Supporting Information

Highly Functionalized Cyclohexanone-Monocyclic Polyprenylated Acylphloroglucinols from *Hypericum perforatum* Induce Leukemia Cell Apoptosis

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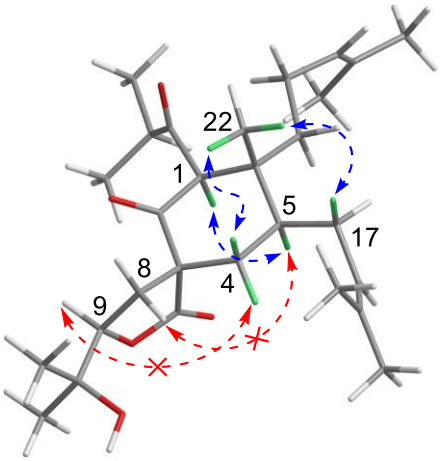


Figure S1. Selected NOESY correlations of **2.** Red arrows indicate selected distances for which no NOESY correlation was observed.

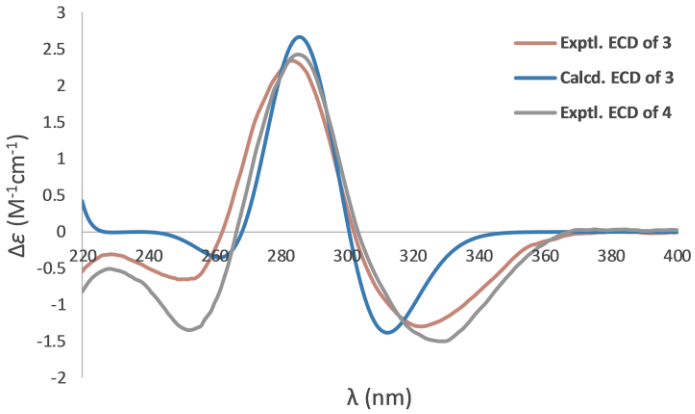


Figure S2. Calculated and experimental ECD spectra of **3** and experimental ECD spectra of **4**.

Table S1. IC_{50} Values (μM) of the isolates on leukemia cell line HL-60 and NB4.

Compound		**1**	**2**	**3**	**4**	**5**	DDP[a]
IC_{50}	HL-60	22.2	31.6	16.2	8.1	33.0	2.8
	NB4	NT[b]	NT	16.8	11.7	NT	0.2

[a]Cisplatin (DDP) was used as positive control. [b]NT for not test.

ECD calculation details of 1, 2, 3, and 5.

The theoretical calculations of compounds **1, 2, 3,** and **5** were performed using Gaussian 09.[1] Conformational analysis was carried out. The optimized conformation geometries and thermodynamic parameters of all conformations were provided. The conformers were optimized at B3LYP/6-31G(d,p) level. The theoretical calculation of ECD was performed using time dependent Density Functional Theory (TDDFT) at B3LYP/6-31G(d,p) level in MeOH with PCM model. The ECD spectra of compounds **1, 2, 3,** and **5** were obtained by weighing the Boltzmann distribution rate of each geometric conformation.

The ECD spectra were simulated by overlapping Gaussian functions for each transition according to:

$$\Delta\varepsilon(E) = \frac{1}{2.297 \times 10^{-39}} \times \frac{1}{\sqrt{2\pi}\sigma} \sum_{i}^{A} \Delta E_i R_i e^{-[(E-E_i)/(2\sigma)]^2}$$

The σ represented the width of the band at 1/e height, and ΔE_i and R_i were the excitation energies and rotational strengths for transition i, respectively. R_{vel} had been used in this work.

References

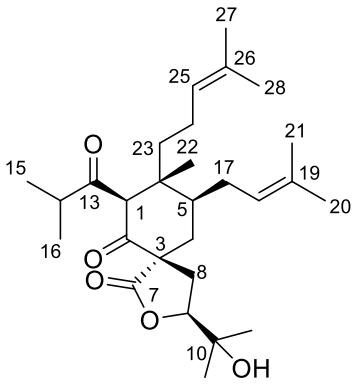
(1) Gaussian 09, Revision C.01,M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J.

Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2010.

(2) (a) Ditchfield, R. *Mol. Phys.* **1974**, *27*, 789.(b) Rohlfing, C. M.; Allen, L. C.; Ditchfield, R. *Chem. Phys.* **1984**, *87*, 9.(c) Wolinski, K.; Hinton, J. F.; Pulay, P. *J. Am. Chem. Soc.* **1990**, *112*, 8251.

(3) (a) Miertus, S.; Scrocc, E.; Tomasi, J. *J. Chem. Phys.* **1981**, *55*, 117. (b) Miertus, S.; Tomasi, J. *J. Chem. Phys.* **1982**, *65*, 239. (c) Cossi, M.; Barone, V.; Cammi, R.; Tomasi, J. *Chem. Phys. Lett.* **1996**, *255*, 327.

(4) Tähtinen, P.; Bagno, A.; Klika, K. D.; Pihlaja, K. *J. Am. Chem. Soc.* **2003**, *125*, 4609−4618.



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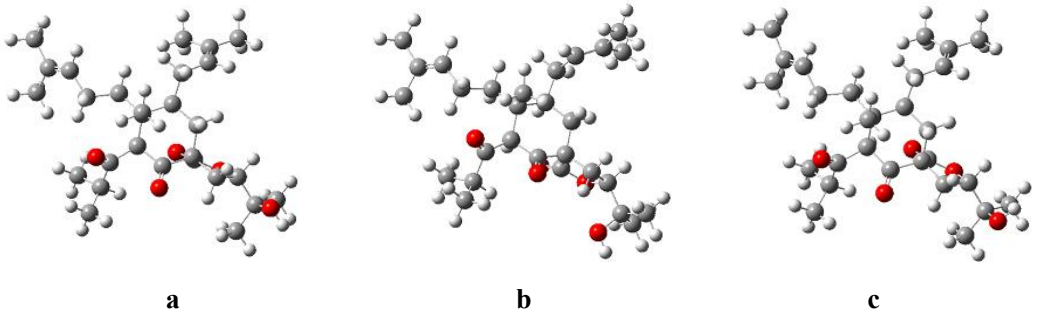
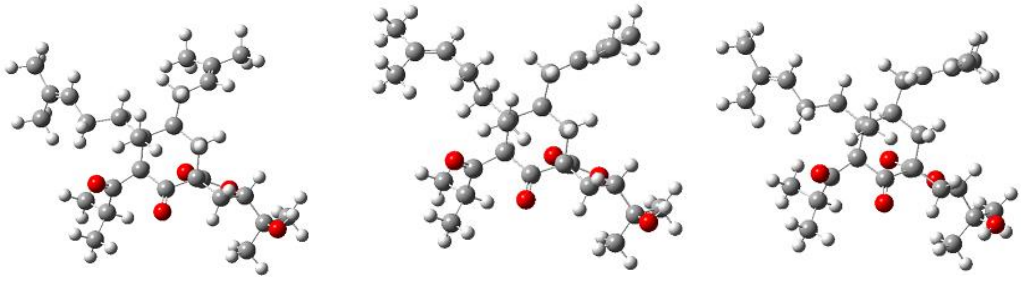
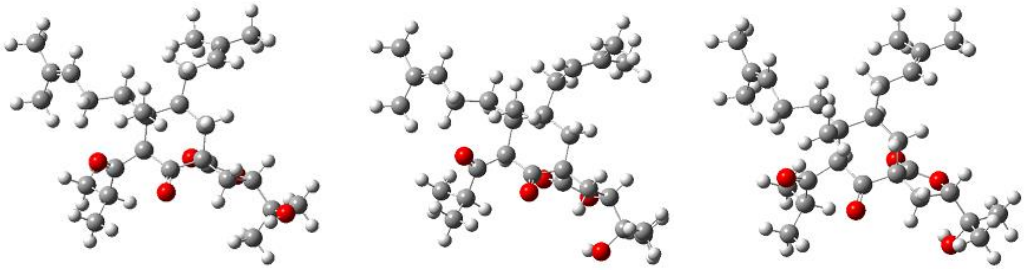


a **b** **c**



d **e** **f**



g **h** **i**

Figure S3. Optimized geometries of predominant conformers for compound **1** at the mPW1PW91/6-31G(d,p) level in the gas phase.

Table S2. Important thermodynamic parameters (a.u.) and Boltzmann distributions of the optimized compound **1** at mPW1PW91/6-31G(d,p) level in the gas phase

Conformations	E+ZPE	G	%
1-a	-1468.976289	-1469.049680	3.6
1-b	-1468.972439	-1469.044660	0
1-c	-1468.972157	-1469.044345	0
1-d	-1468.975648	-1469.048993	1.7
1-e	-1468.978849	-1469.052197	52
1-f	-1468.972723	-1469.044896	0
1-g	-1468.976223	-1469.049560	3.2
1-h	-1468.975963	-1469.047920	0.6
1-i	-1468.979300	-1469.051922	38.9

E+ZPE, G: total energy with zero point energy (ZPE) and Gibbs free energy in the gas phase at mPW1PW91/6-31G(d,p) level., %: Boltzmann distributions, using the relative Gibbs free energies as weighting factors

Table S3. Optimized Z-matrixes of compound **1** in the gas phase (Å) at mPW1PW91/6-31G(d,p) level

1-a				**1-b**			
C	0.807386	-1.37437	0.735556	C	-0.66748	-1.00512	-0.87262
C	1.812846	-0.25365	0.457832	C	-1.71446	-0.21078	-0.08676
C	1.252492	1.052934	1.08335	C	-1.2306	1.265483	-0.03172
C	-0.20834	1.376803	0.72797	C	0.226122	1.455561	0.42122
C	-1.20878	0.202585	1.0796	C	1.268261	0.646765	-0.45291
C	-0.64863	-1.08867	0.362725	C	0.782512	-0.85871	-0.40841
C	-2.59162	0.601381	0.477369	C	2.648634	0.79436	0.255886
C	-1.31242	-0.00604	2.604173	C	1.346907	1.158799	-1.90604
C	-3.81568	-0.33242	0.615284	C	3.908021	0.109224	-0.32169
C	-5.084	0.410119	0.28015	C	5.153886	0.682953	0.303235

