Supporting Information for

Celamonols A−D, four triterpenoid and catechin conjugates with immunosuppressive activities from the stems of *Celastrus monospermus*

Jun-Jun Qin,[‡a,b] Yi-Fan Fu,[‡a,b] Xi Chen,[‡c,d] Yu-Ting Liu,[b,c] Ji-Hui Zhao,[b,c] Jian-Ping Zuo,[c,d] Yi-Ming Li,[*d] Wei-Liang Zhu,[*c] and Wei-Min Zhao[*a]

[a]Department of Natural Products Chemistry, Shanghai Institute of Materia Medica, Chinese Academy of Sciences, Shanghai 201203, People's Republic of China

[b]University of Chinese Academy of Sciences, No. 19A Yuquan Road, Beijing 100049, People's Republic of China

[c]State Key Laboratory of Drug Research, Shanghai Institute of Materia Medica, Chinese Academy of Sciences, Shanghai 201203, People's Republic of China

[d]Shanghai University of Traditional Chinese Medicine, 1200 Cailun Road, Shanghai 201203, People's Republic of China

‡J.-J. Qin, Y.-F. Fu, and X. Chen contributed equally.

List of Supporting Informationn

Figure S1. Key 2D NMR correlations for Celamonol B (**2**)……..3

Figure S2. Key 2D NMR correlations for Celamonol C (**3**)……..3

Figure S3. Key 2D NMR correlations for Celamonol D (**4**)……..3

Figure S4. Atropisomerization barriers……..4

Figure S5. Experimental ECD spectra and Calculated ECD spectra……5

Biological Activity Assay……...6

Computational Section……...6

NMR spectra data for Celamonol A (1)……46

HR-ESIMS of Celamonol A (1)……52

IR spectrum of Celamonol A (1)……...52

UV spectrum of Celamonol A (1)……53

NMR spectra data for Celamonol B (2)……54

HR-ESIMS of Celamonol B (2)……60

IR spectrum of Celamonol B (2)……...60

UV spectrum of Celamonol B (2)……61

NMR spectra data for Celamonol C (3)……62

HR-ESIMS of Celamonol C (3)……68

IR spectrum of Celamonol C (3)……...68

UV spectrum of Celamonol C (3)……69

NMR spectra data for Celamonol D (4)……70

HR-ESIMS of Celamonol D (4)……75

IR spectrum of Celamonol D (4)……...75

UV spectrum of Celamonol D (4)……76

Figure S6. LC-ESIMS monitor compound **1** in the ethanolic crude extract……77

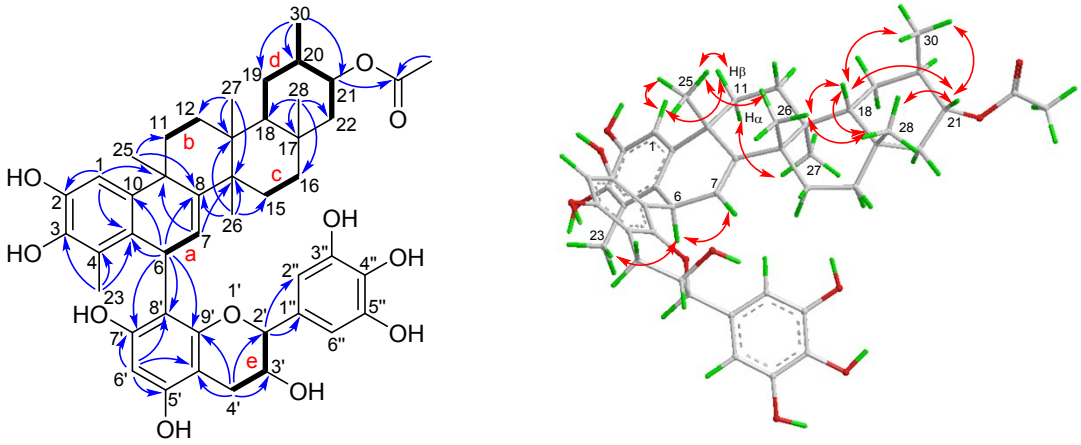


Figure S1. Key 2D NMR correlations for Celamonol B (**2**).

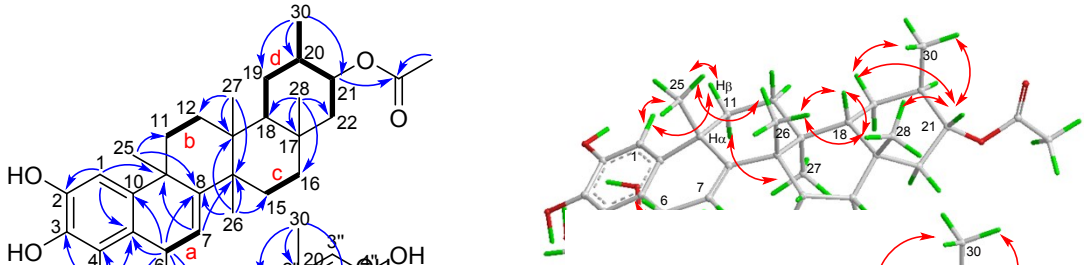


Figure S3. Key 2D NMR correlations for Celamonol D (**4**).

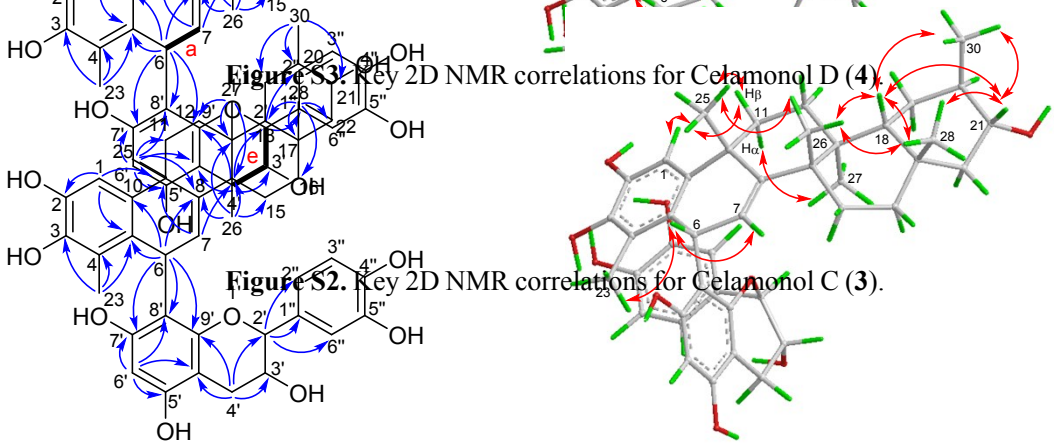


Figure S2. Key 2D NMR correlations for Celamonol C (**3**).

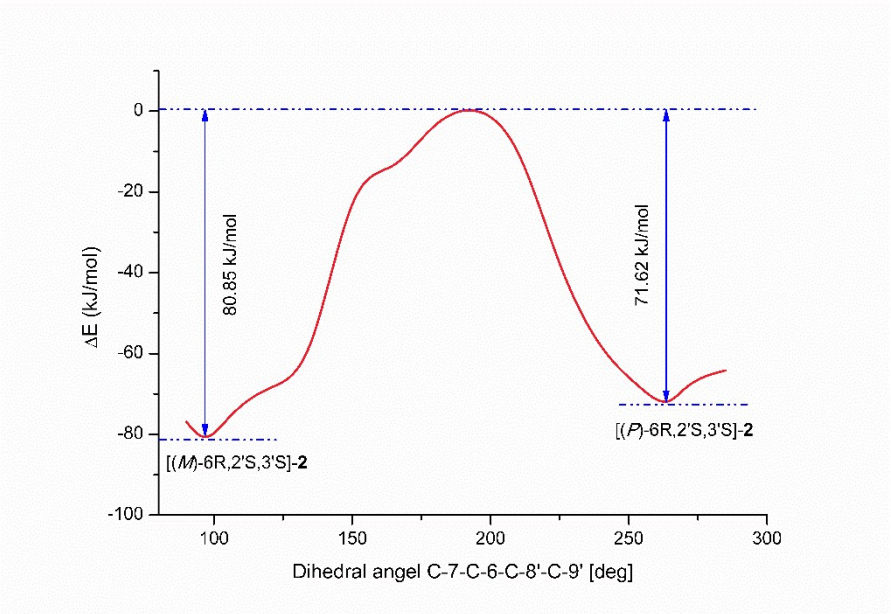


Figure S4. Atropisomerization barriers for [(*M*)-6R,2'S,3'S]-**2** and [(*P*)-6R,2'S,3'S]-**2**.

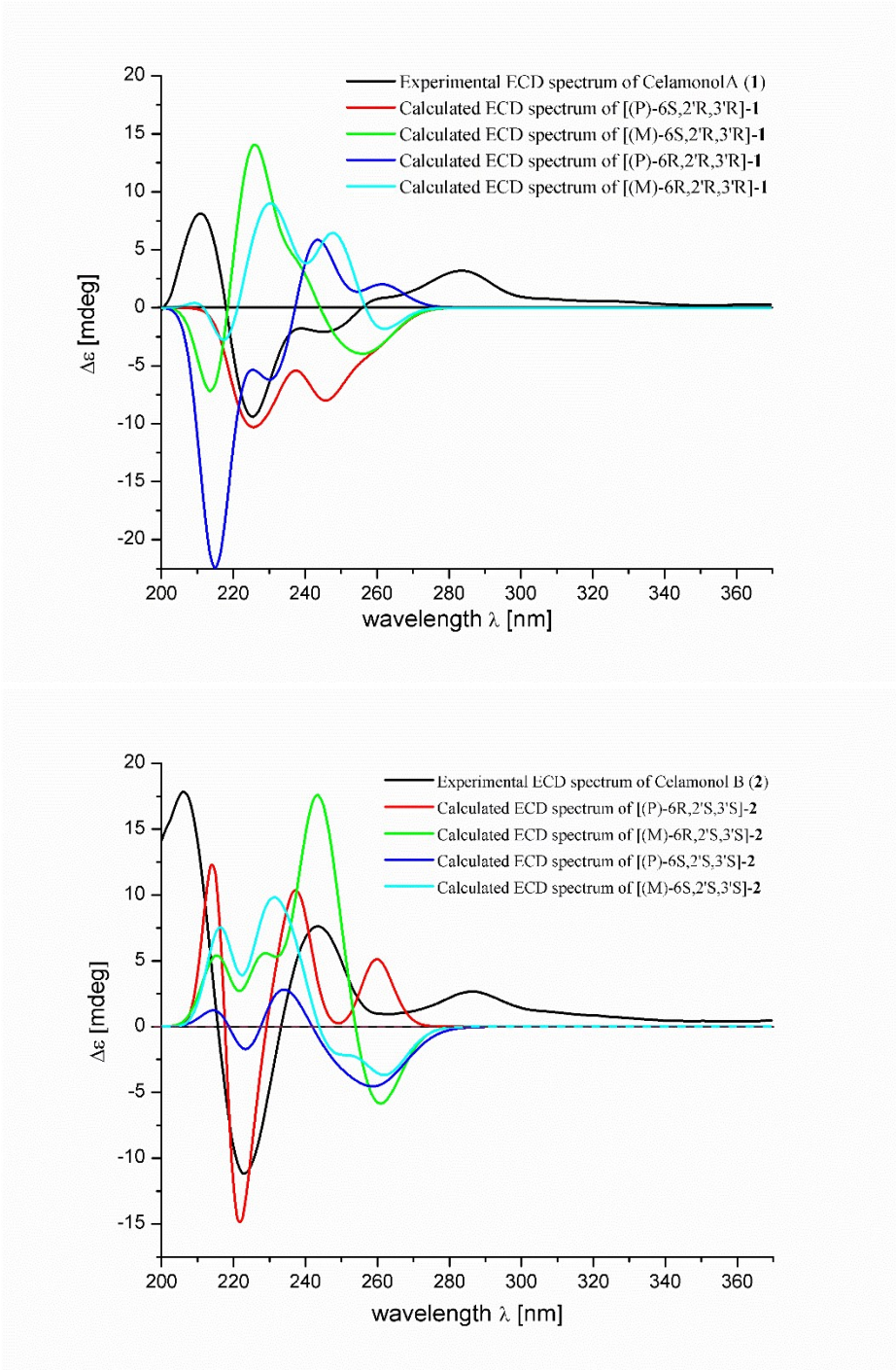


Figure S5. Experimental ECD spectra of Celamonol A and Celamonol B, and calculated ECD spectra of [(*P*)-6S,2'R,3'R]-**1**, [(*M*)-6S,2'R,3'R]-**1**, [(*P*)-6R,2'R,3'R]-**1,** [(*M*)-6R,2R',3R']-**1**, [(*P*)-6R,2'S,3'S]-**2**, [(*M*)-6R,2'S,3'S]-**2**, [(*P*)-6S,2'S,3'S]-**2**, and [(*M*)-6S,2'S,3'S]-**2**.

Experimental Section

Biological Activity Assay

Cytotoxicity assay: Cytotoxicity was assessed with CCK-8 assay. Fresh spleen cells were obtained from female BALB/c mice (18-20 g) and cultured at 37 ℃ for 48 h in 96-well flat plates, in the absence or presence of various concentrations of compounds, in a humidified and 5% CO_2-containing incubator. A certain amount of CCK-8 was added to each well at the final 8-10 h of culture. To the end of the culture, we measured the OD values with microplate reader (Bio-Rad 650) at 450 nm. The cytotoxicity of each compound was expressed as the concentration of compound that reduced cell viability to 50% (CC_{50}).

T cell and B cell function assay: The 5×10^5 spleen cells were obtained and cultured at the same conditions as those mentioned above. The cultures in absence or presence of various concentrations of compounds, were stimulated with 5 μg ml^{-1} of ConA or 10 μg ml^{-1} of LPS to induce T cells or B cells proliferative responses, respectively. Proliferation was assessed in terms of uptake of [^{3}H]-thymidine during 8 h of pulsing with 25 μL/well of [^{3}H]-thymidine, and then cells will be harvested onto glass fiber filters. The incorporated radioactivity was counted using a Beta scintillation counter (MicroBeta Trilux, PerkinElmer Life Sciences). The immunosuppressive activity of each compound was expressed as the concentration of compound that inhibited ConA-induced T cell proliferation or LPS-induced B cell proliferation to 50% (IC_{50}) of the control value.

Computational Section

Optimized Structures and Calculated Energies

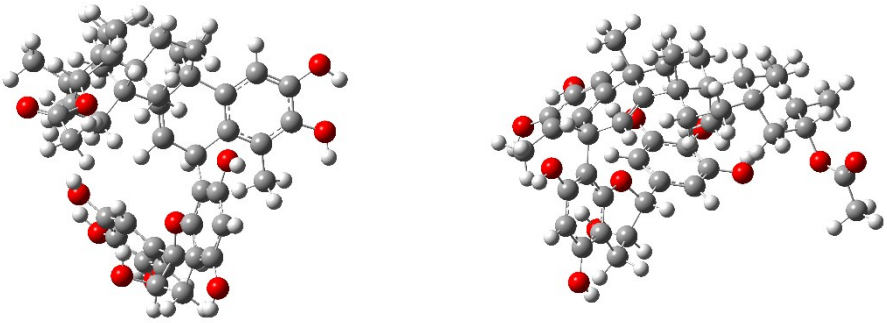


Figure S6. Optimized structures of [(*M*)-6S,2'R,3'R]-**1** and [(*P*)-6S,2'R,3'R]-**1**. Left: [(*M*)-6S,2'R,3'R]-**1**, the C7-C6-C8'-C9' torsion angle is 101.04°; right: [(*P*)-6S,2'R,3'R]-**1**, the C7-C6-C8'-C9' torsion angle is 279.64°.

Table S5. Energy scan at the B3LYP/6-311G(d,p) of (6S,2'R,3'R)-**1**

Dihedral angel	E (au)	ΔE (au)	ΔE (kJ/mol)
45.00	-2575.431932	-0.001832	-4.81
60.00	-2575.442255	-0.012155	-31.92
75.00	-2575.447965	-0.017865	-46.90
90.00	-2575.450689	-0.020589	-54.06
101.04	-2575.453756	-0.023656	-62.11
120.00	-2575.448821	-0.018721	-49.15
135.00	-2575.442387	-0.012287	-32.26
150.00	-2575.439944	-0.009844	-25.84
165.00	-2575.436542	-0.006442	-16.91
180.00	-2575.430155	-0.000050	-0.14
195.00	-2575.430495	-0.000395	-1.04
210.00	-2575.430100	0	0
225.00	-2575.432959	-0.002859	-7.50
240.00	-2575.445037	-0.014937	-39.21
255.00	-2575.45557	-0.025470	-66.87
270.00	-2575.460873	-0.030773	-80.79
279.64	-2575.462578	-0.032478	-85.27
285.00	-2575.462785	-0.032685	-85.82
290.00	-2575.462702	-0.032602	-85.60

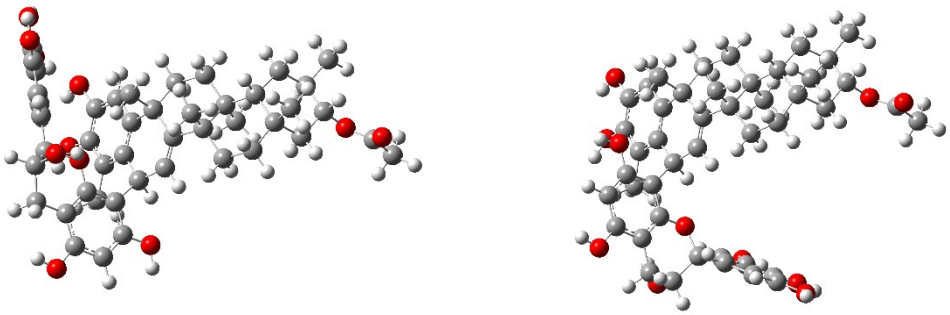


Figure S7. Optimized structures of [(*M*)-6R,2'R,3'R]-**1** and [(*P*)-6R,2'R,3'R]-**1**. Left: [(*M*)-6R,2'R,3'R]-**1**, the C7-C6-C8'-C9' torsion angle is 91.81°; right: [(*P*)-6R,2'R,3'R]-**1**, the C7-C6-C8'-C9' torsion angle is 265.75°.

Table S6. Energy scan at the B3LYP/6-311G(d,p) of (6R,2'R,3'R)-**1**

Dihedral angel	E (au)	ΔE (au)	ΔE (kJ/mol)
45.00	-2575.4167540	-0.0148473	-38.98
60.00	-2575.4261880	-0.0242813	-63.75
75.00	-2575.4309715	-0.0290648	-76.31
90.00	-2575.4323247	-0.0304180	-79.86

91.81	-2575.4325226	-0.0306159	-80.38
105.00	-2575.4310931	-0.0291864	-76.63
120.00	-2575.4258461	-0.0239394	-62.85
135.00	-2575.4215542	-0.0196475	-51.58
150.00	-2575.4110061	-0.0090994	-23.89
165.00	-2575.4087631	-0.0068564	-18.00
180.00	-2575.4055856	-0.0036789	-9.66
195.00	-2575.4019067	0	0
210.00	-2575.4041393	-0.0022326	-5.86
225.00	-2575.4127792	-0.0108725	-28.54
240.00	-2575.4205968	-0.0186901	-49.07
255.00	-2575.4237924	-0.0218857	-57.46
265.75	-2575.4242729	-0.0223662	-58.72
270.00	-2575.4242396	-0.0223329	-58.64
285.00	-2575.4238218	-0.0219151	-57.54
300.00	-2575.4204908	-0.0185841	-48.79
315.00	-2575.4155079	-0.0136012	-35.71

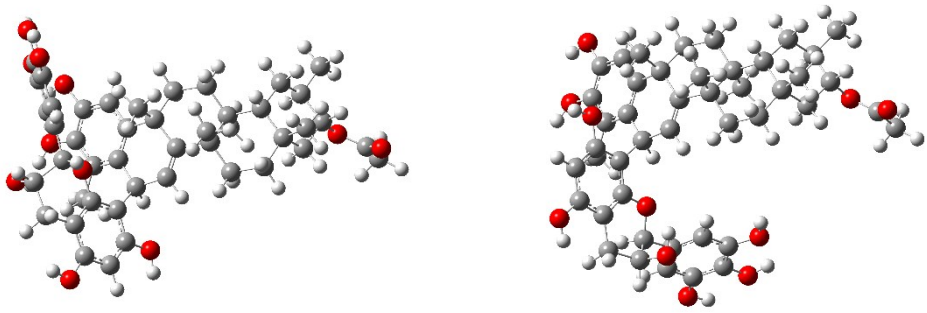


Figure S8. Optimized structures of [(*M*)-6R,2'S,3'S]-**2** and [(*P*)-6R,2'S,3'S]-**2**. Left: [(*M*)-6R,2'S,3'S]-**2**, the C7-C6-C8'-C9' torsion angle is 96.4°; right: [(*P*)-6R,2'S,3'S]-**2**, the C7-C6-C8'-C9' torsion angle is 265.00°.

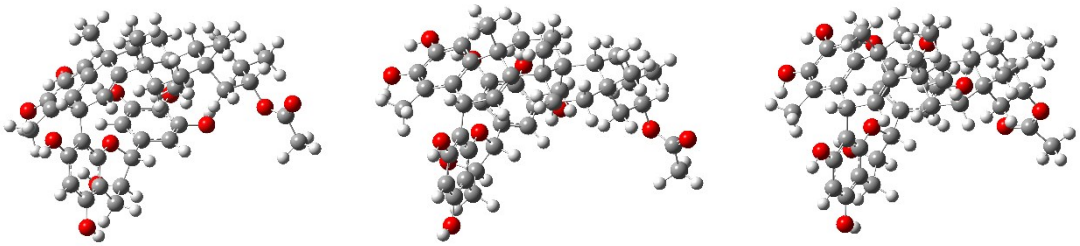
Table S7. Energy scan at the B3LYP/6-311G(d,p) of (6R,2'S,3'S)-**2**

Dihedral angel	E (au)	ΔE (au)	ΔE (kJ/mol)
75.00	-2575.4599998	-0.0271525	-71.29
90.00	-2575.4621423	-0.0292950	-76.91
96.40	-2575.4635663	-0.0307190	-80.65
105.00	-2575.4618536	-0.0290063	-76.16
120.00	-2575.4589818	-0.0261345	-68.62
135.00	-2575.4546890	-0.0218417	-57.35
150.00	-2575.4416452	-0.0087979	-23.10
165.00	-2575.4379357	-0.0050884	-13.36
180.00	-2575.4341844	-0.0013371	-3.51

195.00	-2575.4328473	0	0.00
210.00	-2575.4367902	-0.0039429	-10.35
225.00	-2575.4471752	-0.0143279	-37.62
240.00	-2575.4550072	-0.0221599	-58.18
255.00	-2575.4590869	-0.0262396	-68.89
265.00	-2575.4601279	-0.0272806	-71.63
270.00	-2575.4590869	-0.0262396	-68.89
285.00	-2575.4572989	-0.0244516	-64.20

ECD Calculation

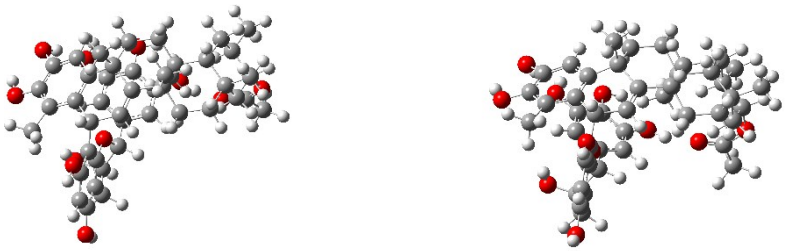
Conformational searches were carried out using the torsional sampling (MCMM) method and OPLS_2005 force field. Conformers above 1% population were re-optimized at the B3LYP/6-311G(d,p) level with IEFPCM (Polarizable Continuum Model using the Integral Equation Formalism variant) solvent model for methanol. For the resulting geometries, ECD spectra were obtained by TDDFT calculations performed with the same functional, basis set and solvent model as the energy optimization. Finally, the Boltzmann-averaged ECD spectra of the eight compounds were obtained with SpecDis 1.62[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 afford 36 conformers for [(*M*)-6S,2R',3R']-**1**, 36 conformers for [(*P*)-6S,2R',3R']-**1**, 35 conformers for [(*M*)-6R,2R',3R']-**1**, 35 conformers for [(*P*)-6R,2R',3R']-**1**, 25 conformers for [(*M*)-6S,2S',3S']-**2**, 25 conformers for [(*P*)-6S,2S',3S']-**2**, 26 conformers for [(*M*)-6R,2S',3S']-**2**, and 26 conformers for [(*P*)-6R,2S',3S']-**2**. The Boltzmann populations of the conformers were obtained based on the potential energy provided by the OPLS_2005 force field, which afford 5 conformers for [(*M*)-6S,2R',3R']-**1**, 7 conformers for [(*P*)-6S,2R',3R']-**1**, 6 conformers for [(*M*)-6R,2R',3R']-**1**, 5 conformers for [(*P*)-6R,2R',3R']-**1**, 5 conformers for [(*M*)-6S,2S',3S']-**2**, 5 conformers for [(*P*)-6S,2S',3S']-**2**, 5 conformers for [(*M*)-6R,2S',3S']-**2**, and 7 conformers for [(*P*)-6R,2S',3S']-**2** for above 1% population for re-optimization. The re-optimization and the following TDDFT calculations of the re-optimized geometries were all performed with Gaussian 09[3] at the B3LYP/6-311G(d,p) level with IEFPCM 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 1.62[5] software was used to obtain the Boltzmann-averaged ECD spectra of the eight compounds and to visualize the results.



Conf.1
8.81%

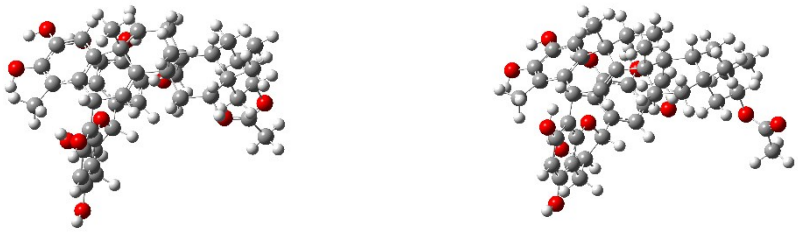
Conf.2
27.55%

Conf.3
0.04%



Conf.4
15.19%

Conf.5
46.37%



Conf.6
0.13%

Conf.7
1.91%

Figure S9. Re-optimized conformers above 1% population (OPLS_2005) of [(*p*)-6S,2R',3R']-**1** calculated at the B3LYP/6-311G(d,p) level with IEFPCM solvent model for Methanol.

