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Supporting Information

Belamchinenin A, an Unprecedented Tricyclic-Fused Triterpenoid with Cytotoxicity from *Belamcanda chinensis*

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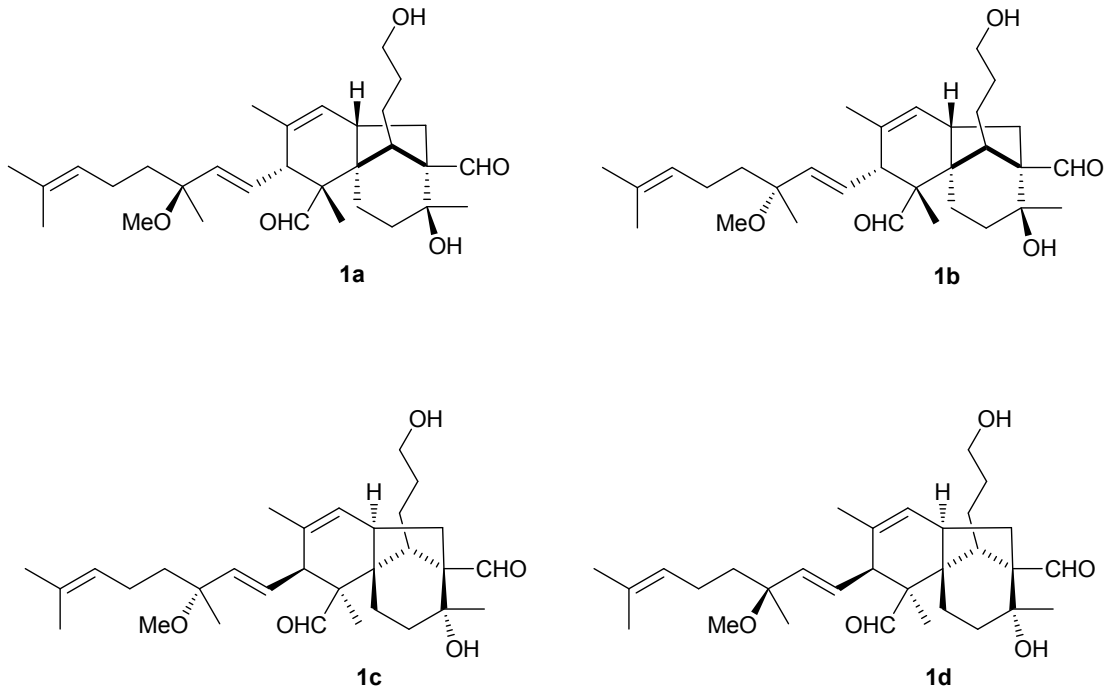


Figure S1. Four possible stereoisomers of compound **1**

Table S1. Energies analysis of **1a**–**1d** at the B3LYP/6-31G(d,p) level with the implicit solvation model in MeOH.

compound	Energy (a.u.)	Imaginary Freg
1a	–1586.19536697	0
1b	–1586.21101471	0
1c	–1586.21092235	0
1d	–1586.21101471	0

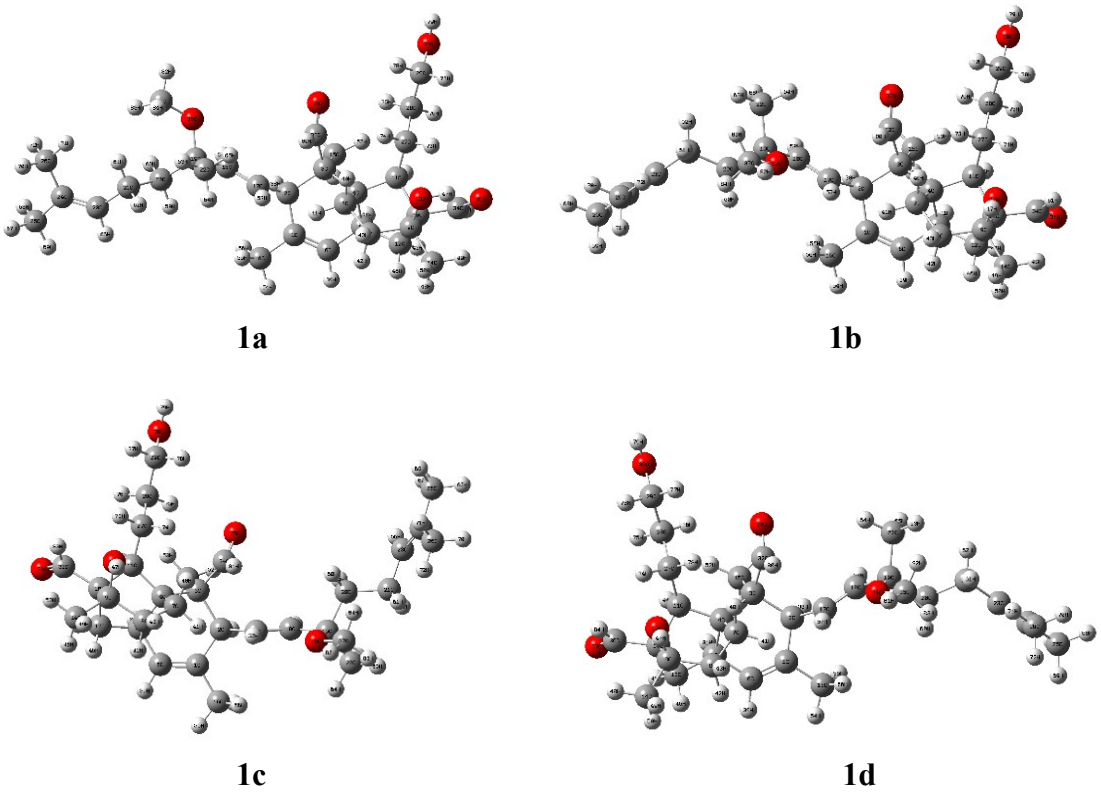


Figure S2. Optimized geometries of **1a**–**1d** at B3LYP/6-31G(d,p) level with the implicit solvation model in MeOH.

Table S2. Z-matrix of optimized 1a at B3LYP/6-31G(d,p) level

Atom	X	Y	Z
C	-0.101295	-2.002823	-1.439038
C	-0.344287	-0.496979	-1.260941
C	0.991395	0.388366	-1.112356
C	2.133634	-0.479812	-0.443687
C	2.356027	-1.699219	-1.376922
C	1.124687	-2.547010	-1.479880
C	1.736778	-0.871869	1.011471
C	2.602771	-1.958452	1.659868
C	4.110230	-1.726742	1.490883
C	4.365000	-1.284171	0.008409
C	3.599970	0.064379	-0.399139
C	3.720018	-2.316578	-0.968049
O	4.471101	-0.694812	2.411858
C	4.888148	-3.001929	1.874449
C	1.350516	0.897037	-2.524737
C	-1.338694	-2.846525	-1.630940
C	-1.419727	-0.239401	-0.213296
C	-2.534515	0.455701	-0.453278
C	-3.676726	0.741995	0.508731
C	-4.935123	-0.002825	-0.041399
C	-6.107392	-0.285800	0.927063
C	-3.342616	0.357210	1.955360
C	-7.226507	-1.011895	0.226919
C	-8.499483	-0.624789	0.050659
C	-9.476063	-1.505003	-0.694071
C	-9.090581	0.670457	0.552758
C	3.936377	1.358802	0.378594
C	4.131596	2.582394	-0.531213
C	4.480918	3.837672	0.257970
O	4.755176	4.878406	-0.676032
H	2.530398	-1.277928	-2.374566
C	0.671114	1.604626	-0.237208
O	0.764172	2.757063	-0.604184
C	5.824547	-1.034421	-0.273193
O	6.654138	-0.716125	0.561050
O	-3.795973	2.177272	0.394675
C	-4.915534	2.822405	0.965644
H	-0.787328	-0.149640	-2.205255
H	1.232316	-3.617842	-1.653349
H	1.794332	0.022626	1.638805
H	0.700404	-1.210624	1.046384

H	2.337834	-2.937726	1.245773
H	2.390124	-2.004791	2.734238
H	3.904774	0.240050	-1.441007
H	4.351330	-2.460413	-1.853808
H	3.616964	-3.299561	-0.503600
H	5.416243	-0.521068	2.248480
H	4.660125	-3.856710	1.229188
H	5.967861	-2.828987	1.843706
H	4.620242	-3.273247	2.900953
H	1.322835	0.089019	-3.261038
H	2.334313	1.370205	-2.563990
H	0.623439	1.654082	-2.830866
H	-1.075192	-3.888316	-1.839598
H	-1.989866	-2.828880	-0.748353
H	-1.945636	-2.474857	-2.468275
H	-1.260409	-0.668121	0.773910
H	-2.693284	0.889283	-1.441521
H	-4.597443	-0.969114	-0.438168
H	-5.299677	0.565479	-0.906459
H	-6.467163	0.636111	1.389345
H	-5.740631	-0.916595	1.749388
H	-4.145118	0.645214	2.639683
H	-3.201217	-0.724310	2.057936
H	-2.426985	0.863974	2.273410
H	-6.937483	-1.976628	-0.195734
H	-10.335587	-1.767665	-0.061133
H	-9.885725	-0.986755	-1.572678
H	-9.010675	-2.434953	-1.035629
H	-9.924834	0.474366	1.240827
H	-8.370545	1.304720	1.075103
H	-9.508461	1.252881	-0.280145
H	4.854450	1.215244	0.952835
H	3.167251	1.569802	1.130008
H	3.232202	2.793492	-1.117715
H	4.946915	2.390096	-1.242618
H	5.355357	3.645720	0.903442
H	3.637839	4.105286	0.915380
H	4.891390	5.696831	-0.175767
H	0.339324	1.385197	0.794472
H	6.119282	-1.094980	-1.345830
H	-4.723818	3.895189	0.871442
H	-5.850524	2.591953	0.434734
H	-5.049943	2.589662	2.032148

Table S3. Z-matrix of optimized **1b** at B3LYP/6-31G(d,p) level

Atom	X	Y	Z
C	-0.107434	-1.873799	-1.549232
C	-0.313957	-0.364318	-1.362974
C	1.039878	0.476279	-1.119682
C	2.113508	-0.44074	-0.405402
C	2.352658	-1.646677	-1.353494
C	1.10309	-2.453892	-1.539505
C	1.618413	-0.864972	1.011062
C	2.414693	-2.002042	1.663865
C	3.936365	-1.787359	1.592884
C	4.292653	-1.322377	0.146584
C	3.590445	0.055024	-0.262867
C	3.672446	-2.312629	-0.88379
O	4.330874	-0.730732	2.487566
C	4.690745	-3.064671	1.999881
C	1.494854	1.001296	-2.497551
C	-1.360746	-2.67377	-1.813538
C	-1.432011	-0.073079	-0.372119
C	-2.504375	0.666134	-0.668538
C	-3.647361	1.011102	0.270145
C	-4.931416	0.313173	-0.278946
C	-6.311407	0.911024	0.081442
C	-3.777049	2.546461	0.322897
C	-7.423554	0.13415	-0.575836
C	-8.429984	-0.545139	-0.00186
C	-9.451206	-1.270353	-0.847951
C	-8.66147	-0.661156	1.485692
C	3.909865	1.325919	0.564888
C	4.165254	2.572724	-0.297156
C	4.524636	3.788388	0.548082
O	4.773727	4.886838	-0.331811
H	2.595176	-1.212707	-2.330769
C	0.683581	1.672079	-0.239059
O	0.732733	2.836236	-0.594043
C	5.790988	-1.149058	-0.015821
O	6.403225	-1.350969	-1.049182
O	-3.249561	0.506002	1.55706
C	-4.193778	0.514716	2.612673
H	-0.686415	0.010197	-2.327103
H	1.188726	-3.52469	-1.724375
H	1.668317	0.00355	1.675233

H	0.571533	-1.168996	0.978808
H	2.155218	-2.95694	1.193745
H	2.122258	-2.094926	2.718326
H	3.969045	0.238729	-1.277038
H	4.360905	-2.434848	-1.723309
H	3.515438	-3.30473	-0.455012
H	4.210378	-1.06213	3.392918
H	5.771431	-2.889016	2.031627
H	4.373267	-3.373664	3.003964
H	4.495595	-3.903103	1.325515
H	1.492237	0.207176	-3.248105
H	0.803091	1.77796	-2.834932
H	2.493179	1.44492	-2.470198
H	-1.119634	-3.720346	-2.025289
H	-1.914079	-2.27012	-2.672941
H	-2.051857	-2.646704	-0.962049
H	-1.354985	-0.489443	0.628463
H	-2.608349	1.087881	-1.669195
H	-4.85977	0.303149	-1.374285
H	-4.885244	-0.738249	0.031876
H	-6.451369	0.959987	1.163685
H	-6.348912	1.948026	-0.280534
H	-4.562844	2.868196	1.012771
H	-2.827936	2.98273	0.650012
H	-4.019049	2.949873	-0.666568
H	-7.377462	0.127363	-1.667249
H	-9.24696	-1.163022	-1.918096
H	-10.465157	-0.892482	-0.654301
H	-9.471581	-2.343236	-0.609557
H	-9.646198	-0.255318	1.756591
H	-8.668487	-1.716194	1.792758
H	-7.909507	-0.142916	2.085185
H	3.106494	1.532596	1.281852
H	4.792644	1.150622	1.183671
H	4.990566	2.377797	-0.995897
H	3.286658	2.824625	-0.900219
H	3.697918	4.020698	1.238205
H	5.412719	3.570823	1.163058
H	4.985335	5.657453	0.217817
H	0.358056	1.435964	0.789038
H	6.324404	-0.770112	0.877792
H	-3.646306	0.216466	3.511476
H	-4.62876	1.507922	2.787043
H	-5.007656	-0.204422	2.450245

Table S4. Z-matrix of optimized 1c at B3LYP/6-31G(d,p) level

Atom	X	Y	Z
C	-0.869048	-2.85281	-1.222581
C	-0.024067	-1.580333	-1.38105
C	-0.849838	-0.200592	-1.265294
C	-2.107811	-0.41048	-0.327373
C	-2.953393	-1.536287	-0.981342
C	-2.197728	-2.829439	-1.034869
C	-1.656935	-0.748222	1.126918
C	-2.764959	-1.282933	2.043574
C	-4.051296	-0.441004	1.986343
C	-4.36319	-0.132352	0.488616
C	-3.206809	0.699476	-0.236534
C	-4.357135	-1.460505	-0.326069
O	-3.847686	0.822351	2.645869
C	-5.212946	-1.164445	2.689846
C	-1.216947	0.224749	-2.701984
C	-0.116682	-4.15551	-1.354419
C	1.236002	-1.653323	-0.529902
C	2.470374	-1.561325	-1.031764
C	3.770012	-1.646486	-0.250063
C	4.453124	-0.244578	-0.326013
C	5.988315	-0.16054	-0.159549
C	4.630344	-2.766096	-0.868725
C	6.468778	1.262026	-0.293599
C	7.12708	2.016217	0.601679
C	7.519653	3.437916	0.270452
C	7.544351	1.562047	1.979896
C	-2.848928	2.104865	0.311
C	-2.662659	3.163192	-0.78826
C	-2.358403	4.540168	-0.211402
O	-2.233957	5.461929	-1.296724
H	-3.11508	-1.222137	-2.019487
C	-5.656452	0.648844	0.35242
O	-6.422239	0.560675	-0.590531
C	0.091914	0.846448	-0.675034
O	0.486145	1.837401	-1.263182
O	3.386143	-2.002103	1.089714
C	4.372903	-1.99322	2.105644
H	0.335241	-1.585465	-2.420092

H	-2.750113	-3.767172	-0.975121
H	-1.24905	0.157722	1.586115
H	-0.848983	-1.480935	1.119015
H	-2.993601	-2.322259	1.78357
H	-2.404198	-1.303027	3.080716
H	-3.60164	0.849485	-1.250189
H	-5.136542	-1.417403	-1.090509
H	-4.576118	-2.326343	0.302812
H	-3.758267	0.637375	3.595351
H	-5.472848	-2.112116	2.21021
H	-4.93021	-1.390308	3.726014
H	-6.108047	-0.533767	2.719325
H	-1.645306	-0.606421	-3.267377
H	-0.313039	0.549557	-3.224549
H	-1.923821	1.057603	-2.725563
H	0.440889	-4.196948	-2.300465
H	-0.803155	-5.00772	-1.326406
H	0.623347	-4.284637	-0.555242
H	1.125879	-1.814394	0.539019
H	2.605811	-1.409306	-2.103496
H	4.208941	0.191412	-1.303176
H	3.959471	0.394765	0.416788
H	6.307238	-0.595485	0.790298
H	6.459693	-0.764401	-0.947784
H	5.57655	-2.898994	-0.336067
H	4.079025	-3.71116	-0.83635
H	4.86755	-2.540587	-1.914256
H	6.229409	1.724766	-1.253811
H	8.609089	3.57158	0.331211
H	7.081804	4.146286	0.987954
H	7.196958	3.728142	-0.734573
H	8.635206	1.629815	2.09512
H	7.112529	2.21769	2.74873
H	7.247022	0.536042	2.208421
H	-3.634347	2.448494	0.987552
H	-1.948131	2.058737	0.934437
H	-1.848111	2.89041	-1.467147
H	-3.577059	3.233519	-1.39345
H	-3.164849	4.848929	0.473112
H	-1.427516	4.501413	0.376587
H	-2.026523	6.330507	-0.918237
H	-5.862822	1.37069	1.166646
H	0.428423	0.66483	0.360722
H	3.893989	-2.409902	2.996474

H	5.243938	-2.615323	1.859458
H	4.718404	-0.978401	2.343153

Table S5. Z-matrix of optimized 1d at B3LYP/6-31G(d,p) level

Atom	X	Y	Z
C	0.10743	-1.873794	-1.549247
C	0.313955	-0.364314	-1.362982
C	-1.03988	0.476282	-1.119684
C	-2.113508	-0.440739	-0.405404
C	-2.352661	-1.646672	-1.3535
C	-1.103094	-2.453887	-1.539519
C	-1.618408	-0.864979	1.011057
C	-2.414686	-2.002052	1.663856
C	-3.936356	-1.787367	1.592884
C	-4.292651	-1.322379	0.146589
C	-3.590445	0.055023	-0.262863
C	-3.672447	-2.312627	-0.883792
O	-4.33086	-0.730741	2.487572
C	-4.690736	-3.064679	1.999882
C	-1.494861	1.001304	-2.49755
C	1.360742	-2.673764	-1.813558
C	1.432008	-0.07308	-0.372125
C	2.504371	0.666136	-0.668539
C	3.647355	1.011101	0.270147
C	4.931412	0.313176	-0.278946
C	6.311402	0.911027	0.081447
C	3.777043	2.546459	0.322907
C	7.42355	0.134157	-0.575833
C	8.429976	-0.545139	-0.001858
C	9.451201	-1.270348	-0.84795
C	8.661455	-0.661168	1.485694
C	-3.909867	1.325916	0.564891
C	-4.165246	2.572725	-0.29715
C	-4.524624	3.788389	0.548088
O	-4.773706	4.886843	-0.331803
H	-2.595183	-1.212698	-2.330772
C	-0.683578	1.672079	-0.239058
O	-0.732729	2.836237	-0.594037
O	3.249554	0.505994	1.557059
C	4.193771	0.514703	2.612673
C	-5.790986	-1.14906	-0.015812

O	-6.403222	-1.350943	-1.04918
H	0.686411	0.010206	-2.32711
H	-1.188731	-3.524683	-1.724392
H	-1.668309	0.00354	1.675233
H	-0.571527	-1.169001	0.978797
H	-2.155215	-2.956947	1.193728
H	-2.122245	-2.094944	2.718314
H	-3.96905	0.238728	-1.277034
H	-4.360908	-2.434844	-1.723309
H	-3.515435	-3.304729	-0.455018
H	-4.21036	-1.062142	3.392922
H	-5.771422	-2.889024	2.031633
H	-4.373254	-3.373673	3.003963
H	-4.495589	-3.90311	1.325514
H	-1.49225	0.207186	-3.248105
H	-2.493184	1.444931	-2.470191
H	-0.803096	1.777967	-2.834932
H	1.119628	-3.720337	-2.025319
H	1.914075	-2.270108	-2.672958
H	2.051852	-2.646706	-0.962069
H	1.354981	-0.489449	0.628455
H	2.608345	1.087889	-1.669193
H	4.859767	0.303157	-1.374285
H	4.88524	-0.738247	0.031872
H	6.451362	0.959986	1.16369
H	6.348906	1.94803	-0.280526
H	4.562837	2.868192	1.012784
H	2.827929	2.982727	0.650023
H	4.019043	2.949876	-0.666556
H	7.377464	0.12738	-1.667247
H	9.246963	-1.163005	-1.918096
H	10.465152	-0.892484	-0.65429
H	9.47157	-2.343234	-0.609567
H	9.64618	-0.25533	1.756602
H	7.909487	-0.142937	2.085188
H	8.668475	-1.716209	1.792751
H	-3.106501	1.532589	1.281864
H	-4.792652	1.150621	1.183667
H	-4.990555	2.377803	-0.995896
H	-3.286645	2.824622	-0.90021
H	-3.697908	4.020692	1.238215
H	-5.41271	3.570828	1.163061
H	-4.985324	5.657453	0.217826
H	-0.358051	1.43596	0.789037

H	3.646299	0.216448	3.511474
H	4.628753	1.507908	2.787048
H	5.00765	-0.204433	2.450242
H	-6.324404	-0.770141	0.877811

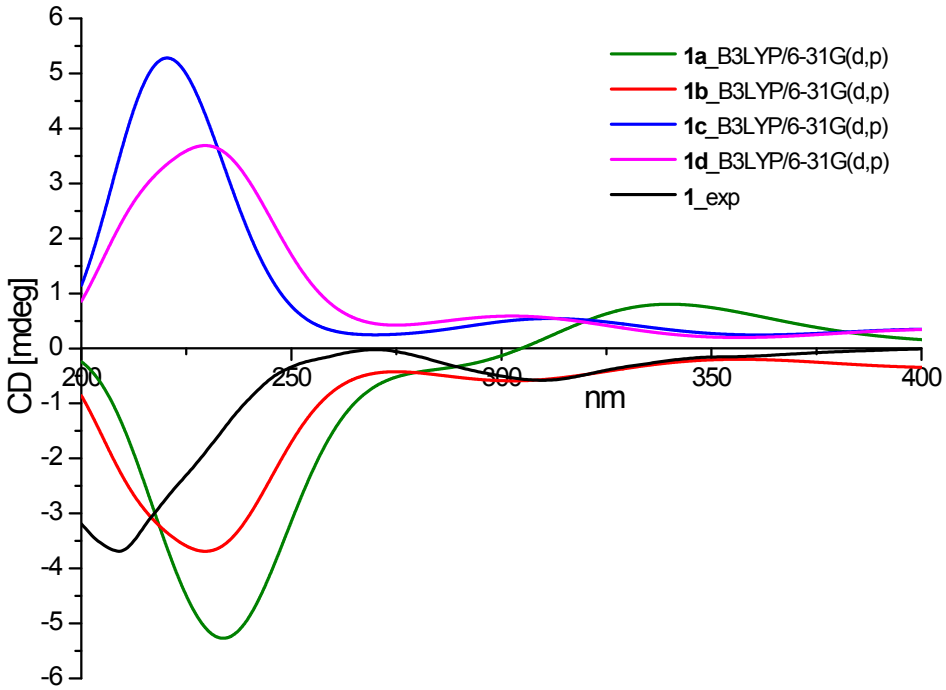
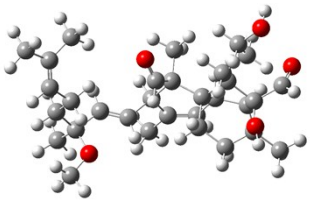
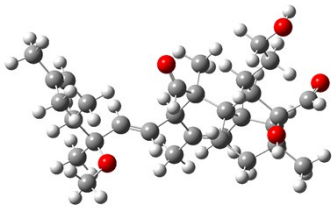


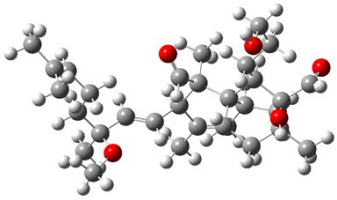
Figure S3. Calculated and experimental ECD spectra of **1**, **1a**, **1b**, **1c**, and **1d** at the B3LYP/6-31G(d,p) level with the implicit solvation model in MeOH.



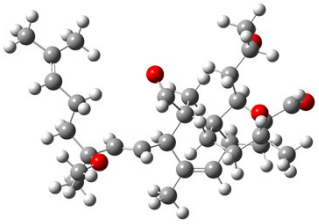
1a1 (18.80%)



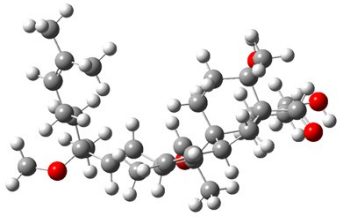
1a2 (23.14%)



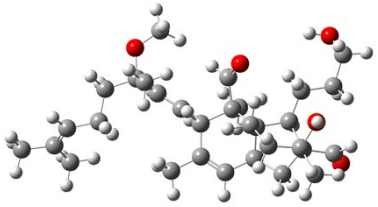
1a3 (11.06%)



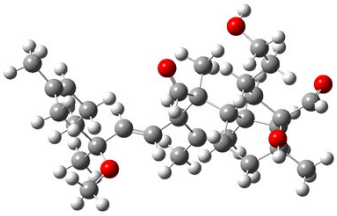
1a4 (0.19%)



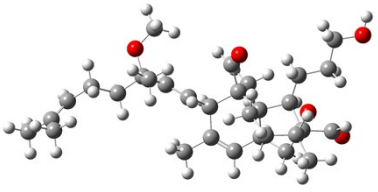
1a5 (1.38%)



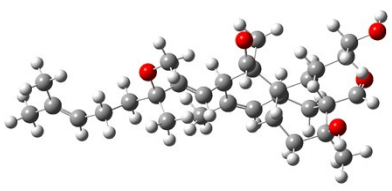
1a6 (0.25%)



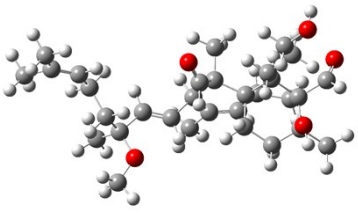
1a7 (19.59%)



1a8 (0.77%)



1a9 (22.09%)



1a10 (2.72%)

Figure S4. Reoptimized geometries of **1a** at B3LYP/6-311+G(d,p) level with the CPCM model in MeOH

Table S6. Z-matrix of optimized conformer 1a1 at B3LYP/6-311+G(d,p) level

Atom	X	Y	Z
C	0.192094	-2.947677	-1.273667
C	-0.597679	-1.632056	-1.276894
C	0.300645	-0.294534	-1.197975
C	1.651749	-0.603142	-0.433777
C	2.347718	-1.742852	-1.217051
C	1.529505	-2.994769	-1.23289
C	1.372353	-0.954296	1.057649
C	2.56817	-1.528269	1.828818
C	3.885095	-0.76418	1.603447
C	4.008412	-0.441651	0.083112
C	2.800132	0.453677	-0.465515
C	3.816003	-1.761665	-0.733102
O	3.865897	0.503952	2.296792
C	5.07281	-1.580488	2.138634
C	0.521541	0.206375	-2.637688
C	-0.633538	-4.206388	-1.382405
C	-1.749504	-1.697926	-0.283507
C	-3.029545	-1.563896	-0.628454
C	-4.23182	-1.700302	0.283521
C	-5.153791	-0.460901	0.152492
C	-4.541108	0.871533	0.618713
C	-5.012067	-2.962016	-0.142663
C	-5.556912	1.982843	0.62039
C	-5.553353	3.125378	-0.081718
C	-6.681135	4.120683	0.056118
C	-4.473611	3.540988	-1.049758
C	2.493757	1.836291	0.129795
C	3.602993	2.884428	-0.035227
C	3.132423	4.276622	0.379868
O	4.166886	5.267187	0.283773
H	2.403589	-1.396301	-2.252861
C	-0.532694	0.745804	-0.452843

O	-1.004164	1.744431	-0.957068
C	5.327788	0.240331	-0.224758
O	5.859573	0.239301	-1.316779
O	-3.716989	-1.839825	1.62182
C	-4.654047	-2.051026	2.670896
H	-1.073173	-1.570711	-2.263003
H	2.035061	-3.95693	-1.276498
H	1.040336	-0.049428	1.570173
H	0.55443	-1.669401	1.134916
H	2.714479	-2.575868	1.553776
H	2.345493	-1.527461	2.901121
H	3.058449	0.623266	-1.517181
H	4.497038	-1.770829	-1.583906
H	4.045533	-2.639794	-0.131174
H	3.94251	0.330296	3.242511
H	5.201319	-2.526149	1.610051
H	6.005136	-1.015383	2.069758
H	4.903137	-1.817667	3.193947
H	0.941204	-0.572135	-3.274825
H	1.179828	1.076408	-2.674624
H	-0.434371	0.505095	-3.070775
H	-1.305139	-4.16244	-2.247595
H	0.010262	-5.081378	-1.493338
H	-1.268143	-4.356135	-0.503944
H	-1.515394	-1.902244	0.756048
H	-3.28567	-1.372905	-1.669477
H	-6.076827	-0.652397	0.710213
H	-5.453172	-0.377983	-0.897627
H	-3.678941	1.118938	-0.002554
H	-4.157885	0.738164	1.637597
H	-5.946056	-3.063414	0.414904
H	-5.265652	-2.905655	-1.203757
H	-4.404235	-3.855361	0.018357
H	-6.40695	1.812683	1.282106
H	-7.164362	4.300446	-0.911662
H	-7.442308	3.778382	0.760475
H	-6.306333	5.091839	0.400869
H	-3.664237	2.816903	-1.135079
H	-4.898098	3.699333	-2.048281
H	-4.037461	4.499834	-0.744987
H	2.229697	1.763004	1.183841
H	1.610445	2.211803	-0.398584
H	3.932747	2.91964	-1.081449
H	4.472411	2.622694	0.573503

H	2.826616	4.278069	1.428844
H	2.265483	4.580567	-0.220219
H	4.429127	5.340678	-0.640884
H	-0.716328	0.547871	0.614574
H	5.798189	0.783287	0.612834
H	-4.069015	-2.120375	3.588777
H	-5.361082	-1.220419	2.771047
H	-5.215627	-2.982301	2.544388

Table S7. Z-matrix of optimized conformer 1a2 at B3LYP/6-311+G(d,p) level

Atom	X	Y	Z
C	0.383444	-3.092159	-0.997045
C	-0.420864	-1.806762	-1.235357
C	0.458718	-0.457749	-1.300767
C	1.751543	-0.62092	-0.40062
C	2.517507	-1.845512	-0.955245
C	1.714946	-3.103932	-0.854352
C	1.364738	-0.760241	1.102251
C	2.506111	-1.183757	2.036863
C	3.828246	-0.433241	1.797853
C	4.059923	-0.332522	0.259316
C	2.885822	0.445844	-0.500319
C	3.944279	-1.762223	-0.365043
O	3.747637	0.920283	2.298256
C	4.982609	-1.139306	2.528119
C	0.784787	-0.186172	-2.781737
C	-0.41685	-4.371599	-0.991683
C	-1.626631	-1.748377	-0.308159
C	-2.888813	-1.709717	-0.733803
C	-4.132074	-1.721257	0.132382
C	-5.076579	-0.559647	-0.270276
C	-4.517477	0.853367	-0.030089
C	-4.856453	-3.066532	-0.083967
C	-5.444517	1.920484	-0.547356
C	-6.056269	2.901865	0.131825
C	-6.961021	3.883936	-0.574089
C	-5.919656	3.141454	1.615038
C	2.517105	1.891105	-0.132551
C	3.624136	2.930644	-0.356126
C	3.105051	4.355971	-0.17955

O	4.134148	5.346924	-0.319576
H	2.650608	-1.649309	-2.022949
C	-0.434987	0.670092	-0.790778
O	-0.887285	1.560707	-1.480771
C	5.389933	0.326801	-0.051834
O	5.994477	0.185741	-1.095773
O	-3.682535	-1.589922	1.495428
C	-4.666053	-1.648028	2.521198
H	-0.838659	-1.896663	-2.245243
H	2.232596	-4.052347	-0.728731
H	0.976301	0.198404	1.451662
H	0.557166	-1.480561	1.223001
H	2.684771	-2.257178	1.93404
H	2.201611	-1.028383	3.077316
H	3.222369	0.470172	-1.543196
H	4.688087	-1.879681	-1.152965
H	4.138122	-2.538204	0.373911
H	3.745186	0.882529	3.262075
H	5.151263	-2.152561	2.161271
H	5.914308	-0.576886	2.433339
H	4.745134	-1.213607	3.594287
H	1.238546	-1.055247	-3.258432
H	1.454379	0.66692	-2.907304
H	-0.134964	0.042445	-3.322372
H	-1.007463	-4.468836	-1.910114
H	0.242514	-5.238709	-0.916402
H	-1.127005	-4.405719	-0.160379
H	-1.44848	-1.773569	0.76149
H	-3.094973	-1.702178	-1.80311
H	-6.026659	-0.670909	0.262437
H	-5.3146	-0.683999	-1.332535
H	-3.553555	0.940163	-0.545133
H	-4.309479	0.987483	1.032588
H	-5.814855	-3.09387	0.439715
H	-5.056166	-3.218581	-1.147188
H	-4.235071	-3.892381	0.270072
H	-5.636746	1.867583	-1.619506
H	-6.600766	4.911398	-0.443791
H	-7.028336	3.678582	-1.644569
H	-7.973538	3.854477	-0.154158
H	-5.280121	2.41398	2.114018
H	-5.508169	4.139989	1.804442
H	-6.903399	3.116367	2.098197
H	2.171528	1.958907	0.897818

H	1.674203	2.168957	-0.775169
H	4.03885	2.82644	-1.367029
H	4.442762	2.776502	0.351578
H	2.706264	4.493294	0.828423
H	2.292612	4.556536	-0.889291
H	4.478482	5.299629	-1.218609
H	-0.683951	0.645256	0.281499
H	5.796078	0.989689	0.731279
H	-4.131955	-1.499497	3.460485
H	-5.419378	-0.859297	2.421129
H	-5.170905	-2.618864	2.556993

Table S8. Z-matrix of optimized conformer **1a3** at B3LYP/6-311+G(d,p) level

Atom	X	Y	Z
C	0.506103	-3.08971	-0.877332
C	-0.336449	-1.838057	-1.160768
C	0.503778	-0.468373	-1.300339
C	1.821058	-0.559945	-0.427873
C	2.605409	-1.788519	-0.946754
C	1.840293	-3.060937	-0.765973
C	1.474585	-0.641584	1.089286
C	2.647945	-1.002668	2.009372
C	3.941928	-0.226451	1.708082
C	4.135287	-0.183698	0.161324
C	2.923044	0.530592	-0.603684
C	4.04462	-1.640611	-0.400189
O	3.832095	1.143202	2.154471
C	5.133622	-0.868441	2.437612
C	0.785051	-0.244125	-2.798668
C	-0.260137	-4.386952	-0.790384
C	-1.528951	-1.769515	-0.217542
C	-2.797609	-1.80088	-0.623772
C	-4.027547	-1.810822	0.260884
C	-5.031577	-0.726029	-0.205958
C	-4.539128	0.726209	-0.077617
C	-4.688728	-3.200741	0.147779
C	-5.523578	1.703735	-0.661741
C	-6.194987	2.688323	-0.046575
C	-7.154909	3.566695	-0.813563
C	-6.077981	3.029842	1.41819

C	2.523191	1.98172	-0.295978
C	3.590073	3.037007	-0.617814
C	3.066655	4.465017	-0.55725
O	2.676974	4.76948	0.793056
H	2.70493	-1.639082	-2.025426
C	-0.411496	0.652318	-0.81241
O	-0.909818	1.499109	-1.525487
C	5.438184	0.498625	-0.20648
O	6.034797	0.318794	-1.249189
O	-3.567947	-1.564648	1.604387
C	-4.533428	-1.607653	2.647959
H	-0.766827	-1.985397	-2.158481
H	2.385699	-3.988421	-0.606039
H	1.078134	0.324635	1.407267
H	0.684196	-1.370452	1.26298
H	2.852061	-2.074257	1.940634
H	2.36546	-0.816582	3.05113
H	3.235973	0.512866	-1.65432
H	4.770401	-1.769716	-1.203012
H	4.280726	-2.379805	0.363877
H	3.844598	1.14504	3.11897
H	5.326138	-1.889253	2.104862
H	6.044857	-0.281601	2.300353
H	4.922209	-0.909363	3.51099
H	1.266618	-1.111021	-3.251456
H	1.413527	0.631363	-2.973171
H	-0.155541	-0.077858	-3.326098
H	-0.874588	-4.540617	-1.685139
H	0.423536	-5.233102	-0.696162
H	-0.944799	-4.400562	0.062651
H	-1.333569	-1.727071	0.848581
H	-3.018414	-1.861713	-1.68841
H	-5.967672	-0.842656	0.349688
H	-5.278344	-0.937461	-1.252359
H	-3.585421	0.821615	-0.610027
H	-4.328354	0.949676	0.969427
H	-5.638602	-3.23785	0.686268
H	-4.893205	-3.435004	-0.89953
H	-4.023971	-3.969845	0.547987
H	-5.709177	1.570483	-1.728053
H	-6.857619	4.620309	-0.750668
H	-7.206837	3.28836	-1.868286
H	-8.164961	3.503348	-0.391437
H	-5.398373	2.374864	1.962569

H	-5.727109	4.061108	1.543147
H	-7.060206	2.977408	1.902264
H	2.209134	2.094798	0.738403
H	1.653588	2.204603	-0.92475
H	3.983019	2.877069	-1.629156
H	4.434702	2.951453	0.071914
H	2.206476	4.581131	-1.229198
H	3.848855	5.160269	-0.884429
H	2.335414	5.669625	0.813627
H	-0.631749	0.663696	0.266327
H	5.830895	1.218198	0.532402
H	-3.998787	-1.356526	3.564823
H	-5.336758	-0.877547	2.502557
H	-4.974995	-2.60289	2.763057

Table S9. Z-matrix of optimized conformer 1a4 at B3LYP/6-311+G(d,p) level

Atom	X	Y	Z
C	0.356356	-2.488031	-1.675182
C	-0.478496	-1.228495	-1.404464
C	0.370859	0.082949	-1.001214
C	1.720464	-0.349513	-0.294079
C	2.466112	-1.260797	-1.299124
C	1.693609	-2.501845	-1.613477
C	1.431706	-1.037072	1.073905
C	2.632379	-1.746897	1.712897
C	3.92726	-0.916801	1.700064
C	4.061443	-0.242164	0.297152
C	2.831366	0.723649	-0.063853
C	3.928246	-1.341052	-0.803678
O	3.864133	0.143999	2.680614
C	5.136497	-1.801057	2.047106
C	0.599376	0.904692	-2.284082
C	-0.421891	-3.715193	-2.083511
C	-1.645928	-1.552464	-0.483326
C	-2.923977	-1.438304	-0.841914
C	-4.132165	-1.833757	-0.017783
C	-5.162291	-0.676458	0.021496
C	-4.690177	0.606935	0.727255
C	-4.778445	-3.068062	-0.682391
C	-5.795262	1.624039	0.832581

C	-5.852682	2.858335	0.311421
C	-7.065599	3.732599	0.526008
C	-4.763626	3.499356	-0.512403
C	2.466915	1.916258	0.839674
C	3.413956	3.133975	0.805091
C	3.212964	4.09427	-0.359911
O	3.554494	3.45063	-1.599339
H	2.521123	-0.687128	-2.228669
C	-0.517572	0.896096	-0.062785
O	-1.03533	1.957777	-0.344531
C	5.366873	0.5205	0.207038
O	6.020397	0.66325	-0.80712
O	-3.642625	-2.156377	1.298327
C	-4.585444	-2.622759	2.255907
H	-0.935329	-0.960853	-2.364803
H	2.233003	-3.41422	-1.858505
H	1.074809	-0.278894	1.77426
H	0.630071	-1.76837	0.976968
H	2.814723	-2.695336	1.201357
H	2.395398	-2.004521	2.750761
H	3.09405	1.138681	-1.039584
H	4.61992	-1.128303	-1.618641
H	4.185357	-2.327305	-0.419339
H	3.94543	-0.254604	3.555211
H	5.300558	-2.593608	1.315825
H	6.049959	-1.20614	2.124487
H	4.968058	-2.2813	3.016619
H	1.038065	0.2969	-3.075803
H	1.246585	1.766524	-2.110934
H	-0.357199	1.279586	-2.651902
H	-1.083301	-3.49754	-2.930047
H	0.255056	-4.520455	-2.376319
H	-1.062282	-4.081162	-1.27563
H	-1.422506	-1.93963	0.505117
H	-3.169748	-1.068893	-1.836489
H	-6.079487	-1.038466	0.498459
H	-5.43796	-0.442837	-1.012326
H	-3.820021	1.013678	0.20945
H	-4.351753	0.344195	1.736718
H	-5.715518	-3.342498	-0.192344
H	-5.00323	-2.856455	-1.730349
H	-4.094319	-3.91878	-0.642377
H	-6.65997	1.289294	1.406618
H	-7.518506	4.014788	-0.431963

H	-7.825882	3.232877	1.130028
H	-6.790036	4.668571	1.026512
H	-3.901783	2.852083	-0.670138
H	-5.152651	3.795917	-1.493568
H	-4.411319	4.418703	-0.029631
H	2.360684	1.588795	1.870387
H	1.483275	2.276425	0.521226
H	4.464021	2.829778	0.839208
H	3.24637	3.720671	1.715269
H	3.844264	4.97963	-0.21595
H	2.167412	4.426889	-0.390024
H	3.383234	4.068285	-2.318313
H	-0.700703	0.459612	0.931528
H	5.712636	0.978647	1.150248
H	-4.022837	-2.795357	3.174172
H	-5.368947	-1.885548	2.461271
H	-5.054289	-3.564155	1.951828

Table S10. Z-matrix of optimized conformer **1a5** at B3LYP/6-311+G(d,p) level

Atom	X	Y	Z
C	-0.73752	0.366176	2.467649
C	-0.79955	-0.915952	1.628361
C	0.603362	-1.370491	0.974291
C	1.49893	-0.094481	0.698662
C	1.688682	0.611367	2.062768
C	0.389713	1.065972	2.648865
C	0.845718	0.814584	-0.385086
C	1.480555	2.201863	-0.54956
C	3.01857	2.186413	-0.59297
C	3.526249	1.210248	0.510939
C	2.998917	-0.28753	0.312297
C	2.865092	1.597524	1.874119
O	3.488476	1.667332	-1.857286
C	3.57156	3.611839	-0.428393
C	1.26301	-2.373979	1.939232
C	-2.023975	0.760357	3.150682
C	-1.97469	-0.883302	0.659734
C	-2.963203	-1.776706	0.678457
C	-4.13701	-1.899283	-0.274111
C	-4.438355	-0.632725	-1.104972

C	-4.93736	0.595512	-0.320198
C	-3.846738	-3.081151	-1.222105
C	-5.37942	1.700464	-1.242456
C	-4.910589	2.952947	-1.340932
C	-5.494267	3.920373	-2.343437
C	-3.798551	3.52933	-0.500422
C	3.290601	-1.076461	-0.973307
C	4.774191	-1.343221	-1.261956
C	4.956671	-2.322963	-2.41927
O	6.335051	-2.542808	-2.754132
H	2.079451	-0.15503	2.73856
C	0.263009	-2.105713	-0.320992
O	0.394992	-3.299847	-0.49403
C	5.041365	1.208482	0.583813
O	5.678144	0.881113	1.564822
O	-5.241143	-2.217382	0.616657
C	-6.492242	-2.556354	0.028291
H	-1.035339	-1.723679	2.33115
H	0.379224	1.941621	3.294098
H	0.899591	0.301048	-1.34672
H	-0.211954	0.962431	-0.173469
H	1.154678	2.854356	0.264429
H	1.111189	2.66434	-1.470996
H	3.477574	-0.841477	1.127883
H	3.590275	1.482796	2.679547
H	2.543621	2.637923	1.880305
H	3.312529	2.32975	-2.535834
H	3.321144	4.046761	0.54018
H	4.657403	3.631568	-0.546757
H	3.139861	4.259489	-1.198536
H	1.338169	-1.969801	2.948742
H	2.261007	-2.668087	1.60826
H	0.658925	-3.280988	1.991894
H	-2.412161	-0.064091	3.760072
H	-1.867337	1.622415	3.80207
H	-2.809921	1.011122	2.432838
H	-1.990367	-0.081621	-0.071818
H	-2.940849	-2.572443	1.421635
H	-5.187174	-0.895241	-1.859722
H	-3.539479	-0.370188	-1.671759
H	-4.167919	0.939314	0.371351
H	-5.786777	0.28686	0.300005
H	-4.677009	-3.258784	-1.909636
H	-2.958697	-2.865268	-1.819762

H	-3.6639	-3.995309	-0.65166
H	-6.189167	1.422234	-1.917742
H	-4.723466	4.275959	-3.037521
H	-6.297668	3.466186	-2.927167
H	-5.894512	4.809597	-1.841965
H	-3.366986	2.813431	0.198256
H	-2.992528	3.906628	-1.14036
H	-4.161869	4.387752	0.076965
H	2.843358	-0.59485	-1.841577
H	2.800435	-2.049508	-0.8562
H	5.263684	-1.753447	-0.369363
H	5.286638	-0.4125	-1.518873
H	4.497831	-1.927061	-3.328445
H	4.469444	-3.278949	-2.189619
H	6.768357	-2.952401	-1.996814
H	-0.142217	-1.489176	-1.138521
H	5.569849	1.50616	-0.33808
H	-7.185237	-2.702453	0.857774
H	-6.882051	-1.759031	-0.613577
H	-6.440147	-3.484462	-0.549729

Table S11. Z-matrix of optimized conformer 1a6 at B3LYP/6-311+G(d,p) level

Atom	X	Y	Z
C	-0.824388	-1.817683	-0.692062
C	-0.830703	-0.301583	-0.92376
C	0.629144	0.365641	-1.089178
C	1.712894	-0.454395	-0.298619
C	1.639775	-1.906459	-0.844508
C	0.302042	-2.537107	-0.632331
C	1.456653	-0.357022	1.232598
C	2.281188	-1.31384	2.104237
C	3.766094	-1.413269	1.71469
C	3.860958	-1.479607	0.16001
C	3.235363	-0.193718	-0.561125
C	2.922718	-2.616705	-0.359447
O	4.486319	-0.229472	2.126094
C	4.415665	-2.62571	2.403535
C	0.931499	0.441291	-2.611658
C	-2.179928	-2.470795	-0.58305
C	-1.71809	0.385288	0.109029

C	-2.810809	1.089051	-0.192462
C	-3.7708	1.769783	0.766693
C	-5.217209	1.29792	0.489968
C	-5.50363	-0.201572	0.688416
C	-3.405028	1.606271	2.244114
C	-6.966249	-0.513501	0.508359
C	-7.548865	-1.303868	-0.40468
C	-9.047543	-1.490394	-0.422096
C	-6.816001	-2.073026	-1.475415
C	3.788124	1.212682	-0.287189
C	5.264131	1.422148	-0.648142
C	5.70921	2.881366	-0.549821
O	5.095495	3.740994	-1.525027
H	1.766144	-1.819494	-1.927592
C	0.433785	1.829848	-0.691247
O	0.979656	2.457293	0.187592
C	5.295714	-1.675211	-0.291644
O	5.6163	-2.134153	-1.36974
O	-3.843708	3.182527	0.410031
C	-2.691193	3.981098	0.659954
H	-1.328083	-0.143044	-1.888252
H	0.242741	-3.615176	-0.499812
H	1.648675	0.67119	1.535681
H	0.406718	-0.552039	1.446552
H	1.842449	-2.314895	2.067294
H	2.218344	-0.999267	3.15174
H	3.416672	-0.386943	-1.625173
H	3.402401	-3.143251	-1.184379
H	2.721558	-3.3541	0.41626
H	4.542497	-0.234463	3.088987
H	3.977111	-3.572108	2.083477
H	5.490976	-2.660536	2.214303
H	4.270392	-2.548315	3.48601
H	0.835972	-0.53339	-3.090626
H	1.934223	0.825427	-2.809434
H	0.217688	1.106617	-3.1049
H	-2.801189	-2.231343	-1.45372
H	-2.080337	-3.556469	-0.523622
H	-2.730406	-2.128573	0.297809
H	-1.442544	0.252455	1.150877
H	-3.084395	1.214945	-1.240195
H	-5.460875	1.575108	-0.540918
H	-5.876492	1.88653	1.136846
H	-5.211968	-0.495538	1.704094

H	-4.885176	-0.788759	0.007996
H	-4.115377	2.163952	2.859273
H	-3.444636	0.557647	2.54322
H	-2.400636	1.973441	2.460953
H	-7.621635	-0.014559	1.222672
H	-9.311604	-2.547997	-0.303012
H	-9.53757	-0.924175	0.372719
H	-9.469981	-1.171361	-1.382327
H	-7.198481	-1.804438	-2.466927
H	-5.740093	-1.9019	-1.471118
H	-6.988204	-3.149532	-1.358718
H	3.626624	1.504896	0.748448
H	3.191399	1.892199	-0.902634
H	5.467831	1.063411	-1.664191
H	5.902511	0.850553	0.03242
H	6.781988	2.955347	-0.738939
H	5.520522	3.269482	0.459052
H	4.166043	3.850648	-1.29821
H	-0.302891	2.339357	-1.343812
H	6.07588	-1.354258	0.419508
H	-1.782589	3.533691	0.246106
H	-2.869827	4.937123	0.165913
H	-2.541987	4.16288	1.729684

Table S12. Z-matrix of optimized conformer **1a7** at B3LYP/6-311+G(d,p) level

Atom	X	Y	Z
C	0.556105	-3.026375	-1.064289
C	-0.291368	-1.763711	-1.273829
C	0.540426	-0.383005	-1.293643
C	1.830191	-0.525436	-0.386403
C	2.643779	-1.706531	-0.966203
C	1.885835	-2.99497	-0.908093
C	1.436079	-0.71894	1.108491
C	2.583509	-1.125011	2.043547
C	3.879778	-0.321349	1.836713
C	4.120423	-0.173125	0.30367
C	2.925149	0.584077	-0.446446
C	4.060857	-1.589245	-0.358765
O	3.745901	1.015063	2.37015
C	5.052645	-1.003916	2.560052

