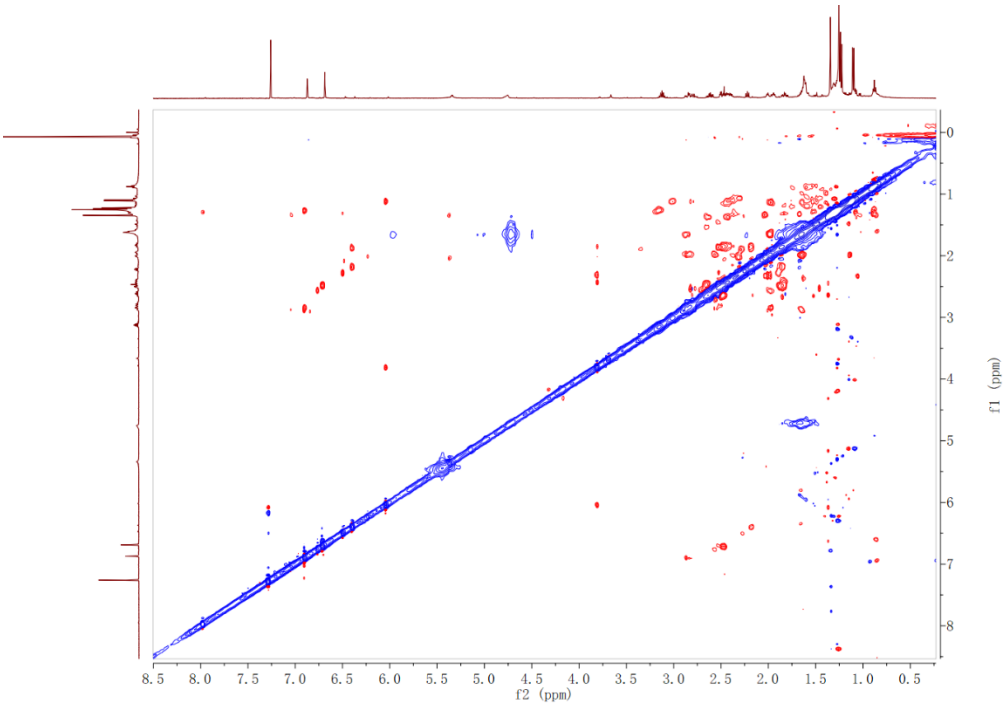
S33. HSQC spectrum of Compound 5 in $CDCl_3$



S34. HMBC spectrum of Compound 5 in $CDCl_3$



S35. NOESY spectrum of Compound 5 in $CDCl_3$

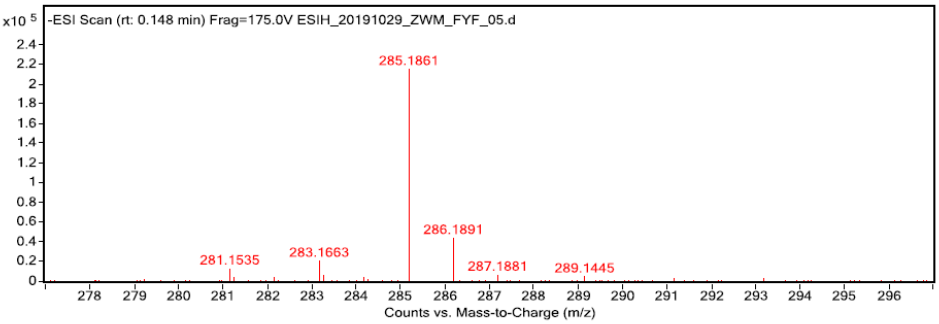


S36. HR-ESIMS of Compound 5

Data Filename	ESIH_20191029_ZWM_FYF_05.d	**Sample Name**	D7-MWD315-1-3
Sample Type	Sample	**Position**	P1-A5
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160324_MS_ESIH_NEG_1min.m
Acquired Time	10/29/2019 16:13:43	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by ZZY

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
175	0	ESI



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
285.1861	285.186	-0.09	-0.31	C19 H25 O2	(M-H)-

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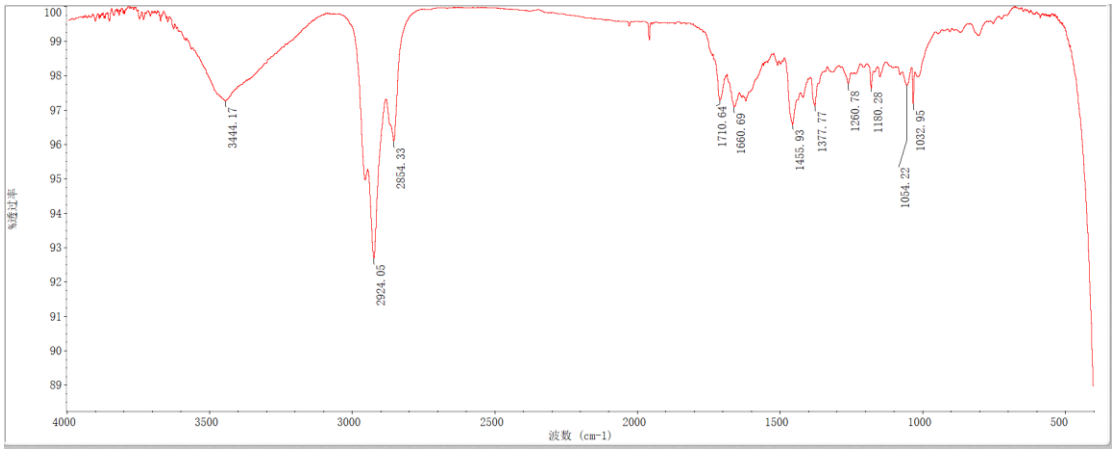
S37. IR spectrum of Compound 5



S38. Computational Section

ECD Calculation

Conformational searches were carried out using the torsional sampling (MCMM) method and OPLS_2005 force field. Conformers that adding up to more than 99% population in reverse order were re-optimized at the B3LYP/6-311G** level and London dispersion corrections[1] with Solvation Model based on Density (SMD) for methanol. Finally, the Boltzmann-averaged ECD spectra of the three compounds were obtained with SpecDis1.71.[1] Torsional sampling (MCMM) conformational searches using OPLS_2005 force field were carried out by means of the conformational search module in the Macromodel 11.0 software[2] applying an energy window of 21 kJ/mol, which afforded 9 conformers for (4R,5R,9S,10R,12R)-**1**, 9 conformers for (4S,5S,9R,10S,12S)-**1**, 16 conformers for (4R,5R,9S,10R,12S)-**2**, 16 conformers for (4S,5R,9S,10R,12S)-**2**, 22 conformers for (4R,5S,10S)-**3**, 22 conformers for (4S,5R,10R)-**3**, 7 conformers for (4R,5R,9R,10R)-**4**, 7 conformers for (4S,5S,9S,10S)-**4**. The Boltzmann populations of the conformers were obtained based on the potential energy provided by the OPLS_2005 force field, which afford 3 conformers for (4R,5R,9S,10R,12R)-**1**, 3 conformers for (4S,5S,9R,10S,12S)-**1**, 5 conformers for (4R,5R,9S,10R,12S)-**2**, 5 conformers for (4S,5R,9S,10R,12S)-**2**, 10 conformers for (4R,5S,10S)-**3**, 10 conformers for (4S,5R,10R)-**3**, 4 conformers for (4R,5R,9R,10R)-**4**, 5 conformers for (4S,5S,9S,10S)-**4**, for adding up to more than 99% population in reverse order for re-optimization. The re-optimization and the following TDDFT calculations of the re-optimized geometries were all performed with Gaussian 16[3] at the B3LYP/6-311G** level and London dispersion correction[4] with SMD solvent model for methanol. Frequency analysis was performed as well to confirm that the re-optimized geometries were at the energy minima. Finally, the SpecDis 1.71[1] software was used to obtain the Boltzmann-averaged ECD spectra of the twelve compounds and to visualize the results.

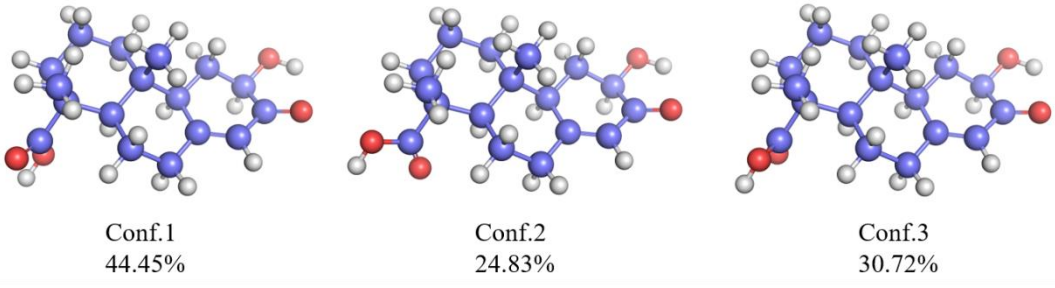
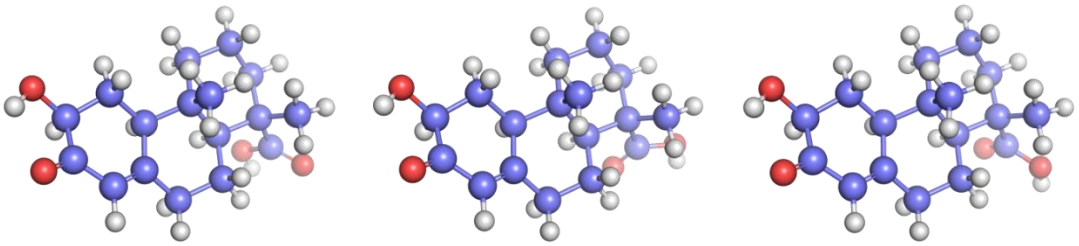


Figure S1. Re-optimized conformers above 1% population (OPLS_2005) of (4R,5R,9S,10R,12R)-**1** calculated at the B3LYP/6-311G** level and London dispersion corrections with SMD solvent model for Methanol.

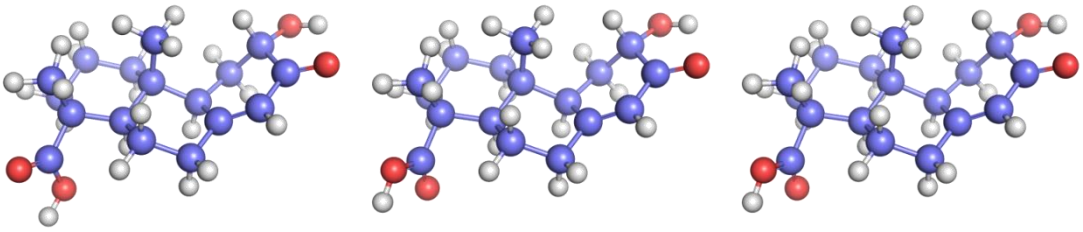


Conf.1
44.45%

Conf.2
24.83%

Conf.3
30.72%

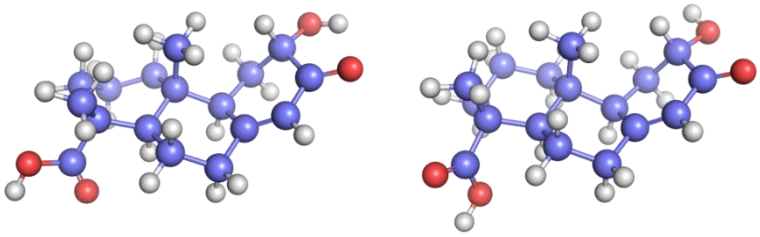
Figure S2. Re-optimized conformers above 1% population (OPLS_2005) of (4S,5S,9R,10S,12S)-**1** calculated at the B3LYP/6-311G** level and London dispersion corrections with SMD solvent model for Methanol.



Conf.1
42.90%

Conf.2
28.00%

Conf.3
28.00%



Conf.4
0.09%

Conf.5
1.01%

Figure S3. Re-optimized conformers above 1% population (OPLS_2005) of (4S,5R,9S,10R,12S)-**2** calculated at the B3LYP/6-311G** level and London dispersion corrections with SMD solvent model for Methanol.

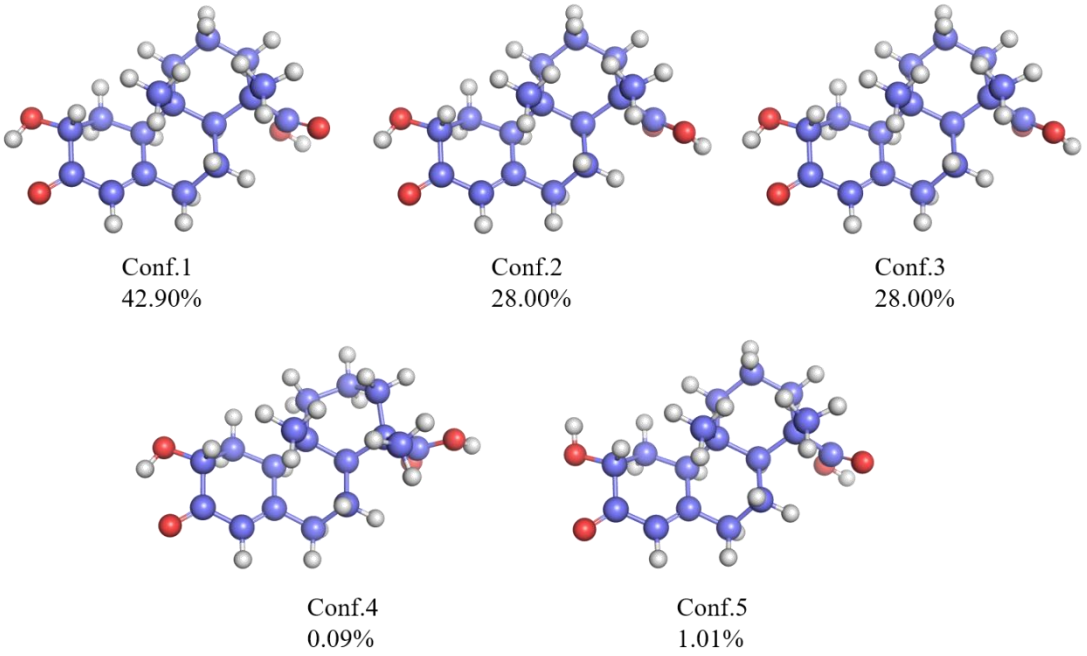


Figure S4. Re-optimized conformers above 1% population (OPLS_2005) of (4S,5R,9S,10R,12S)-**2** calculated at the B3LYP/6-311G** level and London dispersion corrections with SMD solvent model for Methanol.

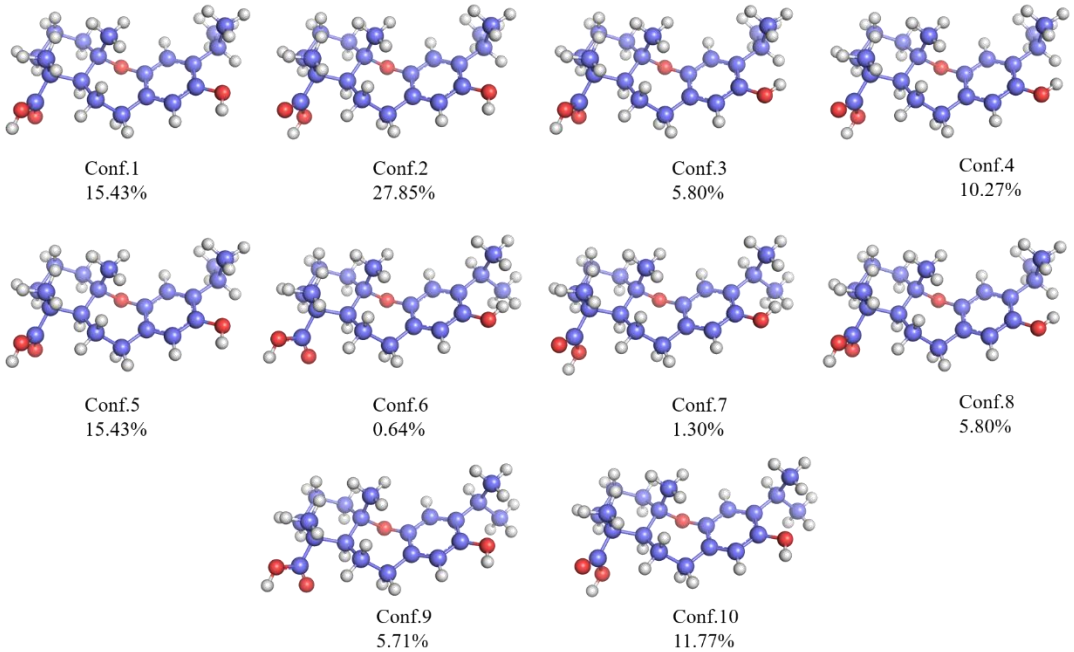


Figure S5. Re-optimized conformers above 1% population (OPLS_2005) of (4R,5S,10S)-**3** calculated at the B3LYP/6-311G** level and London dispersion corrections with SMD solvent model for Methanol.