C	-5.95826	0.184842	-0.71261	C	6.057778	0.080401	1.090998
C	-7.1821	1.055257	-0.87488	C	7.24927	0.842258	1.621427
C	-5.83859	-0.91616	-1.73739	C	6.00316	-1.36511	1.520245
C	-0.56839	2.752444	1.365262	C	0.478059	2.986829	0.625545
C	0.284619	3.898645	0.869327	C	0.064907	3.915994	-0.48864
C	0.039594	4.69521	-0.18353	C	-0.88003	4.870977	-0.46451
C	0.98965	5.808078	-0.55402	C	-1.12514	5.739092	-1.67644
C	-1.16651	4.574449	-1.08201	C	-1.76407	5.19654	0.714788
C	-1.38114	-2.43517	0.528515	C	1.565559	-1.94396	-1.17401
C	-1.13888	-3.45754	-0.59111	C	1.382051	-3.3751	-0.64892
O	-2.10267	-2.70096	1.469759	O	2.283092	-1.71894	-2.1292
C	-1.03239	-4.87399	-0.01694	C	1.3372	-4.37627	-1.80753
C	-2.2799	-3.34458	-1.62352	C	2.527206	-3.69215	0.335674
O	1.158973	-2.4296	1.232372	O	-0.97995	-1.69577	-1.82559
C	2.012195	-0.05885	-1.06044	C	-1.87216	-0.74776	1.350032
O	3.326818	0.124454	-1.3277	O	-3.17918	-0.7654	1.688749
C	4.127819	0.091463	-0.11667	C	-4.03651	-0.35113	0.593772
C	3.23637	-0.58089	0.933184	C	-3.1333	-0.35996	-0.65003
O	1.177038	-0.0445	-1.93317	O	-1.00742	-1.07999	2.126465
C	5.482524	-0.57619	-0.43089	C	-5.26063	-1.28406	0.533362
C	5.334039	-2.0077	-0.96017	C	-5.9592	-1.34742	1.898897
C	6.269992	0.290095	-1.42386	C	-6.22451	-0.78746	-0.55667
O	6.127121	-0.57256	0.850807	O	-4.74264	-2.57054	0.184634
H	1.360974	0.962743	2.171352	H	-1.37516	1.695273	-1.02857
H	1.889093	1.891026	0.780685	H	-1.8922	1.833033	0.634708
H	-0.25863	1.510696	-0.35999	H	0.308601	1.020699	1.425248
H	-0.61657	-0.8548	-0.71151	H	0.767989	-1.1451	0.65297
H	-2.879	1.54889	0.944612	H	2.870989	1.866603	0.28709
H	-2.45158	0.827181	-0.58872	H	2.539012	0.485808	1.304447
H	-0.33563	-0.21111	3.055239	H	0.356523	1.252221	-2.36348
H	-1.7225	0.884419	3.090508	H	1.824884	2.141957	-1.94201
H	-1.95245	-0.856	2.835515	H	1.925955	0.473198	-2.52303
H	-3.70642	-1.21607	-0.01378	H	3.864823	-0.97099	-0.17975
H	-3.88303	-0.70453	1.643984	H	3.947856	0.265419	-1.40569
H	-5.2996	1.248625	0.945841	H	5.320148	1.738995	0.080217
H	-7.22987	1.839047	-0.11396	H	7.252832	1.882261	1.283676
H	-7.19755	1.536889	-1.86186	H	7.263323	0.840775	2.719701
H	-8.10265	0.460018	-0.80744	H	8.191033	0.377404	1.300145
H	-4.94278	-1.52632	-1.61406	H	5.124784	-1.89397	1.14757
H	-6.70849	-1.58458	-1.69072	H	6.893162	-1.90649	1.173038
H	-5.82513	-0.49853	-2.75279	H	6.003275	-1.44233	2.615512
H	-0.45757	2.682351	2.45415	H	1.537851	3.153147	0.846504
H	-1.61983	2.979655	1.182212	H	-0.05059	3.26025	1.544141

H	1.194707	4.094328	1.436175	H	0.623572	3.812843	-1.41644
H	1.848108	5.856888	0.121548	H	-0.46937	5.473274	-2.5098
H	1.367459	5.680458	-1.577	H	-2.1647	5.655078	-2.02048
H	0.483137	6.782121	-0.53103	H	-0.96329	6.799487	-1.44128
H	-1.85035	3.777722	-0.78447	H	-1.58538	4.562364	1.584767
H	-1.73014	5.51631	-1.10224	H	-1.62091	6.239373	1.026624
H	-0.85658	4.377528	-2.11641	H	-2.82317	5.101413	0.441015
H	-0.20143	-3.19796	-1.09715	H	0.438587	-3.41971	-0.09224
H	-0.8931	-5.60409	-0.82068	H	1.238169	-5.39807	-1.42745
H	-0.18623	-4.94655	0.671268	H	0.489449	-4.16493	-2.4645
H	-1.94071	-5.12953	0.534993	H	2.251726	-4.31061	-2.40276
H	-2.10911	-4.04148	-2.44998	H	2.398783	-4.69678	0.750496
H	-2.35308	-2.338	-2.04946	H	2.556549	-2.98951	1.17554
H	-3.24025	-3.59475	-1.16098	H	3.493817	-3.65741	-0.17756
H	4.333172	1.131653	0.163362	H	-4.38828	0.659774	0.834282
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H	3.371034	-1.66377	0.946799	H	-3.21737	-1.31582	-1.16985
H	6.323762	-2.42695	-1.17365	H	-6.82589	-2.01657	1.84618
H	4.848687	-2.65626	-0.22715	H	-5.27101	-1.72241	2.658139
H	4.755959	-2.02844	-1.88785	H	-6.32206	-0.36198	2.209427
H	7.253047	-0.15315	-1.61996	H	-7.09771	-1.447	-0.60872
H	6.423432	1.292904	-1.01409	H	-5.74247	-0.79181	-1.53774
H	5.742129	0.377801	-2.37732	H	-6.58872	0.223891	-0.34701
H	7.005455	-0.95998	0.738964	H	-5.47603	-3.19912	0.196278
1-c				**1-d**			
C	-0.64726	-1.04794	-0.85008	C	0.806084	-1.3726	0.736096
C	-1.7091	-0.24554	-0.08929	C	1.811435	-0.25224	0.454798
C	-1.23663	1.233174	-0.0258	C	1.251851	1.053514	1.082893
C	0.217039	1.435562	0.430843	C	-0.20939	1.377682	0.729218
C	1.266402	0.636554	-0.44336	C	-1.20978	0.203324	1.080723
C	0.7994	-0.87371	-0.38622	C	-0.65009	-1.08808	0.36355
C	2.648641	0.807182	0.256482	C	-2.59262	0.602693	0.478838
C	1.331843	1.138268	-1.90106	C	-1.31315	-0.0056	2.605285
C	3.916055	0.144267	-0.32973	C	-3.81609	-0.33224	0.613917
C	5.15594	0.742459	0.284089	C	-5.08459	0.40996	0.278659
C	6.080773	0.156735	1.060126	C	-5.95699	0.186189	-0.71608
C	7.262292	0.941584	1.579148	C	-7.18155	1.055631	-0.87812
C	6.061067	-1.29085	1.485389	C	-5.83448	-0.91214	-1.7434
C	0.453258	2.968893	0.637643	C	-0.569	2.752806	1.367771
C	0.047738	3.893905	-0.48273	C	0.284002	3.899671	0.873169
C	-0.90578	4.840597	-0.47286	C	0.041664	4.69387	-0.1821
C	-1.14109	5.705622	-1.68892	C	0.990519	5.808432	-0.55053
C	-1.80894	5.159708	0.693587	C	-1.16053	4.568725	-1.08516

C	1.60002	-1.95715	-1.1373	C	-1.38201	-2.43492	0.531074
C	1.450048	-3.38219	-0.58613	C	-1.1381	-3.45888	-0.58658
O	2.305058	-1.73308	-2.10172	O	-2.10426	-2.6992	1.472151
C	1.422315	-4.40485	-1.72638	C	-1.03189	-4.87448	-0.01022
C	2.605227	-3.6575	0.399369	C	-2.2779	-3.3477	-1.6206
O	-0.95124	-1.78015	-1.77457	O	1.158271	-2.42517	1.237684
C	-1.88357	-0.79478	1.342557	C	2.006592	-0.05514	-1.0636
O	-3.20035	-0.85297	1.652737	O	3.320629	0.128932	-1.33415
C	-4.03268	-0.38502	0.556291	C	4.128526	0.086047	-0.12588
C	-3.11978	-0.40205	-0.6756	C	3.23571	-0.58069	0.926867
O	-1.02858	-1.12348	2.130398	O	1.168772	-0.0391	-1.93361
C	-5.32629	-1.23132	0.487826	C	5.486826	-0.58779	-0.43406
C	-5.05184	-2.71678	0.253153	C	5.336174	-2.0274	-0.92532
C	-6.15225	-1.02769	1.763843	C	6.268258	0.253881	-1.45013
O	-6.05549	-0.77601	-0.66086	O	6.199308	-0.66519	0.808913
H	-1.38213	1.666324	-1.02085	H	1.360958	0.961707	2.170792
H	-1.90422	1.793177	0.640926	H	1.887581	1.892519	0.78039
H	0.302573	1.000793	1.434958	H	-0.26032	1.512345	-0.35857
H	0.784981	-1.15011	0.678012	H	-0.61945	-0.8548	-0.71079
H	2.852658	1.883005	0.285061	H	-2.88082	1.549023	0.948027
H	2.551267	0.498199	1.306162	H	-2.45224	0.830758	-0.58672
H	0.338313	1.221804	-2.35359	H	-0.33645	-0.21166	3.056156
H	1.802729	2.124243	-1.94807	H	-1.72268	0.884882	3.092039
H	1.912078	0.451902	-2.51621	H	-1.95363	-0.85527	2.836372
H	3.894436	-0.93628	-0.18641	H	-3.70541	-1.21456	-0.01676
H	3.944432	0.300005	-1.41422	H	-3.88422	-0.70638	1.641806
H	5.297973	1.802154	0.061705	H	-5.30217	1.246521	0.946149
H	7.240673	1.982311	1.244355	H	-7.23137	1.837556	-0.11541
H	7.288992	0.937466	2.67715	H	-7.19605	1.539547	-1.86398
H	8.209609	0.497043	1.245734	H	-8.10149	0.459172	-0.81347
H	5.189025	-1.8365	1.12217	H	-4.93835	-1.52183	-1.62009
H	6.957415	-1.81276	1.125021	H	-6.70385	-1.58144	-1.69988
H	6.076988	-1.37136	2.580293	H	-5.81967	-0.49194	-2.75771
H	1.508311	3.143936	0.873654	H	-0.45857	2.681747	2.456612
H	-0.09049	3.237726	1.548811	H	-1.62039	2.980239	1.184721
H	0.62086	3.795711	-1.40216	H	1.191177	4.098584	1.443689
H	-0.47133	5.444893	-2.51267	H	1.846037	5.860625	0.128584
H	-2.17485	5.612231	-2.04759	H	1.372753	5.68024	-1.57179
H	-0.9918	6.767511	-1.45237	H	0.481534	6.781229	-0.5311
H	-1.63776	4.527504	1.566548	H	-1.84366	3.770926	-0.7889
H	-1.67805	6.203725	1.006754	H	-1.72624	5.509225	-1.10923
H	-2.86329	5.056662	0.404818	H	-0.84605	4.370712	-2.11796
H	0.509846	-3.43629	-0.02456	H	-0.2001	-3.1999	-1.09193