C	0.869212	-0.058331	-2.763312
C	-0.198257	-4.332912	-1.102499
C	-1.50449	-1.775931	-0.3548
C	-2.764328	-1.768859	-0.788929
C	-4.012704	-1.858355	0.065079
C	-4.988895	-0.707541	-0.290377
C	-4.480065	0.708298	0.031559
C	-4.692968	-3.213481	-0.22186
C	-5.4309	1.770536	-0.451795
C	-6.081764	2.702007	0.260507
C	-7.002958	3.689544	-0.415915
C	-5.975188	2.877639	1.755031
C	2.498916	2.004349	-0.047419
C	3.572219	3.086776	-0.216634
C	3.031673	4.5047	-0.038526
O	2.060067	4.876502	-1.029186
H	2.78012	-1.4769	-2.026834
C	-0.399035	0.697289	-0.762745
O	-0.886743	1.582082	-1.435824
C	5.428748	0.540409	0.022629
O	6.051329	0.443793	-1.015891
O	-3.57736	-1.780657	1.436669
C	-4.568441	-1.906377	2.449079
H	-0.698213	-1.839574	-2.289265
H	2.435881	-3.927629	-0.803758
H	1.011261	0.216	1.478707
H	0.654264	-1.470747	1.202537
H	2.802033	-2.188335	1.916202
H	2.263894	-1.007315	3.08449
H	3.270477	0.647166	-1.484939
H	4.816385	-1.659892	-1.141066
H	4.273789	-2.37753	0.361788
H	3.728548	0.951675	3.332459
H	5.263156	-1.9993	2.16681
H	5.963256	-0.404379	2.491033
H	4.807786	-1.117109	3.621126
H	1.364891	-0.893734	-3.258131
H	1.502702	0.825865	-2.857749
H	-0.054057	0.145371	-3.307901
H	-0.777682	-4.424599	-2.028591
H	0.490894	-5.177987	-1.045901
H	-0.913594	-4.416058	-0.279155
H	-1.332651	-1.828915	0.714837
H	-2.963337	-1.732226	-1.85895

H	-5.942131	-0.87711	0.221094
H	-5.20832	-0.783147	-1.361147
H	-3.509827	0.851877	-0.458628
H	-4.296797	0.795436	1.103709
H	-5.653815	-3.296031	0.291327
H	-4.880016	-3.321073	-1.29278
H	-4.048061	-4.035108	0.098385
H	-5.604469	1.761403	-1.528391
H	-6.673746	4.719657	-0.234303
H	-7.047996	3.530586	-1.495422
H	-8.020536	3.613653	-0.014456
H	-6.965937	2.809688	2.219294
H	-5.327957	2.142366	2.232078
H	-5.58902	3.875264	1.995733
H	2.131795	2.034465	0.977955
H	1.663045	2.274456	-0.699747
H	4.040993	3.010573	-1.20657
H	4.367993	2.94902	0.521933
H	3.860356	5.222573	-0.042355
H	2.515007	4.597745	0.920148
H	2.493917	4.879067	-1.890078
H	-0.649559	0.639988	0.308006
H	5.800803	1.201559	0.824133
H	-5.058845	-2.885084	2.429913
H	-4.044849	-1.798739	3.399772
H	-5.332474	-1.124528	2.382062

Table S13. Z-matrix of optimized conformer **1a8** at B3LYP/6-311+G(d,p) level

Atom	X	Y	Z
C	-0.485031	-1.771551	-1.407272
C	-0.552059	-0.239063	-1.380111
C	0.868418	0.50581	-1.220228
C	1.893818	-0.404053	-0.451294
C	1.979099	-1.733912	-1.249621
C	0.667383	-2.446281	-1.325769
C	1.445162	-0.601271	1.025419
C	2.217576	-1.666634	1.815448
C	3.742723	-1.631012	1.613108
C	4.030117	-1.407613	0.09723
C	3.41636	-0.039301	-0.461224

C	3.236221	-2.468151	-0.73317
O	4.329671	-0.514538	2.319327
C	4.379224	-2.921768	2.155956
C	1.357796	0.88136	-2.646077
C	-1.803653	-2.483248	-1.587085
C	-1.607555	0.223483	-0.383472
C	-2.730419	0.853339	-0.730502
C	-3.879995	1.267659	0.171349
C	-5.114535	0.429982	-0.240033
C	-6.424213	0.747535	0.508605
C	-3.572748	1.120173	1.666391
C	-7.600985	0.042652	-0.111877
C	-8.406049	-0.883431	0.429188
C	-9.545365	-1.476786	-0.365436
C	-8.284247	-1.420178	1.833763
C	3.841765	1.31419	0.126311
C	5.334891	1.642172	-0.003203
C	5.629012	3.081505	0.393098
O	7.043419	3.309632	0.273061
H	2.230381	-1.446531	-2.275033
C	0.528453	1.860096	-0.591435
O	0.917692	2.331439	0.452737
C	5.518735	-1.460148	-0.189526
O	5.996286	-1.69948	-1.280583
O	-4.249151	2.633804	-0.154225
C	-3.300129	3.646329	0.161637
H	-0.926951	0.06442	-2.364981
H	0.658996	-3.532362	-1.386046
H	1.53104	0.360636	1.528345
H	0.391458	-0.87579	1.059269
H	1.853055	-2.661491	1.544831
H	2.007458	-1.552247	2.8845
H	3.737028	-0.027645	-1.509858
H	3.845596	-2.814064	-1.567977
H	2.990715	-3.343002	-0.132674
H	4.29945	-0.710063	3.263315
H	4.049653	-3.80907	1.613475
H	5.469841	-2.875505	2.114077
H	4.090837	-3.054163	3.203953
H	1.39713	0.010138	-3.300141
H	2.346007	1.345316	-2.629351
H	0.66566	1.590976	-3.107289
H	-2.330856	-2.114421	-2.474465
H	-1.647612	-3.557538	-1.704205

H	-2.47467	-2.324051	-0.738113
H	-1.432778	-0.02021	0.660085
H	-2.903495	1.084614	-1.781604
H	-4.865836	-0.627341	-0.105679
H	-5.271889	0.582375	-1.313459
H	-6.592498	1.82901	0.463587
H	-6.324278	0.488308	1.563854
H	-4.374818	1.56213	2.259715
H	-3.492268	0.06512	1.937393
H	-2.63653	1.608705	1.942155
H	-7.804743	0.333657	-1.14274
H	-9.44086	-2.56531	-0.446177
H	-10.505929	-1.293099	0.130618
H	-9.597078	-1.061931	-1.374302
H	-8.171762	-2.510459	1.816542
H	-7.442028	-1.003201	2.385179
H	-9.197803	-1.212841	2.403534
H	3.539651	1.402053	1.167609
H	3.287513	2.07948	-0.425052
H	5.672707	1.487289	-1.034652
H	5.92914	0.986347	0.63856
H	5.306947	3.26235	1.426227
H	5.081554	3.774393	-0.258034
H	7.227433	4.219285	0.530522
H	-0.152707	2.453637	-1.233318
H	6.184999	-1.245176	0.66333
H	-2.316157	3.433173	-0.270191
H	-3.681867	4.571645	-0.271611
H	-3.190804	3.784293	1.242748

Table S14. Z-matrix of optimized conformer **1a9** at B3LYP/6-311+G(d,p) level

Atom	X	Y	Z
C	-0.29121	-2.155801	-1.042217
C	-0.53146	-0.641043	-1.100253
C	0.804217	0.262735	-1.128259
C	1.976048	-0.498446	-0.384973
C	2.158811	-1.846131	-1.122966
C	0.932576	-2.699286	-1.041195
C	1.655163	-0.663564	1.130618
C	2.588015	-1.611056	1.896781

C	4.081934	-1.401584	1.593436
C	4.244921	-1.208209	0.055196
C	3.431347	0.050525	-0.505839
C	3.538278	-2.391887	-0.683654
O	4.565439	-0.191369	2.218432
C	4.908034	-2.579218	2.136331
C	1.123174	0.57535	-2.602885
C	-1.532571	-3.014146	-1.049652
C	-1.571222	-0.218477	-0.071502
C	-2.729312	0.361854	-0.387885
C	-3.857887	0.754675	0.549748
C	-5.080803	-0.125608	0.197434
C	-6.374868	0.175501	0.978933
C	-3.488163	0.642647	2.033966
C	-7.505743	-0.719129	0.545904
C	-8.680094	-0.37581	-0.003217
C	-9.699201	-1.428025	-0.371352
C	-9.112487	1.038077	-0.303014
C	3.681609	1.470428	0.021537
C	5.090673	2.028332	-0.222753
C	5.178296	3.513005	0.123325
O	6.500387	4.047251	-0.041654
H	2.287665	-1.588861	-2.177967
C	0.457712	1.57532	-0.427626
O	0.337523	2.646664	-0.985503
C	5.706869	-1.078069	-0.327045
O	6.148731	-1.321131	-1.431929
O	-4.28098	2.103724	0.217753
C	-3.349633	3.149987	0.476132
H	-1.000278	-0.44879	-2.072404
H	1.039199	-3.78173	-1.043394
H	1.701346	0.317351	1.607445
H	0.636871	-1.024625	1.268028
H	2.322371	-2.647575	1.673117
H	2.430642	-1.486077	2.9734
H	3.686532	0.068919	-1.571627
H	4.125787	-2.684897	-1.553557
H	3.456885	-3.269053	-0.043477
H	4.602647	-0.340832	3.170609
H	4.647876	-3.526037	1.660929
H	5.978401	-2.406837	2.002403
H	4.720101	-2.69004	3.20924
H	1.179685	-0.331847	-3.204283
H	2.060184	1.124453	-2.714323

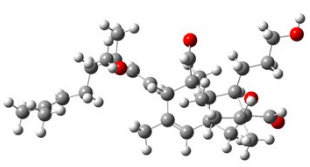
H	0.331427	1.198074	-3.022107
H	-2.176645	-2.766327	-1.901248
H	-1.269819	-4.071824	-1.11628
H	-2.136465	-2.866486	-0.149385
H	-1.354872	-0.441545	0.969034
H	-2.947951	0.56942	-1.435269
H	-4.796067	-1.171997	0.349026
H	-5.278722	-0.005298	-0.872873
H	-6.62957	1.228822	0.861667
H	-6.194013	0.012081	2.047961
H	-4.275665	1.076522	2.652027
H	-3.369677	-0.404521	2.32139
H	-2.554459	1.159614	2.262485
H	-7.325119	-1.782924	0.703534
H	-9.940977	-1.382232	-1.439876
H	-9.344426	-2.435351	-0.143231
H	-10.640571	-1.265873	0.167235
H	-10.028396	1.283317	0.247626
H	-8.358628	1.783494	-0.051551
H	-9.353849	1.145195	-1.366972
H	3.45163	1.542924	1.083399
H	2.977163	2.122967	-0.506218
H	5.371455	1.892842	-1.275103
H	5.825089	1.492519	0.384039
H	4.929645	3.673788	1.175041
H	4.463779	4.087707	-0.479399
H	6.74202	3.971469	-0.971746
H	0.297099	1.518941	0.660412
H	6.382907	-0.713736	0.465342
H	-2.379229	2.961193	0.005104
H	-3.779908	4.055862	0.047021
H	-3.20003	3.309046	1.549644

Table S15. Z-matrix of optimized conformer **1a10** at B3LYP/6-311+G(d,p) level

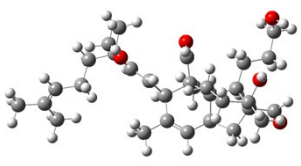
Atom	X	Y	Z
C	0.329187	-2.75641	-1.318797
C	-0.441733	-1.435307	-1.199299
C	0.474316	-0.109292	-1.088781
C	1.871104	-0.480196	-0.445216
C	2.495137	-1.572887	-1.347304

C	1.665397	-2.817118	-1.373977
C	1.694876	-0.92608	1.037034
C	2.93486	-1.562935	1.67789
C	4.241302	-0.794347	1.410546
C	4.25994	-0.369042	-0.089263
C	3.026501	0.567544	-0.489834
C	3.996196	-1.62781	-0.978716
O	4.287601	0.42258	2.188701
C	5.455499	-1.653649	1.800206
C	0.599742	0.49332	-2.500608
C	-0.519102	-3.998991	-1.435825
C	-1.533195	-1.541473	-0.144772
C	-2.825276	-1.335924	-0.398322
C	-3.963839	-1.436022	0.595761
C	-4.648293	-0.052457	0.770418
C	-5.315679	0.555886	-0.480258
C	-4.957099	-2.508164	0.110412
C	-5.857717	1.932866	-0.200184
C	-7.128419	2.358371	-0.246985
C	-7.474862	3.793015	0.073881
C	-8.314876	1.501863	-0.613795
C	2.775417	1.90952	0.214956
C	3.881677	2.960091	0.046528
C	3.448181	4.326848	0.572093
O	4.485262	5.314949	0.479616
H	2.473772	-1.164431	-2.361432
C	-0.295383	0.87926	-0.214376
O	-0.800266	1.908723	-0.613472
C	5.56138	0.325139	-0.44351
O	6.013014	0.398119	-1.568664
O	-3.362486	-1.813512	1.854233
C	-4.221272	-2.19957	2.920875
H	-0.970069	-1.309832	-2.151923
H	2.155857	-3.779466	-1.502401
H	1.41836	-0.05315	1.631329
H	0.871925	-1.633966	1.129242
H	3.047823	-2.589939	1.321556
H	2.789023	-1.63476	2.761015
H	3.212947	0.804981	-1.543547
H	4.609738	-1.575297	-1.877915
H	4.267445	-2.547179	-0.461697
H	4.437016	0.18186	3.110669
H	5.531202	-2.563082	1.202814
H	6.387128	-1.092486	1.697043

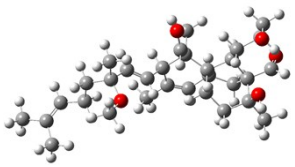
H	5.363674	-1.957837	2.848013
H	0.974223	-0.236241	-3.21883
H	1.255999	1.365441	-2.518959
H	-0.382192	0.820434	-2.846323
H	-1.243809	-3.904422	-2.252821
H	0.103628	-4.874544	-1.630826
H	-1.098647	-4.18513	-0.526674
H	-1.242002	-1.819111	0.862682
H	-3.129444	-1.073657	-1.40897
H	-3.888679	0.63949	1.148888
H	-5.412536	-0.141499	1.548691
H	-6.102277	-0.107617	-0.843809
H	-4.576038	0.633795	-1.285765
H	-5.860934	-2.529309	0.724101
H	-5.259557	-2.308639	-0.919234
H	-4.488697	-3.494969	0.138038
H	-5.100139	2.663171	0.084448
H	-8.179617	3.847187	0.912044
H	-6.589544	4.377739	0.332339
H	-7.968118	4.275603	-0.77825
H	-8.052935	0.465809	-0.826264
H	-9.052398	1.505642	0.197145
H	-8.822567	1.910302	-1.495506
H	2.581142	1.767718	1.277264
H	1.862175	2.323002	-0.227242
H	4.148955	3.057295	-1.013483
H	4.783109	2.657437	0.585658
H	3.200634	4.265355	1.634566
H	2.552491	4.67258	0.040809
H	4.700527	5.439601	-0.451654
H	-0.395689	0.611293	0.848684
H	6.096478	0.805193	0.393638
H	-3.573162	-2.366774	3.782058
H	-4.947288	-1.422098	3.179908
H	-4.757735	-3.128658	2.702907



1b1 (21.88%)



1b2 (17.52%)



1b3 (18.98%)

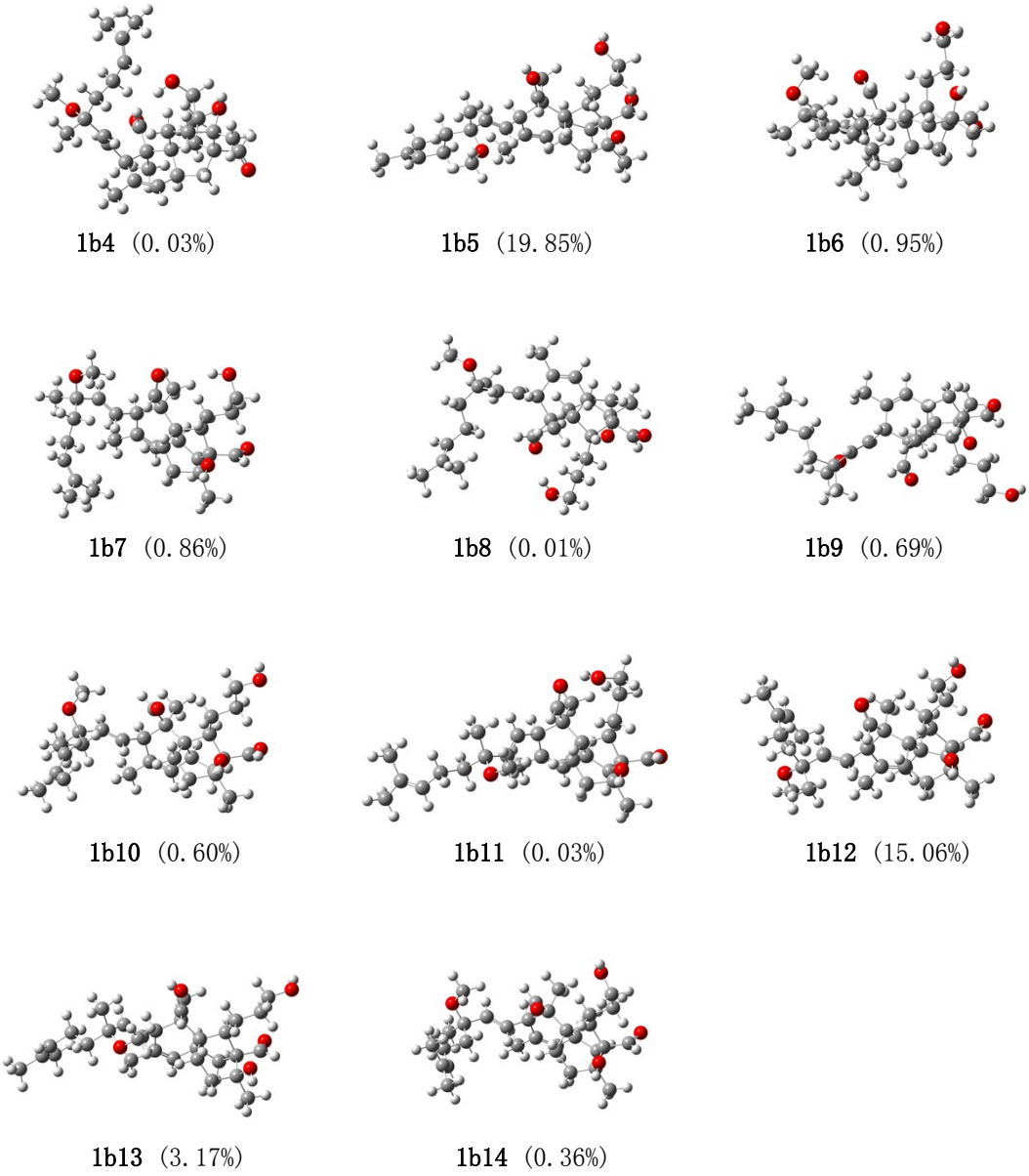


Figure S5. Reoptimized geometries of **1b** at B3LYP/6-311+G(d,p) level with the CPCM model in MeOH

Table S16. Z-matrix of optimized conformer 1b1 at B3LYP/6-311+G(d,p) level

Atom	X	Y	Z
C	-0.646471	-1.73178	-1.213039

C	-0.662409	-0.198823	-1.278489
C	0.791666	0.501461	-1.237917
C	1.802403	-0.417444	-0.437867
C	1.822753	-1.782728	-1.166957
C	0.483272	-2.447657	-1.151157
C	1.389523	-0.519885	1.060408
C	2.133151	-1.588585	1.87236
C	3.6548	-1.605823	1.641857
C	3.918518	-1.450081	0.113492
C	3.327353	-0.090087	-0.488175
C	3.081625	-2.5228	-0.658426
O	4.283215	-0.477629	2.290983
C	4.267237	-2.890241	2.224326
C	1.22833	0.756707	-2.692807
C	-1.996289	-2.401908	-1.287306
C	-1.674415	0.377796	-0.299012
C	-2.700961	1.145299	-0.662908
C	-3.732735	1.770802	0.25296
C	-5.160078	1.363113	-0.196408
C	-5.475172	-0.138906	-0.089089
C	-3.588088	3.304327	0.168567
C	-6.844279	-0.466791	-0.621276
C	-7.89053	-1.00001	0.026659
C	-9.195523	-1.255811	-0.689393
C	-7.894383	-1.397452	1.481978
C	3.765021	1.279936	0.051906
C	5.252949	1.609009	-0.125443
C	5.558022	3.054925	0.23718
O	6.967671	3.278789	0.069272
H	2.042764	-1.553328	-2.213558
C	0.603539	1.852571	-0.550631
O	0.682512	2.929349	-1.105979
C	5.399863	-1.54451	-0.198279
O	5.851206	-1.844056	-1.285336
O	-3.44181	1.296484	1.58229
C	-4.238502	1.79607	2.649331
H	-1.047162	0.054814	-2.273454
H	0.431507	-3.534142	-1.151129
H	1.561844	0.447855	1.535508
H	0.322827	-0.720079	1.151023
H	1.728532	-2.576442	1.636817
H	1.944705	-1.432891	2.939956
H	3.632854	-0.118571	-1.540427
H	3.662172	-2.905518	-1.497554

H	2.83957	-3.373462	-0.022909
H	4.276864	-0.638137	3.242061
H	5.357214	-2.877701	2.152866
H	4.003106	-2.969	3.283871
H	3.898469	-3.789818	1.729643
H	1.177886	-0.151848	-3.292699
H	0.561913	1.48976	-3.149942
H	2.241987	1.157272	-2.754179
H	-2.616669	-2.168167	-0.417086
H	-1.885957	-3.486586	-1.348465
H	-2.554911	-2.063658	-2.167664
H	-1.561453	0.135956	0.752374
H	-2.838097	1.39303	-1.71446
H	-5.893223	1.931326	0.385428
H	-5.285196	1.690838	-1.234244
H	-4.726139	-0.693122	-0.667201
H	-5.36072	-0.46163	0.946765
H	-2.61487	3.615654	0.555062
H	-3.665701	3.631526	-0.870844
H	-4.37255	3.812268	0.734282
H	-6.986604	-0.224869	-1.675006
H	-9.149867	-0.954991	-1.738211
H	-10.01796	-0.710877	-0.210882
H	-9.462156	-2.318683	-0.648602
H	-6.953473	-1.189325	1.990452
H	-8.693016	-0.871975	2.018494
H	-8.105642	-2.468392	1.585403
H	3.195398	2.029855	-0.508321
H	3.497973	1.39285	1.101673
H	5.86447	0.963166	0.510203
H	5.560246	1.435575	-1.163253
H	4.990503	3.736509	-0.408628
H	5.268169	3.253512	1.276546
H	7.160478	4.192653	0.304403
H	0.368351	1.821255	0.52439
H	6.085747	-1.298414	0.630408
H	-4.130404	2.878157	2.77613
H	-5.300149	1.557396	2.524014
H	-3.877124	1.302739	3.552447

Table S17. Z-matrix of optimized conformer **1b2** at B3LYP/6-311+G(d,p)

level

Atom	X	Y	Z
C	-0.683171	-2.049486	-0.298548
C	-0.788257	-0.61072	-0.817326
C	0.619306	0.082316	-1.199396
C	1.774899	-0.534493	-0.311399
C	1.770873	-2.058433	-0.581875
C	0.48138	-2.698955	-0.17686
C	1.574637	-0.167238	1.189422
C	2.476655	-0.922015	2.17522
C	3.952171	-0.995576	1.743394
C	3.997599	-1.323189	0.220288
C	3.259503	-0.222664	-0.678427
C	3.122554	-2.590745	-0.052695
O	4.598872	0.285459	1.912947
C	4.708461	-2.027147	2.597008
C	0.844294	-0.119663	-2.70978
C	-1.995341	-2.724502	0.017626
C	-1.689231	0.224519	0.082007
C	-2.745302	0.906489	-0.359337
C	-3.665518	1.782719	0.465502
C	-5.144092	1.421888	0.173292
C	-5.557106	-0.010169	0.557519
C	-3.410894	3.253557	0.074017
C	-7.032881	-0.239603	0.368862
C	-7.649049	-1.06712	-0.487837
C	-9.156335	-1.151343	-0.53429
C	-6.946693	-1.975299	-1.466588
C	3.682012	1.25392	-0.656455
C	5.113174	1.539723	-1.127975
C	5.406366	3.027428	-1.312738
O	5.297048	3.789373	-0.099841
H	1.840449	-2.164158	-1.668306
C	0.451719	1.57741	-0.935395
O	0.392657	2.430478	-1.797149
C	5.426275	-1.492824	-0.259109
O	5.747001	-2.127708	-1.243715
O	-3.325109	1.548806	1.845863
C	-4.006024	2.31545	2.831684
H	-1.316708	-0.672881	-1.776206
H	0.486689	-3.732913	0.161014
H	1.762716	0.9013	1.309461
H	0.541492	-0.333484	1.491733
H	2.097391	-1.937033	2.318491

H	2.425021	-0.440884	3.157792
H	3.422978	-0.575712	-1.703055
H	3.605738	-3.215444	-0.803725
H	3.010413	-3.198798	0.843721
H	4.711641	0.441468	2.858038
H	5.774204	-2.035404	2.356708
H	4.607333	-1.766729	3.65568
H	4.318341	-3.038303	2.472347
H	0.765094	-1.169617	-2.991659
H	0.084455	0.428845	-3.268616
H	1.817307	0.254121	-3.034271
H	-2.516709	-2.238244	0.847601
H	-1.837519	-3.772859	0.279157
H	-2.674033	-2.684271	-0.842259
H	-1.462777	0.252958	1.142843
H	-2.989661	0.886465	-1.420337
H	-5.791461	2.139862	0.687757
H	-5.318959	1.57665	-0.896637
H	-4.965648	-0.727278	-0.014637
H	-5.302533	-0.173495	1.611325
H	-4.122513	3.927252	0.557239
H	-2.396987	3.548872	0.353668
H	-3.518707	3.378521	-1.005835
H	-7.668927	0.365676	1.015425
H	-9.623692	-0.479823	0.189103
H	-9.498102	-2.172188	-0.325631
H	-9.531716	-0.896327	-1.532497
H	-5.860834	-1.891713	-1.432087
H	-7.212515	-3.021922	-1.276779
H	-7.270939	-1.75498	-2.490413
H	3.008586	1.777164	-1.344965
H	3.536864	1.692779	0.327928
H	5.838673	1.129715	-0.417697
H	5.300364	1.047647	-2.090946
H	6.405584	3.158088	-1.745417
H	4.68469	3.476901	-1.99964
H	5.949697	3.454696	0.525779
H	0.368701	1.875696	0.120922
H	6.199238	-0.973467	0.333171
H	-3.803994	3.387228	2.736372
H	-5.089284	2.154589	2.809407
H	-3.625082	1.974771	3.795222

Table S18. Z-matrix of optimized conformer 1b3 at B3LYP/6-311+G(d,p) level

Atom	X	Y	Z
C	-0.592057	-1.879694	-0.999931
C	-0.636661	-0.364612	-1.236534
C	0.803213	0.36459	-1.307671
C	1.856344	-0.453112	-0.454813
C	1.87612	-1.887064	-1.037606
C	0.551865	-2.567329	-0.898053
C	1.495319	-0.403346	1.059716
C	2.281909	-1.3724	1.951408
C	3.794942	-1.392031	1.672308
C	4.00733	-1.39092	0.127776
C	3.372596	-0.108598	-0.590529
C	3.166928	-2.549875	-0.502537
O	4.424161	-0.193386	2.177678
C	4.449332	-2.599416	2.364215
C	1.195242	0.489906	-2.791724
C	-1.931651	-2.572053	-0.952005
C	-1.639034	0.299438	-0.303172
C	-2.679355	1.016612	-0.725837
C	-3.701939	1.724788	0.138402
C	-5.134456	1.301521	-0.27598
C	-5.464283	-0.186465	-0.06699
C	-3.538264	3.245217	-0.067426
C	-6.839397	-0.534755	-0.570163
C	-7.882105	-1.029461	0.113082
C	-9.193962	-1.316988	-0.577979
C	-7.875041	-1.351435	1.58698
C	3.795685	1.31875	-0.209284
C	5.272251	1.656865	-0.450516
C	5.590375	3.142313	-0.289963
O	5.347047	3.642676	1.034378
H	2.051117	-1.766725	-2.110373
C	0.6038	1.771338	-0.746031
O	0.651429	2.791938	-1.401799
C	5.479639	-1.491532	-0.221293
O	5.903744	-1.892974	-1.286386
O	-3.41385	1.354164	1.500715
C	-4.204866	1.943146	2.525425
H	-1.048438	-0.231437	-2.244193
H	0.521188	-3.647597	-0.774479
H	1.673469	0.610448	1.422574

H	0.43464	-0.603271	1.207125
H	1.886552	-2.384599	1.835788
H	2.126282	-1.108013	3.002969
H	3.646189	-0.240927	-1.643898
H	3.726204	-3.007059	-1.318572
H	2.96236	-3.335526	0.223237
H	4.426531	-0.239952	3.141017
H	5.535369	-2.582117	2.247914
H	4.228486	-2.566548	3.436062
H	4.07594	-3.551721	1.984961
H	1.171999	-0.475043	-3.298275
H	0.488696	1.146296	-3.30228
H	2.189229	0.923332	-2.917968
H	-2.528371	-2.248561	-0.094118
H	-1.804869	-3.655043	-0.893225
H	-2.523267	-2.343675	-1.84611
H	-1.506015	0.164527	0.765115
H	-2.833679	1.155689	-1.794806
H	-5.858818	1.915858	0.26868
H	-5.260487	1.559467	-1.333322
H	-4.723895	-0.78593	-0.610436
H	-5.348624	-0.442374	0.987375
H	-4.317545	3.806784	0.4532
H	-2.561783	3.573708	0.295992
H	-3.609173	3.490241	-1.129733
H	-6.989188	-0.348501	-1.634098
H	-9.156692	-1.069516	-1.640974
H	-10.010731	-0.74618	-0.120396
H	-9.46295	-2.375631	-0.481452
H	-6.92914	-1.120999	2.076188
H	-8.667412	-0.796178	2.102336
H	-8.088829	-2.41492	1.746615
H	3.206367	1.994751	-0.839485
H	3.541762	1.54287	0.82441
H	5.911434	1.089476	0.234172
H	5.565224	1.368835	-1.468187
H	6.632783	3.33128	-0.573425
H	4.953284	3.742355	-0.94477
H	5.922449	3.168913	1.645737
H	0.389855	1.837052	0.331775
H	6.185545	-1.148747	0.554649
H	-4.091796	3.031508	2.562367
H	-5.26786	1.699592	2.423051
H	-3.842545	1.524066	3.464925

Table S19. Z-matrix of optimized conformer 1b4 at B3LYP/6-311+G(d,p) level

Atom	X	Y	Z
C	-0.426488	-3.183739	-0.752573
C	0.026614	-2.569244	0.574273
C	-1.011494	-1.509658	1.20391
C	-1.718726	-0.708796	0.024713
C	-2.465275	-1.769165	-0.816236
C	-1.542344	-2.799426	-1.388449
C	-0.671579	0.105525	-0.789896
C	-1.171729	0.654376	-2.131089
C	-2.536761	1.353602	-2.029361
C	-3.470167	0.460985	-1.148508
C	-2.917921	0.248544	0.337175
C	-3.460553	-0.990752	-1.711897
O	-2.393955	2.62386	-1.357454
C	-3.128375	1.616041	-3.422576
C	-1.997563	-2.310546	2.07738
C	0.360236	-4.381249	-1.236109
C	1.491365	-2.1465	0.63526
C	2.320782	-1.89262	-0.374405
C	3.802003	-1.588843	-0.260922
C	4.13617	-0.255434	-0.978273
C	3.516742	1.004204	-0.348128
C	4.577031	-2.739221	-0.937204
C	3.814298	2.239577	-1.154983
C	4.500222	3.333032	-0.790881
C	4.699266	4.477911	-1.755689
C	5.125219	3.549427	0.565095
C	-2.694278	1.48384	1.241611
C	-3.195863	1.284925	2.681728
C	-2.7505	2.383977	3.644647
O	-1.324482	2.465988	3.792739
H	-3.102895	-2.306389	-0.107231
C	-0.244442	-0.533691	2.08003
O	-0.426388	-0.382212	3.273628
C	-4.852204	1.071259	-1.045234
O	-5.892206	0.444289	-1.041342
O	4.103081	-1.52086	1.145939
C	5.461111	-1.327675	1.521244

H	-0.015422	-3.39977	1.292658
H	-1.850766	-3.328365	-2.287596
H	-0.343256	0.952624	-0.183411
H	0.214041	-0.493625	-0.979982
H	-1.229911	-0.151582	-2.866467
H	-0.442355	1.370097	-2.525556
H	-3.697323	-0.355271	0.814876
H	-4.459232	-1.421205	-1.636607
H	-3.184743	-1.014808	-2.765035
H	-1.942817	3.227928	-1.958994
H	-4.059158	2.184944	-3.352063
H	-2.420283	2.204536	-4.014848
H	-3.327004	0.694931	-3.972301
H	-2.360926	-3.19286	1.55008
H	-1.487681	-2.653608	2.979451
H	-2.859204	-1.722865	2.394757
H	1.401332	-4.146205	-1.463391
H	-0.098639	-4.806603	-2.131093
H	0.377589	-5.159912	-0.464006
H	1.902677	-2.101612	1.640226
H	1.964235	-1.93033	-1.401071
H	5.224126	-0.139436	-1.023745
H	3.802641	-0.347817	-2.017759
H	2.429982	0.86906	-0.292766
H	3.864908	1.106729	0.680687
H	5.649622	-2.535104	-0.9719
H	4.411938	-3.675195	-0.398289
H	4.233299	-2.869837	-1.965949
H	3.419882	2.218796	-2.171377
H	5.766192	4.665703	-1.925254
H	4.280836	5.407492	-1.351706
H	4.22849	4.282261	-2.721463
H	6.201349	3.732492	0.464097
H	4.703426	4.442034	1.042025
H	4.988592	2.708591	1.244462
H	-1.637584	1.758779	1.255569
H	-3.198779	2.355144	0.825569
H	-4.292097	1.25326	2.687742
H	-2.862344	0.325594	3.086814
H	-3.06567	3.367509	3.284909
H	-3.217791	2.222824	4.624512
H	-0.973446	1.570145	3.898336
H	0.517713	0.077469	1.572798
H	-4.873563	2.169631	-0.929154

H	5.874053	-0.393373	1.125742
H	5.468797	-1.27593	2.610646
H	6.099972	-2.159389	1.207047

Table S20. Z-matrix of optimized conformer 1b5 at B3LYP/6-311+G(d,p) level

Atom	X	Y	Z
C	-0.673311	-1.905053	-0.637073
C	-0.74134	-0.395164	-0.899565
C	0.686211	0.336648	-1.086178
C	1.799461	-0.462007	-0.294528
C	1.785817	-1.905697	-0.854181
C	0.477943	-2.58762	-0.606254
C	1.540423	-0.393417	1.239591
C	2.392858	-1.345099	2.088297
C	3.883446	-1.359517	1.707394
C	3.990859	-1.381247	0.151836
C	3.30037	-0.113309	-0.540732
C	3.116351	-2.552954	-0.402741
O	4.537074	-0.149861	2.152854
C	4.592155	-2.552799	2.369744
C	0.971293	0.434242	-2.596925
C	-2.003182	-2.599257	-0.475487
C	-1.677062	0.287071	0.088066
C	-2.732631	1.013611	-0.276199
C	-3.686474	1.749623	0.642033
C	-5.150921	1.374766	0.299186
C	-5.518376	-0.104021	0.514663
C	-3.485144	3.265103	0.431096
C	-6.984539	-0.358608	0.28718
C	-7.566822	-1.133109	-0.639924
C	-9.070307	-1.258845	-0.710386
C	-6.827753	-1.941889	-1.676963
C	3.743344	1.320459	-0.216787
C	5.194507	1.660908	-0.58015
C	5.505578	3.153185	-0.477543
O	4.754529	3.958837	-1.399639
H	1.881387	-1.801568	-1.938367
C	0.522607	1.75464	-0.540535
O	0.50909	2.760343	-1.220444
C	5.437076	-1.478182	-0.293452

O	5.794273	-1.909766	-1.371275
O	-3.340357	1.364688	1.986327
C	-4.055613	1.976294	3.052791
H	-1.222797	-0.282513	-1.87829
H	0.461028	-3.665091	-0.458114
H	1.729974	0.62648	1.579223
H	0.494003	-0.603157	1.458209
H	1.997439	-2.36113	2.012162
H	2.306533	-1.068186	3.144496
H	3.49961	-0.2617	-1.608517
H	3.620126	-3.016456	-1.250837
H	2.970194	-3.331784	0.344512
H	4.604032	-0.183066	3.114501
H	5.668093	-2.527707	2.182354
H	4.441215	-2.508655	3.453319
H	4.203414	-3.512488	2.026221
H	0.91651	-0.53992	-3.0831
H	0.22716	1.078124	-3.068532
H	1.951701	0.868477	-2.802047
H	-2.538049	-2.254002	0.414093
H	-1.868051	-3.680016	-0.39718
H	-2.658273	-2.396408	-1.330585
H	-1.476558	0.164011	1.147196
H	-2.952473	1.143698	-1.334763
H	-5.823424	2.008868	0.886651
H	-5.326391	1.644703	-0.747531
H	-4.899572	-0.731992	-0.128647
H	-5.265772	-0.3788	1.545781
H	-2.48272	3.561557	0.74836
H	-3.598116	3.515414	-0.626298
H	-4.221096	3.849395	0.9885
H	-7.644838	0.173444	0.972787
H	-9.565036	-0.663427	0.059865
H	-9.381778	-2.303288	-0.589462
H	-9.444691	-0.934797	-1.688736
H	-7.052461	-3.00882	-1.561579
H	-7.158458	-1.663608	-2.684402
H	-5.746144	-1.818842	-1.631023
H	3.10158	1.9853	-0.802575
H	3.581667	1.557829	0.834026
H	5.886374	1.139247	0.088508
H	5.423345	1.323006	-1.599426
H	5.242332	3.529756	0.514182
H	6.578908	3.32147	-0.624866

H	5.007861	3.706602	-2.294947
H	0.398208	1.844593	0.549705
H	6.188616	-1.101923	0.421726
H	-3.907454	3.060609	3.083315
H	-5.129637	1.765439	3.008874
H	-3.655339	1.544842	3.971029

Table S21. Z-matrix of optimized conformer 1b6 at B3LYP/6-311+G(d,p) level

Atom	X	Y	Z
C	0.753132	0.143182	-2.662774
C	0.890871	-1.059331	-1.71903
C	-0.472507	-1.501751	-0.980016
C	-1.403059	-0.23613	-0.777588
C	-1.664889	0.343624	-2.18791
C	-0.404287	0.787331	-2.859259
C	-0.744846	0.781968	0.200514
C	-1.421362	2.157286	0.269656
C	-2.955628	2.096823	0.37248
C	-3.467298	1.012401	-0.623908
C	-2.880084	-0.445352	-0.31888
C	-2.869463	1.30263	-2.039858
O	-3.363312	1.676003	1.693273
C	-3.564245	3.48333	0.105533
C	-1.127538	-2.603114	-1.834836
C	1.999316	0.522608	-3.425183
C	2.101187	-0.893399	-0.808365
C	3.156437	-1.70874	-0.829148
C	4.435823	-1.61668	-0.01534
C	4.525173	-0.409545	0.9438
C	4.827515	0.964582	0.308724
C	5.633545	-1.671384	-0.97289
C	4.90325	2.046183	1.354429
C	4.216572	3.195412	1.427396
C	4.442465	4.1592	2.568274
C	3.186504	3.653698	0.425407
C	-3.096884	-1.131066	1.039069
C	-4.556365	-1.448796	1.388303
C	-4.706071	-2.348091	2.61424
O	-4.181006	-1.768084	3.818834
H	-2.051303	-0.489522	-2.782263

C	-0.061119	-2.112966	0.356809
O	-0.127915	-3.293917	0.628848
C	-4.982465	0.955225	-0.637324
O	-5.643347	0.532204	-1.564406
O	4.575687	-2.85441	0.745978
C	3.629137	-3.095808	1.783527
H	1.134099	-1.916096	-2.358239
H	-0.446796	1.604394	-3.576038
H	-0.748857	0.352207	1.203897
H	0.299319	0.944821	-0.061494
H	-1.148127	2.745974	-0.609718
H	-1.035886	2.709394	1.133304
H	-3.367037	-1.082483	-1.066483
H	-3.617865	1.093348	-2.80395
H	-2.5876	2.348856	-2.148124
H	-3.181157	2.39776	2.306765
H	-4.645813	3.477257	0.259248
H	-3.132354	4.209646	0.801535
H	-3.360269	3.840668	-0.904795
H	-1.24701	-2.28936	-2.87172
H	-0.495824	-3.492639	-1.831067
H	-2.1046	-2.897047	-1.446865
H	2.797058	0.871323	-2.763312
H	1.783214	1.313315	-4.146344
H	2.402074	-0.338563	-3.970935
H	2.103709	-0.036286	-0.142512
H	3.143575	-2.561454	-1.508122
H	3.60326	-0.331665	1.527153
H	5.32238	-0.641058	1.658812
H	5.794074	0.911429	-0.205154
H	4.086798	1.203439	-0.455679
H	6.56998	-1.616663	-0.411547
H	5.616037	-2.613	-1.526192
H	5.606269	-0.851171	-1.691811
H	5.621148	1.847377	2.150631
H	3.512483	4.332496	3.122693
H	4.768469	5.13739	2.195173
H	5.195498	3.792587	3.269062
H	2.226633	3.837481	0.921676
H	3.489727	4.606694	-0.024005
H	3.018771	2.941072	-0.381345
H	-2.564442	-2.087884	0.992189
H	-2.653057	-0.556835	1.848752
H	-5.118484	-0.525954	1.56689

H	-5.044786	-1.957757	0.54767
H	-5.761465	-2.610099	2.756057
H	-4.147904	-3.277699	2.476752
H	-4.675936	-0.962395	4.006692
H	0.338504	-1.412724	1.106868
H	-5.486301	1.306396	0.279573
H	2.598961	-3.037143	1.419704
H	3.819785	-4.109874	2.13758
H	3.753295	-2.404312	2.623714

Table S22. Z-matrix of optimized conformer 1b7 at B3LYP/6-311+G(d,p) level

Atom	X	Y	Z
C	-0.691698	0.251448	2.643697
C	-0.82359	-0.976414	1.731718
C	0.529447	-1.404611	0.965771
C	1.430339	-0.125052	0.72206
C	1.711804	0.485331	2.115652
C	0.457324	0.919962	2.804065
C	0.730344	0.862611	-0.258537
C	1.376801	2.249894	-0.366411
C	2.909217	2.2187	-0.502456
C	3.465335	1.162241	0.499682
C	2.900811	-0.311778	0.233183
C	2.893079	1.464728	1.923497
O	3.296098	1.783187	-1.825105
C	3.493985	3.622213	-0.272884
C	1.226626	-2.481095	1.818751
C	-1.930422	0.627203	3.419865
C	-2.060999	-0.863791	0.850101
C	-3.102102	-1.693079	0.934384
C	-4.405072	-1.655138	0.15497
C	-4.540823	-0.494529	-0.854651
C	-4.844956	0.904042	-0.275933
C	-5.574554	-1.685813	1.147859
C	-4.995223	1.927324	-1.371198
C	-4.320284	3.071954	-1.55054
C	-4.623481	3.970722	-2.726023
C	-3.230221	3.585433	-0.643035
C	3.102851	-1.013083	-1.119305
C	4.560974	-1.300651	-1.499401

C	4.705116	-2.15908	-2.756111
O	4.226058	-3.504502	-2.595696
H	2.126224	-0.329154	2.716972
C	0.098821	-2.04293	-0.352499
O	0.199576	-3.223416	-0.616241
C	4.981767	1.136496	0.481483
O	5.669744	0.734616	1.398035
O	-4.546003	-2.9281	-0.546057
C	-3.629149	-3.199793	-1.60249
H	-1.028347	-1.822472	2.398017
H	0.498874	1.753696	3.501405
H	0.721877	0.414838	-1.254014
H	-0.31128	1.008578	0.02346
H	1.110752	2.848514	0.508409
H	0.961704	2.778885	-1.230736
H	3.418555	-0.927238	0.977957
H	3.662266	1.284203	2.674112
H	2.592239	2.506773	2.01972
H	3.087063	2.490844	-2.44638
H	4.571222	3.637137	-0.453657
H	3.028986	4.327586	-0.969104
H	3.30727	3.99156	0.736448
H	1.37331	-2.147225	2.845864
H	0.608344	-3.379568	1.85006
H	2.195479	-2.768354	1.406127
H	-2.743269	0.953867	2.765069
H	-1.713125	1.433335	4.123378
H	-2.312803	-0.229304	3.987055
H	-2.095777	-0.033954	0.151837
H	-3.055233	-2.517665	1.645707
H	-3.63751	-0.430941	-1.468297
H	-5.355236	-0.770289	-1.533605
H	-5.784555	0.858336	0.286142
H	-4.074346	1.198693	0.437536
H	-6.527143	-1.669766	0.611808
H	-5.526365	-2.602284	1.740211
H	-5.540833	-0.835385	1.830509
H	-5.760746	1.683091	-2.108216
H	-3.732592	4.112006	-3.349409
H	-4.927492	4.968485	-2.387871
H	-5.419626	3.564791	-3.353532
H	-2.30493	3.742544	-1.209183
H	-3.508205	4.561222	-0.22753
H	-3.008298	2.917746	0.188657

H	2.584677	-1.974861	-1.038538
H	2.630967	-0.457295	-1.928779
H	5.089127	-0.362191	-1.694826
H	5.08072	-1.800002	-0.673121
H	4.198374	-1.681694	-3.604124
H	5.761271	-2.259285	-3.014102
H	3.2634	-3.491972	-2.579954
H	-0.347131	-1.364828	-1.096771
H	5.459871	1.491935	-0.447449
H	-2.588995	-3.098434	-1.278504
H	-3.805962	-4.234721	-1.898616
H	-3.798981	-2.554855	-2.47123

Table S23. Z-matrix of optimized conformer 1b8 at B3LYP/6-311+G(d,p) level

Atom	X	Y	Z
C	0.501244	-2.735124	-1.306798
C	-0.346866	-1.459436	-1.225727
C	0.510843	-0.099203	-1.157782
C	1.886421	-0.337275	-0.430626
C	2.61001	-1.433912	-1.261972
C	1.839758	-2.715646	-1.30774
C	1.649725	-0.748863	1.051291
C	2.873688	-1.319175	1.780609
C	4.163877	-0.513774	1.561753
C	4.251816	-0.141476	0.047141
C	3.021729	0.751115	-0.450216
C	4.0877	-1.43077	-0.806557
O	4.114313	0.722497	2.307253
C	5.390984	-1.305535	2.041061
C	0.677205	0.382161	-2.629255
C	-0.268515	-4.025726	-1.444435
C	-1.417906	-1.589084	-0.15003
C	-2.724279	-1.643841	-0.407883
C	-3.850834	-1.853758	0.585798
C	-4.902633	-0.725416	0.444282
C	-4.394232	0.706591	0.706221
C	-3.371506	-2.007556	2.032807
C	-5.520119	1.707333	0.700861
C	-5.751002	2.703375	-0.166551
C	-6.945619	3.612408	-0.001533

C	-4.885554	3.027914	-1.358489
C	2.825612	2.124064	0.227666
C	2.288072	3.211689	-0.715171
C	1.936859	4.514761	-0.000807
O	0.926599	4.358706	1.009519
H	2.638786	-1.055917	-2.288099
C	-0.426605	0.928985	-0.536673
O	-0.236082	1.625883	0.436976
C	5.530192	0.619564	-0.242067
O	6.159171	0.550989	-1.278778
O	-4.428519	-3.109493	0.111566
C	-5.588534	-3.611832	0.769255
H	-0.89593	-1.404373	-2.173689
H	2.386524	-3.650551	-1.410423
H	1.280791	0.126512	1.58551
H	0.867023	-1.501162	1.114267
H	3.040974	-2.352821	1.466368
H	2.670086	-1.362909	2.856202
H	3.259266	0.949425	-1.502235
H	4.753157	-1.3877	-1.668967
H	4.352803	-2.326337	-0.246356
H	4.187964	0.504714	3.243884
H	6.300389	-0.70398	1.964367
H	5.259067	-1.579451	3.092926
H	5.538606	-2.229219	1.479856
H	1.010063	-0.433544	-3.271438
H	-0.282527	0.723698	-3.027017
H	1.387014	1.204437	-2.720707
H	0.411843	-4.86492	-1.602067
H	-0.96136	-3.981776	-2.292741
H	-0.874897	-4.235957	-0.558624
H	-1.076095	-1.677586	0.875468
H	-3.065439	-1.570515	-1.440012
H	-5.315861	-0.77719	-0.5689
H	-5.728029	-0.929648	1.133304
H	-3.906411	0.741825	1.687404
H	-3.629817	0.966644	-0.027622
H	-4.218626	-2.117422	2.712661
H	-2.731072	-2.886034	2.135765
H	-2.806999	-1.131782	2.356949
H	-6.235039	1.582157	1.514293
H	-7.546813	3.342664	0.86933
H	-7.589829	3.577218	-0.888081
H	-6.628775	4.656186	0.110735

H	-5.47859	2.992077	-2.279711
H	-4.49436	4.049157	-1.281737
H	-4.040479	2.350632	-1.476575
H	2.174521	2.026512	1.09231
H	3.780944	2.476374	0.6209
H	3.036824	3.441142	-1.483056
H	1.400104	2.871471	-1.254201
H	2.814851	4.923459	0.509059
H	1.604762	5.257238	-0.737393
H	0.34898	3.624609	0.76066
H	-1.372826	1.033877	-1.10103
H	5.86528	1.303994	0.557275
H	-5.807819	-4.570068	0.296467
H	-5.41962	-3.782608	1.837453
H	-6.45646	-2.956529	0.644404

Table S24. Z-matrix of optimized conformer **1b9** at B3LYP/6-311+G(d,p) level

Atom	X	Y	Z
C	-0.802866	-1.911585	-0.565077
C	-0.82654	-0.439965	-0.99139
C	0.624251	0.226513	-1.220384
C	1.706055	-0.46155	-0.310812
C	1.664603	-1.975724	-0.654459
C	0.332159	-2.59683	-0.38528
C	1.428119	-0.156831	1.189508
C	2.256675	-0.966106	2.197324
C	3.748091	-1.098336	1.841326
C	3.862442	-1.377539	0.31216
C	3.228108	-0.213078	-0.584889
C	2.946702	-2.591015	-0.05294
O	4.449951	0.139852	2.095233
C	4.403699	-2.195484	2.697284
C	0.954319	0.105091	-2.733787
C	-2.152529	-2.565028	-0.396543
C	-1.733009	0.362757	-0.067131
C	-2.810947	1.030551	-0.475767
C	-3.736863	1.866336	0.38397
C	-5.211151	1.46657	0.121412
C	-5.575502	0.020122	0.501899
C	-3.534139	3.349456	0.007954