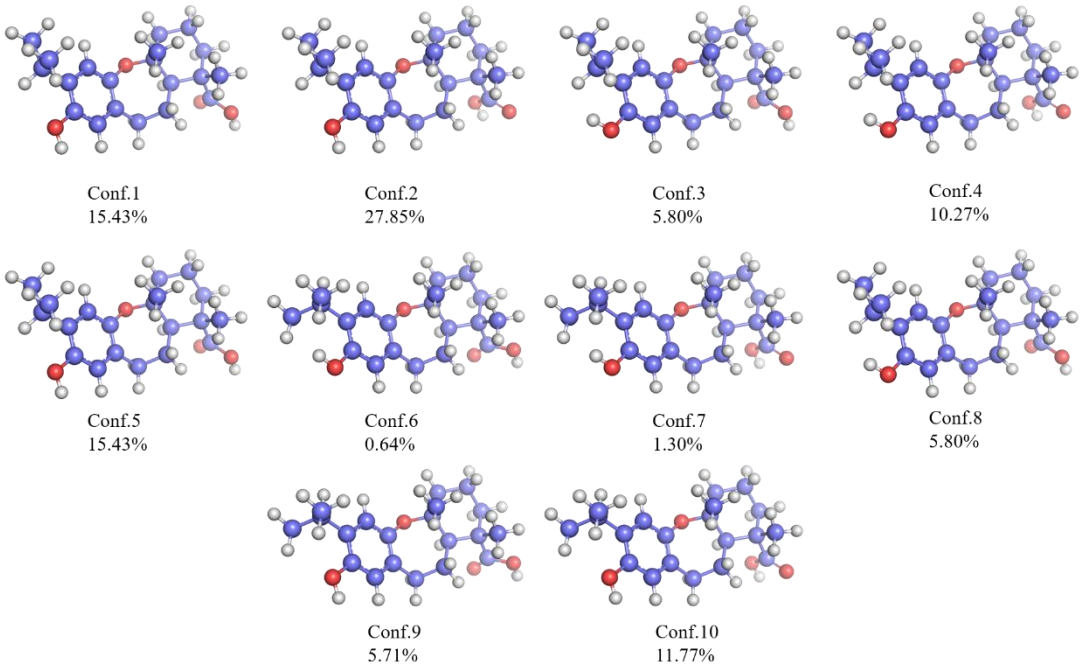


Figure S6. Re-optimized conformers above 1% population (OPLS_2005) of (4S,5R,10R)-**3** calculated at the B3LYP/6-311G** level and London dispersion corrections with SMD solvent model for Methanol.

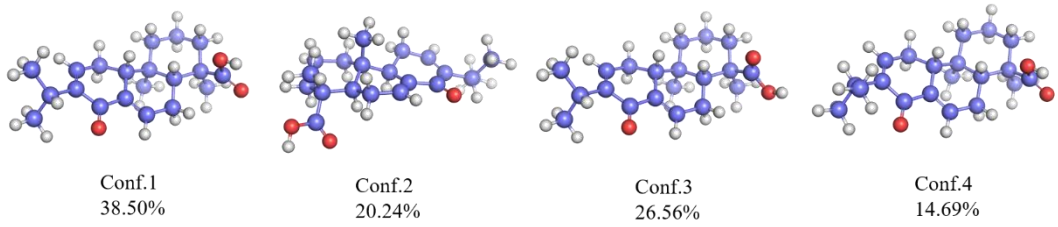


Figure S7. Re-optimized conformers above 1% population (OPLS_2005) of (4R,5R,9R,10R)-**4** calculated at the B3LYP/6-311G** level and London dispersion corrections with SMD solvent model for Methanol.

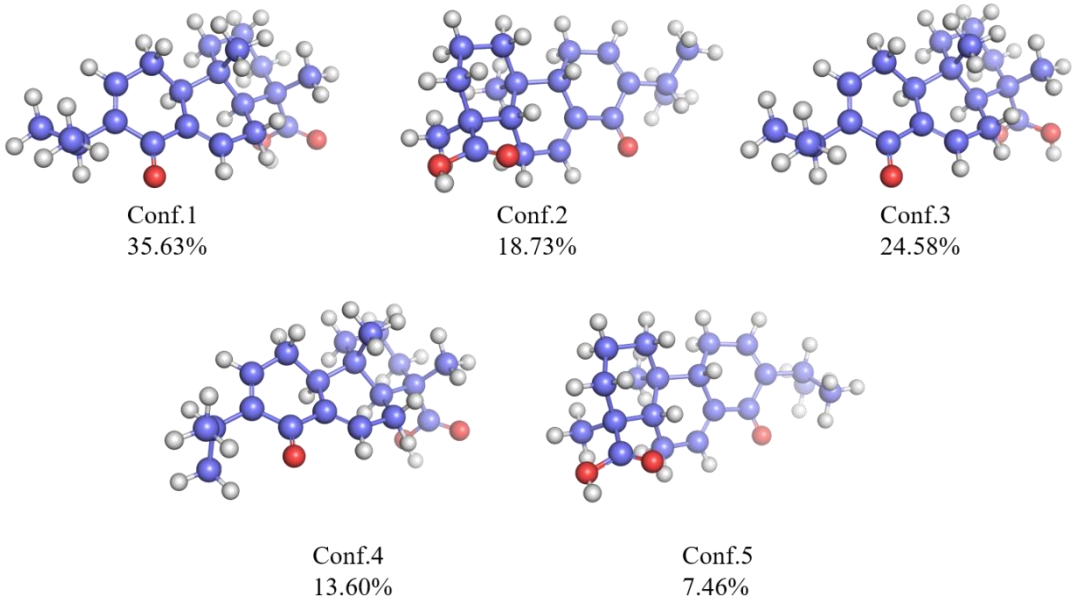


Figure S8. Re-optimized conformers above 1% population (OPLS_2005) of (4S,5S,9S,10S)-**4** calculated at the B3LYP/6-311G** level and London dispersion corrections with SMD solvent model for Methanol.

Table S1. Cartesian coordinates for the re-optimized conformers of (4R,5R,9S,10R,12R)-**1** at the B3LYP/6-311G** level and London dispersion corrections with SMD solvent model for Methanol.

(4R,5R,9S,10R,12R)-1 Conformer 1		Standard Orientation (Ångstroms)		
I	Atom	X	Y	Z
1	C	-1.85393	2.582278	0.059657
2	C	-2.92185	1.594013	-0.40569
3	C	-2.71121	0.18112	0.199834
4	C	-1.24399	-0.29334	-0.08331
5	C	-0.10712	0.714851	0.266799
6	C	-0.45605	2.096622	-0.32424
7	C	-0.9485	-1.67811	0.497097
8	C	0.373232	-2.22083	-0.0547
9	C	1.507679	-1.23694	-0.03348
10	C	1.18861	0.182069	-0.45084
11	C	2.759652	-1.64386	0.269411
12	C	3.917153	-0.79235	0.073883
13	C	3.688255	0.462504	-0.74677
14	C	2.392138	1.126549	-0.30779
15	H	-1.19554	-0.38926	-1.17257
16	C	0.161355	0.83718	1.777493

17	O	5.047927	-1.06054	0.481206
18	O	4.78114	1.357488	-0.61005
19	C	-3.12966	0.170914	1.676983
20	C	-3.63886	-0.785	-0.54057
21	O	-4.52248	-1.44364	-0.03053
22	O	-3.3969	-0.84838	-1.86336
23	H	0.93342	0.125409	-1.51893
24	H	-2.04058	3.554771	-0.40645
25	H	-1.9194	2.74112	1.14003
26	H	-3.92307	1.948408	-0.14129
27	H	-2.88051	1.525268	-1.49591
28	H	0.289272	2.830536	-0.00775
29	H	-0.39706	2.033206	-1.41799
30	H	-0.90774	-1.63837	1.587272
31	H	-1.74721	-2.38067	0.241642
32	H	0.667556	-3.14316	0.450724
33	H	0.218269	-2.47504	-1.11313
34	H	2.948571	-2.6546	0.61804
35	H	3.599685	0.134233	-1.79459
36	H	2.238615	2.027996	-0.9023
37	H	2.524935	1.435451	0.731557
38	H	-0.72322	1.151008	2.326065
39	H	0.504502	-0.10341	2.212985
40	H	0.932925	1.585038	1.968637
41	H	5.512815	0.822824	-0.26063
42	H	-2.92078	-0.78614	2.156735
43	H	-4.20331	0.353093	1.754351
44	H	-2.62406	0.951196	2.239849
45	H	-4.02707	-1.47441	-2.25717

B3LYP/6-311G** Energy = -963.5630621 a.u.; Population = 44.45%

(4R,5R,9S,10R,12R)-1 Conformer 2		Standard Orientation (Ångstroms)		
I	Atom	X	Y	Z
1	C	-1.854532	2.545808	0.03641
2	C	-2.910581	1.547996	-0.431512
3	C	-2.686987	0.130333	0.171161
4	C	-1.218077	-0.323433	-0.079187
5	C	-0.091312	0.703302	0.255184
6	C	-0.453397	2.074333	-0.350662
7	C	-0.907229	-1.688528	0.540403
8	C	0.420685	-2.230853	0.002938
9	C	1.544363	-1.234272	-0.006079

10	C	1.20825	0.171202	-0.455347
11	C	2.802079	-1.619817	0.301799
12	C	3.949294	-0.760879	0.081422
13	C	3.703813	0.472622	-0.766522
14	C	2.401606	1.132087	-0.338898
15	H	-1.159928	-0.450147	-1.164836
16	C	0.181221	0.854376	1.763321
17	O	5.08472	-1.007319	0.489921
18	O	4.787459	1.38216	-0.653067
19	C	-3.132314	0.099368	1.643819
20	C	-3.594888	-0.779122	-0.661566
21	O	-3.256951	-1.407209	-1.64552
22	O	-4.873845	-0.774916	-0.246438
23	H	0.94969	0.087484	-1.520776
24	H	-2.053591	3.518103	-0.424919
25	H	-1.923387	2.696095	1.117911
26	H	-3.916795	1.889529	-0.174547
27	H	-2.86141	1.477104	-1.524162
28	H	0.285503	2.819113	-0.044719
29	H	-0.399401	2.001058	-1.444076
30	H	-0.866371	-1.617732	1.62915
31	H	-1.697534	-2.404204	0.30133
32	H	0.727041	-3.135591	0.532686
33	H	0.266619	-2.51605	-1.047784
34	H	3.003505	-2.619553	0.674455
35	H	3.616316	0.119919	-1.806443
36	H	2.235718	2.017226	-0.95433
37	H	2.53436	1.467535	0.692272
38	H	-0.703355	1.173546	2.309374
39	H	0.531699	-0.075043	2.216224
40	H	0.94859	1.610633	1.938054
41	H	5.524719	0.863793	-0.290958
42	H	-3.022345	-0.896281	2.077893
43	H	-4.179886	0.388663	1.728263
44	H	-2.551676	0.794798	2.244729
45	H	-5.391116	-1.318866	-0.864048

B3LYP/6-311G** Energy = -963.5625129 a.u.; Population = 24.83%

(4R,5R,9S,10R,12R)-1 Conformer 3		Standard Orientation (Ångstroms)		
I	Atom	X	Y	Z
1	C	-1.826958	2.60413	0.088111
2	C	-2.897921	1.634605	-0.40552

3	C	-2.709497	0.206983	0.166313
4	C	-1.239639	-0.272561	-0.109069
5	C	-0.097792	0.720038	0.266201
6	C	-0.431446	2.115717	-0.299274
7	C	-0.957467	-1.669045	0.450237
8	C	0.363792	-2.212186	-0.10222
9	C	1.50515	-1.237367	-0.059174
10	C	1.198425	0.190991	-0.45286
11	C	2.752733	-1.65902	0.241749
12	C	3.917194	-0.812911	0.06629
13	C	3.70057	0.459066	-0.730845
14	C	2.407555	1.123885	-0.284015
15	H	-1.190693	-0.349365	-1.201188
16	C	0.160517	0.810281	1.781178
17	O	5.044561	-1.097368	0.472173
18	O	4.799619	1.343043	-0.573412
19	C	-3.149339	0.163424	1.637187
20	C	-3.580172	-0.723029	-0.684206
21	O	-3.536374	-0.773651	-1.898125
22	O	-4.407867	-1.513476	0.017555
23	H	0.949868	0.155756	-1.523403
24	H	-2.003562	3.588211	-0.357081
25	H	-1.896958	2.739802	1.17153
26	H	-3.89896	1.992713	-0.144712
27	H	-2.846765	1.582361	-1.496422
28	H	0.318797	2.836561	0.035004
29	H	-0.368281	2.073203	-1.393777
30	H	-0.92319	-1.646498	1.541186
31	H	-1.758348	-2.362326	0.178824
32	H	0.648451	-3.144417	0.390486
33	H	0.213106	-2.448872	-1.165286
34	H	2.932502	-2.677183	0.573113
35	H	3.612985	0.151607	-1.785068
36	H	2.26366	2.038436	-0.860563
37	H	2.536518	1.409903	0.76242
38	H	-0.729917	1.104604	2.331505
39	H	0.508025	-0.137495	2.197182
40	H	0.925753	1.55906	1.993423
41	H	5.526888	0.795635	-0.234637
42	H	-2.946755	-0.800399	2.104755
43	H	-4.222594	0.351457	1.708814
44	H	-2.647036	0.933118	2.218544
45	H	-4.897238	-2.07225	-0.610678

B3LYP/6-311G** Energy = -963.5627135 a.u.; Population = 30.72%

Table S2. Cartesian coordinates for the re-optimized conformers of (4S,5S,9R,10S,12S)-**1** at the B3LYP/6-311G** level and London dispersion corrections with SMD solvent model for Methanol.

(4S,5S,9R,10S,12S)-1		Standard Orientation		
Conformer 1		(Ångstroms)		
I	Atom	X	Y	Z
1	C	1.853929	2.582278	0.05966
2	C	2.921855	1.594016	-0.405686
3	C	2.711213	0.181122	0.199839
4	C	1.243987	-0.293341	-0.083306
5	C	0.107117	0.71485	0.266796
6	C	0.456049	2.096621	-0.324247
7	C	0.948494	-1.678114	0.497094
8	C	-0.37323	-2.220827	-0.054714
9	C	-1.507678	-1.23694	-0.033485
10	C	-1.18861	0.182069	-0.450844
11	C	-2.75965	-1.643863	0.269405
12	C	-3.917151	-0.792353	0.073886
13	C	-3.688256	0.462502	-0.746772
14	C	-2.392138	1.126548	-0.307794
15	H	1.195541	-0.389256	-1.172572
16	C	-0.161365	0.83718	1.777489
17	O	-5.047923	-1.060536	0.481218
18	O	-4.781142	1.357486	-0.610043
19	C	3.129662	0.170914	1.676988
20	C	3.638858	-0.784996	-0.540564
21	O	4.522471	-1.443649	-0.030522
22	O	3.396909	-0.848365	-1.863358
23	H	-0.933419	0.125411	-1.51894
24	H	1.919389	2.741119	1.140034
25	H	2.040575	3.554772	-0.406445
26	H	3.923067	1.94841	-0.141276
27	H	2.880514	1.525272	-1.495903
28	H	0.397069	2.033205	-1.417991
29	H	-0.289274	2.830535	-0.007754
30	H	1.747208	-2.380666	0.241642
31	H	0.907734	-1.638372	1.587269
32	H	-0.218262	-2.475033	-1.113141
33	H	-0.667555	-3.143163	0.450706
34	H	-2.948568	-2.654599	0.618032
35	H	-3.59969	0.13423	-1.794591

36	H	-2.524931	1.43545	0.731553
37	H	-2.238617	2.027995	-0.902308
38	H	0.723208	1.150992	2.326068
39	H	-0.932926	1.585047	1.968629
40	H	-0.504527	-0.103409	2.212976
41	H	-5.51281	0.822826	-0.260605
42	H	2.920774	-0.786134	2.156743
43	H	4.203318	0.353083	1.754353
44	H	2.624071	0.951203	2.239852
45	H	4.027074	-1.474394	-2.25717

B3LYP/6-311G** Energy = -963.5630621 a.u.; Population = 44.45%

(4S,5S,9R,10S,12S)-1		Standard Orientation		
Conformer 2		(Ångstroms)		
I	Atom	X	Y	Z
1	C	1.854532	2.545809	0.03641
2	C	2.910582	1.547997	-0.431513
3	C	2.686987	0.130333	0.17116
4	C	1.218078	-0.323433	-0.079188
5	C	0.091312	0.703303	0.255184
6	C	0.453398	2.074333	-0.350662
7	C	0.90723	-1.688527	0.540402
8	C	-0.420685	-2.230853	0.002939
9	C	-1.544363	-1.234272	-0.006078
10	C	-1.20825	0.171203	-0.455346
11	C	-2.802079	-1.619818	0.301798
12	C	-3.949295	-0.76088	0.08142
13	C	-3.703814	0.472622	-0.766521
14	C	-2.401607	1.132087	-0.338895
15	H	1.159929	-0.450146	-1.164837
16	C	-0.181218	0.854375	1.763322
17	O	-5.084721	-1.007322	0.489919
18	O	-4.78746	1.38216	-0.653065
19	C	3.132313	0.099369	1.643819
20	C	3.594888	-0.779121	-0.661568
21	O	3.256952	-1.407194	-1.645531
22	O	4.873842	-0.774932	-0.24643
23	H	-0.949692	0.087485	-1.520775
24	H	1.923387	2.696096	1.117912
25	H	2.053591	3.518105	-0.424918
26	H	3.916796	1.88953	-0.174549
27	H	2.861408	1.477105	-1.524162
28	H	0.399401	2.00106	-1.444075

29	H	-0.285503	2.819114	-0.044718
30	H	1.697535	-2.404203	0.301328
31	H	0.866373	-1.617731	1.629149
32	H	-0.266619	-2.51605	-1.047783
33	H	-0.72704	-3.13559	0.532687
34	H	-3.003505	-2.619554	0.674454
35	H	-3.616315	0.119921	-1.806442
36	H	-2.534361	1.467533	0.692275
37	H	-2.235719	2.017227	-0.954325
38	H	0.703359	1.173547	2.309373
39	H	-0.948588	1.61063	1.938057
40	H	-0.531693	-0.075045	2.216225
41	H	-5.524721	0.863792	-0.29096
42	H	3.022347	-0.896281	2.077893
43	H	4.179884	0.388668	1.728265
44	H	2.551672	0.794796	2.24473
45	H	5.391113	-1.318879	-0.864043

B3LYP/6-311G** Energy = -963.5625129 a.u.; Population = 43.43%

(4S,5S,9R,10S,12S)-1		Standard Orientation		
Conformer 3		(Ångstroms)		
I	Atom	X	Y	Z
1	C	1.827	2.6041	0.0881
2	C	2.8979	1.6346	-0.4055
3	C	2.7095	0.207	0.1663
4	C	1.2396	-0.2726	-0.1091
5	C	0.0978	0.72	0.2662
6	C	0.4314	2.1157	-0.2993
7	C	0.9575	-1.669	0.4502
8	C	-0.3638	-2.2122	-0.1022
9	C	-1.5051	-1.2374	-0.0592
10	C	-1.1984	0.191	-0.4529
11	C	-2.7527	-1.659	0.2417
12	C	-3.9172	-0.8129	0.0663
13	C	-3.7006	0.4591	-0.7309
14	C	-2.4076	1.1239	-0.284
15	H	1.1907	-0.3494	-1.2012
16	C	-0.1605	0.8103	1.7812
17	O	-5.0446	-1.0974	0.4722
18	O	-4.7996	1.343	-0.5734
19	C	3.1493	0.1634	1.6372
20	C	3.5802	-0.723	-0.6842
21	O	3.5364	-0.7737	-1.8981

22	O	4.4079	-1.5135	0.0176
23	H	-0.9499	0.1558	-1.5234
24	H	1.897	2.7398	1.1715
25	H	2.0036	3.5882	-0.3571
26	H	3.899	1.9927	-0.1447
27	H	2.8468	1.5824	-1.4964
28	H	0.3683	2.0732	-1.3938
29	H	-0.3188	2.8366	0.035
30	H	1.7584	-2.3623	0.1788
31	H	0.9232	-1.6465	1.5412
32	H	-0.2131	-2.4489	-1.1653
33	H	-0.6484	-3.1444	0.3905
34	H	-2.9325	-2.6772	0.5731
35	H	-3.613	0.1516	-1.7851
36	H	-2.5365	1.4099	0.7624
37	H	-2.2637	2.0384	-0.8606
38	H	0.7299	1.1046	2.3315
39	H	-0.9258	1.5591	1.9934
40	H	-0.508	-0.1375	2.1972
41	H	-5.5269	0.7956	-0.2346
42	H	2.9468	-0.8004	2.1048
43	H	4.2226	0.3515	1.7088
44	H	2.647	0.9331	2.2185
45	H	4.8972	-2.0722	-0.6107

B3LYP/6-311G** Energy = -963.5627135 a.u.; Population = 24.83%

Table S3. Cartesian coordinates for the re-optimized conformers of (4R,5R,9S,10R,12S)-**2** at the B3LYP/6-311G** level and London dispersion corrections with SMD solvent model for Methanol.