H	1.347014	-5.42158	-1.32774	H	-0.89116	-5.60553	-0.8128
H	0.568122	-4.22399	-2.3841	H	-0.1866	-4.94596	0.679152
H	2.333034	-4.33022	-2.32631	H	-1.94089	-5.12967	0.540755
H	2.497696	-4.65587	0.834644	H	-2.10583	-4.04584	-2.44571
H	2.625445	-2.93767	1.224867	H	-2.35078	-2.34182	-2.04827
H	3.568614	-3.61512	-0.1192	H	-3.23877	-3.59742	-1.1589
H	-4.32302	0.646013	0.804563	H	4.331407	1.130762	0.150844
H	-3.37602	0.390528	-1.38063	H	3.446272	-0.20977	1.931385
H	-3.18425	-1.35039	-1.21131	H	3.369945	-1.66352	0.942423
H	-5.99838	-3.26324	0.254339	H	6.322609	-2.43336	-1.16353
H	-4.57422	-2.88334	-0.71483	H	4.893416	-2.6639	-0.15586
H	-4.4107	-3.12133	1.039996	H	4.712774	-2.06796	-1.82177
H	-7.09322	-1.58015	1.692564	H	7.251985	-0.18999	-1.62597
H	-6.38735	0.034273	1.912421	H	6.413422	1.277169	-1.08028
H	-5.6058	-1.3717	2.645922	H	5.733973	0.319071	-2.40152
H	-6.44855	0.081282	-0.4459	H	6.522695	0.220555	1.02462
1-e				**1-f**			
C	-0.66021	-1.41429	-0.63082	C	-0.66107	-1.03498	-0.83858
C	-1.70373	-0.34329	-0.2741	C	-1.71415	-0.22112	-0.07772
C	-1.09604	1.065901	-0.53704	C	-1.2297	1.253123	-0.01079
C	0.319531	1.271919	0.025549	C	0.226893	1.441248	0.442
C	1.335328	0.191953	-0.49309	C	1.265779	0.635042	-0.438
C	0.738061	-1.20019	-0.06156	C	0.787225	-0.87194	-0.37879
C	2.707412	0.361971	0.250064	C	2.653008	0.794837	0.254164
C	1.488387	0.243606	-2.02921	C	1.327631	1.13592	-1.89614
C	3.853656	1.077859	-0.49991	C	3.912673	0.124565	-0.34038
C	5.055968	1.276247	0.386924	C	5.159866	0.715585	0.265642
C	6.207929	0.587607	0.382431	C	6.085681	0.124958	1.036758
C	7.315745	0.926377	1.350829	C	7.27476	0.903245	1.548326
C	6.520287	-0.55539	-0.55252	C	6.059853	-1.32211	1.463406
C	0.762459	2.738548	-0.21464	C	0.476187	2.972156	0.651713
C	-0.08633	3.734356	0.533315	C	0.081997	3.902733	-0.46819
C	-0.76602	4.789978	0.057323	C	-0.87165	4.849396	-0.46295
C	-1.5369	5.693838	0.99028	C	-1.09539	5.719771	-1.67736
C	-0.8261	5.197332	-1.39456	C	-1.78642	5.162859	0.695889
C	1.582791	-2.45242	-0.35681	C	1.577782	-1.96258	-1.13035
C	1.222922	-3.71314	0.437248	C	1.424662	-3.38422	-0.57156
O	2.525691	-2.45261	-1.12678	O	2.275782	-1.74579	-2.10144
C	1.243568	-4.94857	-0.47042	C	1.393985	-4.41312	-1.70601
C	2.225799	-3.84348	1.603098	C	2.578789	-3.65766	0.415755
O	-0.94446	-2.36494	-1.33711	O	-0.97531	-1.76979	-1.75834
C	-2.09211	-0.45227	1.216211	C	-1.89527	-0.77462	1.35293
O	-3.43136	-0.30599	1.350563	O	-3.21119	-0.83424	1.657755

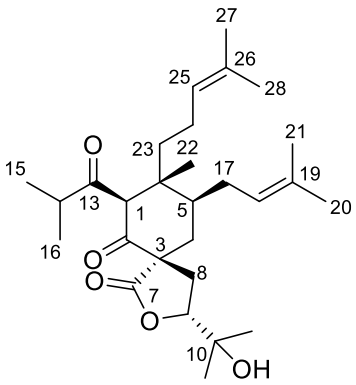
C	-4.07894	-0.09552	0.065652	C	-4.0444	-0.36265	0.562289
C	-3.05267	-0.55325	-0.97748	C	-3.12468	-0.36364	-0.66668
O	-1.36914	-0.62032	2.169326	O	-1.04024	-1.10553	2.14003
C	-5.45876	-0.79564	0.05981	C	-5.32828	-1.22291	0.475048
C	-5.35853	-2.3054	0.27624	C	-5.03361	-2.72027	0.334414
C	-6.37264	-0.15619	1.11231	C	-6.21254	-0.95702	1.694541
O	-6.00504	-0.61773	-1.25495	O	-6.06644	-0.73559	-0.65474
H	-1.09202	1.222474	-1.62239	H	-1.37378	1.691398	-1.00376
H	-1.76236	1.83077	-0.12315	H	-1.89148	1.815474	0.659364
H	0.262452	1.134424	1.113982	H	0.311585	1.003445	1.444816
H	0.593774	-1.15941	1.029086	H	0.772131	-1.14668	0.685883
H	2.523408	0.880018	1.200807	H	2.864138	1.86921	0.282669
H	3.096731	-0.62115	0.523921	H	2.559648	0.485454	1.304075
H	0.541807	0.034799	-2.53774	H	0.332412	1.229198	-2.34306
H	1.830851	1.225416	-2.36586	H	1.8072	2.117463	-1.9459
H	2.203077	-0.5074	-2.3635	H	1.897998	0.444134	-2.51448
H	4.118244	0.499509	-1.38829	H	3.885791	-0.95591	-0.19721
H	3.521644	2.058625	-0.86267	H	3.935132	0.280592	-1.42498
H	4.95118	2.068645	1.130072	H	5.306827	1.774252	0.041665
H	7.048826	1.76325	2.002189	H	7.257372	1.943801	1.212794
H	7.563599	0.0655	1.98596	H	7.307659	0.899867	2.646143
H	8.238351	1.191974	0.81737	H	8.21747	0.452795	1.20988
H	5.679482	-0.83892	-1.18746	H	5.182632	-1.86297	1.105509
H	7.371019	-0.30719	-1.20126	H	6.951157	-1.84955	1.098621
H	6.817779	-1.44429	0.018438	H	6.081319	-1.40172	2.558268
H	0.773601	2.955947	-1.28694	H	1.531921	3.137332	0.89162
H	1.795942	2.850419	0.133449	H	-0.06822	3.243714	1.561637
H	-0.12675	3.563759	1.610869	H	0.664313	3.809112	-1.38235
H	-1.46964	5.361953	2.029775	H	-0.4178	5.462845	-2.49593
H	-1.16302	6.725002	0.938014	H	-2.12577	5.62792	-2.04583
H	-2.59873	5.736734	0.713368	H	-0.94847	6.780527	-1.43449
H	-0.29844	4.51242	-2.0604	H	-1.62071	4.529953	1.569388
H	-1.86786	5.263301	-1.73464	H	-1.66225	6.206846	1.011763
H	-0.39405	6.197087	-1.53297	H	-2.83764	5.055965	0.397665
H	0.219417	-3.58814	0.859411	H	0.484364	-3.43238	-0.00944
H	1.035878	-5.85346	0.109503	H	1.315447	-5.42738	-1.30178
H	0.490678	-4.85978	-1.25798	H	0.540633	-4.23342	-2.36523
H	2.223618	-5.05386	-0.94344	H	2.304915	-4.34477	-2.30633
H	1.986906	-4.72265	2.209519	H	2.467236	-4.65279	0.857359
H	2.205704	-2.96897	2.262665	H	2.601869	-2.93271	1.236612
H	3.243471	-3.95649	1.216872	H	3.542383	-3.62255	-0.10294
H	-4.25454	0.986574	-0.02103	H	-4.35087	0.660151	0.810434
H	-3.13953	0.012459	-1.90666	H	-3.37431	0.444593	-1.35704

H	-3.17092	-1.61003	-1.223	H	-3.17739	-1.30612	-1.21814
H	-6.36336	-2.73463	0.30427	H	-5.97696	-3.26766	0.257818
H	-4.81537	-2.78717	-0.53977	H	-4.44327	-2.94081	-0.56202
H	-4.85401	-2.52868	1.219344	H	-4.48085	-3.09519	1.199378
H	-7.36661	-0.60992	1.069644	H	-7.12797	-1.55103	1.63066
H	-6.47849	0.921944	0.935114	H	-6.49462	0.099452	1.731933
H	-5.96655	-0.28724	2.118703	H	-5.68515	-1.21292	2.617048
H	-6.30598	0.298269	-1.33243	H	-5.66456	-1.10125	-1.45451
1-g				**1-h**			
C	0.815311	-1.35917	0.732771	C	-0.65054	-1.03387	-0.86285
C	1.813369	-0.23123	0.456608	C	-1.71102	-0.24152	-0.09037
C	1.246723	1.070899	1.085294	C	-1.24179	1.238728	-0.0299
C	-0.216	1.385432	0.729419	C	0.212341	1.442	0.426144
C	-1.20886	0.204939	1.081264	C	1.263609	0.644927	-0.44785
C	-0.64196	-1.08276	0.362114	C	0.796636	-0.86591	-0.39851
C	-2.59492	0.595789	0.481468	C	2.6437	0.811902	0.257119
C	-1.30956	-0.00589	2.605745	C	1.333301	1.153097	-1.90299
C	-3.81201	-0.34738	0.617156	C	3.910201	0.141679	-0.32247
C	-5.0861	0.387349	0.286531	C	5.150638	0.733434	0.296404
C	-5.9594	0.160267	-0.70667	C	6.068354	0.143086	1.077389
C	-7.18997	1.022088	-0.86367	C	7.252209	0.921429	1.60084
C	-5.83224	-0.93469	-1.73697	C	6.038035	-1.30381	1.504427
C	-0.58465	2.759573	1.364832	C	0.447994	2.975457	0.633264
C	0.26511	3.9094	0.871125	C	0.034988	3.900885	-0.48409
C	0.026256	4.695379	-0.19108	C	-0.9182	4.847831	-0.46698
C	0.971034	5.813477	-0.55906	C	-1.16156	5.713631	-1.68089
C	-1.1677	4.556565	-1.10306	C	-1.81319	5.166599	0.705836
C	-1.36626	-2.43424	0.527476	C	1.594502	-1.9452	-1.15879
C	-1.122	-3.4526	-0.59516	C	1.435748	-3.37521	-0.62295
O	-2.08174	-2.70586	1.471532	O	2.303999	-1.71493	-2.11837
C	-1.0135	-4.87078	-0.02571	C	1.400865	-4.38522	-1.77428
C	-2.26219	-3.33846	-1.62847	C	2.589866	-3.66818	0.35868
O	1.17626	-2.41266	1.227562	O	-0.95606	-1.74577	-1.80206
C	2.012076	-0.03057	-1.06186	C	-1.87972	-0.78907	1.339629
O	3.32446	0.155663	-1.32922	O	-3.19672	-0.82617	1.660874
C	4.135695	0.106311	-0.12237	C	-4.03753	-0.3552	0.564447
C	3.237263	-0.55409	0.931939	C	-3.12459	-0.40548	-0.66534
O	1.17304	-0.01482	-1.93091	O	-1.02694	-1.13574	2.12172
C	5.484381	-0.58749	-0.43105	C	-5.2882	-1.26151	0.517475
C	5.309508	-1.9845	-1.03626	C	-6.07804	-1.15095	1.83102
C	6.323118	0.301288	-1.35102	C	-6.16363	-0.88617	-0.67981
O	6.202515	-0.65045	0.809538	O	-4.88029	-2.61251	0.300406
H	1.355	0.979732	2.173306	H	-1.38818	1.669519	-1.02591