C	-7.050318	-0.245055	0.358587
C	-7.673099	-1.085328	-0.480746
C	-9.178544	-1.207202	-0.478197
C	-6.980631	-1.972722	-1.485221
C	3.755121	1.22703	-0.493735
C	5.236051	1.410467	-0.850717
C	5.60745	2.887377	-0.961834
O	6.985838	3.094642	-1.308205
H	1.815297	-2.034941	-1.737066
C	0.396974	1.728245	-1.022416
O	0.928087	2.47857	-0.235225
C	5.30509	-1.611181	-0.093715
O	5.645243	-2.212052	-1.093255
O	-3.357265	1.623325	1.752147
C	-4.037256	2.354995	2.764773
H	-1.309953	-0.414966	-1.975678
H	0.287095	-3.647798	-0.108037
H	1.603828	0.906513	1.343357
H	0.377996	-0.331314	1.419868
H	1.832344	-1.968351	2.302681
H	2.177697	-0.503997	3.187489
H	3.42883	-0.544596	-1.610426
H	3.446841	-3.223102	-0.786594
H	2.742224	-3.212522	0.817618
H	4.495527	0.264794	3.050575
H	5.481929	-2.239904	2.527483
H	4.242761	-1.972931	3.757197
H	3.982106	-3.183038	2.504476
H	0.879908	-0.926799	-3.07715
H	0.239426	0.686046	-3.32276
H	1.954465	0.476708	-2.965928
H	-2.730073	-2.106887	0.41142
H	-2.041803	-3.629455	-0.179485
H	-2.754256	-2.461942	-1.307054
H	-1.490092	0.37304	0.989813
H	-3.073368	1.029462	-1.532708
H	-5.865702	2.16171	0.657816
H	-5.415438	1.626391	-0.942584
H	-4.985018	-0.675803	-0.096689
H	-5.282947	-0.147378	1.545139
H	-2.523012	3.670431	0.268854
H	-3.670435	3.485739	-1.06734
H	-4.253546	3.995705	0.516465
H	-7.679996	0.341775	1.027993

H	-9.638356	-0.551602	0.264382
H	-9.487711	-2.237424	-0.264857
H	-9.59294	-0.956243	-1.461893
H	-7.213722	-3.026245	-1.290644
H	-7.343558	-1.757746	-2.497131
H	-5.896662	-1.861968	-1.485809
H	3.170076	1.815453	-1.206683
H	3.563889	1.652451	0.489095
H	5.868394	0.95329	-0.08328
H	5.467521	0.919418	-1.803185
H	5.034367	3.366731	-1.759109
H	5.374613	3.409178	-0.024938
H	7.53223	2.737278	-0.59911
H	-0.34416	2.132194	-1.739783
H	6.072119	-1.179579	0.571741
H	-3.869606	3.433635	2.680787
H	-5.115434	2.161841	2.765163
H	-3.623616	2.012346	3.714016

Table S25. Z-matrix of optimized conformer 1b10 at B3LYP/6-311+G(d,p) level

Atom	X	Y	Z
C	0.102366	-2.647039	-1.431094
C	0.405922	-2.245173	0.017735
C	-0.796342	-1.494113	0.786761
C	-1.717732	-0.726918	-0.22976
C	-2.205226	-1.784954	-1.257183
C	-1.080465	-2.416451	-2.01233
C	-0.942916	0.453759	-0.883335
C	-1.641348	1.122968	-2.074332
C	-3.143268	1.385942	-1.868364
C	-3.770775	0.131694	-1.189345
C	-3.118283	-0.202483	0.233716
C	-3.3878	-1.140587	-2.013912
O	-3.353833	2.497294	-0.968676
C	-3.810072	1.731128	-3.210912
C	-1.569895	-2.568226	1.600259
C	1.207799	-3.375033	-2.156244
C	1.73691	-1.507638	0.094306
C	2.81559	-1.985475	0.715619
C	4.206531	-1.377417	0.783307

C	4.257384	0.080531	0.278454
C	5.628583	0.771056	0.413015
C	5.163262	-2.283571	-0.006223
C	5.547813	2.239418	0.09024
C	6.184864	2.923429	-0.871244
C	5.971445	4.409877	-1.033446
C	7.152425	2.324616	-1.86175
C	-3.165647	0.814172	1.383547
C	-4.572926	1.210262	1.849359
C	-4.529869	2.020983	3.136211
O	-5.874791	2.379727	3.496098
H	-2.659119	-2.58399	-0.663687
C	-0.103793	-0.660534	1.86872
O	-0.134018	0.536706	2.040461
C	-5.272608	0.285218	-1.043359
O	-6.046547	-0.643468	-0.923668
O	4.68755	-1.480275	2.150889
C	3.964724	-0.756396	3.140972
H	0.558304	-3.182996	0.565657
H	-1.253543	-2.756643	-3.030935
H	-0.752782	1.193997	-0.107699
H	0.031455	0.112379	-1.231216
H	-1.514693	0.507119	-2.968898
H	-1.149988	2.076545	-2.296915
H	-3.689927	-1.073236	0.576328
H	-4.235827	-1.824234	-2.049732
H	-3.136755	-0.889113	-3.043339
H	-3.087861	3.304223	-1.425194
H	-4.85735	2.010327	-3.074403
H	-3.294556	2.584894	-3.662879
H	-3.761638	0.907057	-3.924346
H	-1.918399	-3.382449	0.964557
H	-0.914393	-3.013927	2.353253
H	-2.431412	-2.144599	2.120656
H	2.08659	-2.741249	-2.306832
H	0.863453	-3.721213	-3.132844
H	1.546274	-4.246059	-1.583409
H	1.793853	-0.55501	-0.422692
H	2.748209	-2.949519	1.220368
H	3.956772	0.08951	-0.773522
H	3.506587	0.672214	0.811671
H	5.979999	0.652498	1.444829
H	6.362927	0.27065	-0.219724
H	6.198081	-1.96648	0.13647

H	5.07353	-3.316658	0.337427
H	4.927905	-2.25092	-1.072151
H	4.872634	2.803586	0.734373
H	5.586508	4.643095	-2.033318
H	6.917651	4.954437	-0.930413
H	5.268888	4.802951	-0.295567
H	6.822601	2.528263	-2.887087
H	8.141311	2.786567	-1.757549
H	7.271842	1.246932	-1.753904
H	-2.657973	0.345069	2.23145
H	-2.598444	1.709838	1.139219
H	-5.074719	1.811966	1.087005
H	-5.185775	0.317273	2.019759
H	-4.071651	1.432595	3.940882
H	-3.9263	2.925952	2.993106
H	-5.84533	2.890394	4.312198
H	0.469487	-1.294863	2.573769
H	-5.654392	1.320178	-1.030799
H	2.901554	-1.019577	3.14482
H	4.399798	-1.033243	4.101973
H	4.059824	0.327305	3.012135

Table S26. Z-matrix of optimized conformer 1b11 at B3LYP/6-311+G(d,p) level

Atom	X	Y	Z
C	-0.33284	-1.396665	-1.932685
C	-0.319094	0.122332	-1.744897
C	1.142435	0.743118	-1.466747
C	1.989835	-0.286411	-0.598312
C	2.095788	-1.571266	-1.448667
C	0.757803	-2.159179	-1.769766
C	1.320447	-0.5097	0.789508
C	1.851764	-1.707839	1.585091
C	3.386542	-1.76512	1.63784
C	3.929298	-1.473147	0.200577
C	3.514199	-0.029128	-0.34768
C	3.221854	-2.422534	-0.810739
O	3.890133	-0.728413	2.507934
C	3.872226	-3.118511	2.178519
C	1.769528	1.047023	-2.841894
C	-1.608669	-1.988761	-2.488281

C	-1.432349	0.683513	-0.863696
C	-2.183291	0.040986	0.029256
C	-3.371607	0.59732	0.798075
C	-4.630636	-0.16044	0.312627
C	-5.953226	0.206568	1.014988
C	-3.540826	2.115051	0.658861
C	-7.06787	-0.723626	0.615787
C	-8.173992	-0.449108	-0.091298
C	-9.184546	-1.528817	-0.39803
C	-8.53097	0.909688	-0.641176
C	3.959095	1.230173	0.433639
C	4.488014	2.35484	-0.471622
C	4.690122	3.682882	0.255416
O	3.474717	4.225522	0.794506
H	2.512149	-1.251671	-2.409376
C	0.986251	2.040294	-0.690325
O	1.348038	3.132693	-1.084828
C	5.440639	-1.56272	0.1723
O	6.094443	-2.03329	-0.736353
O	-3.238247	0.212595	2.191521
C	-2.177516	0.816399	2.923921
H	-0.567529	0.528366	-2.735224
H	0.699732	-3.222284	-1.993203
H	1.471738	0.387437	1.393982
H	0.245818	-0.626105	0.681895
H	1.466573	-2.638621	1.161639
H	1.46986	-1.66204	2.610717
H	3.998787	0.020593	-1.329235
H	3.933098	-2.744398	-1.571466
H	2.845427	-3.323324	-0.328611
H	3.662418	-0.966702	3.414344
H	4.958612	-3.123795	2.299207
H	3.425528	-3.301605	3.161136
H	3.592041	-3.951483	1.53231
H	1.64893	0.204869	-3.523552
H	1.267186	1.906437	-3.28998
H	2.831009	1.287072	-2.779818
H	-2.468534	-1.848379	-1.831233
H	-1.486682	-3.058457	-2.670121
H	-1.86282	-1.51126	-3.442286
H	-1.647007	1.73198	-1.058956
H	-1.996902	-1.010679	0.237798
H	-4.733434	0.008058	-0.763926
H	-4.441754	-1.231226	0.44659

H	-5.800801	0.136228	2.09723
H	-6.215017	1.244051	0.800869
H	-4.315513	2.469662	1.340589
H	-2.618142	2.65237	0.884814
H	-3.840246	2.374989	-0.358827
H	-6.932643	-1.754654	0.943553
H	-9.312497	-1.649071	-1.480361
H	-10.170784	-1.267671	0.004066
H	-8.889148	-2.493064	0.020984
H	-8.674018	0.855069	-1.726634
H	-9.482751	1.255921	-0.221037
H	-7.776898	1.670063	-0.439521
H	3.137204	1.607963	1.045587
H	4.740071	0.975775	1.148963
H	5.449577	2.05537	-0.905753
H	3.815144	2.529823	-1.315446
H	5.361561	3.560123	1.109885
H	5.150496	4.407784	-0.427919
H	2.78091	4.15316	0.123743
H	0.519098	1.956877	0.302909
H	5.953739	-1.123746	1.046522
H	-2.35402	1.883417	3.097473
H	-2.140806	0.307772	3.888126
H	-1.211902	0.69288	2.421764

Table S27. Z-matrix of optimized conformer **1b12** at B3LYP/6-311+G(d,p) level

Atom	X	Y	Z
C	0.246471	-3.113698	-0.753496
C	-0.525824	-1.824533	-1.063946
C	0.387314	-0.503152	-1.218442
C	1.694439	-0.652867	-0.337499
C	2.413887	-1.929373	-0.835607
C	1.579836	-3.155009	-0.638683
C	1.33681	-0.693721	1.178205
C	2.484843	-1.103708	2.109772
C	3.820789	-0.404378	1.803858
C	4.023393	-0.39428	0.258043
C	2.855692	0.372989	-0.522327
C	3.856571	-1.852223	-0.284103
O	3.784769	0.976037	2.230159

C	4.970867	-1.100409	2.549941
C	0.687244	-0.315907	-2.717925
C	-0.58773	-4.366504	-0.646747
C	-1.725131	-1.679025	-0.135352
C	-2.986498	-1.586877	-0.559755
C	-4.243407	-1.472921	0.283233
C	-5.029679	-0.196939	-0.09765
C	-4.357504	1.147967	0.2319
C	-3.995769	-1.544315	1.792871
C	-5.148219	2.309238	-0.310902
C	-5.730774	3.313417	0.360097
C	-6.48531	4.397562	-0.372498
C	-5.70316	3.482399	1.858929
C	2.534398	1.846991	-0.231871
C	3.663765	2.83896	-0.539928
C	3.187629	4.281218	-0.449122
O	4.302728	5.146479	-0.719598
H	2.525401	-1.801129	-1.915906
C	-0.464762	0.672751	-0.749421
O	-0.90537	1.541543	-1.473346
C	5.364444	0.208836	-0.113946
O	5.945645	-0.009456	-1.157736
O	-5.161365	-2.527164	-0.132462
C	-4.762976	-3.872999	0.110017
H	-0.955671	-1.963685	-2.062911
H	2.073172	-4.108079	-0.461605
H	0.990794	0.296639	1.480212
H	0.507524	-1.376576	1.358064
H	2.631001	-2.185643	2.057623
H	2.207899	-0.887326	3.147089
H	3.169958	0.326818	-1.571349
H	4.577586	-2.031467	-1.081425
H	4.048684	-2.592124	0.491612
H	3.807782	0.991345	3.194293
H	5.913648	-0.566316	2.411355
H	4.750273	-1.114762	3.622202
H	5.109197	-2.134712	2.23246
H	1.11996	-1.215047	-3.156703
H	-0.23968	-0.102517	-3.252487
H	1.366076	0.519451	-2.90016
H	0.049831	-5.245708	-0.534246
H	-1.206402	-4.504152	-1.541055
H	-1.273653	-4.329653	0.204843
H	-1.52355	-1.680502	0.931847

H	-3.185213	-1.600699	-1.631522
H	-5.232801	-0.246973	-1.172891
H	-5.99974	-0.252508	0.406911
H	-4.216674	1.24248	1.309822
H	-3.358174	1.166276	-0.217624
H	-4.951498	-1.498926	2.320705
H	-3.486338	-2.465009	2.08213
H	-3.381069	-0.70821	2.130318
H	-5.252887	2.312081	-1.396146
H	-6.482835	4.236546	-1.452601
H	-6.047327	5.382617	-0.17159
H	-7.527163	4.446224	-0.034258
H	-5.222075	4.430094	2.12838
H	-6.723866	3.530597	2.25577
H	-5.178066	2.679636	2.375766
H	1.685054	2.109467	-0.872275
H	2.212914	1.982813	0.799639
H	4.488818	2.7083	0.165226
H	4.060507	2.664216	-1.546709
H	2.38679	4.463314	-1.17651
H	2.788361	4.485967	0.552164
H	4.000207	6.059123	-0.663058
H	-0.694856	0.704328	0.327099
H	5.802653	0.904397	0.622151
H	-5.499548	-4.503088	-0.390273
H	-3.772835	-4.087868	-0.304234
H	-4.763319	-4.116525	1.177866

Table S28. Z-matrix of optimized conformer **1b13** at B3LYP/6-311+G(d,p) level

Atom	X	Y	Z
C	-0.917035	-1.756895	-0.651755
C	-0.885464	-0.247539	-0.931249
C	0.589179	0.371045	-1.142818
C	1.641479	-0.469509	-0.311908
C	1.54234	-1.924471	-0.830482
C	0.187377	-2.512095	-0.593771
C	1.371606	-0.340424	1.216459
C	2.156246	-1.315733	2.104051
C	3.646241	-1.436463	1.740691
C	3.764379	-1.514022	0.187994

C	3.164097	-0.226971	-0.550317
C	2.81924	-2.644186	-0.336841
O	4.370743	-0.25662	2.155016
C	4.271467	-2.650823	2.447154
C	0.878175	0.378004	-2.656461
C	-2.290206	-2.365352	-0.506687
C	-1.774132	0.500102	0.053975
C	-2.825673	1.235155	-0.308284
C	-3.794102	1.939809	0.630041
C	-5.05396	1.067949	0.863104
C	-5.846393	0.63827	-0.385944
C	-4.178	3.314675	0.059701
C	-7.118105	-0.076463	-0.010748
C	-7.501477	-1.324657	-0.315139
C	-8.830109	-1.862059	0.161638
C	-6.697227	-2.301137	-1.136747
C	3.697802	1.184537	-0.263902
C	5.169849	1.418706	-0.630677
C	5.547409	2.895703	-0.540224
O	6.933667	3.135876	-0.824716
H	1.665446	-1.859249	-1.915
C	0.524891	1.818898	-0.662944
O	0.542424	2.791871	-1.388426
C	5.204309	-1.720274	-0.240941
O	5.538157	-2.201221	-1.305078
O	-3.244098	2.056102	1.962089
C	-2.249879	3.052507	2.182532
H	-1.36734	-0.113473	-1.906915
H	0.096191	-3.584436	-0.435963
H	1.614975	0.675993	1.531362
H	0.313401	-0.4836	1.428971
H	1.697458	-2.306698	2.053884
H	2.077296	-1.000881	3.15009
H	3.363734	-0.420859	-1.61056
H	3.300069	-3.172552	-1.159842
H	2.610535	-3.381279	0.437028
H	4.421283	-0.259207	3.118253
H	5.348005	-2.701805	2.268616
H	4.116793	-2.561722	3.52733
H	3.823187	-3.593974	2.131379
H	0.723272	-0.605087	-3.100957
H	0.200956	1.074029	-3.153611
H	1.89692	0.701888	-2.878537
H	-2.818664	-1.9795	0.369873

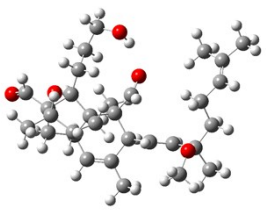
H	-2.223129	-3.451435	-0.416249
H	-2.915928	-2.131892	-1.375697
H	-1.556851	0.394976	1.113133
H	-3.057836	1.336519	-1.367164
H	-4.730678	0.174796	1.406572
H	-5.711985	1.62993	1.535185
H	-6.11189	1.527497	-0.971114
H	-5.220845	0.018314	-1.03052
H	-3.301521	3.943287	-0.108174
H	-4.682769	3.197739	-0.900878
H	-4.856338	3.832299	0.743015
H	-7.803693	0.518924	0.592722
H	-9.379501	-1.124599	0.750472
H	-8.690927	-2.758945	0.776872
H	-9.457962	-2.161202	-0.686084
H	-5.735535	-1.905626	-1.461982
H	-6.511116	-3.217952	-0.565426
H	-7.258551	-2.601944	-2.029222
H	3.097488	1.870893	-0.872119
H	3.544164	1.46085	0.777886
H	5.825395	0.85681	0.039783
H	5.362918	1.065367	-1.651654
H	4.917903	3.491563	-1.213155
H	5.391172	3.266928	0.475406
H	7.104821	2.8692	-1.735051
H	0.444324	1.965509	0.425647
H	5.974514	-1.379953	0.472152
H	-1.448442	3.009657	1.438924
H	-2.677146	4.060501	2.186244
H	-1.826668	2.848613	3.166988

Table S29. Z-matrix of optimized conformer **1b14** at B3LYP/6-311+G(d,p) level

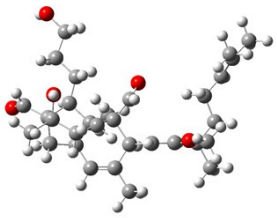
Atom	X	Y	Z
C	-0.218503	-3.067765	-0.513552
C	0.265496	-2.188727	0.646912
C	-0.810183	-1.113548	1.182636
C	-1.800211	-0.693348	0.035556
C	-2.448043	-2.005143	-0.482982
C	-1.445497	-2.964656	-1.037226
C	-1.045844	0.102494	-1.068485

C	-1.832525	0.350588	-2.362489
C	-3.288837	0.795892	-2.1457
C	-3.899406	-0.068362	-1.00156
C	-3.11458	0.083371	0.386895
C	-3.670692	-1.579715	-1.326614
O	-3.346323	2.171673	-1.705916
C	-4.079024	0.686936	-3.461057
C	-1.540559	-1.754527	2.394836
C	0.758928	-4.109371	-1.001349
C	1.627361	-1.588646	0.321167
C	2.755888	-1.924979	0.946414
C	4.171028	-1.464961	0.635658
C	4.214418	-0.258711	-0.326256
C	5.618233	0.307868	-0.612957
C	4.950214	-2.666187	0.078928
C	5.563719	1.463065	-1.577317
C	5.972249	2.727225	-1.39568
C	5.832244	3.750995	-2.497355
C	6.598822	3.260389	-0.131121
C	-2.985844	1.444895	1.084339
C	-4.311584	2.106605	1.481848
C	-4.128199	3.318601	2.384905
O	-3.591555	2.889233	3.648722
H	-2.878403	-2.490227	0.398558
C	0.035935	-0.00519	1.816918
O	0.091963	1.168119	1.527335
C	-5.3665	0.256507	-0.798789
O	-6.171617	-0.498353	-0.290876
O	4.846684	-1.170129	1.887735
C	4.310381	-0.109381	2.671196
H	0.438915	-2.869521	1.489014
H	-1.745841	-3.640506	-1.834984
H	-0.745184	1.055771	-0.637264
H	-0.128293	-0.416638	-1.342878
H	-1.831118	-0.554951	-2.97518
H	-1.321953	1.115081	-2.958453
H	-3.689767	-0.551937	1.071194
H	-4.55059	-2.155312	-1.039594
H	-3.517962	-1.740883	-2.392798
H	-3.083278	2.731488	-2.446003
H	-5.091616	1.081777	-3.350329
H	-3.575554	1.274646	-4.235639
H	-4.145671	-0.339679	-3.824759
H	-1.974058	-2.720765	2.136713

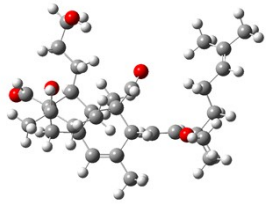
H	-0.833663	-1.933264	3.209577
H	-2.334117	-1.111102	2.779772
H	1.648698	-3.659561	-1.450874
H	0.289533	-4.757575	-1.744002
H	1.110866	-4.735546	-0.173295
H	1.661074	-0.878254	-0.498481
H	2.71257	-2.650009	1.759519
H	3.755151	-0.564957	-1.27144
H	3.583744	0.543092	0.069683
H	6.098998	0.591879	0.324354
H	6.240553	-0.480917	-1.051794
H	6.012162	-2.428717	-0.007578
H	4.84724	-3.524069	0.747358
H	4.569518	-2.945872	-0.905656
H	5.128009	1.218583	-2.546531
H	5.373299	3.325603	-3.392313
H	6.809851	4.162472	-2.77553
H	5.221049	4.599386	-2.167277
H	6.671332	2.517887	0.662945
H	7.607959	3.637756	-0.334697
H	6.022011	4.110673	0.250747
H	-2.421322	1.271635	2.002651
H	-2.40406	2.142956	0.485337
H	-4.847579	2.448773	0.592086
H	-4.963173	1.388804	1.995069
H	-3.447098	4.040594	1.916274
H	-5.093135	3.815088	2.541568
H	-3.454403	3.666652	4.200106
H	0.646121	-0.384304	2.661134
H	-5.689127	1.259781	-1.126001
H	4.873867	-0.102481	3.604964
H	4.427573	0.864493	2.18369
H	3.250343	-0.265468	2.898719



1c1 (1.72%)



1c2 (35.55%)



1c3 (16.94%)

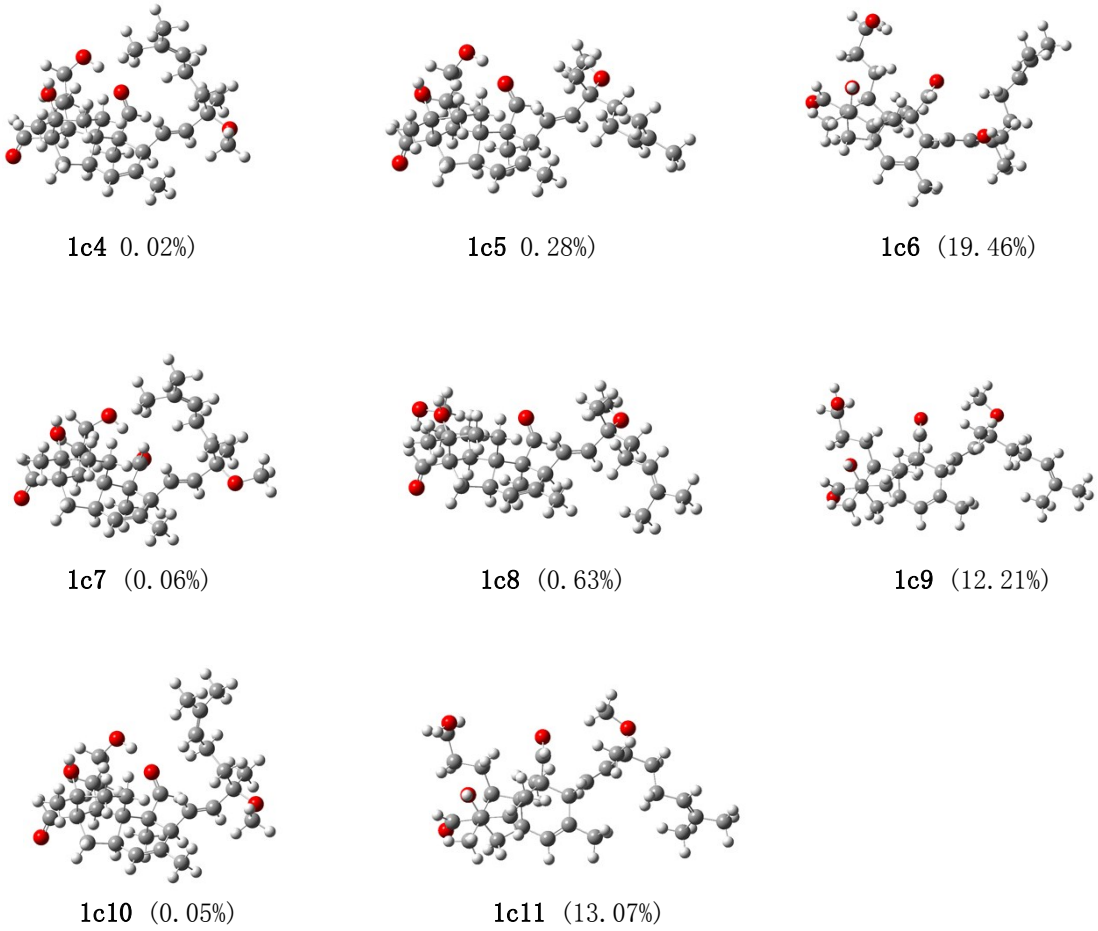


Figure S6. Reoptimized geometries of **1c** at B3LYP/6-311+G(d,p) level with the CPCM model in MeOH

Table S30. Z-matrix of optimized conformer 1c1 at B3LYP/6-311+G(d,p) level

Atom	X	Y	Z
C	-0.635549	-2.822044	-1.278413
C	0.299255	-1.603339	-1.295458
C	-0.459247	-0.18801	-1.243025

C	-1.811056	-0.336564	-0.422819
C	-2.654219	-1.387774	-1.183734
C	-1.970442	-2.719239	-1.221722
C	-1.515672	-0.740273	1.052598
C	-2.733996	-1.219337	1.851733
C	-3.958238	-0.303126	1.703508
C	-4.107626	0.062899	0.190817
C	-2.840369	0.84138	-0.394367
C	-4.102534	-1.247025	-0.651085
O	-3.744704	0.927569	2.428101
C	-5.220003	-0.973961	2.268152
C	-0.673724	0.256591	-2.70406
C	0.040138	-4.164604	-1.411102
C	1.455449	-1.766903	-0.31806
C	2.729777	-1.862416	-0.697786
C	3.939385	-2.080026	0.19647
C	4.863471	-0.838286	0.182688
C	4.268966	0.459586	0.758319
C	4.745966	-3.281128	-0.336421
C	5.321142	1.527765	0.903146
C	5.426165	2.698406	0.257503
C	6.575899	3.636747	0.539417
C	4.456218	3.19985	-0.783166
C	-2.436861	2.196087	0.235764
C	-2.078196	3.273472	-0.800704
C	-1.432402	4.516643	-0.191605
O	-0.184467	4.244101	0.464774
H	-2.705731	-1.035383	-2.217641
C	-5.329627	0.929375	-0.031226
O	-6.069685	0.857003	-0.991261
C	0.446922	0.814648	-0.54738
O	0.865251	1.838108	-1.055134
O	3.560651	-2.256302	1.576199
C	3.083911	-3.537315	1.979498
H	0.769977	-1.612377	-2.285699
H	-2.577827	-3.620492	-1.267368
H	-1.085243	0.118981	1.571333
H	-0.769023	-1.530194	1.092026
H	-3.001951	-2.234125	1.547213
H	-2.472235	-1.281761	2.913419
H	-3.123416	1.04639	-1.433077
H	-4.805254	-1.152196	-1.478926
H	-4.419758	-2.107757	-0.064272
H	-3.776341	0.724317	3.370434

H	-5.488958	-1.88275	1.727677
H	-5.047729	-1.252872	3.312738
H	-6.071959	-0.289677	2.241165
H	-1.088257	-0.552482	-3.305504
H	0.286421	0.532345	-3.144059
H	-1.331853	1.120985	-2.793143
H	0.692182	-4.190768	-2.291789
H	-0.699674	-4.961524	-1.509189
H	0.674487	-4.390186	-0.549011
H	1.223695	-1.842564	0.739567
H	2.970874	-1.795893	-1.758495
H	5.762956	-1.104203	0.749033
H	5.182748	-0.661245	-0.849674
H	3.442051	0.797249	0.132073
H	3.848701	0.239213	1.74552
H	5.605654	-3.476897	0.30972
H	4.140608	-4.186986	-0.401753
H	5.1173	-3.057761	-1.338998
H	6.103033	1.290412	1.625235
H	7.153226	3.832561	-0.372099
H	7.254829	3.234375	1.294357
H	6.210563	4.609367	0.890194
H	3.627112	2.517876	-0.966707
H	4.037277	4.166928	-0.480571
H	4.974454	3.372535	-1.733937
H	-3.245675	2.579694	0.856405
H	-1.601999	2.060086	0.926333
H	-1.399864	2.878522	-1.561819
H	-2.983755	3.588013	-1.333406
H	-1.284349	5.272337	-0.973573
H	-2.078375	4.954621	0.574566
H	0.339595	3.658875	-0.100624
H	-5.508736	1.698128	0.741557
H	0.717154	0.58704	0.494922
H	3.887939	-4.279666	2.010071
H	2.687604	-3.409747	2.987832
H	2.283745	-3.907649	1.331635

Table S31. Z-matrix of optimized conformer **1c2** at B3LYP/6-311+G(d,p) level

Atom	X	Y	Z

C	-0.383441	-3.092237	-0.997025
C	0.420891	-1.806858	-1.235369
C	-0.458662	-0.457818	-1.300771
C	-1.751481	-0.62096	-0.400626
C	-2.517475	-1.845542	-0.955239
C	-1.714943	-3.103979	-0.854316
C	-1.364669	-0.760304	1.102243
C	-2.506043	-1.183825	2.036847
C	-3.828151	-0.433255	1.797864
C	-4.059854	-0.332516	0.259334
C	-2.885744	0.445825	-0.500315
C	-3.944256	-1.762201	-0.365057
O	-3.747468	0.920259	2.298275
C	-4.982524	-1.139275	2.528162
C	-0.784722	-0.186228	-2.781744
C	0.416821	-4.371697	-0.991651
C	1.626659	-1.748493	-0.308178
C	2.888839	-1.709773	-0.733829
C	4.132107	-1.721304	0.13235
C	5.076526	-0.559599	-0.270218
C	4.517344	0.853358	-0.02988
C	4.85656	-3.06652	-0.084121
C	5.444233	1.920565	-0.54724
C	6.055815	2.902116	0.131847
C	6.960414	3.884263	-0.574157
C	5.919161	3.141824	1.615036
C	-2.517004	1.891082	-0.132552
C	-3.624012	2.93064	-0.35616
C	-3.104903	4.355964	-0.179617
O	-4.133984	5.346927	-0.319667
H	-2.650556	-1.64937	-2.022952
C	-5.389858	0.326848	-0.051785
O	-5.994387	0.185891	-1.095749
C	0.435082	0.669995	-0.790776
O	0.887414	1.560603	-1.480759
O	3.682566	-1.590117	1.495412
C	4.666111	-1.648141	2.521161
H	0.838668	-1.896778	-2.245261
H	-2.232611	-4.05238	-0.728657
H	-0.976233	0.198339	1.451664
H	-0.557089	-1.480619	1.222984
H	-2.684735	-2.257237	1.933978
H	-2.201527	-1.028507	3.077304
H	-3.222304	0.470164	-1.543188

H	-4.688045	-1.879596	-1.153008
H	-4.138162	-2.538208	0.373856
H	-3.745057	0.8825	3.262094
H	-5.151215	-2.152532	2.161335
H	-4.745033	-1.213566	3.594327
H	-5.914214	-0.576835	2.433399
H	-1.238487	-1.055294	-3.25845
H	0.135035	0.042384	-3.322373
H	-1.454304	0.666874	-2.907313
H	1.007419	-4.468962	-1.910089
H	-0.242564	-5.238791	-0.916353
H	1.126981	-4.405826	-0.160351
H	1.448512	-1.773715	0.761472
H	3.09499	-1.702163	-1.803137
H	6.026628	-0.670846	0.262459
H	5.314527	-0.683828	-1.332496
H	3.553331	0.94011	-0.544764
H	4.309505	0.987421	1.032837
H	5.814968	-3.093851	0.43955
H	4.235228	-3.892433	0.269858
H	5.056277	-3.218476	-1.147355
H	5.63647	1.86759	-1.619386
H	6.600012	4.911682	-0.443936
H	7.027749	3.678833	-1.64462
H	7.972941	3.854977	-0.154235
H	5.279721	2.414309	2.11408
H	6.902905	3.11691	2.098201
H	5.507532	4.140317	1.804343
H	-2.171442	1.958892	0.897822
H	-1.674085	2.168913	-0.775155
H	-4.038724	2.826418	-1.367061
H	-4.442645	2.776533	0.351545
H	-2.706112	4.493299	0.828353
H	-2.292462	4.556501	-0.889363
H	-4.478311	5.29962	-1.218703
H	-5.795959	0.989763	0.731329
H	0.683999	0.645176	0.281514
H	4.131996	-1.499837	3.460476
H	5.171168	-2.618873	2.556836
H	5.419262	-0.859235	2.421175

Table S32. Z-matrix of optimized conformer **1c3** at B3LYP/6-311+G(d,p)

level

Atom	X	Y	Z
C	-0.312868	-2.97087	-1.179229
C	0.520691	-1.683562	-1.227839
C	-0.334106	-0.316818	-1.230625
C	-1.704312	-0.542745	-0.470608
C	-2.428555	-1.694438	-1.20919
C	-1.651633	-2.97164	-1.157718
C	-1.455387	-0.834932	1.039158
C	-2.679981	-1.329196	1.820799
C	-3.966802	-0.532678	1.541537
C	-4.060455	-0.280183	0.005922
C	-2.816035	0.548111	-0.566717
C	-3.901793	-1.643857	-0.743216
O	-3.911756	0.765769	2.173007
C	-5.188813	-1.281043	2.098728
C	-0.520006	0.115079	-2.697705
C	0.471588	-4.259504	-1.220852
C	1.651633	-1.736775	-0.210031
C	2.941789	-1.671302	-0.536601
C	4.121547	-1.797037	0.405658
C	5.095874	-0.606581	0.213261
C	4.534325	0.777124	0.584663
C	4.856416	-3.113827	0.076169
C	5.591349	1.846281	0.504278
C	5.621726	2.941198	-0.269438
C	6.789277	3.897598	-0.209303
C	4.544073	3.337755	-1.247808
C	-2.47033	1.947974	-0.035239
C	-3.542398	3.021986	-0.267166
C	-3.060311	4.438251	0.043997
O	-2.783491	4.65923	1.436544
H	-2.461621	-1.395243	-2.260665
C	-5.352636	0.42836	-0.352799
O	-5.871391	0.389957	-1.450341
C	0.522993	0.734271	-0.528613
O	1.036202	1.687517	-1.077785
O	3.578547	-1.829785	1.739611
C	4.488893	-2.008477	2.817899
H	1.016142	-1.684778	-2.206049
H	-2.188579	-3.917635	-1.167852
H	-1.094785	0.079096	1.514868
H	-0.666523	-1.57618	1.159223
H	-2.859353	-2.383302	1.594448

H	-2.469712	-1.284024	2.894619
H	-3.05633	0.676281	-1.628491
H	-4.57365	-1.673589	-1.600831
H	-4.165459	-2.483057	-0.101145
H	-4.005193	0.640834	3.124896
H	-5.348349	-2.243502	1.610085
H	-5.037993	-1.477569	3.165201
H	-6.098794	-0.685609	1.995429
H	-0.947001	-0.68522	-3.301952
H	0.449842	0.369098	-3.128356
H	-1.156161	0.99743	-2.791561
H	1.151877	-4.277506	-2.080179
H	-0.199639	-5.117322	-1.297798
H	1.093258	-4.388324	-0.329978
H	1.392074	-1.870108	0.834914
H	3.223999	-1.552502	-1.581691
H	6.003087	-0.799808	0.795884
H	5.41221	-0.602095	-0.83522
H	3.679614	1.011512	-0.051648
H	4.151219	0.73256	1.611345
H	5.774823	-3.216456	0.658706
H	4.209085	-3.969713	0.280748
H	5.131249	-3.135641	-0.98092
H	6.443285	1.685179	1.165895
H	7.264968	3.996147	-1.192389
H	7.546817	3.570488	0.506094
H	6.457816	4.902855	0.077183
H	3.701115	2.648128	-1.269289
H	4.157564	4.334622	-1.004204
H	4.956553	3.406988	-2.261448
H	-2.218209	1.908411	1.023859
H	-1.571408	2.270028	-0.573261
H	-3.861627	3.008309	-1.316794
H	-4.426452	2.819882	0.343985
H	-2.172789	4.679755	-0.554935
H	-3.839281	5.159622	-0.210587
H	-2.013268	4.136765	1.684381
H	-5.814624	1.026894	0.450974
H	0.682574	0.588982	0.551115
H	3.886604	-1.994961	3.727095
H	5.014729	-2.967151	2.762464
H	5.226897	-1.201201	2.87733

Table S33. Z-matrix of optimized conformer **1c4** at B3LYP/6-311+G(d,p) level

Atom	X	Y	Z
C	-0.33996	-2.877693	-0.928492
C	-0.766979	-2.164244	0.358548
C	0.423756	-1.374525	1.104759
C	1.488632	-0.858062	0.067481
C	2.006625	-2.129135	-0.664115
C	0.915844	-2.849736	-1.390556
C	0.843143	0.181896	-0.892885
C	1.660098	0.512957	-2.148032
C	3.147811	0.779156	-1.869014
C	3.653852	-0.30593	-0.865833
C	2.87644	-0.280331	0.531369
C	3.293579	-1.714535	-1.41484
O	3.316953	2.065459	-1.23453
C	3.956321	0.787669	-3.176532
C	1.019561	-2.368156	2.144829
C	-1.415691	-3.673699	-1.624856
C	-2.032911	-1.340327	0.145853
C	-3.163802	-1.547331	0.822593
C	-4.487811	-0.811322	0.710984
C	-4.510826	0.375104	-0.276831
C	-3.836615	1.683172	0.187063
C	-4.939352	-0.392636	2.115711
C	-4.00953	2.776156	-0.835919
C	-3.081902	3.57928	-1.376088
C	-3.466376	4.629814	-2.390848
C	-1.611528	3.546263	-1.04393
C	2.96409	1.014587	1.367183
C	2.978568	0.775186	2.88478
C	2.885716	2.061476	3.702796
O	1.688371	2.815406	3.450353
H	2.352709	-2.803882	0.124513
C	5.131577	-0.124962	-0.582341
O	5.908555	-1.028955	-0.349661
C	-0.267668	-0.318953	1.96173
O	-0.08185	0.879408	1.965209
O	-5.503807	-1.787316	0.323825
C	-5.414307	-2.336745	-0.987289
H	-1.059321	-2.957832	1.056783
H	1.167343	-3.414102	-2.28595
H	0.667663	1.09395	-0.323581

H	-0.131434	-0.166262	-1.228279
H	1.572877	-0.302057	-2.871565
H	1.234703	1.395638	-2.638133
H	3.374245	-1.065474	1.112951
H	4.103434	-2.411697	-1.199287
H	3.160777	-1.706739	-2.49569
H	3.11069	2.745262	-1.886857
H	3.930034	-0.173676	-3.691416
H	3.537575	1.535412	-3.857858
H	5.00014	1.053642	-2.990724
H	1.220595	-3.338508	1.690612
H	0.3044	-2.541929	2.953797
H	1.942991	-1.999035	2.591323
H	-1.895863	-4.376854	-0.934846
H	-0.996651	-4.242577	-2.457202
H	-2.208261	-3.029865	-2.017799
H	-1.992025	-0.556002	-0.603003
H	-3.187068	-2.348448	1.561695
H	-4.072569	0.071883	-1.232226
H	-5.567167	0.586518	-0.476855
H	-4.304747	2.008868	1.123214
H	-2.783211	1.512096	0.41424
H	-5.896543	0.132729	2.065902
H	-5.064243	-1.281691	2.737942
H	-4.205458	0.258311	2.592962
H	-5.039882	2.921389	-1.162009
H	-3.194486	5.631974	-2.038488
H	-4.537966	4.62021	-2.60084
H	-2.929608	4.476295	-3.334558
H	-1.347213	2.771578	-0.325434
H	-1.01722	3.387213	-1.95107
H	-1.293739	4.511187	-0.631381
H	3.879957	1.551734	1.113261
H	2.151855	1.687919	1.105643
H	2.162487	0.117157	3.194578
H	3.904165	0.261568	3.172078
H	2.945687	1.819409	4.771391
H	3.720442	2.728881	3.466877
H	0.987014	2.205804	3.183607
H	5.485391	0.920849	-0.557676
H	-0.993126	-0.755673	2.673674
H	-6.146778	-3.143937	-1.03018
H	-5.65966	-1.600776	-1.760284
H	-4.420829	-2.748851	-1.189101

Table S34. Z-matrix of optimized conformer 1c5 at B3LYP/6-311+G(d,p) level

Atom	X	Y	Z
C	0.525643	-1.707631	-1.350913
C	0.541716	-0.174847	-1.320114
C	-0.921924	0.495127	-1.241811
C	-1.921438	-0.426421	-0.447895
C	-1.949584	-1.772053	-1.226395
C	-0.604412	-2.422907	-1.292631
C	-1.4558	-0.582348	1.028143
C	-2.152526	-1.691997	1.828249
C	-3.678543	-1.734088	1.648739
C	-3.992879	-1.536354	0.131922
C	-3.467179	-0.139207	-0.439483
C	-3.169486	-2.561884	-0.698299
O	-4.298827	-0.643584	2.364336
C	-4.256534	-3.048415	2.198191
C	-1.363417	0.743315	-2.714115
C	1.870505	-2.373704	-1.503077
C	1.532069	0.344734	-0.283422
C	2.603368	1.084056	-0.578231
C	3.653784	1.617996	0.378874
C	5.052696	1.09259	-0.020753
C	5.280284	-0.423845	0.107005
C	3.354705	1.344647	1.855458
C	6.631797	-0.827991	-0.420138
C	7.654148	-1.388079	0.242691
C	8.944275	-1.724546	-0.466882
C	7.644851	-1.739334	1.709906
C	-4.040855	1.144772	0.196535
C	-4.208236	2.30772	-0.793931
C	-4.604432	3.622166	-0.125305
O	-3.645624	4.085573	0.839947
H	-2.216572	-1.511341	-2.254824
C	-5.485722	-1.612958	-0.119304
O	-5.996563	-2.048403	-1.131451
C	-0.688844	1.894098	-0.685788
O	-1.201692	2.409957	0.284247
O	3.794364	3.049776	0.141906
C	2.699217	3.88532	0.502216

H	0.94663	0.142736	-2.28852
H	-0.551944	-3.507468	-1.358892
H	-1.599632	0.375862	1.527608
H	-0.389395	-0.792164	1.063212
H	-1.736083	-2.663098	1.546863
H	-1.930884	-1.568134	2.893907
H	-3.801063	-0.150678	-1.483963
H	-3.771999	-2.933724	-1.527199
H	-2.879824	-3.426434	-0.102841
H	-4.225422	-0.830459	3.30765
H	-3.888296	-3.924296	1.662219
H	-3.967632	-3.161839	3.248196
H	-5.348589	-3.046907	2.151253
H	-1.200956	-0.144249	-3.325539
H	-0.766615	1.544486	-3.159005
H	-2.41268	1.02831	-2.790397
H	2.408757	-1.981824	-2.373632
H	1.755158	-3.452087	-1.629078
H	2.510861	-2.197823	-0.633974
H	1.353391	0.06537	0.749827
H	2.789436	1.35728	-1.617198
H	5.233115	1.400395	-1.056465
H	5.785246	1.623346	0.595793
H	5.159198	-0.73584	1.14545
H	4.507428	-0.947702	-0.467401
H	4.131409	1.799053	2.475367
H	2.389067	1.752865	2.158043
H	3.338531	0.273505	2.062119
H	6.780464	-0.623279	-1.48052
H	9.7915	-1.202591	-0.006451
H	8.90947	-1.454804	-1.524494
H	9.162745	-2.79655	-0.393178
H	6.718646	-1.467871	2.215612
H	7.802493	-2.815713	1.846451
H	8.471719	-1.238036	2.226266
H	-5.024887	0.934174	0.619324
H	-3.425838	1.456823	1.036727
H	-3.294114	2.481201	-1.367551
H	-4.982363	2.060142	-1.530362
H	-4.750769	4.392642	-0.892883
H	-5.549433	3.509491	0.415236
H	-2.769242	3.765758	0.58641
H	-6.124109	-1.201468	0.682396
H	0.0211	2.480879	-1.299614

H	2.927991	4.875284	0.105475
H	1.756665	3.539968	0.065933
H	2.580569	3.96266	1.588106

Table S35. Z-matrix of optimized conformer 1c6 at B3LYP/6-311+G(d,p) level

Atom	X	Y	Z
C	-0.50964	-3.090649	-0.87513
C	0.333784	-1.840124	-1.160604
C	-0.504812	-0.469575	-1.300241
C	-1.821658	-0.55913	-0.426725
C	-2.607695	-1.787476	-0.943815
C	-1.84366	-3.060454	-0.762441
C	-1.474483	-0.639638	1.090322
C	-2.648047	-0.997144	2.011643
C	-3.940952	-0.219409	1.709517
C	-4.135681	-0.179815	0.162792
C	-2.923507	0.531385	-0.603579
C	-4.046309	-1.63785	-0.396093
O	-3.827478	1.151544	2.15195
C	-5.133119	-0.857071	2.441687
C	-0.786928	-0.245264	-2.798375
C	0.255514	-4.38846	-0.787602
C	1.527422	-1.771883	-0.218776
C	2.795627	-1.802887	-0.626446
C	4.026486	-1.812718	0.256924
C	5.029024	-0.726368	-0.209577
C	4.535355	0.725228	-0.078896
C	4.68893	-3.201837	0.141443
C	5.518928	1.704626	-0.661378
C	6.18898	2.689151	-0.044639
C	7.14816	3.569672	-0.810085
C	6.070994	3.028632	1.420529
C	-2.524743	1.983792	-0.297644
C	-3.590109	3.039973	-0.622496
C	-3.062989	4.472818	-0.556804
O	-2.67925	4.885982	0.764864
H	-2.708036	-1.638899	-2.02253
C	-5.438896	0.502453	-0.205787
O	-6.035291	0.320822	-1.248126
C	0.411552	0.65051	-0.812913

O	0.90455	1.500847	-1.525409
O	3.567996	-1.568661	1.60117
C	4.534593	-1.611813	2.64373
H	0.762766	-1.988708	-2.158711
H	-2.389987	-3.987102	-0.601023
H	-1.074953	0.325687	1.407432
H	-0.685598	-1.37012	1.264008
H	-2.853858	-2.068492	1.945017
H	-2.36479	-0.80951	3.052865
H	-3.235826	0.514181	-1.654186
H	-4.772947	-1.768112	-1.197908
H	-4.282015	-2.375257	0.369772
H	-3.843817	1.15705	3.116386
H	-5.328183	-1.878023	2.110851
H	-4.92043	-0.896678	3.514837
H	-6.043233	-0.268535	2.304499
H	-1.270754	-1.111314	-3.250359
H	0.153582	-0.081377	-3.326701
H	-1.413504	0.631536	-2.973092
H	0.869075	-4.543423	-1.682731
H	-0.42881	-5.233916	-0.692026
H	0.940867	-4.40184	0.064875
H	1.333206	-1.72985	0.847589
H	3.015261	-1.863312	-1.691343
H	5.965744	-0.842865	0.345033
H	5.274984	-0.936261	-1.256473
H	3.581604	0.820692	-0.611215
H	4.324354	0.946827	0.968498
H	5.639237	-3.238654	0.679174
H	4.025265	-3.97214	0.541143
H	4.892863	-3.434488	-0.906327
H	5.705076	1.573003	-1.727794
H	6.849409	4.62281	-0.746138
H	7.201041	3.292621	-1.865094
H	8.158051	3.507209	-0.387455
H	5.391845	2.372254	1.963795
H	7.053069	2.976622	1.904943
H	5.719011	4.059377	1.546677
H	-2.215358	2.086412	0.741257
H	-1.651832	2.204694	-0.922746
H	-3.974999	2.880626	-1.637652
H	-4.438002	2.953458	0.062669
H	-2.218508	4.599425	-1.24637
H	-3.846352	5.170674	-0.859024

H	-1.891783	4.396054	1.02474
H	-5.831838	1.222665	0.532302
H	0.637239	0.658393	0.264727
H	4.00057	-1.362396	3.561416
H	4.977395	-2.606687	2.757179
H	5.33695	-0.880632	2.498399

Table S36. Z-matrix of optimized conformer 1c7 at B3LYP/6-311+G(d,p) level

Atom	X	Y	Z
C	-0.233394	-1.491837	-2.534143
C	-0.656071	-1.799312	-1.092185
C	0.534544	-1.709877	-0.014352
C	1.593105	-0.625321	-0.482692
C	2.118382	-1.108406	-1.857143
C	1.02245	-1.173336	-2.875375
C	0.941733	0.788653	-0.537071
C	1.761925	1.855761	-1.27211
C	3.238965	1.882729	-0.848835
C	3.750426	0.406949	-0.785868
C	2.955888	-0.487231	0.274031
C	3.414703	-0.305068	-2.128766
O	3.363262	2.43994	0.477484
C	4.07183	2.74698	-1.808104
C	1.125275	-3.128275	0.113533
C	-1.317169	-1.641445	-3.573864
C	-1.943143	-1.070642	-0.724601
C	-3.021114	-1.701572	-0.259775
C	-4.376998	-1.12417	0.098715
C	-4.519638	0.397494	-0.118192
C	-3.885334	1.331255	0.934507
C	-4.720358	-1.550423	1.536153
C	-4.217383	2.773358	0.652108
C	-3.388524	3.810154	0.463906
C	-3.932546	5.192404	0.190264
C	-1.883239	3.733712	0.507129
C	2.961338	-0.071206	1.764569
C	3.170931	-1.248902	2.730049
C	2.921469	-0.892399	4.194152
O	1.570748	-0.480315	4.455598
H	2.459024	-2.136105	-1.700295