(4R,5R,9S,10R,12S)-2		Standard Orientation		
Conformer 1		(Ångstroms)		
I	Atom	X	Y	Z
1	C	-1.760165	2.592886	-0.069029
2	C	-2.901503	1.611961	-0.330237
3	C	-2.635862	0.223047	0.309609
4	C	-1.229372	-0.292063	-0.147064
5	C	-0.034068	0.698627	0.035743
6	C	-0.429314	2.050752	-0.594427
7	C	-0.905779	-1.690334	0.388174
8	C	0.310109	-2.27843	-0.347143
9	C	1.461841	-1.322365	-0.306524
10	C	1.156326	0.074066	-0.793123
11	C	2.674062	-1.70669	0.144946

12	C	3.798406	-0.79558	0.231528
13	C	3.494538	0.685437	0.110787
14	C	2.426574	0.935039	-0.947127
15	H	-1.323029	-0.392085	-1.232636
16	C	0.406357	0.909483	1.492632
17	O	4.95735	-1.161737	0.431344
18	O	4.67485	1.409647	-0.212941
19	C	-2.851258	0.282721	1.82812
20	C	-3.674497	-0.74657	-0.259137
21	O	-4.524359	-1.325995	0.386102
22	O	-3.580498	-0.908549	-1.592301
23	H	0.742927	-0.051222	-1.800588
24	H	-1.985432	3.541056	-0.567085
25	H	-1.684244	2.817636	0.99871
26	H	-3.84818	2.005878	0.052521
27	H	-3.015187	1.489492	-1.410654
28	H	0.357176	2.787793	-0.416022
29	H	-0.506078	1.921176	-1.681094
30	H	-0.704589	-1.659342	1.461588
31	H	-1.75649	-2.363367	0.247029
32	H	0.596484	-3.243144	0.076326
33	H	0.032267	-2.441039	-1.396249
34	H	2.85661	-2.735763	0.438975
35	H	3.138374	0.993303	1.102462
36	H	2.885279	0.697479	-1.912132
37	H	2.184617	1.997513	-0.966233
38	H	1.22432	1.631536	1.528423
39	H	-0.391205	1.310061	2.113145
40	H	0.755881	-0.013733	1.958374
41	H	5.411659	0.834596	0.050148
42	H	-2.572833	-0.652036	2.317206
43	H	-3.905057	0.469217	2.042442
44	H	-2.277467	1.087234	2.280798
45	H	-4.272927	-1.531076	-1.869457

B3LYP/6-311G** Energy = -963.5617364 a.u.; Population = 42.90%

(4R,5R,9S,10R,12S)-2		Standard Orientation		
Conformer 2		(Ångstroms)		
I	Atom	X	Y	Z
1	C	-1.729278	2.616986	-0.023315
2	C	-2.876957	1.654916	-0.319468
3	C	-2.636701	0.2447	0.276314
4	C	-1.226894	-0.270863	-0.181395

5	C	-0.024681	0.70444	0.034639
6	C	-0.402257	2.077194	-0.559326
7	C	-0.916142	-1.684564	0.321199
8	C	0.30115	-2.2632	-0.419487
9	C	1.459248	-1.317191	-0.347323
10	C	1.166575	0.092379	-0.802152
11	C	2.664982	-1.720007	0.105321
12	C	3.793734	-0.818059	0.224606
13	C	3.499891	0.667352	0.13546
14	C	2.443914	0.947512	-0.926754
15	H	-1.322268	-0.34236	-1.27065
16	C	0.403877	0.870071	1.501146
17	O	4.948403	-1.195745	0.427574
18	O	4.687867	1.391354	-0.159308
19	C	-2.869757	0.256715	1.794163
20	C	-3.63123	-0.694083	-0.414314
21	O	-3.754267	-0.787649	-1.620163
22	O	-4.368714	-1.440695	0.422506
23	H	0.758783	-0.005295	-1.814938
24	H	-1.943306	3.581673	-0.493841
25	H	-1.655181	2.809874	1.050981
26	H	-3.823457	2.047995	0.065317
27	H	-2.983054	1.559211	-1.40337
28	H	0.391456	2.80022	-0.357301
29	H	-0.476316	1.978707	-1.649415
30	H	-0.722262	-1.680239	1.396432
31	H	-1.768969	-2.349178	0.158658
32	H	0.577248	-3.239884	-0.017107
33	H	0.030092	-2.398612	-1.474203
34	H	2.83853	-2.756882	0.376529
35	H	3.135456	0.9545	1.130376
36	H	2.90956	0.726937	-1.892487
37	H	2.209835	2.011864	-0.92554
38	H	-0.400351	1.248645	2.127007
39	H	0.751919	-0.066464	1.940417
40	H	1.21972	1.59248	1.566674
41	H	5.418355	0.80465	0.09566
42	H	-2.597386	-0.689444	2.262937
43	H	-3.923592	0.446235	2.00721
44	H	-2.296687	1.047661	2.272281
45	H	-4.951272	-2.006199	-0.112403

B3LYP/6-311G** Energy = -963.5613339 a.u.; Population = 28.00%

(4R,5R,9S,10R,12S)-2		Standard Orientation		
Conformer 3		(Ångstroms)		
I	Atom	X	Y	Z
1	C	-1.729275	2.616986	-0.023299
2	C	-2.876955	1.654918	-0.319457
3	C	-2.636697	0.244699	0.276318
4	C	-1.226894	-0.270862	-0.181397
5	C	-0.024679	0.704438	0.034642
6	C	-0.402254	2.077197	-0.559314
7	C	-0.916144	-1.684567	0.321187
8	C	0.301148	-2.2632	-0.419504
9	C	1.459245	-1.31719	-0.347334
10	C	1.166573	0.092381	-0.802158
11	C	2.664977	-1.720007	0.105316
12	C	3.793728	-0.81806	0.224615
13	C	3.499892	0.667352	0.135448
14	C	2.443911	0.947514	-0.92676
15	H	-1.322269	-0.342351	-1.270652
16	C	0.403887	0.870059	1.501147
17	O	4.94839	-1.195746	0.42762
18	O	4.687869	1.391344	-0.159349
19	C	-2.869747	0.256708	1.794168
20	C	-3.63123	-0.694078	-0.414314
21	O	-3.754264	-0.787641	-1.620164
22	O	-4.368722	-1.440687	0.422502
23	H	0.758777	-0.005288	-1.814942
24	H	-1.943304	3.581675	-0.493821
25	H	-1.655179	2.809869	1.050998
26	H	-3.823454	2.047995	0.065331
27	H	-2.983052	1.559217	-1.40336
28	H	0.39146	2.800221	-0.357282
29	H	-0.476312	1.978718	-1.649403
30	H	-0.722264	-1.68025	1.39642
31	H	-1.768973	-2.349177	0.15864
32	H	0.577246	-3.239885	-0.017128
33	H	0.03009	-2.398606	-1.47422
34	H	2.838522	-2.756881	0.376527
35	H	3.13547	0.954515	1.130367
36	H	2.909555	0.72694	-1.892494
37	H	2.209832	2.011866	-0.925542
38	H	1.219738	1.59246	1.566673
39	H	-0.400334	1.248639	2.127014
40	H	0.751922	-0.066481	1.940413

41	H	5.418358	0.804682	0.095715
42	H	-2.597389	-0.689459	2.262934
43	H	-3.923577	0.446244	2.007222
44	H	-2.296661	1.047642	2.272289
45	H	-4.951283	-2.006187	-0.112411

B3LYP/6-311G** Energy = -963.5613339 a.u.; Population = 28.00%

(4R,5R,9S,10R,12S)-2		Standard Orientation		
Conformer 4		(Ångstroms)		
I	Atom	X	Y	Z
1	C	-1.990844	2.228307	-0.684541
2	C	-2.729218	1.585454	0.481611
3	C	-2.55516	0.033777	0.47679
4	C	-1.191428	-0.364574	-0.172944
5	C	-0.035204	0.660563	0.033583
6	C	-0.470459	2.039741	-0.558333
7	C	-0.796198	-1.803736	0.174079
8	C	0.424899	-2.260108	-0.639134
9	C	1.543157	-1.284155	-0.458353
10	C	1.194225	0.140875	-0.804772
11	C	2.757083	-1.672133	-0.014766
12	C	3.840516	-0.733186	0.199802
13	C	3.478351	0.739663	0.229145
14	C	2.428209	1.066236	-0.826655
15	H	-1.372668	-0.354727	-1.25035
16	C	0.362575	0.829512	1.508289
17	O	5.008753	-1.072966	0.392585
18	O	4.636234	1.540082	0.025981
19	C	-2.760472	-0.504012	1.905839
20	C	-3.672175	-0.49576	-0.425781
21	O	-3.567891	-0.772841	-1.604415
22	O	-4.856677	-0.582109	0.206209
23	H	0.812235	0.097671	-1.831429
24	H	-2.35025	1.792354	-1.622305
25	H	-2.220933	3.296413	-0.733314
26	H	-2.338496	1.971922	1.426711
27	H	-3.793553	1.833507	0.464569
28	H	-0.065172	2.834273	0.074359
29	H	-0.022998	2.174855	-1.546396
30	H	-0.570234	-1.900585	1.238712
31	H	-1.632488	-2.476623	-0.036415
32	H	0.735512	-3.265247	-0.346714
33	H	0.150697	-2.28587	-1.701163

34	H	2.974266	-2.719884	0.169104
35	H	3.083179	0.920676	1.237221
36	H	2.922011	0.964794	-1.798088
37	H	2.135062	2.111993	-0.72642
38	H	-0.467464	1.202891	2.106558
39	H	0.707708	-0.105532	1.955564
40	H	1.164364	1.564028	1.600547
41	H	5.3882	0.966353	0.245981
42	H	-2.872971	-1.58933	1.924185
43	H	-3.658054	-0.067741	2.346876
44	H	-1.91399	-0.239344	2.537555
45	H	-5.524468	-0.862982	-0.441369

B3LYP/6-311G** Energy = -963.5559344 a.u.; Population = 0.09%

(4R,5R,9S,10R,12S)-2		Standard Orientation		
Conformer 5		(Ångstroms)		
I	Atom	X	Y	Z
1	C	-1.74994	2.594262	-0.069497
2	C	-2.895163	1.616247	-0.325108
3	C	-2.63019	0.226604	0.313464
4	C	-1.227366	-0.29222	-0.150195
5	C	-0.028638	0.694929	0.028827
6	C	-0.42274	2.048036	-0.600009
7	C	-0.905813	-1.692921	0.380436
8	C	0.303259	-2.283464	-0.363887
9	C	1.458583	-1.33092	-0.323973
10	C	1.157167	0.067547	-0.802842
11	C	2.669575	-1.715832	0.125266
12	C	3.811736	-0.818673	0.235013
13	C	3.508397	0.662912	0.115684
14	C	2.435096	0.917869	-0.943386
15	H	-1.325979	-0.389998	-1.235611
16	C	0.417939	0.904739	1.483978
17	O	4.947838	-1.226335	0.462623
18	O	4.719034	1.349597	-0.190478
19	C	-2.837766	0.28696	1.833094
20	C	-3.674068	-0.740466	-0.249908
21	O	-4.521645	-1.318416	0.399671
22	O	-3.587697	-0.902248	-1.583625
23	H	0.745327	-0.047188	-1.812396
24	H	-1.974954	3.542702	-0.567197
25	H	-1.66895	2.819428	0.997797
26	H	-3.838885	2.012878	0.062155

27	H	-3.014446	1.494012	-1.404952
28	H	0.366656	2.783024	-0.425288
29	H	-0.504331	1.918193	-1.686306
30	H	-0.697589	-1.664539	1.452668
31	H	-1.760499	-2.361918	0.243809
32	H	0.588024	-3.250794	0.054884
33	H	0.018508	-2.441788	-1.411831
34	H	2.846744	-2.746502	0.418269
35	H	3.152612	0.968057	1.107332
36	H	2.894757	0.686033	-1.90944
37	H	2.199312	1.982747	-0.954668
38	H	-0.375865	1.306889	2.108261
39	H	0.767729	-0.019371	1.947675
40	H	1.237559	1.625216	1.516462
41	H	4.535003	2.294519	-0.128479
42	H	-2.556393	-0.647404	2.321264
43	H	-3.890491	0.473204	2.052836
44	H	-2.261941	1.091957	2.282316
45	H	-4.282568	-1.523798	-1.856837

B3LYP/6-311G** Energy = -963.5582007 a.u.; Population = 1.01%

Table S4. Cartesian coordinates for the re-optimized conformers of (4S,5R,9S,10R,12S)-**2** at the B3LYP/6-311G** level and London dispersion corrections with SMD solvent model for Methanol.

(4S,5R,9S,10R,12S)-2		Standard Orientation		
Conformer 1		(Ångstroms)		
I	Atom	X	Y	Z
1	C	1.760165	2.592886	-0.069029
2	C	2.901503	1.61196	-0.330237
3	C	2.635862	0.223047	0.309609
4	C	1.229372	-0.292063	-0.147064
5	C	0.034068	0.698627	0.035743
6	C	0.429314	2.050752	-0.594428
7	C	0.905779	-1.690334	0.388175
8	C	-0.310109	-2.27843	-0.347142
9	C	-1.461841	-1.322366	-0.306523
10	C	-1.156326	0.074065	-0.793123
11	C	-2.674062	-1.70669	0.144947
12	C	-3.798406	-0.79558	0.231528
13	C	-3.494538	0.685437	0.110788
14	C	-2.426574	0.935039	-0.947127
15	H	1.323029	-0.392085	-1.232636
16	C	-0.406357	0.909484	1.492632
17	O	-4.95735	-1.161737	0.431343

18	O	-4.67485	1.409647	-0.21294
19	C	2.851259	0.282721	1.82812
20	C	3.674497	-0.74657	-0.259137
21	O	4.52436	-1.325993	0.386102
22	O	3.580496	-0.908551	-1.592301
23	H	-0.742927	-0.051223	-1.800587
24	H	1.684245	2.817636	0.998709
25	H	1.985432	3.541056	-0.567086
26	H	3.848181	2.005878	0.05252
27	H	3.015187	1.489492	-1.410655
28	H	0.506078	1.921175	-1.681094
29	H	-0.357176	2.787793	-0.416023
30	H	1.75649	-2.363367	0.24703
31	H	0.704589	-1.659341	1.461589
32	H	-0.032267	-2.44104	-1.396248
33	H	-0.596484	-3.243144	0.076327
34	H	-2.85661	-2.735763	0.438976
35	H	-3.138374	0.993303	1.102462
36	H	-2.885279	0.697479	-1.912132
37	H	-2.184617	1.997513	-0.966233
38	H	0.391205	1.310062	2.113145
39	H	-1.22432	1.631537	1.528422
40	H	-0.755881	-0.013732	1.958374
41	H	-5.411659	0.834595	0.050146
42	H	2.572833	-0.652036	2.317206
43	H	3.905058	0.469218	2.042441
44	H	2.277468	1.087234	2.280798
45	H	4.272927	-1.531077	-1.869457

B3LYP/6-311G** Energy = -963.5617364 a.u.; Population = 42.90%

(4S,5R,9S,10R,12S)-2		Standard Orientation		
Conformer 2		(Ångstroms)		
I	Atom	X	Y	Z
1	C	1.729276	2.616986	-0.023303
2	C	2.876955	1.654918	-0.319459
3	C	2.636698	0.2447	0.276317
4	C	1.226894	-0.270862	-0.181396
5	C	0.02468	0.704439	0.034642
6	C	0.402254	2.077197	-0.559315
7	C	0.916144	-1.684566	0.321189
8	C	-0.301148	-2.2632	-0.419501
9	C	-1.459245	-1.31719	-0.347332
10	C	-1.166573	0.09238	-0.802156