H	1.878301	1.913036	0.783388	H	-1.90942	1.79929	0.636195
H	-0.26629	1.51822	-0.35856	H	0.298446	1.006936	1.43019
H	-0.61217	-0.84691	-0.71176	H	0.785031	-1.14906	0.663864
H	-2.88845	1.539536	0.952403	H	2.852039	1.886967	0.284595
H	-2.45757	0.826315	-0.58394	H	2.540924	0.505036	1.306923
H	-0.33121	-0.20578	3.055892	H	0.341187	1.235881	-2.35876
H	-1.72411	0.881793	3.093261	H	1.801817	2.140462	-1.9436
H	-1.94451	-0.85962	2.83704	H	1.917479	0.471024	-2.51908
H	-3.69705	-1.22747	-0.01592	H	3.881878	-0.93856	-0.17734
H	-3.87549	-0.72429	1.644345	H	3.944322	0.29535	-1.40705
H	-5.30745	1.220897	0.956511	H	5.300013	1.791954	0.073331
H	-7.24297	1.802036	-0.09917	H	7.238405	1.961848	1.264704
H	-7.21009	1.507989	-1.84844	H	7.27391	0.918455	2.698952
H	-8.10582	0.419481	-0.798	H	8.198278	0.47072	1.272237
H	-4.93162	-1.53854	-1.61767	H	5.164794	-1.845	1.137419
H	-6.69689	-1.61002	-1.69269	H	6.933193	-1.83137	1.149405
H	-5.82312	-0.51195	-2.75027	H	6.047819	-1.38291	2.599502
H	-0.47836	2.690887	2.454219	H	1.504261	3.151192	0.863259
H	-1.63639	2.981513	1.176899	H	-0.09081	3.243197	1.547639
H	1.166247	4.117276	1.447834	H	0.601652	3.802916	-1.40752
H	1.821016	5.875121	0.126076	H	-0.49788	5.452891	-2.50956
H	1.361925	5.681083	-1.57646	H	-2.19796	5.6213	-2.03206
H	0.455762	6.783104	-0.54974	H	-1.00972	6.77524	-1.44478
H	-1.84941	3.757742	-0.80611	H	-1.63597	4.534206	1.577451
H	-1.73791	5.493916	-1.13958	H	-1.68002	6.21051	1.018333
H	-0.84345	4.351835	-2.13151	H	-2.8695	5.063622	0.424433
H	-0.18465	-3.18966	-1.0998	H	0.495468	-3.42989	-0.06153
H	-0.87192	-5.59774	-0.83183	H	1.319613	-5.40567	-1.38653
H	-0.16805	-4.94461	0.663303	H	0.547135	-4.19205	-2.42904
H	-1.92187	-5.1301	0.52432	H	2.311639	-4.30964	-2.37398
H	-2.08886	-4.0323	-2.45691	H	2.477928	-4.67144	0.781459
H	-2.337	-2.33073	-2.0513	H	2.613612	-2.95882	1.193125
H	-3.22253	-3.59228	-1.16796	H	3.553263	-3.6236	-0.15965
H	4.356283	1.142443	0.159546	H	-4.3377	0.670406	0.81202
H	3.442185	-0.17146	1.933885	H	-3.37144	0.366253	-1.39768
H	3.359291	-1.64038	0.95473	H	-3.20779	-1.38227	-1.14763
H	6.293584	-2.4311	-1.20234	H	-6.9316	-1.83329	1.801615
H	4.744869	-2.65139	-0.37501	H	-5.45023	-1.4136	2.687521
H	4.781668	-1.93649	-1.99195	H	-6.45257	-0.13384	1.988112
H	7.281924	-0.17844	-1.56426	H	-7.05071	-1.52463	-0.69506
H	6.523436	1.261277	-0.86589	H	-5.6267	-1.03446	-1.6199
H	5.799288	0.485739	-2.29237	H	-6.48981	0.156814	-0.61839
H	5.843042	-1.3842	1.326467	H	-4.32792	-2.86525	1.0546

1-i							
C	0.804387	-1.3769	0.745106				
C	1.811517	-0.25985	0.461152				
C	1.25852	1.039716	1.108947				
C	-0.20053	1.372842	0.753691				
C	-1.20786	0.200967	1.094022				
C	-0.6516	-1.09045	0.372961				
C	-2.58555	0.609989	0.486878				
C	-1.31964	-0.01416	2.617084				
C	-3.81142	-0.32426	0.602237				
C	-5.07507	0.42166	0.257077				
C	-5.93695	0.20391	-0.74814				
C	-7.15791	1.076524	-0.91999				
C	-5.80555	-0.89026	-1.77881				
C	-0.55576	2.746202	1.398177				
C	0.300746	3.89205	0.906818				
C	0.064082	4.684984	-0.15072				
C	1.015792	5.797896	-0.51667				
C	-1.13434	4.559678	-1.05881				
C	-1.38527	-2.4366	0.539814				
C	-1.13296	-3.46503	-0.57193				
O	-2.11583	-2.69734	1.475374				
C	-1.0209	-4.87691	0.012702				
C	-2.27113	-3.36531	-1.60886				
O	1.154663	-2.42398	1.258598				
C	2.000624	-0.03922	-1.05141				
O	3.311792	0.183975	-1.31611				
C	4.128923	0.117479	-0.108				
C	3.239004	-0.59783	0.913822				
O	1.167733	-0.03421	-1.92588				
C	5.447349	-0.59561	-0.48317				
C	6.207456	0.213675	-1.54552				
C	6.307621	-0.80279	0.764825				
O	5.14876	-1.90103	-0.97869				
H	1.364312	0.931061	2.195657				
H	1.898281	1.880336	0.819945				
H	-0.24744	1.514569	-0.33342				
H	-0.6232	-0.85586	-0.7011				
H	-2.87522	1.552011	0.963905				
H	-2.43689	0.84855	-0.57525				
H	-0.34688	-0.23171	3.071052				
H	-1.72276	0.878008	3.106026				
H	-1.96903	-0.85872	2.841623				

H	-3.6945	-1.20223	-0.03347				
H	-3.89135	-0.70552	1.62666				
H	-5.29846	1.255519	0.925997				
H	-7.21462	1.855497	-0.15476				
H	-7.16052	1.564454	-1.90398				
H	-8.07969	0.481683	-0.86799				
H	-4.91334	-1.50393	-1.64713				
H	-6.67781	-1.5565	-1.74898				
H	-5.77669	-0.46568	-2.791				
H	-0.44493	2.670758	2.486613				
H	-1.60665	2.977286	1.216555				
H	1.205395	4.09074	1.481372				
H	1.868391	5.850241	0.166045				
H	1.40237	5.667592	-1.53603				
H	0.507751	6.771243	-0.50112				
H	-1.81982	3.763319	-0.7641				
H	-1.69869	5.500853	-1.08699				
H	-0.81564	4.359545	-2.08991				
H	-0.19496	-3.20444	-1.0764				
H	-0.87404	-5.61162	-0.78539				
H	-0.17702	-4.94	0.704565				
H	-1.93023	-5.13366	0.562397				
H	-2.09514	-4.06869	-2.42869				
H	-2.34677	-2.36268	-2.04376				
H	-3.23187	-3.61503	-1.14699				
H	4.343728	1.151444	0.188747				
H	3.441209	-0.27756	1.938303				
H	3.394429	-1.67748	0.850414				
H	7.109385	-0.32941	-1.83984				
H	5.588807	0.371029	-2.4339				
H	6.50356	1.196446	-1.16349				
H	7.246214	-1.28658	0.482499				
H	5.801111	-1.44753	1.487124				
H	6.542647	0.152045	1.245517				
H	4.608002	-1.78316	-1.77334				