C	5.219747	0.366368	-0.420533
O	6.02966	-0.414926	-0.87676
C	-0.064002	-1.295571	1.321278
O	-0.030224	-1.966832	2.334981
O	-5.249447	-1.798869	-0.863176
C	-6.649067	-1.822378	-0.599635
H	-0.929687	-2.860834	-1.084992
H	1.267883	-1.015472	-3.923228
H	0.776289	1.13559	0.484868
H	-0.037924	0.744097	-1.008458
H	1.695439	1.698097	-2.351612
H	1.327196	2.843166	-1.083911
H	3.456785	-1.45984	0.214034
H	4.228864	-0.977144	-2.400207
H	3.304927	0.404229	-2.947684
H	3.170079	3.383239	0.421597
H	4.081313	2.352286	-2.82504
H	3.648796	3.755808	-1.851947
H	5.104452	2.832679	-1.460042
H	1.313973	-3.565608	-0.86695
H	0.412565	-3.774235	0.629363
H	2.055239	-3.149796	0.681722
H	-1.78003	-2.633426	-3.517427
H	-0.910502	-1.510274	-4.578593
H	-2.122642	-0.914138	-3.432889
H	-1.971691	0.00276	-0.884624
H	-2.973992	-2.781578	-0.123746
H	-4.130738	0.642832	-1.111036
H	-5.590558	0.619727	-0.149996
H	-4.285161	1.072656	1.921956
H	-2.807066	1.174704	0.990603
H	-5.676924	-1.139659	1.867527
H	-4.765917	-2.640281	1.603607
H	-3.950027	-1.203626	2.226895
H	-5.286727	2.979474	0.596115
H	-3.599381	5.902566	0.956423
H	-5.024224	5.202509	0.166273
H	-3.564222	5.574772	-0.769158
H	-1.506336	2.730469	0.702092
H	-1.455191	4.079388	-0.440966
H	-1.489905	4.398916	1.2848
H	3.745936	0.661383	1.949858
H	2.034746	0.44875	2.016887
H	2.522324	-2.090418	2.47229

H	4.199558	-1.618881	2.64131
H	3.178188	-1.750424	4.82836
H	3.54986	-0.052161	4.502738
H	0.969846	-1.093568	4.009089
H	5.533326	1.09381	0.34933
H	-0.542758	-0.30536	1.352452
H	-7.113978	-2.258566	-1.484715
H	-6.894879	-2.4442	0.267217
H	-7.066526	-0.820967	-0.447809

Table S37. Z-matrix of optimized conformer 1c8 at B3LYP/6-311+G(d,p) level

Atom	X	Y	Z
C	0.908585	-1.732294	-0.802273
C	0.877171	-0.214431	-1.021656
C	-0.600959	0.423395	-1.139007
C	-1.645655	-0.431526	-0.332502
C	-1.555547	-1.873992	-0.901082
C	-0.200052	-2.477465	-0.727315
C	-1.35162	-0.351223	1.193167
C	-2.130929	-1.340824	2.069607
C	-3.623206	-1.465329	1.718238
C	-3.758546	-1.509508	0.165563
C	-3.179572	-0.20061	-0.551851
C	-2.811124	-2.618671	-0.396238
O	-4.355543	-0.302854	2.166926
C	-4.229157	-2.701526	2.404508
C	-0.945571	0.515267	-2.651243
C	2.27907	-2.357868	-0.726974
C	1.774479	0.490033	-0.009926
C	2.867318	1.184454	-0.332016
C	3.828558	1.88874	0.608766
C	5.262654	1.340743	0.41774
C	5.483988	-0.148546	0.738207
C	3.409404	1.847196	2.081207
C	6.942312	-0.518438	0.660254
C	7.550733	-1.350751	-0.196983
C	9.039664	-1.591078	-0.116761
C	6.857266	-2.117067	-1.29569
C	-3.754893	1.189101	-0.243361
C	-5.245158	1.37012	-0.562547

C	-5.669989	2.833142	-0.455778
O	-7.074938	3.02579	-0.681592
H	-1.708965	-1.775678	-1.979682
C	-5.20057	-1.727871	-0.250717
O	-5.540498	-2.173974	-1.328335
C	-0.427275	1.886053	-0.722841
O	-0.953515	2.484689	0.187321
O	3.974184	3.268274	0.159252
C	2.841228	4.120889	0.288098
H	1.344069	-0.039944	-1.998687
H	-0.11387	-3.55534	-0.608768
H	-1.560107	0.66704	1.517594
H	-0.292106	-0.524414	1.376885
H	-1.671799	-2.331047	2.003473
H	-2.046606	-1.04287	3.120556
H	-3.384442	-0.383106	-1.613526
H	-3.300759	-3.141529	-1.217667
H	-2.57588	-3.364334	0.361723
H	-4.379881	-0.319683	3.130974
H	-3.777956	-3.633182	2.059635
H	-4.058875	-2.636822	3.48415
H	-5.307802	-2.757671	2.241179
H	-0.847233	-0.450731	-3.146816
H	-0.256272	1.199339	-3.153585
H	-1.959389	0.885562	-2.81649
H	2.883424	-2.086663	-1.600172
H	2.203182	-3.446413	-0.689556
H	2.833325	-2.022902	0.154164
H	1.501472	0.38531	1.035686
H	3.141457	1.28111	-1.382747
H	5.551096	1.528644	-0.621515
H	5.923431	1.95227	1.04144
H	5.129013	-0.357919	1.754213
H	4.882177	-0.763237	0.067594
H	4.121446	2.422059	2.678347
H	2.413126	2.264417	2.237292
H	3.397533	0.823492	2.458531
H	7.570284	-0.024861	1.402242
H	9.2561	-2.654247	0.042024
H	9.500583	-1.023537	0.694355
H	9.531902	-1.310816	-1.055612
H	7.308646	-1.882501	-2.266642
H	6.983463	-3.196207	-1.14853
H	5.790012	-1.908391	-1.361389

H	-3.571887	1.468293	0.791842
H	-3.197265	1.898595	-0.861908
H	-5.460689	1.013184	-1.578128
H	-5.861393	0.787621	0.127179
H	-5.484705	3.210458	0.552752
H	-5.090469	3.450458	-1.153913
H	-7.27745	2.738986	-1.579229
H	-5.967538	-1.435507	0.486491
H	0.271047	2.424839	-1.394001
H	3.092192	5.042777	-0.238118
H	1.946213	3.686315	-0.167918
H	2.624982	4.362687	1.33412

Table S38. Z-matrix of optimized conformer 1c9 at B3LYP/6-311+G(d,p) level

Atom	X	Y	Z
C	0.734246	-1.95525	-0.421446
C	0.817174	-0.456415	-0.741195
C	-0.595916	0.256889	-1.056291
C	-1.757825	-0.508223	-0.301269
C	-1.707617	-1.974671	-0.794876
C	-0.41611	-2.640224	-0.43881
C	-1.598915	-0.371963	1.241902
C	-2.506398	-1.286404	2.075466
C	-3.969237	-1.320829	1.597886
C	-3.972566	-1.413285	0.041698
C	-3.23918	-0.175443	-0.660059
C	-3.063006	-2.606337	-0.399103
O	-4.64915	-0.094147	1.944573
C	-4.721021	-2.484763	2.264198
C	-0.777444	0.275631	-2.586181
C	2.051518	-2.63767	-0.144348
C	1.684837	0.267747	0.2785
C	2.801455	0.925975	-0.035789
C	3.757295	1.622676	0.916781
C	5.077388	0.824384	1.046908
C	5.834765	0.538517	-0.263428
C	3.174572	1.840056	2.319698
C	7.198537	-0.042752	-0.000123
C	7.675869	-1.25003	-0.336182
C	9.086796	-1.65162	0.023667

C	6.902414	-2.307454	-1.084319
C	-3.702619	1.270677	-0.430896
C	-5.119706	1.590077	-0.92657
C	-5.435749	3.078864	-0.938034
O	-5.419453	3.575776	0.411284
H	-1.737025	-1.918314	-1.886551
C	-5.386394	-1.535888	-0.493486
O	-5.671591	-2.025992	-1.567675
C	-0.473196	1.701223	-0.573816
O	-0.411332	2.670828	-1.301457
O	4.160731	2.887475	0.330969
C	3.139788	3.862371	0.141841
H	1.366066	-0.381357	-1.68713
H	-0.406598	-3.710883	-0.247252
H	-1.806444	0.661681	1.524905
H	-0.570111	-0.571739	1.538962
H	-2.10736	-2.30431	2.069406
H	-2.488643	-0.962447	3.121444
H	-3.366596	-0.37435	-1.730683
H	-3.510983	-3.111215	-1.254772
H	-2.965496	-3.347352	0.393219
H	-4.802614	-0.095953	2.89682
H	-4.31243	-3.457783	1.988172
H	-4.640386	-2.392922	3.352261
H	-5.7825	-2.468996	2.006454
H	-0.673139	-0.720418	-3.016297
H	-0.012082	0.909728	-3.036336
H	-1.747497	0.681055	-2.880145
H	2.76728	-2.456243	-0.954291
H	1.913664	-3.716278	-0.045062
H	2.519023	-2.265902	0.772421
H	1.376679	0.206832	1.317949
H	3.104589	0.972777	-1.080311
H	5.728775	1.393684	1.719794
H	4.8514	-0.121795	1.548144
H	5.243675	-0.121851	-0.900291
H	5.949652	1.482084	-0.808187
H	3.87699	2.425932	2.917204
H	2.218197	2.365639	2.293688
H	3.017933	0.884398	2.824352
H	7.870666	0.620344	0.545368
H	9.089881	-2.551757	0.649834
H	9.610842	-0.858704	0.561515
H	9.665361	-1.896939	-0.874997

H	5.877409	-2.015349	-1.310689
H	7.402086	-2.550266	-2.02963
H	6.869573	-3.237166	-0.504486
H	-3.617593	1.554198	0.615079
H	-3.014881	1.909613	-0.996612
H	-5.251321	1.220784	-1.950822
H	-5.865951	1.086407	-0.305252
H	-4.696028	3.618439	-1.54338
H	-6.423932	3.244089	-1.383584
H	-5.605457	4.520308	0.387788
H	-6.182986	-1.122727	0.148691
H	-0.426687	1.847807	0.516687
H	3.588105	4.667132	-0.442392
H	2.284464	3.457717	-0.40933
H	2.786256	4.275661	1.092831

Table S39. Z-matrix of optimized conformer 1c10 at B3LYP/6-311+G(d,p) level

Atom	X	Y	Z
C	0.087600	-2.949576	-0.887582
C	-0.389476	-2.258831	0.3938
C	0.727551	-1.339989	1.105883
C	1.705377	-0.71844	0.040494
C	2.339335	-1.933709	-0.695879
C	1.319295	-2.783778	-1.384454
C	0.931995	0.241252	-0.907902
C	1.683637	0.659038	-2.178606
C	3.143294	1.074639	-1.935317
C	3.780721	0.049581	-0.944155
C	3.036402	0.001745	0.47077
C	3.553602	-1.391409	-1.482797
O	3.19644	2.373264	-1.305449
C	3.915281	1.161987	-3.261878
C	1.453569	-2.260557	2.130883
C	-0.907557	-3.876995	-1.540051
C	-1.732013	-1.570837	0.17579
C	-2.822691	-1.831962	0.89805
C	-4.20708	-1.219688	0.771784
C	-4.346865	-0.123847	-0.306118
C	-3.742762	1.256214	0.034386
C	-4.654841	-0.716749	2.149812

C	-3.758039	2.175515	-1.158321
C	-4.432478	3.322836	-1.321887
C	-4.318238	4.109858	-2.605938
C	-5.343443	3.944553	-0.292766
C	3.01272	1.302588	1.301577
C	3.080683	1.070583	2.818844
C	2.873845	2.3419	3.639256
O	1.599637	2.967536	3.414757
H	2.777233	-2.556275	0.089863
C	5.238812	0.379126	-0.694944
O	6.105765	-0.441603	-0.471539
C	-0.052809	-0.360553	1.975584
O	0.011238	0.850479	1.978096
O	-5.149663	-2.300245	0.497573
C	-5.032128	-2.965616	-0.75653
H	-0.592409	-3.061562	1.113082
H	1.612726	-3.331784	-2.277237
H	0.660467	1.127825	-0.335013
H	-0.001128	-0.216601	-1.228143
H	1.662526	-0.158619	-2.904037
H	1.159562	1.495101	-2.654735
H	3.624721	-0.725608	1.042674
H	4.437281	-2.000108	-1.290519
H	3.389488	-1.400239	-2.559426
H	2.91519	3.027411	-1.955996
H	3.978547	0.201004	-3.774178
H	3.405112	1.858939	-3.934787
H	4.92945	1.536534	-3.101026
H	1.737337	-3.208038	1.672388
H	0.786193	-2.501235	2.963184
H	2.348646	-1.796654	2.545286
H	-1.29043	-4.611896	-0.822763
H	-0.446544	-4.416824	-2.369615
H	-1.775795	-3.334943	-1.927023
H	-1.785079	-0.841211	-0.625412
H	-2.758288	-2.578561	1.689904
H	-3.914414	-0.477186	-1.247052
H	-5.418765	0.004358	-0.490065
H	-4.282151	1.696808	0.873702
H	-2.70641	1.12994	0.367716
H	-5.661848	-0.295856	2.089331
H	-4.668987	-1.548241	2.858045
H	-3.976975	0.048207	2.531735
H	-3.139966	1.840991	-1.991778

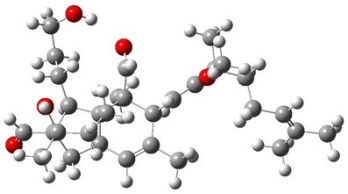
H	-5.300901	4.238079	-3.075091
H	-3.656368	3.62203	-3.324569
H	-3.932379	5.117998	-2.413072
H	-5.43226	3.356096	0.619989
H	-4.985219	4.943748	-0.018339
H	-6.349119	4.079766	-0.707402
H	3.867228	1.924833	1.028796
H	2.1339	1.892689	1.055251
H	2.34169	0.333959	3.144141
H	4.058992	0.65422	3.088148
H	2.983229	2.109173	4.70606
H	3.629076	3.092123	3.384941
H	0.957295	2.286937	3.172089
H	5.488961	1.454665	-0.687665
H	-0.720053	-0.868212	2.697461
H	-5.725357	-3.807001	-0.720455
H	-5.31139	-2.318134	-1.594468
H	-4.019744	-3.347361	-0.922152

Table S40. Z-matrix of optimized conformer **1c11** at B3LYP/6-311+G(d,p) level

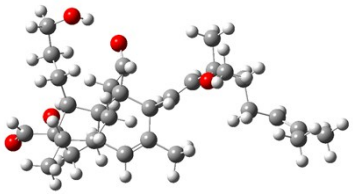
Atom	X	Y	Z
C	0.835222	-1.821853	-0.696066
C	0.84047	-0.310015	-0.963932
C	-0.617967	0.348855	-1.17501
C	-1.69924	-0.484011	-0.372554
C	-1.623413	-1.931993	-0.914696
C	-0.286192	-2.552668	-0.664972
C	-1.445506	-0.385644	1.160648
C	-2.259537	-1.360015	2.021806
C	-3.747075	-1.445035	1.638882
C	-3.849067	-1.492459	0.083791
C	-3.213936	-0.204679	-0.625034
C	-2.922222	-2.632284	-0.45174
O	-4.453692	-0.259159	2.066038
C	-4.403588	-2.659296	2.316819
C	-0.893137	0.396258	-2.690475
C	2.191044	-2.462704	-0.532959
C	1.733971	0.419536	0.030797
C	2.807275	1.131571	-0.316773
C	3.765507	1.869946	0.599895

C	5.198219	1.306725	0.443701
C	5.410586	-0.167172	0.833188
C	3.333239	1.894393	2.069271
C	6.867548	-0.54725	0.780223
C	7.478875	-1.410847	-0.043249
C	8.965484	-1.657055	0.059373
C	6.790877	-2.208875	-1.122628
C	-3.721433	1.212736	-0.321457
C	-5.183722	1.482124	-0.699095
C	-5.569032	2.958146	-0.617327
O	-5.450102	3.509822	0.703709
H	-1.727023	-1.845494	-1.999623
C	-5.287895	-1.661405	-0.364463
O	-5.619774	-2.114947	-1.441231
C	-0.529407	1.785265	-0.663296
O	-0.552456	2.77282	-1.368685
O	3.922518	3.228213	0.095652
C	2.78012	4.078719	0.139447
H	1.33107	-0.180002	-1.93568
H	-0.221337	-3.628242	-0.516683
H	-1.672824	0.630321	1.488553
H	-0.392914	-0.554345	1.383204
H	-1.81957	-2.358839	1.960261
H	-2.187288	-1.06472	3.073995
H	-3.404397	-0.377788	-1.690715
H	-3.403729	-3.133185	-1.291382
H	-2.739801	-3.389658	0.309204
H	-4.518413	-0.279583	3.028198
H	-3.972094	-3.6056	1.987421
H	-4.256884	-2.593397	3.399835
H	-5.479216	-2.684527	2.127789
H	-0.768495	-0.581956	-3.154849
H	-0.188665	1.078691	-3.168427
H	-1.898218	0.759591	-2.913255
H	2.839996	-2.231368	-1.385412
H	2.098058	-3.548145	-0.459751
H	2.708283	-2.102118	0.360761
H	1.481182	0.322478	1.08245
H	3.066644	1.215744	-1.372209
H	5.493877	1.445643	-0.601209
H	5.858086	1.943235	1.042985
H	5.05094	-0.328528	1.85621
H	4.808387	-0.809248	0.189009
H	4.044073	2.489847	2.647346

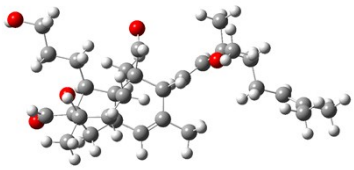
H	2.33877	2.325924	2.195632
H	3.309597	0.888814	2.492035
H	7.491944	-0.032552	1.510758
H	9.173625	-2.715313	0.257337
H	9.42219	-1.064268	0.854696
H	9.468389	-1.412743	-0.883831
H	5.725803	-1.995299	-1.205924
H	7.253176	-2.009463	-2.096299
H	6.908224	-3.283378	-0.938706
H	-3.569479	1.47433	0.722807
H	-3.107215	1.896826	-0.918306
H	-5.376593	1.149438	-1.726765
H	-5.857812	0.911766	-0.051157
H	-4.903902	3.561193	-1.240711
H	-6.591724	3.096913	-0.988068
H	-6.057646	3.036666	1.283619
H	-6.059152	-1.320766	0.347427
H	-0.425427	1.909849	0.426091
H	2.512174	4.354689	1.164983
H	3.055868	4.98446	-0.402446
H	1.911112	3.626026	-0.34777



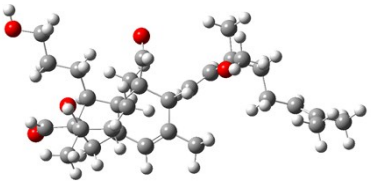
1d1 (7.70%)



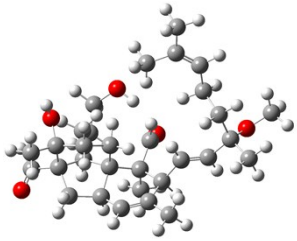
1d2 (9.31%)

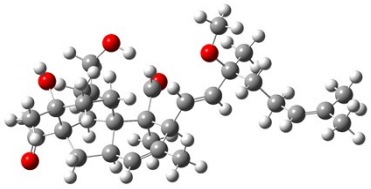


1d3 (35.37%)



1d4 (26.86%)





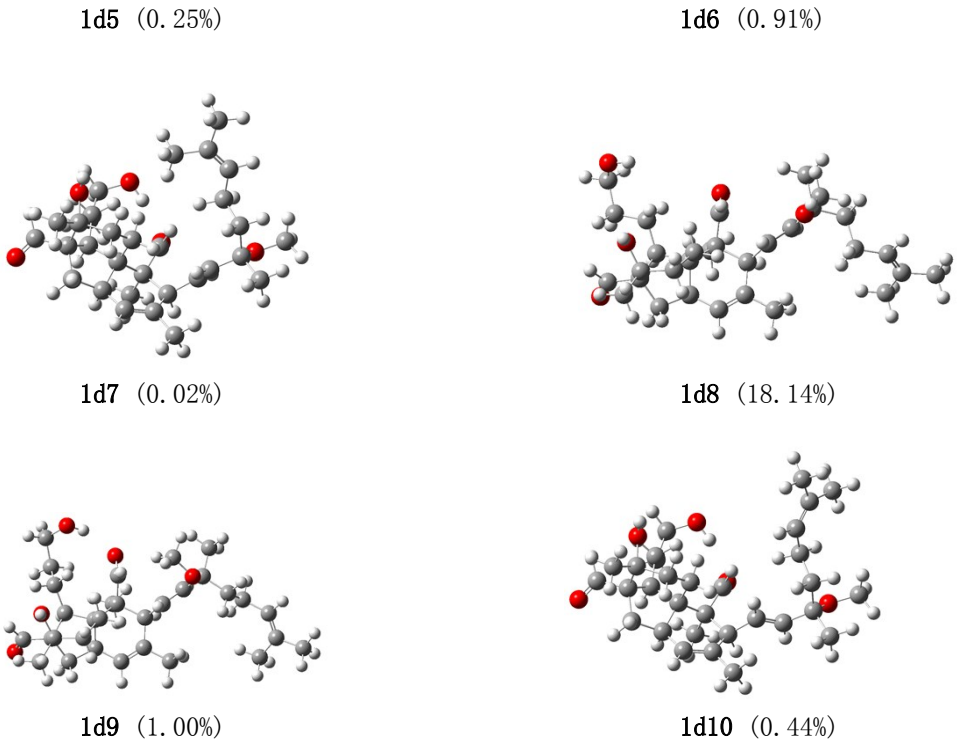


Figure S7. Reoptimized geometries of **1d** at B3LYP/6-311+G(d,p) level with the CPCM model in MeOH.

Table S41. Z-matrix of optimized conformer 1d1 at B3LYP/6-311+G(d,p) level

Atom	X	Y	Z
C	0.510648	-1.965505	-0.680424
C	0.618011	-0.454465	-0.922789
C	-0.792475	0.286943	-1.144511
C	-1.924752	-0.473941	-0.333884
C	-1.955863	-1.914663	-0.899949
C	-0.656811	-2.622634	-0.667183
C	-1.629596	-0.424659	1.194693
C	-2.465275	-1.384234	2.049459
C	-3.964473	-1.344048	1.718059
C	-4.11658	-1.347503	0.161744
C	-3.427192	-0.086544	-0.538827
C	-3.296619	-2.532966	-0.428533
O	-4.5461	-0.115164	2.204888
C	-4.706433	-2.516574	2.377918
C	-1.043742	0.321864	-2.665639

C	1.823333	-2.692214	-0.522642
C	1.54764	0.213607	0.079434
C	2.611597	0.93339	-0.274746
C	3.56301	1.659867	0.653331
C	5.026888	1.267639	0.327796
C	5.374785	-0.214695	0.551647
C	3.381267	3.177173	0.437797
C	6.841442	-0.485604	0.348133
C	7.429651	-1.27758	-0.560245
C	8.932787	-1.417624	-0.607383
C	6.698235	-2.093525	-1.59715
C	-3.906963	1.336277	-0.163887
C	-4.068435	2.268466	-1.375772
C	-4.284175	3.732757	-0.998222
O	-3.17829	4.302186	-0.280403
H	-2.065369	-1.806887	-1.98269
C	-0.667278	1.712335	-0.627001
O	-0.801243	2.710989	-1.309236
O	3.197438	1.280457	1.993864
C	3.906388	1.886308	3.067894
C	-5.578688	-1.357271	-0.232507
O	-6.039582	-1.955669	-1.183397
H	1.122534	-0.346556	-1.890303
H	-0.661559	-3.70286	-0.539252
H	-1.809069	0.591053	1.552275
H	-0.581319	-0.640992	1.388497
H	-2.095349	-2.405613	1.933525
H	-2.336111	-1.135145	3.108276
H	-3.6557	-0.227786	-1.601258
H	-3.834608	-2.964521	-1.27265
H	-3.156465	-3.332037	0.298136
H	-4.578242	-0.163663	3.167615
H	-5.784062	-2.440956	2.211416
H	-4.532251	-2.497129	3.458624
H	-4.366543	-3.485846	2.010362
H	-0.870818	-0.655833	-3.115636
H	-2.053724	0.642309	-2.921427
H	-0.350656	1.023894	-3.132828
H	1.664103	-3.770288	-0.454044
H	2.485576	-2.49638	-1.373889
H	2.362901	-2.366636	0.371743
H	1.338564	0.092133	1.136799
H	2.842389	1.062882	-1.331081
H	5.699451	1.895582	0.921758

H	5.217752	1.533064	-0.717391
H	4.759657	-0.837314	-0.100345
H	5.102588	-0.484467	1.579159
H	4.116977	3.753926	1.003253
H	2.378544	3.485645	0.742562
H	3.509881	3.424533	-0.618502
H	7.496848	0.048697	1.036678
H	9.324083	-1.108676	-1.584008
H	9.421763	-0.817372	0.162781
H	9.233127	-2.463235	-0.469596
H	7.04517	-1.83103	-2.603366
H	6.912583	-3.160642	-1.464934
H	5.617075	-1.961486	-1.567915
H	-3.225993	1.789849	0.559241
H	-4.86358	1.286989	0.355104
H	-4.925188	1.943586	-1.978544
H	-3.196883	2.215854	-2.034193
H	-5.150256	3.841937	-0.339317
H	-4.480403	4.318776	-1.905166
H	-2.357344	4.038598	-0.720161
H	-0.459122	1.824422	0.447522
H	3.766591	2.971766	3.096836
H	4.979039	1.666782	3.035165
H	3.492917	1.458138	3.981781
H	-6.239273	-0.731724	0.393991

Table S42. Z-matrix of optimized conformer **1d2** at B3LYP/6-311+G(d,p) level

Atom	X	Y	Z
C	0.402919	-1.732275	-1.325547
C	0.461991	-0.198499	-1.290586
C	-0.9745	0.52004	-1.21038
C	-1.991401	-0.41397	-0.427763
C	-2.072607	-1.728114	-1.242447
C	-0.746049	-2.421072	-1.299115
C	-1.518511	-0.635014	1.040282
C	-2.240829	-1.759666	1.792439
C	-3.769603	-1.708854	1.644607
C	-4.100001	-1.433673	0.141146
C	-3.510719	-0.045035	-0.386185
C	-3.339859	-2.466211	-0.742332

O	-4.305044	-0.610169	2.413924
C	-4.416097	-3.005905	2.154456
C	-1.405959	0.818797	-2.660029
C	1.733188	-2.43068	-1.461757
C	1.491942	0.30442	-0.290524
C	2.527768	1.07263	-0.626542
C	3.579028	1.633898	0.308307
C	4.993381	1.207627	-0.164386
C	5.268727	-0.30568	-0.12191
C	3.47275	3.172852	0.285471
C	6.62959	-0.64656	-0.667024
C	7.662577	-1.228277	-0.039939
C	8.961002	-1.48897	-0.766161
C	7.656813	-1.67903	1.399734
C	-3.956925	1.270867	0.296051
C	-4.299207	2.39204	-0.698608
C	-4.492031	3.757109	-0.040898
O	-3.31247	4.240188	0.620772
H	-2.313208	-1.42963	-2.266495
C	-0.811608	1.833078	-0.459915
O	-1.045363	2.931771	-0.927811
O	3.281071	1.114766	1.618885
C	4.099816	1.545103	2.699406
C	-5.597491	-1.419401	-0.082289
O	-6.161283	-1.872374	-1.057839
H	0.849834	0.103944	-2.270576
H	-0.72148	-3.505794	-1.376376
H	-1.659249	0.29324	1.598052
H	-0.453466	-0.854106	1.069132
H	-1.875446	-2.729877	1.44695
H	-1.991071	-1.704843	2.857435
H	-3.85911	0.002088	-1.424149
H	-3.966913	-2.75991	-1.58426
H	-3.105088	-3.37601	-0.191483
H	-4.244327	-0.844975	3.347461
H	-5.50669	-2.935616	2.129915
H	-4.114921	-3.180109	3.19256
H	-4.112971	-3.879373	1.575695
H	-1.278181	-0.0561	-3.297393
H	-2.442371	1.147908	-2.7335
H	-0.780778	1.615243	-3.067862
H	1.595085	-3.506991	-1.583448
H	2.287271	-2.055293	-2.329856
H	2.371195	-2.262348	-0.589149

H	1.385763	0.014488	0.749105
H	2.660625	1.368993	-1.666043
H	5.743154	1.730583	0.438356
H	5.124482	1.575717	-1.187836
H	4.506872	-0.814729	-0.724184
H	5.143341	-0.669867	0.898929
H	4.273892	3.639273	0.863348
H	2.51064	3.492187	0.69279
H	3.550041	3.538755	-0.740956
H	6.777703	-0.369617	-1.711294
H	9.203259	-2.558445	-0.762554
H	8.9217	-1.150958	-1.803842
H	9.796025	-0.979987	-0.270177
H	6.72223	-1.464558	1.917174
H	7.839213	-2.758356	1.463366
H	8.469702	-1.195437	1.953903
H	-3.187541	1.618887	0.988433
H	-4.830083	1.095052	0.923001
H	-5.222683	2.139901	-1.233898
H	-3.52356	2.492968	-1.463192
H	-5.2649	3.711395	0.731624
H	-4.818852	4.483471	-0.795895
H	-2.550222	4.085385	0.044751
H	-0.475119	1.758637	0.584987
H	4.031642	2.624818	2.867149
H	5.151498	1.273188	2.558947
H	3.724798	1.031707	3.585601
H	-6.185601	-0.917798	0.70695

Table S43. Z-matrix of optimized conformer **1d3** at B3LYP/6-311+G(d,p) level

Atom	X	Y	Z
C	0.645215	-1.725713	-1.22387
C	0.660841	-0.192423	-1.282005
C	-0.79338	0.506919	-1.236652
C	-1.80211	-0.415272	-0.437905
C	-1.824031	-1.777548	-1.172668
C	-0.484271	-2.442131	-1.162954
C	-1.385522	-0.52425	1.058875
C	-2.127491	-1.596126	1.86818
C	-3.649672	-1.612306	1.641207

C	-3.916837	-1.450458	0.114108
C	-3.327233	-0.088114	-0.483388
C	-3.081513	-2.519984	-0.664015
O	-4.276505	-0.486555	2.29603
C	-4.260774	-2.898977	2.220092
C	-1.232454	0.76654	-2.690069
C	1.994995	-2.395241	-1.304017
C	1.673606	0.38013	-0.300955
C	2.7001	1.148793	-0.662552
C	3.732316	1.770879	0.255145
C	5.159389	1.362691	-0.194688
C	5.472876	-0.139899	-0.090527
C	3.589354	3.30476	0.174321
C	6.842093	-0.468013	-0.622294
C	7.887516	-1.002888	0.025618
C	9.192824	-1.258619	-0.689881
C	7.890097	-1.402333	1.480394
C	-3.764734	1.279579	0.062839
C	-5.253998	1.609434	-0.106267
C	-5.558017	3.060429	0.261066
O	-6.954571	3.379073	0.168757
H	-2.046787	-1.543833	-2.217719
C	-0.605156	1.856004	-0.545401
O	-0.685217	2.93438	-1.097471
O	3.440447	1.293687	1.583222
C	4.237225	1.790055	2.651708
C	-5.398859	-1.543753	-0.194847
O	-5.852434	-1.836447	-1.28286
H	1.044469	0.066041	-2.276154
H	-0.432231	-3.52859	-1.168151
H	-1.555647	0.441543	1.538781
H	-0.318781	-0.725755	1.145588
H	-1.723585	-2.583038	1.627452
H	-1.936382	-1.444961	2.935941
H	-3.635077	-0.112558	-1.535081
H	-3.66388	-2.899658	-1.503273
H	-2.83771	-3.37299	-0.032326
H	-4.26772	-0.650337	3.24653
H	-5.350937	-2.886037	2.151681
H	-3.993764	-2.982038	3.278588
H	-3.893459	-3.796579	1.72075
H	-1.18144	-0.139834	-3.2932
H	-2.246779	1.165841	-2.748756
H	-0.567725	1.502163	-3.145521

H	1.884756	-3.479644	-1.370029
H	2.551809	-2.052751	-2.183873
H	2.617003	-2.165456	-0.433919
H	1.561121	0.134647	0.74962
H	2.83689	1.400287	-1.713257
H	5.892923	1.928823	0.388689
H	5.285252	1.692583	-1.231745
H	4.723774	-0.69204	-0.670516
H	5.357211	-0.464825	0.944502
H	4.374229	3.810554	0.741376
H	2.61639	3.616254	0.561318
H	3.667559	3.634265	-0.864315
H	6.985321	-0.22468	-1.675576
H	9.1481	-0.956344	-1.73832
H	10.015307	-0.714906	-0.21006
H	9.458695	-2.32173	-0.650345
H	6.948976	-1.194285	1.988506
H	8.100606	-2.473545	1.582517
H	8.688691	-0.878098	2.018181
H	-3.198067	2.032418	-0.496574
H	-3.494861	1.389533	1.112245
H	-5.864015	0.962416	0.529363
H	-5.561783	1.434581	-1.145204
H	-4.974868	3.743405	-0.369476
H	-5.285178	3.254639	1.301072
H	-7.228252	3.27266	-0.7493
H	-0.369049	1.821673	0.529339
H	4.129916	2.87191	2.781108
H	5.298723	1.550881	2.526097
H	3.875217	1.294811	3.553523
H	-6.083093	-1.3035	0.636911

Table S44. Z-matrix of optimized conformer **1d4** at B3LYP/6-311+G(d,p) level

Atom	X	Y	Z
C	0.646452	-1.731737	-1.213144
C	0.662392	-0.198778	-1.2785
C	-0.791722	0.501465	-1.23796
C	-1.802422	-0.417438	-0.437886
C	-1.822778	-1.782744	-1.166919
C	-0.483275	-2.447629	-1.151204

C	-1.389523	-0.519841	1.060393
C	-2.133149	-1.588503	1.872406
C	-3.654797	-1.60572	1.641937
C	-3.918522	-1.450085	0.113569
C	-3.327373	-0.090095	-0.488184
C	-3.081618	-2.522821	-0.658292
O	-4.283173	-0.477455	2.290983
C	-4.267266	-2.890083	2.22449
C	-1.228351	0.756647	-2.692871
C	1.996276	-2.401845	-1.28752
C	1.674374	0.377776	-0.298965
C	2.700942	1.145277	-0.6628
C	3.732719	1.770673	0.253147
C	5.160065	1.363102	-0.196281
C	5.475234	-0.138913	-0.089103
C	3.588014	3.304208	0.168994
C	6.844343	-0.466692	-0.621358
C	7.890667	-0.999839	0.02651
C	9.195648	-1.255516	-0.68961
C	7.894615	-1.397346	1.481815
C	-3.765071	1.279948	0.051818
C	-5.253004	1.608984	-0.125534
C	-5.55808	3.054932	0.236951
O	-6.967748	3.278739	0.069109
H	-2.042869	-1.553383	-2.213512
C	-0.603565	1.852592	-0.550734
O	-0.68251	2.929342	-1.106129
O	3.44184	1.296136	1.582413
C	4.238463	1.795689	2.649521
C	-5.399862	-1.544522	-0.198187
O	-5.851219	-1.844271	-1.28518
H	1.047163	0.054944	-2.273431
H	-0.431476	-3.534113	-1.151238
H	-1.56182	0.447916	1.535461
H	-0.322832	-0.720053	1.150993
H	-1.728549	-2.576374	1.636903
H	-1.944689	-1.432754	2.939989
H	-3.63289	-0.118662	-1.540425
H	-3.662187	-2.905605	-1.497371
H	-2.839528	-3.373432	-0.022721
H	-4.276976	-0.637975	3.242055
H	-5.357241	-2.877535	2.152997
H	-4.003157	-2.968763	3.284046
H	-3.898497	-3.7897	1.729886

H	-1.177841	-0.151933	-3.292713
H	-2.242026	1.157157	-2.754288
H	-0.561953	1.489719	-3.149994
H	1.885948	-3.486517	-1.348787
H	2.554871	-2.063497	-2.167856
H	2.616685	-2.168186	-0.417299
H	1.561427	0.135868	0.752403
H	2.838107	1.393084	-1.714329
H	5.893199	1.931296	0.385587
H	5.28514	1.690933	-1.234088
H	4.726204	-0.693111	-0.667232
H	5.360833	-0.461716	0.946732
H	4.372481	3.812097	0.734751
H	2.614796	3.615428	0.555568
H	3.665573	3.631557	-0.870372
H	6.986608	-0.224723	-1.675087
H	9.462346	-2.318377	-0.64891
H	9.149934	-0.954616	-1.738402
H	10.018077	-0.71058	-0.211089
H	6.953678	-1.1894	1.990314
H	8.106048	-2.468256	1.585192
H	8.693173	-0.871767	2.018341
H	-3.195463	2.02984	-0.508465
H	-3.498014	1.392932	1.101575
H	-5.864497	0.963194	0.51019
H	-5.560317	1.435444	-1.163322
H	-4.990618	3.736462	-0.408964
H	-5.268162	3.253641	1.276276
H	-7.160555	4.192636	0.304096
H	-0.368395	1.821312	0.52429
H	5.300169	1.557338	2.524082
H	3.877273	1.302048	3.552544
H	4.130079	2.877719	2.776573
H	-6.085739	-1.298342	0.63048

Table S45. Z-matrix of optimized conformer **1d5** at B3LYP/6-311+G(d,p) level

Atom	X	Y	Z
C	0.066236	-2.858255	-1.218935
C	-0.520499	-2.215442	0.044891
C	0.545171	-1.39567	0.926082

C	1.653991	-0.773439	-0.023978
C	2.329046	-1.974131	-0.7292
C	1.354347	-2.740662	-1.56883
C	1.018108	0.241204	-1.020008
C	1.924251	0.672062	-2.180413
C	3.343025	1.058757	-1.734948
C	3.835861	-0.014073	-0.710809
C	2.921267	-0.099326	0.596617
C	3.650185	-1.431288	-1.330541
O	3.318357	2.330516	-1.051634
C	4.284854	1.185477	-2.942022
C	1.11368	-2.383171	1.965547
C	-0.891805	-3.70306	-2.022888
C	-1.835332	-1.504873	-0.253374
C	-2.976957	-1.81713	0.359332
C	-4.374801	-1.298287	0.083368
C	-4.447442	0.02249	-0.713185
C	-3.902164	1.280106	-0.008695
C	-5.133429	-2.402114	-0.682976
C	-4.337585	2.540116	-0.709858
C	-3.587698	3.475865	-1.309792
C	-4.228165	4.679108	-1.960588
C	-2.082799	3.448658	-1.403064
C	2.757732	1.155219	1.487488
C	2.869935	0.856824	2.991696
C	2.461617	2.029107	3.881739
O	1.088471	2.416191	3.716804
H	2.647237	-2.647817	0.071586
C	-0.192611	-0.281542	1.651507
O	-0.268708	-0.171923	2.860411
O	-4.924648	-1.135487	1.419347
C	-6.302721	-0.797872	1.5353
C	5.254098	0.28038	-0.268473
O	6.107543	-0.558067	-0.06069
H	-0.803089	-3.05091	0.695858
H	1.717961	-3.263565	-2.450625
H	0.725673	1.137136	-0.468637
H	0.106981	-0.167441	-1.451548
H	1.982981	-0.126902	-2.923517
H	1.474585	1.528611	-2.693903
H	3.421685	-0.858414	1.208364
H	4.48809	-2.068127	-1.046756
H	3.63284	-1.398502	-2.418859
H	3.148947	3.01636	-1.708362

H	5.270062	1.544451	-2.633103
H	3.872891	1.908959	-3.652928
H	4.41201	0.241529	-3.473979
H	1.39641	-3.326449	1.498338
H	1.982113	-1.988516	2.492641
H	0.349827	-2.603351	2.71329
H	-0.371005	-4.208746	-2.838478
H	-1.365987	-4.465081	-1.393693
H	-1.701907	-3.105312	-2.451759
H	-1.831172	-0.748694	-1.032827
H	-2.965174	-2.588456	1.128176
H	-5.496996	0.194968	-0.973657
H	-3.934021	-0.119806	-1.669406
H	-2.816367	1.226608	0.075328
H	-4.287082	1.294765	1.017222
H	-6.169147	-2.115359	-0.879068
H	-5.130847	-3.335483	-0.114365
H	-4.649116	-2.583439	-1.644739
H	-5.41773	2.689151	-0.725947
H	-3.972089	4.731022	-3.02545
H	-5.316303	4.659501	-1.870486
H	-3.863368	5.608829	-1.50784
H	-1.638832	2.559424	-0.957587
H	-1.765524	3.496852	-2.451188
H	-1.651724	4.32688	-0.908162
H	1.803595	1.64501	1.282213
H	3.509337	1.901518	1.233948
H	3.904834	0.58936	3.237255
H	2.259375	-0.006797	3.26945
H	3.048846	2.920656	3.644234
H	2.652875	1.774626	4.93199
H	0.542406	1.617323	3.70295
H	-0.672379	0.478582	1.016771
H	-6.956359	-1.578954	1.134028
H	-6.542644	0.152577	1.046536
H	-6.498529	-0.696383	2.603441
H	5.481332	1.347721	-0.096569

Table S46. Z-matrix of optimized conformer **1d6** at B3LYP/6-311+G(d,p) level

Atom	X	Y	Z

C	0.213921	-2.110436	-0.834101
C	0.463254	-0.598455	-0.926991
C	-0.86899	0.287534	-1.093924
C	-2.083015	-0.43879	-0.373824
C	-2.232771	-1.810474	-1.074957
C	-1.008532	-2.655044	-0.899464
C	-1.821468	-0.559413	1.1573
C	-2.761908	-1.514399	1.902901
C	-4.243331	-1.302147	1.554063
C	-4.35607	-1.146725	0.002512
C	-3.537282	0.103574	-0.564258
C	-3.633512	-2.344585	-0.681416
O	-4.719112	-0.074572	2.147676
C	-5.107398	-2.454992	2.087672
C	-1.084229	0.490004	-2.606966
C	1.451138	-2.968473	-0.734291
C	1.428587	-0.119636	0.146428
C	2.600007	0.453473	-0.129311
C	3.619702	0.948303	0.875624
C	4.884561	0.047255	0.846516
C	5.636007	-0.05134	-0.496885
C	3.95819	2.417255	0.561114
C	6.799773	-1.003052	-0.407183
C	8.104908	-0.749223	-0.581663
C	9.130774	-1.849157	-0.443608
C	8.686187	0.600189	-0.923508
C	-3.893047	1.525068	-0.066535
C	-3.961747	2.569294	-1.192797
C	-4.059157	4.008611	-0.69086
O	-2.922337	4.416578	0.086016
H	-2.311389	-1.591755	-2.143631
C	-0.626339	1.639156	-0.439402
O	-0.657078	2.707096	-1.021739
O	2.99381	0.826589	2.172093
C	3.664747	1.380081	3.298223
C	-5.802419	-0.983418	-0.415323
O	-6.295861	-1.45842	-1.418095
H	0.996674	-0.447209	-1.872956
H	-1.114013	-3.737494	-0.87949
H	-1.917237	0.430323	1.609104
H	-0.802007	-0.887622	1.347627
H	-2.48339	-2.549983	1.691495
H	-2.635394	-1.381626	2.982749
H	-3.749774	0.080125	-1.63901

H	-4.188871	-2.64921	-1.568499
H	-3.581731	-3.213223	-0.026615
H	-4.771251	-0.20798	3.10156
H	-6.169042	-2.260162	1.914854
H	-4.957406	-2.554557	3.167501
H	-4.852999	-3.413212	1.632531
H	-0.996555	-0.453043	-3.146419
H	-2.053538	0.929344	-2.84241
H	-0.318074	1.162871	-2.996506
H	1.191929	-4.028153	-0.780514
H	2.148514	-2.749628	-1.551182
H	1.996925	-2.788368	0.196876
H	1.157056	-0.264808	1.186205
H	2.88531	0.597784	-1.168736
H	4.573475	-0.954514	1.161083
H	5.588568	0.413986	1.599911
H	5.96572	0.939112	-0.81507
H	4.949153	-0.415828	-1.269785
H	4.776372	2.784615	1.184907
H	3.08126	3.048933	0.722362
H	4.263343	2.523809	-0.48163
H	6.522707	-2.027997	-0.159799
H	9.85896	-1.607865	0.339768
H	8.668998	-2.807868	-0.19848
H	9.701664	-1.970118	-1.371898
H	7.938497	1.389182	-0.999081
H	9.420497	0.900746	-0.167147
H	9.225662	0.553146	-1.876783
H	-3.178369	1.851792	0.691632
H	-4.853182	1.515998	0.447841
H	-4.834836	2.370952	-1.826016
H	-3.088966	2.500364	-1.84819
H	-4.924854	4.134953	-0.034515
H	-4.187975	4.685206	-1.545272
H	-2.118663	4.117179	-0.362387
H	-0.427996	1.626351	0.642756
H	3.75233	2.469415	3.232529
H	4.660897	0.951239	3.44806
H	3.04926	1.133535	4.164271
H	-6.414878	-0.34713	0.248267

Table S47. Z-matrix of optimized conformer **1d7** at B3LYP/6-311+G(d,p)

level

Atom	X	Y	Z
C	0.010173	-2.927019	-1.402792
C	-0.343938	-2.613723	0.05342
C	0.798946	-1.812695	0.861577
C	1.551816	-0.830043	-0.137301
C	2.176562	-1.729681	-1.228116
C	1.143989	-2.507035	-1.981967
C	0.566935	0.233909	-0.701606
C	1.086352	1.029225	-1.905967
C	2.512931	1.566815	-1.708471
C	3.378778	0.42176	-1.088989
C	2.840584	-0.075584	0.332493
C	3.223257	-0.856691	-1.963257
O	2.503688	2.659881	-0.764541
C	3.095665	2.086771	-3.031379
C	1.725857	-2.866429	1.497957
C	-0.90606	-3.892041	-2.121413
C	-1.766673	-2.116161	0.294204
C	-2.606472	-1.55367	-0.572033
C	-4.058391	-1.201884	-0.310407
C	-4.335426	0.283018	-0.660065
C	-3.613015	1.316867	0.222488
C	-4.931252	-2.105504	-1.207128
C	-4.152934	2.706118	0.008315
C	-3.511944	3.808497	-0.405887
C	-4.247578	5.118675	-0.559573
C	-2.045305	3.876817	-0.749224
C	2.751233	0.936544	1.499574
C	3.267263	0.377687	2.835881
C	2.950919	1.26906	4.035288
O	1.542815	1.439053	4.260137
H	2.774324	-2.472298	-0.690564
C	0.137562	-0.996697	1.960802
O	0.356558	-1.129293	3.150329
O	-4.304493	-1.467698	1.083538
C	-5.629774	-1.286951	1.567733
C	4.813617	0.872201	-0.910442
O	5.790204	0.171897	-1.085174
H	-0.34549	-3.59328	0.551036
H	1.374241	-2.830222	-2.99487
H	0.333996	0.944546	0.094418
H	-0.375804	-0.227747	-0.981947
H	1.051924	0.410035	-2.805669

H	0.42005	1.876631	-2.098831
H	3.570258	-0.837266	0.629673
H	4.178539	-1.378013	-2.025187
H	2.92735	-0.616889	-2.983265
H	2.090155	3.417992	-1.194067
H	4.079275	2.537216	-2.875189
H	2.435881	2.857861	-3.442148
H	3.189419	1.302915	-3.784204
H	2.000881	-3.633938	0.774452
H	2.640932	-2.435604	1.904369
H	1.205423	-3.362246	2.319453
H	-0.499779	-4.145743	-3.102689
H	-1.006456	-4.820818	-1.54701
H	-1.915785	-3.501747	-2.259172
H	-2.140245	-2.305327	1.297112
H	-2.28943	-1.349119	-1.591877
H	-5.415709	0.45479	-0.60654
H	-4.063043	0.439365	-1.70908
H	-2.537531	1.27035	0.042167
H	-3.760736	1.036707	1.272269
H	-5.987993	-1.836651	-1.141957
H	-4.813347	-3.15242	-0.917914
H	-4.62919	-2.001489	-2.251844
H	-5.217706	2.806535	0.221688
H	-5.305248	5.023779	-0.304764
H	-3.808075	5.891956	0.081762
H	-4.174081	5.490191	-1.588658
H	-1.531257	2.923309	-0.634888
H	-1.909426	4.214488	-1.783332
H	-1.5376	4.612329	-0.114199
H	1.724219	1.286805	1.622138
H	3.321434	1.834754	1.265777
H	4.35527	0.249594	2.785595
H	2.852962	-0.614628	3.034815
H	3.348673	2.276999	3.886898
H	3.423926	0.853886	4.934361
H	1.111211	0.576667	4.178015
H	-0.580094	-0.23044	1.630049
H	-5.596487	-1.5237	2.631854
H	-6.343763	-1.960295	1.082681
H	-5.978674	-0.255203	1.451738
H	4.940343	1.911726	-0.559052

Table S48. Z-matrix of optimized conformer 1d8 at B3LYP/6-311+G(d,p) level

Atom	X	Y	Z
C	0.680667	-2.047213	-0.307509
C	0.785275	-0.605023	-0.816753
C	-0.622435	0.091101	-1.192364
C	-1.777502	-0.531654	-0.307664
C	-1.773631	-2.053953	-0.587909
C	-0.483839	-2.697139	-0.188274
C	-1.576492	-0.173949	1.195398
C	-2.477578	-0.935648	2.176606
C	-3.953269	-1.005315	1.744919
C	-3.99996	-1.324446	0.219789
C	-3.262551	-0.219129	-0.672463
C	-3.124934	-2.589955	-0.061275
O	-4.597561	0.275972	1.921637
C	-4.710679	-2.040691	2.592591
C	-0.849269	-0.099369	-2.703949
C	1.993135	-2.72467	0.002081
C	1.687691	0.223589	0.087251
C	2.743617	0.908084	-0.350518
C	3.665828	1.777159	0.479668
C	5.143641	1.418193	0.181506
C	5.556754	-0.017452	0.551917
C	3.411063	3.25128	0.100771
C	7.032023	-0.245945	0.358142
C	7.645884	-1.066223	-0.50713
C	9.153008	-1.151254	-0.557251
C	6.94093	-1.965273	-1.49243
C	-3.6897	1.256659	-0.642724
C	-5.119946	1.539655	-1.122108
C	-5.409786	3.025979	-1.325504
O	-5.400013	3.787534	-0.106909
H	-1.84391	-2.152676	-1.67499
C	-0.454766	1.584144	-0.917029
O	-0.403336	2.44454	-1.771961
O	3.327927	1.532125	1.858714
C	4.012879	2.28868	2.849536
C	-5.429579	-1.491131	-0.258987
O	-5.751809	-2.125448	-1.243345
H	1.312418	-0.660697	-1.776716
H	-0.489124	-3.733238	0.142894
H	-1.764398	0.893856	1.322949