11	C	-2.664978	-1.720007	0.105317
12	C	-3.793729	-0.81806	0.224613
13	C	-3.499891	0.667352	0.135451
14	C	-2.443911	0.947514	-0.926758
15	H	1.322269	-0.342352	-1.270652
16	C	-0.403885	0.870061	1.501148
17	O	-4.948392	-1.195746	0.427609
18	O	-4.687868	1.391346	-0.159339
19	C	2.86975	0.256709	1.794167
20	C	3.631229	-0.694079	-0.414313
21	O	3.754265	-0.787641	-1.620164
22	O	4.368717	-1.440691	0.422503
23	H	-0.758777	-0.005289	-1.814941
24	H	1.65518	2.809872	1.050993
25	H	1.943304	3.581674	-0.493827
26	H	3.823455	2.047994	0.065327
27	H	2.983053	1.559215	-1.403362
28	H	0.476312	1.978716	-1.649405
29	H	-0.391459	2.800221	-0.357285
30	H	1.768972	-2.349177	0.158641
31	H	0.722265	-1.680249	1.396421
32	H	-0.030091	-2.398607	-1.474217
33	H	-0.577246	-3.239885	-0.017124
34	H	-2.838523	-2.756881	0.376528
35	H	-3.135466	0.954511	1.130369
36	H	-2.909555	0.72694	-1.892493
37	H	-2.209832	2.011866	-0.925542
38	H	0.400339	1.248636	2.127014
39	H	-1.219732	1.592466	1.566675
40	H	-0.751924	-0.066477	1.940413
41	H	-5.418357	0.804673	0.0957
42	H	2.597389	-0.689456	2.262935
43	H	3.923581	0.446242	2.007218
44	H	2.296667	1.047645	2.272288
45	H	4.951277	-2.006192	-0.112409

B3LYP/6-311G** Energy = -963.5613339 a.u.; Population = 28.00%

(4S,5R,9S,10R,12S)-2		Standard Orientation		
Conformer 3		(Ångstroms)		
I	Atom	X	Y	Z
1	C	1.729271	2.616986	-0.023288
2	C	2.876952	1.65492	-0.319448
3	C	2.636692	0.244699	0.276322

4	C	1.226892	-0.27086	-0.181401
5	C	0.024677	0.704436	0.034641
6	C	0.40225	2.0772	-0.559306
7	C	0.916146	-1.684569	0.32117
8	C	-0.301144	-2.263199	-0.419525
9	C	-1.459242	-1.31719	-0.347348
10	C	-1.166571	0.092382	-0.802167
11	C	-2.66497	-1.720007	0.105311
12	C	-3.793719	-0.81806	0.224627
13	C	-3.499889	0.667352	0.135439
14	C	-2.443909	0.947514	-0.926767
15	H	1.322272	-0.34234	-1.270656
16	C	-0.403898	0.870047	1.501144
17	O	-4.948374	-1.195747	0.42767
18	O	-4.687867	1.391334	-0.159381
19	C	2.869732	0.256703	1.794173
20	C	3.63123	-0.694074	-0.414308
21	O	3.754259	-0.787642	-1.620159
22	O	4.368732	-1.440672	0.422507
23	H	-0.758771	-0.00528	-1.814951
24	H	1.655174	2.809865	1.051009
25	H	1.9433	3.581677	-0.493807
26	H	3.82345	2.047995	0.065344
27	H	2.983051	1.559223	-1.403351
28	H	0.476309	1.978727	-1.649396
29	H	-0.391465	2.800222	-0.357271
30	H	1.768977	-2.349176	0.158618
31	H	0.722265	-1.680263	1.396403
32	H	-0.030087	-2.398598	-1.474243
33	H	-0.577242	-3.239887	-0.017156
34	H	-2.838512	-2.756881	0.376526
35	H	-3.135477	0.954529	1.130357
36	H	-2.909553	0.72694	-1.892501
37	H	-2.20983	2.011866	-0.92555
38	H	0.400318	1.248627	2.127017
39	H	-1.219753	1.592444	1.566669
40	H	-0.751931	-0.066497	1.940402
41	H	-5.418356	0.804714	0.095776
42	H	2.597384	-0.68947	2.262932
43	H	3.923558	0.446253	2.007235
44	H	2.29663	1.047626	2.272294
45	H	4.951295	-2.006169	-0.112405

B3LYP/6-311G** Energy = -963.5613339 a.u.; Population = 28.00%

(4S,5R,9S,10R,12S)-2		Standard Orientation		
Conformer 4		(Ångstroms)		
I	Atom	X	Y	Z
1	C	1.990843	2.22831	-0.684542
2	C	2.729215	1.585456	0.48161
3	C	2.555156	0.03378	0.47679
4	C	1.191427	-0.364571	-0.172949
5	C	0.035202	0.660564	0.033578
6	C	0.470457	2.039743	-0.558336
7	C	0.796198	-1.803734	0.174072
8	C	-0.424897	-2.260106	-0.639144
9	C	-1.543155	-1.284154	-0.458361
10	C	-1.194225	0.140875	-0.80478
11	C	-2.757078	-1.672133	-0.014765
12	C	-3.840509	-0.733186	0.19981
13	C	-3.478347	0.739663	0.229143
14	C	-2.42821	1.066234	-0.826663
15	H	1.37267	-0.354723	-1.250353
16	C	-0.36258	0.829511	1.508282
17	O	-5.008743	-1.072968	0.392608
18	O	-4.636233	1.540078	0.025976
19	C	2.760459	-0.504008	1.905841
20	C	3.672174	-0.495763	-0.425773
21	O	3.567893	-0.772862	-1.604402
22	O	4.856677	-0.582097	0.206218
23	H	-0.812234	0.097672	-1.831435
24	H	2.220931	3.296415	-0.733315
25	H	2.350249	1.792356	-1.622305
26	H	2.338493	1.971925	1.426709
27	H	3.793549	1.833509	0.464569
28	H	0.022998	2.174859	-1.546399
29	H	0.06517	2.834274	0.074356
30	H	1.632489	-2.476619	-0.036421
31	H	0.570231	-1.900583	1.238704
32	H	-0.150693	-2.285865	-1.701172
33	H	-0.735508	-3.265246	-0.346727
34	H	-2.974259	-2.719883	0.169108
35	H	-3.083173	0.920684	1.237215
36	H	-2.922015	0.964785	-1.798093
37	H	-2.135064	2.111992	-0.726435
38	H	0.46746	1.202883	2.106555
39	H	-1.164364	1.564031	1.60054

40	H	-0.707719	-0.105532	1.955555
41	H	-5.388195	0.966355	0.246
42	H	2.872955	-1.589326	1.924189
43	H	3.65804	-0.067739	2.346881
44	H	1.913975	-0.239338	2.537552
45	H	5.524468	-0.862978	-0.441355

B3LYP/6-311G** Energy = -963.5559344 a.u.; Population = 0.09%

(4S,5R,9S,10R,12S)-2		Standard Orientation		
Conformer 5		(Ångstroms)		
I	Atom	X	Y	Z
1	C	1.749941	2.594261	-0.069499
2	C	2.895163	1.616246	-0.325108
3	C	2.63019	0.226603	0.313464
4	C	1.227365	-0.29222	-0.150195
5	C	0.028638	0.694929	0.028827
6	C	0.42274	2.048036	-0.60001
7	C	0.905812	-1.692921	0.380437
8	C	-0.303259	-2.283465	-0.363886
9	C	-1.458584	-1.33092	-0.323973
10	C	-1.157167	0.067546	-0.802841
11	C	-2.669576	-1.715832	0.125267
12	C	-3.811737	-0.818673	0.235013
13	C	-3.508397	0.662913	0.115684
14	C	-2.435096	0.917869	-0.943385
15	H	1.325978	-0.389999	-1.235611
16	C	-0.417938	0.90474	1.483978
17	O	-4.947839	-1.226335	0.462622
18	O	-4.719034	1.349597	-0.190476
19	C	2.837765	0.28696	1.833094
20	C	3.674068	-0.740466	-0.249908
21	O	4.52165	-1.318409	0.399671
22	O	3.587694	-0.902253	-1.583624
23	H	-0.745327	-0.047189	-1.812396
24	H	1.668951	2.819428	0.997795
25	H	1.974955	3.542702	-0.567199
26	H	3.838885	2.012877	0.062154
27	H	3.014446	1.49401	-1.404952
28	H	0.504331	1.918191	-1.686307
29	H	-0.366656	2.783023	-0.42529
30	H	1.760498	-2.361918	0.243811
31	H	0.697588	-1.664538	1.452669
32	H	-0.018508	-2.441789	-1.41183

33	H	-0.588024	-3.250794	0.054885
34	H	-2.846744	-2.746502	0.41827
35	H	-3.152611	0.968056	1.107332
36	H	-2.894757	0.686033	-1.909439
37	H	-2.199312	1.982747	-0.954668
38	H	0.375865	1.30689	2.108261
39	H	-1.237558	1.625218	1.516461
40	H	-0.767729	-0.019369	1.947675
41	H	-4.534998	2.294519	-0.128493
42	H	2.556393	-0.647404	2.321264
43	H	3.89049	0.473205	2.052836
44	H	2.261939	1.091957	2.282315
45	H	4.282568	-1.5238	-1.856836

B3LYP/6-311G** Energy = -963.5582007 a.u.; Population = 1.01%

Table S5. Cartesian coordinates for the re-optimized conformers of (4R,5S,10S)-**3** at the B3LYP/6-311G** level and London dispersion corrections with SMD solvent model for Methanol.

(4R,5S,10S)-3		Standard Orientation		
Conformer 1		(Ångstroms)		
I	Atom	X	Y	Z
1	C	-2.912336	2.654047	0.042269
2	C	-3.89679	1.509	-0.184824
3	C	-3.368574	0.153846	0.355227
4	C	-1.941108	-0.129058	-0.23497
5	C	-0.937487	1.046251	-0.093035
6	C	-1.567413	2.342625	-0.612033
7	C	-1.392365	-1.489052	0.22323
8	C	-0.251892	-2.037566	-0.648666
9	C	1.078698	-1.354123	-0.47042
10	C	1.222412	0.019393	-0.678915
11	O	0.147889	0.800715	-1.065398
12	C	2.217092	-2.077046	-0.10815
13	C	3.459144	-1.46003	0.025992
14	C	3.612396	-0.084282	-0.20703
15	C	2.466463	0.632461	-0.55258
16	C	4.971004	0.569711	-0.025089
17	C	5.14242	1.863568	-0.825349
18	C	5.247887	0.815132	1.469278
19	O	4.577489	-2.172953	0.389884
20	C	-0.329753	1.254937	1.291199
21	H	-2.099496	-0.200803	-1.315605
22	C	-3.436443	0.124424	1.888497
23	C	-4.275069	-0.920537	-0.253542

24	O	-4.905169	-1.693116	0.644549
25	O	-4.431838	-1.079233	-1.44831
26	H	-2.782917	2.846144	1.111365
27	H	-3.322904	3.571615	-0.38907
28	H	-4.074523	1.407368	-1.258865
29	H	-4.860785	1.72696	0.285306
30	H	-0.85722	3.160838	-0.461957
31	H	-1.710949	2.229395	-1.691923
32	H	-1.070533	-1.451365	1.266869
33	H	-2.205155	-2.220636	0.184708
34	H	-0.555892	-1.963119	-1.700325
35	H	-0.124224	-3.101048	-0.433046
36	H	2.137759	-3.145915	0.067574
37	H	2.521823	1.698208	-0.734768
38	H	5.719264	-0.144595	-0.383374
39	H	6.172331	2.22061	-0.737232
40	H	4.926954	1.711652	-1.886785
41	H	4.487813	2.658631	-0.456494
42	H	6.250128	1.230522	1.613773
43	H	5.179286	-0.11227	2.042653
44	H	4.522761	1.524802	1.880488
45	H	4.34308	-3.103391	0.502454
46	H	0.059244	0.335074	1.72717
47	H	0.492439	1.97035	1.21616
48	H	-1.06489	1.668524	1.978921
49	H	-3.035052	-0.801976	2.300222
50	H	-4.472125	0.219067	2.219931
51	H	-2.879689	0.953358	2.319543
52	H	-5.453222	-2.3335	0.159976

B3LYP/6-311G** Energy = -1080.3472777 a.u.; Population = 15.43%

(4R,5S,10S)-3		Standard Orientation		
Conformer 2		(Ångstroms)		
I	Atom	X	Y	Z
1	C	-2.930166	2.634442	0.031033
2	C	-3.910837	1.481683	-0.177737
3	C	-3.370261	0.139208	0.385658
4	C	-1.944536	-0.148489	-0.201476
5	C	-0.946177	1.033787	-0.079642
6	C	-1.583861	2.318674	-0.618513
7	C	-1.391009	-1.497484	0.281352
8	C	-0.249342	-2.058058	-0.580695
9	C	1.078546	-1.363808	-0.422906

10	C	1.215665	0.005986	-0.659541
11	O	0.136575	0.777668	-1.052167
12	C	2.222853	-2.075134	-0.055838
13	C	3.464191	-1.451793	0.053379
14	C	3.611026	-0.081137	-0.211397
15	C	2.459145	0.624929	-0.558729
16	C	4.96994	0.580267	-0.061511
17	C	5.131338	1.849796	-0.901996
18	C	5.260625	0.870949	1.42198
19	O	4.588181	-2.15334	0.42188
20	C	-0.33441	1.268115	1.298517
21	H	-2.09281	-0.23802	-1.280883
22	C	-3.435257	0.136974	1.918665
23	C	-4.308109	-0.95924	-0.118556
24	O	-4.289058	-1.100637	-1.456562
25	O	-5.029576	-1.643109	0.578548
26	H	-2.801827	2.842786	1.097138
27	H	-3.344547	3.543507	-0.414424
28	H	-4.09276	1.368466	-1.249749
29	H	-4.873607	1.701286	0.29368
30	H	-0.877911	3.142905	-0.481999
31	H	-1.727048	2.187699	-1.696484
32	H	-1.068819	-1.439539	1.323919
33	H	-2.202087	-2.232037	0.256948
34	H	-0.556639	-2.009049	-1.632989
35	H	-0.11477	-3.115769	-0.342077
36	H	2.148922	-3.140455	0.14251
37	H	2.509109	1.686767	-0.76406
38	H	5.716047	-0.143172	-0.405559
39	H	6.161888	2.209768	-0.835947
40	H	4.904403	1.665966	-1.955988
41	H	4.480279	2.655325	-0.549964
42	H	6.263239	1.292576	1.544182
43	H	5.199794	-0.038939	2.023646
44	H	4.537815	1.591125	1.818741
45	H	4.358159	-3.082193	0.554625
46	H	0.05902	0.356941	1.748605
47	H	0.48523	1.984764	1.20829
48	H	-1.068426	1.690959	1.98181
49	H	-3.034611	-0.785833	2.34032
50	H	-4.47265	0.229488	2.24519
51	H	-2.880532	0.971586	2.340245
52	H	-4.920033	-1.799566	-1.695588

B3LYP/6-311G** Energy = -1080.3478351 a.u.; Population = 27.85%

(4R,5S,10S)-3		Standard Orientation		
Conformer 3		(Ångstroms)		
I	Atom	X	Y	Z
1	C	-2.905788	2.65542	0.032258
2	C	-3.892975	1.511744	-0.189678
3	C	-3.36781	0.157696	0.355733
4	C	-1.941084	-0.131201	-0.233888
5	C	-0.934776	1.042434	-0.097403
6	C	-1.561962	2.338101	-0.621449
7	C	-1.395332	-1.49036	0.230149
8	C	-0.257288	-2.045942	-0.640357
9	C	1.075247	-1.365459	-0.466634
10	C	1.222422	0.008284	-0.681517
11	O	0.149689	0.790787	-1.069569
12	C	2.211828	-2.088161	-0.107716
13	C	3.456826	-1.475362	0.023469
14	C	3.614522	-0.100226	-0.212457
15	C	2.466855	0.617385	-0.559603
16	C	4.963864	0.574593	-0.020029
17	C	5.123097	1.871059	-0.819144
18	C	5.227395	0.823157	1.476723
19	O	4.496576	-2.294631	0.401755
20	C	-0.32558	1.255239	1.285486
21	H	-2.100166	-0.207258	-1.31413
22	C	-3.435149	0.134683	1.889151
23	C	-4.276586	-0.917426	-0.248308
24	O	-4.904488	-1.688008	0.652993
25	O	-4.436407	-1.078596	-1.442335
26	H	-2.77537	2.851663	1.100484
27	H	-3.31438	3.572154	-0.402711
28	H	-4.071393	1.406071	-1.263207
29	H	-4.856287	1.733917	0.279898
30	H	-0.849769	3.155267	-0.475215
31	H	-1.706393	2.22066	-1.700767
32	H	-1.072328	-1.448601	1.273256
33	H	-2.209879	-2.220143	0.195949
34	H	-0.562093	-1.975375	-1.692053
35	H	-0.131688	-3.10862	-0.419918
36	H	2.142795	-3.156081	0.069403
37	H	2.52346	1.682614	-0.743226
38	H	5.740637	-0.110138	-0.386823

39	H	6.147894	2.239992	-0.72463
40	H	4.914066	1.716824	-1.881174
41	H	4.456512	2.655634	-0.450405
42	H	6.222481	1.251657	1.629028
43	H	5.165119	-0.104951	2.051158
44	H	4.487622	1.521362	1.880056
45	H	5.335405	-1.821419	0.346744
46	H	0.062408	0.336388	1.724492
47	H	0.49759	1.969197	1.20722
48	H	-1.059602	1.672289	1.972318
49	H	-3.035187	-0.790651	2.304595
50	H	-4.470584	0.232455	2.2205
51	H	-2.876855	0.96445	2.316597
52	H	-5.453339	-2.329725	0.171093

B3LYP/6-311G** Energy = -1080.3463546 a.u.; Population = 5.80%

(4R,5S,10S)-3		Standard Orientation		
Conformer 4		(Ångstroms)		
I	Atom	X	Y	Z
1	C	-2.923837	2.635509	0.017139
2	C	-3.907112	1.483393	-0.182575
3	C	-3.367955	0.143252	0.387852
4	C	-1.944091	-0.150697	-0.200762
5	C	-0.943194	1.030242	-0.087196
6	C	-1.579205	2.313139	-0.632665
7	C	-1.392371	-1.498436	0.287782
8	C	-0.254751	-2.066499	-0.574745
9	C	1.075358	-1.375562	-0.422884
10	C	1.215566	-0.005594	-0.665837
11	O	0.137935	0.766712	-1.060254
12	C	2.217935	-2.086461	-0.059253
13	C	3.461982	-1.467006	0.048327
14	C	3.612723	-0.096727	-0.218098
15	C	2.459046	0.609695	-0.568142
16	C	4.961392	0.586812	-0.054413
17	C	5.108647	1.864855	-0.885016
18	C	5.238418	0.870799	1.433368
19	O	4.507393	-2.275291	0.434777
20	C	-0.328389	1.271126	1.288354
21	H	-2.094869	-0.245584	-1.279354
22	C	-3.429621	0.150438	1.921013
23	C	-4.308806	-0.956538	-0.107709
24	O	-4.29364	-1.105258	-1.445021