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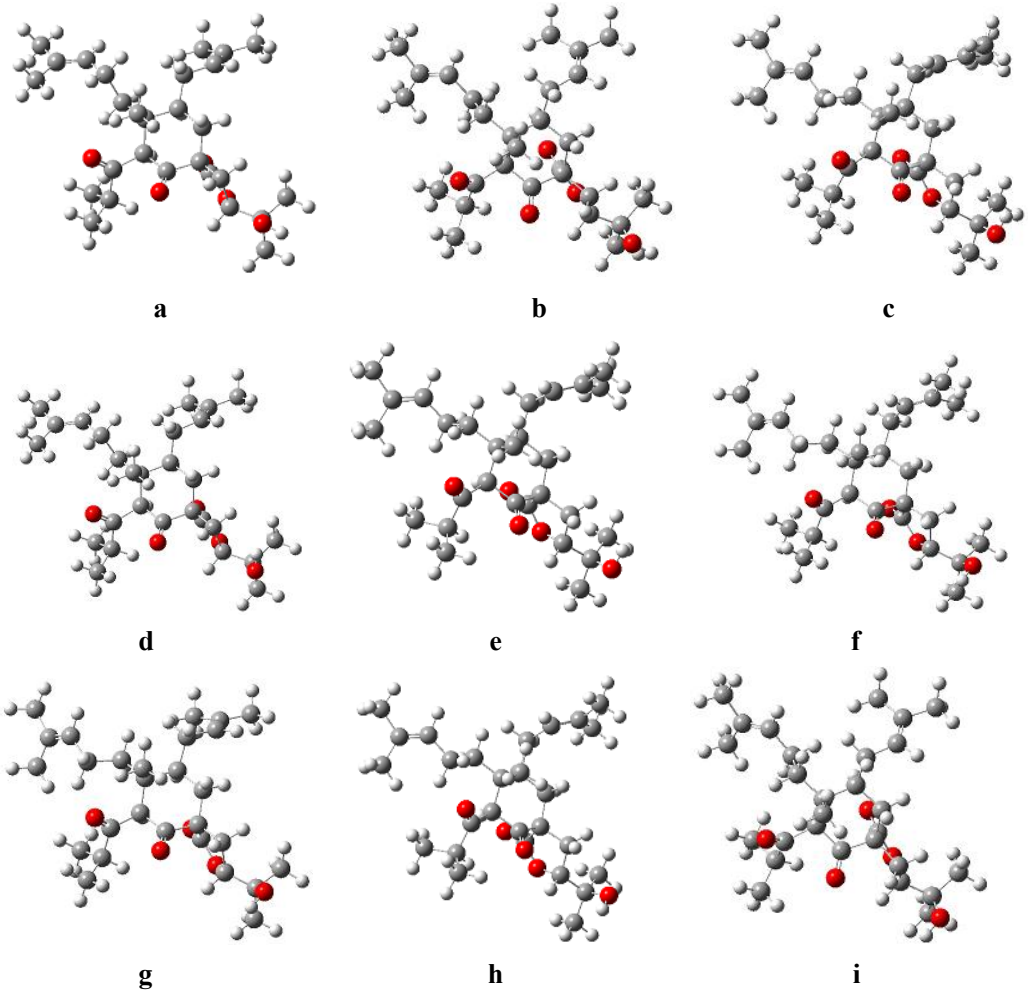


Figure S4. Optimized geometries of predominant conformers for compound **2** at the mPW1PW91/6-31G(d,p) level in the gas phase.

Table S4. Important thermodynamic parameters (a.u.) and Boltzmann distributions of the optimized compound **2** at mPW1PW91/6-31G(d,p) level in the gas phase

Conformations	E+ZPE	G	%
2-a	-1468.977978	-1469.050829	2.7
2-b	-1468.981122	-1469.053382	40.7

2-c	-1468.972796	-1469.045745	0
2-d	-1468.977359	-1469.049858	1
2-e	-1468.977457	-1469.049469	0.6
2-f	-1468.973568	-1469.046564	0
2-g	-1468.976692	-1469.049767	0.9
2-h	-1468.978285	-1469.050120	1.3
2-i	-1468.981384	-1469.053628	52.8

E+ZPE, G: total energy with zero point energy (ZPE) and Gibbs free energy in the gas phase at mPW1PW91/6-31G(d,p) level., %: Boltzmann distributions, using the relative Gibbs free energies as weighting factors

Table S5. Optimized Z-matrixes of compound **2** in the gas phase (Å) at mPW1PW91/6-31G(d,p) level.

2-a				**2-b**			
C	0.970306	-1.2562	0.549229	C	1.021412	-1.18797	0.808719
C	1.834885	0.015365	0.431139	C	1.787765	0.100044	0.445346
C	1.03136	1.248347	0.912406	C	1.035281	1.333829	1.002643
C	-0.42589	1.330028	0.425305	C	-0.49238	1.334846	0.81026
C	-1.24167	0.019534	0.717919	C	-1.16193	0.009379	1.324391
C	-0.45065	-1.14308	0.008558	C	-0.47732	-1.16485	0.526116
C	-2.64906	0.111897	0.030323	C	-2.69736	0.011784	1.072213
C	-1.34392	-0.27079	2.231504	C	-0.94791	-0.19312	2.842382
C	-3.86252	0.486854	0.910812	C	-3.19295	0.19423	-0.37809
C	-5.11422	0.64793	0.08649	C	-4.68671	0.387386	-0.4245
C	-6.13312	-0.21578	-0.04405	C	-5.61996	-0.35561	-1.03837
C	-7.31798	0.11223	-0.9206	C	-7.08072	0.019343	-0.95373
C	-6.21266	-1.55735	0.643095	C	-5.34374	-1.59482	-1.85292
C	-1.09459	2.622593	0.9704	C	-1.09995	2.626124	1.429432
C	-0.35822	3.895879	0.625231	C	-0.47729	3.908597	0.930173
C	-0.57429	4.706975	-0.42268	C	-0.92077	4.713407	-0.04884
C	0.254584	5.952641	-0.62332	C	-0.16676	5.968405	-0.41765
C	-1.6248	4.476168	-1.48051	C	-2.16754	4.470764	-0.86246
C	-1.08469	-2.54666	0.023392	C	-1.02362	-2.59194	0.713762
C	-0.55932	-3.53767	-1.0216	C	-0.58538	-3.63165	-0.32744
O	-1.98843	-2.85931	0.775893	O	-1.79133	-2.90027	1.605719
C	-0.3726	-4.92789	-0.40289	C	-0.19446	-4.94475	0.362773
C	-1.5569	-3.56345	-2.19891	C	-1.739	-3.83997	-1.32969
O	1.409621	-2.27974	1.042914	O	1.589343	-2.1497	1.29471
C	2.242216	0.127877	-1.05448	C	1.897248	0.131415	-1.09432
O	3.519506	-0.28809	-1.21505	O	3.137604	-0.25128	-1.47622
C	4.105023	-0.72307	0.044539	C	3.96729	-0.59499	-0.33023
C	3.191172	-0.14934	1.133517	C	3.259655	0.027414	0.878622

O	1.565725	0.501827	-1.98215	O	1.040128	0.42569	-1.89249
C	5.588233	-0.29994	0.069577	C	5.414346	-0.14482	-0.61623
C	6.372083	-1.09908	-0.98073	C	6.001625	-0.98688	-1.75733
C	5.78156	1.206981	-0.14417	C	5.52179	1.351281	-0.93857
O	5.99758	-0.67847	1.391033	O	6.081442	-0.44381	0.617734
H	1.059053	1.246681	2.009463	H	1.277515	1.404928	2.070515
H	1.565312	2.148573	0.592795	H	1.454875	2.227945	0.531666
H	-0.3885	1.433628	-0.66568	H	-0.66646	1.38953	-0.2694
H	-0.34155	-0.84966	-1.047	H	-0.56994	-0.92517	-0.54358
H	-2.57764	0.821671	-0.8047	H	-3.10645	-0.92193	1.464733
H	-2.89599	-0.85011	-0.4242	H	-3.1325	0.805636	1.691009
H	-0.35658	-0.40327	2.685774	H	0.110358	-0.21465	3.121597
H	-1.83975	0.544049	2.764424	H	-1.42306	0.610491	3.412601
H	-1.90422	-1.18923	2.404141	H	-1.39032	-1.13929	3.156358
H	-3.99956	-0.27919	1.677783	H	-2.71679	1.075162	-0.83012
H	-3.67418	1.425188	1.446655	H	-2.88988	-0.65874	-0.99286
H	-5.17219	1.577347	-0.48272	H	-5.03801	1.25743	0.13385
H	-7.22054	1.095475	-1.38918	H	-7.23734	0.923842	-0.35972
H	-7.44075	-0.63437	-1.71656	H	-7.50368	0.190665	-1.95269
H	-8.25148	0.102605	-0.34199	H	-7.67035	-0.79009	-0.50304
H	-5.3096	-1.81382	1.199191	H	-4.28797	-1.86761	-1.88345
H	-7.0634	-1.59062	1.336864	H	-5.89963	-2.45164	-1.45061
H	-6.38468	-2.35306	-0.09303	H	-5.68644	-1.46215	-2.88761
H	-1.17541	2.556105	2.062767	H	-0.98339	2.590791	2.520174
H	-2.11717	2.673599	0.589873	H	-2.17551	2.637059	1.238275
H	0.438012	4.180984	1.312871	H	0.441657	4.209427	1.433465
H	1.002265	6.078621	0.164587	H	0.728273	6.102174	0.19606
H	0.777553	5.927612	-1.58845	H	0.141766	5.948135	-1.4712
H	-0.37885	6.84955	-0.63781	H	-0.79866	6.858371	-0.29724
H	-2.23514	3.590352	-1.29624	H	-2.7188	3.580474	-0.55518
H	-2.296	5.341528	-1.55611	H	-2.84775	5.32986	-0.7955
H	-1.15738	4.358523	-2.46658	H	-1.91705	4.356777	-1.92508
H	0.405001	-3.17543	-1.39643	H	0.279551	-3.24052	-0.87521
H	-0.04613	-5.64497	-1.16284	H	0.077402	-5.70068	-0.3809
H	0.377703	-4.89748	0.391535	H	0.657242	-4.79018	1.030002
H	-1.31369	-5.27934	0.028404	H	-1.03126	-5.32293	0.956071
H	-1.20072	-4.24211	-2.98005	H	-1.45862	-4.5897	-2.07602
H	-1.68594	-2.57384	-2.65096	H	-1.98878	-2.91759	-1.86518
H	-2.53643	-3.9129	-1.85852	H	-2.63623	-4.1894	-0.80992
H	4.058885	-1.81664	0.060406	H	3.960078	-1.68618	-0.24182
H	3.549459	0.825749	1.473529	H	3.634524	1.03464	1.07854
H	3.135511	-0.81842	1.991631	H	3.399266	-0.58116	1.771463
H	7.433934	-0.82805	-0.95468	H	7.041734	-0.69876	-1.94957