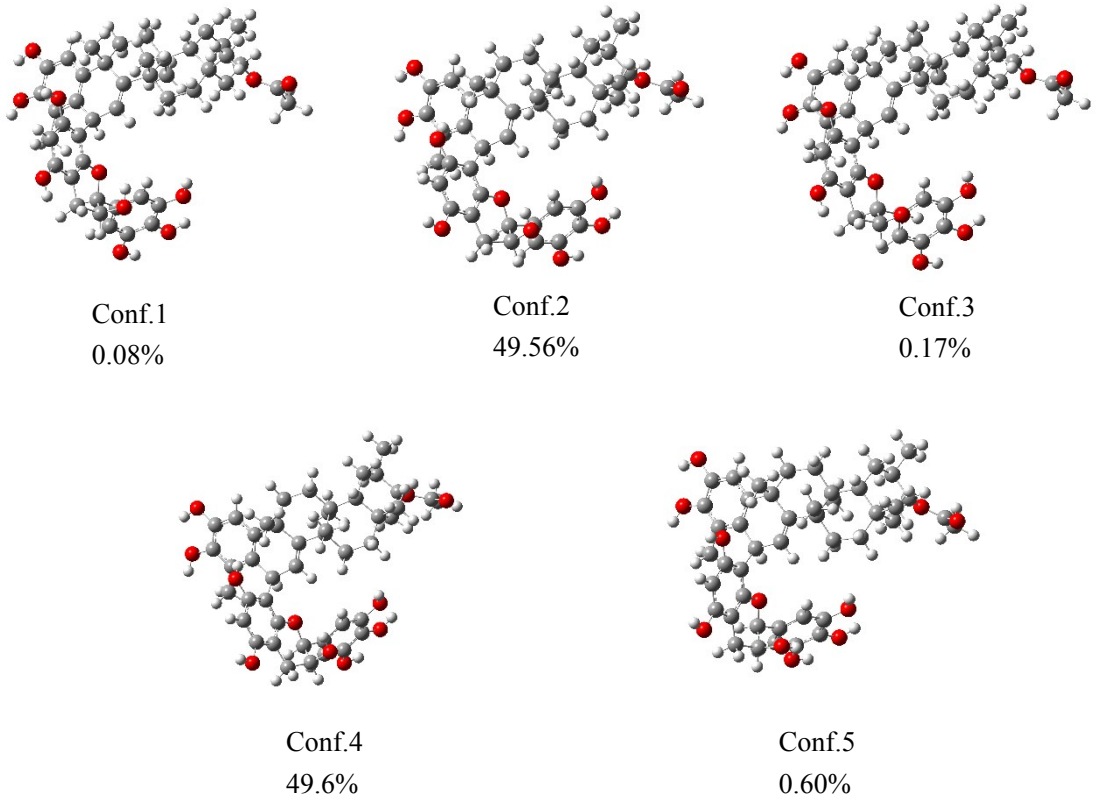


Figure S10. Re-optimized conformers above 1% population (OPLS_2005) of [(*p*)-6R,2S',3S']-**2** calculated at the B3LYP/6-311G(d,p) level with IEFPCM solvent model for Methanol.

Table S8. Cartesian coordinates for the re-optimized conformers of [(*p*)-6S,2R',3R']-**1** at the B3LYP/6-311G(d,p) level with IEFPCM solvent model for Methanol.

[(*P*)-6S,2R',3R']-**1** Conformer 1		Standard Orientation (Ångstroms)		
I	Atom	X	Y	Z
1	C	3.935848	1.508145	-2.25633
2	C	4.7569	0.568809	-1.63635
3	C	4.253554	-0.67844	-1.27163
4	C	2.881265	-0.9481	-1.48609
5	C	2.087985	-0.05312	-2.21844
6	C	2.638358	1.180359	-2.59431
7	C	2.265895	-2.21311	-0.91391
8	C	0.773577	-2.29765	-1.11843
9	C	0.017824	-1.51604	-1.89185
10	C	0.680072	-0.41583	-2.74561

11	C	-1.51701	-1.7299	-1.97238
12	C	-2.24024	-0.3357	-1.76311
13	C	-1.72641	0.613825	-2.87225
14	C	-0.21423	0.85867	-2.79943
15	C	-2.04255	-2.69465	-0.88107
16	C	-3.55508	-2.93451	-0.9803
17	C	-4.46229	-1.67719	-1.07153
18	C	-3.79982	-0.50944	-1.89616
19	C	-4.84131	-1.23589	0.367537
20	C	-5.67556	0.040561	0.428359
21	C	-5.00833	1.214228	-0.28201
22	C	-4.62126	0.798775	-1.71684
23	C	-5.90583	2.457548	-0.30477
24	C	-5.75967	-2.11936	-1.79326
25	C	-1.82716	0.276207	-0.40097
26	C	-1.84853	-2.38725	-3.34464
27	C	5.216009	-1.68369	-0.67798
28	C	2.568268	-2.47053	0.570527
29	C	2.942422	-3.76264	0.969509
30	C	3.194443	-4.08908	2.299421
31	C	3.081982	-3.10398	3.272323
32	C	2.716664	-1.79271	2.940924
33	C	2.443322	-1.5077	1.590788
34	O	4.403902	2.78956	-2.48545
35	O	6.064291	0.972167	-1.44301
36	O	3.05998	-4.71282	-0.01146
37	C	2.648455	-0.71694	4.004735
38	C	2.648582	0.678139	3.378094
39	C	1.632146	0.681429	2.223187
40	O	2.083263	-0.23854	1.200802
41	C	1.408697	2.04162	1.605369
42	C	0.329657	2.804718	2.059432
43	C	0.126362	4.092734	1.567618
44	C	0.994644	4.615232	0.609471
45	C	2.066644	3.848458	0.144262
46	C	2.286367	2.569689	0.653654
47	O	2.836918	4.467421	-0.80259
48	O	0.743683	5.876923	0.134535
49	O	-0.93627	4.830094	2.009261
50	O	3.947222	1.072282	2.945079
51	O	3.350483	-3.48053	4.558377

52	O	-5.84508	0.423016	1.83187
53	C	-6.90654	-0.05824	2.504376
54	C	-6.91945	0.447684	3.924443
55	O	-7.73836	-0.79539	2.023259
56	C	0.933768	-0.92215	-4.20204
57	H	2.056479	1.921425	-3.12481
58	H	2.705576	-3.06713	-1.44219
59	H	0.314799	-3.09018	-0.54165
60	H	-2.00964	0.227529	-3.85528
61	H	-2.21199	1.589404	-2.78651
62	H	-0.00343	1.469333	-1.9189
63	H	0.074008	1.464262	-3.66366
64	H	-1.55462	-3.66924	-0.97628
65	H	-1.77632	-2.31777	0.109302
66	H	-3.87527	-3.53066	-0.11812
67	H	-3.75068	-3.56552	-1.85059
68	H	-3.94637	-0.77969	-2.94717
69	H	-5.40694	-2.04676	0.837052
70	H	-3.94815	-1.08708	0.978566
71	H	-6.67378	-0.13353	0.023471
72	H	-4.10539	1.458069	0.283587
73	H	-4.10059	1.636879	-2.18439
74	H	-5.55129	0.690053	-2.28685
75	H	-5.39367	3.29592	-0.78524
76	H	-6.82772	2.263833	-0.86357
77	H	-6.18016	2.7659	0.706353
78	H	-5.53688	-2.46643	-2.80633
79	H	-6.22966	-2.94734	-1.25293
80	H	-6.49812	-1.31963	-1.87424
81	H	-0.75084	0.209158	-0.24399
82	H	-2.29919	-0.21189	0.447969
83	H	-2.09451	1.334585	-0.36264
84	H	-1.60786	-1.76075	-4.19738
85	H	-1.2737	-3.31219	-3.44295
86	H	-2.90189	-2.64629	-3.43618
87	H	6.200436	-1.58227	-1.14378
88	H	5.345963	-1.55878	0.402247
89	H	4.883812	-2.70742	-0.84333
90	H	3.475942	-5.09542	2.587227
91	H	5.340796	2.801459	-2.23694
92	H	6.440934	0.545735	-0.66559

93	H	3.354076	-5.54285	0.381291
94	H	1.749281	-0.82878	4.623326
95	H	3.511848	-0.77475	4.677037
96	H	2.346564	1.420356	4.117802
97	H	0.679004	0.313061	2.619091
98	H	-0.36993	2.411894	2.788208
99	H	3.118697	1.983533	0.292199
100	H	3.407121	3.844031	-1.29094
101	H	1.379395	6.057474	-0.57186
102	H	-0.93399	5.672296	1.534622
103	H	4.206961	0.497141	2.215683
104	H	3.223059	-2.73706	5.157889
105	H	-7.76324	0.017552	4.459734
106	H	-5.98555	0.181822	4.423741
107	H	-6.99552	1.537369	3.928083
108	H	0.016193	-1.03072	-4.77823
109	H	1.567694	-0.20486	-4.72913
110	H	1.447421	-1.88654	-4.19253

B3LYP/6-311G(d,p) Energy = -2575.4625782 a.u.; Population = 8.81%.

[(*P*)-6S,2R',3R']-**1** Conformer 2		Standard Orientation (Ångstroms)		
I	Atom	X	Y	Z
1	C	3.93427	1.508244	-2.25556
2	C	4.755031	0.566201	-1.63944
3	C	4.250803	-0.68132	-1.27711
4	C	2.877753	-0.94844	-1.48957
5	C	2.084538	-0.05074	-2.21863
6	C	2.635777	1.183013	-2.59237
7	C	2.261667	-2.21338	-0.91814
8	C	0.769216	-2.29648	-1.12188
9	C	0.013465	-1.51303	-1.89346
10	C	0.675735	-0.41105	-2.74509
11	C	-1.52151	-1.72606	-1.97387
12	C	-2.24419	-0.33214	-1.76104
13	C	-1.7302	0.619934	-2.86793
14	C	-0.2179	0.864076	-2.79471
15	C	-2.04698	-2.69314	-0.88464
16	C	-3.55952	-2.93265	-0.98429
17	C	-4.46652	-1.67496	-1.07257
18	C	-3.80388	-0.50511	-1.8942

19	C	-4.84553	-1.23738	0.367611
20	C	-5.6796	0.038985	0.431778
21	C	-5.01193	1.214429	-0.27522
22	C	-4.62484	0.802925	-1.71115
23	C	-5.90912	2.458039	-0.29453
24	C	-5.7639	-2.11502	-1.79558
25	C	-1.8308	0.276341	-0.39749
26	C	-1.85389	-2.37997	-3.34759
27	C	5.213252	-1.68997	-0.68928
28	C	2.566005	-2.47045	0.565924
29	C	2.942846	-3.75983	0.964179
30	C	3.201487	-4.08488	2.296265
31	C	3.091606	-3.09636	3.266636
32	C	2.719197	-1.78873	2.934242
33	C	2.441597	-1.50552	1.587572
34	O	4.40436	2.789208	-2.48281
35	O	6.063872	0.96675	-1.44793
36	O	3.05947	-4.71212	-0.01533
37	C	2.653843	-0.72063	4.003127
38	C	2.650838	0.67415	3.381498
39	C	1.633656	0.682845	2.226201
40	O	2.076119	-0.2381	1.199284
41	C	1.412699	2.043848	1.60947
42	C	0.333561	2.807978	2.061797
43	C	0.132605	4.096762	1.570995
44	C	1.003167	4.619182	0.61498
45	C	2.075245	3.851606	0.151378
46	C	2.292715	2.572188	0.660001
47	O	2.848561	4.470736	-0.79332
48	O	0.754551	5.88173	0.140353
49	O	-0.93029	4.834985	2.011278
50	O	3.949325	1.074912	2.946834
51	O	3.340902	-3.34479	4.587177
52	O	-5.84931	0.417614	1.836301
53	C	-6.911	-0.06515	2.507255
54	C	-6.92634	0.440003	3.927564
55	O	-7.74217	-0.8019	2.024361
56	C	0.927633	-0.91353	-4.2032
57	H	2.053975	1.926018	-3.12024
58	H	2.700176	-3.06755	-1.44717
59	H	0.310332	-3.08979	-0.54621

60	H	-2.01358	0.236018	-3.85186
61	H	-2.2155	1.59544	-2.77978
62	H	-0.00659	1.471988	-1.9124
63	H	0.070352	1.472155	-3.65719
64	H	-1.55908	-3.66753	-0.98202
65	H	-1.78065	-2.31835	0.106498
66	H	-3.87973	-3.53065	-0.12339
67	H	-3.75527	-3.5617	-1.85596
68	H	-3.95072	-0.77251	-2.94589
69	H	-5.41123	-2.04941	0.835005
70	H	-3.95236	-1.09022	0.979035
71	H	-6.67777	-0.13382	0.026198
72	H	-4.10901	1.45643	0.291205
73	H	-4.10375	1.642149	-2.17624
74	H	-5.55485	0.696275	-2.28158
75	H	-5.39679	3.297598	-0.77274
76	H	-6.83109	2.266053	-0.85382
77	H	-6.18331	2.763661	0.717453
78	H	-5.54096	-2.45985	-2.80938
79	H	-6.23434	-2.94407	-1.25727
80	H	-6.502	-1.3148	-1.87491
81	H	-0.75454	0.208285	-0.24068
82	H	-2.30315	-0.21345	0.450286
83	H	-2.09763	1.334765	-0.3567
84	H	-1.61202	-1.75202	-4.19891
85	H	-1.28055	-3.30563	-3.44784
86	H	-2.90767	-2.63703	-3.43996
87	H	6.196926	-1.58703	-1.15626
88	H	5.345122	-1.57	0.391205
89	H	4.879568	-2.71261	-0.85852
90	H	3.485198	-5.09658	2.568704
91	H	5.341586	2.7984	-2.23526
92	H	6.437664	0.545797	-0.66612
93	H	3.359324	-5.54069	0.375865
94	H	1.755679	-0.8446	4.619774
95	H	3.508134	-0.80978	4.677961
96	H	2.348375	1.416954	4.120921
97	H	0.679828	0.317404	2.623361
98	H	-0.36791	2.415193	2.788826
99	H	3.126054	1.985698	0.301372
100	H	3.414507	3.845795	-1.28455

101	H	1.392017	6.061637	-0.56461
102	H	-0.92585	5.677631	1.537478
103	H	4.225419	0.476273	2.243063
104	H	3.616815	-4.26194	4.698505
105	H	-5.98432	0.195389	4.42217
106	H	-7.02662	1.527857	3.930638
107	H	-7.7584	-0.00716	4.467265
108	H	0.00953	-1.01907	-4.7791
109	H	1.562228	-0.19563	-4.72863
110	H	1.43993	-1.87867	-4.19687

B3LYP/6-311G(d,p) Energy = -2575.4636537 a.u.; Population = 27.55%.

[(*P*)-6S,2R',3R']-**1** Conformer 3		Standard Orientation (Ångstroms)		
I	Atom	X	Y	Z
1	C	3.549405	1.321098	-2.68774
2	C	4.485678	0.596159	-1.95442
3	C	4.130948	-0.6086	-1.3491
4	C	2.788634	-1.04505	-1.43803
5	C	1.882645	-0.38372	-2.2814
6	C	2.284976	0.807992	-2.89943
7	C	2.320963	-2.23092	-0.6095
8	C	0.829421	-2.45386	-0.68256
9	C	-0.02449	-1.91335	-1.55347
10	C	0.513554	-0.99004	-2.66593
11	C	-1.537	-2.25367	-1.49697
12	C	-2.37183	-0.91247	-1.60654
13	C	-1.9826	-0.2486	-2.94919
14	C	-0.50135	0.141954	-3.00657
15	C	-1.94416	-2.9484	-0.17491
16	C	-3.42899	-3.33077	-0.14632
17	C	-4.4442	-2.20458	-0.48238
18	C	-3.91629	-1.22413	-1.59827
19	C	-4.78939	-1.46124	0.837887
20	C	-5.71249	-0.26185	0.638289
21	C	-5.16702	0.762575	-0.35674
22	C	-4.83065	0.031735	-1.67634
23	C	-6.16432	1.89858	-0.6173
24	C	-5.72469	-2.90433	-1.00043
25	C	-1.96342	0.059111	-0.47129
26	C	-1.84732	-3.25949	-2.64444

27	C	5.21802	-1.39475	-0.64907
28	C	2.733008	-2.19613	0.869402
29	C	3.267409	-3.35346	1.454712
30	C	3.615875	-3.41463	2.801623
31	C	3.437943	-2.29167	3.600046
32	C	2.913846	-1.10259	3.076377
33	C	2.551543	-1.08753	1.717971
34	O	3.867793	2.581091	-3.16154
35	O	5.749092	1.153675	-1.90317
36	O	3.446151	-4.44315	0.642436
37	C	2.772193	0.129836	3.945215
38	C	2.579308	1.387325	3.095452
39	C	1.524002	1.079876	2.018151
40	O	2.041362	0.051988	1.141224
41	C	1.125146	2.279798	1.191839
42	C	-0.00116	3.009887	1.580025
43	C	-0.36011	4.162852	0.883997
44	C	0.398666	4.579145	-0.20971
45	C	1.516841	3.841275	-0.60827
46	C	1.89168	2.701552	0.101195
47	O	2.167012	4.346474	-1.70126
48	O	-0.00482	5.706191	-0.87948
49	O	-1.46748	4.869248	1.261788
50	O	3.803123	1.841516	2.524459
51	O	3.805161	-2.40788	4.911341
52	O	-6.10679	0.329569	1.927291
53	C	-5.21528	0.90833	2.748812
54	C	-5.89759	1.406894	3.999904
55	O	-4.0296	1.018345	2.524806
56	C	0.805266	-1.80657	-3.96655
57	H	1.611624	1.376308	-3.5259
58	H	2.796402	-3.13201	-1.01439
59	H	0.466702	-3.13163	0.079199
60	H	-2.24556	-0.90594	-3.78248
61	H	-2.56097	0.667081	-3.09843
62	H	-0.34075	0.975997	-2.32075
63	H	-0.28508	0.52725	-4.00745
64	H	-1.37114	-3.87068	-0.04335
65	H	-1.69406	-2.30971	0.675655
66	H	-3.6734	-3.72974	0.844638
67	H	-3.58799	-4.16306	-0.83646

68	H	-4.08729	-1.74756	-2.54477
69	H	-5.2843	-2.17037	1.510487
70	H	-3.88047	-1.13494	1.340482
71	H	-6.68249	-0.6089	0.275404
72	H	-4.25999	1.191744	0.065637
73	H	-4.40661	0.762269	-2.36847
74	H	-5.77988	-0.27273	-2.13297
75	H	-5.75014	2.618597	-1.32879
76	H	-7.09888	1.511888	-1.03836
77	H	-6.40832	2.439053	0.300151
78	H	-5.50995	-3.47282	-1.90985
79	H	-6.10097	-3.60698	-0.24983
80	H	-6.5332	-2.20883	-1.23287
81	H	-0.88152	0.09248	-0.34642
82	H	-2.38788	-0.20104	0.494336
83	H	-2.29153	1.074424	-0.70568
84	H	-1.61531	-2.87465	-3.63216
85	H	-1.24789	-4.16206	-2.4957
86	H	-2.89397	-3.56011	-2.66349
87	H	6.165296	-1.28062	-1.18391
88	H	5.379973	-1.07191	0.384646
89	H	4.989893	-2.45912	-0.61983
90	H	4.022088	-4.32103	3.235905
91	H	4.805768	2.731777	-2.96891
92	H	6.189939	0.920318	-1.07898
93	H	3.85147	-5.15598	1.149458
94	H	1.923478	0.03121	4.633395
95	H	3.668149	0.282221	4.557431
96	H	2.222214	2.207853	3.718827
97	H	0.6357	0.685302	2.524089
98	H	-0.6215	2.690715	2.409576
99	H	2.755756	2.132692	-0.21082
100	H	2.790839	3.710933	-2.09924
101	H	0.569976	5.812783	-1.65004
102	H	-1.57457	5.607945	0.647434
103	H	4.085662	1.193315	1.868543
104	H	3.635072	-1.58319	5.379887
105	H	-5.16496	1.872469	4.65574
106	H	-6.67452	2.128473	3.738567
107	H	-6.38222	0.574551	4.514757
108	H	-0.104	-2.1369	-4.46737

109	H	1.356807	-1.17857	-4.67098
110	H	1.414546	-2.68657	-3.74708

B3LYP/6-311G(d,p) Energy = -2575.4575839 a.u.; Population = 0.04%.

[(*P*)-6S,2R',3R']-**1** Conformer 4		Standard Orientation (Ångstroms)		
I	Atom	X	Y	Z
1	C	2.984885	1.598912	-2.94518
2	C	4.105035	1.122494	-2.26688
3	C	4.058425	-0.09775	-1.58561
4	C	2.833482	-0.79755	-1.5358
5	C	1.74908	-0.39365	-2.33769
6	C	1.847931	0.815028	-3.03602
7	C	2.64396	-1.97536	-0.58081
8	C	1.185427	-2.34569	-0.40639
9	C	0.186351	-2.05299	-1.24059
10	C	0.526051	-1.31424	-2.55315
11	C	-1.25759	-2.54469	-0.96006
12	C	-2.2907	-1.4167	-1.36482
13	C	-2.06319	-1.11718	-2.86491
14	C	-0.67959	-0.51049	-3.1181
15	C	-1.49235	-2.87349	0.533749
16	C	-2.90321	-3.41152	0.800467
17	C	-4.08528	-2.55984	0.267445
18	C	-3.7684	-1.91306	-1.1333
19	C	-4.44921	-1.49234	1.339061
20	C	-5.53726	-0.5237	0.881644
21	C	-5.23425	0.184285	-0.43979
22	C	-4.8721	-0.88134	-1.49827
23	C	-6.42121	1.030446	-0.91816
24	C	-5.28738	-3.52388	0.11502
25	C	-1.97978	-0.11874	-0.57894
26	C	-1.45014	-3.86615	-1.76067
27	C	5.34188	-0.59088	-0.95409
28	C	3.258056	-1.79001	0.811223
29	C	4.085394	-2.78157	1.354498
30	C	4.621164	-2.67918	2.637192
31	C	4.336793	-1.55788	3.407949
32	C	3.51963	-0.52901	2.920966
33	C	2.980211	-0.6833	1.633025
34	O	3.085668	2.855885	-3.52863

35	O	5.247794	1.878756	-2.24419
36	O	4.365428	-3.86909	0.568584
37	C	3.248778	0.715005	3.742764
38	C	2.689406	1.846308	2.873693
39	C	1.583227	1.258563	1.982829
40	O	2.176044	0.285884	1.08799
41	C	0.814057	2.246617	1.139431
42	C	1.402829	2.881109	0.04184
43	C	0.646246	3.740278	-0.74545
44	C	-0.6887	3.997263	-0.43347
45	C	-1.27531	3.374958	0.671386
46	C	-0.52432	2.500592	1.45453
47	O	-2.59204	3.673602	0.880414
48	O	-1.3942	4.835257	-1.25537
49	O	1.207141	4.321722	-1.86265
50	O	3.708971	2.487657	2.111778
51	O	4.897532	-1.51227	4.65408
52	O	-5.89761	0.411179	1.972356
53	C	-5.07555	1.366958	2.395687
54	C	-5.71482	2.228866	3.45198
55	O	-3.94589	1.54476	1.966857
56	C	0.966274	-2.34425	-3.6413
57	H	1.036637	1.185209	-3.64756
58	H	3.150471	-2.84938	-1.00786
59	H	0.991514	-2.90876	0.497586
60	H	-2.21584	-2.02207	-3.45988
61	H	-2.8012	-0.39443	-3.22275
62	H	-0.67668	0.49108	-2.68792
63	H	-0.54166	-0.37452	-4.1954
64	H	-0.78898	-3.64128	0.866595
65	H	-1.28951	-1.98948	1.143966
66	H	-3.03498	-3.55011	1.879786
67	H	-2.97823	-4.41447	0.37118
68	H	-3.90047	-2.72136	-1.86014
69	H	-4.80677	-2.01265	2.234119
70	H	-3.56673	-0.92977	1.637738
71	H	-6.47962	-1.06433	0.773741
72	H	-4.38159	0.842093	-0.28641
73	H	-4.61295	-0.36158	-2.42288
74	H	-5.78614	-1.43863	-1.73351
75	H	-6.18183	1.528529	-1.86169

76	H	-7.30601	0.406253	-1.08369
77	H	-6.68755	1.802491	-0.1923
78	H	-5.06139	-4.30515	-0.61616
79	H	-5.50022	-4.01345	1.070717
80	H	-6.2033	-3.02708	-0.20998
81	H	-0.90865	0.073501	-0.5277
82	H	-2.3432	-0.13116	0.443032
83	H	-2.43586	0.743946	-1.07033
84	H	-1.22504	-3.75939	-2.81843
85	H	-0.76942	-4.62211	-1.35969
86	H	-2.46256	-4.26304	-1.6885
87	H	6.190235	-0.27632	-1.56512
88	H	5.505245	-0.1881	0.050335
89	H	5.361963	-1.67749	-0.87759
90	H	5.25643	-3.45818	3.042764
91	H	2.430214	3.431223	-3.09446
92	H	5.044166	2.679589	-2.75146
93	H	4.954863	-4.46492	1.045195
94	H	2.539563	0.505892	4.553242
95	H	4.168857	1.085639	4.208532
96	H	2.261946	2.625003	3.506678
97	H	0.877053	0.734969	2.636554
98	H	2.429947	2.690374	-0.23118
99	H	-1.00069	1.998683	2.288922
100	H	-3.03205	2.969641	1.399482
101	H	-2.31588	4.829933	-0.96076
102	H	0.533442	4.869743	-2.28949
103	H	4.057299	1.848782	1.478492
104	H	4.626538	-0.70909	5.112247
105	H	-6.45712	1.672319	4.021778
106	H	-4.9455	2.630834	4.109601
107	H	-6.21758	3.06589	2.958446
108	H	0.13455	-2.96372	-3.98091
109	H	1.35699	-1.8087	-4.5111
110	H	1.75119	-3.00524	-3.26717

B3LYP/6-311G(d,p) Energy = -2575.4575839 a.u.; Population = 15.19%.