25	O	-5.029564	-1.635418	0.59502
26	H	-2.793264	2.85047	1.081644
27	H	-3.337183	3.542524	-0.433425
28	H	-4.091463	1.364018	-1.253467
29	H	-4.868459	1.707769	0.289478
30	H	-0.871544	3.136873	-0.502234
31	H	-1.724438	2.175978	-1.709566
32	H	-1.066842	-1.435694	1.328997
33	H	-2.205225	-2.23113	0.269833
34	H	-0.564512	-2.021107	-1.626446
35	H	-0.122258	-3.123379	-0.331618
36	H	2.154476	-3.150841	0.139883
37	H	2.509964	1.671119	-0.774136
38	H	5.737027	-0.103451	-0.412842
39	H	6.133604	2.237881	-0.810419
40	H	4.888375	1.685614	-1.940843
41	H	4.444517	2.656537	-0.527203
42	H	6.233022	1.306971	1.565863
43	H	5.186097	-0.043895	2.029779
44	H	4.499604	1.575043	1.827854
45	H	5.344535	-1.801251	0.364086
46	H	0.064128	0.361781	1.742909
47	H	0.492406	1.985731	1.192671
48	H	-1.060252	1.699208	1.970673
49	H	-3.029338	-0.770309	2.347455
50	H	-4.466179	0.246341	2.24914
51	H	-2.872894	0.986757	2.336425
52	H	-4.926439	-1.804372	-1.678556

B3LYP/6-311G** Energy = -1080.3468942 a.u.; Population = 10.27%

(4R,5S,10S)-3		Standard Orientation		
Conformer 5		(Ångstroms)		
I	Atom	X	Y	Z
1	C	-2.912337	2.654047	0.042265
2	C	-3.89679	1.508999	-0.184827
3	C	-3.368575	0.153847	0.355227
4	C	-1.941109	-0.129058	-0.234969
5	C	-0.937487	1.046251	-0.093034
6	C	-1.567413	2.342625	-0.612034
7	C	-1.392365	-1.489052	0.223232
8	C	-0.251892	-2.037566	-0.648665
9	C	1.078698	-1.354123	-0.470419
10	C	1.222412	0.019393	-0.678914

11	O	0.147889	0.800714	-1.065397
12	C	2.217092	-2.077046	-0.108151
13	C	3.459145	-1.46003	0.025991
14	C	3.612397	-0.084282	-0.20703
15	C	2.466463	0.632461	-0.552579
16	C	4.971004	0.569711	-0.025089
17	C	5.142419	1.863569	-0.825349
18	C	5.247887	0.815132	1.469278
19	O	4.577491	-2.172954	0.389881
20	C	-0.329753	1.25494	1.291199
21	H	-2.099496	-0.200803	-1.315604
22	C	-3.436447	0.124428	1.888497
23	C	-4.275068	-0.920539	-0.253542
24	O	-4.905167	-1.693117	0.64455
25	O	-4.431835	-1.079238	-1.448309
26	H	-2.782921	2.846145	1.111361
27	H	-3.322905	3.571614	-0.389076
28	H	-4.074522	1.407366	-1.258869
29	H	-4.860786	1.72696	0.285301
30	H	-0.857221	3.160838	-0.461957
31	H	-1.710947	2.229394	-1.691924
32	H	-1.070534	-1.451365	1.26687
33	H	-2.205155	-2.220636	0.184709
34	H	-0.555892	-1.96312	-1.700324
35	H	-0.124225	-3.101049	-0.433044
36	H	2.13776	-3.145916	0.067572
37	H	2.521823	1.698208	-0.734766
38	H	5.719264	-0.144594	-0.383375
39	H	6.17233	2.220611	-0.737231
40	H	4.926952	1.711654	-1.886785
41	H	4.487812	2.658632	-0.456492
42	H	6.250128	1.230522	1.613773
43	H	5.179287	-0.112271	2.042653
44	H	4.522761	1.524801	1.88049
45	H	4.343079	-3.103389	0.502464
46	H	0.059245	0.335078	1.727172
47	H	0.492438	1.970354	1.21616
48	H	-1.064891	1.668527	1.978921
49	H	-3.035053	-0.801969	2.300224
50	H	-4.47213	0.219068	2.219928
51	H	-2.879697	0.953365	2.319542
52	H	-5.453218	-2.333503	0.159977

B3LYP/6-311G** Energy = -1080.3472777 a.u.; Population = 15.43%

(4R,5S,10S)-3		Standard Orientation		
Conformer 6		(Ångstroms)		
I	Atom	X	Y	Z
1	C	-3.071306	2.578107	-0.097277
2	C	-4.002619	1.384165	-0.290772
3	C	-3.422642	0.071923	0.314344
4	C	-1.975495	-0.170809	-0.219778
5	C	-1.029582	1.057262	-0.130118
6	C	-1.707423	2.295746	-0.723768
7	C	-1.374543	-1.467861	0.343669
8	C	-0.18758	-2.019476	-0.4611
9	C	1.103547	-1.256014	-0.318525
10	C	1.183777	0.104866	-0.631496
11	O	0.079792	0.808208	-1.075596
12	C	2.269958	-1.8875	0.108385
13	C	3.486261	-1.210451	0.203006
14	C	3.581111	0.146509	-0.145226
15	C	2.398529	0.775124	-0.549342
16	C	4.868027	0.958667	-0.10018
17	C	5.407182	1.145879	1.328606
18	C	5.944304	0.429891	-1.064554
19	O	4.549221	-1.970464	0.642352
20	C	-0.449379	1.373577	1.246198
21	H	-2.094519	-0.320314	-1.296359
22	C	-3.528074	0.088089	1.847533
23	C	-4.315462	-1.023575	-0.272848
24	O	-5.368268	-1.330057	0.503148
25	O	-4.160727	-1.539889	-1.361827
26	H	-2.966181	2.81424	0.965687
27	H	-3.515197	3.45959	-0.568915
28	H	-4.155273	1.233313	-1.364632
29	H	-4.983155	1.576122	0.153495
30	H	-1.035443	3.151094	-0.609336
31	H	-1.834506	2.121819	-1.79761
32	H	-1.081897	-1.342669	1.389083
33	H	-2.152103	-2.236831	0.334202
34	H	-0.472273	-2.043208	-1.5206
35	H	-0.008934	-3.054765	-0.161
36	H	2.250397	-2.939789	0.371158
37	H	2.420188	1.826875	-0.812764
38	H	4.596305	1.955265	-0.459291
39	H	6.272045	1.815547	1.320447

40	H	4.641981	1.584796	1.974296
41	H	5.727136	0.207578	1.792387
42	H	6.795293	1.116713	-1.088834
43	H	5.545469	0.345944	-2.078916
44	H	6.329246	-0.553926	-0.779965
45	H	5.342223	-1.433555	0.736966
46	H	-0.039117	0.497697	1.74794
47	H	0.351248	2.108588	1.135454
48	H	-1.206815	1.809932	1.89495
49	H	-3.218052	-0.864277	2.280932
50	H	-4.55603	0.279269	2.156895
51	H	-2.904478	0.869376	2.275636
52	H	-5.919227	-1.971521	0.023534

B3LYP/6-311G** Energy = -1080.3442745 a.u.; Population = 0.64%

(4R,5S,10S)-3		Standard Orientation		
Conformer 7		(Ångstroms)		
I	Atom	X	Y	Z
1	C	-3.096632	2.586822	-0.084282
2	C	-4.025124	1.387383	-0.264956
3	C	-3.438848	0.089665	0.355105
4	C	-1.992264	-0.159441	-0.197516
5	C	-1.047036	1.06866	-0.11006
6	C	-1.729662	2.304417	-0.705244
7	C	-1.390554	-1.461496	0.352205
8	C	-0.209943	-2.008879	-0.464428
9	C	1.083086	-1.248836	-0.321554
10	C	1.163584	0.114299	-0.624163
11	O	0.058715	0.821545	-1.0599
12	C	2.250611	-1.88544	0.094279
13	C	3.468436	-1.210852	0.187474
14	C	3.563323	0.14872	-0.150576
15	C	2.379504	0.782364	-0.542991
16	C	4.851841	0.958423	-0.107817
17	C	5.400943	1.133712	1.318584
18	C	5.920592	0.435292	-1.083596
19	O	4.53259	-1.976096	0.61429
20	C	-0.464329	1.380849	1.265269
21	H	-2.117595	-0.300101	-1.274292
22	C	-3.530614	0.139179	1.885799
23	C	-4.323225	-1.062757	-0.124711
24	O	-4.272243	-1.251492	-1.456041
25	O	-5.032851	-1.746922	0.584089

26	H	-2.992396	2.83786	0.975271
27	H	-3.541784	3.461585	-0.567122
28	H	-4.184318	1.228521	-1.334712
29	H	-5.00376	1.582921	0.183746
30	H	-1.060367	3.161985	-0.591467
31	H	-1.852901	2.127529	-1.77905
32	H	-1.091068	-1.345015	1.396577
33	H	-2.169163	-2.230787	0.345786
34	H	-0.500354	-2.022588	-1.522563
35	H	-0.03215	-3.047033	-0.174183
36	H	2.230932	-2.939755	0.348717
37	H	2.401439	1.835982	-0.798752
38	H	4.579316	1.958169	-0.457417
39	H	6.267406	1.801277	1.30957
40	H	4.641161	1.56967	1.972611
41	H	5.721543	0.1912	1.773305
42	H	6.772406	1.121042	-1.108694
43	H	5.514581	0.359536	-2.095758
44	H	6.305968	-0.551166	-0.809032
45	H	5.32709	-1.441459	0.709181
46	H	-0.042157	0.504505	1.756486
47	H	0.327624	2.125622	1.15747
48	H	-1.224297	1.800738	1.921569
49	H	-3.1086	-0.754901	2.346576
50	H	-4.575934	0.209624	2.19192
51	H	-3.009731	1.005242	2.286772
52	H	-4.874708	-1.978996	-1.682925

B3LYP/6-311G** Energy = -1080.3449438 a.u.; Population = 1.30%

(4R,5S,10S)-3		Standard Orientation		
Conformer 8		(Ångstroms)		
I	Atom	X	Y	Z
1	C	-2.905786	2.655419	0.032262
2	C	-3.892973	1.511744	-0.189673
3	C	-3.367806	0.157695	0.355735
4	C	-1.941083	-0.131201	-0.233889
5	C	-0.934775	1.042433	-0.097406
6	C	-1.56196	2.338101	-0.621449
7	C	-1.395331	-1.490361	0.230144
8	C	-0.257289	-2.045941	-0.640367
9	C	1.075246	-1.36546	-0.46664
10	C	1.222421	0.008283	-0.681525
11	O	0.149688	0.790783	-1.069579

12	C	2.211826	-2.088161	-0.107718
13	C	3.456823	-1.475361	0.023471
14	C	3.614519	-0.100226	-0.212457
15	C	2.466854	0.617384	-0.55961
16	C	4.963862	0.574593	-0.020026
17	C	5.123095	1.871061	-0.819137
18	C	5.227393	0.82315	1.476726
19	O	4.496572	-2.294625	0.40177
20	C	-0.325573	1.255237	1.28548
21	H	-2.100167	-0.207257	-1.314131
22	C	-3.435139	0.134681	1.889154
23	C	-4.276587	-0.917424	-0.248303
24	O	-4.904501	-1.687994	0.652999
25	O	-4.436402	-1.078601	-1.44233
26	H	-2.775364	2.851661	1.100487
27	H	-3.314378	3.572154	-0.402705
28	H	-4.071394	1.406072	-1.263201
29	H	-4.856284	1.733916	0.279906
30	H	-0.849767	3.155267	-0.475217
31	H	-1.706394	2.220661	-1.700767
32	H	-1.072323	-1.448604	1.273251
33	H	-2.209879	-2.220143	0.195945
34	H	-0.562096	-1.975368	-1.692061
35	H	-0.131689	-3.10862	-0.419933
36	H	2.142794	-3.156081	0.069401
37	H	2.523459	1.682613	-0.743235
38	H	5.740634	-0.110137	-0.386822
39	H	6.147893	2.239994	-0.72462
40	H	4.914067	1.71683	-1.881168
41	H	4.45651	2.655635	-0.450397
42	H	6.222479	1.251649	1.629032
43	H	5.165116	-0.10496	2.051157
44	H	4.48762	1.521354	1.880062
45	H	5.335406	-1.821426	0.34671
46	H	0.062412	0.336385	1.724486
47	H	0.497601	1.96919	1.207209
48	H	-1.059589	1.672293	1.972313
49	H	-3.035184	-0.790657	2.304594
50	H	-4.470572	0.232463	2.220507
51	H	-2.876835	0.964442	2.316598
52	H	-5.453356	-2.329708	0.1711

B3LYP/6-311G** Energy = -1080.3463546 a.u.; Population = 5.80%

(4R,5S,10S)-3		Standard Orientation		
Conformer 9		(Ångstroms)		
I	Atom	X	Y	Z
1	C	-3.088273	2.571582	-0.104622
2	C	-4.011004	1.370252	-0.293736
3	C	-3.42176	0.064403	0.316235
4	C	-1.973195	-0.169363	-0.21747
5	C	-1.035615	1.065209	-0.129946
6	C	-1.721646	2.2968	-0.72846
7	C	-1.362588	-1.461613	0.346717
8	C	-0.177215	-2.008641	-0.463723
9	C	1.111458	-1.239786	-0.326442
10	C	1.18368	0.122058	-0.629773
11	O	0.076247	0.821388	-1.072983
12	C	2.285544	-1.872557	0.08598
13	C	3.498027	-1.189342	0.176929
14	C	3.579093	0.174799	-0.14616
15	C	2.395337	0.801291	-0.540411
16	C	4.867951	0.975986	-0.070997
17	C	5.417059	1.068567	1.36185
18	C	5.935209	0.464385	-1.051903
19	O	4.642124	-1.835823	0.582317
20	C	-0.4588	1.389425	1.245818
21	H	-2.091535	-0.321082	-1.293821
22	C	-3.527312	0.085237	1.849265
23	C	-4.306821	-1.039502	-0.266887
24	O	-5.360391	-1.346709	0.507846
25	O	-4.146202	-1.561861	-1.352164
26	H	-2.985935	2.813276	0.957351
27	H	-3.538143	3.447671	-0.580657
28	H	-4.162461	1.214228	-1.367048
29	H	-4.992937	1.556994	0.149651
30	H	-1.056091	3.157456	-0.616324
31	H	-1.846089	2.118123	-1.801843
32	H	-1.064715	-1.331865	1.390127
33	H	-2.13606	-2.234703	0.343863
34	H	-0.467172	-2.034061	-1.521754
35	H	0.006487	-3.043347	-0.164376
36	H	2.260553	-2.929686	0.334824
37	H	2.409332	1.856629	-0.789876
38	H	4.606605	1.992698	-0.381602
39	H	6.287396	1.73147	1.391106
40	H	4.662578	1.471999	2.043439

41	H	5.723894	0.089823	1.735619
42	H	6.8079	1.124707	-1.03881
43	H	5.546134	0.439898	-2.073916
44	H	6.267937	-0.542008	-0.790966
45	H	4.441584	-2.764681	0.756138
46	H	-0.042216	0.517707	1.749667
47	H	0.336517	2.129923	1.133406
48	H	-1.219545	1.821987	1.893233
49	H	-3.207225	-0.862209	2.286217
50	H	-4.557137	0.266919	2.158069
51	H	-2.911976	0.87467	2.274342
52	H	-5.906679	-1.993643	0.030239

B3LYP/6-311G** Energy = -1080.3463402 a.u.; Population = 5.71%

(4R,5S,10S)-3		Standard Orientation		
Conformer 10		(Ångstroms)		
I	Atom	X	Y	Z
1	C	-3.114185	2.580054	-0.090742
2	C	-4.033868	1.373267	-0.267953
3	C	-3.438388	0.082013	0.356533
4	C	-1.990197	-0.158013	-0.195647
5	C	-1.05343	1.076576	-0.109331
6	C	-1.744245	2.30574	-0.708793
7	C	-1.379134	-1.455666	0.354266
8	C	-0.199557	-1.997654	-0.467614
9	C	1.090773	-1.231929	-0.329068
10	C	1.163357	0.132102	-0.621707
11	O	0.055168	0.835699	-1.056345
12	C	2.265869	-1.869802	0.072374
13	C	3.479844	-1.18913	0.162083
14	C	3.561266	0.177414	-0.151111
15	C	2.376381	0.808983	-0.533446
16	C	4.852246	0.975462	-0.07929
17	C	5.412309	1.056115	1.349981
18	C	5.910855	0.469031	-1.072226
19	O	4.625073	-1.840528	0.555759
20	C	-0.474715	1.395744	1.265978
21	H	-2.114819	-0.300377	-1.272305
22	C	-3.530572	0.136033	1.88697
23	C	-4.313646	-1.079002	-0.119387
24	O	-4.262469	-1.270628	-1.450285
25	O	-5.01661	-1.767489	0.591902
26	H	-3.013151	2.836046	0.967939

27	H	-3.565217	3.449599	-0.577585
28	H	-4.191455	1.209699	-1.33725
29	H	-5.014111	1.563282	0.179662
30	H	-1.081438	3.168551	-0.596595
31	H	-1.864456	2.124787	-1.782296
32	H	-1.07523	-1.335397	1.396981
33	H	-2.153527	-2.229265	0.353225
34	H	-0.49465	-2.012549	-1.524456
35	H	-0.016535	-3.035336	-0.178629
36	H	2.240533	-2.92881	0.313003
37	H	2.39075	1.866091	-0.775299
38	H	4.590636	1.994986	-0.380303
39	H	6.284382	1.716815	1.37751
40	H	4.663887	1.456227	2.040155
41	H	5.71962	0.073901	1.714083
42	H	6.784987	1.127481	-1.060933
43	H	5.513841	0.453057	-2.09137
44	H	6.243482	-0.539977	-0.821404
45	H	4.423707	-2.770032	0.725527
46	H	-0.046423	0.523204	1.758783
47	H	0.311938	2.146009	1.157313
48	H	-1.238162	1.81135	1.92097
49	H	-3.097331	-0.750975	2.351102
50	H	-4.576646	0.19474	2.193005
51	H	-3.020572	1.010135	2.284531
52	H	-4.859105	-2.0037	-1.674822

B3LYP/6-311G** Energy = -1080.3470229 a.u.; Population = 11.77%

Table S6. Cartesian coordinates for the re-optimized conformers of (4S,5R,10R)-**3** at the B3LYP/6-311G** level and London dispersion corrections with SMD solvent model for Methanol.