H	6.287047	-2.17127	-0.78104	H	5.983252	-2.04819	-1.49256
H	5.997578	-0.89931	-1.98843	H	5.436052	-0.84639	-2.68251
H	6.849646	1.449989	-0.11417	H	6.568554	1.613029	-1.12942
H	5.288988	1.788653	0.639292	H	5.174469	1.965393	-0.10385
H	5.392603	1.522051	-1.11578	H	4.943961	1.607639	-1.83032
H	6.946817	-0.51128	1.463083	H	7.02273	-0.26287	0.493701
2-c				**2-d**			
C	-0.75653	-0.92111	-0.76008	C	0.973875	-1.24258	0.557682
C	-1.74776	-0.02799	0.006925	C	1.8336	0.031432	0.428779
C	-1.16224	1.396523	0.114369	C	1.026166	1.259294	0.917311
C	0.31831	1.481538	0.521137	C	-0.43212	1.33519	0.431436
C	1.275871	0.617272	-0.39363	C	-1.2427	0.020736	0.720933
C	0.703937	-0.85536	-0.30944	C	-0.44511	-1.13894	0.012716
C	2.694582	0.695767	0.246102	C	-2.64836	0.107482	0.028763
C	1.31278	1.102987	-1.85764	C	-1.34817	-0.2706	2.234021
C	3.894839	-0.03316	-0.39981	C	-3.86704	0.472651	0.906102
C	5.192866	0.482179	0.167306	C	-5.1169	0.627507	0.077765
C	6.126847	-0.17482	0.871967	C	-6.12948	-0.24277	-0.05821
C	7.372392	0.533278	1.350315	C	-7.31348	0.079318	-0.93807
C	6.057833	-1.6338	1.250401	C	-6.2024	-1.5864	0.625626
C	0.67403	2.988849	0.743674	C	-1.10571	2.623765	0.97993
C	0.374326	3.956653	-0.37376	C	-0.37703	3.901213	0.633335
C	-0.53166	4.948923	-0.39226	C	-0.59689	4.708324	-0.4169
C	-0.65593	5.853055	-1.5962	C	0.2238	5.959017	-0.6195
C	-1.48264	5.283919	0.730848	C	-1.64436	4.467758	-1.4755
C	1.410002	-2.00379	-1.0603	C	-1.07213	-2.54605	0.028805
C	1.185098	-3.40571	-0.47797	C	-0.53336	-3.5385	-1.00768
O	2.093188	-1.84081	-2.05176	O	-1.98028	-2.85948	0.775471
C	1.079539	-4.44807	-1.59522	C	-0.34544	-4.92562	-0.38227
C	2.334966	-3.72886	0.49933	C	-1.52076	-3.57349	-2.19344
O	-1.12952	-1.64388	-1.66697	O	1.414145	-2.25636	1.070214
C	-1.97316	-0.68161	1.388653	C	2.233259	0.15009	-1.05936
O	-3.15532	-1.33588	1.401054	O	3.51013	-0.25918	-1.22732
C	-3.83629	-1.24621	0.113652	C	4.103926	-0.70708	0.027251
C	-3.15248	-0.08013	-0.6126	C	3.194847	-0.13154	1.12169
O	-1.2368	-0.65827	2.345703	O	1.548434	0.526935	-1.97972
C	-5.36194	-1.14523	0.347778	C	5.597782	-0.3071	0.056994
C	-5.88094	-2.46305	0.926133	C	6.365619	-1.11111	-0.994
C	-5.75081	0.032095	1.249213	C	5.817691	1.196658	-0.14496
O	-5.97159	-1.02442	-0.94477	O	6.116024	-0.73492	1.324188
H	-1.31276	1.890803	-0.85165	H	1.054472	1.253204	2.014484
H	-1.76138	1.962747	0.837135	H	1.554811	2.163551	0.599927
H	0.394073	1.028729	1.516416	H	-0.39498	1.441544	-0.65913

H	0.6908	-1.1161	0.759012	H	-0.33702	-0.84565	-1.04284
H	2.962876	1.757251	0.271678	H	-2.57796	0.820329	-0.80368
H	2.624064	0.385476	1.29764	H	-2.88802	-0.85435	-0.42988
H	0.30907	1.267146	-2.26311	H	-0.36159	-0.3961	2.692021
H	1.858872	2.046633	-1.93692	H	-1.85192	0.540617	2.764916
H	1.806	0.367738	-2.49234	H	-1.90263	-1.19291	2.404655
H	3.815048	-1.11247	-0.27002	H	-4.00186	-0.29601	1.670842
H	3.887806	0.137065	-1.48281	H	-3.68641	1.410966	1.444719
H	5.376971	1.540705	-0.02832	H	-5.17915	1.557904	-0.48935
H	7.385088	1.58506	1.051651	H	-7.22126	1.064418	-1.40377
H	7.457729	0.488707	2.444397	H	-7.42821	-0.66606	-1.73635
H	8.276852	0.055589	0.950436	H	-8.24887	0.061617	-0.36276
H	5.138267	-2.12197	0.9244	H	-5.29932	-1.83862	1.183646
H	6.9024	-2.18661	0.818165	H	-7.05485	-1.62657	1.316895
H	6.135756	-1.75381	2.338961	H	-6.36742	-2.38141	-0.11282
H	1.733939	3.074857	1.005915	H	-1.18324	2.555879	2.072431
H	0.133363	3.2918	1.646015	H	-2.12967	2.669442	0.602468
H	0.994368	3.853627	-1.26192	H	0.415962	4.193461	1.3218
H	0.044737	5.577775	-2.389	H	0.969031	6.092683	0.169466
H	-1.67157	5.821334	-2.01269	H	0.748728	5.934721	-1.58355
H	-0.4673	6.900039	-1.32394	H	-0.41589	6.85134	-0.63793
H	-1.3865	4.626449	1.596483	H	-2.24953	3.578754	-1.28952
H	-1.3246	6.314599	1.074288	H	-2.32075	5.328707	-1.55456
H	-2.52303	5.232831	0.383704	H	-1.17475	4.350166	-2.4605
H	0.250335	-3.3927	0.096071	H	0.43244	-3.17335	-1.37598
H	0.946328	-5.44939	-1.17371	H	-0.00999	-5.64382	-1.13714
H	0.23002	-4.22808	-2.2471	H	0.398593	-4.88959	0.417832
H	1.984952	-4.44309	-2.20758	H	-1.28834	-5.27964	0.042891
H	2.170666	-4.70662	0.962571	H	-1.15451	-4.2536	-2.96856
H	2.41539	-2.99043	1.304469	H	-1.65048	-2.58636	-2.65066
H	3.290891	-3.76222	-0.03341	H	-2.50151	-3.92625	-1.86008
H	-3.63658	-2.17945	-0.42212	H	4.044993	-1.79994	0.038899
H	-3.66359	0.868553	-0.41539	H	3.54496	0.851648	1.45396
H	-3.11615	-0.24949	-1.68918	H	3.136359	-0.8001	1.981243
H	-6.96191	-2.40547	1.078374	H	7.425556	-0.84503	-0.96845
H	-5.67747	-3.28313	0.231414	H	6.27747	-2.18118	-0.78499
H	-5.39673	-2.68276	1.880878	H	5.971814	-0.91465	-1.9943
H	-6.83676	0.049368	1.374128	H	6.88873	1.413656	-0.112
H	-5.44998	0.994925	0.819827	H	5.333731	1.792118	0.638183
H	-5.28557	-0.05582	2.234189	H	5.422583	1.526248	-1.10906
H	-5.83953	-0.11898	-1.25655	H	5.817519	-0.10966	1.998327
2-e				**2-f**			
C	0.768206	-0.90377	0.871814	C	-0.78266	-0.92076	-0.72333

C	1.671116	0.000331	0.005712	C	-1.76053	0.004901	0.021935
C	1.057075	1.418492	-0.09372	C	-1.1492	1.41708	0.143234
C	-0.46266	1.468586	-0.32682	C	0.330881	1.465801	0.555564
C	-1.2633	0.609839	0.716699	C	1.267839	0.596677	-0.37516
C	-0.71951	-0.86236	0.54105	C	0.681778	-0.86903	-0.28023
C	-2.79217	0.666649	0.437038	C	2.698305	0.669937	0.237249
C	-1.0469	1.060202	2.180166	C	1.281147	1.075015	-1.84225
C	-3.29323	0.206918	-0.94885	C	3.879657	-0.08192	-0.41715
C	-4.7502	0.540752	-1.1418	C	5.192627	0.429565	0.1181
C	-5.79188	-0.28534	-1.32174	C	6.133398	-0.22528	0.815708
C	-7.18869	0.263489	-1.49268	C	7.394165	0.478204	1.259802
C	-5.70475	-1.79026	-1.37653	C	6.057717	-1.67751	1.218131
C	-0.90813	2.950189	-0.53752	C	0.721204	2.957767	0.815203
C	-0.59287	3.952358	0.544727	C	0.519668	3.95029	-0.30222
C	0.323504	4.934949	0.526576	C	-0.3886	4.937395	-0.38305
C	0.465916	5.875806	1.69981	C	-0.40942	5.866023	-1.5744
C	1.270608	5.220912	-0.61318	C	-1.44257	5.240058	0.653967
C	-1.42012	-1.99981	1.305681	C	1.370704	-2.02898	-1.0287
C	-1.09405	-3.42878	0.84903	C	1.148624	-3.42355	-0.42763
O	-2.22318	-1.80752	2.199084	O	2.037593	-1.87971	-2.03338
C	-0.82332	-4.32679	2.063562	C	1.034813	-4.47945	-1.53106
C	-2.27287	-3.95711	0.006616	C	2.30363	-3.73669	0.546828
O	1.231002	-1.592	1.763745	O	-1.17085	-1.66827	-1.60433
C	1.787792	-0.68034	-1.37614	C	-2.01792	-0.64665	1.399577
O	2.974524	-1.31813	-1.47768	O	-3.20885	-1.28836	1.389717
C	3.764841	-1.18516	-0.25827	C	-3.86495	-1.17947	0.092167
C	3.125003	-0.01442	0.500334	C	-3.1581	-0.01867	-0.61537
O	0.970605	-0.68679	-2.26558	O	-1.29962	-0.63514	2.370103
C	5.261228	-1.05997	-0.62979	C	-5.39303	-1.06208	0.295938
C	5.757918	-2.38271	-1.21619	C	-5.93857	-2.35913	0.906447
C	5.542356	0.098742	-1.5933	C	-5.78754	0.143338	1.149446
O	5.979242	-0.88952	0.600124	O	-5.96885	-0.83385	-0.99797
H	1.310788	1.956781	0.825777	H	-1.28703	1.924732	-0.81758
H	1.561256	1.952663	-0.90748	H	-1.73994	1.98554	0.87057
H	-0.63619	0.991047	-1.29687	H	0.394295	0.991946	1.542101
H	-0.79136	-1.10949	-0.52837	H	0.669175	-1.12556	0.78944
H	-3.30145	0.077463	1.203087	H	2.976574	1.729299	0.239602
H	-3.11496	1.702701	0.597569	H	2.643756	0.378092	1.295112
H	0.011083	1.134222	2.450208	H	0.270858	1.22937	-2.23483
H	-1.49895	2.037838	2.358983	H	1.817823	2.022012	-1.93695
H	-1.51464	0.344529	2.857661	H	1.769623	0.338065	-2.47887
H	-2.71885	0.704352	-1.74234	H	3.791443	-1.15802	-0.26739
H	-3.1193	-0.86582	-1.07644	H	3.855107	0.069982	-1.5026