[(*P*)-6S,2R',3R']-**1** Conformer 5		Standard Orientation (Ångstroms)		
I	Atom	X	Y	Z
1	C	2.966387	1.604638	-2.94942

2	C	4.08963	1.129184	-2.27574
3	C	4.047724	-0.0921	-1.59591
4	C	2.824206	-0.79409	-1.54269
5	C	1.736743	-0.39156	-2.34144
6	C	1.830766	0.818525	-3.03798
7	C	2.639328	-1.97412	-0.58914
8	C	1.18142	-2.3447	-0.4094
9	C	0.179769	-2.05329	-1.24092
10	C	0.516049	-1.31567	-2.55503
11	C	-1.26307	-2.54577	-0.95627
12	C	-2.29834	-1.42034	-1.36258
13	C	-2.07394	-1.12532	-2.86401
14	C	-0.69208	-0.51644	-3.12094
15	C	-1.49472	-2.87027	0.538937
16	C	-2.9045	-3.40907	0.809851
17	C	-4.08855	-2.56039	0.276488
18	C	-3.77496	-1.91798	-1.12695
19	C	-4.45165	-1.48967	1.345098
20	C	-5.54118	-0.52328	0.886304
21	C	-5.24166	0.180061	-0.43843
22	C	-4.88072	-0.8892	-1.49361
23	C	-6.43047	1.023239	-0.91745
24	C	-5.2899	-3.52625	0.129721
25	C	-1.98728	-0.11958	-0.58116
26	C	-1.45516	-3.86981	-1.7527
27	C	5.334499	-0.58286	-0.96955
28	C	3.259864	-1.79125	0.800197
29	C	4.097064	-2.77712	1.333372
30	C	4.642473	-2.67433	2.615147
31	C	4.353183	-1.5566	3.390074
32	C	3.522019	-0.5361	2.91274
33	C	2.977512	-0.68826	1.629522
34	O	3.06266	2.862578	-3.53233
35	O	5.231087	1.887412	-2.25647
36	O	4.38247	-3.85994	0.542335
37	C	3.250008	0.6963	3.747865
38	C	2.692375	1.831576	2.887327
39	C	1.582681	1.254163	1.9925
40	O	2.161746	0.275032	1.093882
41	C	0.819834	2.248796	1.150901
42	C	1.417421	2.893551	0.063895

43	C	0.666208	3.757409	-0.72335
44	C	-0.67202	4.009633	-0.42179
45	C	-1.26728	3.37847	0.673284
46	C	-0.52188	2.498491	1.455595
47	O	-2.58606	3.674316	0.873421
48	O	-1.37131	4.853603	-1.24335
49	O	1.235793	4.348622	-1.83149
50	O	3.712919	2.478576	2.127352
51	O	4.862181	-1.39481	4.648452
52	O	-5.89964	0.415329	1.974329
53	C	-5.07692	1.373036	2.392307
54	C	-5.7146	2.238776	3.446435
55	O	-3.94819	1.549301	1.960603
56	C	0.958009	-2.34654	-3.64163
57	H	1.017121	1.188117	-3.64672
58	H	3.143807	-2.84715	-1.0206
59	H	0.990527	-2.90689	0.495774
60	H	-2.22549	-2.03257	-3.45566
61	H	-2.81399	-0.40533	-3.22317
62	H	-0.69133	0.48642	-2.69394
63	H	-0.55563	-0.38329	-4.1988
64	H	-0.78984	-3.63621	0.872859
65	H	-1.29175	-1.98415	1.146021
66	H	-3.03413	-3.54469	1.889819
67	H	-2.9792	-4.41336	0.383559
68	H	-3.90703	-2.72901	-1.85078
69	H	-4.80743	-2.00723	2.242464
70	H	-3.56912	-0.92554	1.640603
71	H	-6.48344	-1.06489	0.782353
72	H	-4.3893	0.839248	-0.28948
73	H	-4.6242	-0.37272	-2.42077
74	H	-5.7946	-1.44851	-1.72464
75	H	-6.19338	1.518324	-1.86314
76	H	-7.31489	0.397518	-1.0792
77	H	-6.69632	1.797495	-0.19377
78	H	-5.06482	-4.30949	-0.59965
79	H	-5.4999	-4.01319	1.087396
80	H	-6.20718	-3.03147	-0.19451
81	H	-0.91616	0.073366	-0.53182
82	H	-2.34931	-0.12896	0.441317
83	H	-2.44442	0.741396	-1.0746

84	H	-1.2305	-3.76604	-2.81091
85	H	-0.77365	-4.62403	-1.34976
86	H	-2.46724	-4.26734	-1.67895
87	H	6.179937	-0.26453	-1.58266
88	H	5.499292	-0.18085	0.034873
89	H	5.358119	-1.66948	-0.89504
90	H	5.286894	-3.45857	2.999745
91	H	2.422689	3.441933	-3.08027
92	H	5.024481	2.687086	-2.7645
93	H	4.980227	-4.45289	1.011884
94	H	2.540542	0.469858	4.55265
95	H	4.169155	1.035359	4.231057
96	H	2.264597	2.609538	3.521592
97	H	0.87233	0.735649	2.645905
98	H	2.448594	2.708802	-0.19756
99	H	-1.00484	1.989414	2.281842
100	H	-3.02779	2.97106	1.391768
101	H	-2.29531	4.845683	-0.95632
102	H	0.566275	4.90385	-2.25562
103	H	4.103132	1.825887	1.534069
104	H	5.43958	-2.1369	4.862181
105	H	-4.94404	2.646172	4.099207
106	H	-6.2217	3.071715	2.950479
107	H	-6.45327	1.683041	4.021765
108	H	0.127503	-2.9691	-3.97866
109	H	1.345975	-1.81172	-4.51313
110	H	1.74531	-3.00455	-3.26729

B3LYP/6-311G(d,p) Energy = -2575.4641449 a.u.; Population = 46.37%.

[(*P*)-6S,2R',3R']-**1** Conformer 6		Standard Orientation (Ångstroms)		
I	Atom	X	Y	Z
1	C	3.539296	1.322757	-2.6945
2	C	4.477753	0.599104	-1.96282
3	C	4.125783	-0.60581	-1.35628
4	C	2.783764	-1.04379	-1.44215
5	C	1.875414	-0.38376	-2.28405
6	C	2.274966	0.808197	-2.90339
7	C	2.318736	-2.22969	-0.612
8	C	0.827065	-2.45292	-0.6809
9	C	-0.02897	-1.91423	-1.55084

10	C	0.506409	-0.99216	-2.66564
11	C	-1.54104	-2.25595	-1.49133
12	C	-2.37764	-0.91601	-1.60238
13	C	-1.99087	-0.25408	-2.94671
14	C	-0.51018	0.138129	-3.00664
15	C	-1.94551	-2.94849	-0.16731
16	C	-3.42986	-3.3326	-0.1359
17	C	-4.44698	-2.20854	-0.47324
18	C	-3.92167	-1.22967	-1.59175
19	C	-4.79192	-1.46285	0.845785
20	C	-5.71702	-0.26527	0.644539
21	C	-5.17395	0.757876	-0.35309
22	C	-4.83788	0.024716	-1.67148
23	C	-6.17311	1.891901	-0.61509
24	C	-5.72702	-2.91118	-0.98848
25	C	-1.96897	0.058131	-0.46939
26	C	-1.8517	-3.26439	-2.63641
27	C	5.215694	-1.39014	-0.65867
28	C	2.735827	-2.19343	0.865266
29	C	3.274722	-3.3472	1.448528
30	C	3.632478	-3.40464	2.796095
31	C	3.458675	-2.27806	3.591059
32	C	2.926406	-1.09376	3.068046
33	C	2.555741	-1.08231	1.714615
34	O	3.855786	2.582646	-3.16968
35	O	5.741038	1.157735	-1.91459
36	O	3.451469	-4.43932	0.638532
37	C	2.793731	0.134772	3.940319
38	C	2.595442	1.390303	3.09286
39	C	1.532367	1.085915	2.02124
40	O	2.037395	0.053892	1.140121
41	C	1.129992	2.284843	1.195323
42	C	0.005057	3.015437	1.586819
43	C	-0.3569	4.167655	0.891057
44	C	0.397262	4.58277	-0.20618
45	C	1.514	3.844601	-0.60815
46	C	1.891816	2.705648	0.100926
47	O	2.16005	4.349147	-1.70419
48	O	-0.00893	5.709217	-0.87582
49	O	-1.46292	4.874522	1.272665
50	O	3.815707	1.846387	2.510366

51	O	3.798807	-2.26519	4.914725
52	O	-6.11111	0.328212	1.932663
53	C	-5.21971	0.91031	2.752029
54	C	-5.90179	1.411389	4.002242
55	O	-4.03443	1.021552	2.526679
56	C	0.797077	-1.81044	-3.96541
57	H	1.599639	1.375492	-3.52865
58	H	2.793083	-3.13082	-1.01817
59	H	0.466397	-3.12969	0.082723
60	H	-2.2541	-0.91325	-3.77851
61	H	-2.57054	0.66062	-3.09686
62	H	-0.34956	0.973398	-2.32231
63	H	-0.29566	0.52214	-4.0084
64	H	-1.37123	-3.86984	-0.0347
65	H	-1.69494	-2.3078	0.681601
66	H	-3.67247	-3.72965	0.856274
67	H	-3.58869	-4.16665	-0.82396
68	H	-4.093	-1.75528	-2.53699
69	H	-5.28509	-2.17126	1.520414
70	H	-3.88299	-1.13411	1.346767
71	H	-6.68683	-0.61451	0.28324
72	H	-4.2671	1.189164	0.06754
73	H	-4.41564	0.75438	-2.36562
74	H	-5.78715	-0.28211	-2.12645
75	H	-5.76067	2.611019	-1.32849
76	H	-7.10753	1.502977	-1.03442
77	H	-6.41702	2.43396	0.301448
78	H	-5.51242	-3.48143	-1.89684
79	H	-6.10165	-3.61265	-0.23594
80	H	-6.53666	-2.21725	-1.22167
81	H	-0.88693	0.092845	-0.34607
82	H	-2.39184	-0.2008	0.49726
83	H	-2.29863	1.072621	-0.70521
84	H	-1.62107	-2.88128	-3.62513
85	H	-1.25117	-4.16605	-2.48651
86	H	-2.89805	-3.56616	-2.65377
87	H	6.161628	-1.27343	-1.19527
88	H	5.378946	-1.06727	0.374848
89	H	4.989697	-2.45496	-0.62941
90	H	4.040714	-4.31846	3.216402
91	H	4.793957	2.733956	-2.97834

92	H	6.180498	0.93196	-1.08752
93	H	3.864269	-5.14959	1.142894
94	H	1.950134	0.027496	4.632461
95	H	3.687294	0.257417	4.556528
96	H	2.243063	2.213973	3.715306
97	H	0.646236	0.694721	2.53369
98	H	-0.61175	2.697216	2.419399
99	H	2.755709	2.137216	-0.21229
100	H	2.782193	3.713167	-2.10391
101	H	0.563382	5.814995	-1.64831
102	H	-1.57225	5.612648	0.658054
103	H	4.111544	1.178984	1.880302
104	H	4.186963	-3.11379	5.157999
105	H	-5.1684	1.874896	4.658683
106	H	-6.67571	2.135738	3.739493
107	H	-6.39015	0.581104	4.516807
108	H	-0.11259	-2.14255	-4.46437
109	H	1.346882	-1.18296	-4.67166
110	H	1.40764	-2.68944	-3.7455

B3LYP/6-311G(d,p) Energy = -2575.458609 a.u.; Population = 0.13%.

[(*P*)-6S,2R',3R']-**1** Conformer 7		Standard Orientation (Ångstroms)		
I	Atom	X	Y	Z
1	C	3.723936	1.551935	-2.4531
2	C	4.632669	0.725504	-1.79661
3	C	4.239758	-0.52728	-1.32739
4	C	2.886494	-0.91014	-1.47236
5	C	2.008376	-0.13974	-2.25047
6	C	2.448453	1.100966	-2.73057
7	C	2.370711	-2.16732	-0.78475
8	C	0.870978	-2.32238	-0.87614
9	C	0.047372	-1.67036	-1.69803
10	C	0.633367	-0.67028	-2.71522
11	C	-1.47423	-1.97265	-1.69397
12	C	-2.27876	-0.60872	-1.72537
13	C	-1.83424	0.149406	-2.99848
14	C	-0.34495	0.511399	-2.98155
15	C	-1.92613	-2.74941	-0.43371
16	C	-3.41929	-3.10004	-0.46495
17	C	-4.40602	-1.93697	-0.76089

18	C	-3.827	-0.89352	-1.79046
19	C	-4.79751	-1.27721	0.588386
20	C	-5.70475	-0.05878	0.447683
21	C	-5.11062	1.010114	-0.46357
22	C	-4.72272	0.377172	-1.81684
23	C	-6.0726	2.185553	-0.67462
24	C	-5.67792	-2.5793	-1.36781
25	C	-1.88742	0.260996	-0.50373
26	C	-1.77667	-2.88741	-2.91788
27	C	5.302266	-1.41336	-0.71406
28	C	2.797038	-2.33515	0.680939
29	C	3.299527	-3.56161	1.141137
30	C	3.672941	-3.76051	2.471298
31	C	3.547619	-2.71732	3.375569
32	C	3.039064	-1.4714	2.9838
33	C	2.652103	-1.31208	1.646634
34	O	4.08135	2.845382	-2.78296
35	O	5.910941	1.236987	-1.6797
36	O	3.486482	-4.64972	0.328834
37	C	2.947518	-0.33859	3.981287
38	C	2.778155	1.001987	3.270824
39	C	1.693071	0.841024	2.190464
40	O	2.148707	-0.11323	1.1999
41	C	1.318804	2.130702	1.499326
42	C	0.215017	2.842545	1.976098
43	C	-0.11884	4.073934	1.415057
44	C	0.643564	4.5894	0.367285
45	C	1.740733	3.872726	-0.1192
46	C	2.089432	2.651697	0.455427
47	O	2.398885	4.479871	-1.15421
48	O	0.26581	5.793918	-0.16921
49	O	-1.20398	4.762497	1.880613
50	O	4.004944	1.480657	2.72175
51	O	3.905382	-2.84545	4.687979
52	O	-5.8839	0.546946	1.768724
53	C	-6.89949	0.116085	2.539229
54	C	-6.92592	0.849446	3.85614
55	O	-7.68491	-0.74453	2.208775
56	C	0.931745	-1.38272	-4.07403
57	H	1.798488	1.754473	-3.29556
58	H	2.809619	-3.00684	-1.34792

59	H	0.476735	-3.05303	-0.18226
60	H	-2.0822	-0.43666	-3.88766
61	H	-2.39076	1.085317	-3.09375
62	H	-0.18635	1.280846	-2.22355
63	H	-0.09186	0.974404	-3.93983
64	H	-1.3777	-3.69216	-0.35584
65	H	-1.68047	-2.1777	0.464685
66	H	-3.69712	-3.55144	0.494001
67	H	-3.57487	-3.88756	-1.20658
68	H	-3.96983	-1.35075	-2.77492
69	H	-5.30788	-2.02706	1.201087
70	H	-3.90767	-0.97598	1.146132
71	H	-6.69441	-0.35439	0.094997
72	H	-4.21366	1.390509	0.031731
73	H	-4.26068	1.150776	-2.43361
74	H	-5.65374	0.121432	-2.33559
75	H	-5.6143	2.952872	-1.30487
76	H	-6.99304	1.853699	-1.16709
77	H	-6.3447	2.649206	0.275954
78	H	-5.44099	-3.08621	-2.30753
79	H	-6.08839	-3.32595	-0.68062
80	H	-6.4683	-1.85559	-1.57554
81	H	-0.80925	0.261315	-0.34374
82	H	-2.34285	-0.07451	0.424285
83	H	-2.18974	1.298895	-0.66079
84	H	-1.5256	-2.4338	-3.87149
85	H	-1.18967	-3.80553	-2.82726
86	H	-2.82582	-3.17334	-2.973
87	H	6.255923	-1.25899	-1.22633
88	H	5.46221	-1.21437	0.350566
89	H	5.055343	-2.46962	-0.8073
90	H	4.052106	-4.72992	2.773461
91	H	5.019664	2.94896	-2.56184
92	H	6.327068	0.931691	-0.86613
93	H	3.107209	-4.49138	-0.54215
94	H	2.10689	-0.49485	4.667672
95	H	3.849077	-0.3059	4.597078
96	H	2.457089	1.767408	3.978561
97	H	0.8015	0.427883	2.675656
98	H	-0.40125	2.453123	2.778211
99	H	2.940296	2.102464	0.080085

100	H	3.017259	3.881513	-1.61325
101	H	0.845573	5.977319	-0.9213
102	H	-1.29422	5.569135	1.35551
103	H	4.296607	0.851148	2.052159
104	H	4.27269	-3.72451	4.837018
105	H	-5.96964	0.728554	4.369189
106	H	-7.07287	1.917765	3.682347
107	H	-7.732	0.462306	4.475749
108	H	0.023102	-1.64305	-4.61522
109	H	1.51358	-0.71332	-4.7127
110	H	1.512174	-2.29535	-3.91993

B3LYP/6-311G(d,p) Energy = -2575.4611344 a.u.; Population = 1.91%.

Table S9. Cartesian coordinates for the re-optimized conformers of [(*p*)-6R,2S',3S']-**2** at the B3LYP/6-311G(d,p) level with IEFPCM solvent model for Methanol.

[(*P*)-6R,2S',3S']-**2** Conformer 1		Standard Orientation (Ångstroms)		
I	Atom	X	Y	Z
1	C	0.383139	2.960891	4.880976
2	C	0.516746	3.837747	3.800674
3	C	0.100126	3.469401	2.524042
4	C	-0.51032	2.203889	2.336648
5	C	-0.6253	1.307911	3.40868
6	C	-0.17194	1.711495	4.675636
7	C	-0.95166	1.799333	0.943459
8	C	-1.31429	0.342432	0.837339
9	C	-1.43816	-0.5389	1.832333
10	C	-1.28176	-0.08987	3.300479
11	C	-1.72135	-2.03378	1.522404
12	C	-0.61972	-2.91935	2.243628
13	C	-0.68393	-2.59697	3.756001
14	C	-0.40111	-1.12246	4.07244
15	C	-1.64781	-2.35292	0.008421
16	C	-1.95385	-3.82373	-0.30762
17	C	-1.19626	-4.89824	0.522111
18	C	-0.93137	-4.44659	2.009417
19	C	0.118146	-5.25846	-0.22157
20	C	1.004897	-6.2529	0.522937
21	C	1.351499	-5.7906	1.93485
22	C	0.056106	-5.43354	2.692814

23	C	2.154107	-6.84657	2.704506
24	C	-2.09785	-6.15777	0.538564
25	C	0.793615	-2.51795	1.749296
26	C	-3.17183	-2.37267	1.975003
27	C	0.337173	4.443045	1.390919
28	C	-2.02994	2.6689	0.280971
29	C	-3.22145	3.054805	0.911765
30	C	-4.182	3.826826	0.257854
31	C	-3.97938	4.212967	-1.06158
32	C	-2.82131	3.83963	-1.75588
33	C	-1.87125	3.081449	-1.05531
34	O	0.798852	3.334915	6.129842
35	O	1.130223	5.042434	4.104013
36	O	-3.41719	2.662719	2.203856
37	C	-2.61595	4.223953	-3.20773
38	C	-1.46013	3.442989	-3.84292
39	C	-0.29169	3.425169	-2.8409
40	O	-0.71047	2.673554	-1.67886
41	C	0.990591	2.824632	-3.36034
42	C	1.985712	3.68074	-3.83642
43	C	3.165225	3.159708	-4.36582
44	C	3.357756	1.778614	-4.41078
45	C	2.364793	0.925221	-3.92535
46	C	1.180784	1.439771	-3.40536
47	O	2.662657	-0.40977	-4.0118
48	O	4.538975	1.315929	-4.92959
49	O	4.13359	4.003921	-4.82641
50	O	-1.84521	2.126776	-4.22623
51	O	-4.96611	4.960509	-1.64101
52	O	2.265875	-6.39418	-0.20865
53	C	2.353417	-7.34178	-1.15991
54	C	3.722164	-7.34597	-1.79189
55	O	1.449598	-8.09088	-1.45777
56	C	-2.66167	0.022077	4.023016
57	H	-0.26256	1.063778	5.537798
58	H	-0.07953	1.918417	0.292717
59	H	-1.43731	0.016922	-0.1881
60	H	-1.65427	-2.8962	4.162654
61	H	0.059503	-3.18932	4.296096
62	H	0.650719	-0.90798	3.86721
63	H	-0.53415	-0.97448	5.147523

64	H	-2.37717	-1.74559	-0.53651
65	H	-0.66719	-2.07459	-0.38456
66	H	-1.75388	-4.00447	-1.36981
67	H	-3.02768	-3.98885	-0.19043
68	H	-1.88063	-4.60377	2.532209
69	H	-0.14378	-5.68354	-1.19568
70	H	0.708898	-4.36218	-0.42348
71	H	0.539365	-7.23966	0.547584
72	H	1.974293	-4.89802	1.834497
73	H	0.329801	-5.06584	3.683634
74	H	-0.48146	-6.37059	2.87789
75	H	2.414683	-6.4833	3.702581
76	H	1.574124	-7.76799	2.824538
77	H	3.08161	-7.09513	2.184303
78	H	-2.31573	-6.47893	-0.48496
79	H	-1.64539	-7.0042	1.058571
80	H	-3.05045	-5.94044	1.03004
81	H	0.912289	-1.43488	1.726119
82	H	1.016404	-2.88053	0.749418
83	H	1.557632	-2.91393	2.422131
84	H	-3.48746	-3.35887	1.640157
85	H	-3.31237	-2.35043	3.050578
86	H	-3.86062	-1.64429	1.538378
87	H	1.227868	5.047146	1.581702
88	H	0.492753	3.932047	0.441663
89	H	-0.50652	5.12789	1.252857
90	H	-5.09319	4.125175	0.764215
91	H	1.107444	4.249714	6.062268
92	H	0.77185	5.749521	3.557088
93	H	-4.25334	3.021863	2.523107
94	H	-3.51467	4.018469	-3.80008
95	H	-2.40866	5.297366	-3.29999
96	H	-1.13927	3.935607	-4.76143
97	H	-0.10006	4.458793	-2.53201
98	H	1.865859	4.757148	-3.79827
99	H	0.419584	0.766052	-3.03399
100	H	1.935113	-0.93876	-3.66578
101	H	4.539498	0.35083	-4.88158
102	H	4.876723	3.469124	-5.13718
103	H	-2.06019	1.633347	-3.42549
104	H	-4.71782	5.202589	-2.53996

105	H	3.753709	-8.07911	-2.59503
106	H	3.957619	-6.35356	-2.18122
107	H	4.475019	-7.59096	-1.03911
108	H	-3.07522	-0.95047	4.283872
109	H	-2.53556	0.576138	4.955764
110	H	-3.38023	0.559713	3.405798

B3LYP/6-311G(d,p) Energy = -2574.7525275 a.u.; Population = 0.08%.

[(*P*)-6R,2S',3S']-**2** Conformer 2		Standard Orientation (Ångstroms)		
I	Atom	X	Y	Z
1	C	0.1858	2.737619	5.274276
2	C	0.458506	3.709003	4.302587
3	C	0.146231	3.489937	2.964928
4	C	-0.48791	2.272237	2.596019
5	C	-0.74047	1.281172	3.56081
6	C	-0.40025	1.543549	4.898645
7	C	-0.81512	2.021796	1.134623
8	C	-1.12687	0.576642	0.847465
9	C	-1.3774	-0.38961	1.73329
10	C	-1.43618	-0.06503	3.241895
11	C	-1.6173	-1.8468	1.255075
12	C	-0.65972	-2.81505	2.067282
13	C	-0.98753	-2.62666	3.568513
14	C	-0.74302	-1.19629	4.064791
15	C	-1.29999	-2.03652	-0.24861
16	C	-1.56415	-3.46696	-0.73722
17	C	-0.95566	-4.62359	0.10385
18	C	-0.93366	-4.3087	1.648352
19	C	0.459425	-4.94281	-0.44786
20	C	1.206511	-6.01782	0.336285
21	C	1.32352	-5.68832	1.821058
22	C	-0.07445	-5.36918	2.391768
23	C	1.982023	-6.82558	2.611398
24	C	-1.85404	-5.86247	-0.13546
25	C	0.819132	-2.39712	1.862895
26	C	-3.12544	-2.18442	1.437715
27	C	0.502278	4.569084	1.967728
28	C	-1.8787	2.936042	0.500708
29	C	-2.97519	3.489945	1.175173
30	C	-3.91084	4.292842	0.514745

31	C	-3.77284	4.542694	-0.8431
32	C	-2.70208	4.010127	-1.57519
33	C	-1.78017	3.223262	-0.87862
34	O	0.494924	2.966953	6.58277
35	O	1.076987	4.842436	4.783531
36	O	-3.21311	3.296937	2.50752
37	C	-2.5701	4.255639	-3.06232
38	C	-1.62858	3.233947	-3.70154
39	C	-0.3577	3.135507	-2.83557
40	O	-0.71598	2.638629	-1.52446
41	C	0.726059	2.241971	-3.38589
42	C	1.824266	2.81958	-4.02554
43	C	2.820175	2.012716	-4.57457
44	C	2.72818	0.624182	-4.47181
45	C	1.63368	0.049707	-3.82199
46	C	0.630665	0.850081	-3.28555
47	O	1.64799	-1.32078	-3.76837
48	O	3.739949	-0.12387	-5.01571
49	O	3.88991	2.585722	-5.19989
50	O	-2.2565	1.964539	-3.87373
51	O	-4.66261	5.315164	-1.53576
52	O	2.568271	-6.12314	-0.19181
53	C	2.796814	-6.96999	-1.21229
54	C	4.250346	-6.95356	-1.61182
55	O	1.943129	-7.65589	-1.72953
56	C	-2.90914	0.081449	3.738085
57	H	-0.59637	0.822221	5.680358
58	H	0.096536	2.232579	0.566105
59	H	-1.10399	0.349882	-0.20942
60	H	-2.01813	-2.93366	3.768151
61	H	-0.35942	-3.28461	4.174692
62	H	0.332841	-1.00834	4.078523
63	H	-1.07353	-1.13669	5.105296
64	H	-1.92664	-1.36966	-0.84858
65	H	-0.26622	-1.74582	-0.4506
66	H	-1.20044	-3.56024	-1.76685
67	H	-2.64435	-3.61733	-0.80409
68	H	-1.95579	-4.49293	1.994346
69	H	0.356361	-5.2741	-1.48587
70	H	1.080294	-4.04448	-0.47002
71	H	0.734768	-6.99221	0.198237

72	H	1.962146	-4.80489	1.902452
73	H	0.041022	-5.09201	3.441421
74	H	-0.64143	-6.30701	2.408315
75	H	2.083101	-6.5563	3.666516
76	H	1.381082	-7.73964	2.555235
77	H	2.978297	-7.05045	2.224657
78	H	-1.9023	-6.09347	-1.20446
79	H	-1.49767	-6.75751	0.377688
80	H	-2.87353	-5.66913	0.210316
81	H	0.944216	-1.32049	1.978541
82	H	1.209183	-2.65509	0.881412
83	H	1.456488	-2.87808	2.608382
84	H	-3.38548	-3.15166	1.011675
85	H	-3.44485	-2.20438	2.474458
86	H	-3.72439	-1.42789	0.923429
87	H	1.47003	5.016969	2.212044
88	H	0.573994	4.185155	0.952479
89	H	-0.24205	5.373292	1.954747
90	H	-4.73452	4.709998	1.082979
91	H	0.852852	3.863931	6.644642
92	H	0.92598	5.592182	4.197979
93	H	-2.43505	2.888121	2.917747
94	H	-3.54757	4.189397	-3.54538
95	H	-2.19512	5.267555	-3.25546
96	H	-1.34231	3.557485	-4.7034
97	H	0.042413	4.149093	-2.71972
98	H	1.927696	3.895592	-4.10247
99	H	-0.21903	0.392272	-2.797
100	H	0.83948	-1.64858	-3.35859
101	H	3.536245	-1.05936	-4.88523
102	H	4.476262	1.878845	-5.50205
103	H	-2.59311	1.678632	-3.0161
104	H	-5.36576	5.606101	-0.94343
105	H	4.397403	-7.58279	-2.48706
106	H	4.569556	-5.93185	-1.82581
107	H	4.86253	-7.32361	-0.78597
108	H	-3.42943	-0.87332	3.784029
109	H	-2.91129	0.500831	4.747135
110	H	-3.47971	0.750573	3.091918

B3LYP/6-311G(d,p) Energy = -2574.7536827 a.u.; Population = 49.56%.