(4S,5R,10R)-3		Standard Orientation		
Conformer 1		(Ångstroms)		
I	Atom	X	Y	Z
1	C	2.912335	2.654047	0.042278
2	C	3.89679	1.509	-0.184816
3	C	3.368573	0.153844	0.355227
4	C	1.941107	-0.129059	-0.234971
5	C	0.937486	1.046249	-0.093036
6	C	1.567415	2.342625	-0.612029
7	C	1.392364	-1.489051	0.223231
8	C	0.251892	-2.037566	-0.648664
9	C	-1.078698	-1.354122	-0.470419
10	C	-1.222413	0.019393	-0.678916

11	O	-0.14789	0.800718	-1.065397
12	C	-2.217091	-2.077044	-0.108146
13	C	-3.459144	-1.460029	0.025993
14	C	-3.612397	-0.084281	-0.207032
15	C	-2.466465	0.632461	-0.552584
16	C	-4.971007	0.56971	-0.025093
17	C	-5.24789	0.815129	1.469275
18	C	-5.142423	1.863569	-0.82535
19	O	-4.577488	-2.172953	0.389888
20	C	0.329754	1.254933	1.291201
21	H	2.099495	-0.200803	-1.315606
22	C	3.436439	0.124412	1.888498
23	C	4.275072	-0.920534	-0.253548
24	O	4.905178	-1.693111	0.64454
25	O	4.43184	-1.079224	-1.448315
26	H	3.322903	3.571618	-0.389053
27	H	2.782912	2.846138	1.111375
28	H	4.860785	1.726959	0.285314
29	H	4.074523	1.407375	-1.258858
30	H	0.85722	3.160837	-0.461956
31	H	1.710956	2.229395	-1.691919
32	H	2.205155	-2.220635	0.184711
33	H	1.070532	-1.451362	1.26687
34	H	0.124223	-3.101048	-0.433042
35	H	0.555892	-1.963121	-1.700323
36	H	-2.137758	-3.145913	0.067581
37	H	-2.521824	1.698207	-0.734775
38	H	-5.719265	-0.144595	-0.38338
39	H	-6.250131	1.230519	1.613772
40	H	-5.179289	-0.112274	2.042649
41	H	-4.522763	1.524798	1.880486
42	H	-6.172333	2.220611	-0.737231
43	H	-4.926958	1.711655	-1.886787
44	H	-4.487814	2.65863	-0.456494
45	H	-4.343087	-3.103396	0.502424
46	H	-0.059245	0.335069	1.727168
47	H	1.064891	1.668515	1.978924
48	H	-0.492438	1.970347	1.216164
49	H	3.035059	-0.801995	2.300214
50	H	4.472119	0.219066	2.219934
51	H	2.879674	0.953336	2.319548
52	H	5.453237	-2.333489	0.159967

B3LYP/6-311G** Energy = -1080.3472777 a.u.; Population = 15.43%

(4S,5R,10R)-3		Standard Orientation		
Conformer 2		(Ångstroms)		
I	Atom	X	Y	Z
1	C	2.93017	2.634441	0.03103
2	C	3.910839	1.481682	-0.177744
3	C	3.370265	0.139208	0.385654
4	C	1.944537	-0.148489	-0.201474
5	C	0.946179	1.033788	-0.079638
6	C	1.583863	2.318674	-0.618512
7	C	1.39101	-1.497482	0.281359
8	C	0.249341	-2.058059	-0.580681
9	C	-1.078547	-1.363807	-0.422898
10	C	-1.215665	0.005987	-0.659533
11	O	-0.136576	0.777672	-1.052158
12	C	-2.222857	-2.075133	-0.055838
13	C	-3.464195	-1.451793	0.053373
14	C	-3.611028	-0.081136	-0.211399
15	C	-2.459146	0.624931	-0.558724
16	C	-4.969942	0.580269	-0.061515
17	C	-5.260631	0.870942	1.421977
18	C	-5.131334	1.849804	-0.901992
19	O	-4.588189	-2.153342	0.421858
20	C	0.334417	1.268117	1.298523
21	H	2.092807	-0.238022	-1.280882
22	C	3.435266	0.136976	1.918661
23	C	4.308108	-0.959244	-0.118561
24	O	4.289057	-1.100636	-1.456567
25	O	5.029568	-1.64312	0.578542
26	H	3.344551	3.543506	-0.414429
27	H	2.801836	2.842785	1.097135
28	H	4.873612	1.701284	0.293668
29	H	4.092757	1.368463	-1.249757
30	H	0.877915	3.142906	-0.481996
31	H	1.727047	2.187698	-1.696483
32	H	2.202087	-2.232036	0.256955
33	H	1.068824	-1.439533	1.323927
34	H	0.114767	-3.115768	-0.342055
35	H	0.556636	-2.009059	-1.632977
36	H	-2.148925	-3.140455	0.142507
37	H	-2.509108	1.686769	-0.764054
38	H	-5.716049	-0.143166	-0.40557
39	H	-6.263246	1.292569	1.544178

40	H	-5.199803	-0.03895	2.023638
41	H	-4.537823	1.591115	1.818745
42	H	-6.161883	2.20978	-0.835943
43	H	-4.904398	1.66598	-1.955985
44	H	-4.480273	2.655328	-0.549954
45	H	-4.358158	-3.082185	0.554656
46	H	-0.059015	0.356944	1.748611
47	H	1.068436	1.690957	1.981815
48	H	-0.48522	1.984769	1.208299
49	H	3.034618	-0.785829	2.340319
50	H	4.47266	0.229488	2.245183
51	H	2.880545	0.971592	2.340242
52	H	4.920025	-1.79957	-1.695595

B3LYP/6-311G** Energy = -1080.3478351 a.u.; Population = 27.85%

(4S,5R,10R)-3		Standard Orientation		
Conformer 3		(Ångstroms)		
I	Atom	X	Y	Z
1	C	2.905786	2.655421	0.032258
2	C	3.892974	1.511746	-0.189671
3	C	3.367807	0.157697	0.355736
4	C	1.941085	-0.131201	-0.233892
5	C	0.934776	1.042433	-0.097408
6	C	1.561961	2.338101	-0.621452
7	C	1.39533	-1.490361	0.230141
8	C	0.257288	-2.04594	-0.640371
9	C	-1.075247	-1.36546	-0.466643
10	C	-1.222422	0.008283	-0.681524
11	O	-0.149688	0.790783	-1.069579
12	C	-2.211826	-2.088162	-0.107722
13	C	-3.456823	-1.475361	0.023469
14	C	-3.614519	-0.100226	-0.212455
15	C	-2.466853	0.617385	-0.559605
16	C	-4.963861	0.574593	-0.020023
17	C	-5.227391	0.823155	1.476728
18	C	-5.123094	1.87106	-0.819136
19	O	-4.496572	-2.294629	0.401761
20	C	0.325577	1.255236	1.285479
21	H	2.10017	-0.207257	-1.314133
22	C	3.435138	0.134683	1.889155
23	C	4.276585	-0.917425	-0.248299
24	O	4.904479	-1.688011	0.653004
25	O	4.436419	-1.078591	-1.442326

26	H	3.314378	3.572154	-0.402712
27	H	2.775363	2.851667	1.100483
28	H	4.856282	1.73392	0.279911
29	H	4.0714	1.406072	-1.263199
30	H	0.849767	3.155267	-0.47522
31	H	1.706394	2.22066	-1.70077
32	H	2.209877	-2.220143	0.195944
33	H	1.072321	-1.448603	1.273247
34	H	0.13169	-3.10862	-0.419938
35	H	0.562096	-1.975367	-1.692065
36	H	-2.142794	-3.156082	0.069395
37	H	-2.523459	1.682614	-0.743227
38	H	-5.740635	-0.110136	-0.386817
39	H	-6.222476	1.251656	1.629034
40	H	-5.165117	-0.104954	2.051162
41	H	-4.487618	1.521358	1.880063
42	H	-6.147892	2.239994	-0.72462
43	H	-4.914067	1.716827	-1.881168
44	H	-4.456508	2.655634	-0.450398
45	H	-5.335403	-1.821421	0.346738
46	H	-0.062408	0.336385	1.724485
47	H	1.059596	1.67229	1.972312
48	H	-0.497595	1.969192	1.207211
49	H	3.035167	-0.790648	2.304596
50	H	4.470572	0.232448	2.220509
51	H	2.876847	0.964454	2.316597
52	H	5.453333	-2.329727	0.171106

B3LYP/6-311G** Energy = -1080.3463546 a.u.; Population = 5.80%

(4S,5R,10R)-3		Standard Orientation		
Conformer 4		(Ångstroms)		
I	Atom	X	Y	Z
1	C	2.923835	2.635512	0.017139
2	C	3.907111	1.483396	-0.182572
3	C	3.367955	0.143255	0.387854
4	C	1.944092	-0.150696	-0.200764
5	C	0.943194	1.030242	-0.087198
6	C	1.579203	2.31314	-0.632666
7	C	1.392371	-1.498436	0.287775
8	C	0.254752	-2.066498	-0.574753
9	C	-1.075358	-1.375563	-0.422889
10	C	-1.215566	-0.005594	-0.66584
11	O	-0.137934	0.766711	-1.060258

12	C	-2.217934	-2.086462	-0.059258
13	C	-3.46198	-1.467007	0.048326
14	C	-3.612721	-0.096728	-0.218097
15	C	-2.459046	0.609695	-0.568141
16	C	-4.961389	0.586812	-0.054409
17	C	-5.238409	0.870804	1.433373
18	C	-5.108649	1.864852	-0.885015
19	O	-4.507391	-2.275293	0.434775
20	C	0.328388	1.271123	1.288351
21	H	2.094873	-0.245581	-1.279356
22	C	3.429618	0.150442	1.921014
23	C	4.308802	-0.956541	-0.107704
24	O	4.293659	-1.105242	-1.445017
25	O	5.029535	-1.635442	0.59503
26	H	3.337181	3.542526	-0.433425
27	H	2.793261	2.850473	1.081644
28	H	4.868457	1.707774	0.289481
29	H	4.091464	1.364021	-1.253465
30	H	0.871541	3.136873	-0.502235
31	H	1.724438	2.17598	-1.709567
32	H	2.205225	-2.23113	0.269825
33	H	1.066842	-1.435697	1.32899
34	H	0.12226	-3.123379	-0.331627
35	H	0.564513	-2.021103	-1.626453
36	H	-2.154475	-3.150843	0.139877
37	H	-2.509963	1.67112	-0.774133
38	H	-5.737026	-0.103451	-0.412831
39	H	-6.233011	1.306979	1.565871
40	H	-5.186088	-0.043889	2.029786
41	H	-4.499591	1.575047	1.827854
42	H	-6.133606	2.237876	-0.810418
43	H	-4.888379	1.685607	-1.940842
44	H	-4.444519	2.656536	-0.527208
45	H	-5.34453	-1.801245	0.364111
46	H	-0.064133	0.361778	1.742902
47	H	1.060252	1.699199	1.970673
48	H	-0.492404	1.985731	1.192671
49	H	3.029322	-0.770299	2.347458
50	H	4.466177	0.246333	2.249143
51	H	2.872901	0.98677	2.336423
52	H	4.92645	-1.804365	-1.67855

B3LYP/6-311G** Energy = -1080.3468942 a.u.; Population = 10.27%

(4S,5R,10R)-3		Standard Orientation		
Conformer 5		(Ångstroms)		
I	Atom	X	Y	Z
1	C	2.912367	2.65404	0.042246
2	C	3.896785	1.50898	-0.184989
3	C	3.368658	0.15387	0.355155
4	C	1.941096	-0.129085	-0.234915
5	C	0.937485	1.046253	-0.092974
6	C	1.567414	2.342627	-0.611995
7	C	1.392397	-1.489053	0.223345
8	C	0.251869	-2.037613	-0.648462
9	C	-1.078697	-1.354107	-0.47028
10	C	-1.222407	0.019398	-0.67879
11	O	-0.14789	0.800753	-1.065261
12	C	-2.217147	-2.077041	-0.108118
13	C	-3.459201	-1.460029	0.025947
14	C	-3.612421	-0.084259	-0.207012
15	C	-2.466474	0.63247	-0.552513
16	C	-4.971034	0.569727	-0.025145
17	C	-5.247919	0.815093	1.469242
18	C	-5.142407	1.863603	-0.825396
19	O	-4.577618	-2.172933	0.389605
20	C	0.329775	1.254949	1.291286
21	H	2.099415	-0.200831	-1.315565
22	C	3.436655	0.124544	1.88843
23	C	4.275085	-0.920562	-0.253641
24	O	4.905072	-1.693243	0.644473
25	O	4.431885	-1.079247	-1.448384
26	H	3.322924	3.571621	-0.389067
27	H	2.783017	2.846094	1.111363
28	H	4.860868	1.726942	0.284959
29	H	4.074339	1.407369	-1.25907
30	H	0.857213	3.160834	-0.461923
31	H	1.710916	2.22939	-1.691895
32	H	2.205168	-2.220661	0.184831
33	H	1.070612	-1.451346	1.267004
34	H	0.124147	-3.101066	-0.432739
35	H	0.555854	-1.963293	-1.70014
36	H	-2.137812	-3.145913	0.067577
37	H	-2.521801	1.698216	-0.734727
38	H	-5.719296	-0.144564	-0.38346
39	H	-6.250162	1.23047	1.61376
40	H	-5.179304	-0.112342	2.042564

41	H	-4.522792	1.52475	1.880478
42	H	-6.172284	2.220712	-0.737203
43	H	-4.92702	1.711647	-1.886843
44	H	-4.487714	2.658627	-0.456607
45	H	-4.343116	-3.103267	0.502778
46	H	-0.059405	0.335106	1.727149
47	H	1.064977	1.668308	1.979067
48	H	-0.492298	1.970505	1.21629
49	H	3.035192	-0.801777	2.300254
50	H	4.47238	0.219086	2.219775
51	H	2.880039	0.953579	2.319463
52	H	5.453084	-2.333671	0.159927

B3LYP/6-311G** Energy = -1080.3472777 a.u.; Population = 15.43%

(4S,5R,10R)-3		Standard Orientation		
Conformer 6		(Ångstroms)		
I	Atom	X	Y	Z
1	C	3.07131	2.578105	-0.097311
2	C	4.002621	1.384156	-0.290762
3	C	3.422626	0.071931	0.314369
4	C	1.97549	-0.1708	-0.219777
5	C	1.029583	1.057276	-0.130154
6	C	1.707439	2.295739	-0.723824
7	C	1.374521	-1.467841	0.343679
8	C	0.187597	-2.019472	-0.461141
9	C	-1.103538	-1.256022	-0.318585
10	C	-1.183768	0.104862	-0.631536
11	O	-0.079783	0.808201	-1.075643
12	C	-2.269948	-1.887517	0.108311
13	C	-3.48625	-1.210467	0.20295
14	C	-3.581093	0.146508	-0.145223
15	C	-2.398514	0.775127	-0.549341
16	C	-4.867996	0.958684	-0.100092
17	C	-5.944306	0.429985	-1.06447
18	C	-5.407131	1.145793	1.328711
19	O	-4.549215	-1.970494	0.642249
20	C	0.449367	1.373627	1.246146
21	H	2.094534	-0.320325	-1.296353
22	C	3.528035	0.088119	1.847556
23	C	4.315439	-1.023588	-0.272797
24	O	5.368179	-1.330143	0.503259
25	O	4.160748	-1.539858	-1.361803
26	H	3.515215	3.459575	-0.568961

27	H	2.966164	2.814265	0.965646
28	H	4.983148	1.57612	0.153526
29	H	4.155299	1.233279	-1.364614
30	H	1.035463	3.151095	-0.609424
31	H	1.83454	2.121785	-1.797659
32	H	2.152088	-2.236805	0.334269
33	H	1.081823	-1.342626	1.389076
34	H	0.008952	-3.054766	-0.161059
35	H	0.472329	-2.043185	-1.52063
36	H	-2.250389	-2.939812	0.371057
37	H	-2.420172	1.826886	-0.812726
38	H	-4.596263	1.955304	-0.459133
39	H	-6.795299	1.116806	-1.088672
40	H	-5.54551	0.346105	-2.078852
41	H	-6.32923	-0.553849	-0.779919
42	H	-6.271949	1.815519	1.320614
43	H	-4.641903	1.584598	1.974446
44	H	-5.727155	0.207469	1.7924
45	H	-5.342216	-1.433582	0.736856
46	H	0.039099	0.497759	1.747905
47	H	1.206799	1.81	1.894891
48	H	-0.351258	2.108636	1.135373
49	H	3.217953	-0.864223	2.280966
50	H	4.555996	0.27925	2.156931
51	H	2.904474	0.869449	2.275634
52	H	5.919136	-1.971621	0.02366

B3LYP/6-311G** Energy = -1080.3442745 a.u.; Population = 0.64%

(4S,5R,10R)-3		Standard Orientation		
Conformer 7		(Ångstroms)		
I	Atom	X	Y	Z
1	C	3.096663	2.586935	-0.083914
2	C	4.025167	1.387523	-0.264939
3	C	3.439091	0.089721	0.35498
4	C	1.992316	-0.15945	-0.19751
5	C	1.047092	1.068648	-0.109884
6	C	1.729711	2.304548	-0.704884
7	C	1.390632	-1.461429	0.352367
8	C	0.209982	-2.008824	-0.464209
9	C	-1.083043	-1.248659	-0.321444
10	C	-1.163568	0.114452	-0.623969
11	O	-0.058726	0.82185	-1.059573
12	C	-2.250637	-1.885364	0.0943