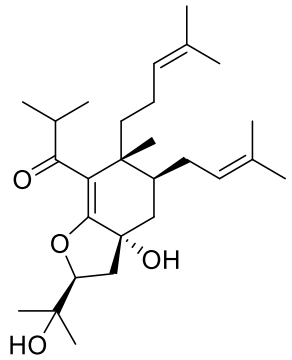
H	-4.96657	1.610558	-1.11852	H	5.38284	1.483102	-0.09757
H	-7.20756	1.355778	-1.44698	H	7.410724	1.525165	0.944839
H	-7.6191	-0.04441	-2.455	H	7.499808	0.449523	2.352639
H	-7.86202	-0.12146	-0.71527	H	8.286556	-0.01392	0.850383
H	-4.69261	-2.17146	-1.2342	H	5.129049	-2.16239	0.913727
H	-6.34331	-2.24065	-0.60554	H	6.890764	-2.24442	0.781833
H	-6.07298	-2.16484	-2.34071	H	6.151224	-1.78136	2.307162
H	-1.98883	2.964585	-0.72035	H	1.766317	3.003051	1.139374
H	-0.4519	3.271365	-1.47982	H	0.139283	3.266717	1.689659
H	-1.21315	3.888571	1.436714	H	1.221336	3.872275	-1.1305
H	-0.23038	5.632649	2.506799	H	0.3635	5.611391	-2.30449
H	1.484571	5.847499	2.109035	H	-1.38202	5.83586	-2.08327
H	0.284735	6.915323	1.395738	H	-0.25547	6.908283	-1.2647
H	1.138877	4.554859	-1.46751	H	-1.40272	4.581024	1.52283
H	1.144327	6.251816	-0.96858	H	-1.34426	6.273131	1.011985
H	2.313504	5.137088	-0.27991	H	-2.44711	5.160536	0.218014
H	-0.20134	-3.40268	0.213489	H	0.217313	-3.40145	0.151705
H	-0.63211	-5.35555	1.742145	H	0.902278	-5.47542	-1.09669
H	0.045504	-3.96901	2.621715	H	0.182108	-4.26552	-2.18084
H	-1.68688	-4.3249	2.734114	H	1.936505	-4.48365	-2.14887
H	-2.07467	-4.9837	-0.31678	H	2.139139	-4.70713	1.025243
H	-2.43816	-3.35348	-0.8925	H	2.391968	-2.98705	1.340676
H	-3.19344	-3.95327	0.598022	H	3.256104	-3.78121	0.008718
H	3.633219	-2.10907	0.313496	H	-3.65698	-2.1155	-0.44149
H	3.599368	0.937503	0.23837	H	-3.66796	0.928119	-0.41875
H	3.186297	-0.15938	1.579401	H	-3.11771	-0.17399	-1.69311
H	6.819519	-2.30686	-1.46575	H	-7.02603	-2.2994	1.003847
H	5.636289	-3.18624	-0.48399	H	-5.69658	-3.22019	0.270751
H	5.196637	-2.6406	-2.11777	H	-5.50366	-2.54299	1.892544
H	6.613729	0.13942	-1.80711	H	-6.87218	0.152813	1.283735
H	5.250489	1.066496	-1.16886	H	-5.50789	1.081593	0.66386
H	5.001669	-0.03101	-2.5341	H	-5.31068	0.09475	2.131156
H	5.85582	0.022151	0.896988	H	-5.89119	-1.65194	-1.5087
2-g				**2-h**			
C	0.94644	-1.15691	0.729981	C	0.786657	-0.89809	0.8516
C	1.842337	0.059723	0.445245	C	1.678221	0.024039	-0.00675
C	1.147823	1.329869	0.981677	C	1.045844	1.433298	-0.11449
C	-0.34681	1.482536	0.646021	C	-0.47424	1.461505	-0.34627
C	-1.21259	0.218511	1.037261	C	-1.25889	0.599404	0.706269
C	-0.52436	-1.01753	0.334954	C	-0.70382	-0.86779	0.529113
C	-2.63877	0.451076	0.451176	C	-2.79044	0.645058	0.440926
C	-1.27067	0.02775	2.566572	C	-1.03107	1.053305	2.167101
C	-3.76362	-0.58758	0.668501	C	-3.30022	0.178639	-0.9396

C	-5.10978	0.019868	0.366439	C	-4.75988	0.505731	-1.1232
C	-5.99239	-0.31343	-0.58772	C	-5.79905	-0.32477	-1.29716
C	-7.30288	0.425792	-0.72004	C	-7.19926	0.217989	-1.45952
C	-5.79876	-1.41991	-1.59501	C	-5.70571	-1.82929	-1.35335
C	-0.84487	2.823478	1.262881	C	-0.94311	2.933854	-0.56939
C	-0.10354	4.043079	0.762993	C	-0.67415	3.945327	0.516574
C	-0.41401	4.802817	-0.29954	C	0.240003	4.930048	0.528294
C	0.428036	5.999204	-0.67079	C	0.333653	5.879027	1.699822
C	-1.5916	4.556411	-1.20982	C	1.232442	5.208665	-0.57403
C	-1.12413	-2.42871	0.505083	C	-1.39116	-2.01068	1.296963
C	-0.80598	-3.41977	-0.62305	C	-1.06491	-3.43691	0.831196
O	-1.79384	-2.76327	1.461977	O	-2.18417	-1.82528	2.200773
C	-0.61125	-4.83335	-0.06627	C	-0.78707	-4.34055	2.039757
C	-1.93992	-3.36832	-1.66844	C	-2.24657	-3.9633	-0.00844
O	1.397204	-2.17336	1.228949	O	1.260676	-1.59982	1.727802
C	2.06945	0.100463	-1.08212	C	1.809361	-0.66129	-1.38496
O	3.290793	-0.40294	-1.37725	O	3.001736	-1.29432	-1.47332
C	3.998794	-0.82878	-0.17629	C	3.780844	-1.14036	-0.25035
C	3.26668	-0.1427	0.981714	C	3.130293	0.031452	0.492859
O	1.308196	0.486594	-1.93588	O	1.000698	-0.67916	-2.28167
C	5.50835	-0.53487	-0.33596	C	5.279189	-1.00803	-0.60824
C	6.09155	-1.39956	-1.4606	C	5.787026	-2.31908	-1.22103
C	5.802764	0.94427	-0.58573	C	5.565058	0.169	-1.54099
O	6.128574	-0.85382	0.917561	O	5.974929	-0.72061	0.612899
H	1.285068	1.336542	2.070672	H	1.293582	1.980333	0.801406
H	1.686605	2.202064	0.598865	H	1.543208	1.967979	-0.93185
H	-0.41924	1.584856	-0.44288	H	-0.64255	0.973839	-1.31241
H	-0.51271	-0.78532	-0.74033	H	-0.7773	-1.11669	-0.53995
H	-3.00635	1.387921	0.881547	H	-3.28952	0.05464	1.212808
H	-2.54543	0.639746	-0.62725	H	-3.11789	1.679658	0.601486
H	-0.27044	-0.02215	3.010673	H	0.029158	1.124188	2.428978
H	-1.80027	0.86039	3.039473	H	-1.47686	2.033337	2.347164
H	-1.78021	-0.89986	2.823422	H	-1.49588	0.340333	2.849527
H	-3.59607	-1.47971	0.064554	H	-2.7336	0.675703	-1.7389
H	-3.75416	-0.92736	1.710577	H	-3.12262	-0.8938	-1.06475
H	-5.38329	0.84809	1.023663	H	-4.98083	1.57457	-1.0983
H	-7.40379	1.217373	0.027508	H	-7.22269	1.310154	-1.41298
H	-7.40171	0.881699	-1.71436	H	-7.63395	-0.09116	-2.41953
H	-8.15527	-0.2576	-0.60772	H	-7.86638	-0.17039	-0.67845
H	-4.83443	-1.92178	-1.50443	H	-4.69099	-2.20601	-1.21778
H	-6.58403	-2.18043	-1.49172	H	-6.33741	-2.28296	-0.57861
H	-5.88072	-1.02897	-2.6177	H	-6.07842	-2.20495	-2.31541
H	-0.73936	2.776808	2.353701	H	-2.01943	2.926039	-0.77678

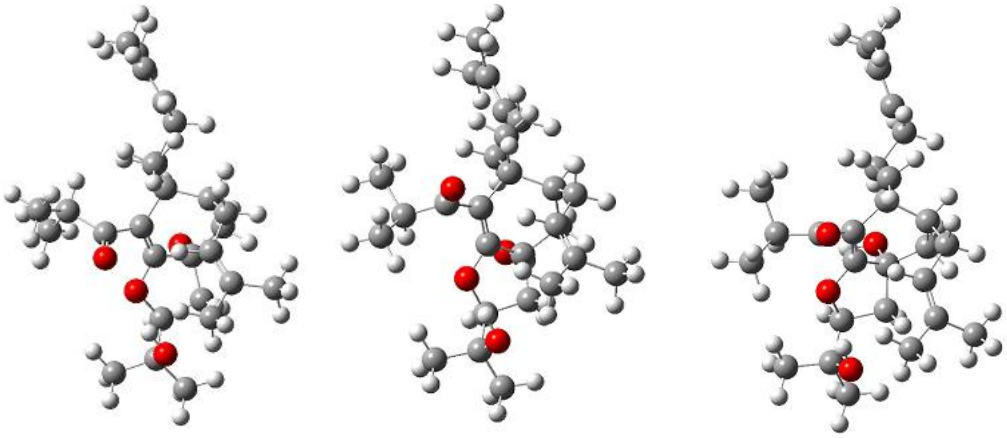
H	-1.91149	2.946328	1.066698	H	-0.47217	3.261438	-1.50233
H	0.778096	4.330564	1.335549	H	-1.33121	3.887107	1.382423
H	1.269851	6.135309	0.013702	H	-0.39469	5.640313	2.479437
H	0.828326	5.899679	-1.68829	H	1.334802	5.854236	2.150232
H	-0.17022	6.920009	-0.66238	H	0.164201	6.916259	1.381453
H	-2.20354	3.705161	-0.90605	H	1.125847	4.545622	-1.43416
H	-2.23926	5.441733	-1.25445	H	1.130198	6.241579	-0.93121
H	-1.25026	4.370274	-2.23628	H	2.260998	5.112603	-0.20199
H	0.118469	-3.09264	-1.11471	H	-0.1753	-3.40551	0.191626
H	-0.41014	-5.54056	-0.87722	H	-0.59555	-5.36754	1.712695
H	0.22728	-4.8588	0.63471	H	0.083457	-3.98344	2.595765
H	-1.50742	-5.15879	0.468276	H	-1.64744	-4.34325	2.714344
H	-1.7096	-4.03346	-2.50642	H	-2.04851	-4.98824	-0.33723
H	-2.08325	-2.36125	-2.07482	H	-2.41648	-3.35604	-0.90419
H	-2.88454	-3.69797	-1.22384	H	-3.16473	-3.9634	0.58676
H	3.863813	-1.91557	-0.10371	H	3.642039	-2.06381	0.326023
H	3.716214	0.827685	1.208314	H	3.607137	0.977845	0.225121
H	3.284722	-0.75356	1.883852	H	3.195173	-0.0965	1.573084
H	7.168777	-1.23097	-1.54313	H	6.857726	-2.24573	-1.43038
H	5.924223	-2.46523	-1.25927	H	5.627648	-3.15802	-0.53188
H	5.62161	-1.16609	-2.41976	H	5.259158	-2.54937	-2.15043
H	6.879068	1.081702	-0.71718	H	6.632692	0.195043	-1.77346
H	5.49352	1.559097	0.26295	H	5.307547	1.120863	-1.06998
H	5.28968	1.294607	-1.48425	H	5.003037	0.070063	-2.47251
H	6.116745	-1.81572	1.021767	H	5.969563	-1.5207	1.156966
2-i							
C	1.036926	-1.16012	0.805063				
C	1.784604	0.13696	0.437347				
C	1.018284	1.363127	0.991275				
C	-0.50982	1.34302	0.803568				
C	-1.16028	0.0102	1.323206				
C	-0.46229	-1.15757	0.52657				
C	-2.69625	-0.00851	1.07523				
C	-0.93946	-0.18555	2.841113				
C	-3.19882	0.167632	-0.37342				
C	-4.69555	0.337976	-0.41472				
C	-5.61909	-0.4165	-1.02923				
C	-7.08517	-0.06435	-0.93883				
C	-5.32625	-1.64747	-1.85036				
C	-1.13298	2.627739	1.420887				
C	-0.52477	3.917089	0.921299				
C	-0.97646	4.715633	-0.0591				
C	-0.23724	5.979471	-0.42757				