H	-0.543006	-0.341616	1.495732
H	-2.098241	-1.95165	2.312419
H	-2.425304	-0.461381	3.162422
H	-3.425616	-0.564665	-1.699586
H	-3.608369	-3.21008	-0.815903
H	-3.012369	-3.203323	0.831439
H	-4.717523	0.423801	2.867161
H	-5.776614	-2.045615	2.353082
H	-4.608167	-1.78722	3.652797
H	-4.322325	-3.051647	2.461062
H	-0.771703	-1.147327	-2.993579
H	-1.821987	0.27815	-3.024985
H	-0.089235	0.452246	-3.259478
H	1.835305	-3.774409	0.257965
H	2.669955	-2.67996	-0.859055
H	2.516537	-2.24335	0.833627
H	1.462774	0.244286	1.1486
H	2.986508	0.895787	-1.411969
H	5.792269	2.131223	0.701226
H	5.316571	1.582507	-0.887309
H	4.96383	-0.729081	-0.025534
H	5.304368	-0.190369	1.604742
H	4.124202	3.920727	0.587639
H	2.397996	3.544793	0.385317
H	3.516329	3.384893	-0.978297
H	7.669762	0.353056	1.008868
H	9.526711	-0.887891	-1.553912
H	9.622346	-0.4865	0.171082
H	9.494271	-2.174176	-0.358142
H	5.855219	-1.880764	-1.455521
H	7.263849	-1.736732	-2.514866
H	7.205814	-3.013758	-1.311837
H	-3.011714	1.787054	-1.321383
H	-3.548352	1.677763	0.351767
H	-5.848358	1.142539	-0.409822
H	-5.296606	1.039254	-2.082603
H	-6.413524	3.155311	-1.73513
H	-4.698725	3.45886	-2.040887
H	-4.498454	3.818217	0.230432
H	-0.365143	1.873791	0.141144
H	3.631687	1.942203	3.810904
H	3.814959	3.361934	2.762552
H	5.095467	2.123714	2.824775
H	-6.200913	-0.97018	0.333832

Table S49. Z-matrix of optimized conformer 1d9 at B3LYP/6-311+G(d,p) level

Atom	X	Y	Z
C	0.646992	-1.903875	-0.600143
C	0.709795	-0.388417	-0.839032
C	-0.718931	0.298043	-1.108341
C	-1.844995	-0.495053	-0.32038
C	-1.814878	-1.938428	-0.878827
C	-0.497753	-2.60013	-0.614258
C	-1.589122	-0.428829	1.214423
C	-2.41561	-1.409248	2.054703
C	-3.90658	-1.418971	1.685088
C	-4.018482	-1.436468	0.125477
C	-3.352826	-0.157761	-0.56567
C	-3.145411	-2.598028	-0.435004
O	-4.539174	-0.206575	2.149064
C	-4.627992	-2.610497	2.333556
C	-0.925943	0.305212	-2.63643
C	1.979049	-2.58734	-0.412344
C	1.598352	0.298317	0.189385
C	2.657707	1.039391	-0.136607
C	3.635821	1.692022	0.827022
C	4.927278	0.84225	0.942237
C	5.669852	0.516348	-0.36748
C	3.962638	3.120598	0.361
C	6.981325	-0.174145	-0.098527
C	7.367584	-1.407644	-0.455001
C	8.737414	-1.925425	-0.085305
C	6.525967	-2.385443	-1.236837
C	-3.885078	1.252391	-0.214347
C	-4.061296	2.163073	-1.440592
C	-4.330971	3.624232	-1.086189
O	-3.257093	4.239535	-0.357804
H	-1.902951	-1.839231	-1.964265
C	-0.66285	1.732474	-0.607795
O	-0.798084	2.71814	-1.307717
O	3.1299	1.679876	2.180827
C	2.134112	2.637875	2.527248
C	-5.468889	-1.495168	-0.305901
O	-5.888077	-2.123145	-1.257003

H	1.239264	-0.262598	-1.790652
H	-0.467703	-3.679993	-0.487083
H	-1.807524	0.582519	1.562504
H	-0.539997	-0.612908	1.434698
H	-2.009935	-2.418783	1.955155
H	-2.32105	-1.149584	3.114596
H	-3.54858	-0.313194	-1.632497
H	-3.647273	-3.054127	-1.288428
H	-2.996904	-3.386597	0.30137
H	-4.588728	-0.247893	3.111443
H	-5.703019	-2.568222	2.140532
H	-4.481054	-2.580277	3.41805
H	-4.250343	-3.570871	1.979769
H	-0.698037	-0.6692	-3.068236
H	-1.940686	0.579158	-2.924855
H	-0.250019	1.031317	-3.091666
H	1.853257	-3.670086	-0.348588
H	2.653852	-2.368894	-1.247957
H	2.486961	-2.246657	0.494862
H	1.375808	0.145147	1.241266
H	2.889481	1.188446	-1.190012
H	4.652611	-0.09349	1.438603
H	5.602594	1.376392	1.619728
H	5.876089	1.446909	-0.909932
H	5.03429	-0.087413	-1.017486
H	4.652335	3.598773	1.06151
H	3.065228	3.736454	0.276385
H	4.433951	3.099637	-0.623307
H	7.694163	0.424329	0.469121
H	9.306405	-2.200413	-0.981374
H	9.314943	-1.185651	0.472888
H	8.660328	-2.833393	0.524505
H	5.529367	-2.011323	-1.469234
H	7.019207	-2.644438	-2.181172
H	6.414551	-3.322599	-0.679362
H	-3.227678	1.737377	0.510395
H	-4.845321	1.178198	0.294467
H	-4.898797	1.801895	-2.049663
H	-3.18025	2.130258	-2.087976
H	-5.211073	3.71297	-0.443012
H	-4.531321	4.19167	-2.003962
H	-2.420319	4.000442	-0.78123
H	-0.507038	1.864099	0.473706
H	1.300664	2.645704	1.818227

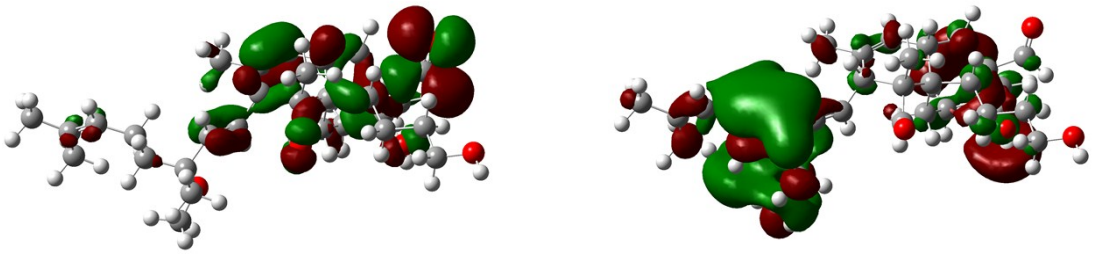
H	2.54811	3.648756	2.598824
H	1.757212	2.343907	3.507681
H	-6.162513	-0.877308	0.291969

Table S50. Z-matrix of optimized conformer **1d10** at B3LYP/6-311+G(d,p) level

Atom	X	Y	Z
C	0.437474	-3.076307	-0.717961
C	-0.236541	-2.256426	0.390503
C	0.734298	-1.199264	1.114423
C	1.817409	-0.676072	0.078547
C	2.60689	-1.926729	-0.37702
C	1.7212	-2.91731	-1.068004
C	1.130922	0.077325	-1.09907
C	2.032562	0.361162	-2.307358
C	3.402722	0.940552	-1.923279
C	3.950345	0.121885	-0.709061
C	3.007941	0.205774	0.579344
C	3.895979	-1.396658	-1.054102
O	3.257963	2.310709	-1.491039
C	4.364987	0.91811	-3.120804
C	1.346187	-1.924055	2.330088
C	-0.425605	-4.136542	-1.357122
C	-1.588516	-1.71952	-0.062671
C	-2.726593	-1.975085	0.582523
C	-4.140867	-1.599749	0.180178
C	-4.236211	-0.442639	-0.837121
C	-3.807802	0.942922	-0.319675
C	-4.811233	-2.8612	-0.401332
C	-3.798647	1.972719	-1.417763
C	-4.518649	3.099664	-1.51716
C	-4.365999	4.011862	-2.711268
C	-5.51957	3.579096	-0.495526
C	2.721845	1.586358	1.216628
C	2.799525	1.581178	2.752337
C	2.267653	2.860249	3.396235
O	0.876173	3.093461	3.128176
H	2.955966	-2.408798	0.540682
C	-0.111704	-0.034004	1.602565
O	-0.25011	0.28337	2.768427
O	-4.749827	-1.234645	1.448561

C	-6.149517	-0.975945	1.459056
C	5.327557	0.611479	-0.313146
O	6.238574	-0.098591	0.06159
H	-0.476038	-2.972512	1.184934
H	2.150941	-3.563583	-1.830157
H	0.748427	1.030983	-0.729957
H	0.27001	-0.48171	-1.458825
H	2.176197	-0.553701	-2.887436
H	1.531264	1.067487	-2.977731
H	3.550226	-0.381488	1.328853
H	4.774278	-1.897209	-0.646494
H	3.904634	-1.567334	-2.129454
H	3.055896	2.845923	-2.267636
H	5.311069	1.405584	-2.871791
H	3.917904	1.463086	-3.958401
H	4.57769	-0.094385	-3.466689
H	1.726527	-2.906629	2.051089
H	2.156468	-1.36253	2.794583
H	0.576424	-2.074465	3.089179
H	0.155029	-4.736364	-2.060883
H	-0.84738	-4.80804	-0.600233
H	-1.274123	-3.703186	-1.895386
H	-1.610101	-1.135074	-0.977708
H	-2.694906	-2.573418	1.491998
H	-5.267356	-0.380717	-1.199748
H	-3.639154	-0.712728	-1.714184
H	-2.800541	0.868132	0.104172
H	-4.458411	1.241631	0.503026
H	-5.85437	-2.674748	-0.666929
H	-4.775107	-3.682278	0.319137
H	-4.286069	-3.173863	-1.30624
H	-3.112546	1.751305	-2.23583
H	-4.05202	5.015179	-2.39949
H	-3.632005	3.630432	-3.424287
H	-5.321908	4.134156	-3.234332
H	-5.637512	2.899055	0.347479
H	-5.223834	4.558644	-0.101593
H	-6.502744	3.716806	-0.960318
H	1.743856	1.9563	0.902581
H	3.427666	2.328134	0.845053
H	3.841437	1.449951	3.068425
H	2.246265	0.737038	3.172921
H	2.792461	3.738253	3.009259
H	2.436926	2.82204	4.479821

H	0.393893	2.264903	3.260103
H	-0.611869	0.561998	0.82443
H	-6.433269	-0.185436	0.756185
H	-6.387172	-0.64229	2.469916
H	-6.737993	-1.873032	1.240931
H	5.464533	1.707078	-0.346629



MO137 **MO144**

Figure S8. Molecular orbitals involved in the key transitions in ECD of conformer **1b1** at the B3LYP/6-311+G(d,p) level with the CPCM model in MeOH.

Table S51. Energies analysis of reoptimized conformers of **1a**–**1b** at the B3LYP/6-311+G(d,p) level with the CPCM model in MeOH.

conformers	Energy (a.u.)	Boltzmann distribution (%)	Imaginary Freg
1a1	−1586.67964708	18.80	0
1a2	−1586.67984314	23.14	0
1a3	−1586.67914658	11.06	0
1a4	−1586.67533632	0.19	0
1a5	−1586.67718531	1.38	0
1a6	−1586.67556266	0.25	0
1a7	−1586.67968622	19.59	0
1a8	−1586.67663514	0.77	0
1a9	−1586.67979925	22.09	0
1a10	−1586.67782404	2.72	0
1b1	−1586.67976536	21.88	0
1b2	−1586.67955622	17.52	0
1b3	−1586.67963133	18.98	0
1b4	−1586.67363193	0.03	0
1b5	−1586.67967375	19.85	0
1b6	−1586.67681010	0.95	0
1b7	−1586.67670819	0.86	0
1b8	−1586.67281835	0.01	0
1b9	−1586.67650970	0.69	0
1b10	−1586.67638081	0.60	0
1b11	−1586.67358310	0.03	0

1b12	−1586.67941321	15.06	0
1b13	−1586.67794354	3.17	0
1b14	−1586.67588177	0.36	0

Table S52. Energies analysis of reoptimized conformers of **1c**–**1d** at the B3LYP/6-311+G(d,p) level with the CPCM model in MeOH.

conformers	Energy (a.u.)	Boltzmann distribution (%)	Imaginary Freg
1c1	−1586.67698847	1.72	0
1c2	−1586.67984313	35.55	0
1c3	−1586.67914371	16.94	0
1c4	−1586.67297391	0.02	0
1c5	−1586.67527432	0.28	0
1c6	−1586.67927494	19.46	0
1c7	−1586.67380903	0.06	0
1c8	−1586.67604351	0.63	0
1c9	−1586.67883494	12.21	0
1c10	−1586.67364045	0.05	0
1c11	−1586.67889932	13.07	0
1d1	−1586.67858682	7.70	0
1d2	−1586.67876605	9.31	0
1d3	−1586.68002523	35.37	0
1d4	−1586.67976535	26.86	0
1d5	−1586.67536498	0.25	0
1d6	−1586.67657031	0.91	0
1d7	−1586.67306308	0.02	0
1d8	−1586.67939499	18.14	0
1d9	−1586.67665993	1.00	0
1d10	−1586.67589328	0.44	0

Table S53. Key Transition, Oscillator Strengths, and Rotatory Strengths of Conformer **1b1** at the B3LYP/6-311+G(d,p) level with the CPCM model in MeOH.

Species	Exited State	ΔE^a(eV)	λ^b(nm)	f^c	$R_{vel}{}^d$	$R_{len}{}^e$
	134→138	4.1275	304.39	0.0005	–4.9810	–3.9450
	135→139	4.1419	303.34	0.0024	–4.0947	–3.3933
1b1	137→144	6.0590	208.63	0.0522	–22.2792	–20.4217
	131→139	6.0923	207.51	0.0103	–11.2585	–11.2268
	129→138	6.0955	207.40	0.0181	–16.7409	–16.9347

[a]Excitation energy. [b]Wavelength. [c]Oscillator strength. [d]Rotatory strength in velocity form (10^{-40} cgs). [e]Rotatory strength in length form (10^{-40} cgs).

Figure S9. The UV spectrum of belamchinenin A (1) in MeOH

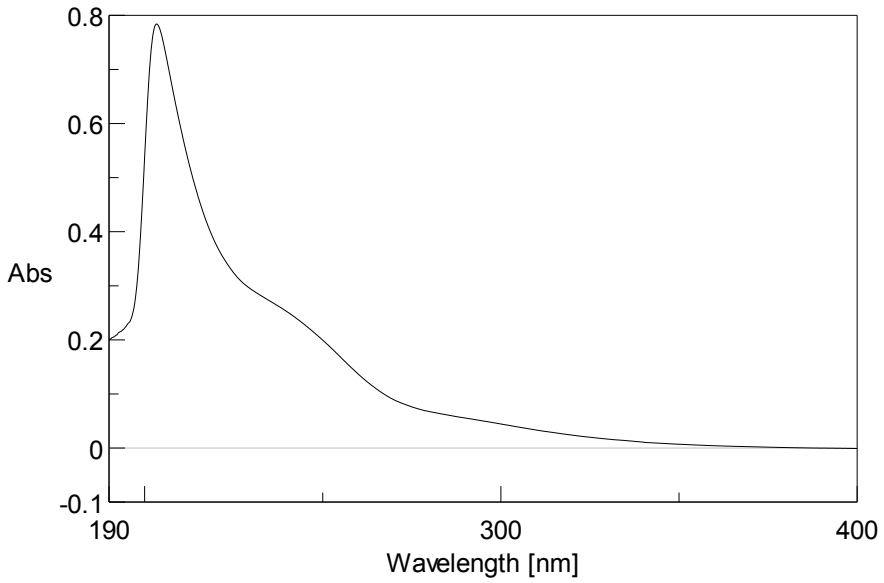
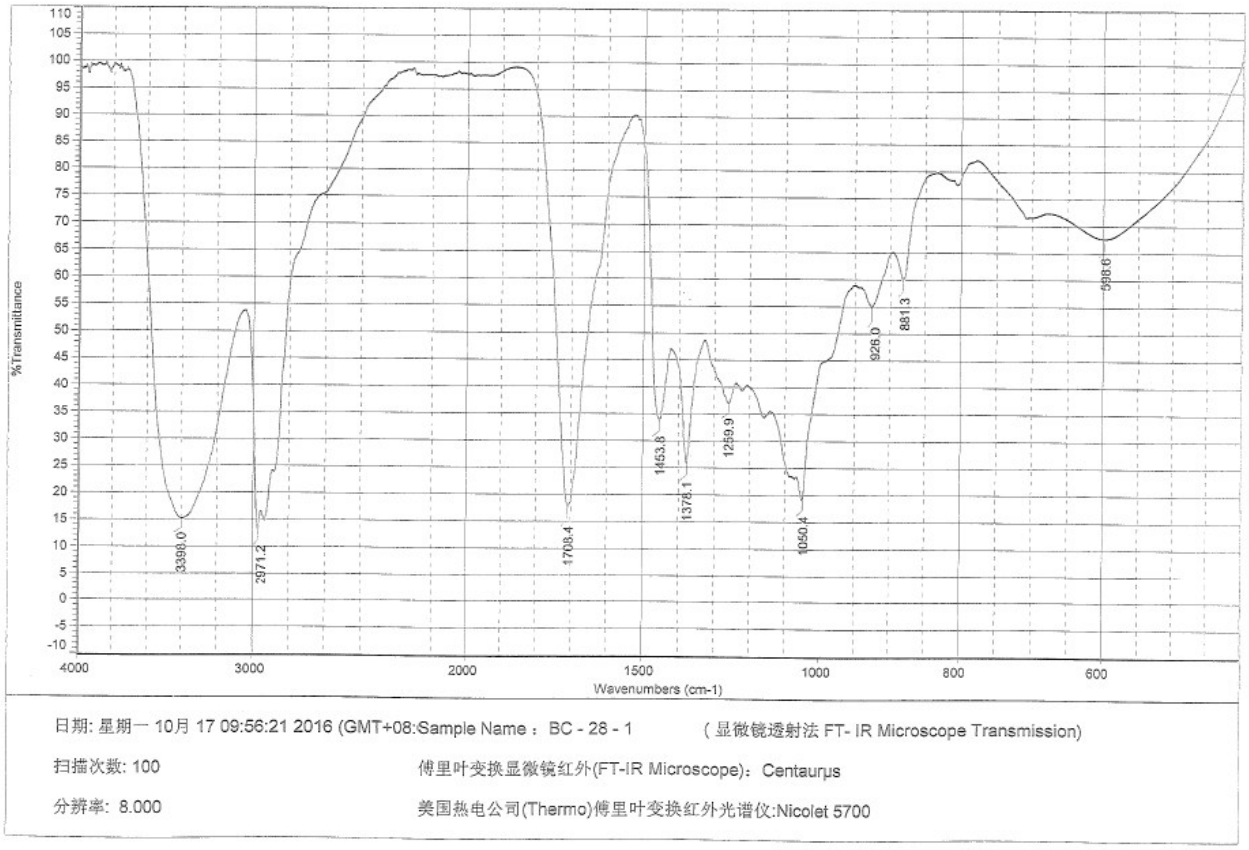


Figure S10. The IR spectrum of belamchinenin A (1)



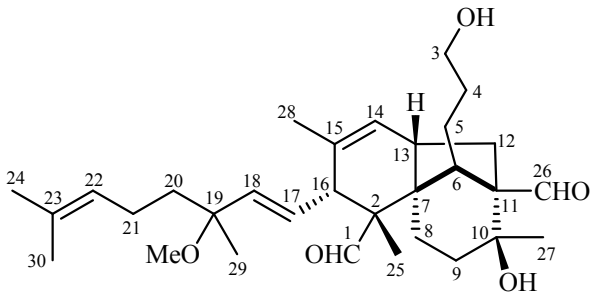
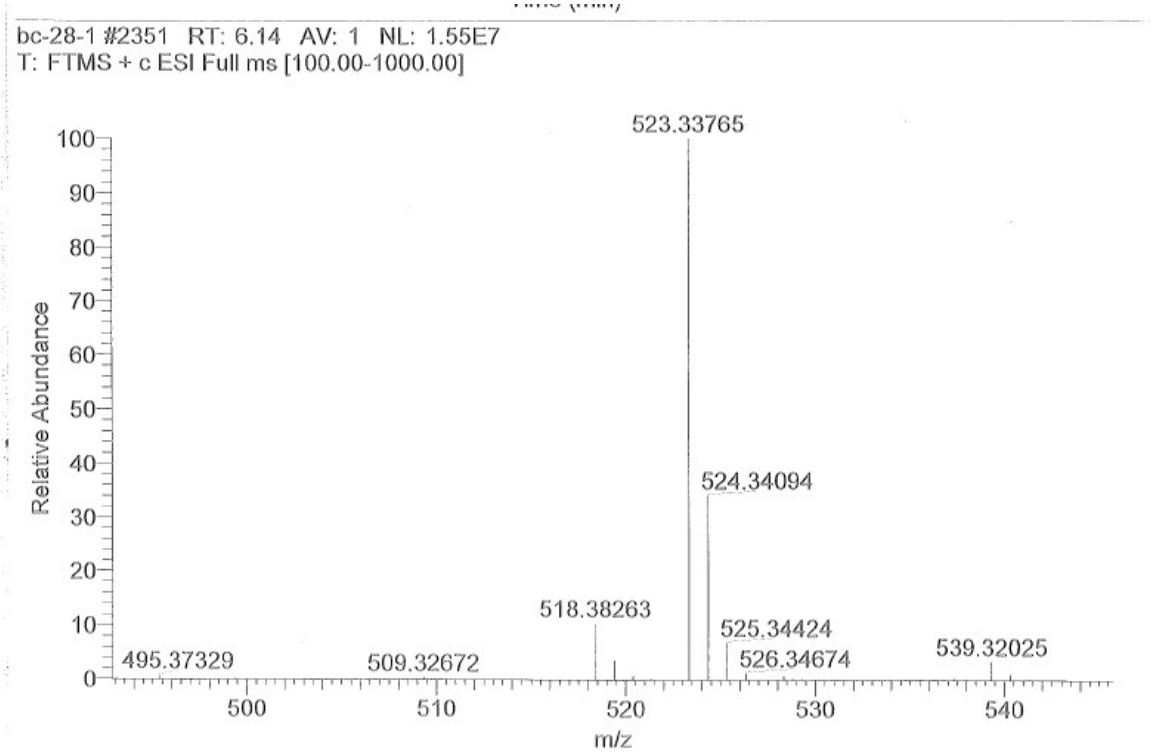


Figure S11. The HRESI spectrum of belamchinenin A (1)



Elemental composition search on mass 523.34

m/z= 518.34-528.34

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
523.33765	523.33940	-3.34	7.5	$C_{31}H_{48}O_5Na$

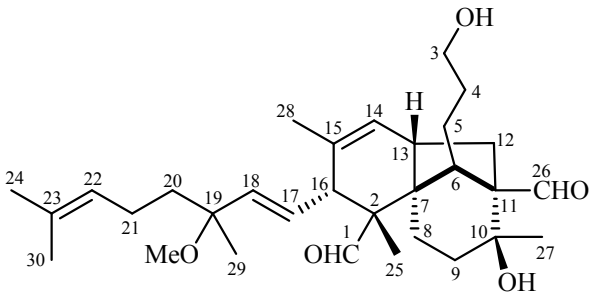
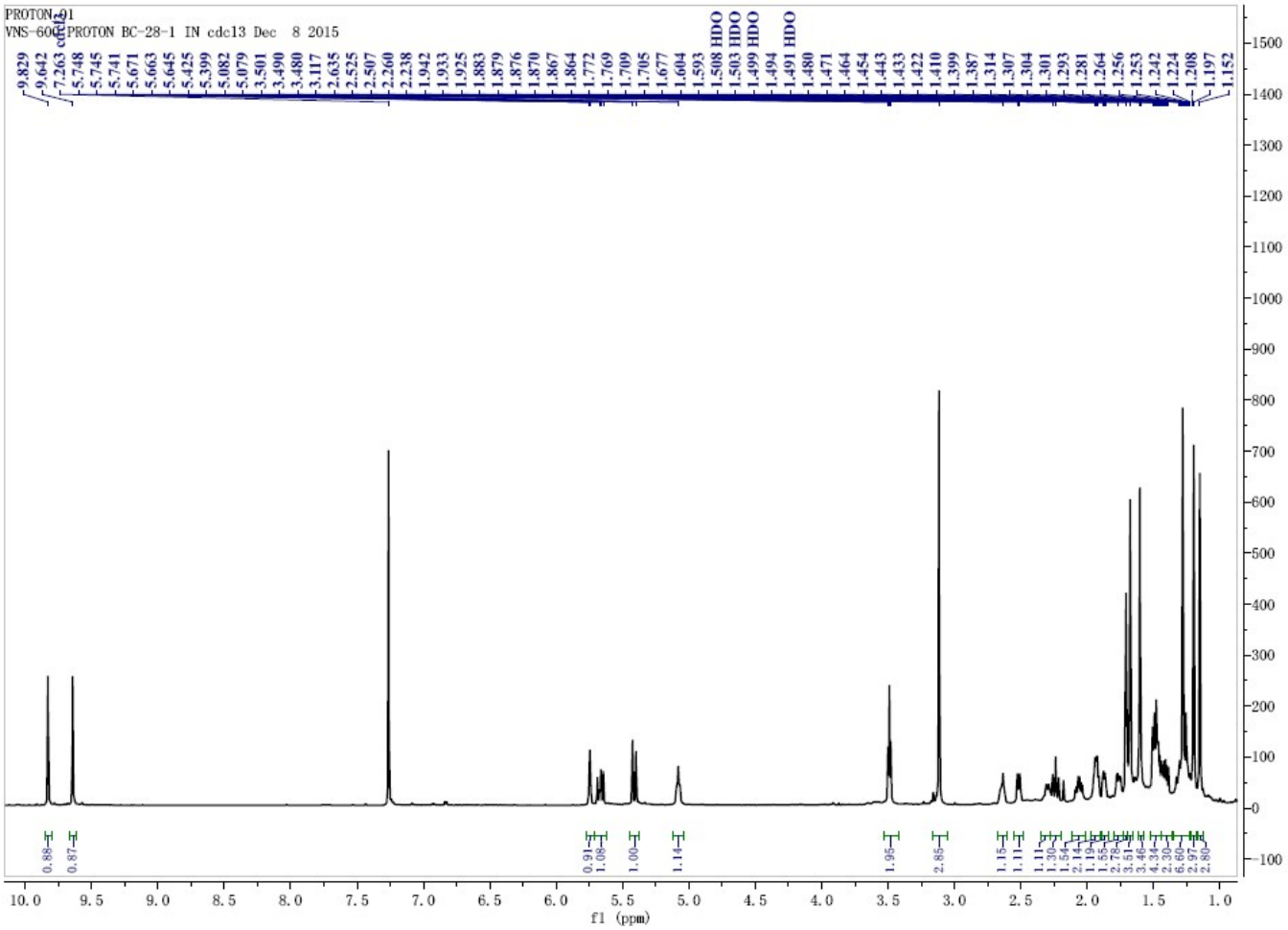


Figure S12. The ^{1}H NMR spectrum of belamchinenin A (1)



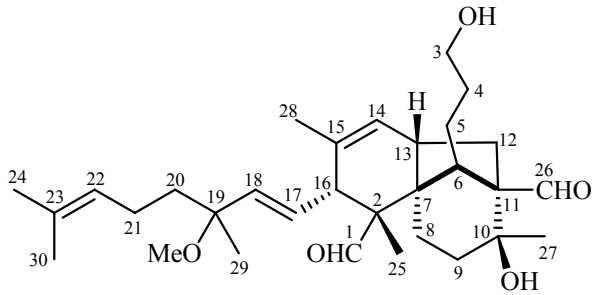
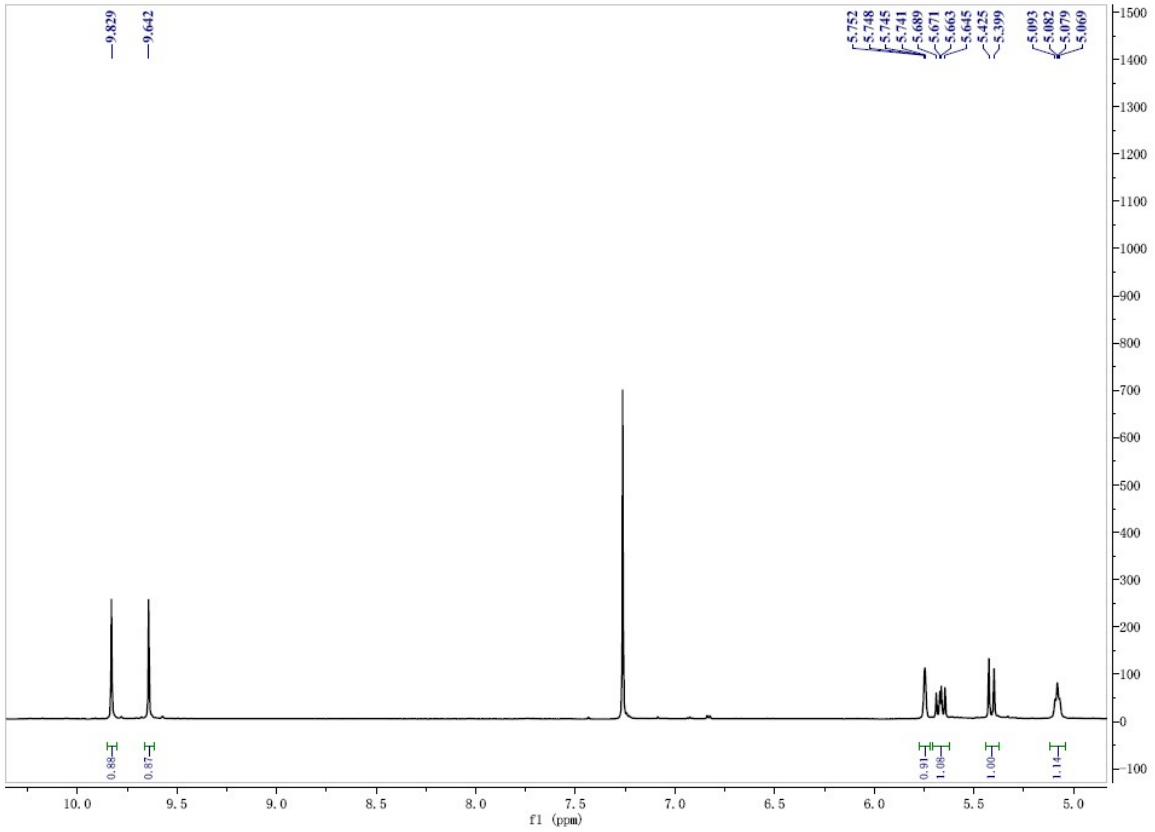


Figure S13. The enlarged ^{1}H NMR spectrum of belamchinenin A (1)



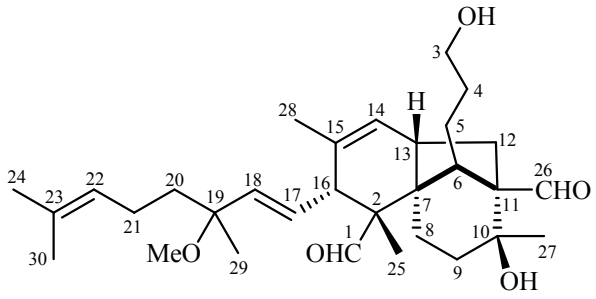
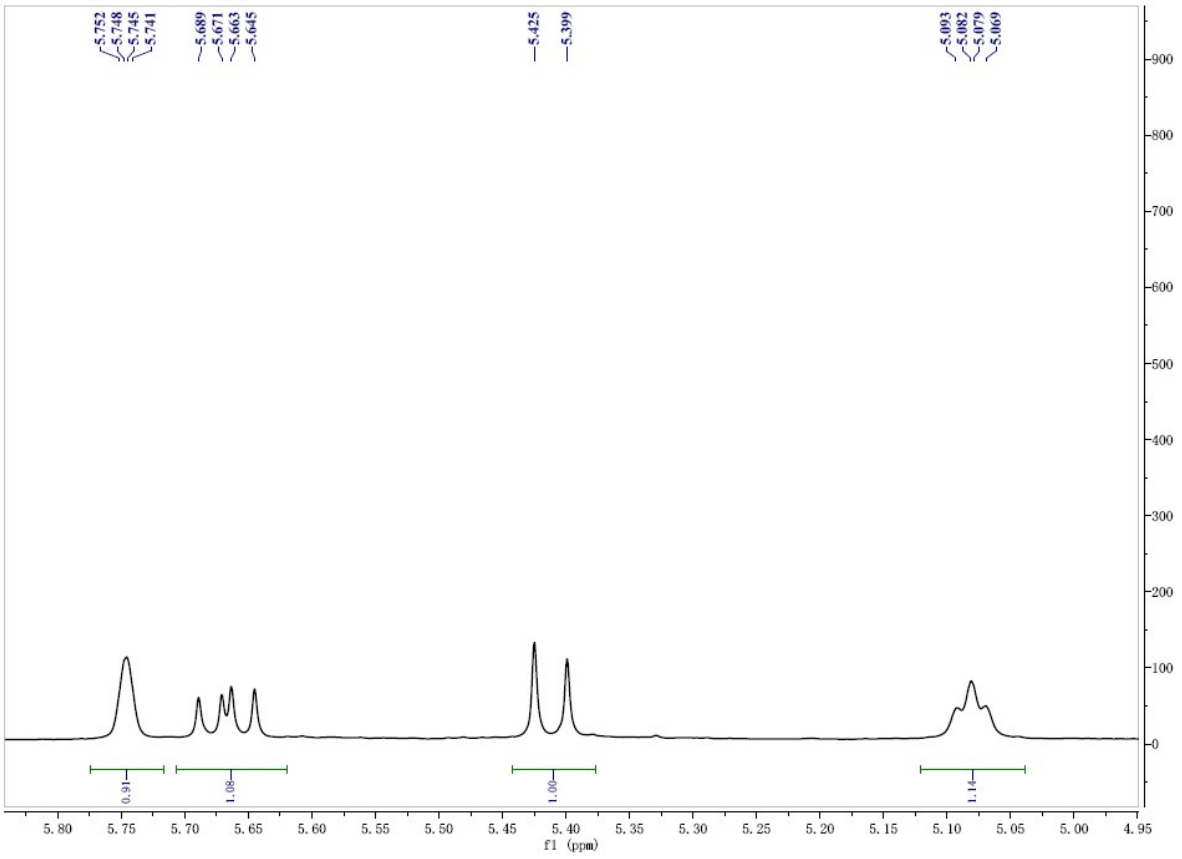


Figure S14. The enlarged ^{1}H NMR spectrum of belamchinenin A (1)



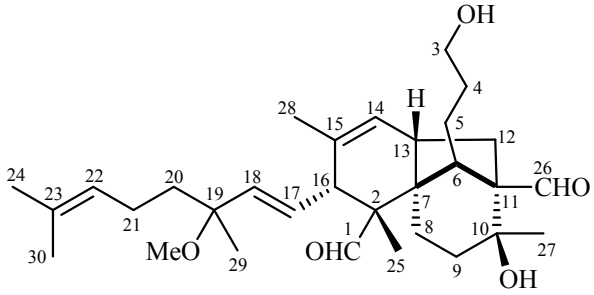
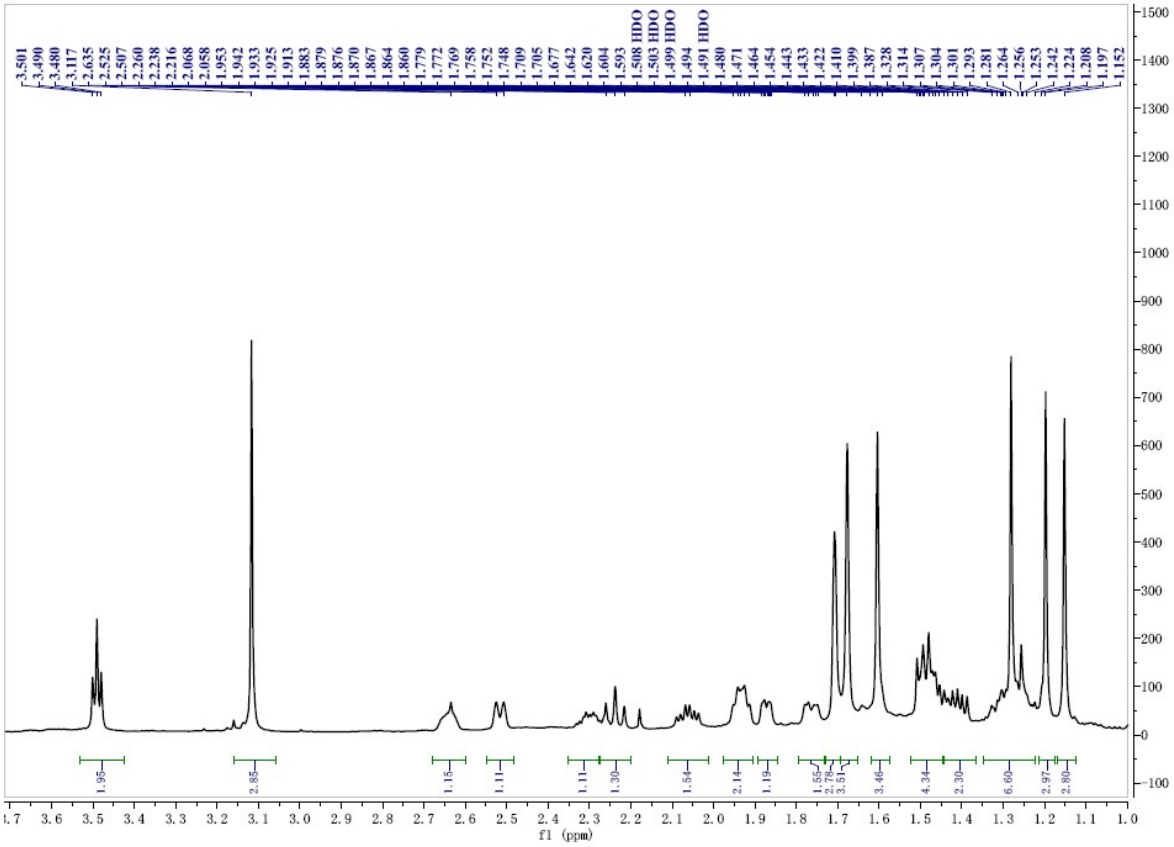


Figure S15. The enlarged ^{1}H NMR spectrum of belamchinenin A (1)



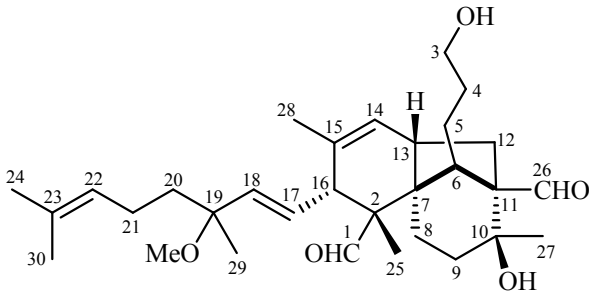
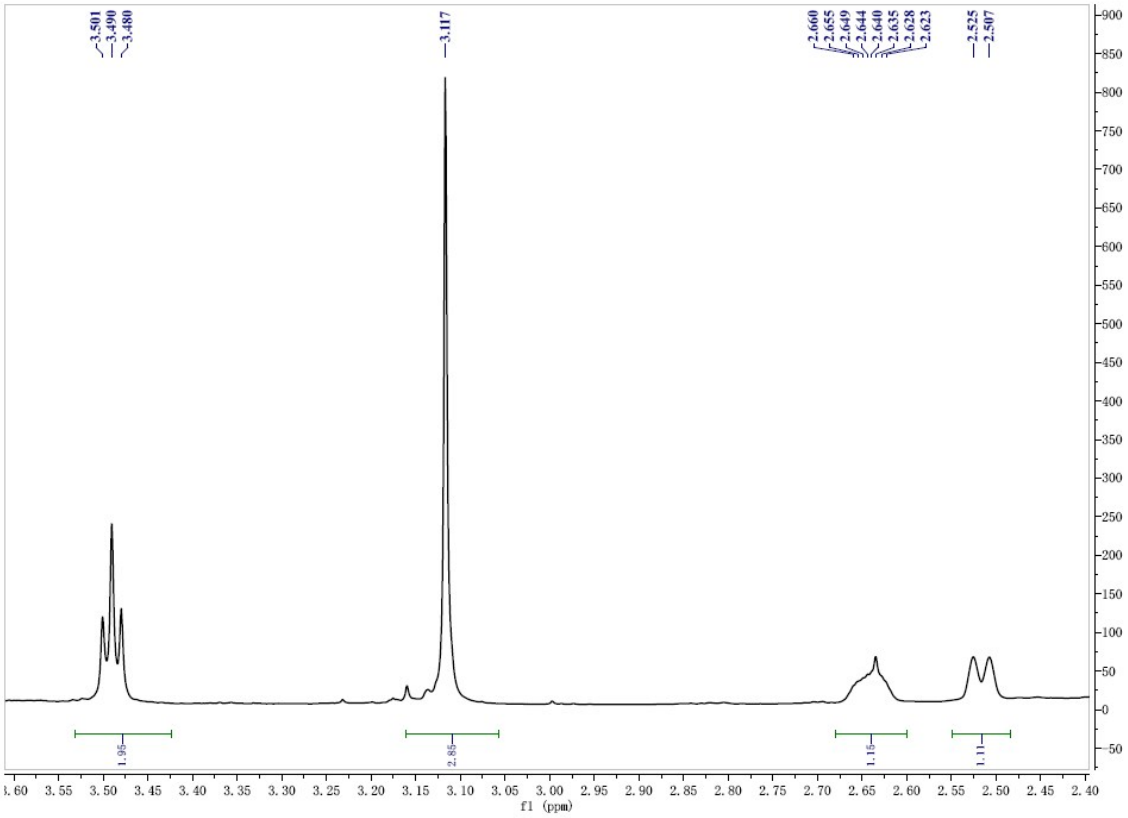


Figure S16. The enlarged ^{1}H NMR spectrum of belamchinenin A (1)



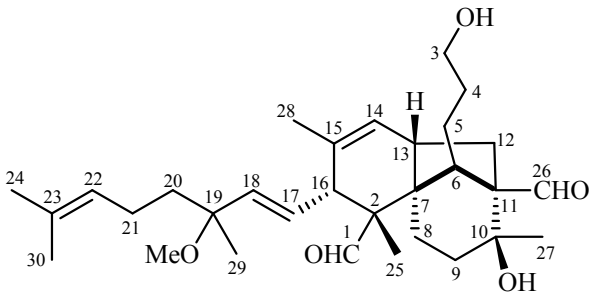
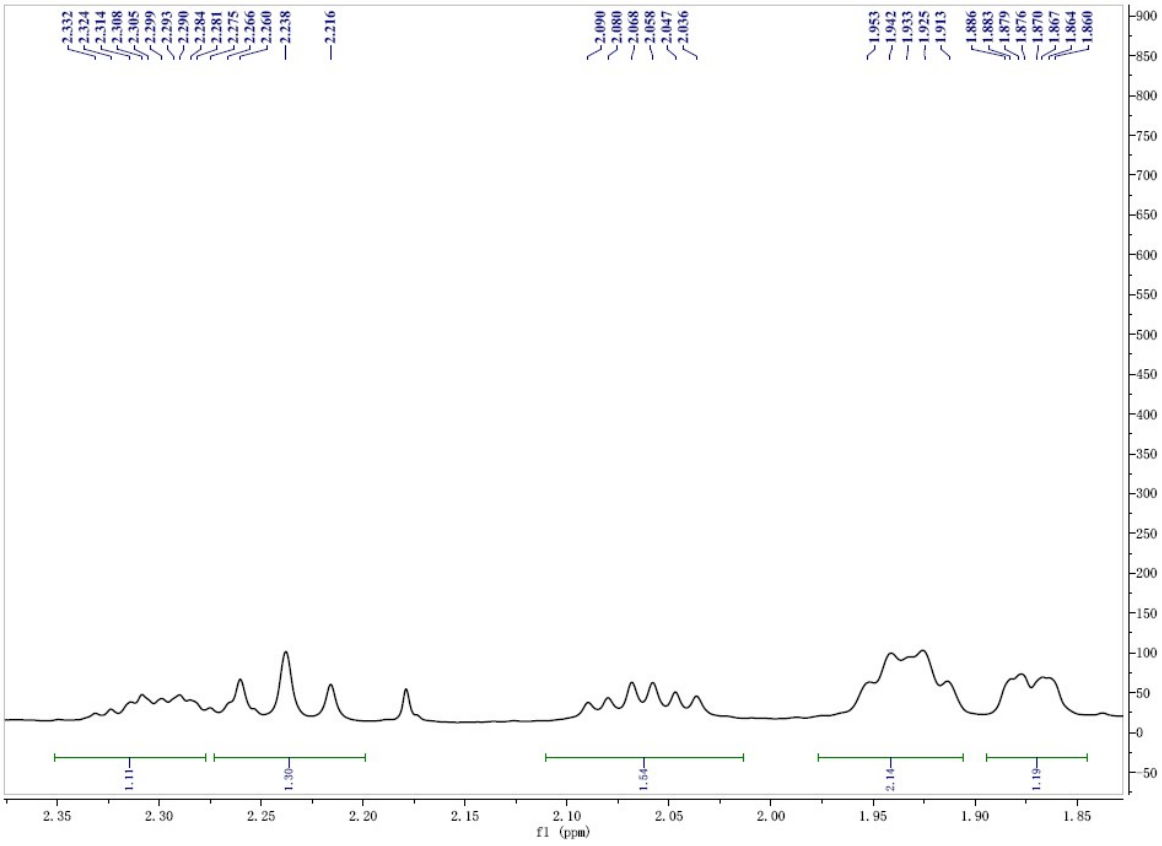


Figure S17. The enlarged ^{1}H NMR spectrum of belamchinenin A (1)



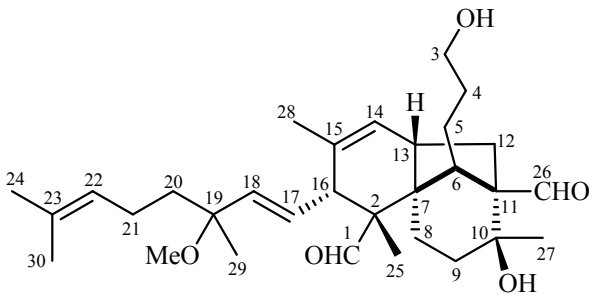
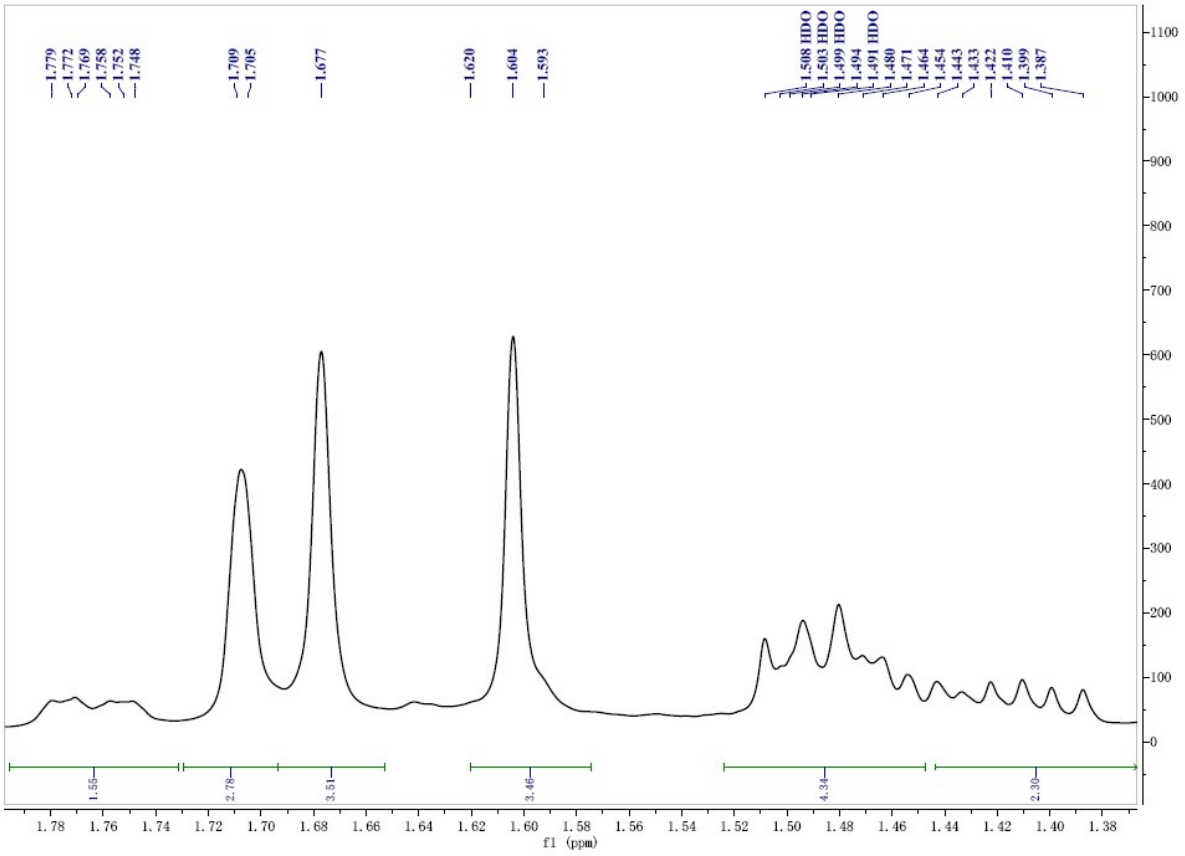