[(*P*)-6R,2S',3S']-**2** Conformer 3		Standard Orientation (Ångstroms)		
I	Atom	X	Y	Z
1	C	0.39011	2.810363	4.933728
2	C	0.530088	3.726183	3.887052
3	C	0.124154	3.403708	2.594628
4	C	-0.48255	2.144825	2.356648
5	C	-0.60359	1.210325	3.394554
6	C	-0.16054	1.568223	4.678778
7	C	-0.91217	1.790249	0.94623
8	C	-1.27676	0.339038	0.785729
9	C	-1.40327	-0.57909	1.74648
10	C	-1.25551	-0.18432	3.231071
11	C	-1.6806	-2.06231	1.380616
12	C	-0.57759	-2.97005	2.072311
13	C	-0.64969	-2.70506	3.59554
14	C	-0.37598	-1.2424	3.969019
15	C	-1.60138	-2.32545	-0.14388
16	C	-1.90014	-3.78438	-0.51421
17	C	-1.13723	-4.88501	0.274691
18	C	-0.87965	-4.48934	1.778706
19	C	0.181188	-5.2067	-0.47938
20	C	1.072599	-6.22398	0.227947
21	C	1.410834	-5.8174	1.659153
22	C	0.111801	-5.49601	2.426865
23	C	2.215303	-6.90036	2.388422
24	C	-2.03006	-6.1502	0.238252
25	C	0.835836	-2.54397	1.599692
26	C	-3.13143	-2.42324	1.81589
27	C	0.366979	4.417991	1.498886
28	C	-1.97976	2.686963	0.303052
29	C	-3.17835	3.047636	0.933985
30	C	-4.1295	3.848117	0.301293
31	C	-3.90844	4.284415	-0.99981
32	C	-2.74274	3.937493	-1.69329
33	C	-1.80194	3.149853	-1.01562
34	O	0.795652	3.139621	6.198575
35	O	1.139573	4.920158	4.238825
36	O	-3.39119	2.600303	2.206475
37	C	-2.52109	4.374039	-3.12514
38	C	-1.40495	3.580647	-3.79513
39	C	-0.22023	3.460484	-2.81696

40	O	-0.63031	2.771661	-1.62418
41	C	0.960208	2.718739	-3.39968
42	C	1.95429	3.439297	-4.0645
43	C	3.018057	2.770374	-4.66697
44	C	3.094553	1.37741	-4.60217
45	C	2.10346	0.660058	-3.93125
46	C	1.031598	1.322276	-3.33522
47	O	2.284523	-0.69713	-3.91783
48	O	4.16733	0.771454	-5.20096
49	O	3.988456	3.480458	-5.30939
50	O	-1.93066	2.305277	-4.1482
51	O	-4.8879	5.056488	-1.56211
52	O	2.337649	-6.32639	-0.50317
53	C	2.436663	-7.23469	-1.49098
54	C	3.808395	-7.20381	-2.11568
55	O	1.539859	-7.97775	-1.82316
56	C	-2.6396	-0.10269	3.949669
57	H	-0.25618	0.889362	5.516121
58	H	-0.03254	1.927693	0.309563
59	H	-1.39605	0.052265	-0.25165
60	H	-1.62017	-3.02481	3.985845
61	H	0.094656	-3.31361	4.115998
62	H	0.676374	-1.01563	3.77998
63	H	-0.51664	-1.13612	5.04811
64	H	-2.33124	-1.7012	-0.66854
65	H	-0.6205	-2.02941	-0.52332
66	H	-1.69919	-3.92455	-1.58239
67	H	-2.97312	-3.95948	-0.40375
68	H	-1.82966	-4.67263	2.291569
69	H	-0.07566	-5.59521	-1.47003
70	H	0.766634	-4.29966	-0.64534
71	H	0.614027	-7.21411	0.210295
72	H	2.030342	-4.919	1.597276
73	H	0.381763	-5.1641	3.431289
74	H	-0.42146	-6.44193	2.576447
75	H	2.469652	-6.57723	3.401785
76	H	1.639129	-7.82855	2.467781
77	H	3.146334	-7.12315	1.862861
78	H	-2.24671	-6.42838	-0.79797
79	H	-1.57142	-7.01528	0.720482
80	H	-2.98371	-5.96036	0.738922

81	H	0.949939	-1.46031	1.616582
82	H	1.064284	-2.86786	0.58799
83	H	1.598958	-2.96142	2.260458
84	H	-3.44362	-3.39726	1.443967
85	H	-3.27518	-2.44172	2.891103
86	H	-3.82125	-1.68104	1.404911
87	H	0.533242	3.941804	0.533454
88	H	-0.47929	5.102762	1.377197
89	H	1.252453	5.019408	1.719998
90	H	-5.04673	4.127753	0.807419
91	H	1.10335	4.056651	6.165782
92	H	0.776789	5.647865	3.722697
93	H	-4.2356	2.939326	2.525783
94	H	-3.4268	4.228453	-3.72454
95	H	-2.27038	5.440057	-3.1765
96	H	-1.0566	4.115991	-4.68584
97	H	0.09024	4.476992	-2.54724
98	H	1.924208	4.521263	-4.11759
99	H	0.278954	0.759274	-2.79751
100	H	1.575353	-1.12748	-3.42689
101	H	4.101694	-0.18241	-5.06086
102	H	4.647133	2.857439	-5.64564
103	H	-1.22288	1.794576	-4.56014
104	H	-4.63143	5.325379	-2.45094
105	H	3.849606	-7.90507	-2.9464
106	H	4.037762	-6.1953	-2.46529
107	H	4.559565	-7.47176	-1.36909
108	H	-3.05174	-1.08533	4.171886
109	H	-2.52025	0.416615	4.903105
110	H	-3.35636	0.455523	3.34873

B3LYP/6-311G(d,p) Energy = -2574.7534216 a.u.; Population = 0.17%.

[(*P*)-6R,2S',3S']-**2** Conformer 4		Standard Orientation (Ångstroms)		
I	Atom	X	Y	Z
1	C	0.185712	2.737931	5.274154
2	C	0.458263	3.709352	4.302449
3	C	0.146221	3.490111	2.964758
4	C	-0.48781	2.272303	2.595946
5	C	-0.74027	1.281251	3.560764
6	C	-0.40007	1.543708	4.898586

7	C	-0.81504	2.021871	1.134575
8	C	-1.12683	0.57672	0.847387
9	C	-1.37721	-0.38955	1.733234
10	C	-1.43586	-0.065	3.24186
11	C	-1.61714	-1.84677	1.255064
12	C	-0.65947	-2.81501	2.06718
13	C	-0.98706	-2.62659	3.568447
14	C	-0.74256	-1.19621	4.064678
15	C	-1.29999	-2.03648	-0.24866
16	C	-1.56408	-3.46696	-0.73725
17	C	-0.95564	-4.62361	0.103844
18	C	-0.9335	-4.30865	1.648328
19	C	0.459393	-4.94298	-0.44795
20	C	1.206508	-6.01794	0.336242
21	C	1.323668	-5.68824	1.820964
22	C	-0.07428	-5.36913	2.391721
23	C	1.982324	-6.82536	2.611371
24	C	-1.85415	-5.86242	-0.13537
25	C	0.819368	-2.39711	1.862551
26	C	-3.12526	-2.18438	1.437878
27	C	0.502021	4.568914	1.967119
28	C	-1.87856	2.936234	0.500747
29	C	-2.97514	3.489919	1.175222
30	C	-3.91096	4.292672	0.514831
31	C	-3.77293	4.542687	-0.84297
32	C	-2.70201	4.010439	-1.57506
33	C	-1.77997	3.223675	-0.87853
34	O	0.494657	2.967445	6.582643
35	O	1.076622	4.842897	4.783509
36	O	-3.21299	3.296943	2.507582
37	C	-2.57003	4.25613	-3.06217
38	C	-1.62863	3.234378	-3.70143
39	C	-0.35762	3.135995	-2.83562
40	O	-0.71565	2.639283	-1.52437
41	C	0.72605	2.242389	-3.38597
42	C	1.824455	2.819887	-4.0254
43	C	2.820271	2.012915	-4.57444
44	C	2.728078	0.624394	-4.47175
45	C	1.633349	0.050028	-3.82222
46	C	0.630354	0.850493	-3.2859
47	O	1.647275	-1.32048	-3.76895

48	O	3.739936	-0.12379	-5.01531
49	O	3.890162	2.585802	-5.19959
50	O	-2.25663	1.964972	-3.87341
51	O	-4.66285	5.315025	-1.5356
52	O	2.56818	-6.1234	-0.192
53	C	2.796671	-6.97078	-1.21203
54	C	4.25042	-6.95564	-1.61082
55	O	1.942892	-7.65666	-1.72913
56	C	-2.9088	0.081315	3.738152
57	H	-0.59608	0.822386	5.68033
58	H	0.096598	2.232636	0.566029
59	H	-1.10407	0.349966	-0.20951
60	H	-2.01761	-2.93363	3.768264
61	H	-0.35883	-3.28449	4.17455
62	H	0.333293	-1.00821	4.078295
63	H	-1.07295	-1.13662	5.105218
64	H	-1.92678	-1.36971	-0.84858
65	H	-0.26628	-1.74568	-0.4508
66	H	-1.20031	-3.56022	-1.76686
67	H	-2.64427	-3.61735	-0.80418
68	H	-1.95561	-4.49283	1.994422
69	H	0.356228	-5.27437	-1.48592
70	H	1.080319	-4.04469	-0.47026
71	H	0.73469	-6.99232	0.19839
72	H	1.962242	-4.80476	1.902197
73	H	0.041213	-5.09197	3.44137
74	H	-0.64125	-6.30697	2.408283
75	H	2.083525	-6.55594	3.666439
76	H	1.381424	-7.73946	2.555407
77	H	2.978558	-7.05023	2.224532
78	H	-1.9025	-6.09345	-1.20435
79	H	-1.49781	-6.75747	0.377777
80	H	-2.87359	-5.66899	0.210464
81	H	0.944462	-1.32046	1.97802
82	H	1.209288	-2.65521	0.881055
83	H	1.456837	-2.87796	2.608012
84	H	-3.38544	-3.15139	1.011397
85	H	-3.44444	-2.2049	2.47469
86	H	-3.72432	-1.42759	0.924124
87	H	1.466732	5.021429	2.214702
88	H	0.579981	4.18312	0.952973

89	H	-0.24572	5.36981	1.949108
90	H	-4.73472	4.709605	1.083092
91	H	0.852564	3.864443	6.644356
92	H	0.922973	5.59335	4.199571
93	H	-2.43511	2.887696	2.917691
94	H	-3.54751	4.190063	-3.5452
95	H	-2.19492	5.268017	-3.2552
96	H	-1.34247	3.5578	-4.70336
97	H	0.042507	4.149599	-2.71999
98	H	1.92802	3.895891	-4.10223
99	H	-0.21955	0.392816	-2.79758
100	H	0.838987	-1.64807	-3.35858
101	H	3.534779	-1.05929	-4.88725
102	H	4.476024	1.878834	-5.50247
103	H	-2.59402	1.679651	-3.0159
104	H	-5.36622	5.605534	-0.94335
105	H	4.395958	-7.57865	-2.49074
106	H	4.573543	-5.93345	-1.81624
107	H	4.860608	-7.33475	-0.78754
108	H	-3.42903	-0.87348	3.783966
109	H	-2.91093	0.500564	4.747257
110	H	-3.47949	0.750458	3.092106

B3LYP/6-311G(d,p) Energy = -2574.7583956 a.u.; Population = 49.6%.

[(*P*)-6R,2S',3S']-**2** Conformer 5		Standard Orientation (Ångstroms)		
I	Atom	X	Y	Z
1	C	0.382702	2.822818	4.938737
2	C	0.522585	3.736783	3.890402
3	C	0.117767	3.41149	2.598328
4	C	-0.48747	2.151529	2.362267
5	C	-0.60866	1.218989	3.401942
6	C	-0.16687	1.579814	4.685813
7	C	-0.91446	1.793351	0.952015
8	C	-1.27754	0.341476	0.794321
9	C	-1.40614	-0.57432	1.757006
10	C	-1.25983	-0.17631	3.240834
11	C	-1.68395	-2.05815	1.394157
12	C	-0.58194	-2.96503	2.088459
13	C	-0.65441	-2.69631	3.611049
14	C	-0.38042	-1.23278	3.981232

15	C	-1.60402	-2.32458	-0.12972
16	C	-1.90372	-3.78406	-0.49714
17	C	-1.14263	-4.88366	0.295013
18	C	-0.88522	-4.48472	1.798265
19	C	0.175752	-5.20882	-0.45764
20	C	1.065547	-6.22545	0.252553
21	C	1.404049	-5.81538	1.682661
22	C	0.105085	-5.49077	2.449164
23	C	2.207312	-6.89715	2.414989
24	C	-2.03702	-6.14783	0.261293
25	C	0.832029	-2.54133	1.615368
26	C	-3.13524	-2.41746	1.829304
27	C	0.360108	4.424086	1.500903
28	C	-1.98238	2.686019	0.303771
29	C	-3.18329	3.043038	0.928199
30	C	-4.13953	3.834894	0.285911
31	C	-3.91433	4.263262	-1.01777
32	C	-2.74239	3.923063	-1.70133
33	C	-1.80149	3.145756	-1.01781
34	O	0.787174	3.154767	6.2033
35	O	1.130474	4.931869	4.240569
36	O	-3.39926	2.602115	2.202766
37	C	-2.52609	4.358765	-3.13176
38	C	-1.40452	3.572	-3.79717
39	C	-0.21933	3.459893	-2.81754
40	O	-0.62519	2.773257	-1.6206
41	C	0.96644	2.722924	-3.39543
42	C	1.957807	3.446911	-4.06074
43	C	3.026118	2.78233	-4.65993
44	C	3.11025	1.390012	-4.59142
45	C	2.122083	0.669105	-3.92013
46	C	1.045796	1.327022	-3.32728
47	O	2.310373	-0.68723	-3.90303
48	O	4.187282	0.788217	-5.18725
49	O	3.993638	3.496069	-5.30299
50	O	-1.91831	2.290038	-4.15023
51	O	-4.82115	5.029026	-1.69754
52	O	2.330496	-6.33174	-0.47822
53	C	2.42766	-7.2422	-1.46424
54	C	3.79859	-7.21356	-2.09077
55	O	1.529661	-7.98481	-1.79419

56	C	-2.64436	-0.09346	3.958426
57	H	-0.26257	0.902522	5.524427
58	H	-0.03405	1.930406	0.316319
59	H	-1.39511	0.052286	-0.24258
60	H	-1.62511	-3.01477	4.00187
61	H	0.089568	-3.30387	4.133198
62	H	0.671948	-1.00655	3.791556
63	H	-0.521	-1.12407	5.060094
64	H	-2.33303	-1.70084	-0.65616
65	H	-0.62269	-2.03013	-0.5092
66	H	-1.70177	-3.92675	-1.56479
67	H	-2.97699	-3.95793	-0.38749
68	H	-1.83558	-4.66594	2.311229
69	H	-0.08114	-5.59937	-1.44747
70	H	0.762385	-4.30287	-0.62545
71	H	0.605562	-7.21497	0.237545
72	H	2.024397	-4.91772	1.618509
73	H	0.375025	-5.15664	3.452856
74	H	-0.4291	-6.43583	2.600838
75	H	2.461756	-6.57159	3.427547
76	H	1.630247	-7.82459	2.496679
77	H	3.138229	-7.12223	1.890206
78	H	-2.25315	-6.42861	-0.77434
79	H	-1.5799	-7.01215	0.746339
80	H	-2.99085	-5.95542	0.760647
81	H	0.947024	-1.45772	1.629611
82	H	1.06058	-2.868	0.604582
83	H	1.594525	-2.9578	2.277481
84	H	-3.44812	-3.39148	1.457998
85	H	-3.27933	-2.43509	2.904491
86	H	-3.82432	-1.675	1.417548
87	H	1.246756	5.024736	1.719644
88	H	0.524121	3.946709	0.535722
89	H	-0.48552	5.109783	1.379771
90	H	-5.05774	4.101761	0.800626
91	H	1.094444	4.071864	6.169151
92	H	0.772806	5.657261	3.717698
93	H	-4.24466	2.940732	2.519588
94	H	-3.44241	4.222955	-3.71081
95	H	-2.2867	5.427113	-3.17741
96	H	-1.05529	4.105821	-4.68889

97	H	0.085387	4.478869	-2.55055
98	H	1.921711	4.528554	-4.11693
99	H	0.295255	0.761265	-2.78948
100	H	1.601169	-1.12012	-3.41441
101	H	4.125423	-0.16574	-5.04619
102	H	4.65571	2.875582	-5.6372
103	H	-1.20402	1.785243	-4.558
104	H	-5.59938	5.174124	-1.14724
105	H	3.841533	-7.92444	-2.91317
106	H	4.022614	-6.20836	-2.45334
107	H	4.552203	-7.46855	-1.3422
108	H	-3.05674	-1.07563	4.182223
109	H	-2.52565	0.427609	4.91098
110	H	-3.36068	0.463661	3.35591

B3LYP/6-311G(d,p) Energy = -2574.7546688 a.u.; Population = 0.60%.

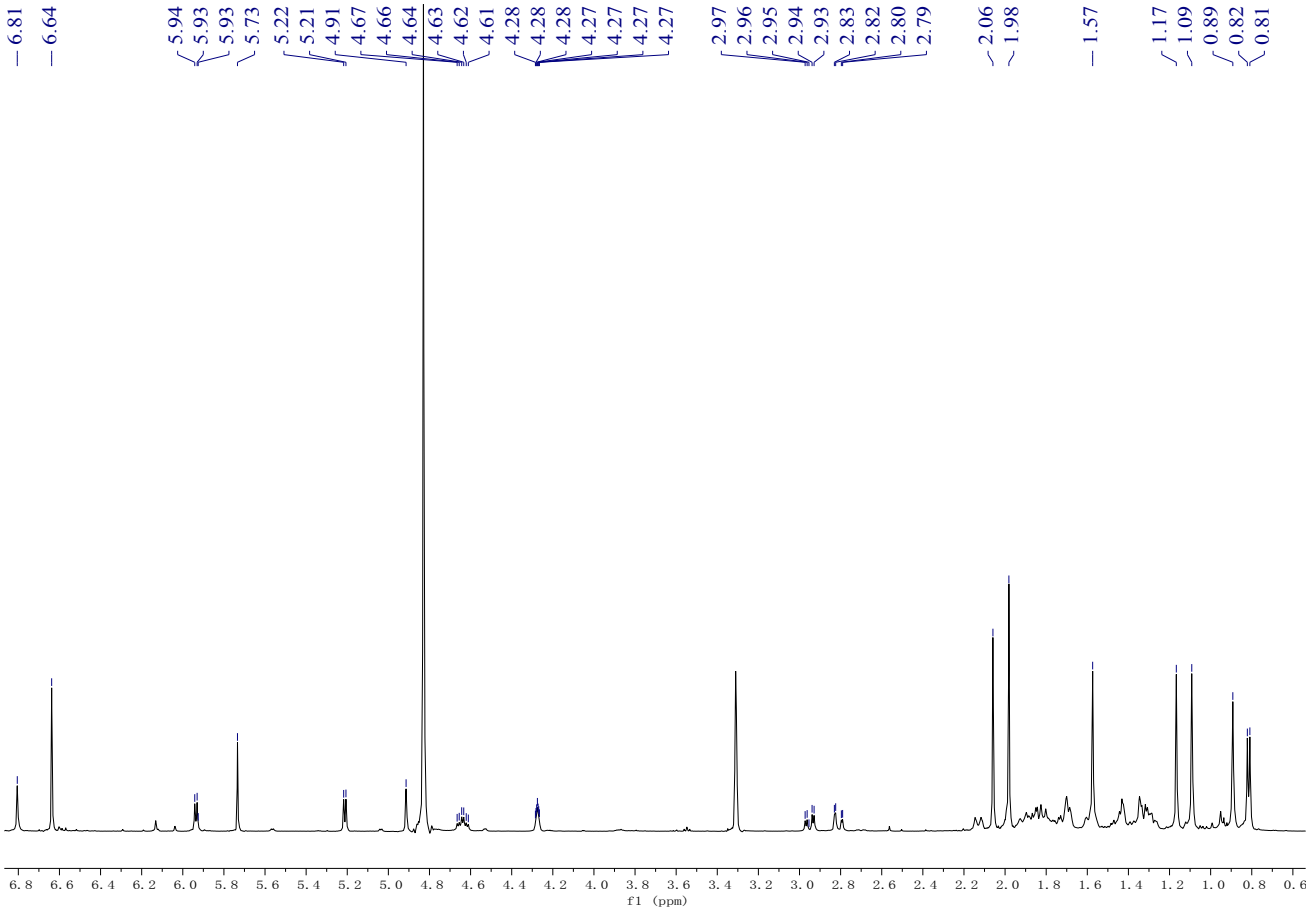
Reference

1. Bruhn, T.; Schaumuloffel, A.; Hemnerger, Y.; Bringmsnn, G., SpecDis: quantifying the comparison of calculated and experimental electronic circular dichroism spectra. *Chirality* **2013**, *25* (4), 243-249.
2. MacroModel, Schrödinger LLC, **2010**.
3. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A. et al. Gaussian 09, revision C.01; Gaussian, Inc.: Wallingford, CT, **2009**.

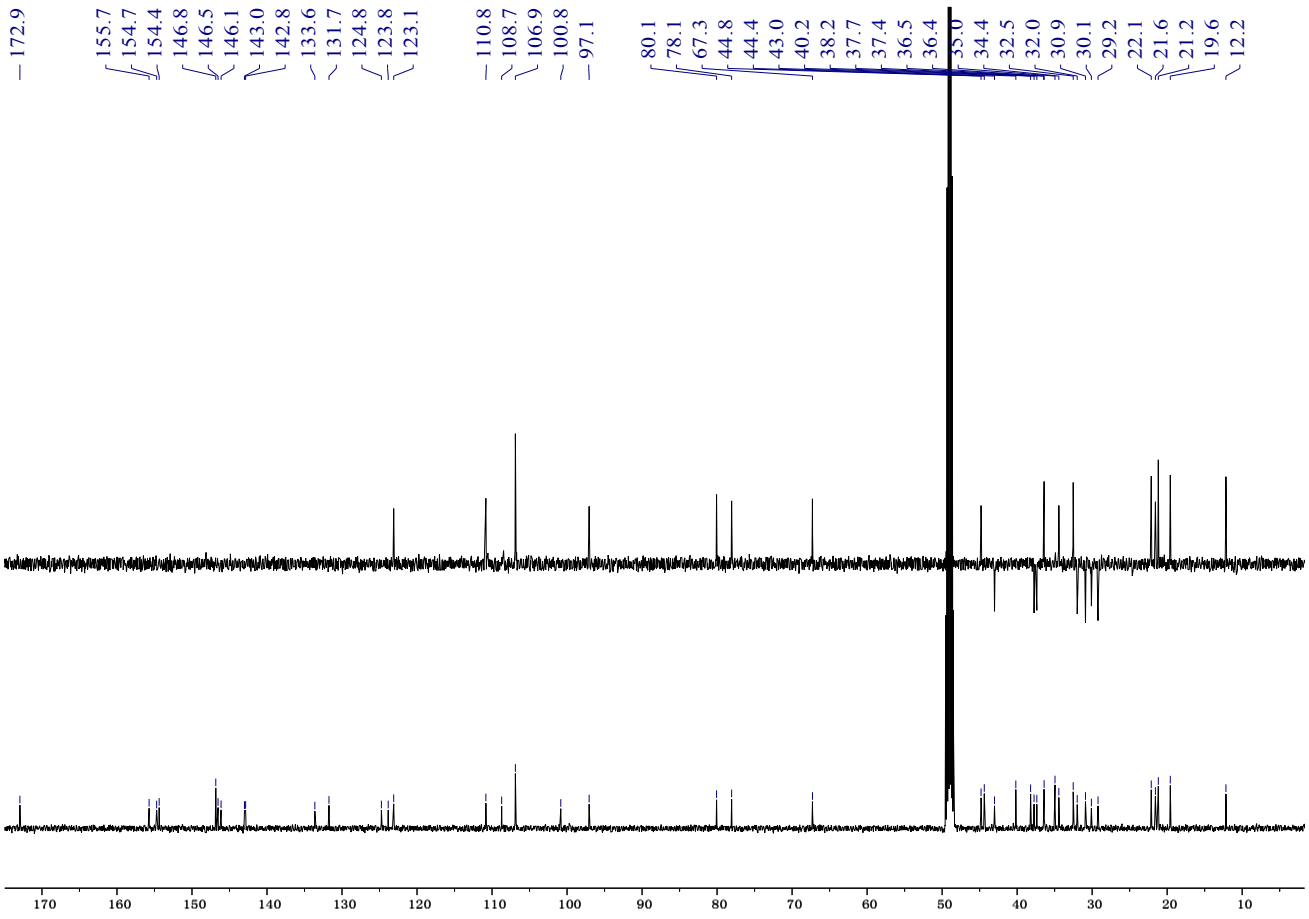
Original spectra for Celamonol A-D

NMR spectra for Celamonol A

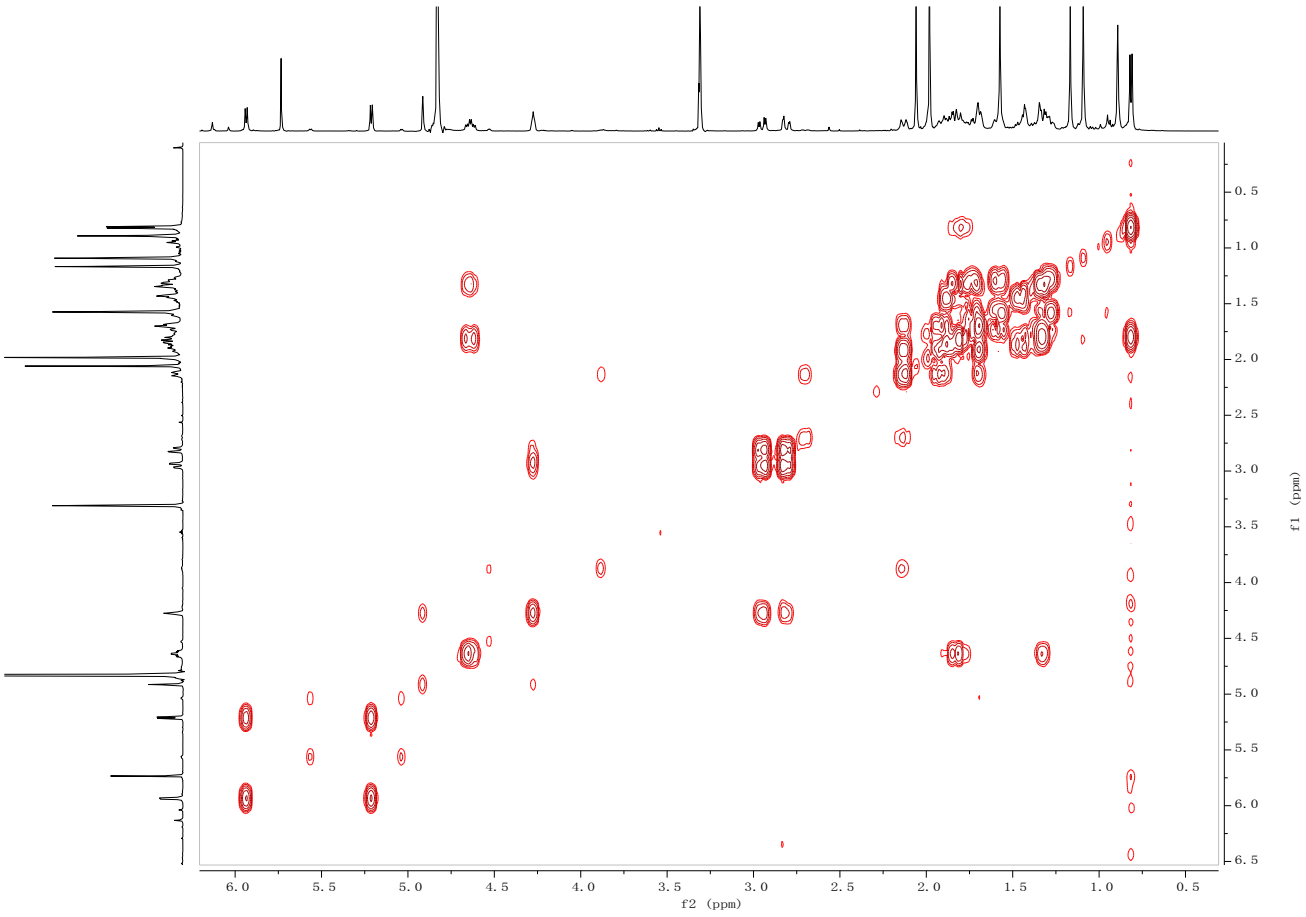
^{1}H NMR spectrum (500 MHz) of Celamonol A (**1**) in CD_3OD