13	C	-3.468464	-1.210851	0.187381
14	C	-3.563378	0.148804	-0.150653
15	C	-2.379578	0.782505	-0.542879
16	C	-4.852027	0.958374	-0.107923
17	C	-5.920642	0.435251	-1.083879
18	C	-5.401241	1.13348	1.318494
19	O	-4.532677	-1.976063	0.61403
20	C	0.464512	1.380504	1.265635
21	H	2.117604	-0.30013	-1.274308
22	C	3.531041	0.139049	1.885697
23	C	4.323194	-1.06293	-0.125055
24	O	4.273076	-1.250504	-1.456569
25	O	5.031605	-1.748253	0.583797
26	H	3.541746	3.461832	-0.566569
27	H	2.992459	2.837748	0.975701
28	H	5.003892	1.583013	0.183595
29	H	4.18417	1.228911	-1.334763
30	H	1.060322	3.162029	-0.591017
31	H	1.852958	2.127788	-1.778719
32	H	2.169194	-2.230761	0.346069
33	H	1.091164	-1.344843	1.396751
34	H	0.032084	-3.04694	-0.173911
35	H	0.500404	-2.022638	-1.522347
36	H	-2.230831	-2.93969	0.348701
37	H	-2.401485	1.836144	-0.798583
38	H	-4.579607	1.958204	-0.457371
39	H	-6.772697	1.120708	-1.108781
40	H	-5.514589	0.359952	-2.096059
41	H	-6.305717	-0.551439	-0.809726
42	H	-6.267642	1.801123	1.309528
43	H	-4.641456	1.56923	1.972647
44	H	-5.721991	0.190889	1.77295
45	H	-5.327229	-1.441431	0.708446
46	H	0.041759	0.504108	1.756274
47	H	1.224752	1.799419	1.922221
48	H	-0.326986	2.125824	1.158228
49	H	3.108348	-0.754691	2.34651
50	H	4.57646	0.208641	2.191706
51	H	3.010931	1.005537	2.286783
52	H	4.874814	-1.978508	-1.683695

B3LYP/6-311G** Energy = -1080.3449437 a.u.; Population = 1.30%

(4S,5R,10R)-3	Standard Orientation

Conformer 8		(Ångstroms)		
I	Atom	X	Y	Z
1	C	2.905786	2.655419	0.032261
2	C	3.892974	1.511744	-0.189674
3	C	3.367806	0.157694	0.355735
4	C	1.941083	-0.131201	-0.233889
5	C	0.934775	1.042433	-0.097406
6	C	1.561961	2.338101	-0.621449
7	C	1.395331	-1.490361	0.230146
8	C	0.257288	-2.045942	-0.640364
9	C	-1.075246	-1.36546	-0.466639
10	C	-1.222421	0.008283	-0.681524
11	O	-0.149688	0.790784	-1.069577
12	C	-2.211826	-2.088161	-0.107717
13	C	-3.456824	-1.475361	0.023471
14	C	-3.61452	-0.100226	-0.212457
15	C	-2.466854	0.617384	-0.559609
16	C	-4.963863	0.574593	-0.020028
17	C	-5.227394	0.823151	1.476725
18	C	-5.123095	1.871061	-0.819138
19	O	-4.496573	-2.294626	0.401767
20	C	0.325574	1.255237	1.285481
21	H	2.100166	-0.207258	-1.31413
22	C	3.435141	0.134681	1.889153
23	C	4.276586	-0.917424	-0.248304
24	O	4.904502	-1.687994	0.652997
25	O	4.4364	-1.078602	-1.442332
26	H	3.314378	3.572154	-0.402706
27	H	2.775365	2.851661	1.100487
28	H	4.856285	1.733916	0.279905
29	H	4.071394	1.406071	-1.263202
30	H	0.849768	3.155267	-0.475216
31	H	1.706394	2.220661	-1.700767
32	H	2.209879	-2.220143	0.195947
33	H	1.072324	-1.448603	1.273252
34	H	0.131689	-3.10862	-0.41993
35	H	0.562096	-1.97537	-1.692059
36	H	-2.142794	-3.156081	0.069402
37	H	-2.52346	1.682613	-0.743234
38	H	-5.740635	-0.110137	-0.386824
39	H	-6.22248	1.25165	1.629031
40	H	-5.165118	-0.104959	2.051156
41	H	-4.487621	1.521355	1.88006

42	H	-6.147893	2.239994	-0.724622
43	H	-4.914066	1.716829	-1.88117
44	H	-4.45651	2.655634	-0.450398
45	H	-5.335405	-1.821425	0.346717
46	H	-0.06241	0.336386	1.724489
47	H	1.059591	1.672295	1.972313
48	H	-0.4976	1.969191	1.207211
49	H	3.035186	-0.790658	2.304594
50	H	4.470574	0.232462	2.220506
51	H	2.876837	0.964442	2.316598
52	H	5.453357	-2.329708	0.171097

B3LYP/6-311G** Energy = -1080.3463546 a.u.; Population = 5.80%

(4S,5R,10R)-3		Standard Orientation		
Conformer 9		(Ångstroms)		
I	Atom	X	Y	Z
1	C	3.088274	2.571581	-0.104622
2	C	4.011005	1.370252	-0.293737
3	C	3.421761	0.064402	0.316234
4	C	1.973196	-0.169363	-0.21747
5	C	1.035616	1.065209	-0.129945
6	C	1.721646	2.2968	-0.72846
7	C	1.362588	-1.461613	0.346717
8	C	0.177215	-2.008641	-0.463722
9	C	-1.111458	-1.239786	-0.326441
10	C	-1.18368	0.122058	-0.629772
11	O	-0.076247	0.821389	-1.072982
12	C	-2.285544	-1.872556	0.085981
13	C	-3.498027	-1.189342	0.176929
14	C	-3.579093	0.174799	-0.14616
15	C	-2.395337	0.801291	-0.54041
16	C	-4.867952	0.975986	-0.070998
17	C	-5.935209	0.464384	-1.051904
18	C	-5.417061	1.068568	1.361849
19	O	-4.642125	-1.835823	0.582317
20	C	0.458801	1.389425	1.24582
21	H	2.091534	-0.321081	-1.293822
22	C	3.527313	0.085237	1.849264
23	C	4.306822	-1.039502	-0.266888
24	O	5.360391	-1.346709	0.507845
25	O	4.146202	-1.561861	-1.352165
26	H	3.538144	3.447671	-0.580657
27	H	2.985937	2.813275	0.957351

28	H	4.992938	1.556993	0.14965
29	H	4.162461	1.214227	-1.367049
30	H	1.056091	3.157457	-0.616323
31	H	1.846089	2.118124	-1.801842
32	H	2.13606	-2.234704	0.343862
33	H	1.064717	-1.331865	1.390128
34	H	-0.006488	-3.043347	-0.164373
35	H	0.46717	-2.034062	-1.521753
36	H	-2.260553	-2.929685	0.334826
37	H	-2.409332	1.856629	-0.789876
38	H	-4.606606	1.992698	-0.381604
39	H	-6.8079	1.124706	-1.038812
40	H	-5.546133	0.439896	-2.073917
41	H	-6.267937	-0.542009	-0.790967
42	H	-6.287398	1.731469	1.391104
43	H	-4.66258	1.472	2.043438
44	H	-5.723896	0.089823	1.735617
45	H	-4.441586	-2.764682	0.756132
46	H	0.042219	0.517707	1.749669
47	H	1.219546	1.821988	1.893233
48	H	-0.336517	2.129922	1.133408
49	H	3.207227	-0.86221	2.286216
50	H	4.557137	0.26692	2.158069
51	H	2.911976	0.874668	2.274341
52	H	5.906679	-1.993643	0.030237

B3LYP/6-311G** Energy = -1080.3463402 a.u.; Population = 5.71%

(4S,5R,10R)-3		Standard Orientation		
Conformer 10		(Ångstroms)		
I	Atom	X	Y	Z
1	C	3.114183	2.580052	-0.090735
2	C	4.033867	1.373266	-0.267952
3	C	3.438386	0.08201	0.356531
4	C	1.990197	-0.158013	-0.195648
5	C	1.053429	1.076575	-0.109328
6	C	1.744243	2.305741	-0.708785
7	C	1.379136	-1.455667	0.354265
8	C	0.199554	-1.997656	-0.467608
9	C	-1.090773	-1.231929	-0.329063
10	C	-1.163358	0.132102	-0.621703
11	O	-0.055168	0.835698	-1.056342
12	C	-2.26587	-1.869801	0.072379
13	C	-3.479845	-1.189129	0.162085

14	C	-3.561267	0.177414	-0.151112
15	C	-2.376382	0.808983	-0.533444
16	C	-4.852246	0.975462	-0.079293
17	C	-5.91085	0.46904	-1.072238
18	C	-5.412318	1.056105	1.349975
19	O	-4.625073	-1.840526	0.555766
20	C	0.474714	1.395739	1.265982
21	H	2.114816	-0.300375	-1.272307
22	C	3.53057	0.136025	1.886967
23	C	4.313652	-1.078996	-0.119395
24	O	4.26246	-1.270631	-1.450291
25	O	5.016636	-1.767467	0.591889
26	H	3.565214	3.449599	-0.577576
27	H	3.013151	2.83604	0.967947
28	H	5.01411	1.56328	0.179664
29	H	4.191452	1.209701	-1.337249
30	H	1.081436	3.168551	-0.596583
31	H	1.864452	2.124792	-1.782289
32	H	2.153529	-2.229266	0.353218
33	H	1.075237	-1.335399	1.396982
34	H	0.016532	-3.035336	-0.178614
35	H	0.494644	-2.01256	-1.52445
36	H	-2.240534	-2.928808	0.31301
37	H	-2.39075	1.86609	-0.775298
38	H	-4.590634	1.994988	-0.380297
39	H	-6.78498	1.127493	-1.060947
40	H	-5.513829	0.453071	-2.091379
41	H	-6.243482	-0.539968	-0.821424
42	H	-6.284391	1.716805	1.377505
43	H	-4.6639	1.45621	2.040157
44	H	-5.719631	0.073887	1.714067
45	H	-4.423711	-2.770035	0.725515
46	H	0.046437	0.523195	1.758793
47	H	1.238158	1.811359	1.920969
48	H	-0.311949	2.145992	1.157317
49	H	3.097348	-0.750996	2.351095
50	H	4.576642	0.194753	2.193004
51	H	3.02055	1.010113	2.284533
52	H	4.85911	-2.00369	-1.674831

B3LYP/6-311G** Energy = -1080.3470229 a.u.; Population = 11.77%

Table S7. Cartesian coordinates for the re-optimized conformers of (4R,5R,9R,10R)-**4** at the B3LYP/6-311G** level and London dispersion corrections with SMD solvent model for Methanol.

(4R,5R,9R,10R)-4		Standard Orientation		
Conformer 1		(Ångstroms)		
I	Atom	X	Y	Z
1	C	2.839359	2.456558	0.280755
2	C	3.614608	1.238698	0.781433
3	C	3.253734	-0.043655	-0.013294
4	C	1.698871	-0.243821	0.008905
5	C	0.825779	0.993118	-0.361714
6	C	1.33328	2.229782	0.410244
7	C	1.252064	-1.485006	-0.770503
8	C	-0.226437	-1.670721	-0.717491
9	C	-1.077444	-0.723956	-0.296684
10	C	-0.612114	0.650517	0.142871
11	C	-2.522731	-1.066408	-0.18159
12	C	-3.464558	0.00195	0.216639
13	C	-3.047474	1.279922	0.189212
14	C	-1.668883	1.711068	-0.197609
15	O	-2.932456	-2.21259	-0.397869
16	C	-4.890082	-0.413737	0.531878
17	C	-5.593514	0.524192	1.516295
18	C	-5.707854	-0.553577	-0.764432
19	H	1.462798	-0.43665	1.059723
20	C	3.893764	0.010415	-1.408331
21	C	3.859153	-1.243181	0.717195
22	O	3.439923	-1.35903	1.991042
23	O	4.641624	-2.038068	0.236872
24	C	0.802813	1.283536	-1.872453
25	H	-0.557559	0.626926	1.239974
26	H	3.105943	2.683224	-0.755692
27	H	3.127886	3.331331	0.871835
28	H	3.378164	1.08502	1.837495
29	H	4.693811	1.407177	0.712197
30	H	0.792493	3.118127	0.072588
31	H	1.09544	2.097972	1.473017
32	H	1.568607	-1.439678	-1.819393
33	H	1.731633	-2.384278	-0.365539
34	H	-0.627713	-2.63325	-1.019135
35	H	-3.75399	2.07238	0.417609
36	H	-1.675239	1.92468	-1.273066
37	H	-1.43171	2.65418	0.298522
38	H	-4.832598	-1.405628	0.990783
39	H	-6.572613	0.116824	1.783884
40	H	-5.01444	0.646522	2.436096

41	H	-5.759497	1.51598	1.085525
42	H	-6.713132	-0.92764	-0.547284
43	H	-5.231796	-1.246356	-1.461627
44	H	-5.805567	0.417582	-1.260203
45	H	3.608596	-0.839492	-2.028895
46	H	4.981169	-0.004126	-1.310135
47	H	3.624752	0.922729	-1.934746
48	H	3.86175	-2.14459	2.376697
49	H	0.341252	0.471614	-2.438408
50	H	0.23337	2.19266	-2.076535
51	H	1.801458	1.440094	-2.273602

B3LYP/6-311G** Energy = -1005.0786947 a.u.; Population = 38.50%

(4R,5R,9R,10R)-4		Standard Orientation		
Conformer 2		(Ångstroms)		
I	Atom	X	Y	Z
1	C	-2.825	2.431813	-0.280841
2	C	-3.595624	1.211034	-0.77734
3	C	-3.219758	-0.079342	0.008386
4	C	-1.673015	-0.260122	0.005522
5	C	-0.802924	0.988992	0.350885
6	C	-1.32017	2.213938	-0.430922
7	C	-1.219292	-1.474723	0.822528
8	C	0.25955	-1.657625	0.767386
9	C	1.105543	-0.720119	0.316009
10	C	0.632282	0.640877	-0.157115
11	C	2.550948	-1.060924	0.203057
12	C	3.487038	-0.001782	-0.232024
13	C	3.065957	1.275138	-0.239843
14	C	1.688778	1.713477	0.144053
15	O	2.966368	-2.198753	0.451242
16	C	4.912054	-0.422306	-0.54336
17	C	5.607937	0.489933	-1.556785
18	C	5.737005	-0.52454	0.752
19	H	-1.428936	-0.481966	-1.037488
20	C	-3.870277	-0.060377	1.40329
21	C	-3.822047	-1.214717	-0.822912
22	O	-5.122578	-1.431051	-0.558492
23	O	-3.244222	-1.841245	-1.689123
24	C	-0.767977	1.310785	1.855471
25	H	0.567273	0.587661	-1.252615
26	H	-3.081627	2.647919	0.760592
27	H	-3.129515	3.306798	-0.863531

28	H	-3.360229	1.058428	-1.836813
29	H	-4.674901	1.368977	-0.70473
30	H	-0.779098	3.108262	-0.109882
31	H	-1.096479	2.071496	-1.495441
32	H	-1.529505	-1.39449	1.871441
33	H	-1.699425	-2.384652	0.446699
34	H	0.666215	-2.610127	1.093011
35	H	3.768391	2.062684	-0.496213
36	H	1.703238	1.959185	1.212588
37	H	1.445233	2.640976	-0.377866
38	H	4.854777	-1.426693	-0.974334
39	H	6.586647	0.077682	-1.818267
40	H	5.023746	0.585679	-2.476499
41	H	5.773717	1.493529	-1.154171
42	H	6.74218	-0.901746	0.539816
43	H	5.2664	-1.199388	1.470158
44	H	5.834625	0.460052	1.220585
45	H	-3.706027	-0.997044	1.939126
46	H	-4.946648	0.088622	1.314688
47	H	-3.476111	0.749158	2.012402
48	H	-5.443251	-2.115553	-1.169564
49	H	-0.327051	0.501405	2.440685
50	H	-0.175163	2.209508	2.037675
51	H	-1.761083	1.505587	2.254268

B3LYP/6-311G** Energy = -1005.0780882 a.u.; Population = 20.24%

(4R,5R,9R,10R)-4		Standard Orientation		
Conformer 3		(Ångstroms)		
I	Atom	X	Y	Z
1	C	2.816126	2.488654	0.246798
2	C	3.596461	1.288421	0.778746
3	C	3.251602	-0.017154	0.020022
4	C	1.69527	-0.225474	0.038843
5	C	0.816262	0.996457	-0.364341
6	C	1.311784	2.255139	0.378514
7	C	1.256764	-1.487404	-0.712174
8	C	-0.220789	-1.680478	-0.658225
9	C	-1.078396	-0.728846	-0.263119
10	C	-0.622331	0.659107	0.141289
11	C	-2.521821	-1.076833	-0.141624
12	C	-3.472332	-0.001739	0.215793
13	C	-3.061572	1.277037	0.152868
14	C	-1.682148	1.704602	-0.234514

15	O	-2.92285	-2.232474	-0.320407
16	C	-4.898237	-0.415132	0.532243
17	C	-5.617947	0.553406	1.474304
18	C	-5.701964	-0.608271	-0.765982
19	H	1.46393	-0.394479	1.096251
20	C	3.901863	0.002173	-1.372101
21	C	3.802455	-1.177439	0.853233
22	O	4.514153	-2.076155	0.154369
23	O	3.609237	-1.31187	2.045778
24	C	0.801918	1.247597	-1.882402
25	H	-0.573892	0.665588	1.238895
26	H	3.083182	2.692204	-0.794563
27	H	3.09794	3.379523	0.816642
28	H	3.355326	1.152815	1.836436
29	H	4.675022	1.463107	0.712076
30	H	0.765078	3.130751	0.01796
31	H	1.072311	2.147074	1.443549
32	H	1.575879	-1.463801	-1.761046
33	H	1.739364	-2.374749	-0.286368
34	H	-0.615218	-2.653013	-0.935785
35	H	-3.774168	2.072117	0.351121
36	H	-1.681375	1.890428	-1.315175
37	H	-1.453714	2.661571	0.238665
38	H	-4.839051	-1.388841	1.028357
39	H	-6.596507	0.14867	1.747759
40	H	-5.048734	0.714434	2.39429
41	H	-5.787156	1.527125	1.005284
42	H	-6.707007	-0.980723	-0.545037
43	H	-5.2147	-1.322981	-1.432552
44	H	-5.800792	0.343394	-1.298029
45	H	3.611681	-0.851255	-1.984607
46	H	4.989059	-0.015828	-1.270173
47	H	3.642794	0.910129	-1.91211
48	H	4.797648	-2.777348	0.765526
49	H	0.340208	0.422694	-2.429114
50	H	0.237112	2.153197	-2.113292
51	H	1.80365	1.389243	-2.281891