Figure S18. The enlarged ^{1}H NMR spectrum of belamchinenin A (1)



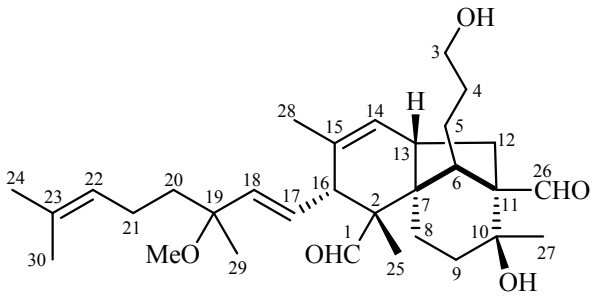
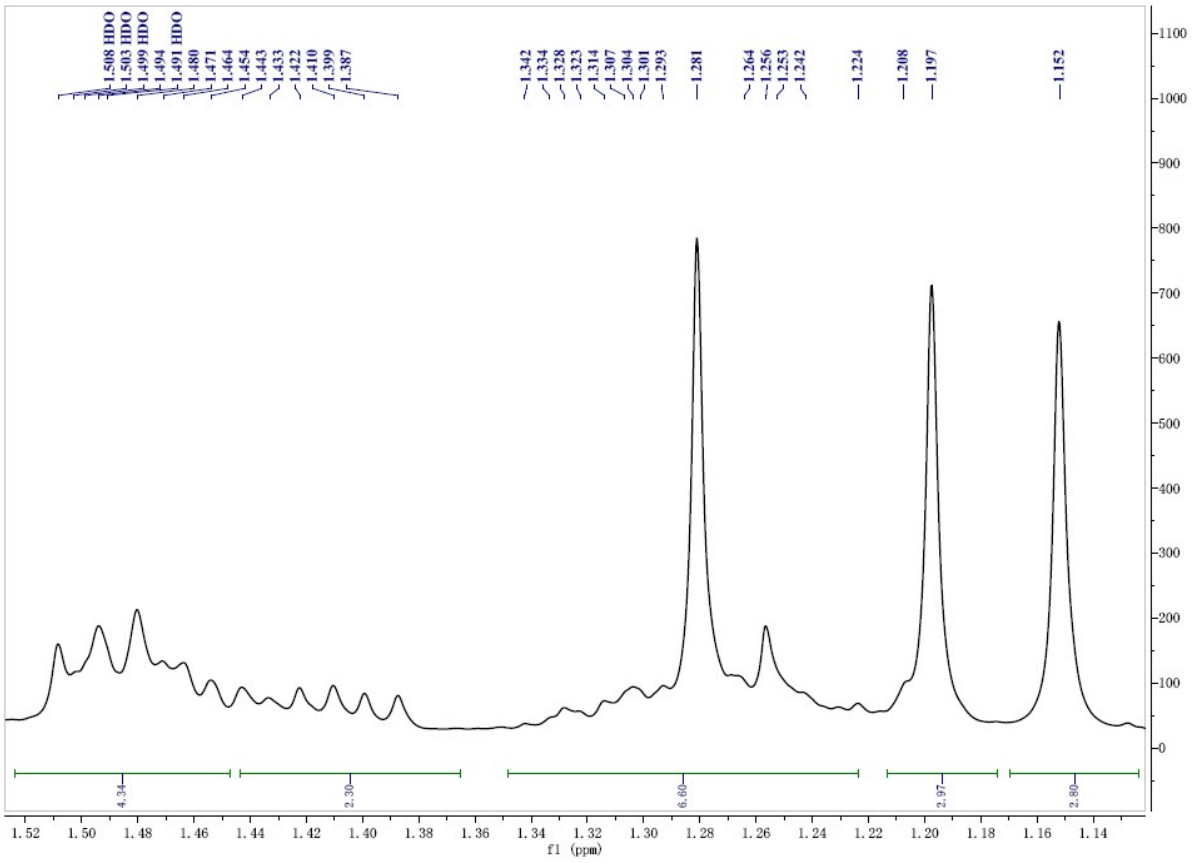


Figure S19. The enlarged ^{1}H NMR spectrum of belamchinenin A (1)



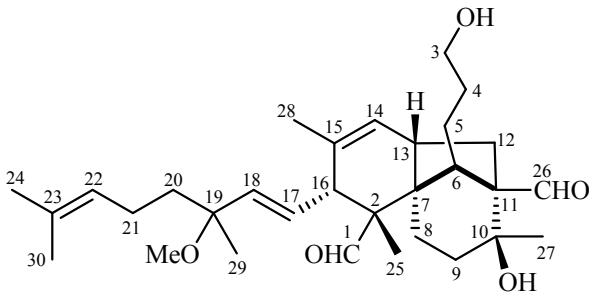
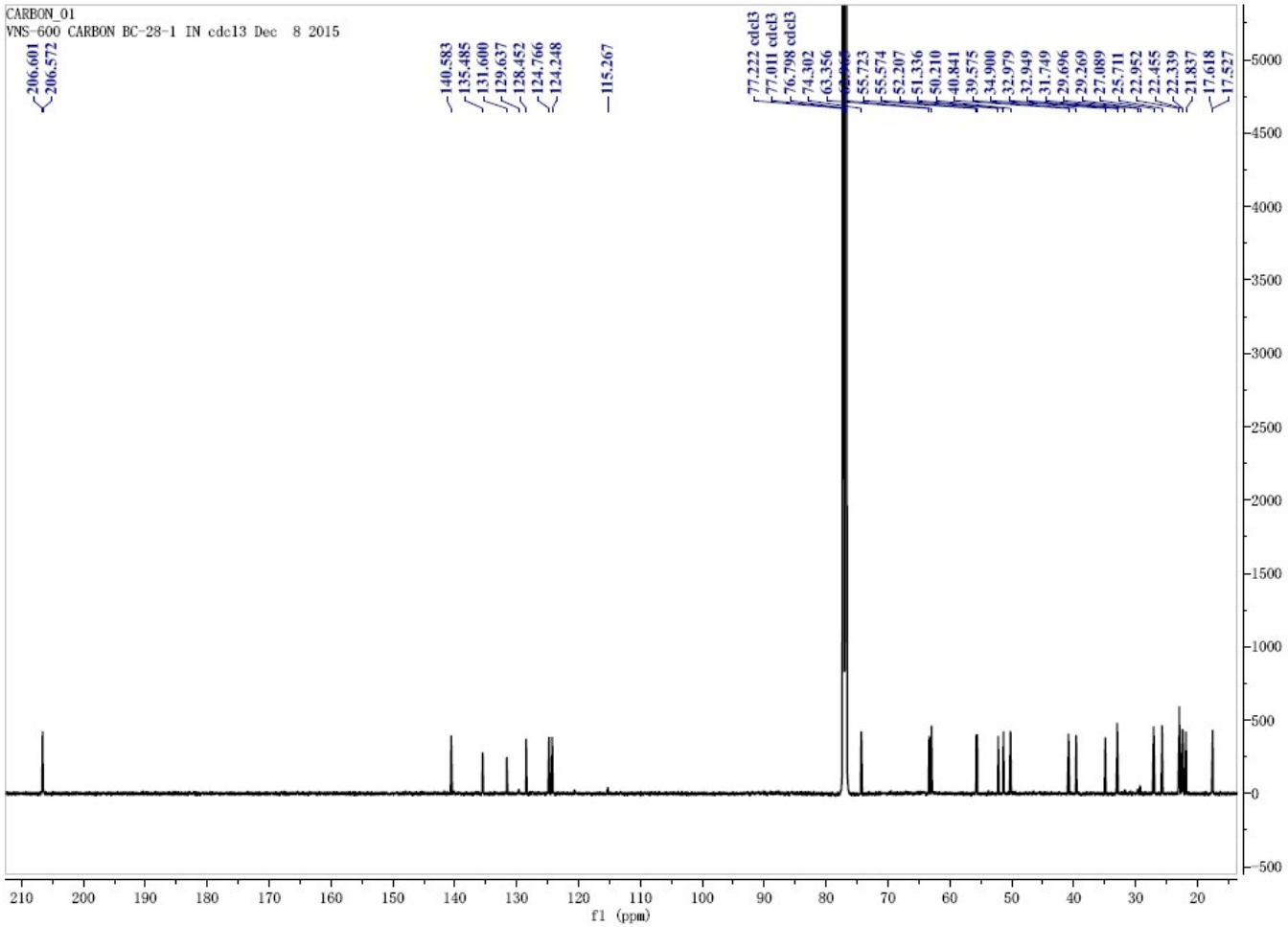


Figure S20. The ^{13}C NMR spectrum of belamchinenin A (1)



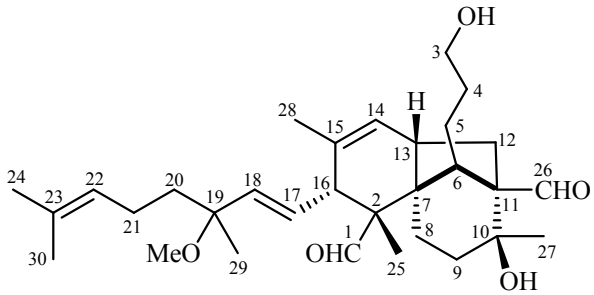
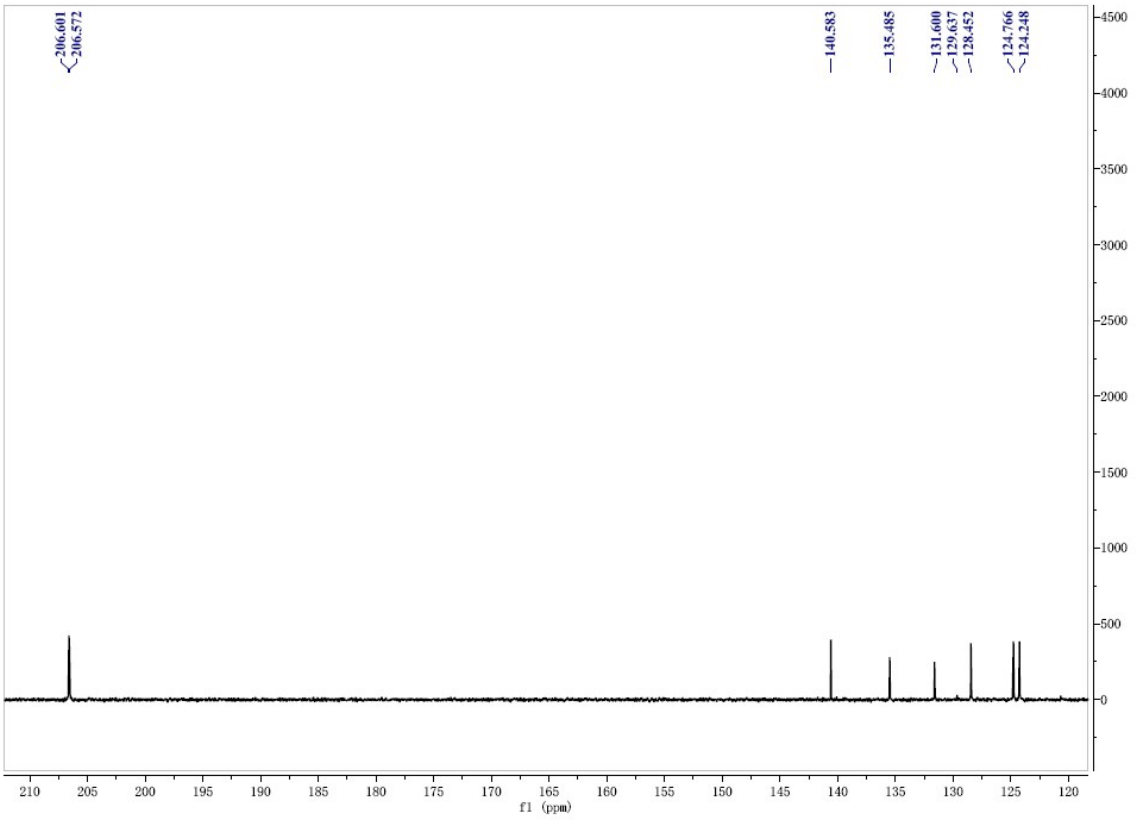


Figure S21. The enlarged ^{13}C NMR spectrum of belamchinenin A (1)



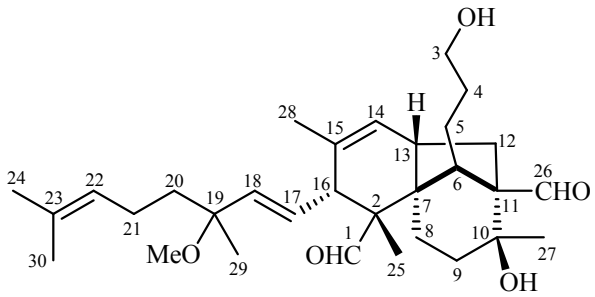
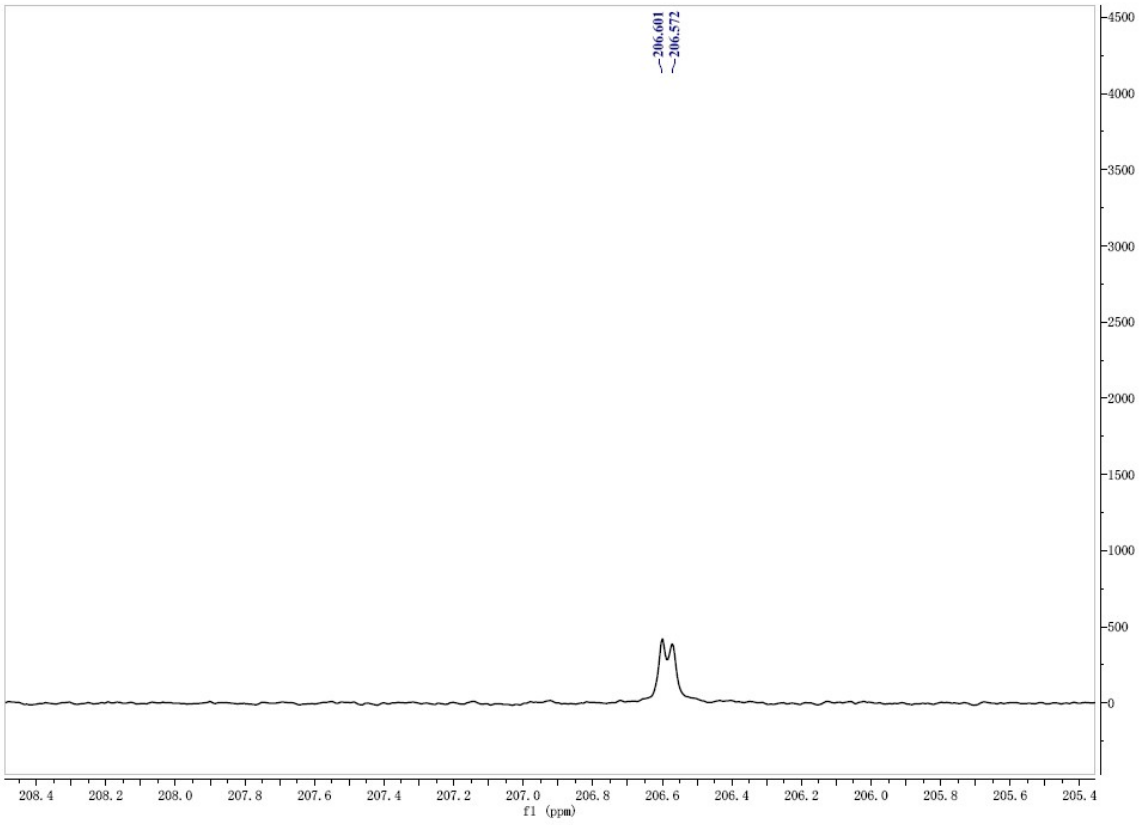


Figure S22. The enlarged ^{13}C NMR spectrum of belamchinenin A (1)



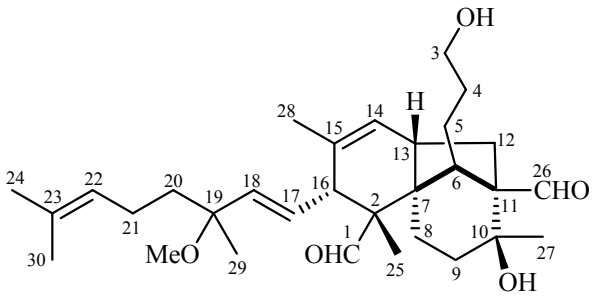
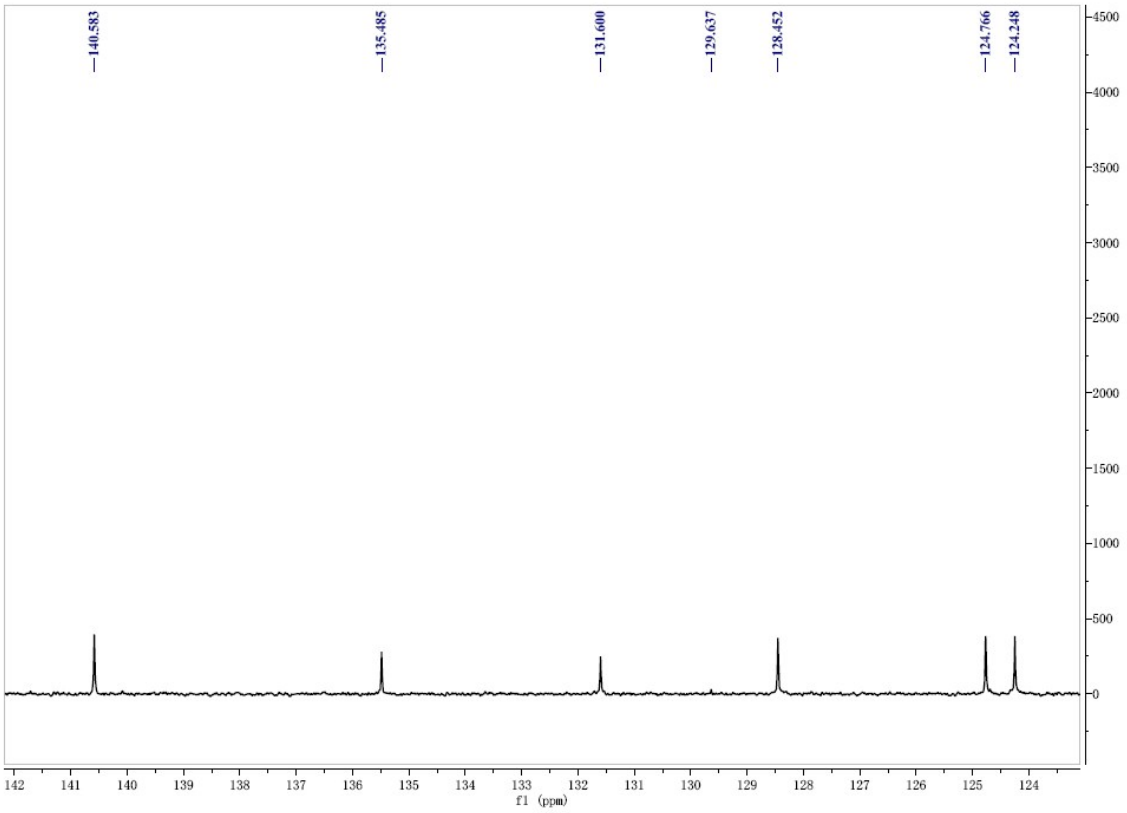


Figure S23. The enlarged ^{13}C NMR spectrum of belamchinenin A (1)



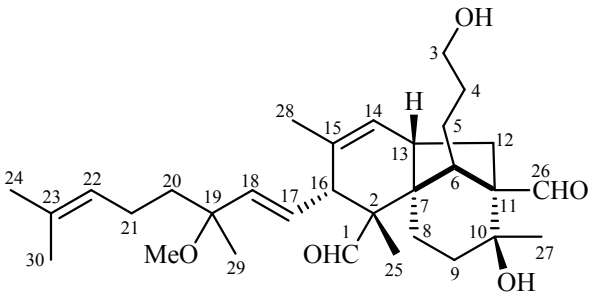
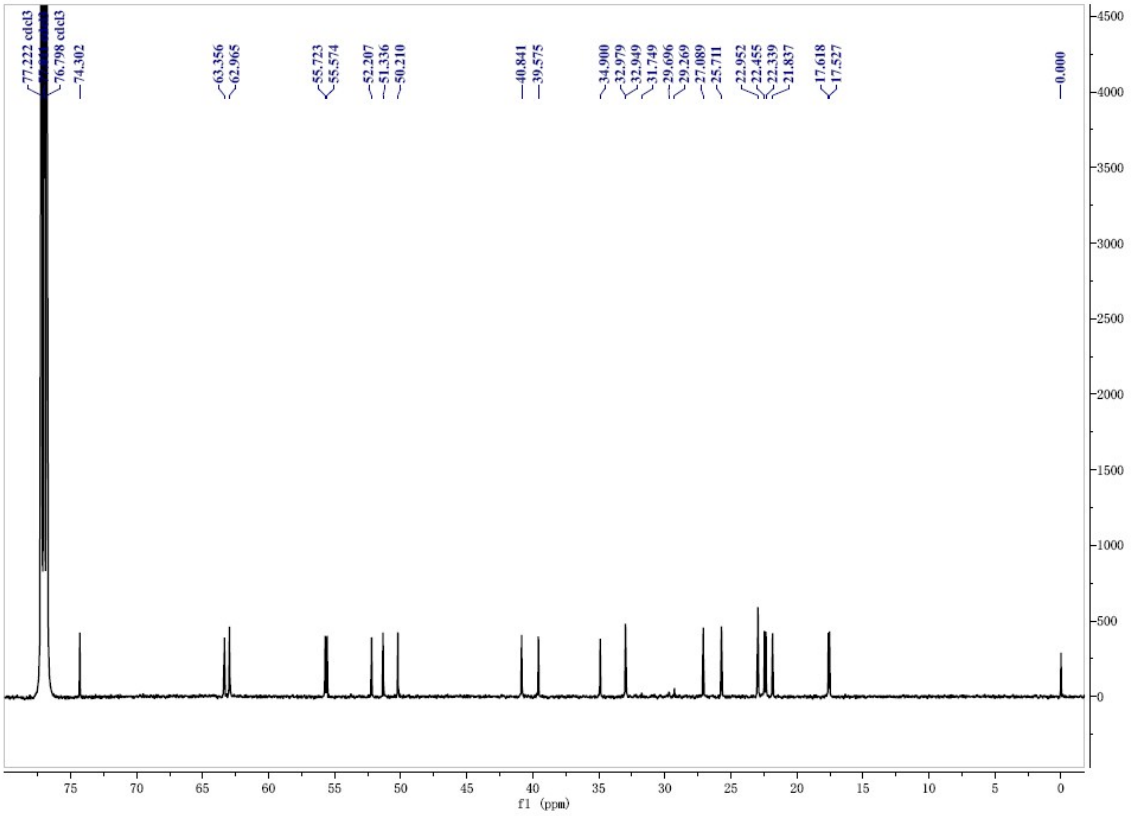


Figure S24. The enlarged ^{13}C NMR spectrum of belamchinenin A (1)



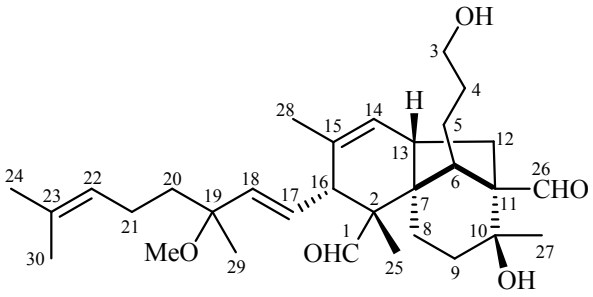
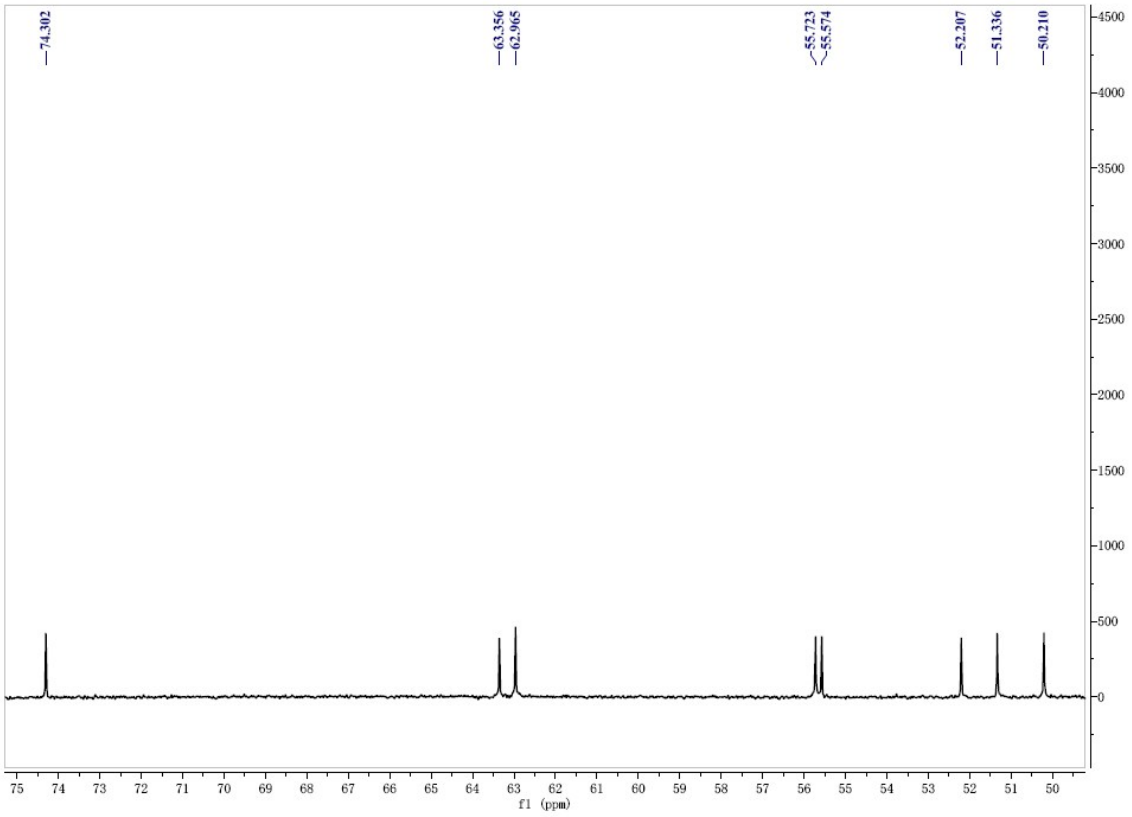


Figure S25. The enlarged ^{13}C NMR spectrum of belamchinenin A (1)



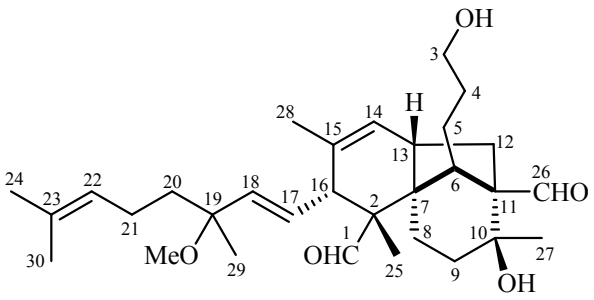
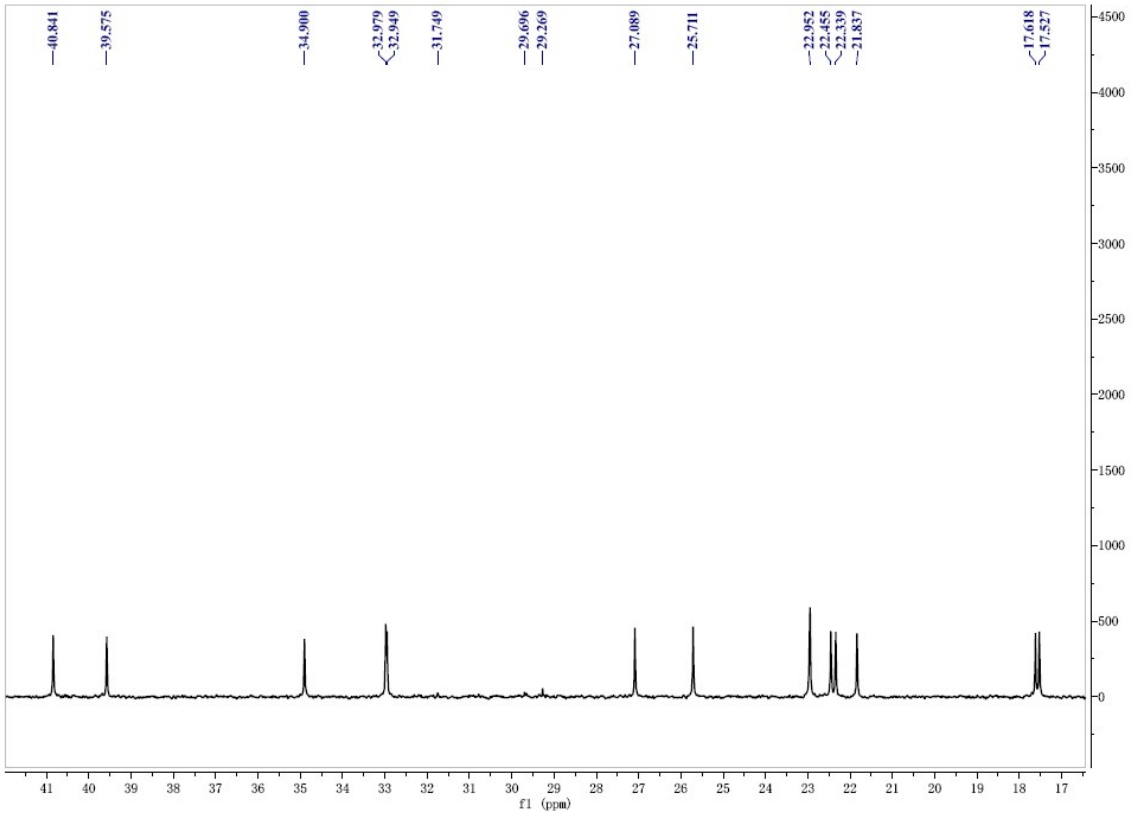


Figure S26. The enlarged ^{13}C NMR spectrum of belamchinenin A (1)



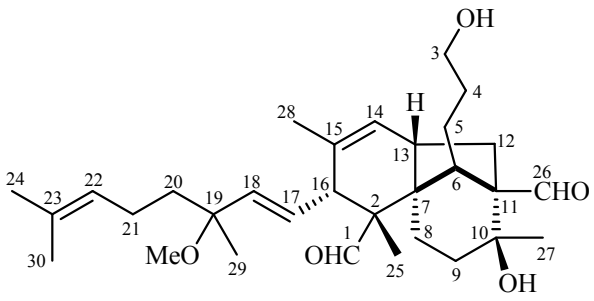
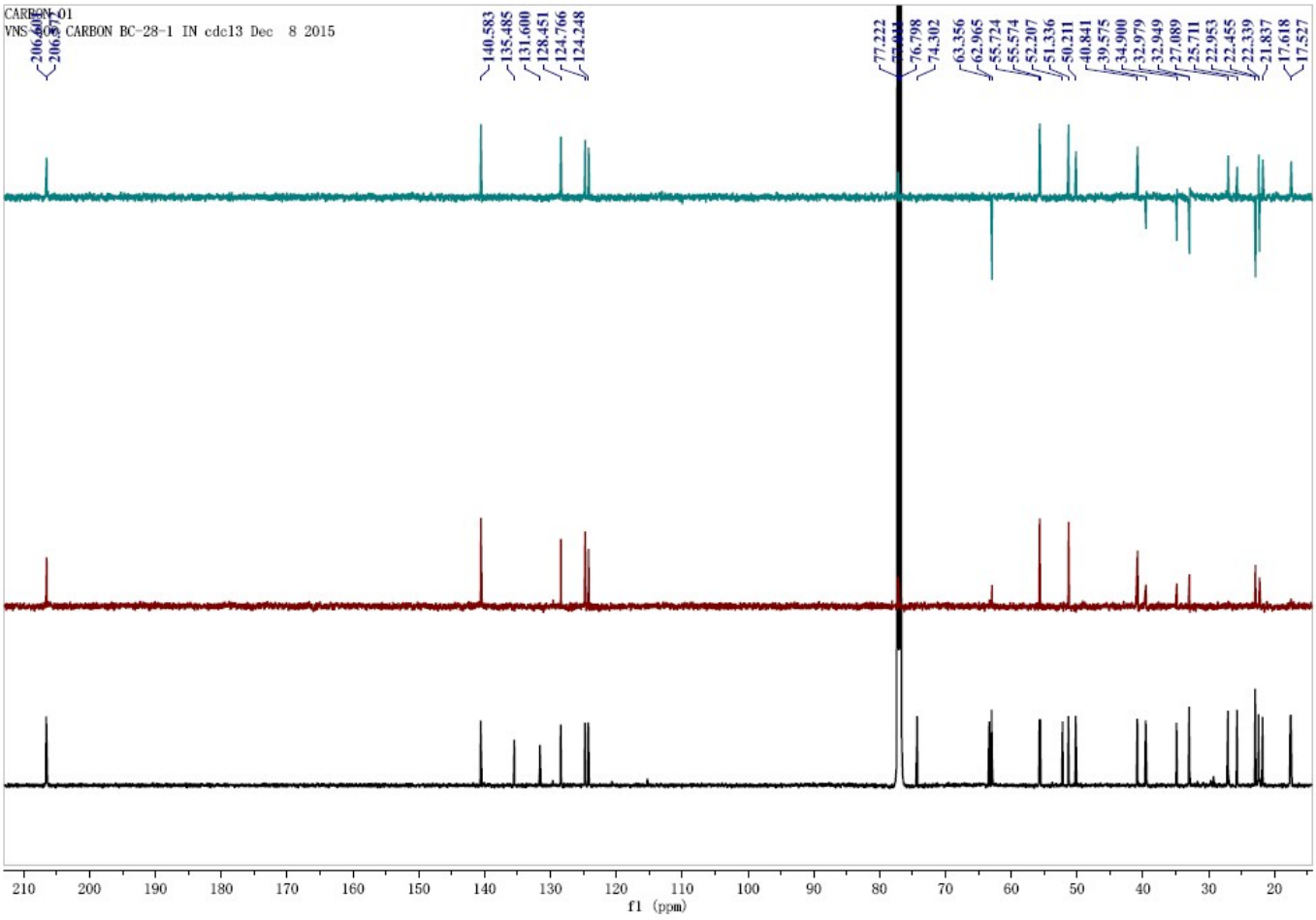


Figure S27. The DEPT spectrum of belamchinenin A (1)



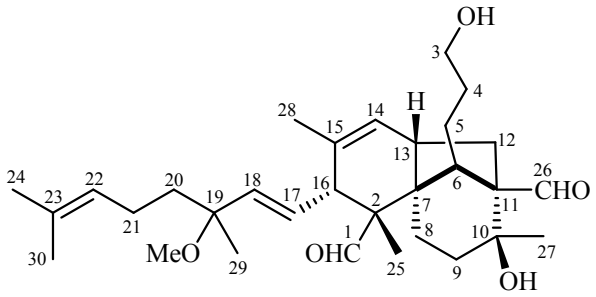
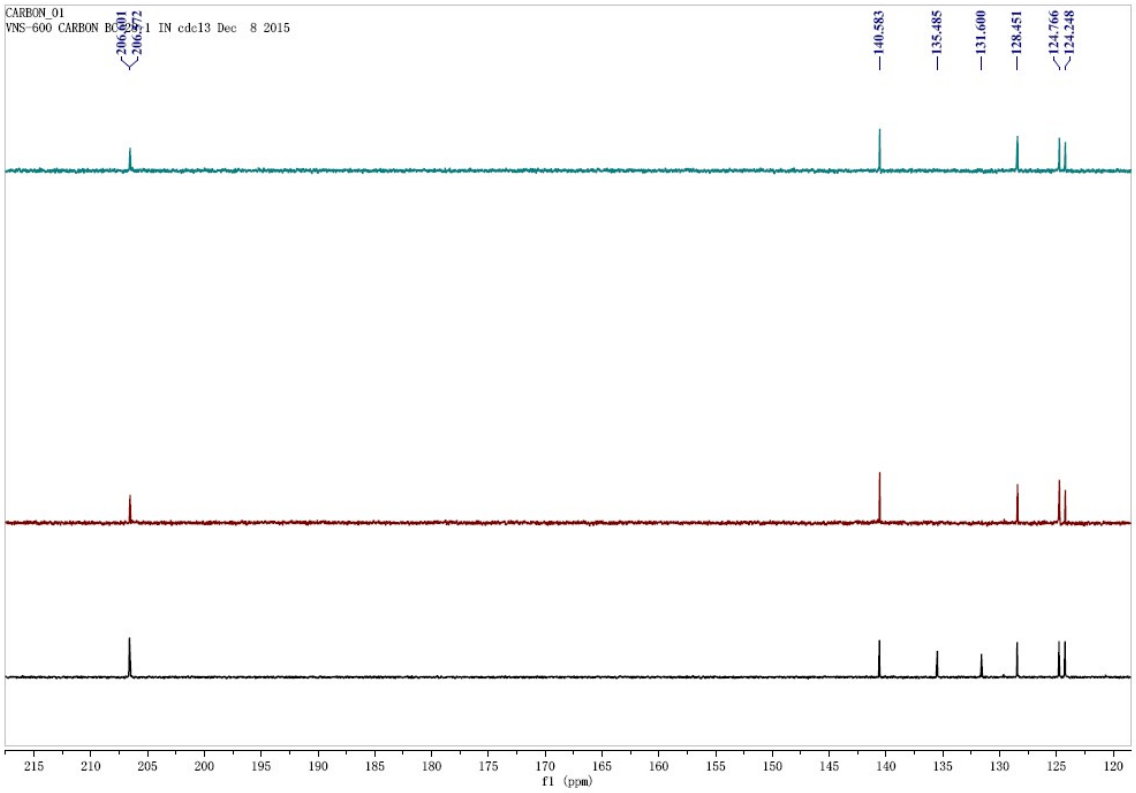


Figure S28. The enlarged DEPT spectrum of belamchinenin A (1)



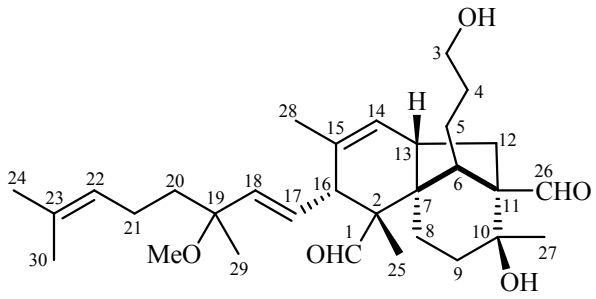
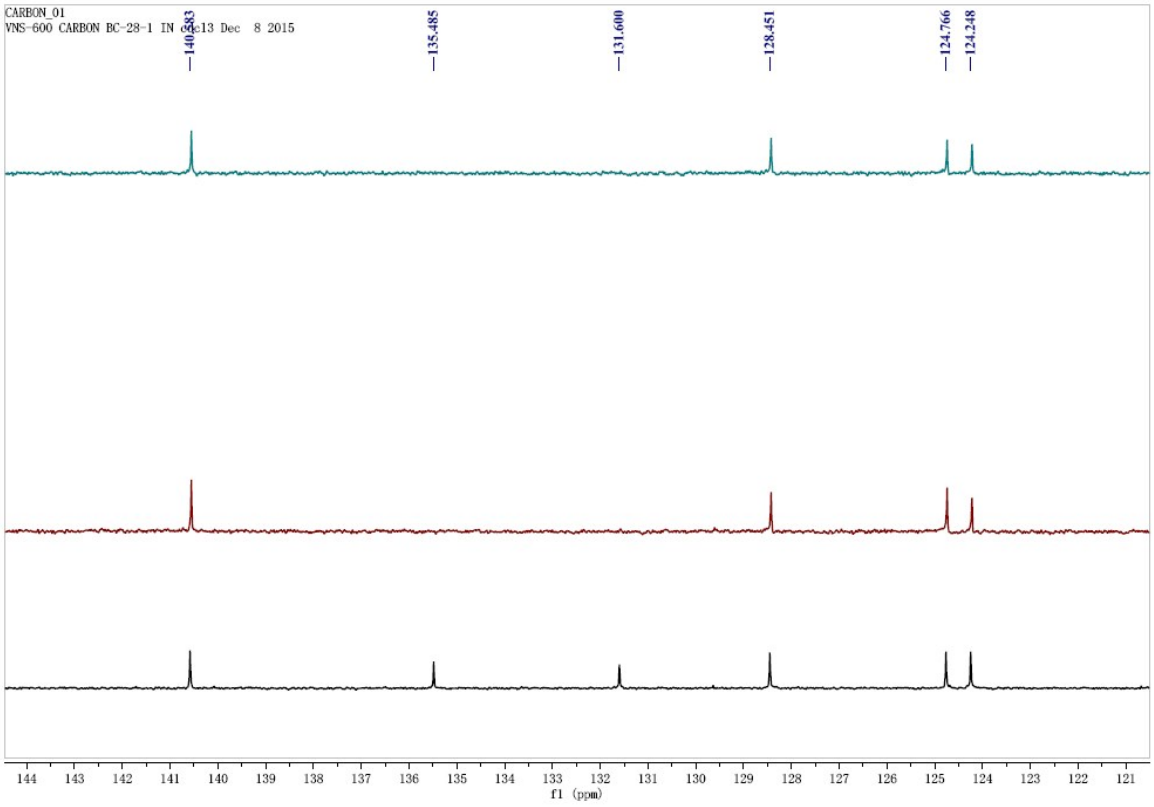


Figure S29. The enlarged DEPT spectrum of belamchinenin A (1)



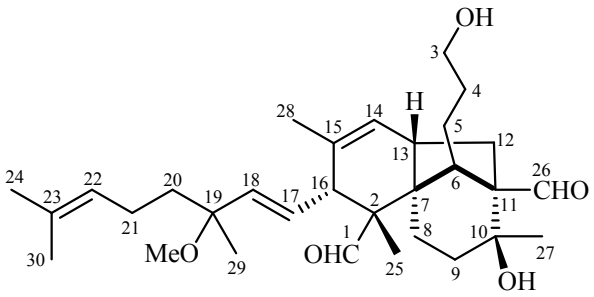
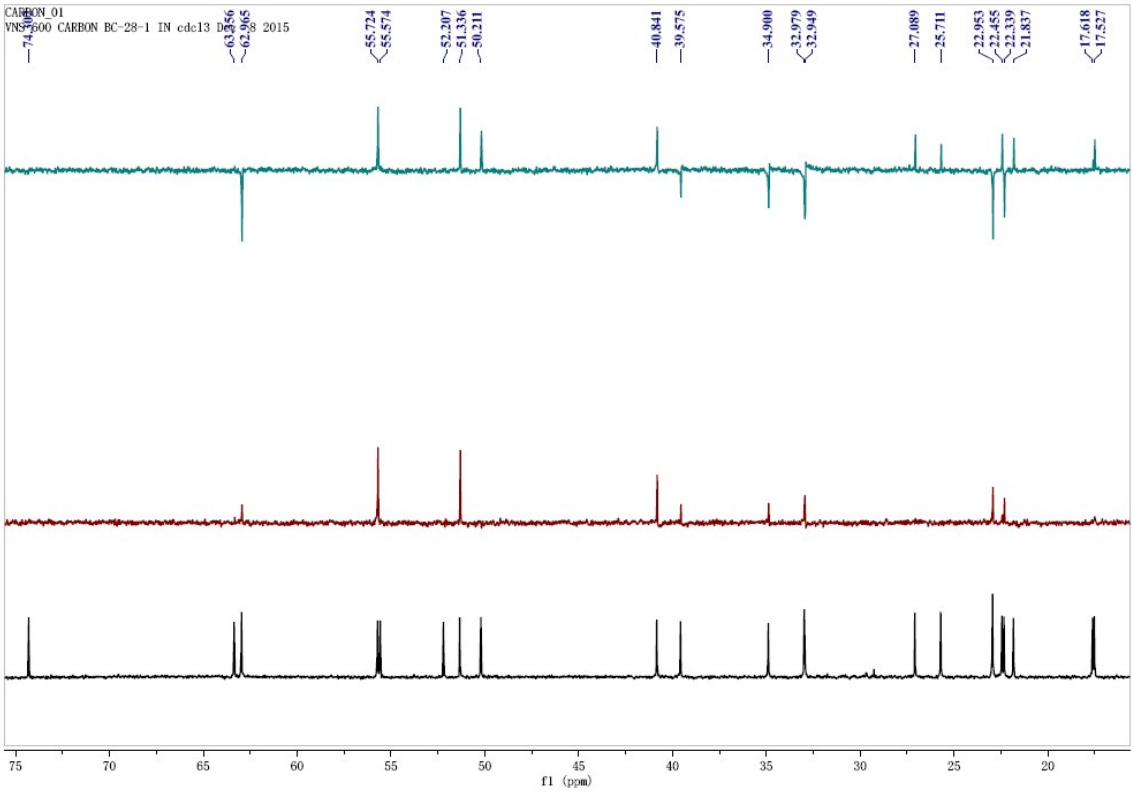


Figure S30. The enlarged DEPT spectrum of belamchinenin A (1)



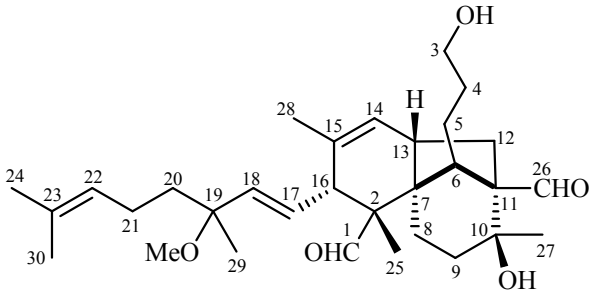
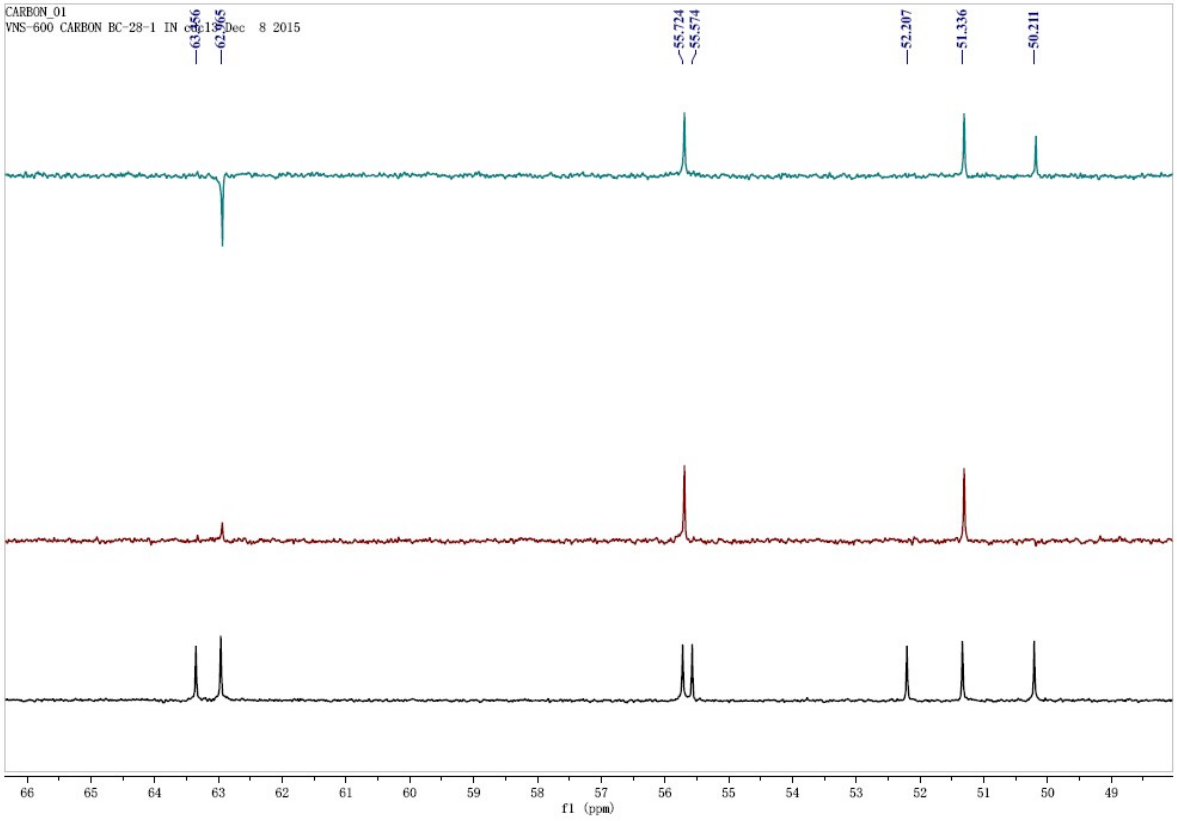


Figure S31. The enlarged DEPT spectrum of belamchinenin A (1)