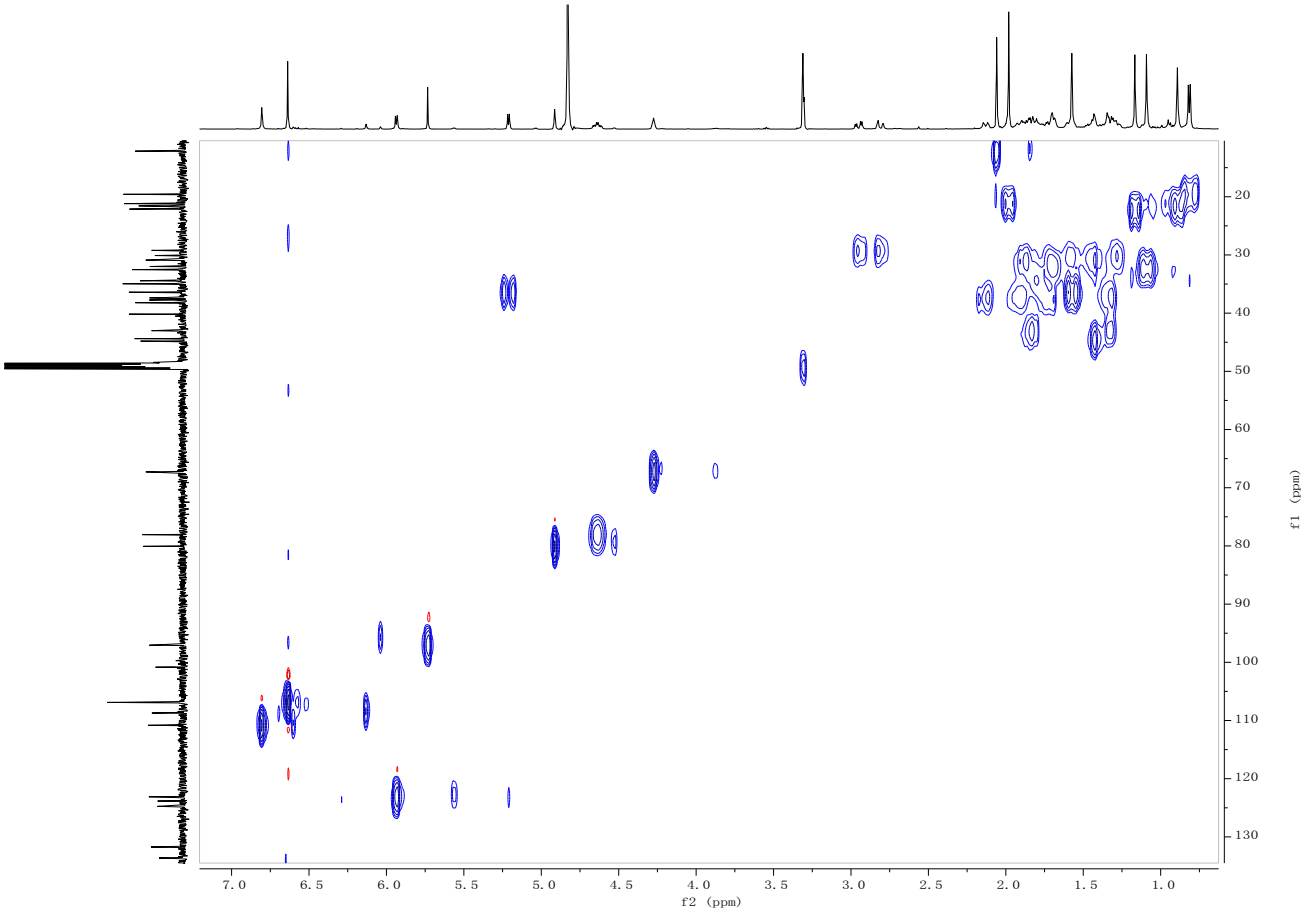
^{13}C NMR (BB+DEPT) spectrum (125 MHz) of Celamonol A (**1**) in CD_3OD



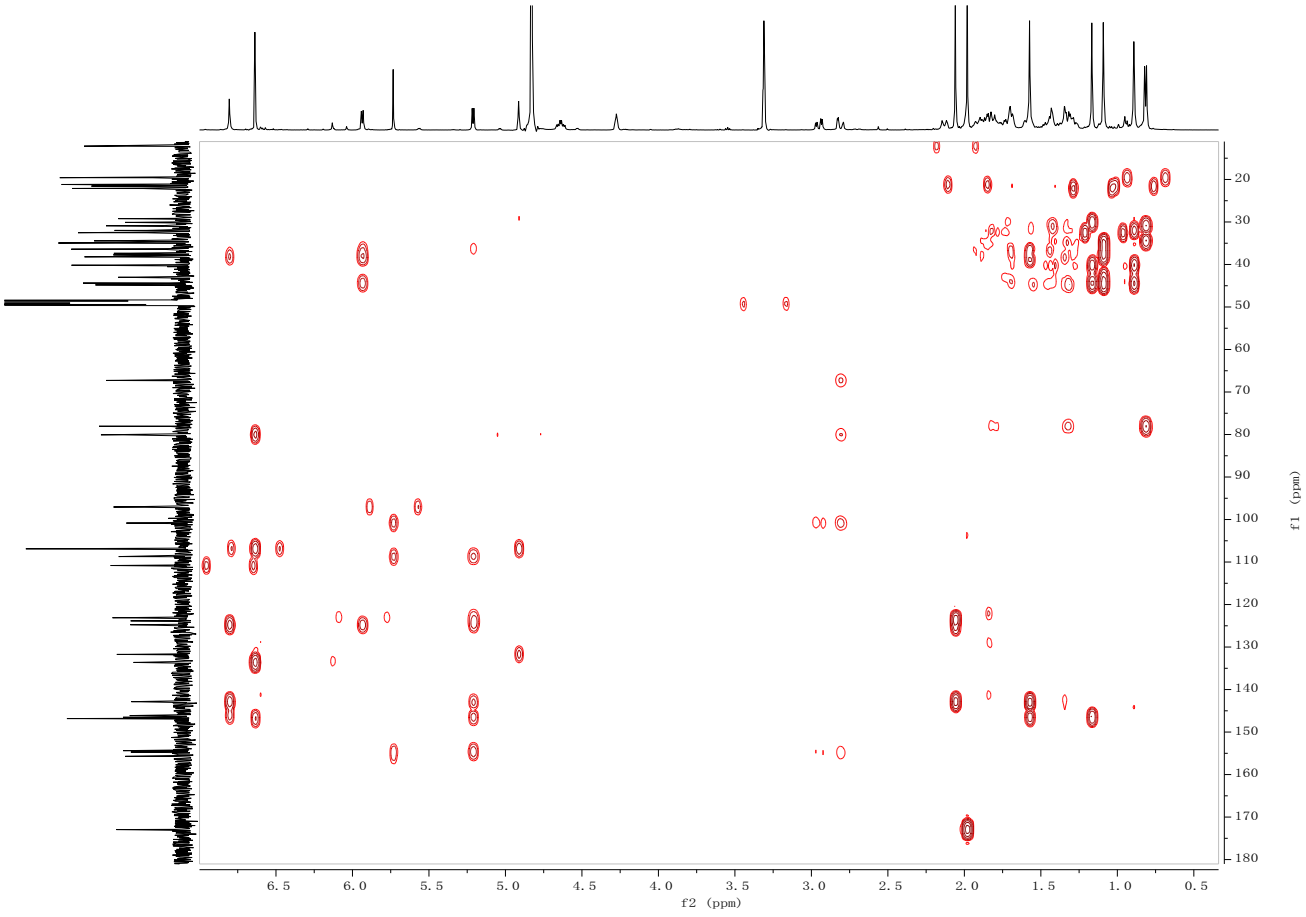
^{1}H-^{1}H COSY spectrum (500 MHz) of Celamonol A (**1**) in CD_3OD



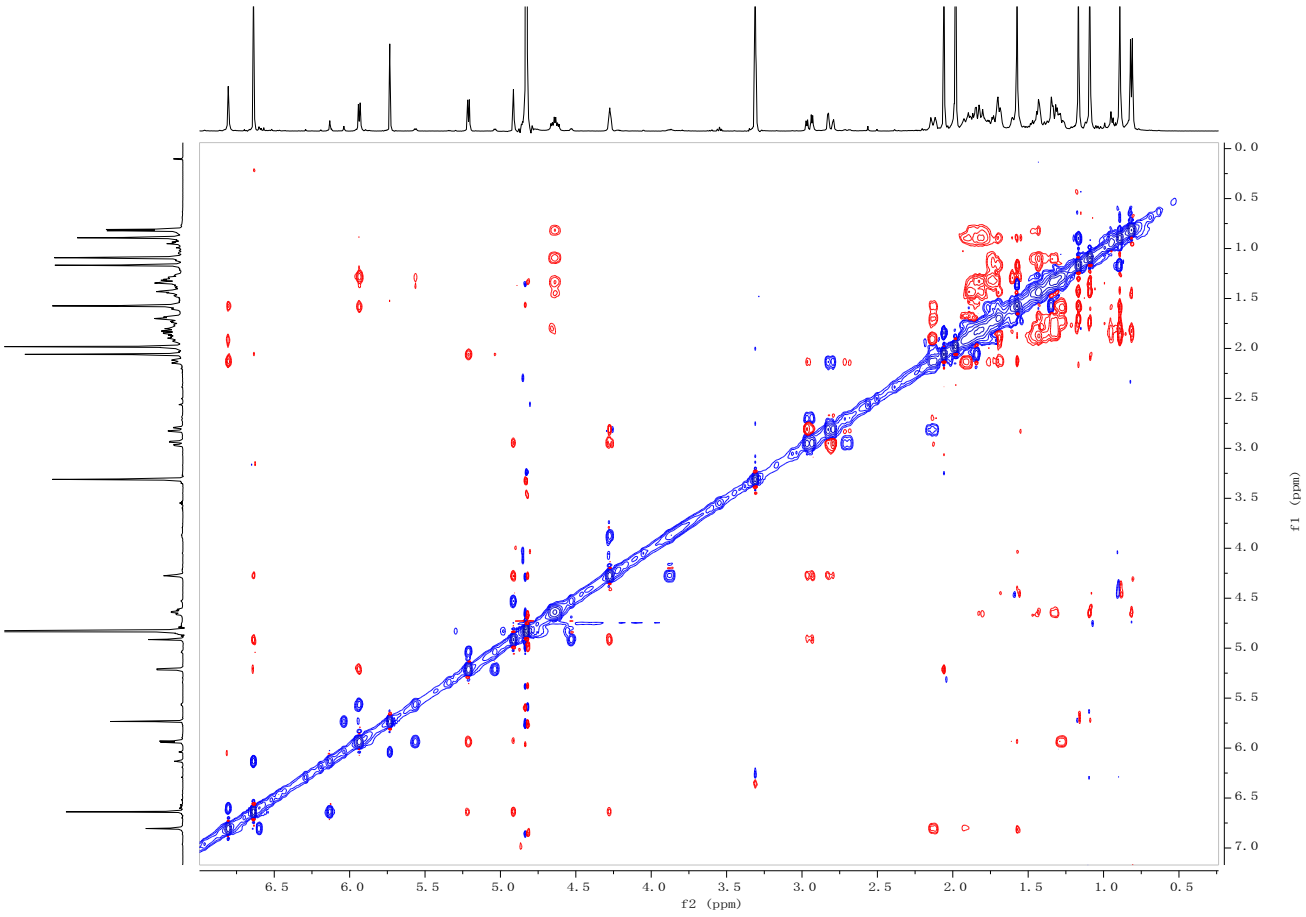
HSQC spectrum (500 MHz) of Celamonol A (**1**) in CD_3OD



HMBC spectrum (500 MHz) of Celamonol A (**1**) in CD_3OD



ROESY spectrum (500 MHz) of Celamonol A (**1**) in CD_3OD



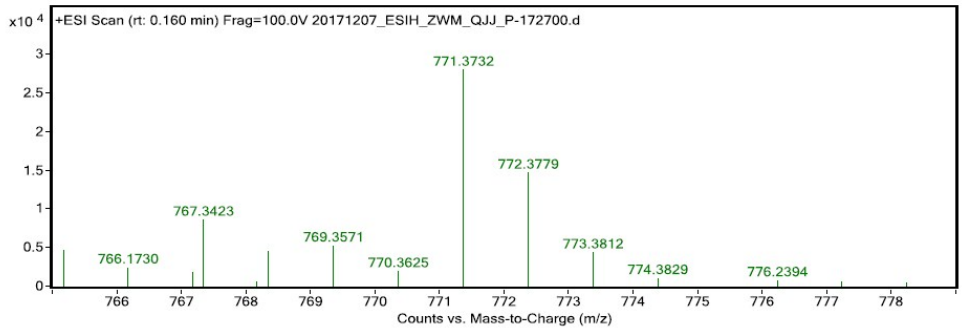
HR-ESIMS of Celamonol A (**1**)

Qualitative Analysis Report

Data Filename	20171207_ESIH_ZWM_QJJ_P-172700.d	**Sample Name**	8904-3
Sample Type	Sample	**Position**	P1-D2
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	12/7/2017 10:08:43 AM	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by ZZY

User Spectra

Spectrum Source	Fragmentor Voltage	Collision Energy	Ionization Mode
	100	0	ESI

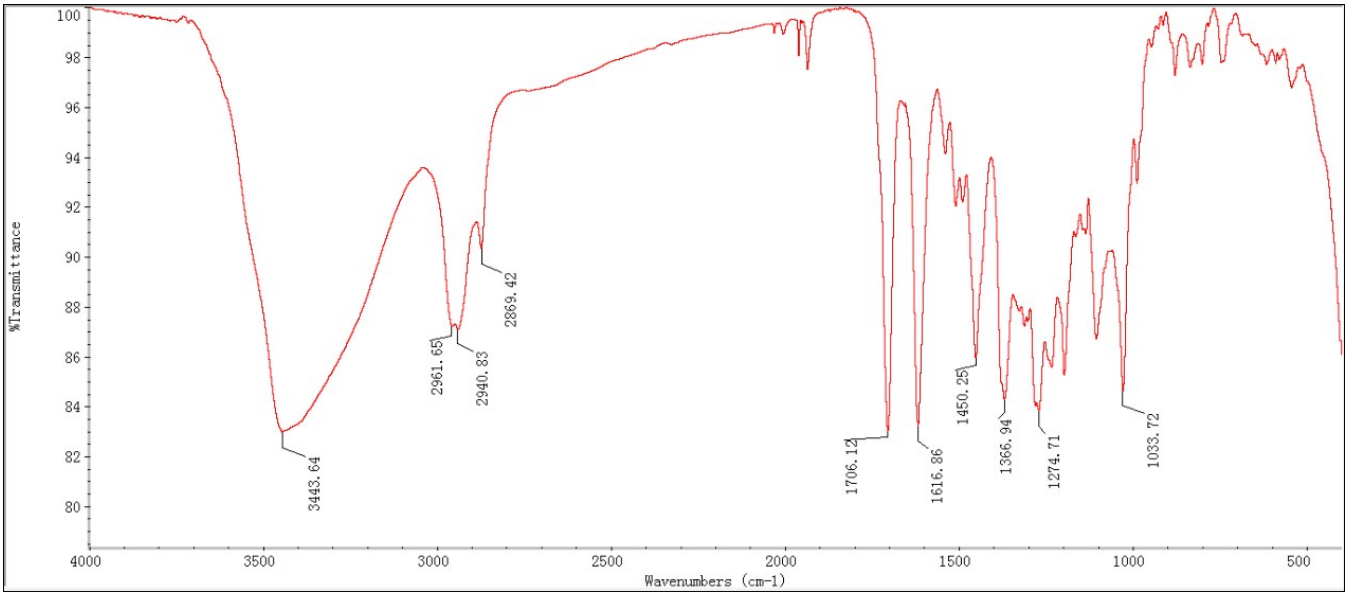


Formula Calculator Results

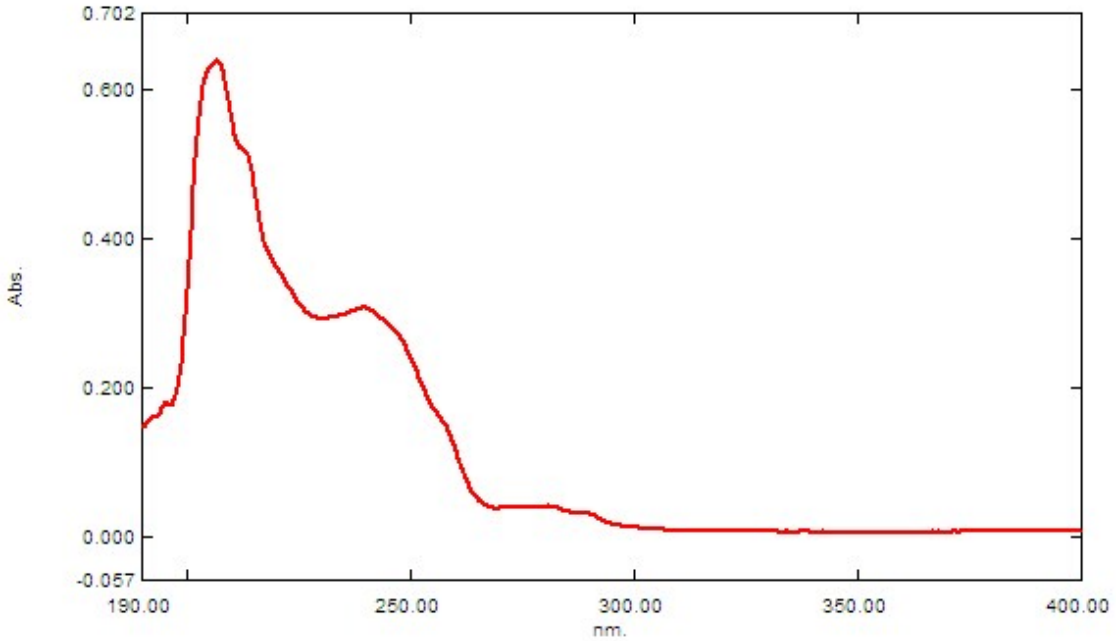
m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
771.3732	771.3739	0.71	0.92	C45 H55 O11	(M+H)+

--- End Of Report ---

IR spectrum of Celamonol A (**1**)

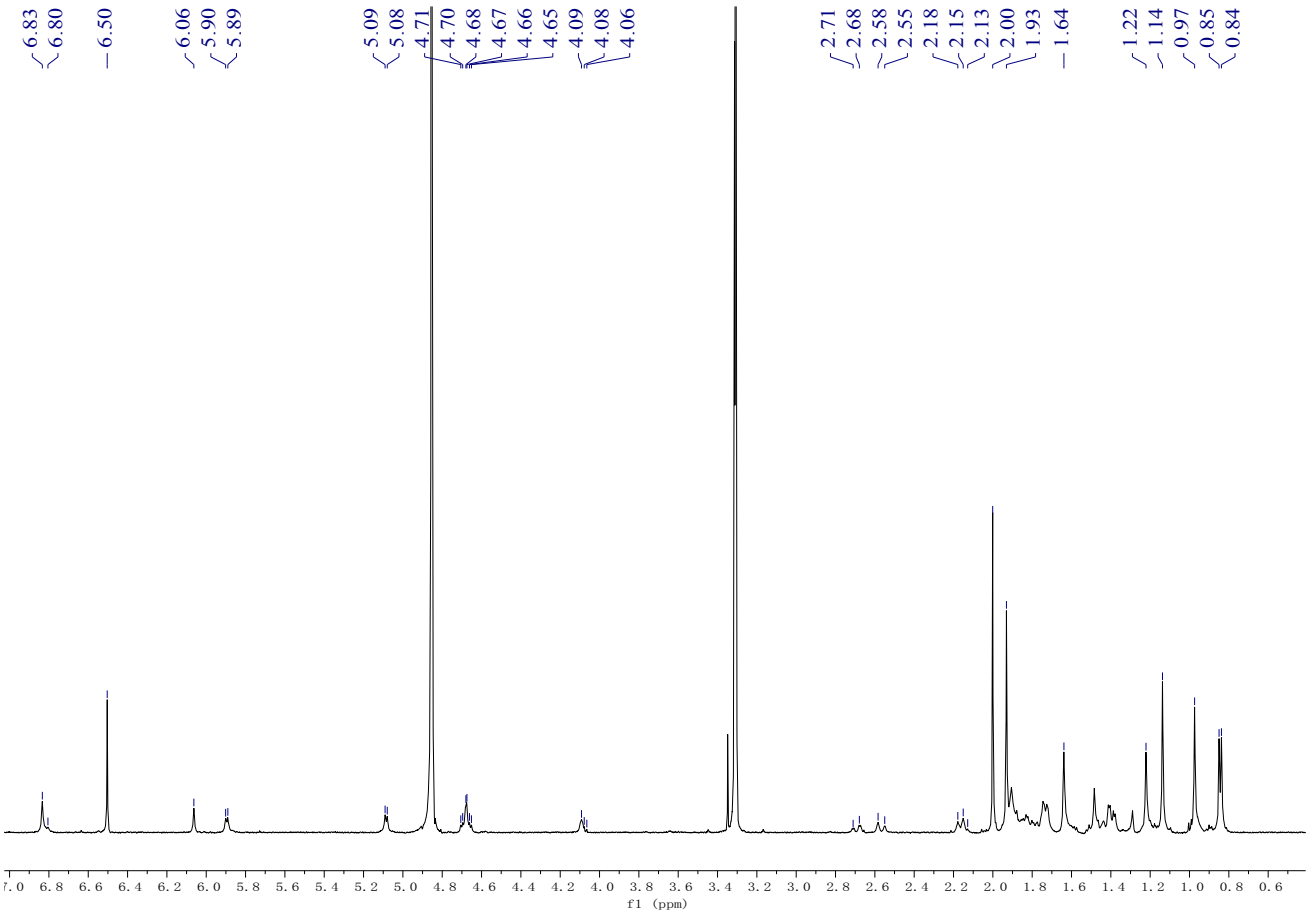


UV spectrum of Celamonol A (**1**)

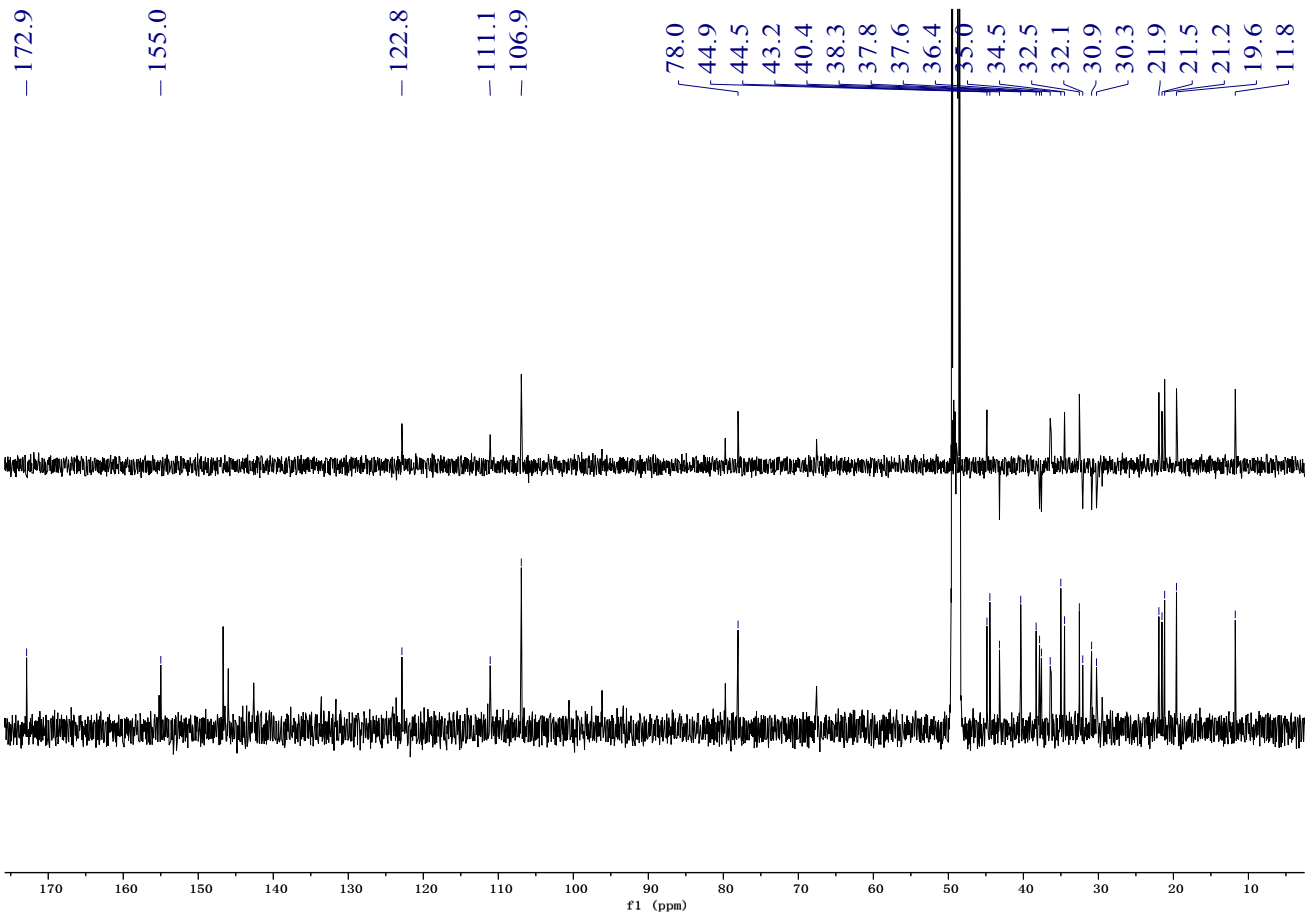


NMR spectra for Celamonol B

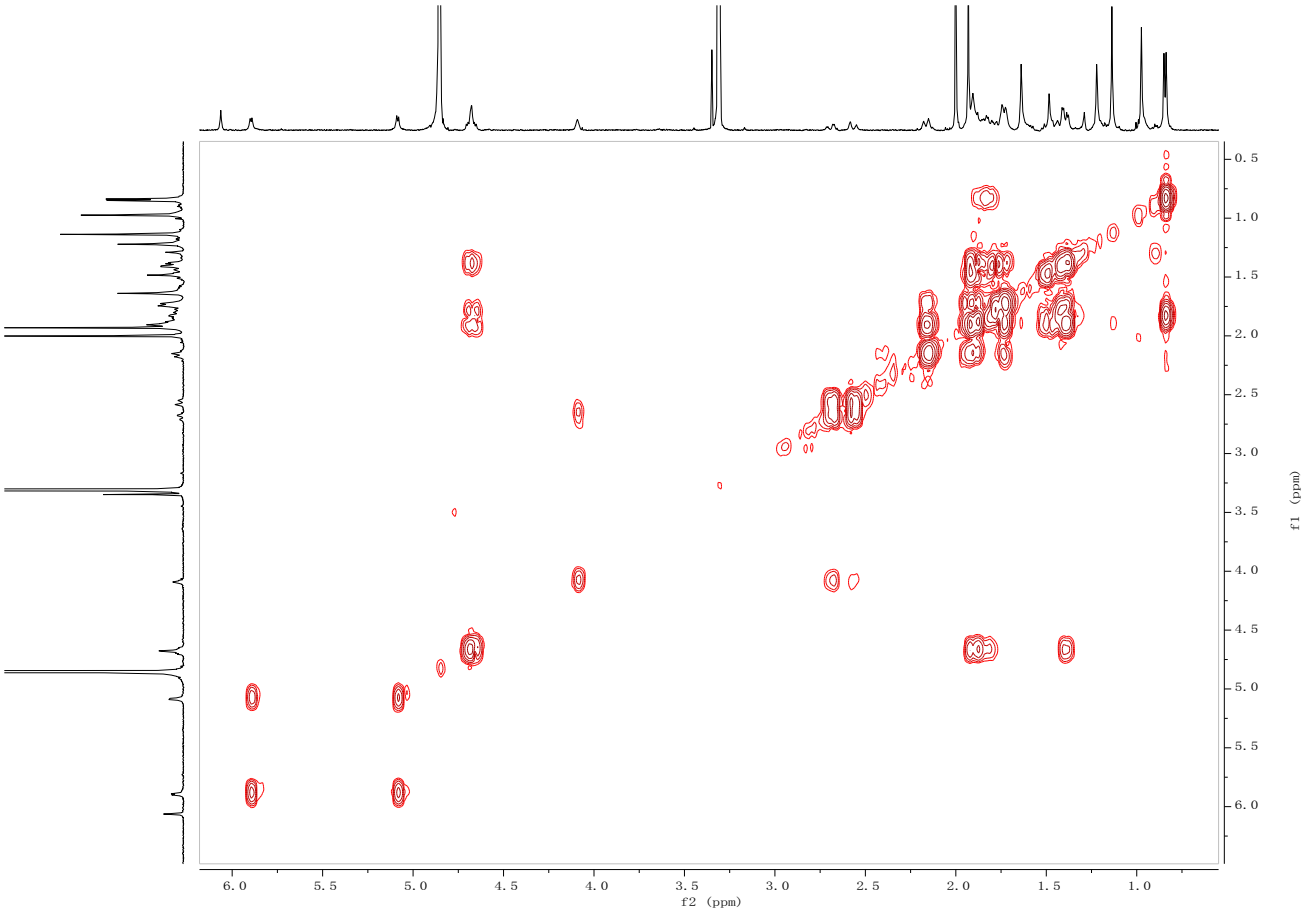
^{1}H NMR spectrum (500 MHz) of Celamonol B (**2**) in CD_3OD