B3LYP/6-311G** Energy = -1005.0783444 a.u.; Population = 26.56%

(4R,5R,9R,10R)-4		Standard Orientation		
Conformer 4		(Ångstroms)		
I	Atom	X	Y	Z
1	C	2.971102	2.300468	0.623347

2	C	3.655373	0.972341	0.943819
3	C	3.216489	-0.1564	-0.026477
4	C	1.651773	-0.247747	-0.037964
5	C	0.870945	1.088026	-0.228687
6	C	1.451841	2.161635	0.716002
7	C	1.129506	-1.327924	-0.990776
8	C	-0.359042	-1.413629	-0.97128
9	C	-1.148347	-0.480656	-0.419685
10	C	-0.593393	0.778321	0.216752
11	C	-2.617847	-0.734688	-0.366202
12	C	-3.481318	0.316427	0.216458
13	C	-2.973639	1.55328	0.36875
14	C	-1.572382	1.946065	0.027632
15	O	-3.097175	-1.792778	-0.787938
16	C	-4.930232	0.015516	0.561362
17	C	-5.799982	-0.216295	-0.685401
18	C	-5.066417	-1.140102	1.564535
19	H	1.388745	-0.572438	0.973145
20	C	3.876263	0.047667	-1.397961
21	C	3.735867	-1.483068	0.530919
22	O	3.272738	-1.762879	1.763525
23	O	4.494432	-2.237949	-0.04306
24	C	0.887461	1.594811	-1.681171
25	H	-0.555337	0.594246	1.299217
26	H	3.264696	2.656696	-0.368464
27	H	3.311789	3.057965	1.336125
28	H	3.397515	0.685978	1.966783
29	H	4.744273	1.073509	0.900498
30	H	0.976225	3.124623	0.510895
31	H	1.192883	1.893097	1.747623
32	H	1.462084	-1.152627	-2.020897
33	H	1.538718	-2.308923	-0.72069
34	H	-0.821854	-2.290541	-1.413066
35	H	-3.629755	2.34084	0.732369
36	H	-1.562439	2.299938	-1.010028
37	H	-1.274091	2.796638	0.643358
38	H	-5.308684	0.917684	1.05379
39	H	-6.851829	-0.308332	-0.397117
40	H	-5.713992	0.622016	-1.382888
41	H	-5.510069	-1.127637	-1.210356
42	H	-6.109797	-1.245868	1.87659
43	H	-4.46473	-0.955515	2.459431
44	H	-4.746232	-2.088369	1.128847

45	H	3.550858	-0.693946	-2.128011
46	H	4.9597	-0.042774	-1.297488
47	H	3.665907	1.035635	-1.799292
48	H	3.649043	-2.614655	2.040734
49	H	0.387539	0.903034	-2.362331
50	H	0.375357	2.556468	-1.753899
51	H	1.899394	1.747812	-2.048921

B3LYP/6-311G** Energy = -1005.0777859 a.u.; Population = 14.69%

Table S8. Cartesian coordinates for the re-optimized conformers of (4S,5S,9S,10S)-**4** at the B3LYP/6-311G** level and London dispersion corrections with SMD solvent model for Methanol.

(4S,5S,9S,10S)-4		Standard Orientation		
Conformer 1		(Ångstroms)		
I	Atom	X	Y	Z
1	C	-2.839358	2.456558	0.280751
2	C	-3.61461	1.238699	0.781428
3	C	-3.253735	-0.043655	-0.013299
4	C	-1.698873	-0.243821	0.008906
5	C	-0.825778	0.993117	-0.361712
6	C	-1.33328	2.229782	0.410244
7	C	-1.252063	-1.485009	-0.770497
8	C	0.226437	-1.670723	-0.717482
9	C	1.077444	-0.723957	-0.296676
10	C	0.612113	0.650515	0.142879
11	C	2.522731	-1.06641	-0.181581
12	C	3.464559	0.00195	0.216641
13	C	3.047474	1.279922	0.189217
14	C	1.668882	1.711069	-0.197596
15	O	2.932455	-2.212593	-0.397854
16	C	4.890086	-0.413736	0.531871
17	C	5.707847	-0.553581	-0.764445
18	C	5.593526	0.524198	1.516278
19	H	-1.462804	-0.436648	1.059725
20	C	-3.893762	0.010417	-1.408338
21	C	-3.859157	-1.243178	0.71719
22	O	-3.439924	-1.35903	1.991036
23	O	-4.641633	-2.038062	0.236869
24	C	-0.802807	1.283534	-1.872451
25	H	0.557553	0.626923	1.239981
26	H	-3.127887	3.331332	0.87183
27	H	-3.10594	2.683224	-0.755696
28	H	-4.693813	1.407178	0.712189
29	H	-3.378168	1.08502	1.837491

30	H	-1.095442	2.097972	1.473017
31	H	-0.792492	3.118126	0.072589
32	H	-1.731632	-2.38428	-0.36553
33	H	-1.568604	-1.439685	-1.819388
34	H	0.627714	-2.633252	-1.019124
35	H	3.75399	2.07238	0.417609
36	H	1.431709	2.654176	0.298543
37	H	1.675236	1.92469	-1.273051
38	H	4.832605	-1.405624	0.990782
39	H	6.713127	-0.927644	-0.547303
40	H	5.231784	-1.246363	-1.461633
41	H	5.805557	0.417575	-1.26022
42	H	6.572627	0.11683	1.783861
43	H	5.01446	0.646533	2.436083
44	H	5.759507	1.515983	1.085502
45	H	-3.608596	-0.839493	-2.0289
46	H	-4.981167	-0.004121	-1.310143
47	H	-3.624745	0.922728	-1.934752
48	H	-3.861755	-2.144588	2.376692
49	H	-0.341245	0.471612	-2.438405
50	H	-1.801451	1.440094	-2.273603
51	H	-0.233363	2.192658	-2.076532

B3LYP/6-311G** Energy = -1005.0786947 a.u.; Population = 35.63%

(4S,5S,9S,10S)-4		Standard Orientation		
Conformer 2		(Ångstroms)		
I	Atom	X	Y	Z
1	C	2.825	2.431813	-0.280828
2	C	3.595621	1.211036	-0.777337
3	C	3.219759	-0.079342	0.008388
4	C	1.673016	-0.260121	0.005527
5	C	0.802923	0.988991	0.350892
6	C	1.320169	2.213941	-0.430907
7	C	1.219294	-1.474727	0.822525
8	C	-0.259549	-1.657627	0.767385
9	C	-1.105541	-0.72012	0.316008
10	C	-0.632278	0.640874	-0.157119
11	C	-2.550947	-1.060924	0.20306
12	C	-3.487036	-0.001783	-0.232027
13	C	-3.065953	1.275136	-0.239858
14	C	-1.688773	1.713479	0.144031
15	O	-2.966366	-2.198752	0.451249
16	C	-4.912052	-0.422308	-0.543356

17	C	-5.736998	-0.524537	0.752007
18	C	-5.607938	0.489931	-1.55678
19	H	1.428938	-0.481961	-1.037485
20	C	3.870284	-0.060378	1.403287
21	C	3.822042	-1.214713	-0.822919
22	O	5.122564	-1.431076	-0.558481
23	O	3.244218	-1.841211	-1.689154
24	C	0.767966	1.310779	1.855479
25	H	-0.567257	0.587653	-1.252618
26	H	3.129514	3.306801	-0.863514
27	H	3.081631	2.647912	0.760606
28	H	4.674899	1.368979	-0.704731
29	H	3.360221	1.058432	-1.836809
30	H	1.096475	2.071507	-1.495427
31	H	0.779099	3.108264	-0.109859
32	H	1.699424	-2.384654	0.446686
33	H	1.529511	-1.394504	1.871438
34	H	-0.666215	-2.610127	1.093012
35	H	-3.768387	2.062681	-0.496234
36	H	-1.445227	2.640969	-0.377905
37	H	-1.703236	1.959209	1.212561
38	H	-4.854777	-1.426696	-0.974329
39	H	-6.742174	-0.901742	0.539827
40	H	-5.26639	-1.199385	1.470164
41	H	-5.834615	0.460055	1.220591
42	H	-6.58665	0.07768	-1.818257
43	H	-5.02375	0.585674	-2.476496
44	H	-5.773715	1.493528	-1.154168
45	H	3.706033	-0.997045	1.939125
46	H	4.946656	0.088618	1.314681
47	H	3.476121	0.749158	2.012399
48	H	5.443235	-2.115568	-1.169566
49	H	0.327059	0.501387	2.44069
50	H	1.761067	1.505606	2.254278
51	H	0.17513	2.209487	2.037683

B3LYP/6-311G** Energy = -1005.0780882 a.u.; Population = 18.73%

(4S,5S,9S,10S)-4		Standard Orientation		
Conformer 3		(Ångstroms)		
I	Atom	X	Y	Z
1	C	-2.816127	2.488655	0.246805
2	C	-3.596464	1.288422	0.778746
3	C	-3.251604	-0.017148	0.020018

4	C	-1.695272	-0.225474	0.038845
5	C	-0.816264	0.996457	-0.364331
6	C	-1.311786	2.255138	0.378526
7	C	-1.256763	-1.487401	-0.712174
8	C	0.220789	-1.680476	-0.658211
9	C	1.078392	-0.728846	-0.263097
10	C	0.622329	0.65911	0.141301
11	C	2.521816	-1.076837	-0.141582
12	C	3.472332	-0.001734	0.215797
13	C	3.061572	1.27704	0.152854
14	C	1.682144	1.704603	-0.234511
15	O	2.922838	-2.232485	-0.320323
16	C	4.898241	-0.415123	0.532232
17	C	5.701936	-0.608313	-0.766006
18	C	5.61798	0.553442	1.474242
19	H	-1.463937	-0.394483	1.096254
20	C	-3.90186	0.002189	-1.372107
21	C	-3.802458	-1.177442	0.853217
22	O	-4.514095	-2.076185	0.154326
23	O	-3.609283	-1.311861	2.045768
24	C	-0.801916	1.247599	-1.882392
25	H	0.57389	0.665597	1.238907
26	H	-3.097941	3.379523	0.816652
27	H	-3.083179	2.692209	-0.794556
28	H	-4.675024	1.463108	0.712073
29	H	-3.355333	1.152811	1.836436
30	H	-1.072318	2.147067	1.443561
31	H	-0.765075	3.130748	0.017977
32	H	-1.739365	-2.374747	-0.286374
33	H	-1.575872	-1.463794	-1.761047
34	H	0.61522	-2.653012	-0.935763
35	H	3.774173	2.072123	0.351078
36	H	1.453714	2.661571	0.238672
37	H	1.68136	1.890432	-1.315171
38	H	4.839061	-1.388813	1.028382
39	H	6.706982	-0.980764	-0.545072
40	H	5.214651	-1.323043	-1.432539
41	H	5.800757	0.343334	-1.298087
42	H	6.596541	0.148705	1.74769
43	H	5.048787	0.714508	2.394234
44	H	5.787188	1.527143	1.005184
45	H	-3.611655	-0.85122	-1.984629
46	H	-4.989056	-0.01584	-1.270182

47	H	-3.64281	0.910163	-1.912095
48	H	-4.79759	-2.777389	0.765471
49	H	-0.340188	0.422704	-2.429099
50	H	-1.803647	1.389228	-2.281887
51	H	-0.237123	2.153209	-2.113277

B3LYP/6-311G** Energy = -1005.0783444 a.u.; Population = 24.58%

(4S,5S,9S,10S)-4		Standard Orientation		
Conformer 4		(Ångstroms)		
I	Atom	X	Y	Z
1	C	-2.971072	2.30053	0.623096
2	C	-3.655434	0.972455	0.943606
3	C	-3.216483	-0.156416	-0.026512
4	C	-1.651768	-0.247767	-0.037921
5	C	-0.870934	1.087987	-0.228716
6	C	-1.451829	2.161633	0.715904
7	C	-1.129504	-1.327955	-0.990708
8	C	0.359037	-1.413679	-0.971192
9	C	1.148347	-0.480697	-0.419629
10	C	0.593388	0.778294	0.216772
11	C	2.61782	-0.734723	-0.366115
12	C	3.481322	0.316432	0.21639
13	C	2.973645	1.55329	0.368674
14	C	1.572359	1.946052	0.027686
15	O	3.097106	-1.792899	-0.787718
16	C	4.930281	0.015609	0.561177
17	C	5.066592	-1.139633	1.564775
18	C	5.79988	-0.21666	-0.685604
19	H	-1.388767	-0.572402	0.973207
20	C	-3.876161	0.047386	-1.398065
21	C	-3.73589	-1.482967	0.531043
22	O	-3.272984	-1.76252	1.76379
23	O	-4.494269	-2.238009	-0.042964
24	C	-0.887461	1.59468	-1.681234
25	H	0.555292	0.594218	1.299233
26	H	-3.311786	3.058093	1.335784
27	H	-3.264552	2.656704	-0.368765
28	H	-4.744324	1.073647	0.90016
29	H	-3.397696	0.686174	1.966622
30	H	-1.192978	1.893096	1.747551
31	H	-0.976139	3.124584	0.510816
32	H	-1.538737	-2.308949	-0.72065
33	H	-1.462051	-1.152631	-2.020835

34	H	0.82184	-2.290624	-1.412922
35	H	3.62979	2.340881	0.732168
36	H	1.274091	2.79657	0.643491
37	H	1.562367	2.300004	-1.009944
38	H	5.3088	0.917955	1.053217
39	H	6.110018	-1.245338	1.876685
40	H	4.465074	-0.95467	2.459705
41	H	4.746278	-2.088041	1.1295
42	H	6.851768	-0.30847	-0.397408
43	H	5.713731	0.621337	-1.383446
44	H	5.509988	-1.128251	-1.210132
45	H	-3.550662	-0.694349	-2.127948
46	H	-4.959602	-0.04308	-1.297658
47	H	-3.665802	1.035284	-1.799551
48	H	-3.649283	-2.61426	2.041086
49	H	-0.387374	0.90295	-2.362321
50	H	-1.899393	1.747462	-2.049075
51	H	-0.375529	2.556422	-1.753999

B3LYP/6-311G** Energy = -1005.0777859 a.u.; Population = 13.60%

(4S,5S,9S,10S)-4		Standard Orientation		
Conformer 5		(Ångstroms)		
I	Atom	X	Y	Z
1	C	2.953384	2.285253	-0.62134
2	C	3.632645	0.956246	-0.942245
3	C	3.182846	-0.178255	0.024139
4	C	1.627325	-0.252601	0.050204
5	C	0.847029	1.088074	0.218692
6	C	1.435032	2.152386	-0.730705
7	C	1.104046	-1.308426	1.029556
8	C	-0.384489	-1.394887	1.007627
9	C	-1.172019	-0.475098	0.431144
10	C	-0.613791	0.769551	-0.231384
11	C	-2.640879	-0.730458	0.377784
12	C	-3.501819	0.304683	-0.236582
13	C	-2.994075	1.537498	-0.418465
14	C	-1.595369	1.940298	-0.078679
15	O	-3.122785	-1.776906	0.825396
16	C	-4.948719	-0.006025	-0.581374
17	C	-5.078552	-1.18624	-1.556308
18	C	-5.824966	-0.208204	0.666028
19	H	1.357585	-0.60113	-0.950972
20	C	3.848594	0.002338	1.399298

21	C	3.694327	-1.460565	-0.637164
22	O	4.954969	-1.77253	-0.290496
23	O	3.082371	-2.12632	-1.449219
24	C	0.851285	1.620365	1.662735
25	H	-0.566144	0.560131	-1.308836
26	H	3.307173	3.045487	-1.324708
27	H	3.240061	2.62901	0.377025
28	H	4.721256	1.048797	-0.898865
29	H	3.37108	0.669562	-1.966961
30	H	1.186187	1.877123	-1.763048
31	H	0.960303	3.118198	-0.537036
32	H	1.516408	-2.292674	0.781461
33	H	1.433665	-1.10594	2.05582
34	H	-0.84956	-2.261181	1.467774
35	H	-3.648673	2.314694	-0.806359
36	H	-1.29365	2.775135	-0.714027
37	H	-1.593304	2.32087	0.949543
38	H	-5.325356	0.883402	-1.097768
39	H	-6.120117	-1.300829	-1.871321
40	H	-4.472079	-1.023481	-2.452187
41	H	-4.759962	-2.122937	-1.095185
42	H	-6.875413	-0.306053	0.374563
43	H	-5.741841	0.645838	1.344525
44	H	-5.538523	-1.107466	1.213158
45	H	3.624362	-0.828675	2.070364
46	H	4.931819	0.058931	1.289179
47	H	3.519592	0.920576	1.879176
48	H	5.222079	-2.555606	-0.800614
49	H	0.374384	0.928143	2.35938
50	H	1.859365	1.812522	2.023674
51	H	0.311845	2.568001	1.719023

B3LYP/6-311G** Energy = -1005.0772191 a.u.; Population = 7.46%

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S39. Raw bioactivity data

compound	PDE4D inhibition		compound	PDE4D inhibition	
	10 μM	5 μM		10 μM	5 μM
1	5.1%		**16**	17.0%	
2	3.3%		**17**	49.7%	
3	17.5%		**18**	3.4%	
4	66.2%	55.0%	**19**	15.3%	
5	63.7%	41.3%	**20**	58.8%	25.7%
6	4.2%		**21**	10.6%	
7	17.4%		**22**	54.5%	30.3%
8	4.7%		**23**	79.1%	36.0%
9	26.1%		**24**	31.3%	
10	11.3%		**25**	68.3%	39.2%
11	25.7%		**26**	19.1%	
12	64.5%	27.0%	**27**	58.3%	23.3%
13	80.2%		**28**	30.5%	
14	75.5%	15.2%	**29**	-0.7%	
15	6.1%		**30**	8.7%	
apremilast	98.9%	96.3%			