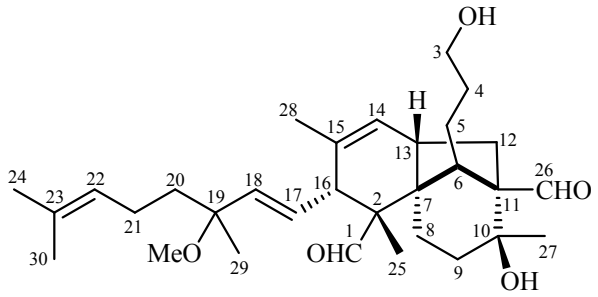
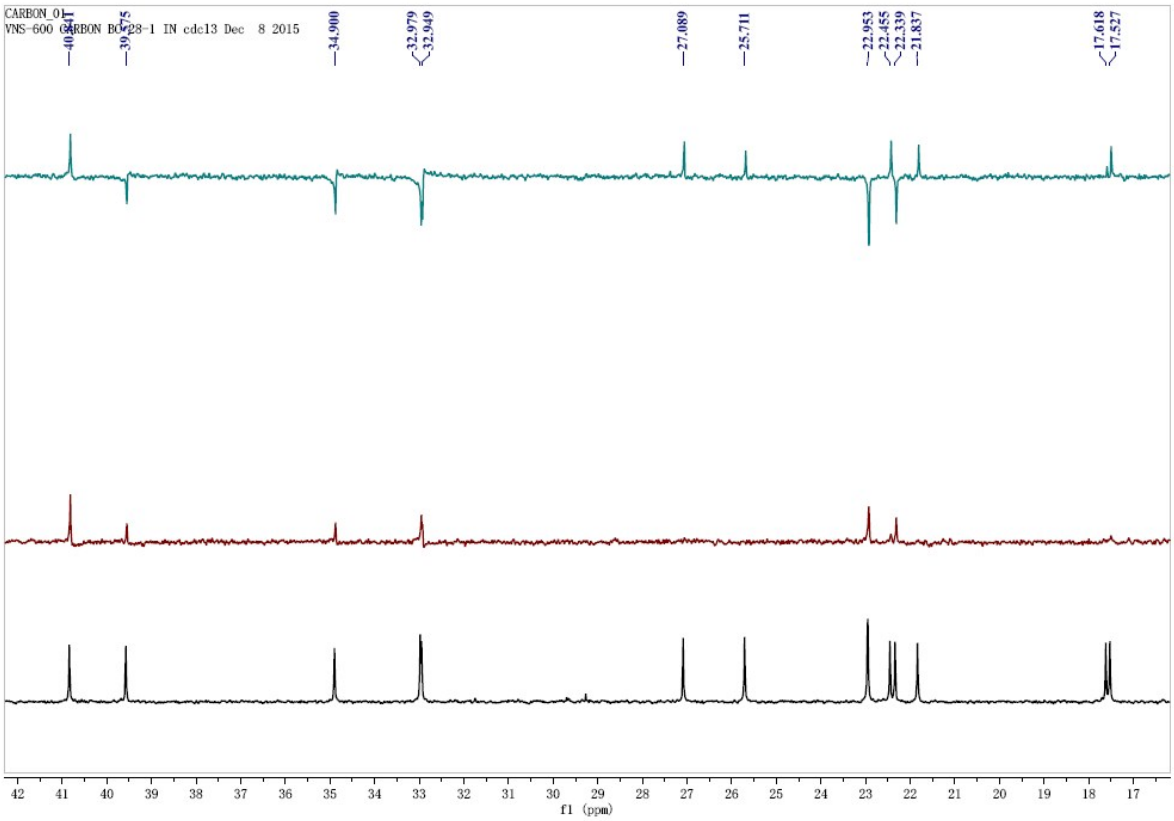


Figure S32. The enlarged DEPT spectrum of belamchinenin A (1)



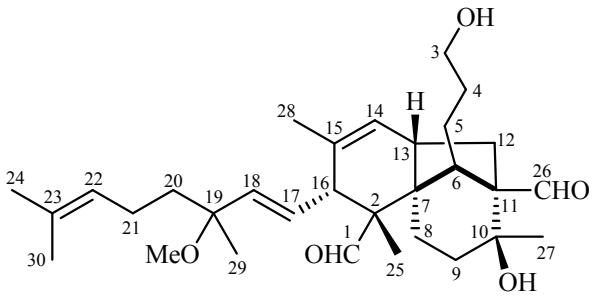
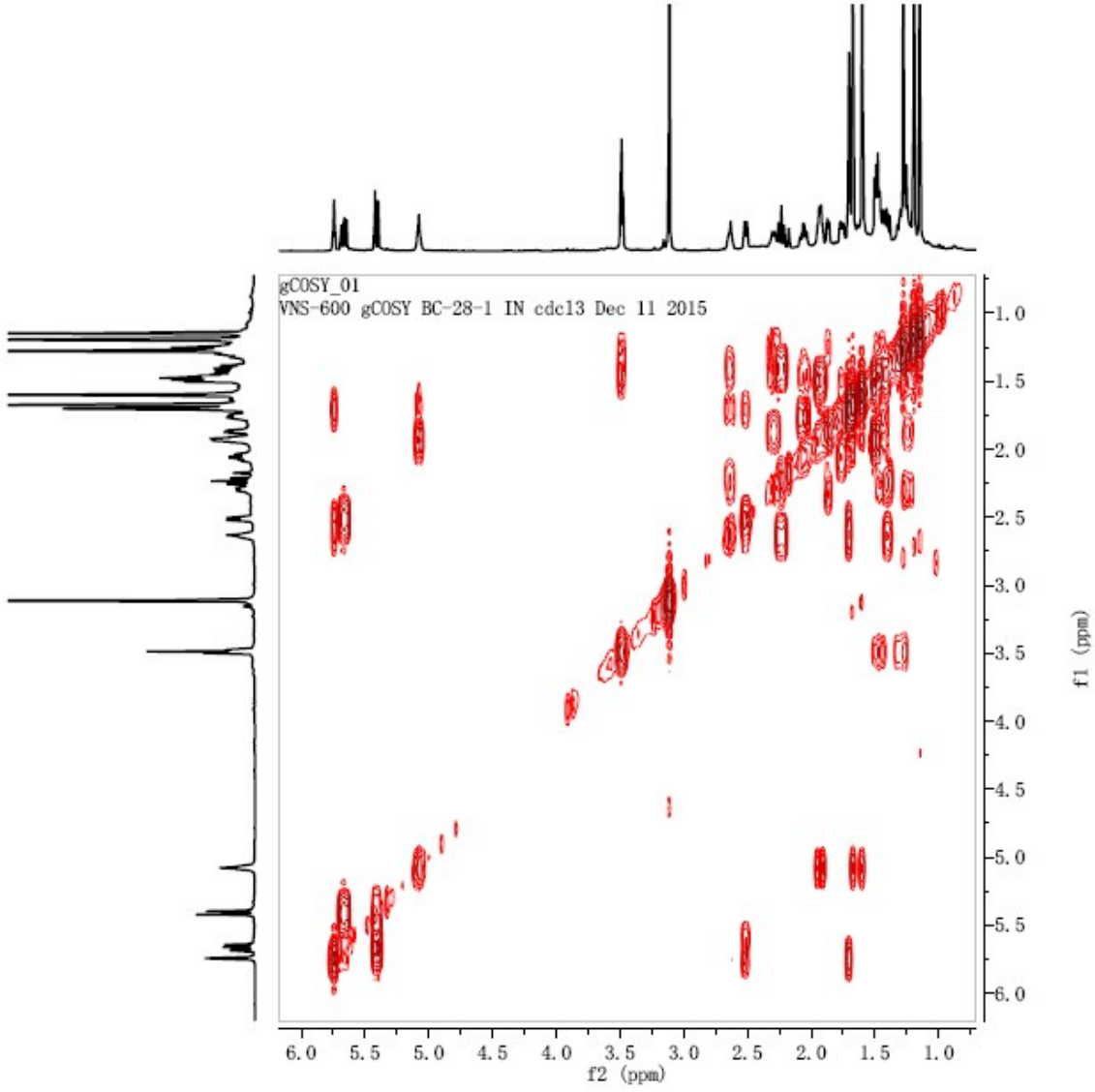


Figure S33. The ^{1}H-^{1}H COSY spectrum of belamchinenin A (1)



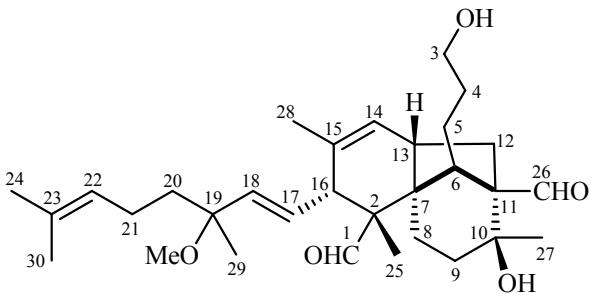
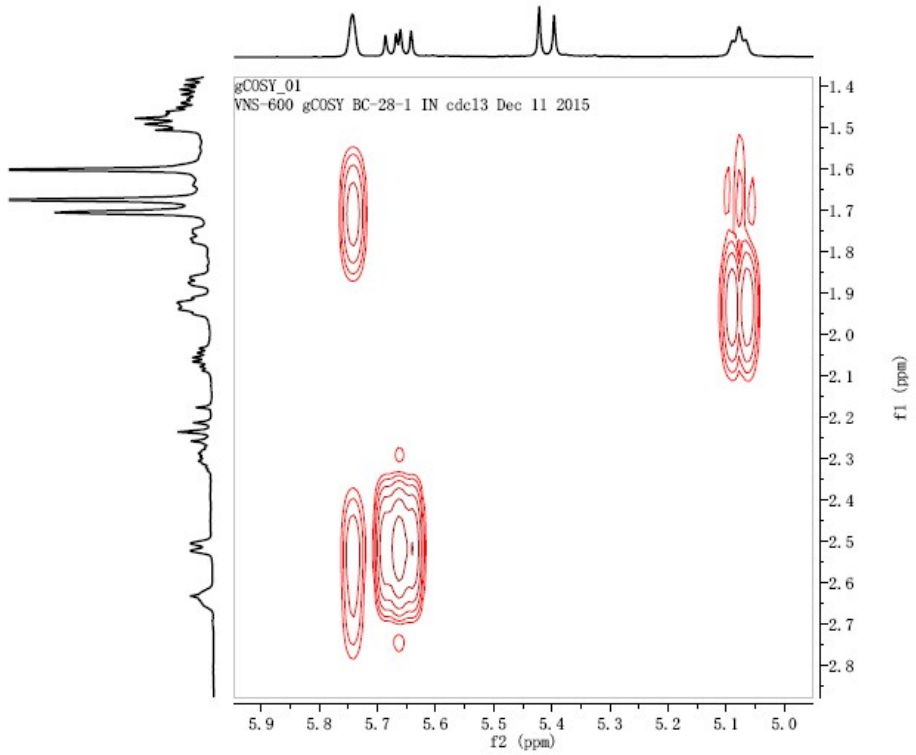


Figure S34. The enlarged ^{1}H-^{1}H COSY spectrum of belamchinenin A (1)



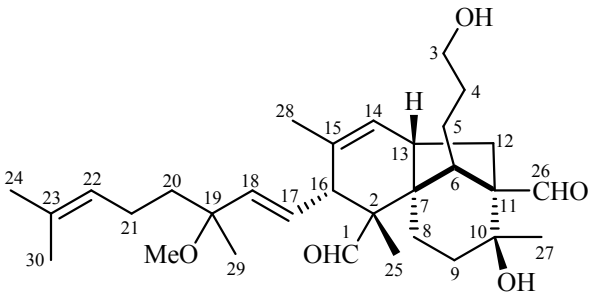
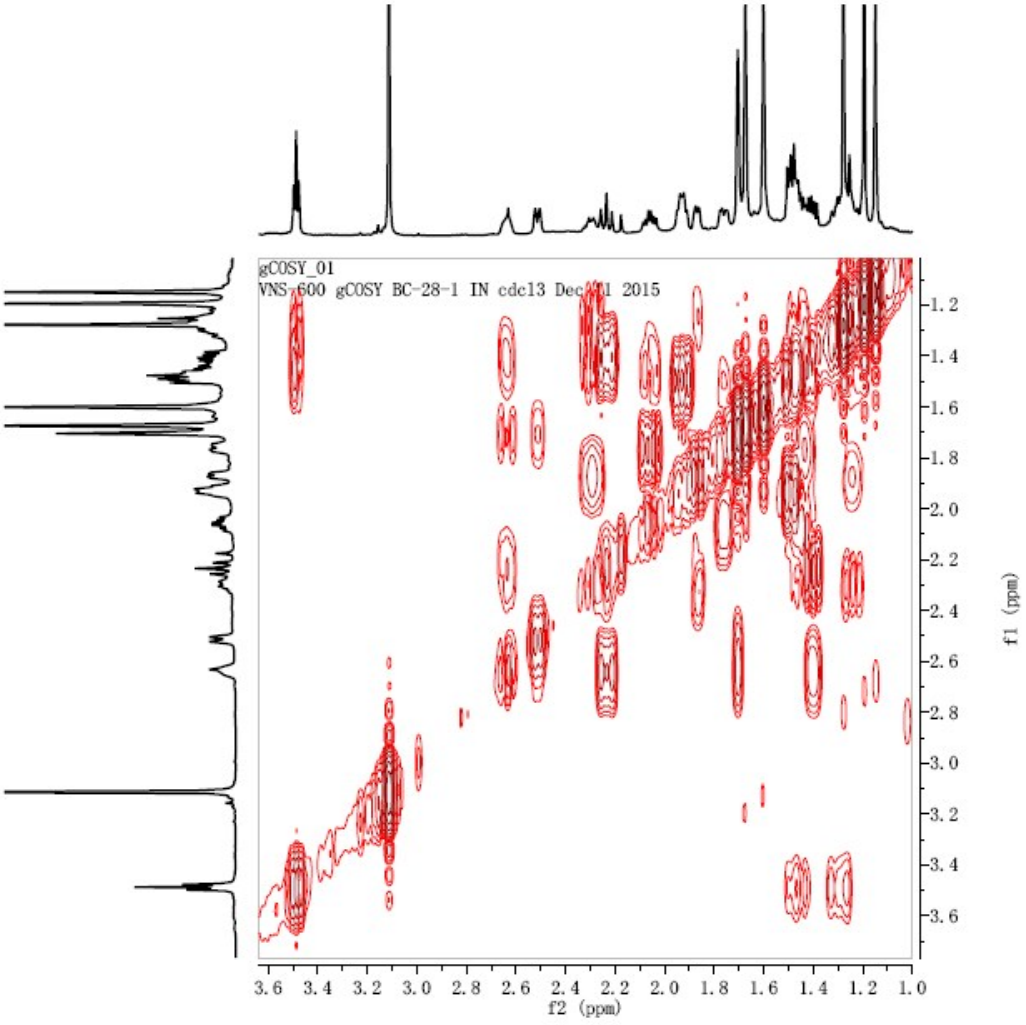


Figure S35. The enlarged ^{1}H-^{1}H COSY spectrum of belamchinenin A (1)



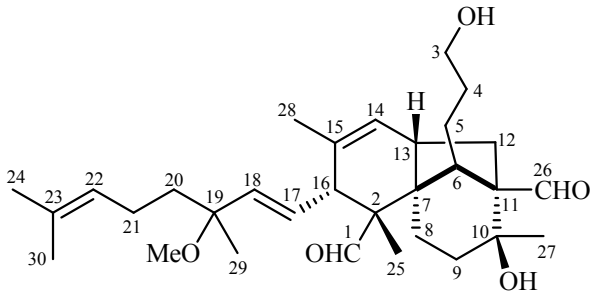
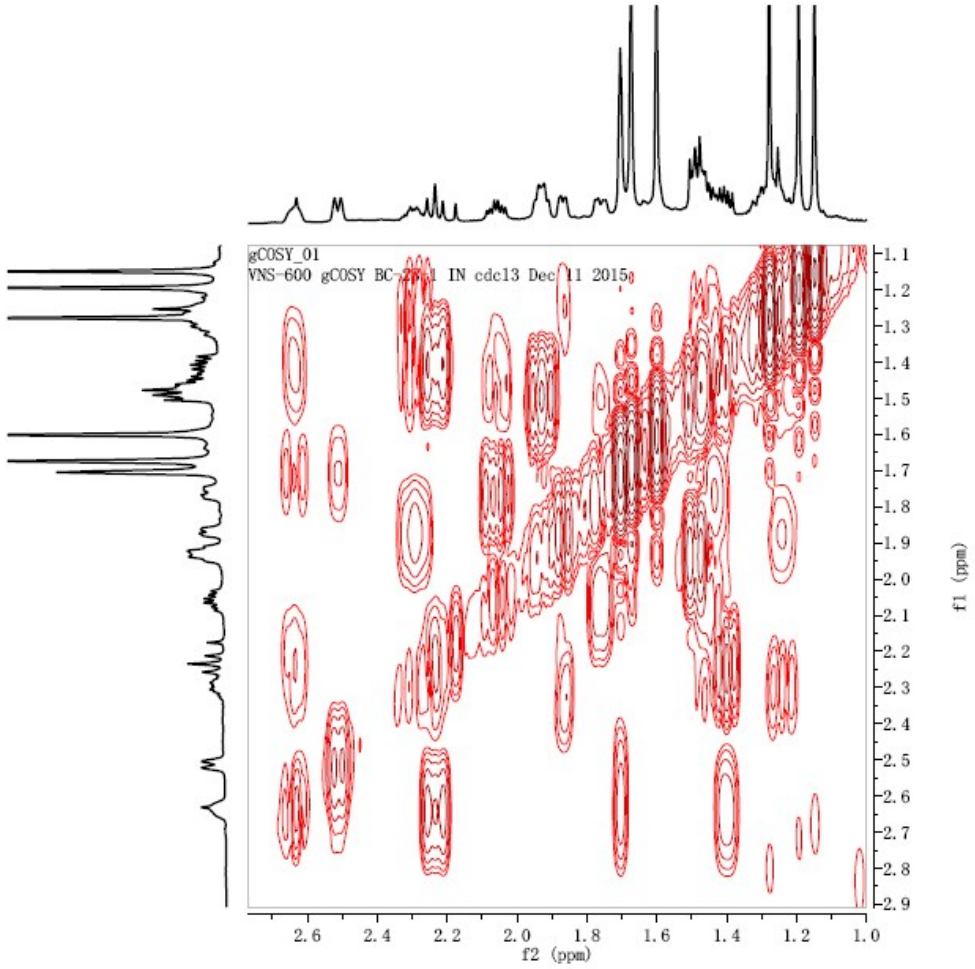


Figure S36. The enlarged ^{1}H-^{1}H COSY spectrum of belamchinenin A (1)



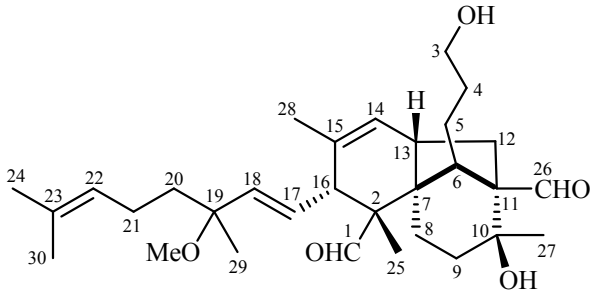
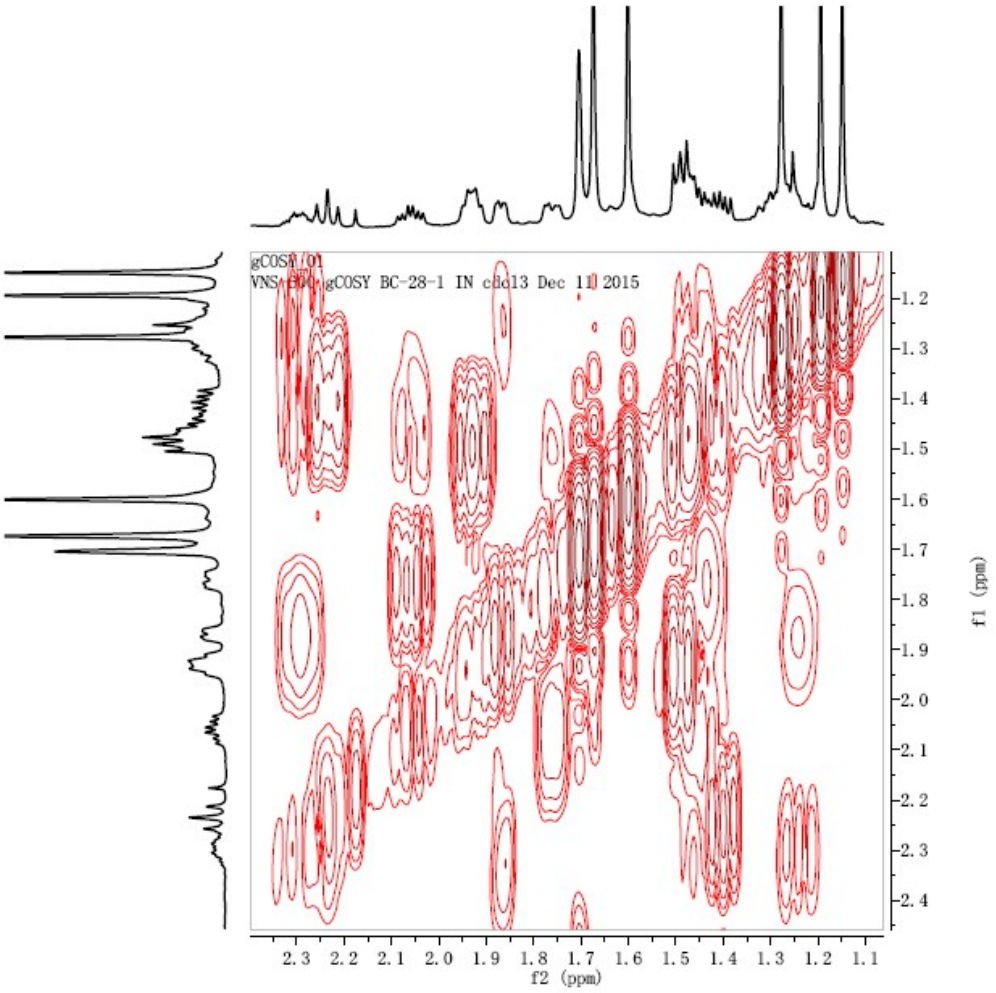


Figure S37. The enlarged ^{1}H-^{1}H COSY spectrum of belamchinenin A (1)



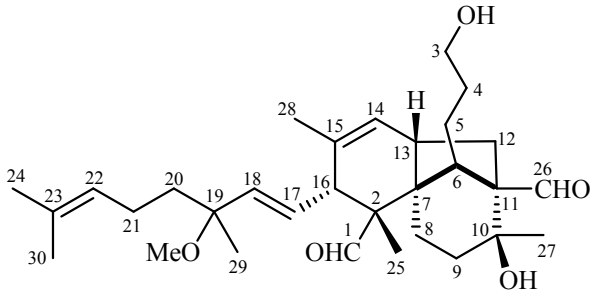
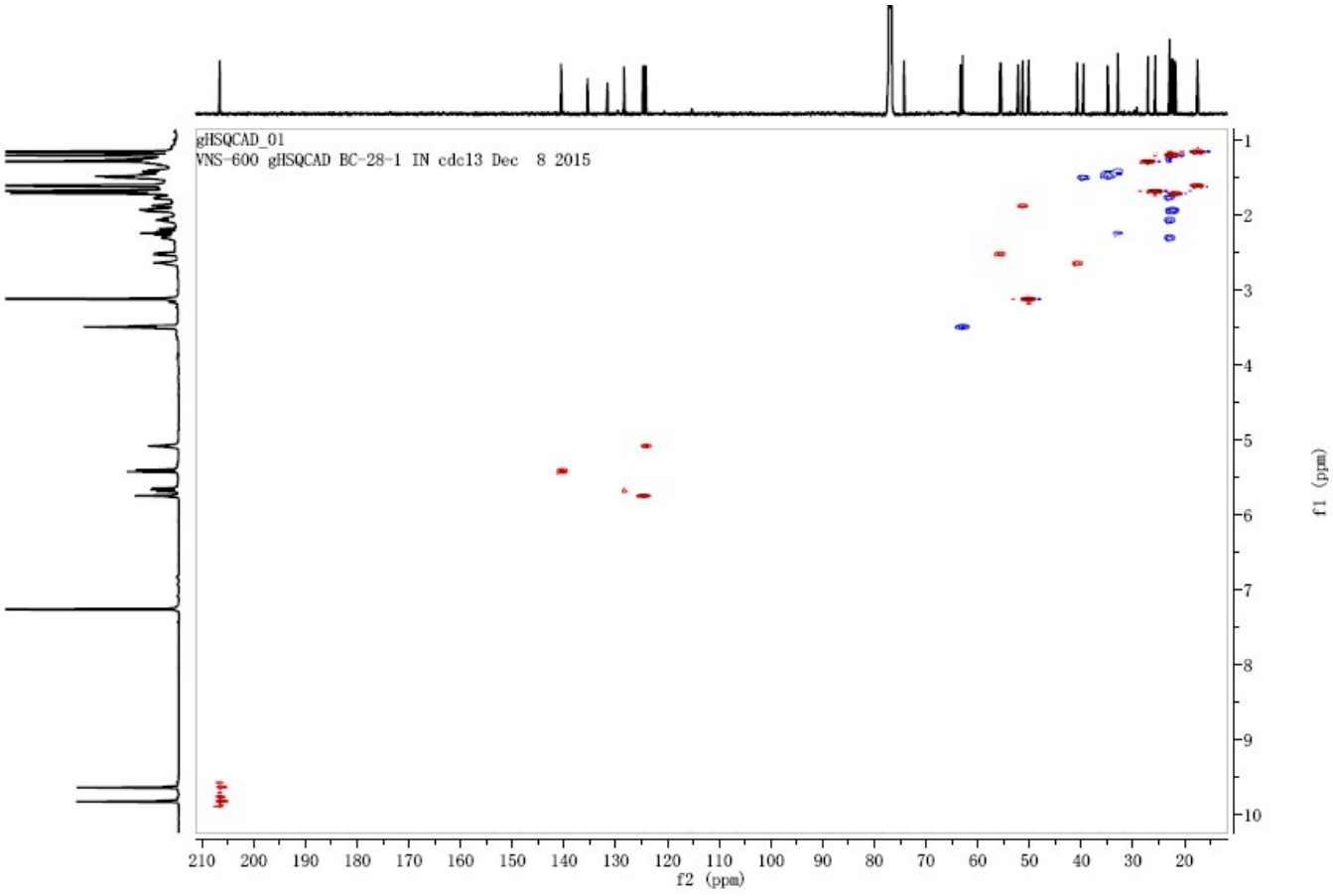


Figure S38. The HSQC spectrum of belamchinenin A (1)



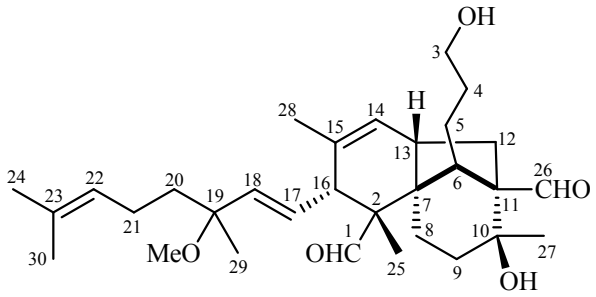
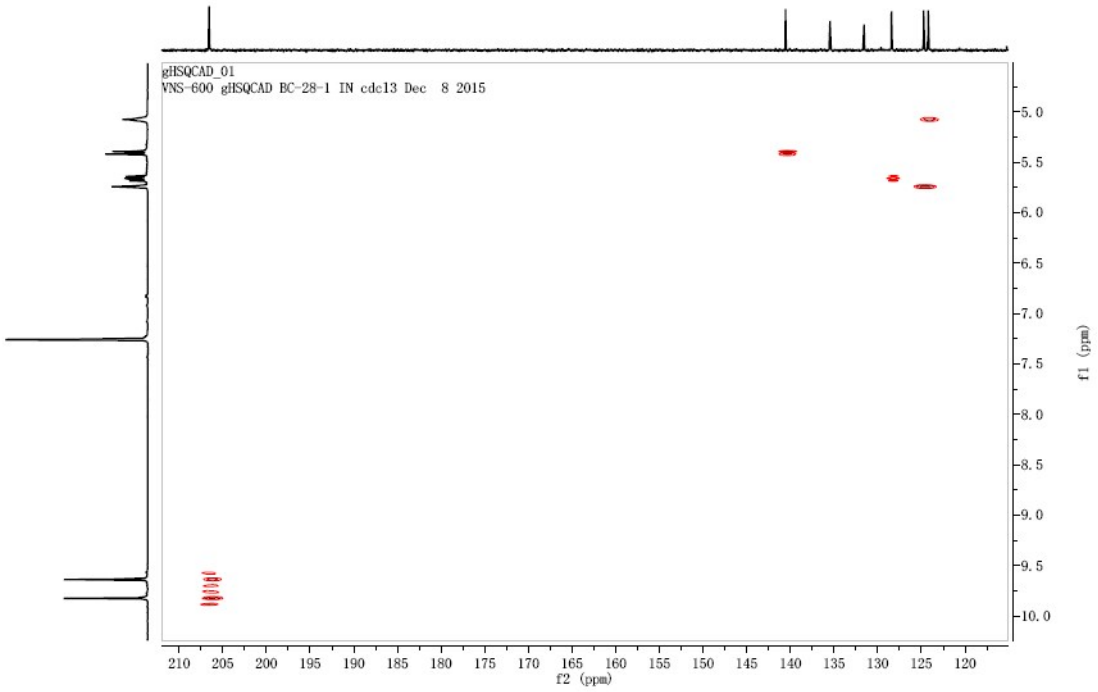


Figure S39. The enlarged HSQC spectrum of belamchinenin A (1)



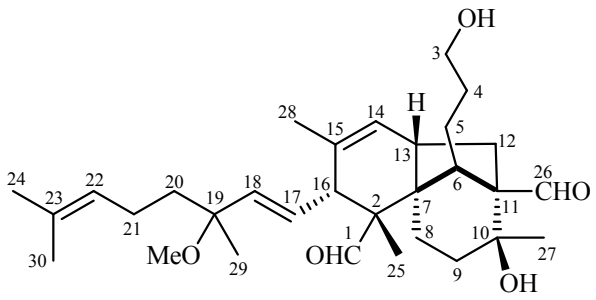
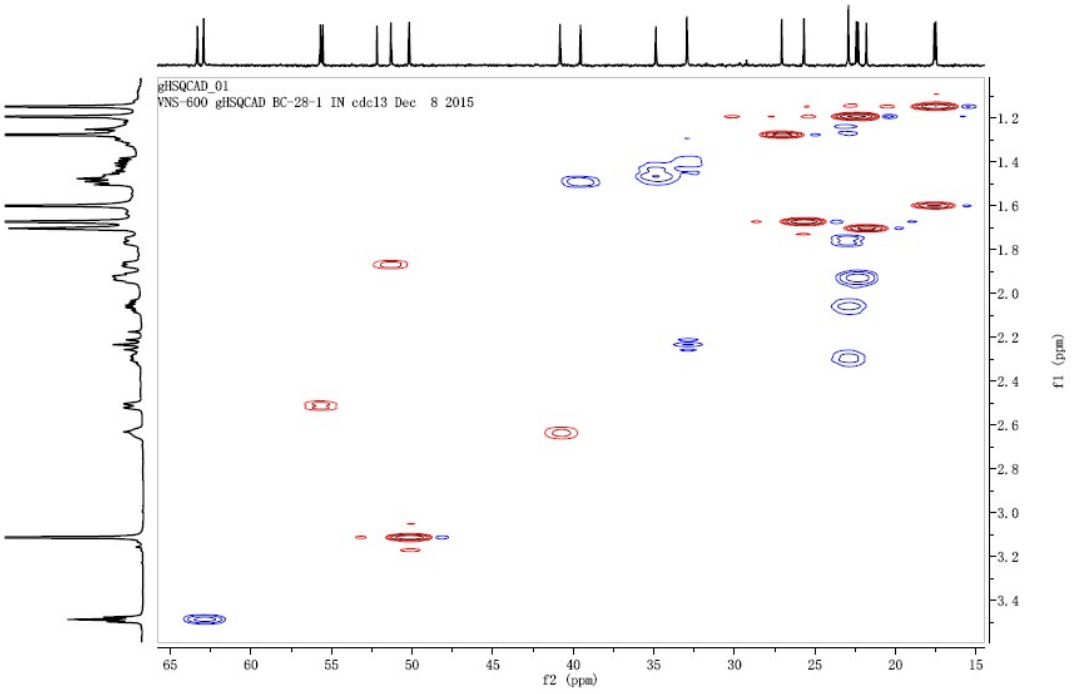


Figure S40. The enlarged HSQC spectrum of belamchinenin A (1)



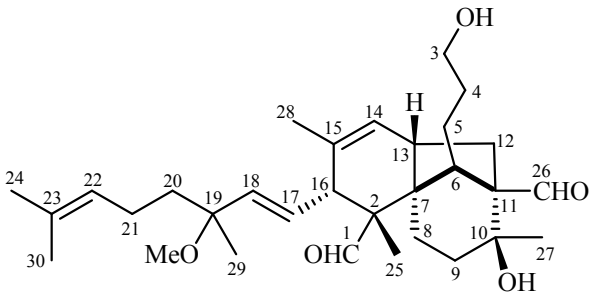
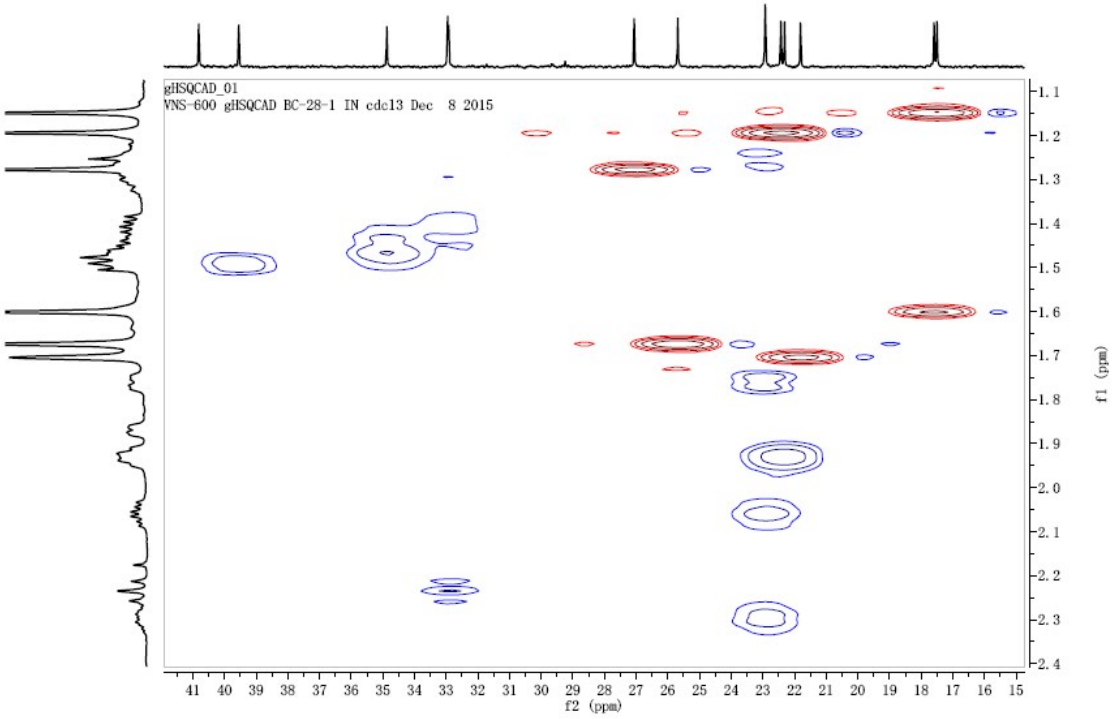


Figure S41. The enlarged HSQC spectrum of belamchinenin A (1)



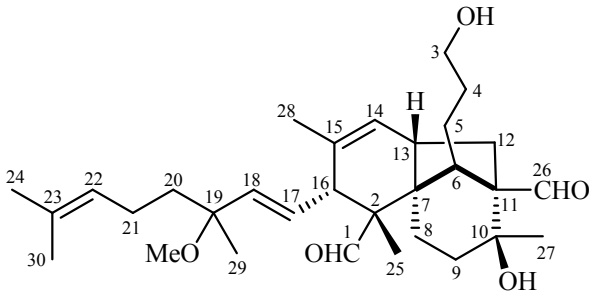
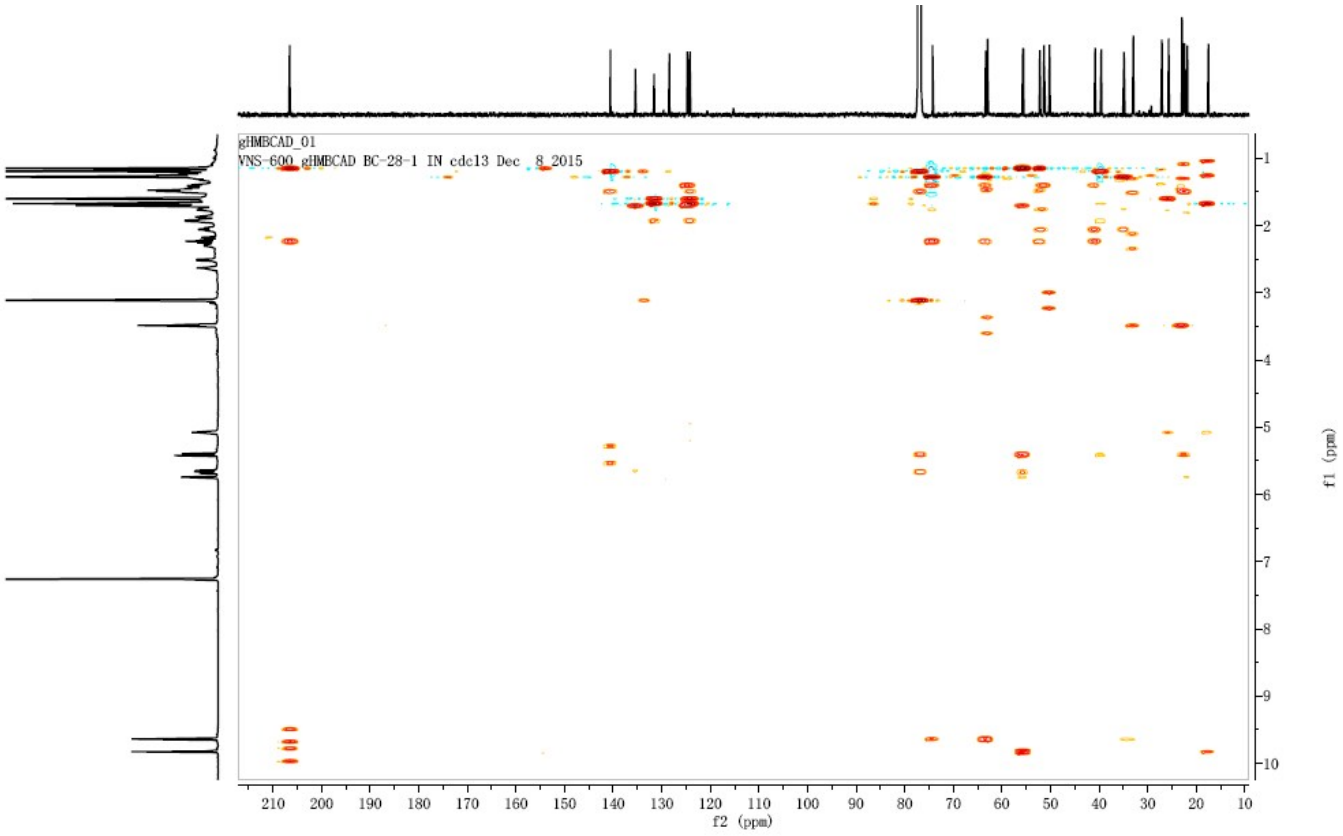


Figure S42. The HMBC spectrum of belamchinenin A (1)



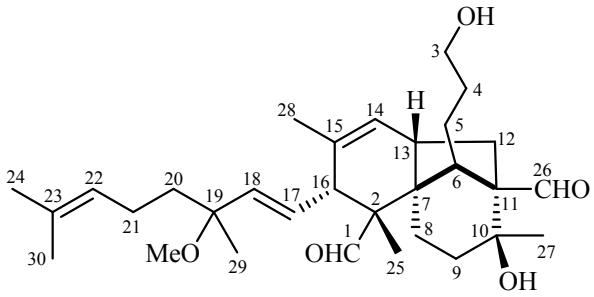
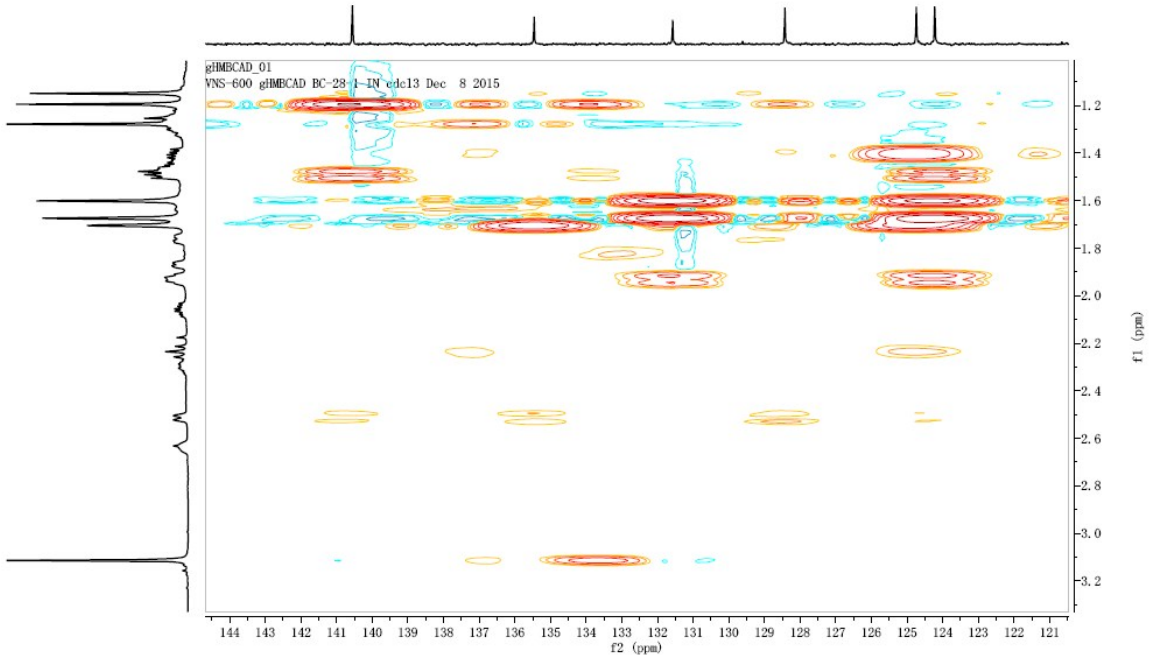


Figure S43. The enlarged HMBC spectrum of belamchinenin A (1)



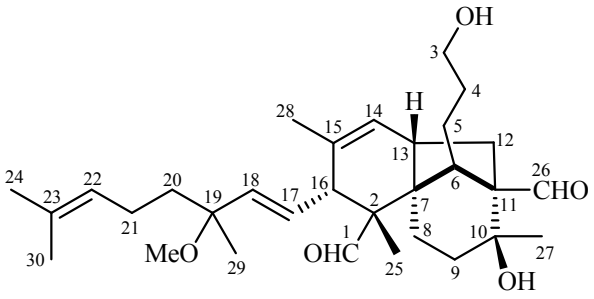
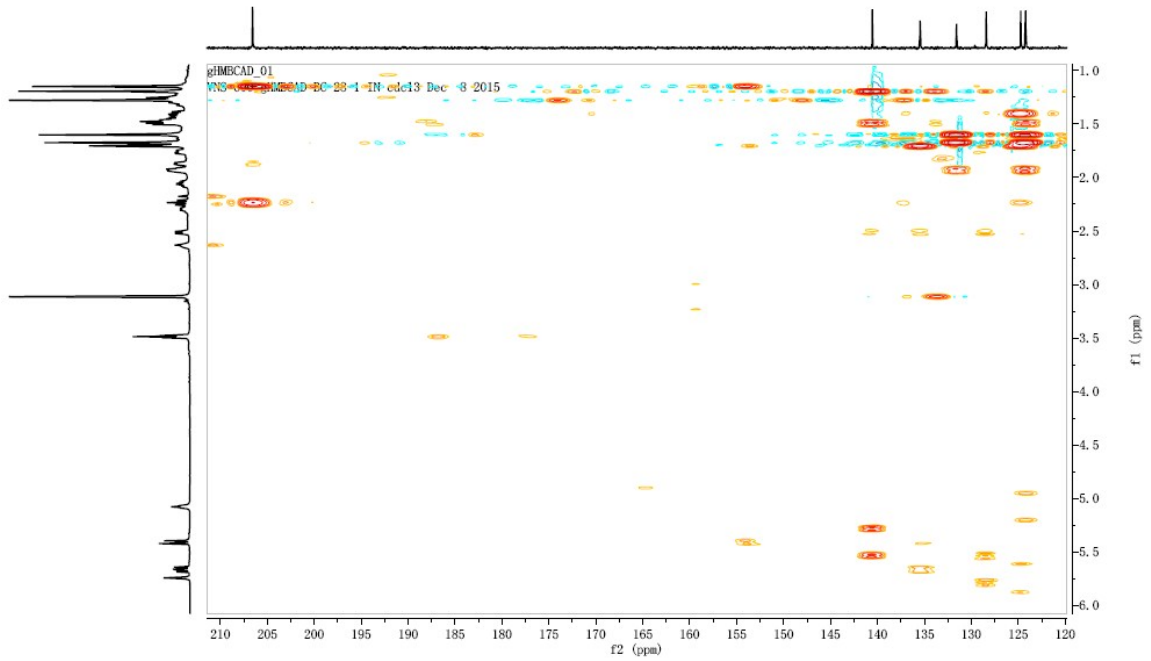


Figure S44. The enlarged HMBC spectrum of belamchinenin A (1)



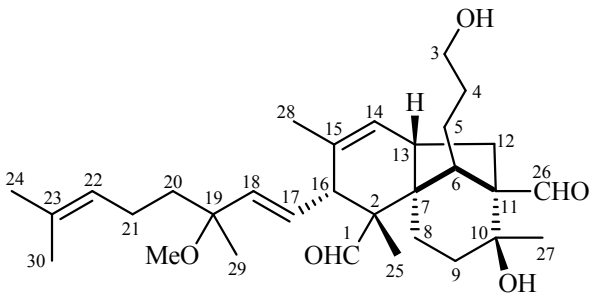


Figure S45. The enlarged HMBC spectrum of belamchinenin A (1)

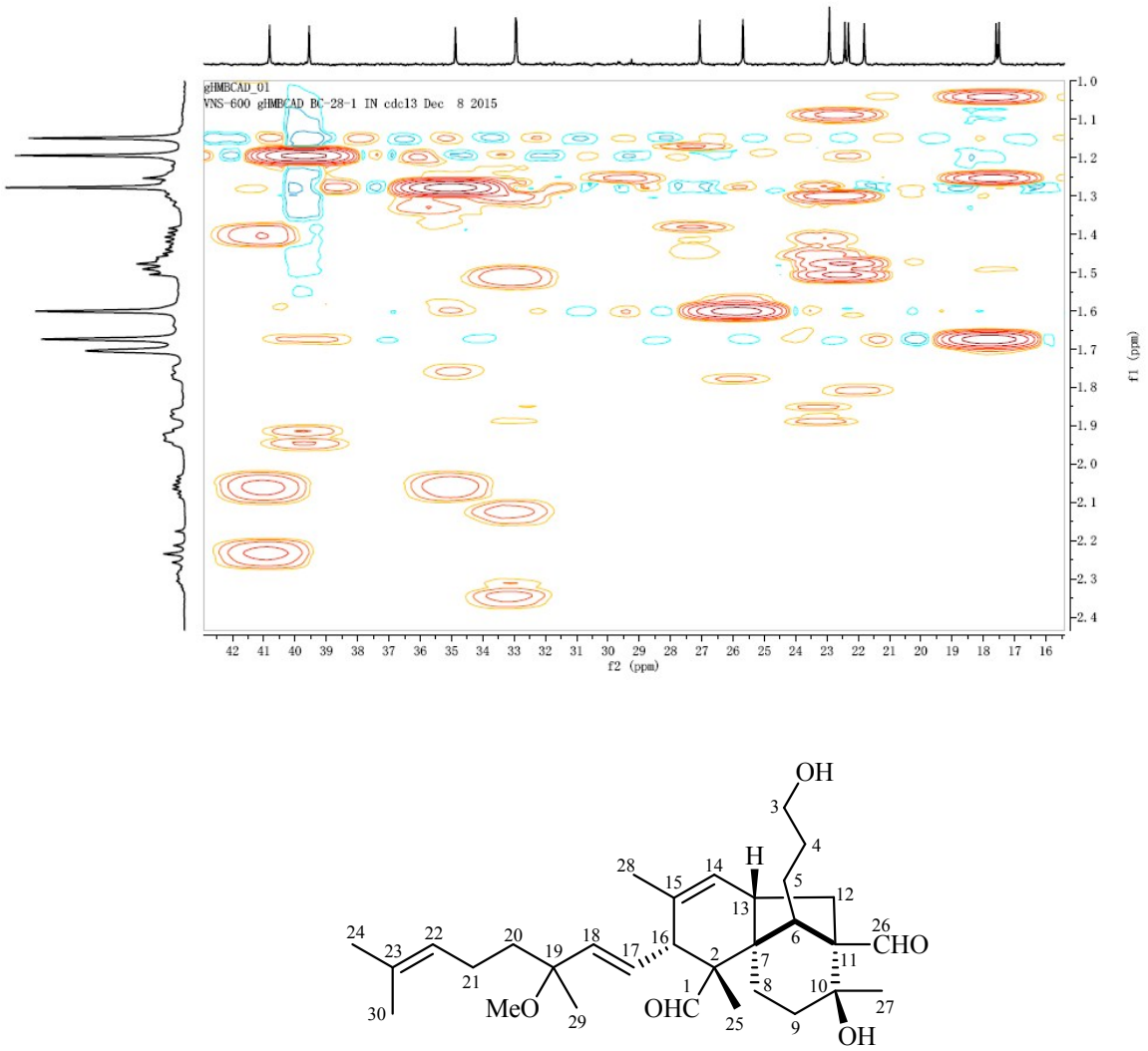
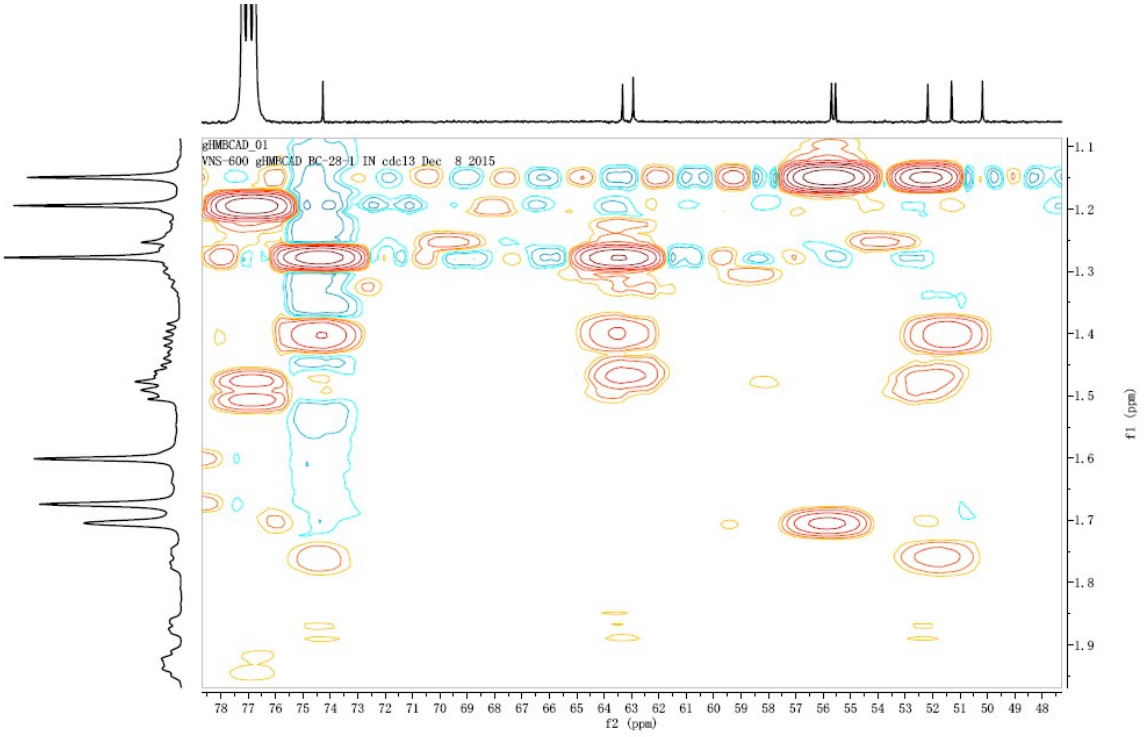