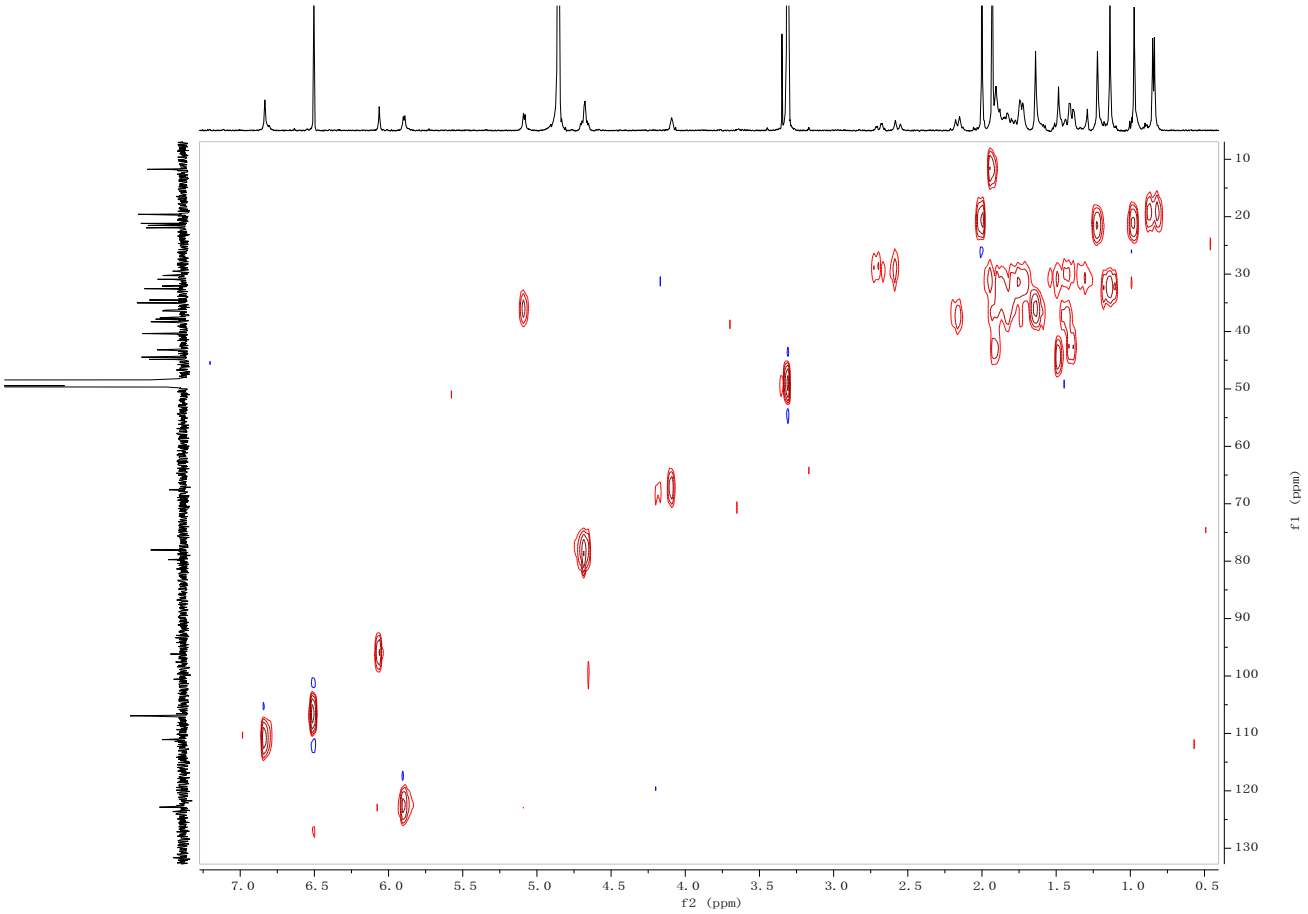
^{13}C NMR (BB+DEPT) spectrum (125 MHz) of Celamonol B (**2**) in CD_3OD



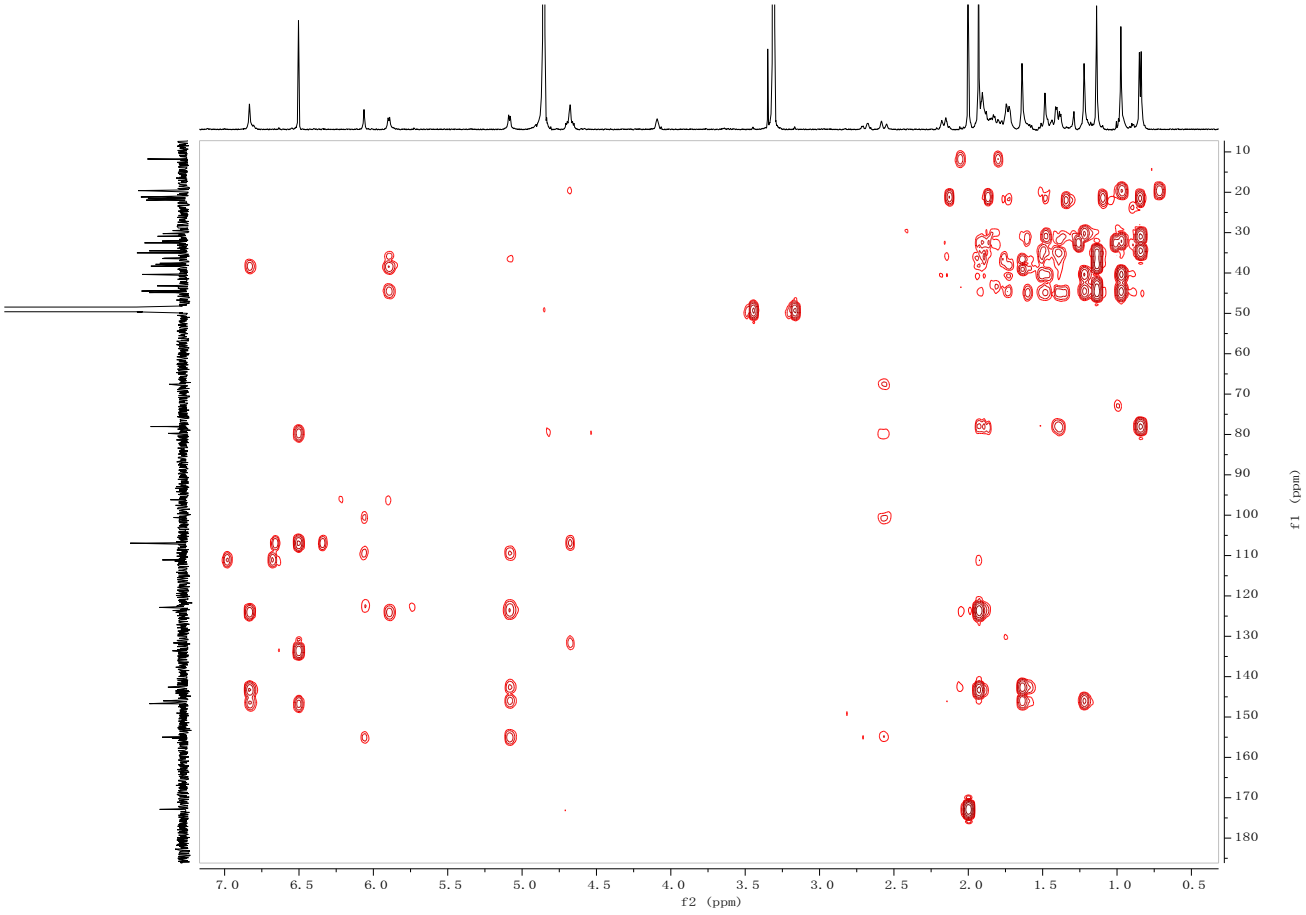
^{1}H-^{1}H COSY spectrum (500 MHz) of Celamonol B (**2**) in CD_3OD



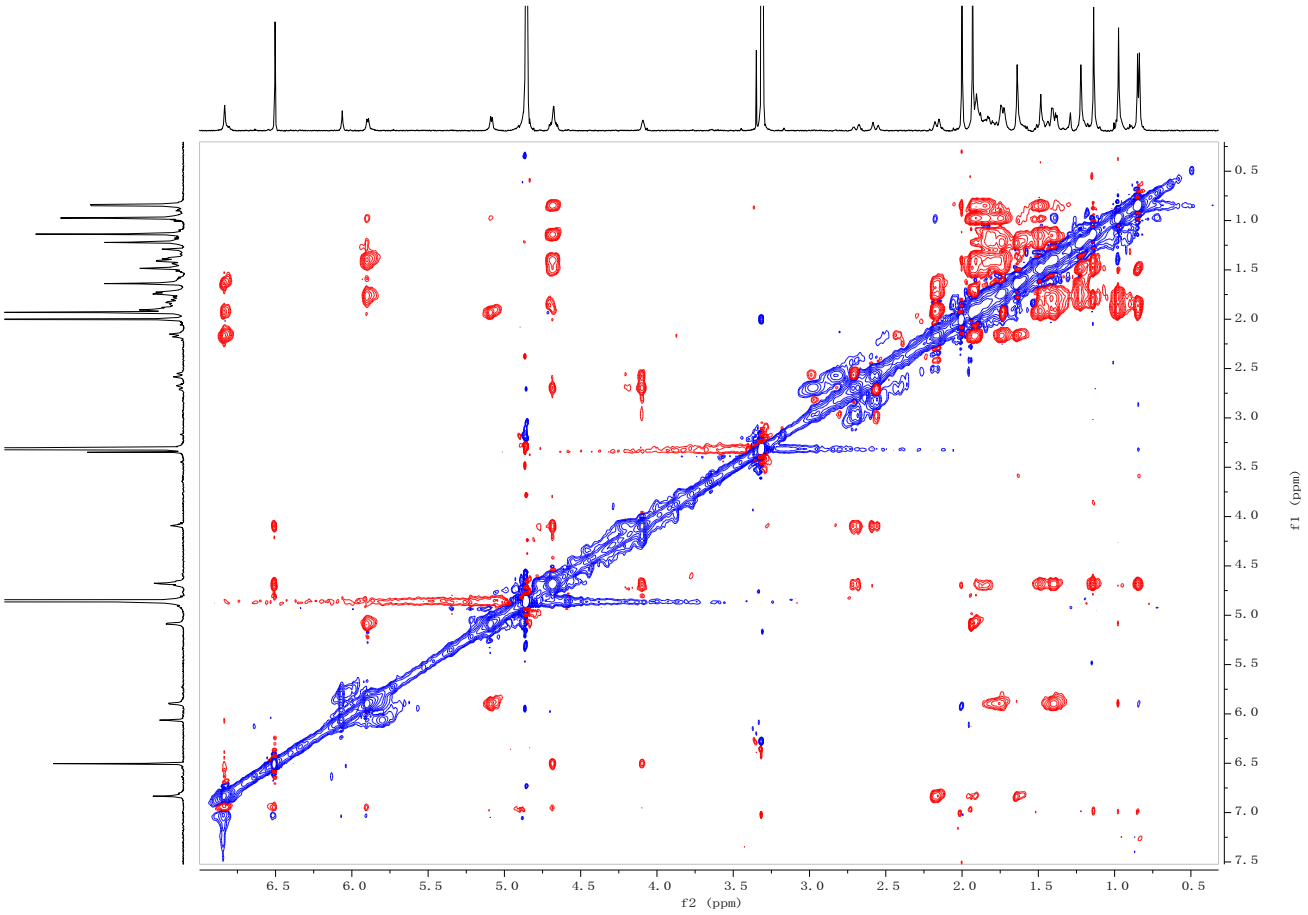
HSQC spectrum (500 MHz) of Celamonol B (**2**) in CD_3OD



HMBC spectrum (500 MHz) of Celamonol B (**2**) in CD_3OD



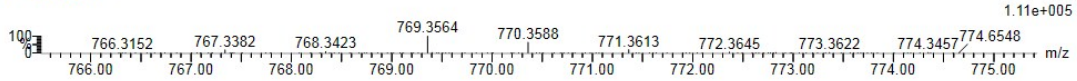
ROESY spectrum (500 MHz) of Celamonol B (**2**) in CD_3OD



HR-ESIMS of Celamonol B (**2**)

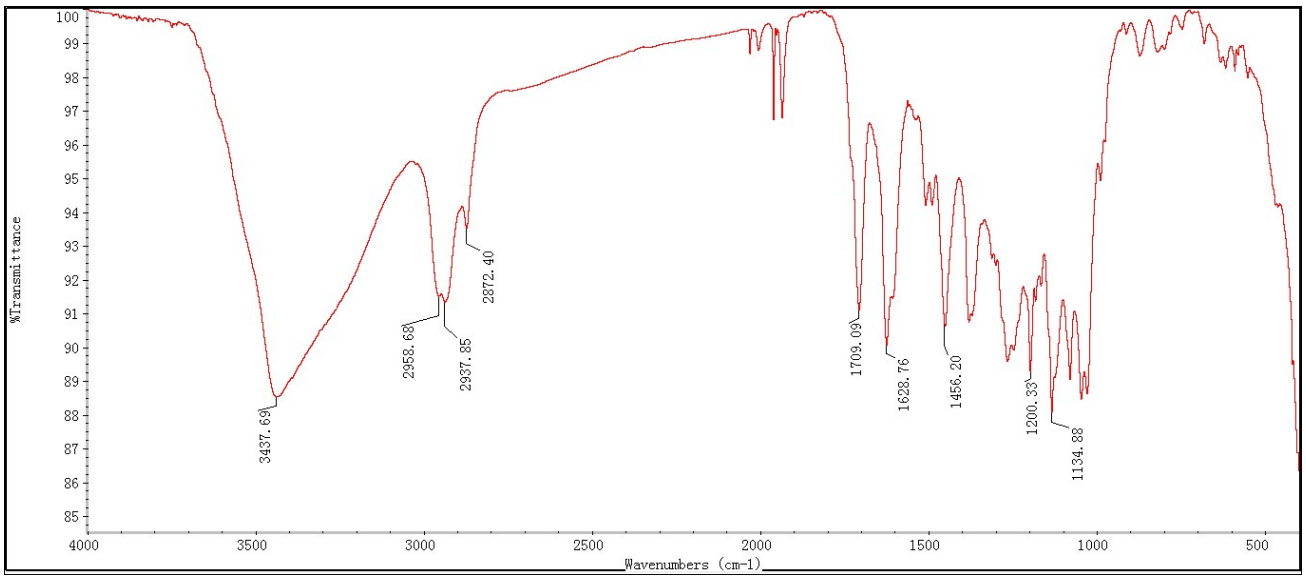
Single Mass Analysis
Tolerance = 4.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
265 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 10-70 H: 0-200 O: 0-120
9A56-5 275 (2.235)
1: TOF MS ES-

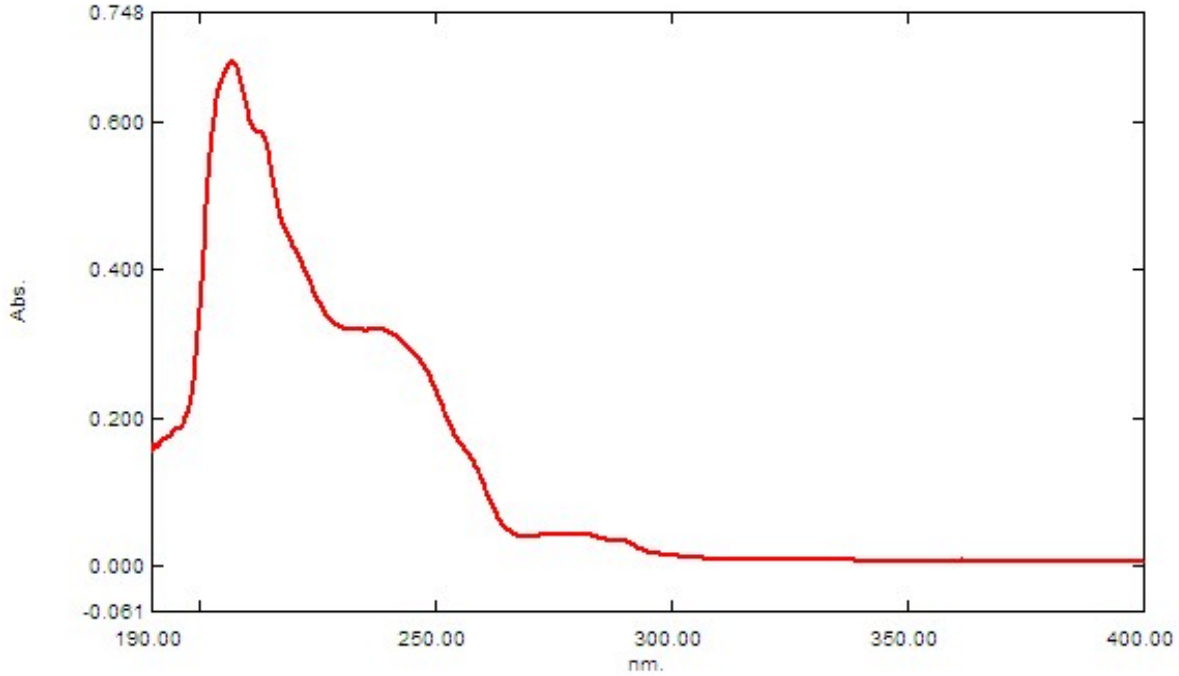


Minimum:				-1.5				
Maximum:		5.0	4.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
769.3564	769.3588	-2.4	-3.1	19.5	374.4	n/a	n/a	C45 H53 O11

IR spectrum of Celamonol B (**2**)

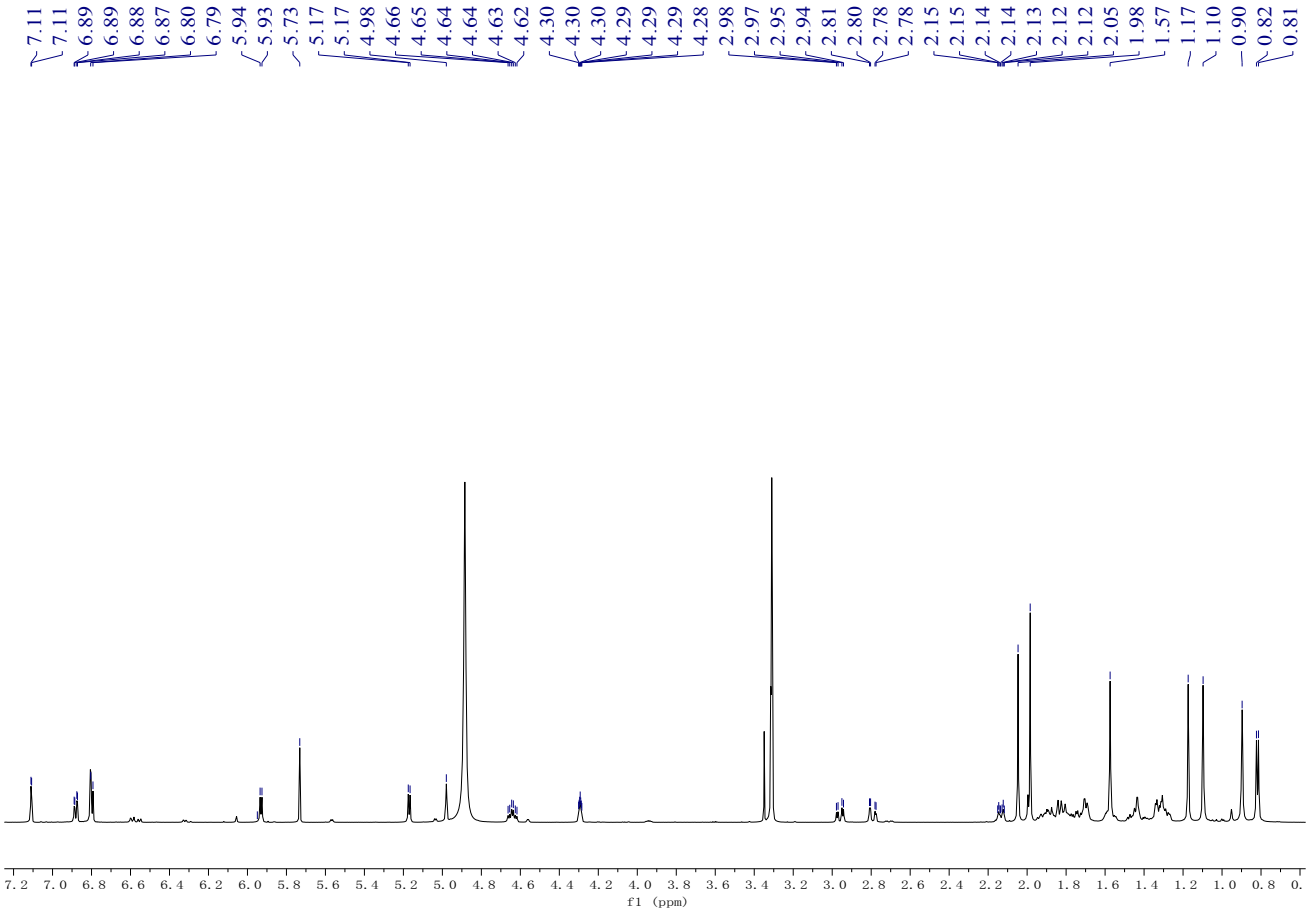


UV spectrum of Celamonol B (**2**)

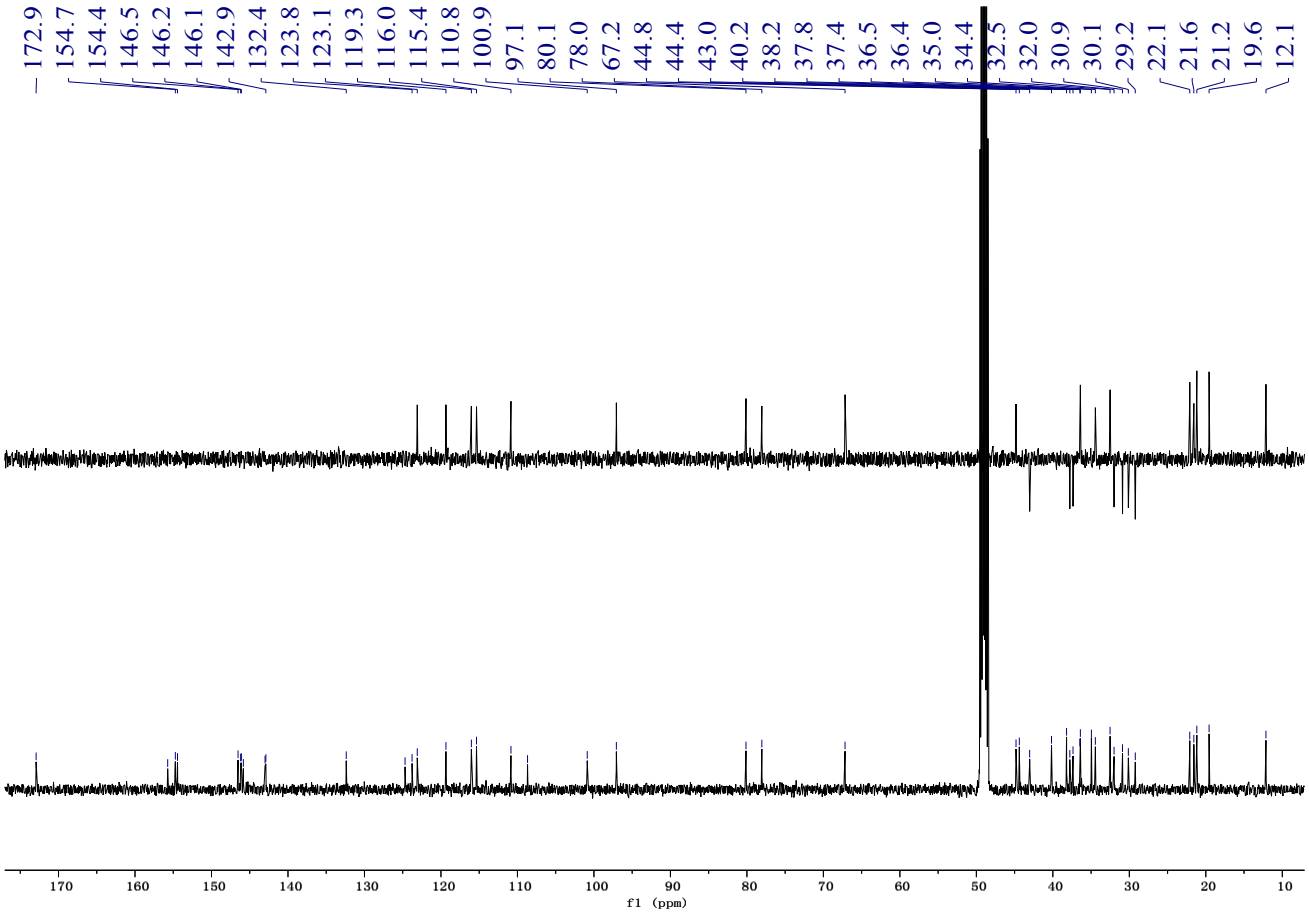


NMR spectra for Celamonol C

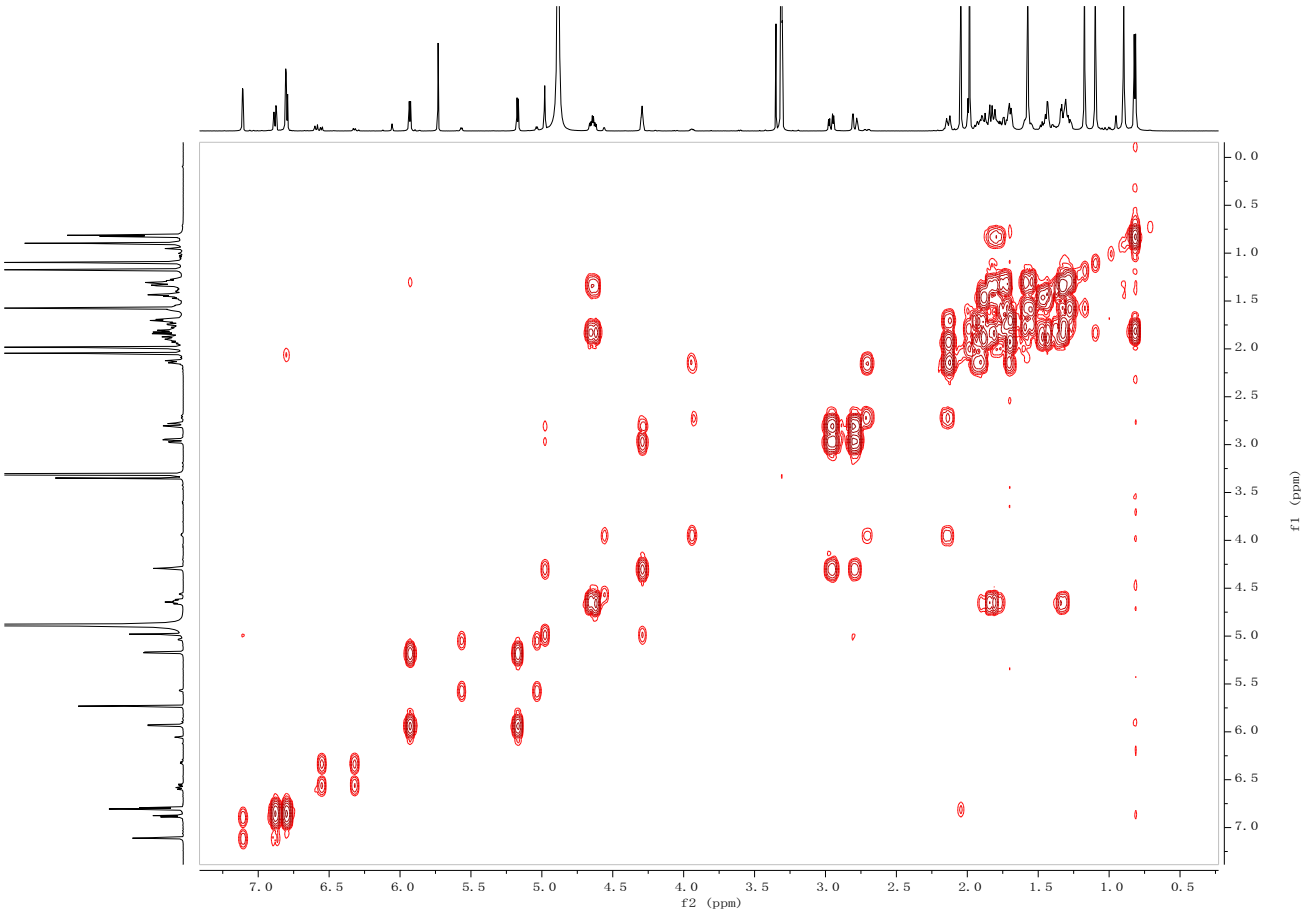
^{1}H NMR spectrum (500 MHz) of Celamonol C (**3**) in CD_3OD



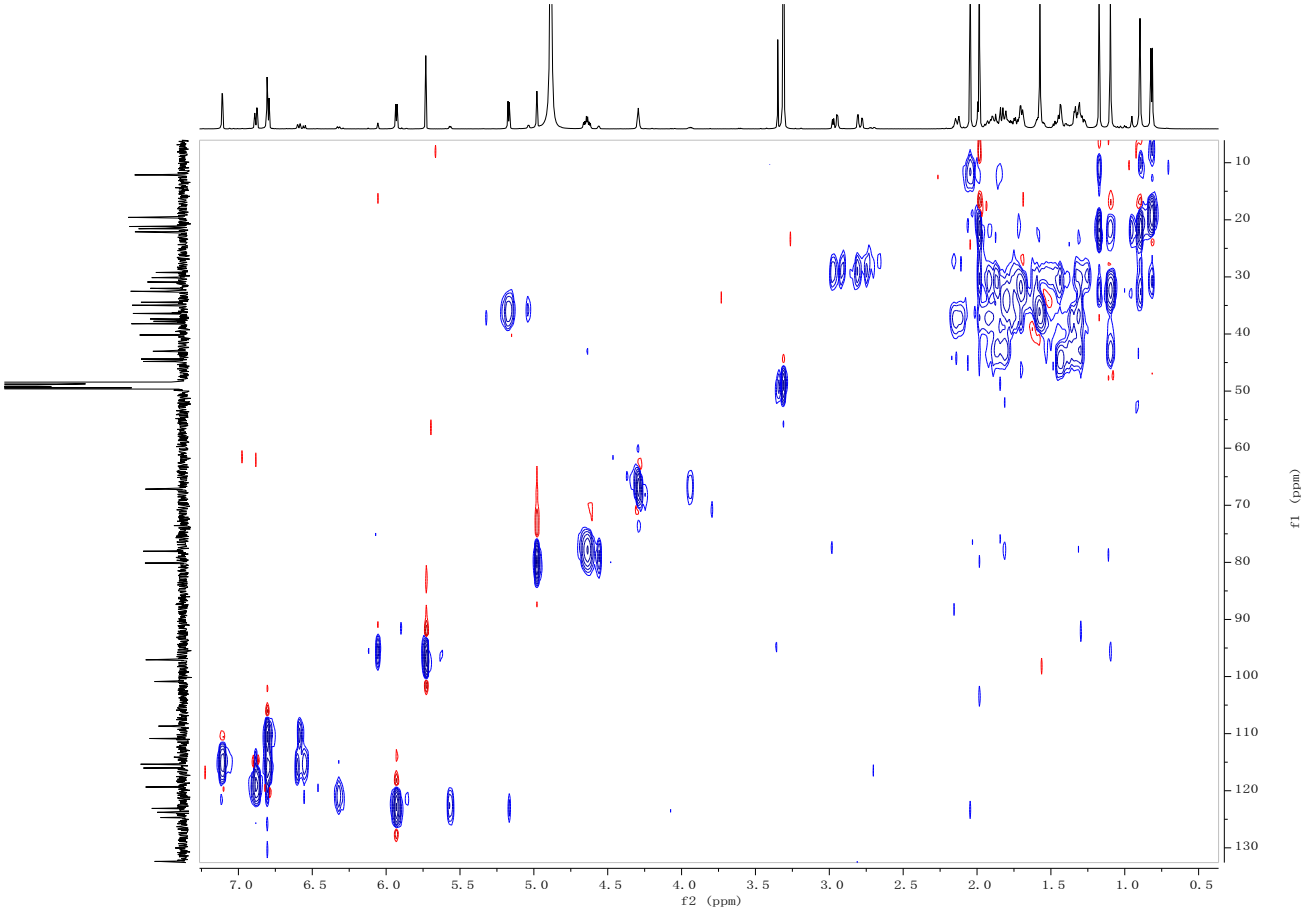
^{13}C NMR (BB+DEPT) spectrum (125 MHz) of Celamonol C (**3**) in CD_3OD



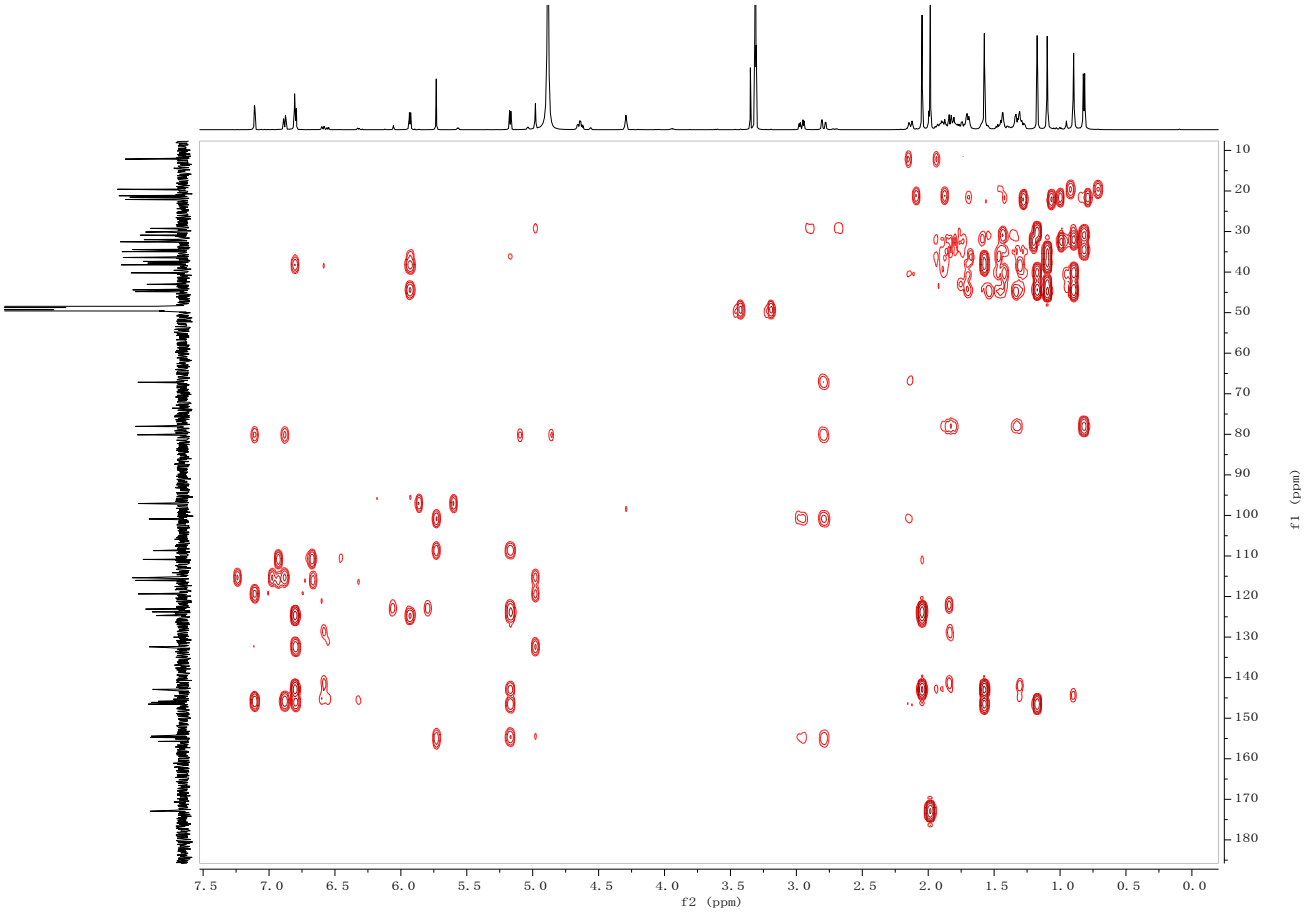
^{1}H-^{1}H COSY spectrum (500 MHz) of Celamonol C (**3**) in CD_3OD



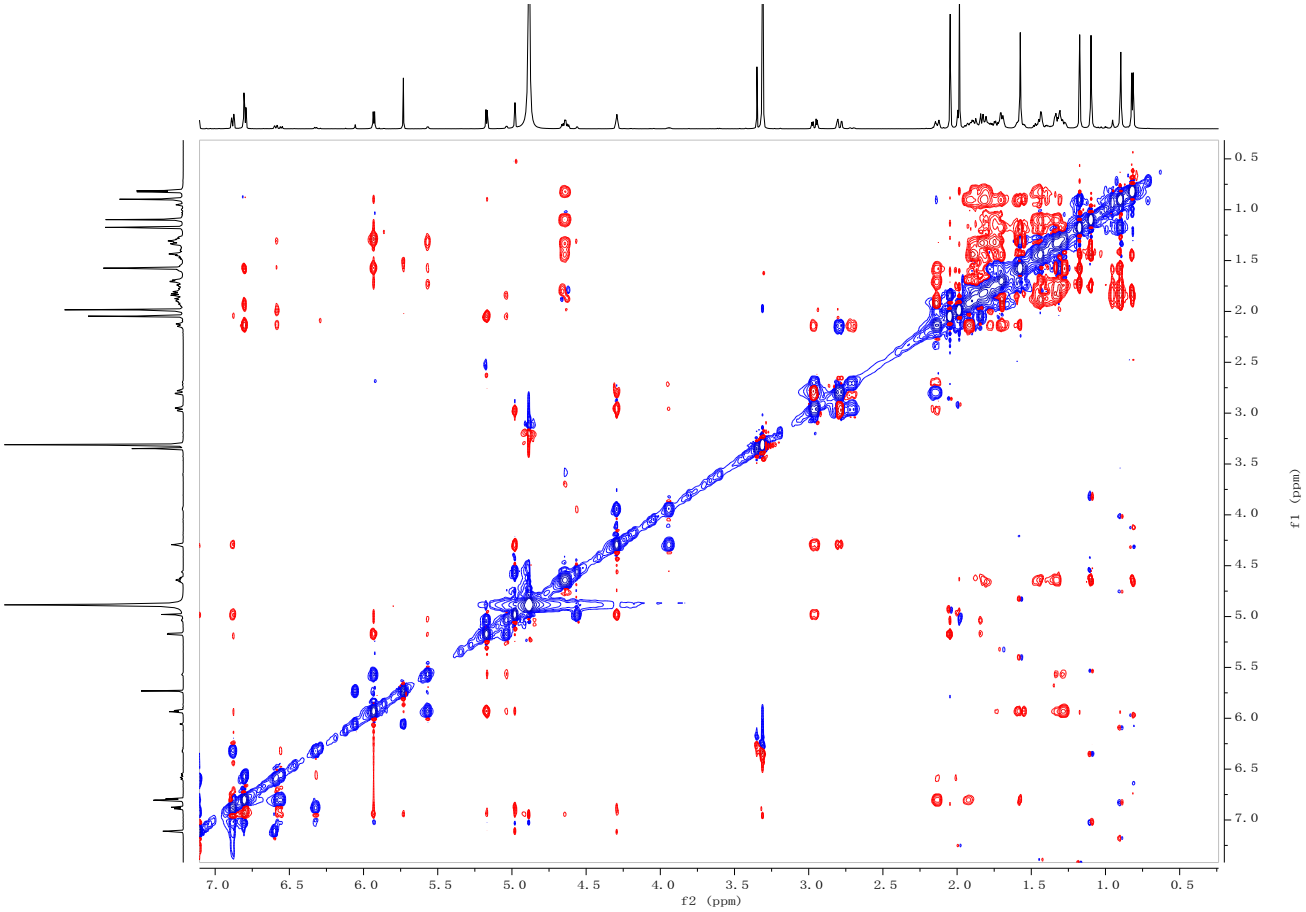
HSQC spectrum (500 MHz) of Celamonol C (**3**) in CD_3OD



HMBC spectrum (500 MHz) of Celamonol C (**3**) in CD_3OD



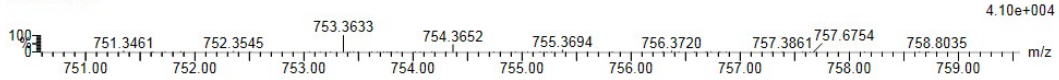
ROESY spectrum (500 MHz) of Celamonol C (**3**) in CD_3OD



HR-ESIMS of Celamonol C (**3**)

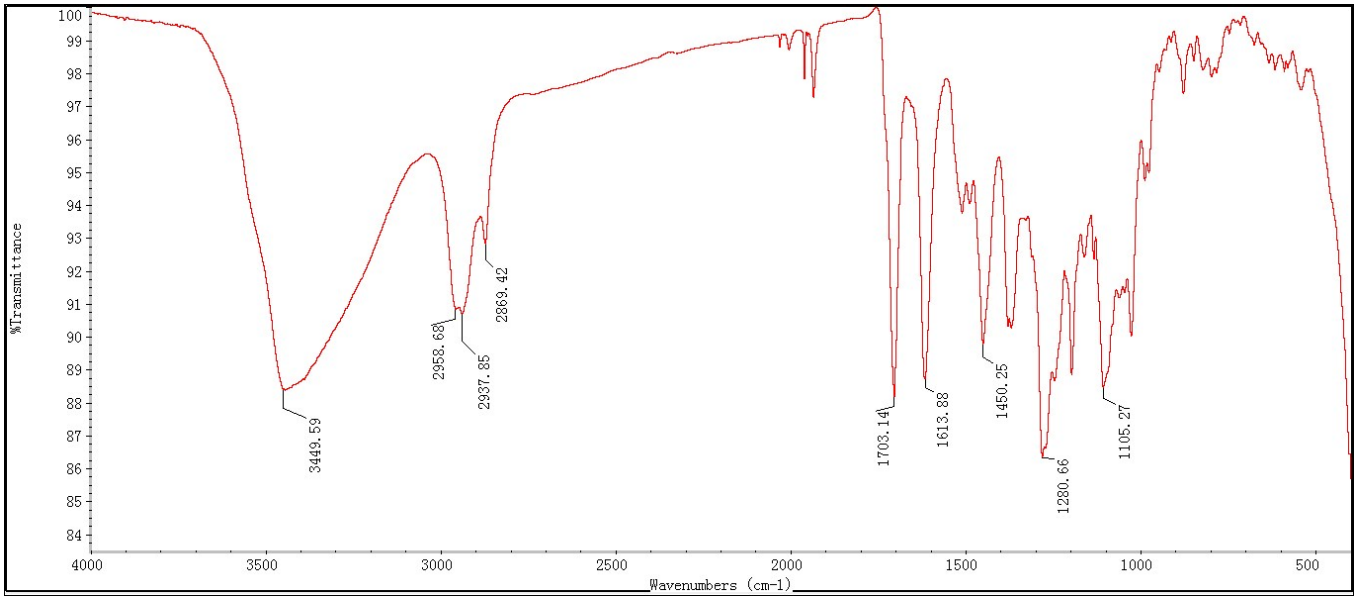
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
255 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 10-70 H: 0-200 O: 0-120
9A5-3-neg 266 (2.151)
1: TOF MS ES-

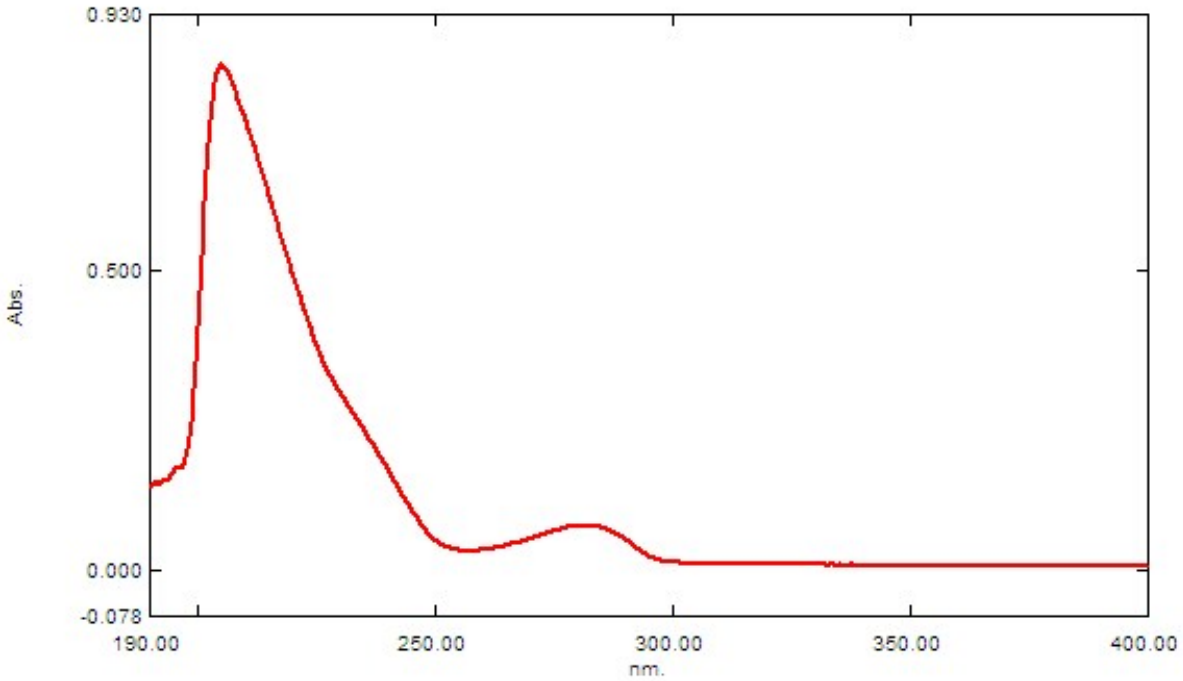


Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
753.3633	753.3639	-0.6	-0.8	19.5	222.6	n/a	n/a	C45 H53 O10

IR spectrum of Celamonol C (**3**)

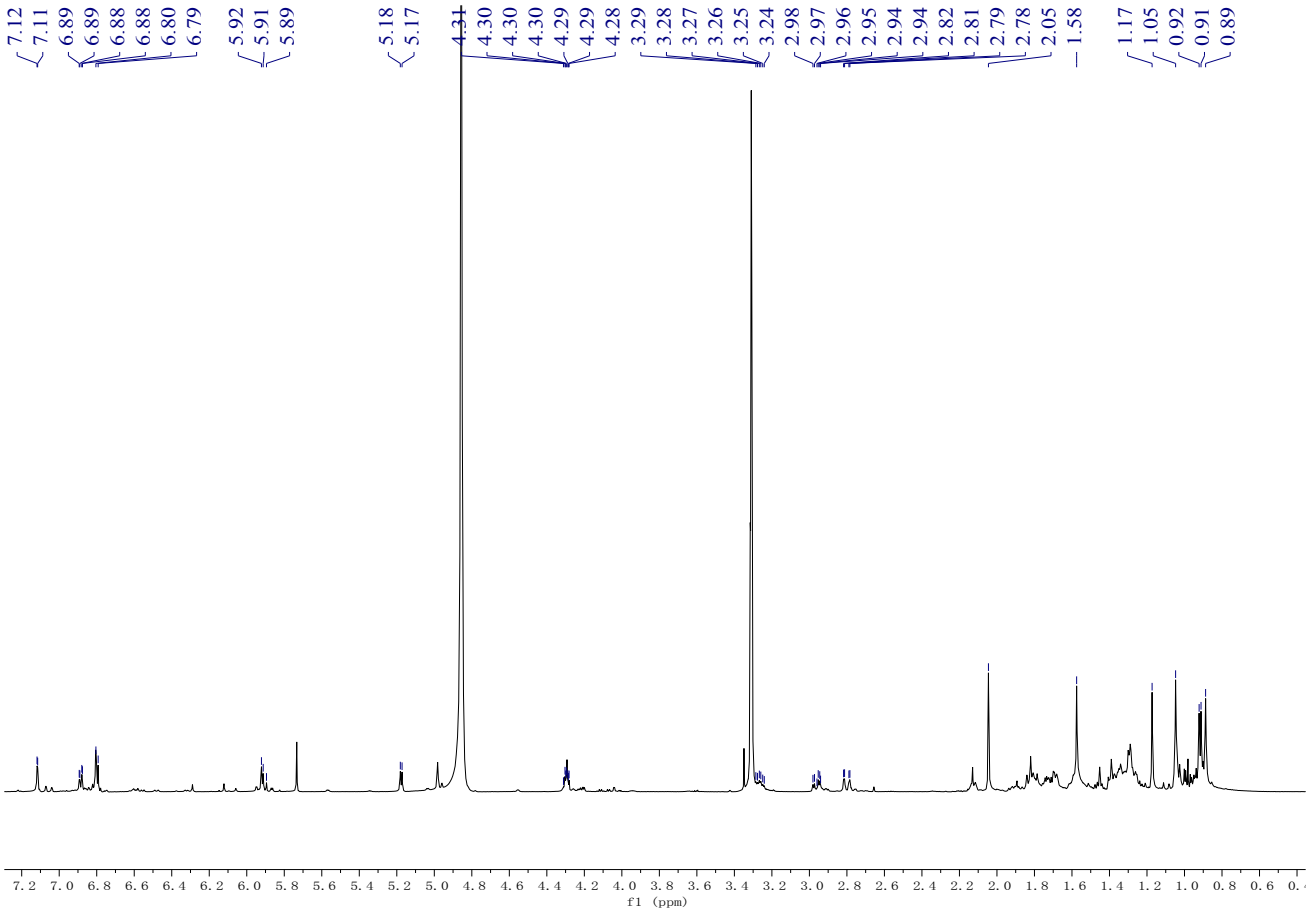


UV spectrum of Celamonol C (**3**)