Figure S46. The enlarged HMBC spectrum of belamchinenin A (1)



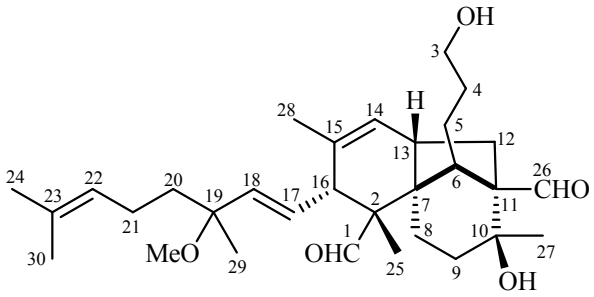
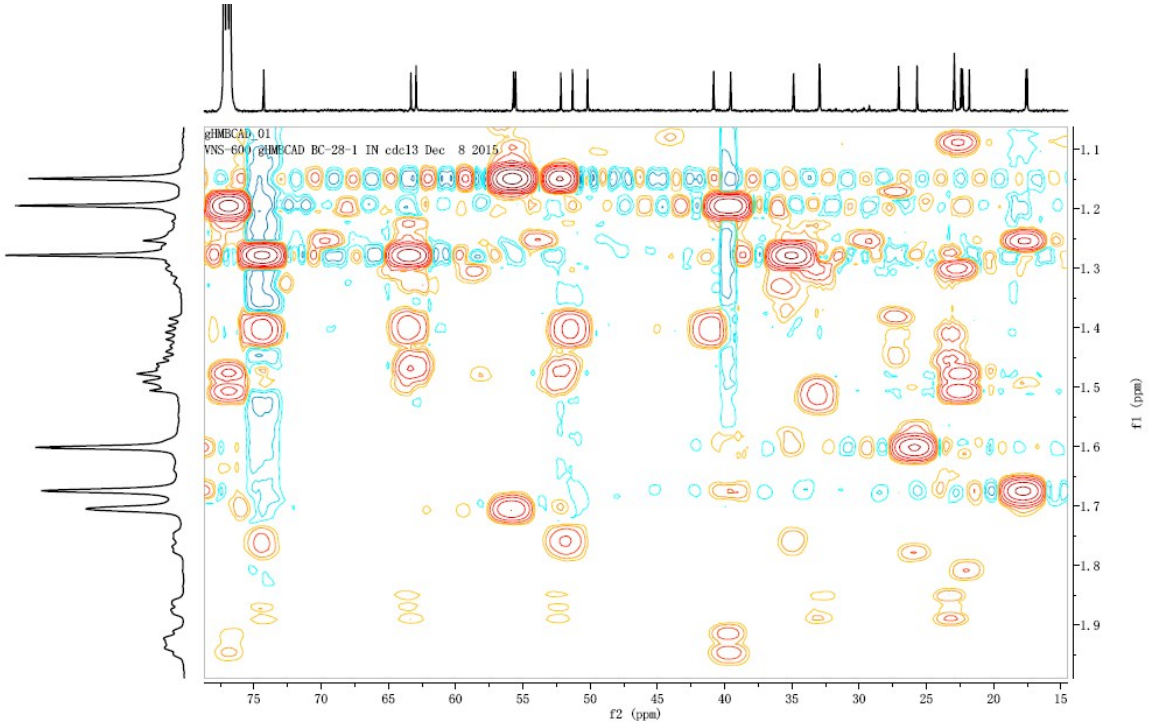


Figure S47. The enlarged HMBC spectrum of belamchinenin A (1)



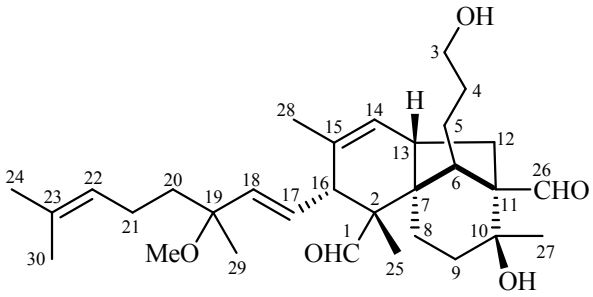
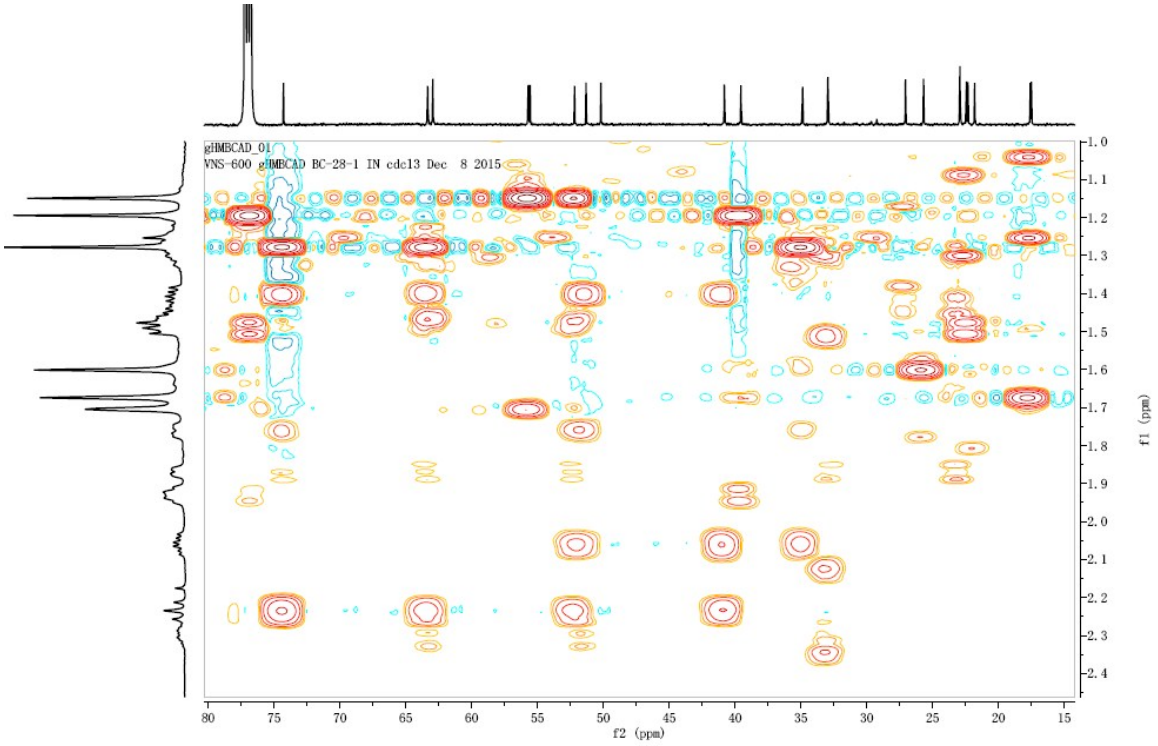


Figure S48. The enlarged HMBC spectrum of belamchinenin A (1)



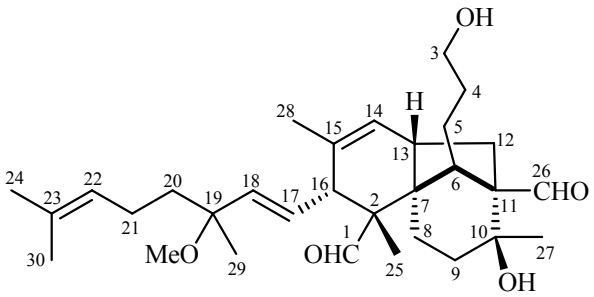
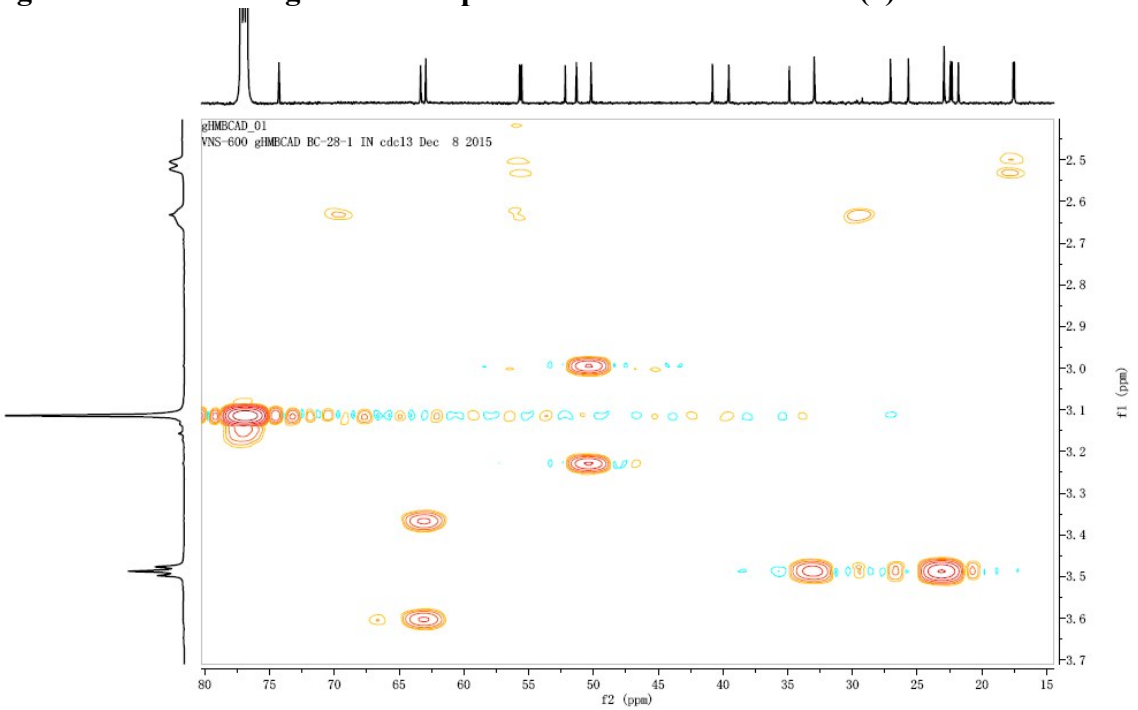


Figure S49. The enlarged HMBC spectrum of belamchinenin A (1)



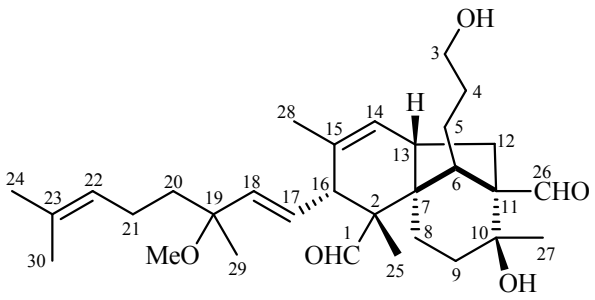
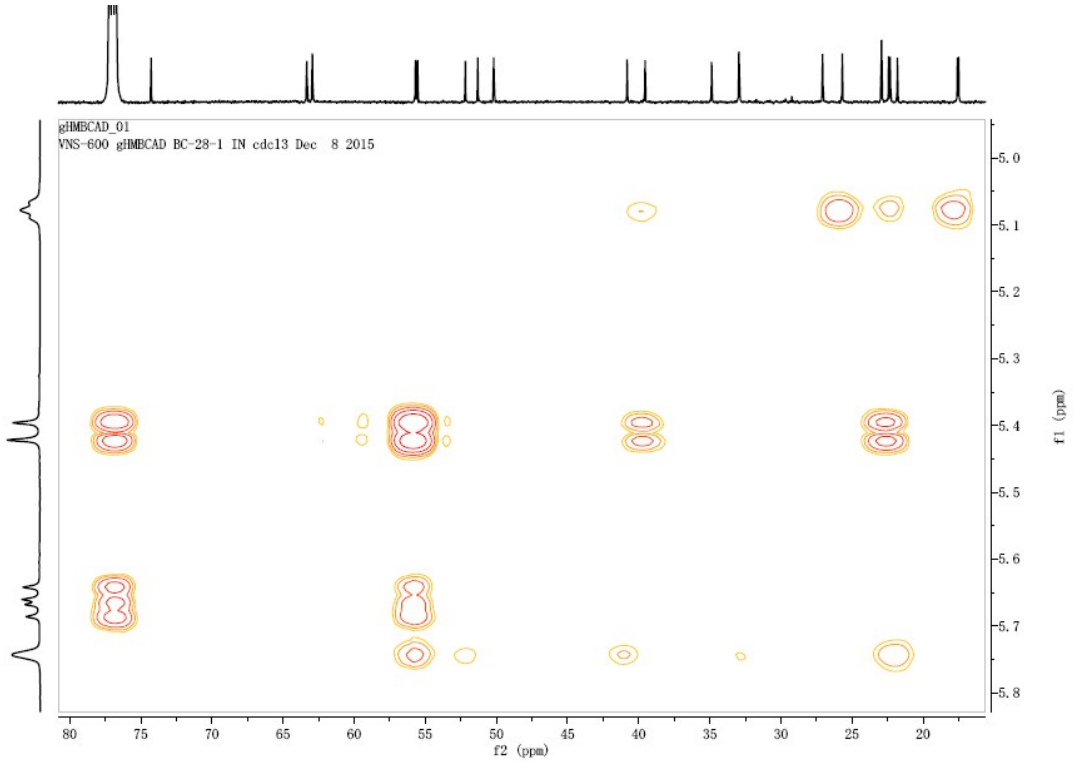


Figure S50. The enlarged HMBC spectrum of belamchinenin A (1)



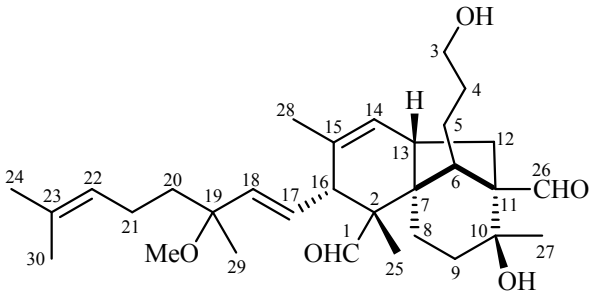
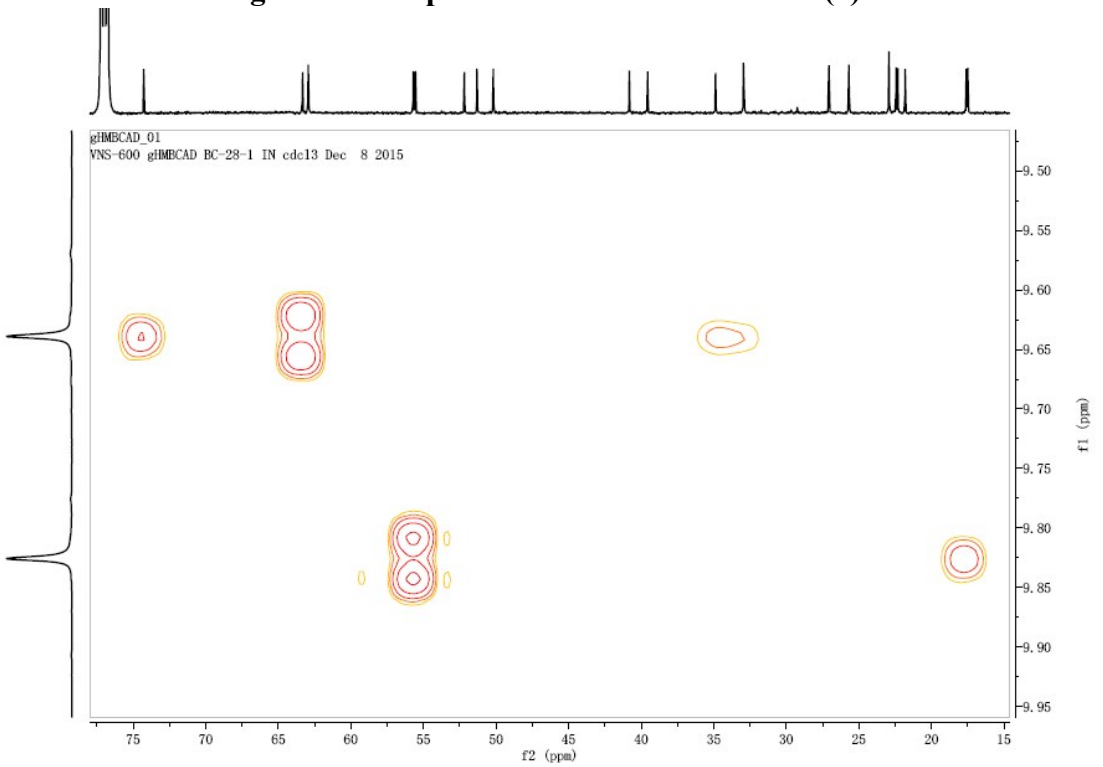


Figure S51. The enlarged HMBC spectrum of belamchinenin A (1)



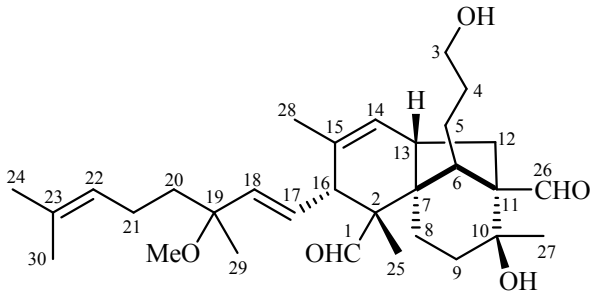
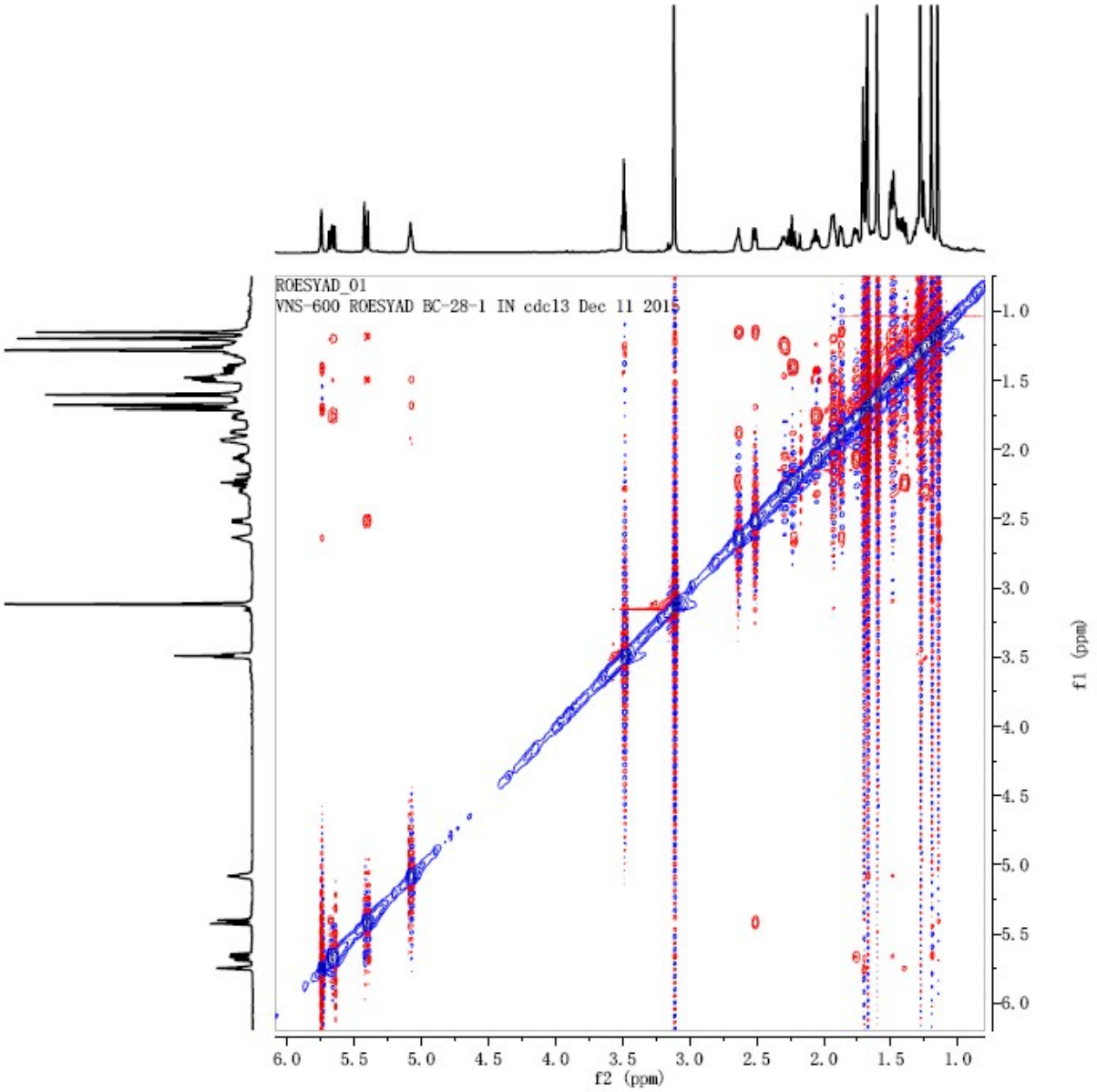


Figure S52. The ROESY spectrum of belamchinenin A (1)



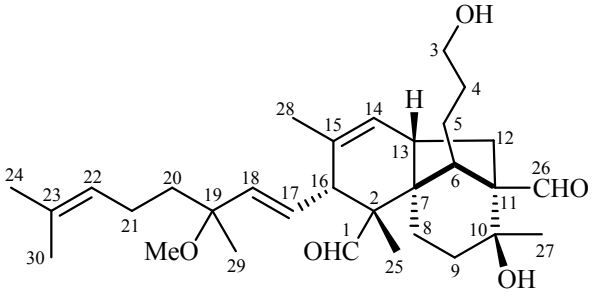
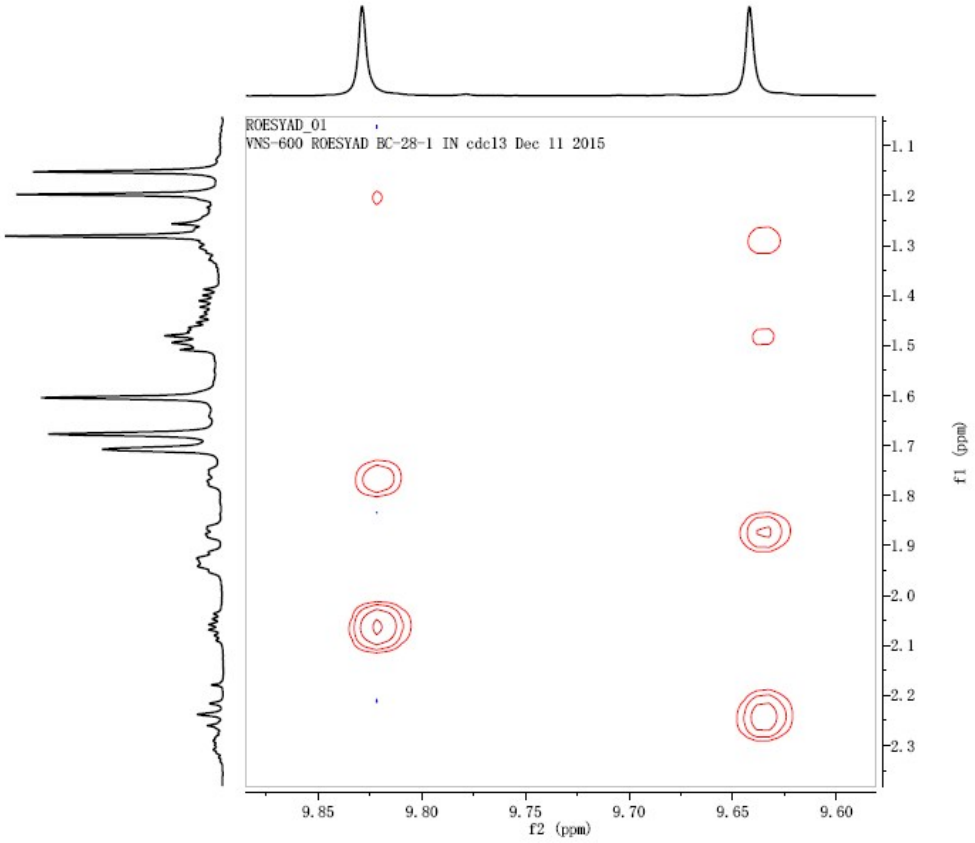


Figure S53. The ROESY spectrum of belamchinenin A (1)



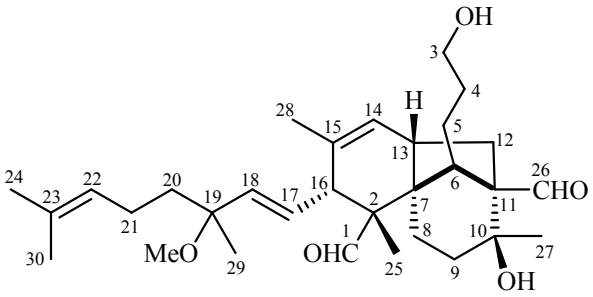
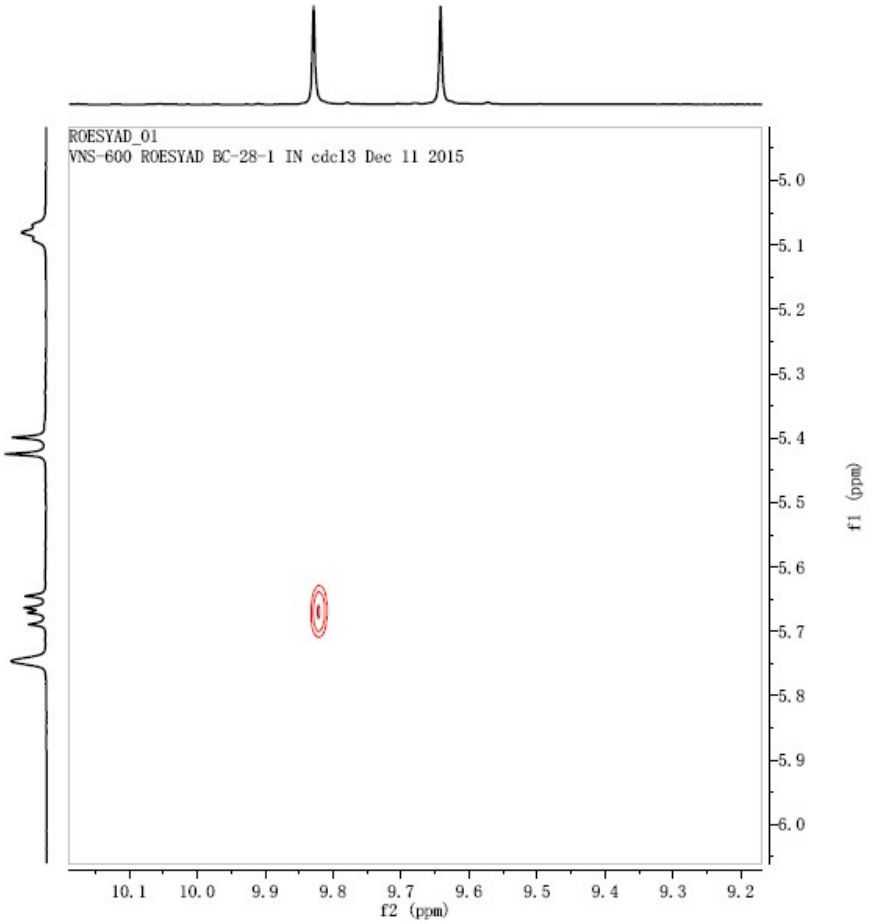


Figure S54. The ROESY spectrum of belamchinenin A (1)



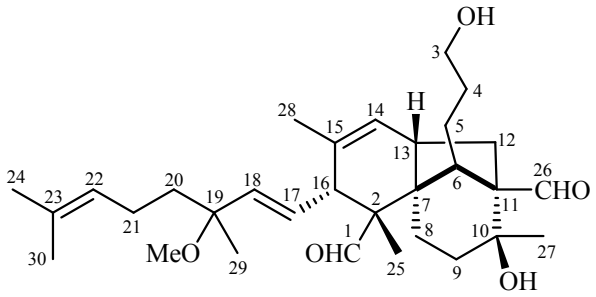


Figure S55. The ROESY spectrum of belamchinenin A (1)

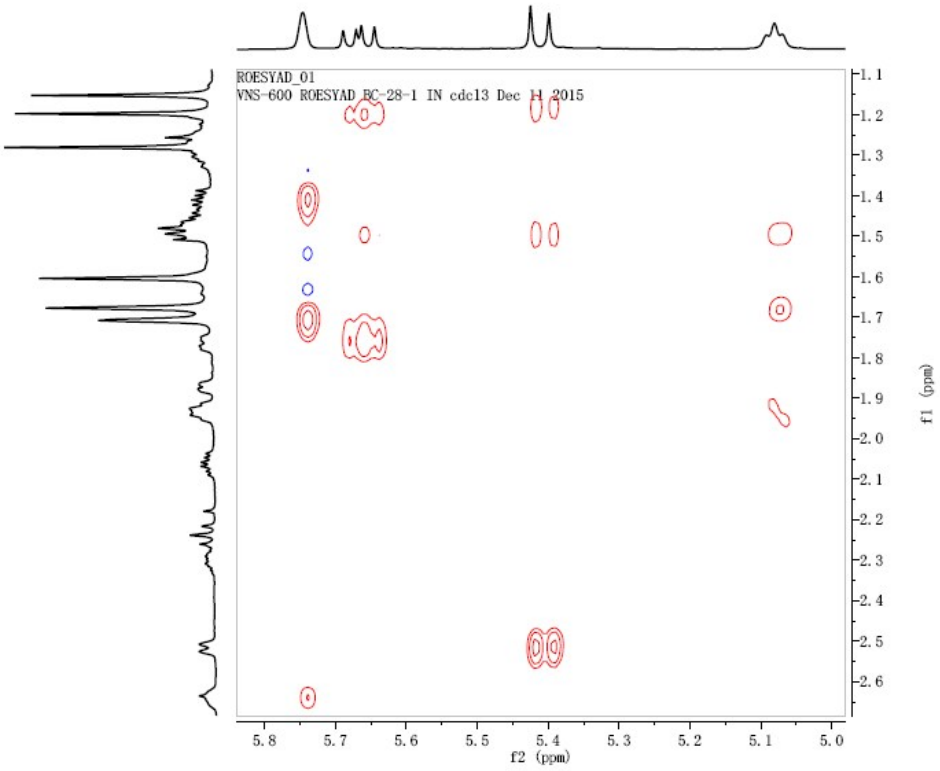
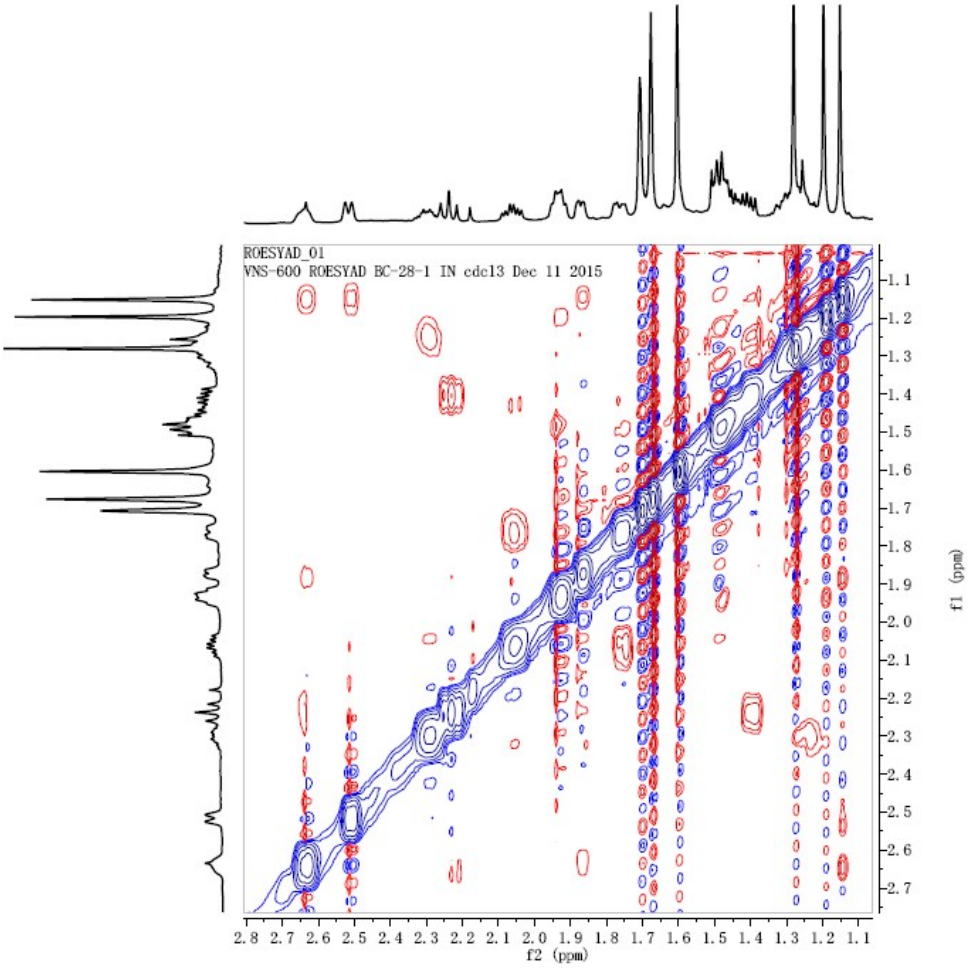


Figure S56. The ROESY spectrum of belamchinenin A (1)



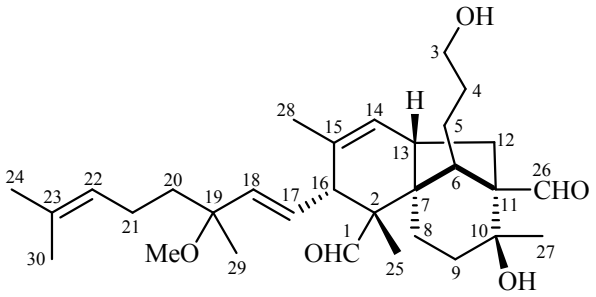
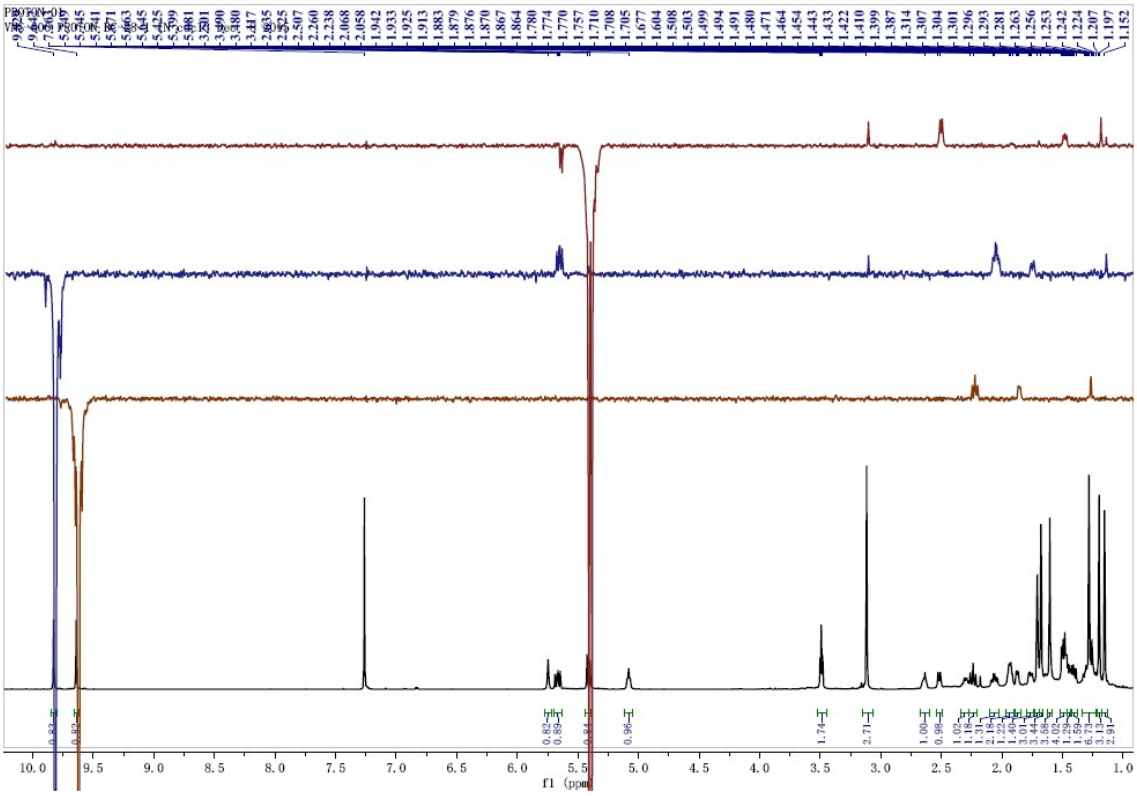


Figure S57. The 1D NOESY spectra of belamchinenin A (1)



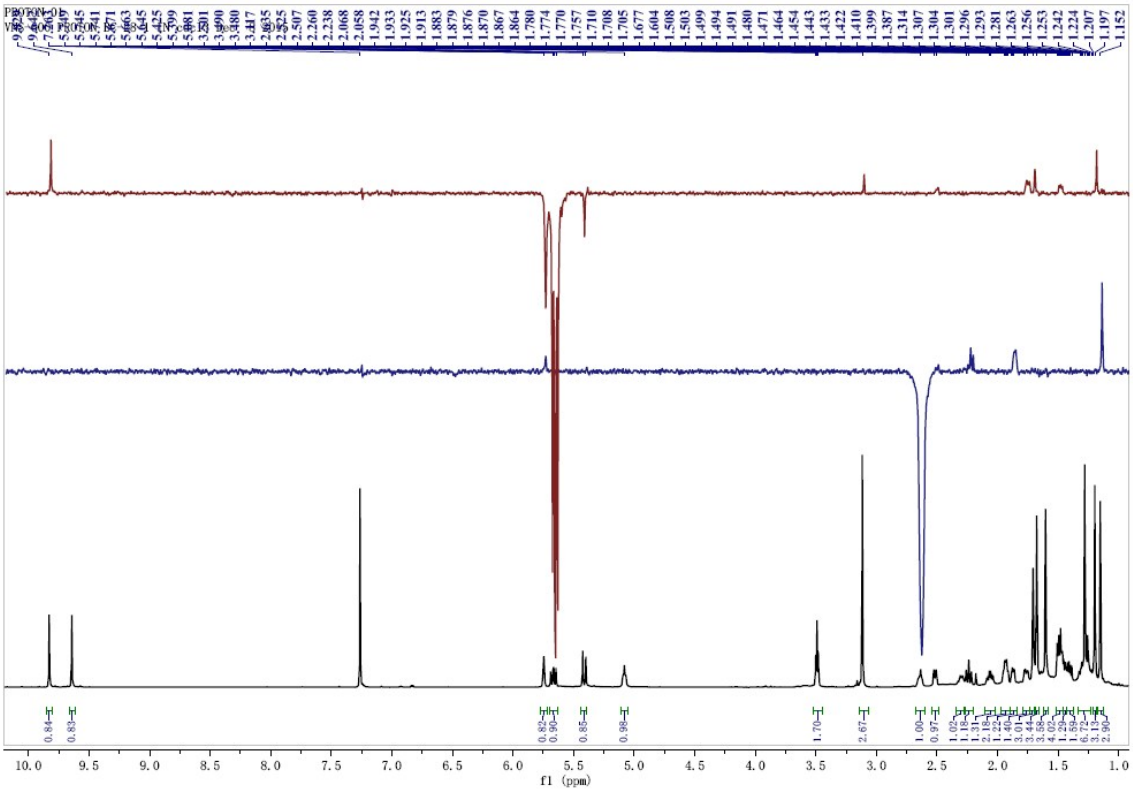


Figure S58. The 1D NOESY spectra of belamchinenin A (1)

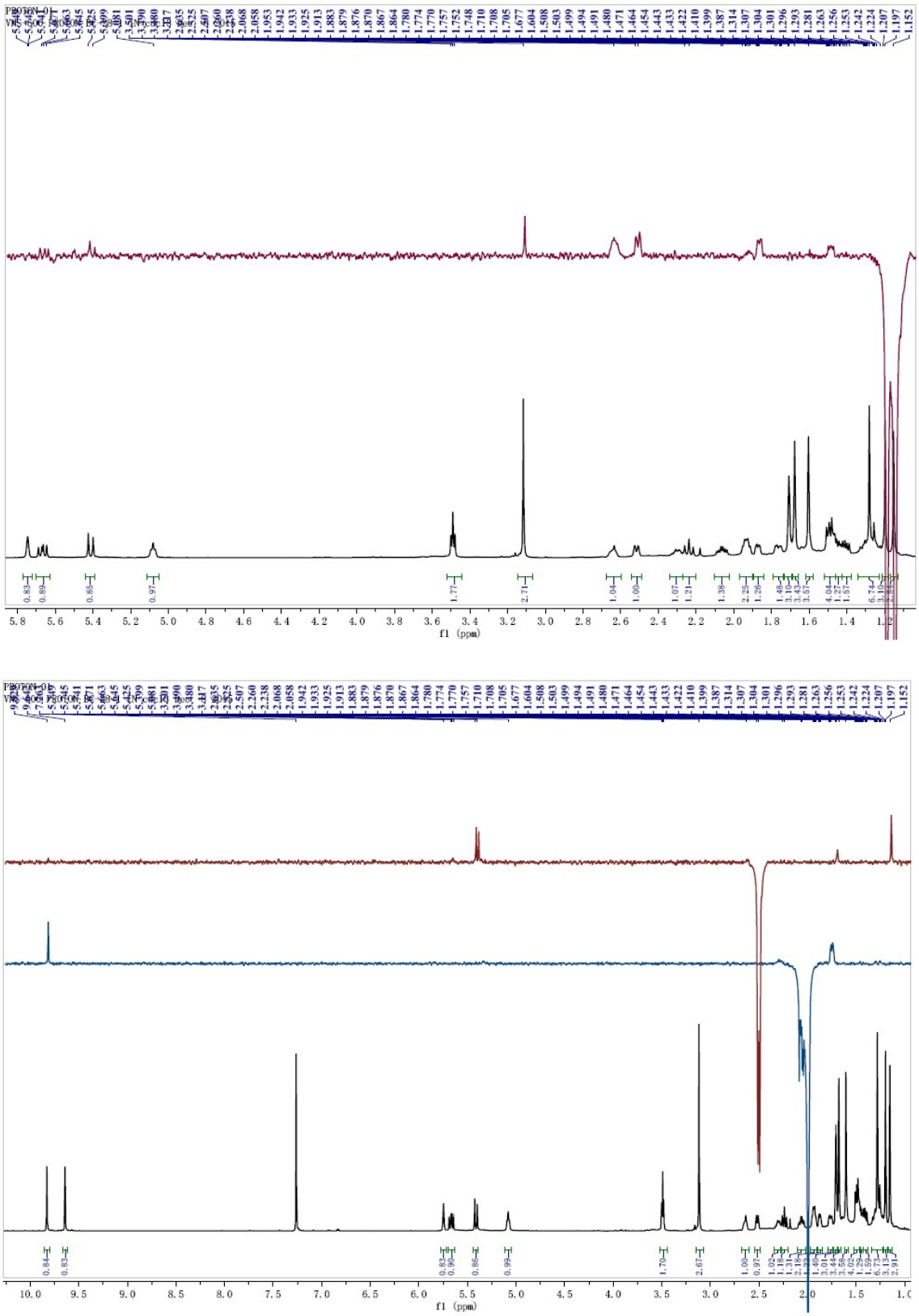
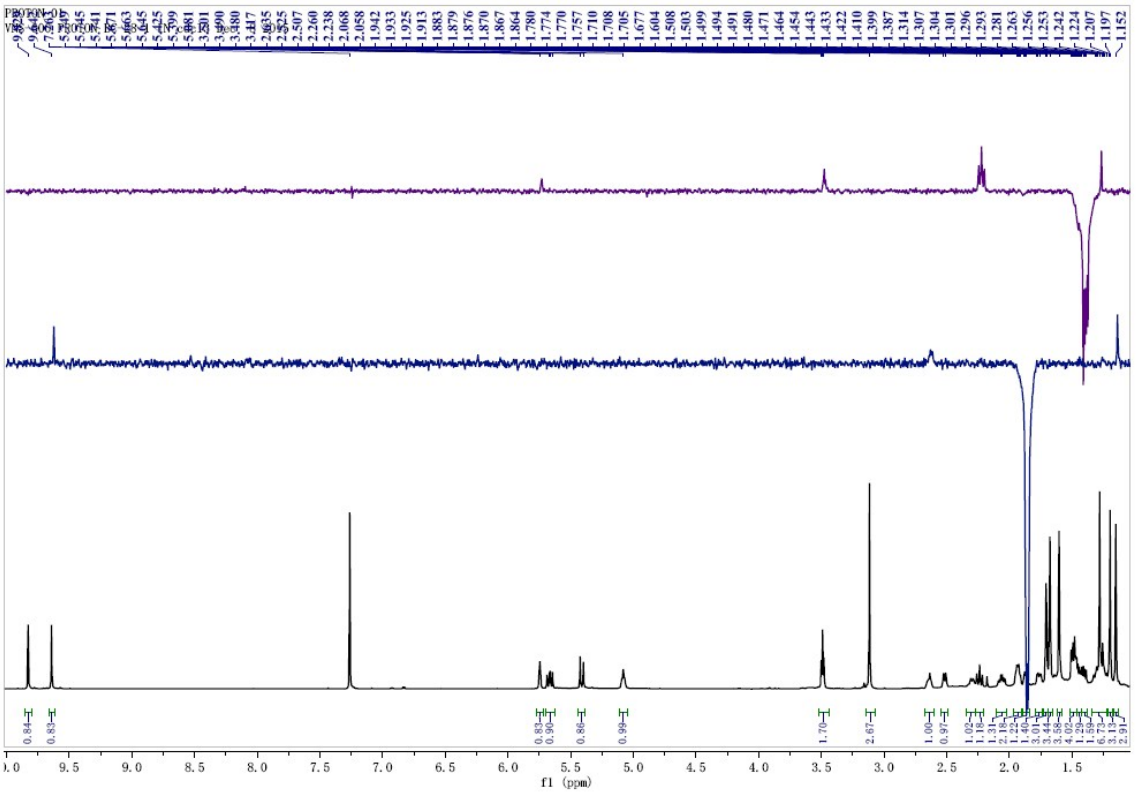


Figure S59. The 1D NOESY spectra of belamchinenin A (1)



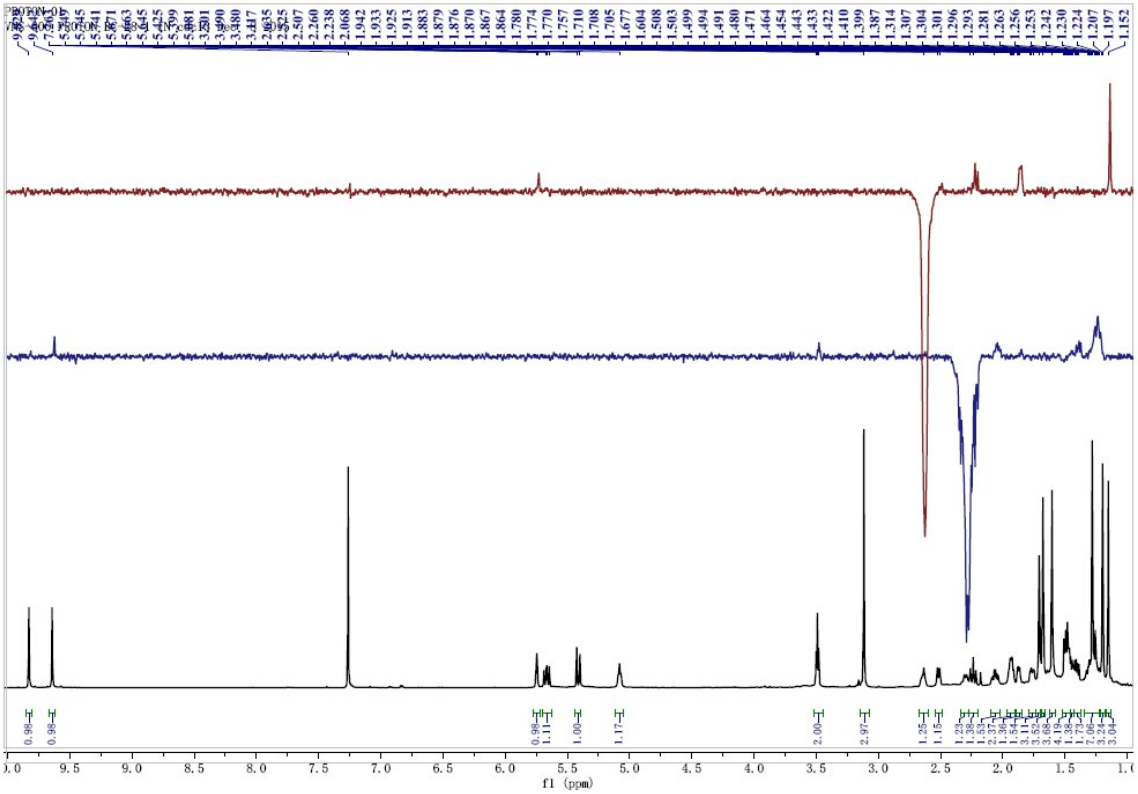


Figure S60. The 1D NOESY spectra of belamchinenin A (1)