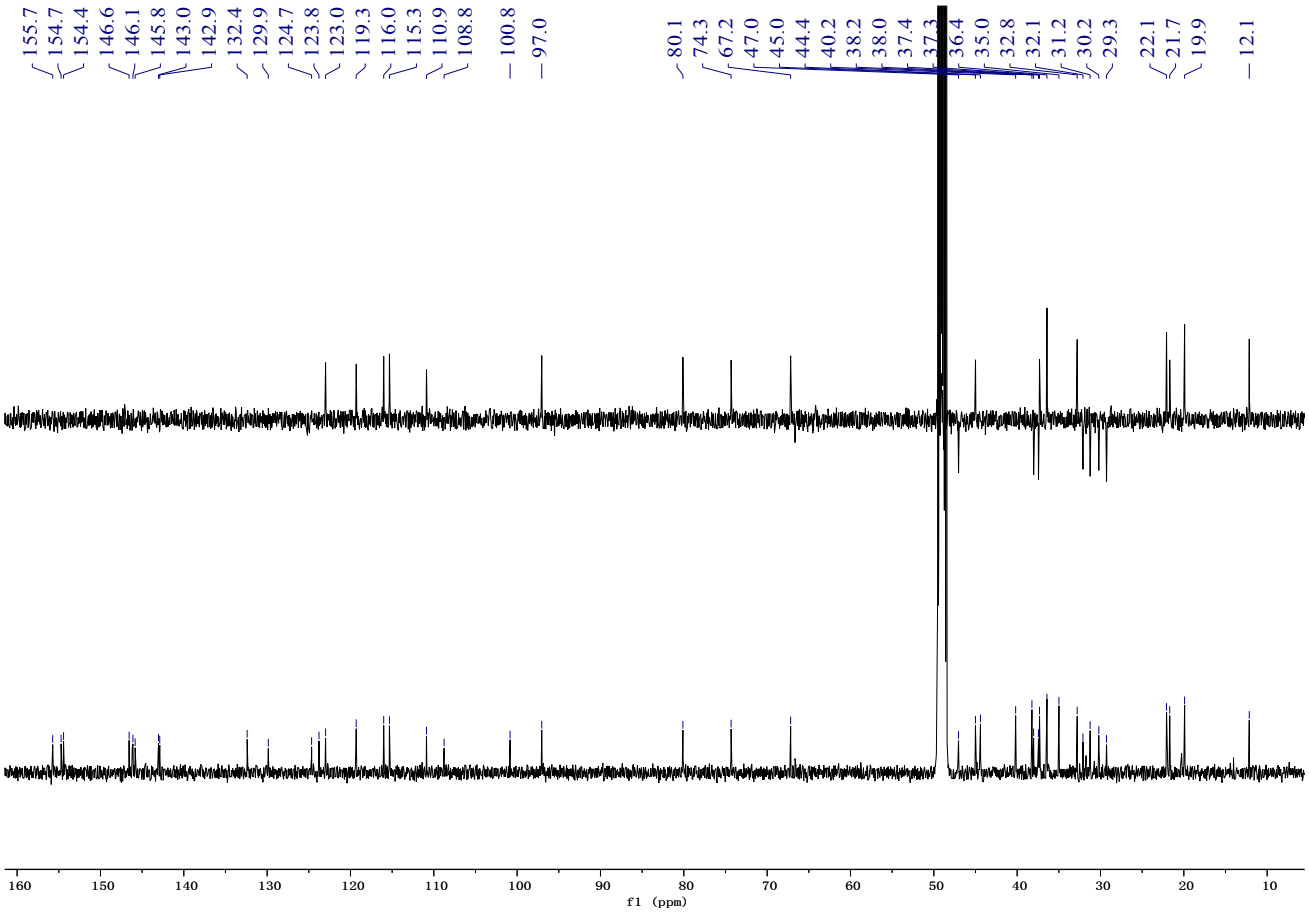


NMR spectra for Celamonol D

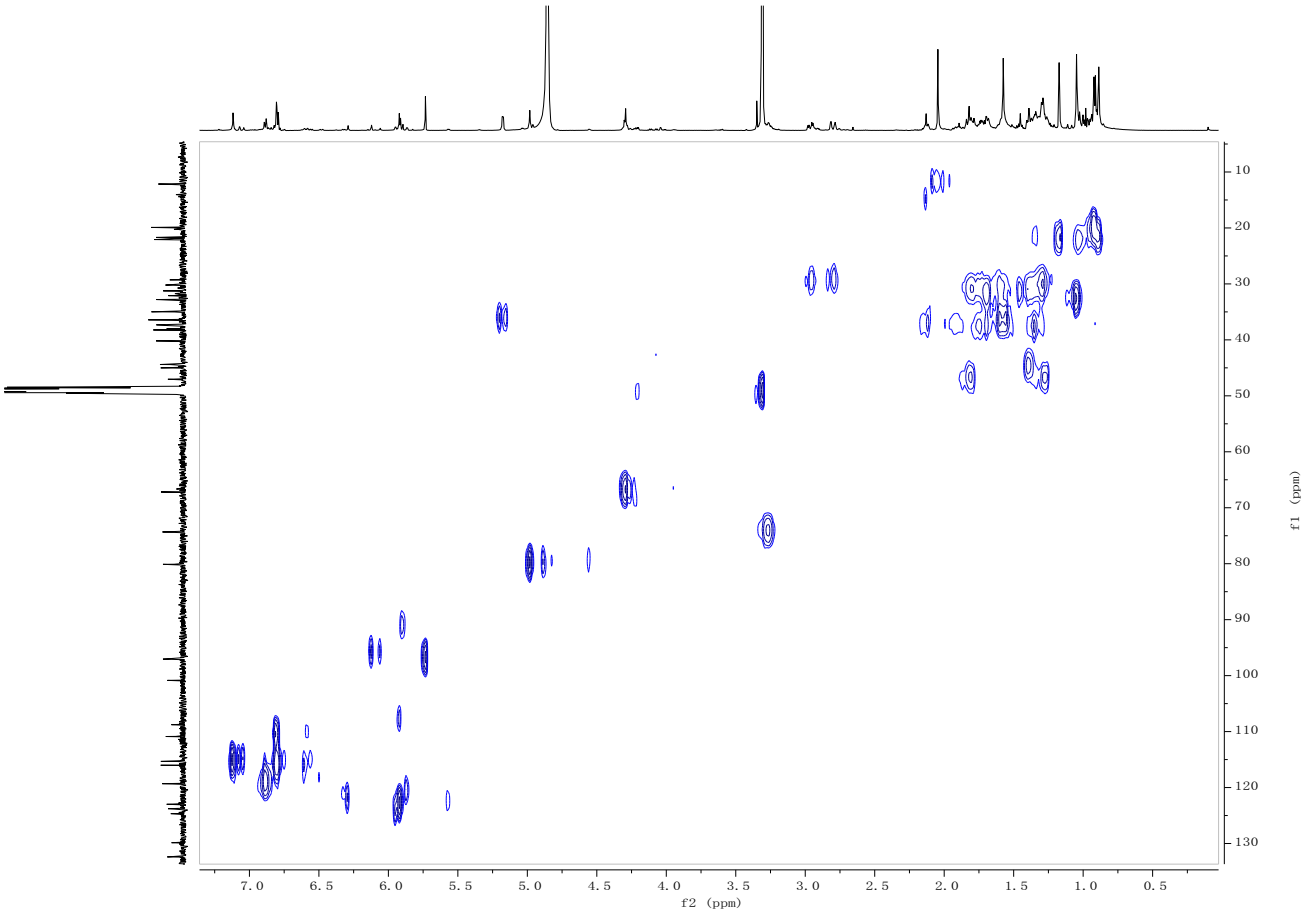
^{1}H NMR spectrum (500 MHz) of Celamonol D (**4**) in CD_3OD



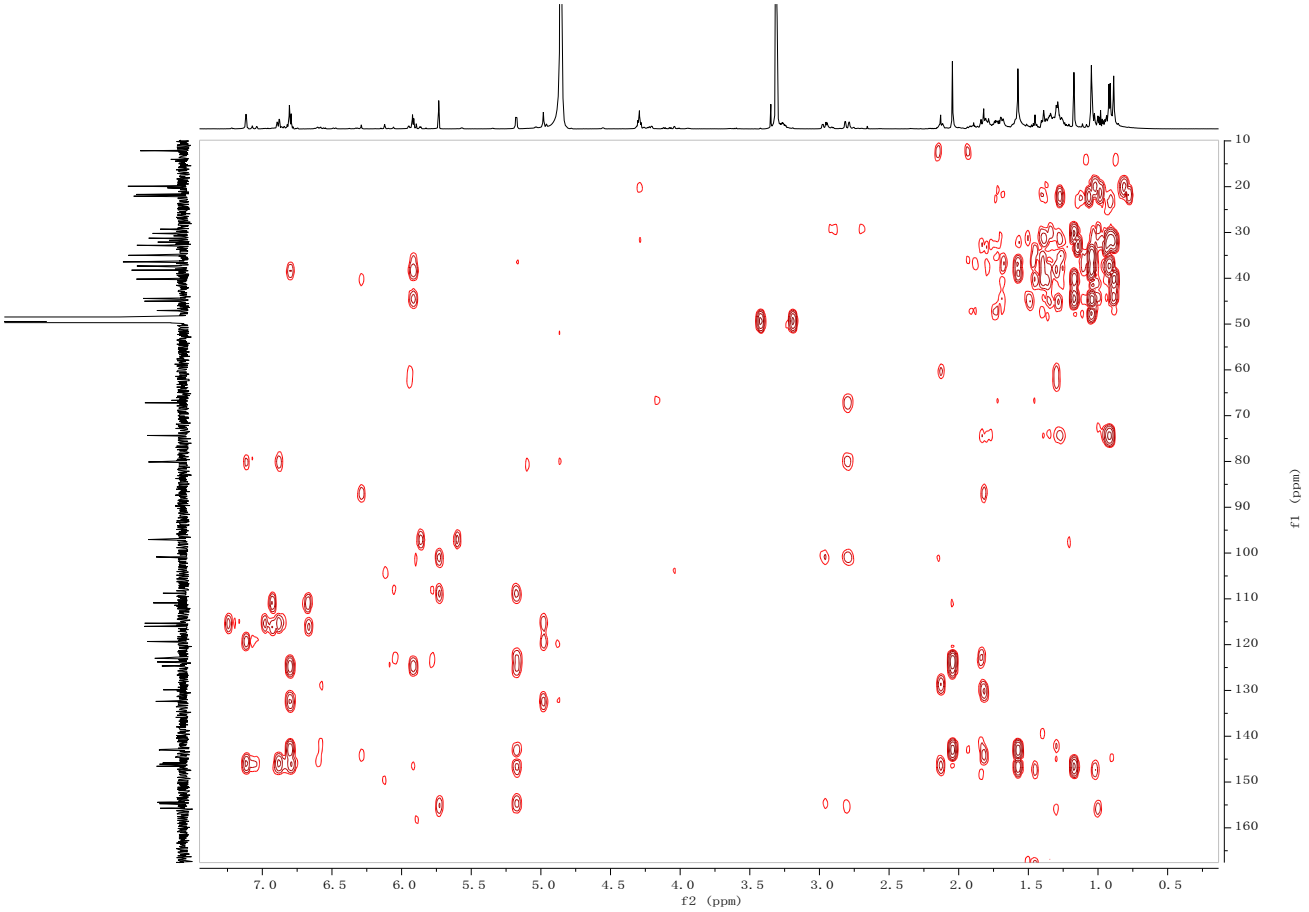
^{13}C NMR (BB+DEPT) spectrum (125 MHz) of Celamonol D (**4**) in CD_3OD



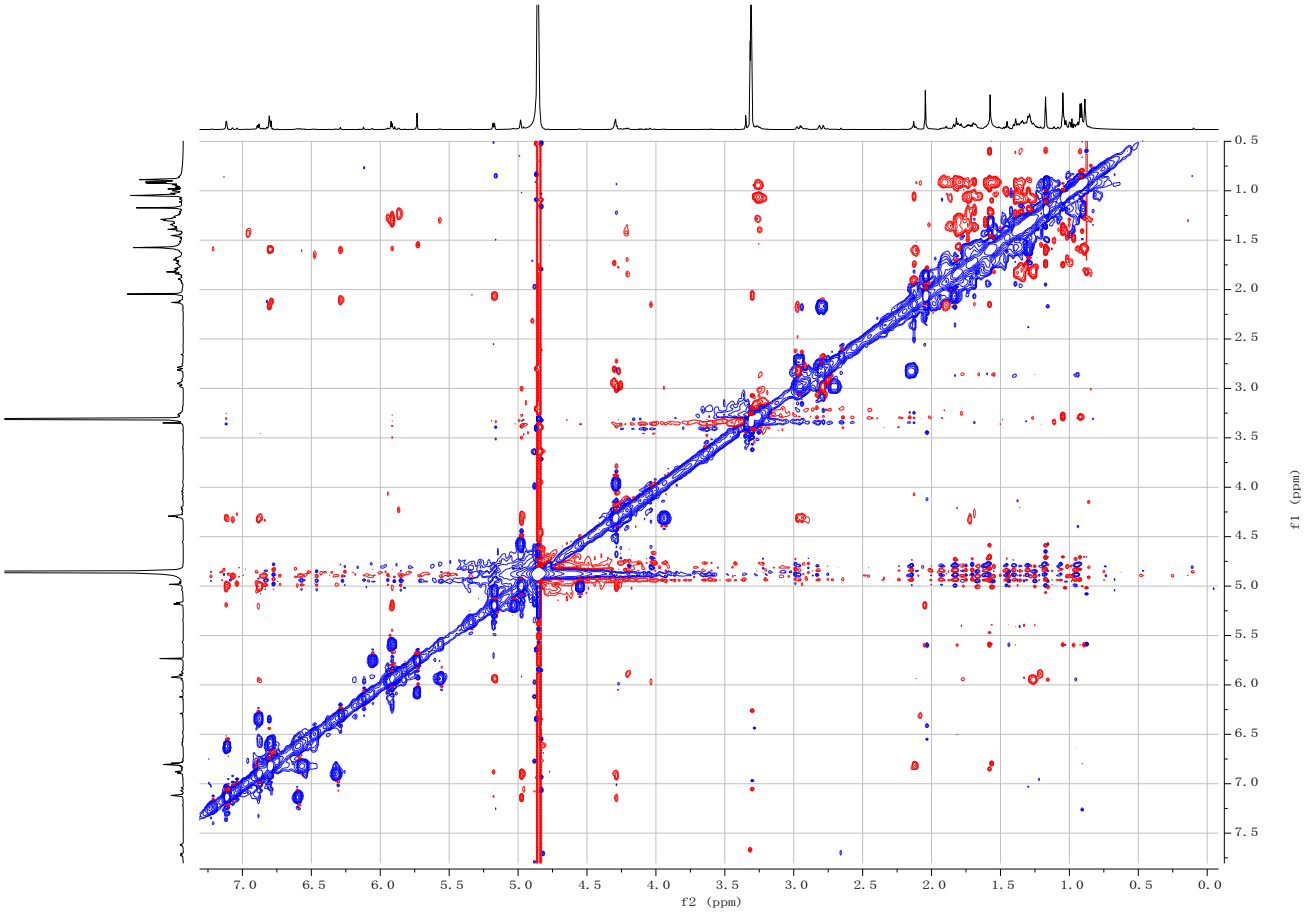
HSQC spectrum (500 MHz) of Celamonol D (**4**) in CD_3OD



HMBC spectrum (500 MHz) of Celamonol D (**4**) in CD_3OD



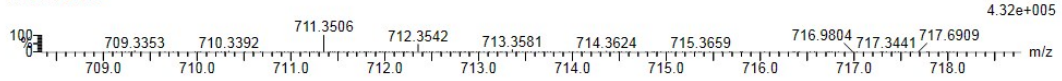
ROESY spectrum (500 MHz) of Celamonol D (**4**) in CD_3OD



HR-ESIMS of Celamonol D (**4**)

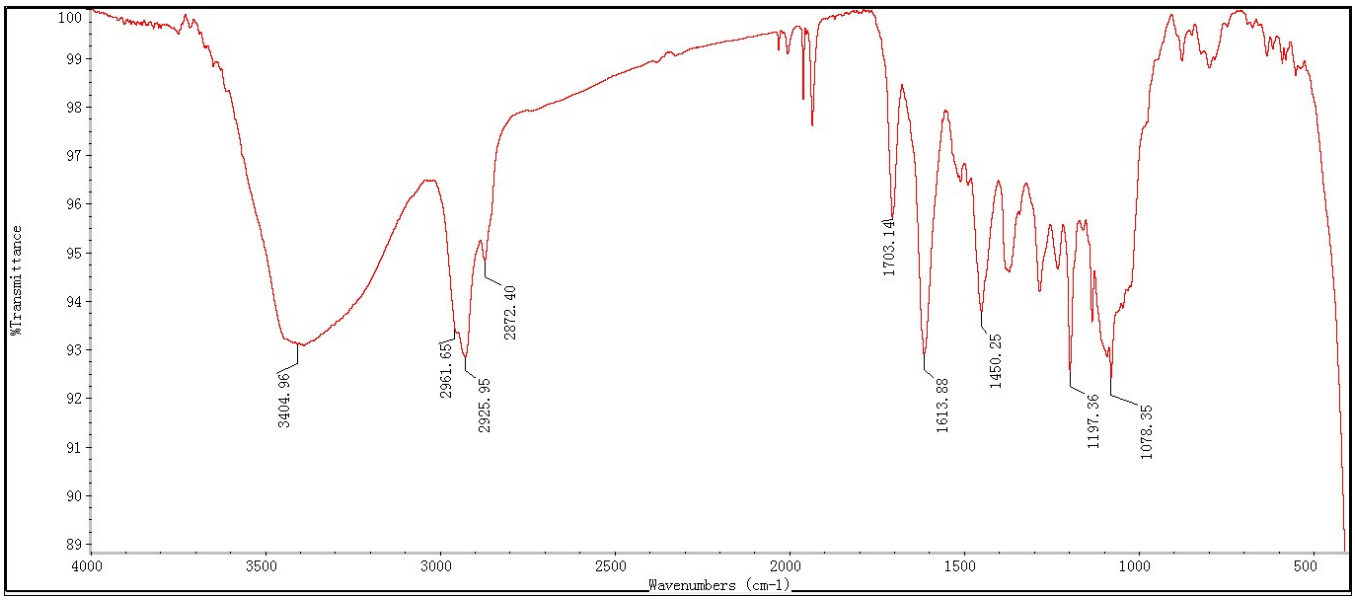
Single Mass Analysis
Tolerance = 4.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
235 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 10-70 H: 0-200 O: 0-120
9A34-1 203 (1.642)
1: TOF MS ES-



Minimum:				-1.5				
Maximum:		5.0	4.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
711.3506	711.3533	-2.7	-3.8	18.5	641.3	n/a	n/a	C43 H51 O9

IR spectrum of Celamonol D (**4**)



UV spectrum of Celamonol D (**4**)

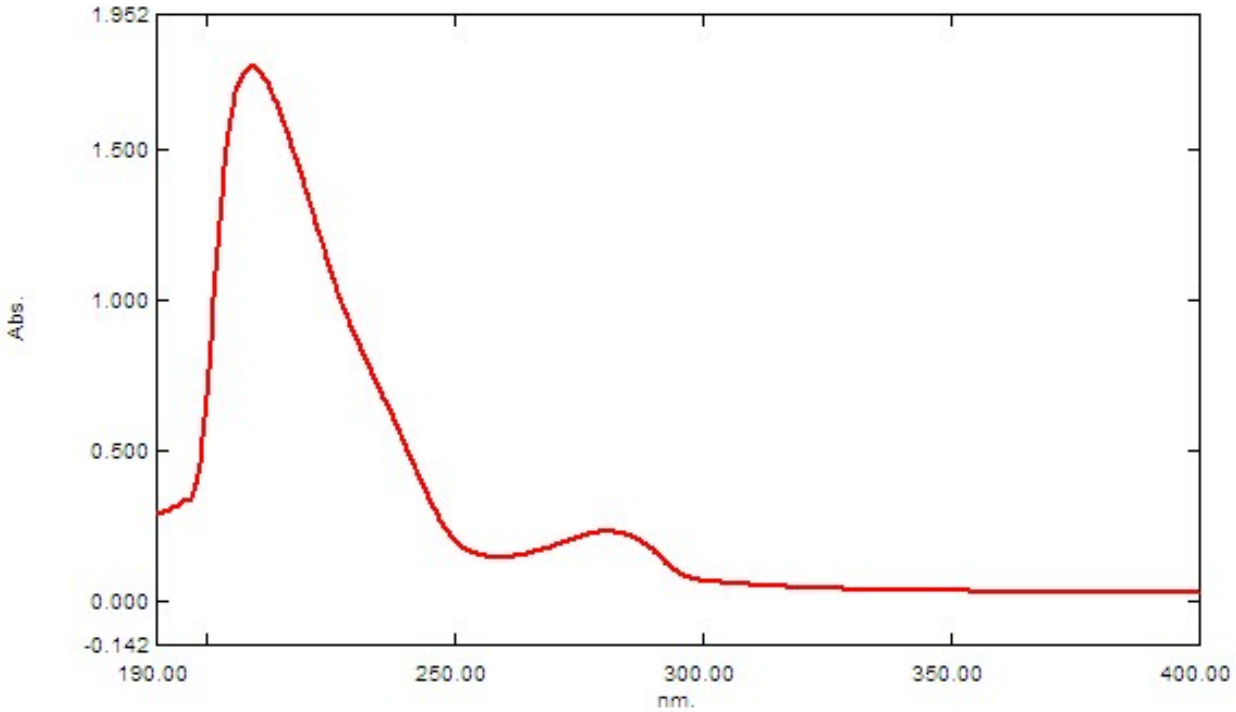
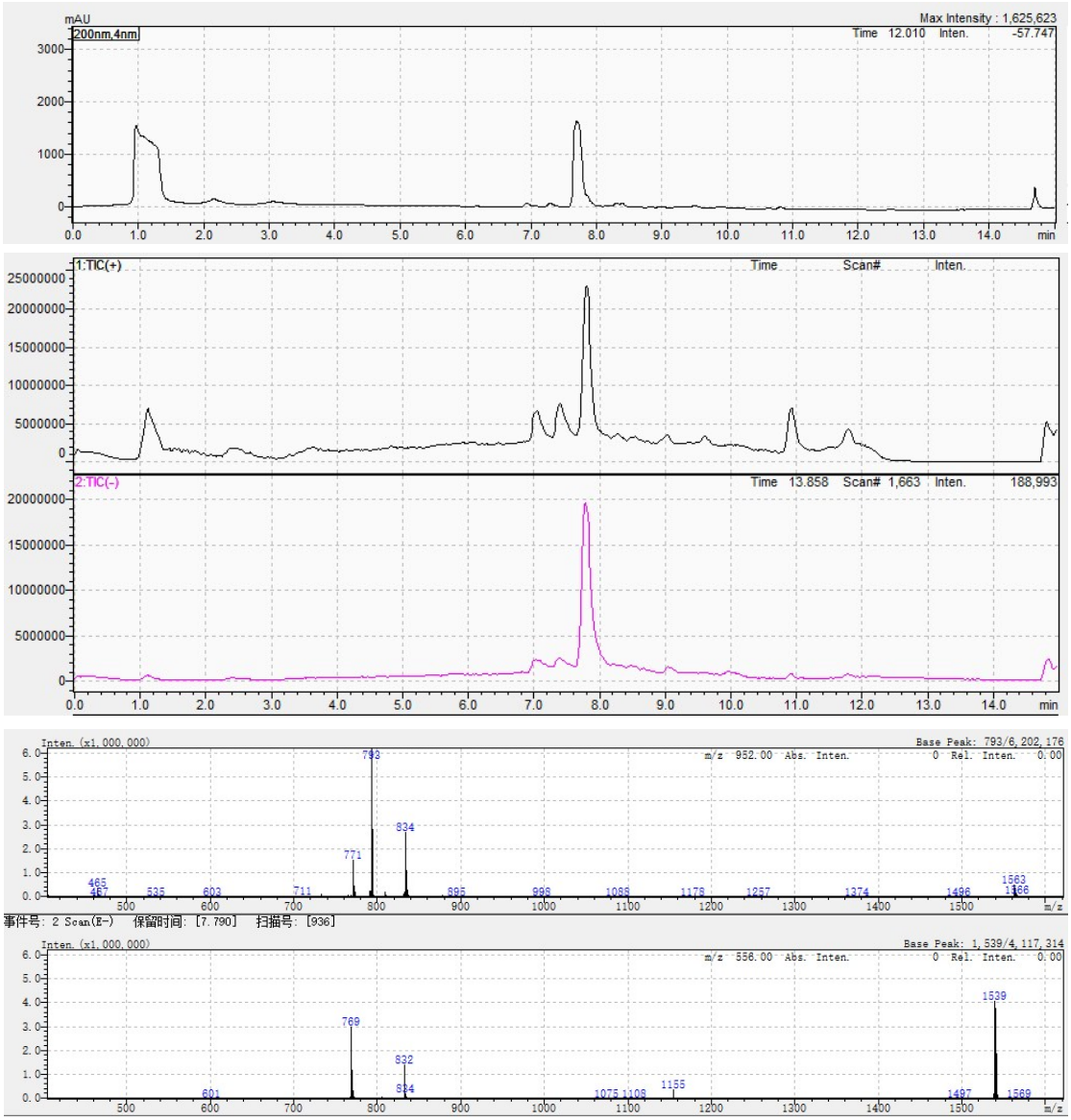
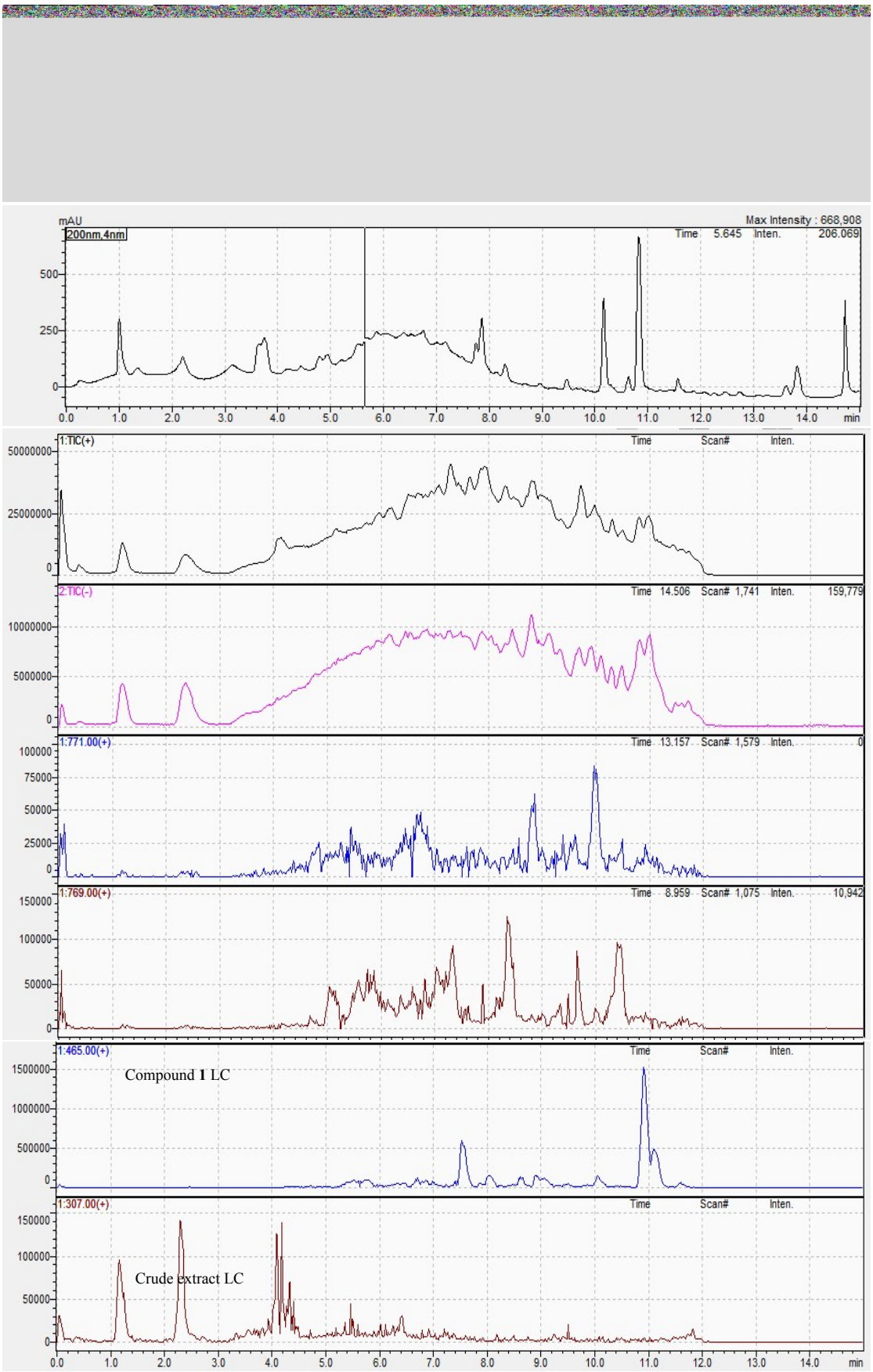


Figure S6. LC-ESIMS monitors compound **1** in the ethanolic crude extract. (A) LC-ESI(+)MS chromatogram of authentic compound **1**. (B) LC-ESI(+)MS chromatogram of ethanolic crude extract.



(A) LC-ESI(+)MS chromatogram of authentic compound **1**



(B) LC-ESI(+)MS chromatogram of ethanolic crude extract.

Crude extract MS (+)

The results and discussion

The LC-ESIMS analysis on the authentic sample of compound **1** is clear. The triterpenoid part (A) and the catechin part (B) were observed by selective ion monitoring mode, however, the molecular ion peaks for compound **1** was not detected in the mass spectra of the ethanolic crude extract acquired around the corresponding retention times of authentic sample (t_R = 7.65 min). Thus, we cannot fully exclude the possibility that these four compounds are artefact, and we gave the hypothetical biosynthetic pathway to explain it as bellow.