C	-2.21891	4.456879	-0.87432				
C	-0.98976	-2.59119	0.718943				
C	-0.5449	-3.62616	-0.32419				
O	-1.74739	-2.90819	1.616333				
C	-0.14166	-4.93667	0.363675				
C	-1.69849	-3.84301	-1.32473				
O	1.620427	-2.11434	1.288953				
C	1.892684	0.161685	-1.10323				
O	3.133037	-0.22394	-1.48344				
C	3.963375	-0.55911	-0.33273				
C	3.257888	0.081614	0.867077				
O	1.034677	0.452856	-1.90121				
C	5.423701	-0.13446	-0.60959				
C	5.999062	-0.96792	-1.76146				
C	5.563062	1.359592	-0.90248				
O	6.161334	-0.36846	0.598295				
H	1.262815	1.442848	2.058				
H	1.424477	2.260255	0.514493				
H	-0.6875	1.39226	-0.27577				
H	-0.55982	-0.9216	-0.54355				
H	-3.09165	-0.94761	1.469015				
H	-3.14016	0.779328	1.695439				
H	0.119802	-0.1921	3.117573				
H	-1.42363	0.613215	3.410438				
H	-1.36844	-1.13661	3.158911				
H	-2.73775	1.056367	-0.82581				
H	-2.88451	-0.67988	-0.99016				
H	-5.05832	1.200342	0.148145				
H	-7.25401	0.834786	-0.34006				
H	-7.51341	0.105205	-1.93582				
H	-7.66108	-0.88485	-0.49044				
H	-4.26633	-1.90297	-1.88623				
H	-5.86677	-2.51495	-1.44993				
H	-5.675	-1.51564	-2.88312				
H	-1.01714	2.594705	2.511767				
H	-2.20841	2.625881	1.228574				
H	0.389615	4.2293	1.425874				
H	0.655458	6.124207	0.187005				
H	0.072612	5.962554	-1.48076				
H	-0.87996	6.861762	-0.30808				
H	-2.75868	3.559368	-0.56769				
H	-2.91039	5.306973	-0.80811				
H	-1.96554	4.346318	-1.93659				

H	0.315528	-3.22688	-0.87325				
H	0.135135	-5.68957	-0.38124				
H	0.709805	-4.77572	1.029811				
H	-0.97395	-5.32253	0.958298				
H	-1.41326	-4.58979	-2.07216				
H	-1.95658	-2.92227	-1.859				
H	-2.59204	-4.20015	-0.8039				
H	3.933784	-1.65192	-0.23474				
H	3.629133	1.094372	1.044228				
H	3.400197	-0.50582	1.773769				
H	7.04774	-0.70606	-1.92672				
H	5.943799	-2.03957	-1.53182				
H	5.441294	-0.79837	-2.6864				
H	6.60983	1.589773	-1.11671				
H	5.263015	1.961926	-0.04152				
H	4.9554	1.644254	-1.76453				
H	6.249607	-1.32481	0.715458				



3



a **b** **c**

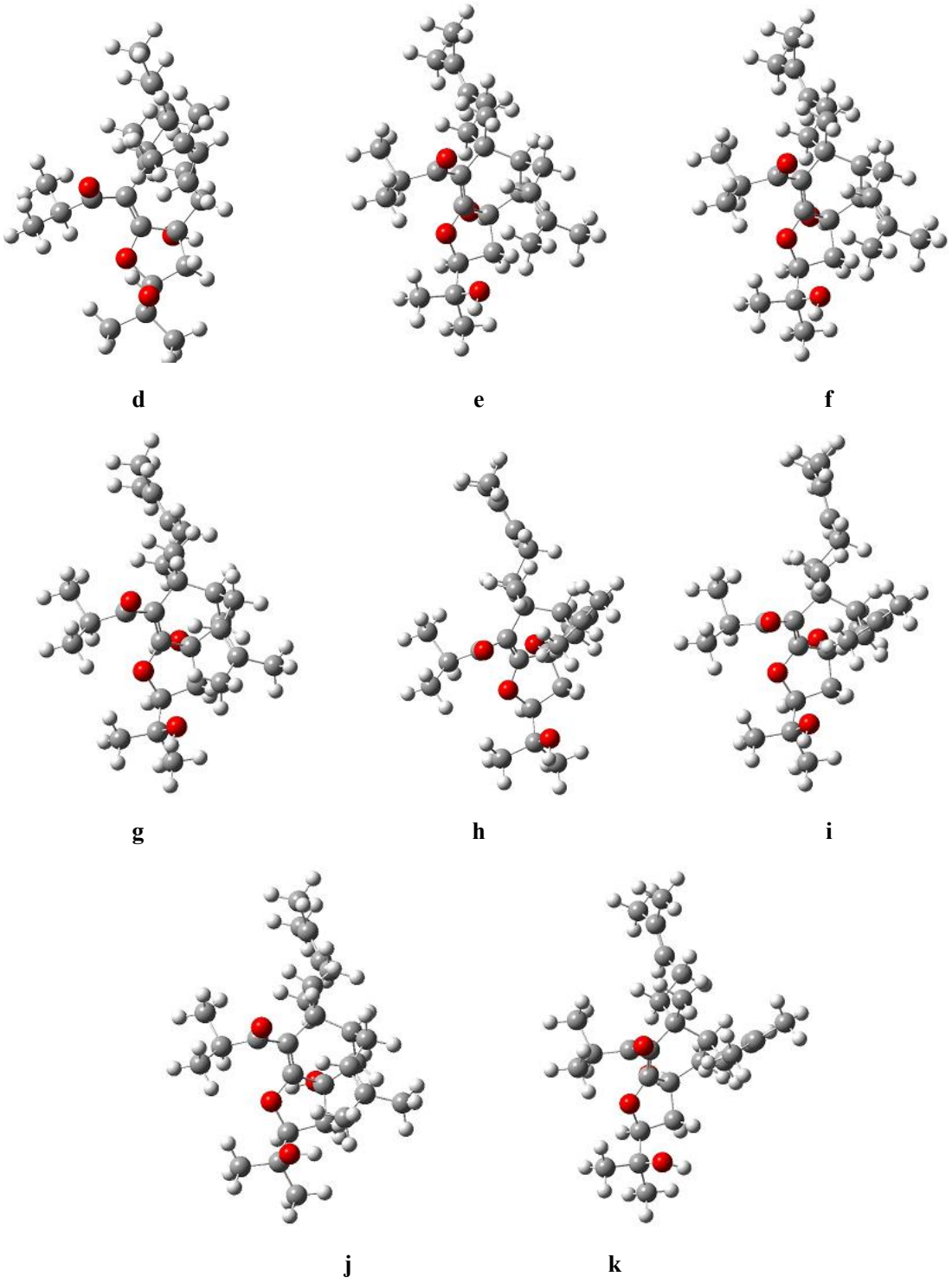


Figure S5. Optimized geometries of predominant conformers for compound **3** at the B3LYP/6-31G(d,p) level in the gas phase.

Table S6. Important thermodynamic parameters (a.u.) and Boltzmann distributions of the optimized compound **3** at B3LYP/6-31G(d,p) level in the gas phase

compound	E+ZPE	G	%
3-a	-1355.618468	-1355.687860	4.5
3-b	-1355.619924	-1355.689748	32.8
3-c	-1355.620265	-1355.688711	10.9
3-d	-1355.619792	-1355.690152	50.3
3-e	-1355.614319	-1355.683871	0.1
3-f	-1355.614660	-1355.683799	0.0
3-g	-1355.615132	-1355.685435	0.4
3-h	-1355.616079	-1355.686388	0.9
3-i	-1355.613187	-1355.683310	0.0
3-j	-1355.614010	-1355.684038	0.1
3-k	-1355.613297	-1355.683118	0.0

E+ZPE, G: total energy with zero point energy (ZPE) and Gibbs free energy in the gas phase at B3LYP/6-31G(d,p) level., %: Boltzmann distributions, using the relative Gibbs free energies as weighting factors

Table S7. Optimized Z-matrixes of compound **3** in the gas phase (Å) at B3LYP/6-31G(d,p) level

3-a				**3-b**			
C	0.214848	0.450253	0.544982	C	-0.25095	0.403549	-0.65273
C	-0.60336	0.460463	-0.51384	C	0.545527	0.423673	0.429489
C	-0.60592	-0.53404	-1.64298	C	0.473621	-0.52354	1.603174
C	0.007604	-1.90115	-1.26283	C	-0.16613	-1.88871	1.262323
C	0.673514	-2.00381	0.141573	C	-0.80253	-2.02729	-0.15088
C	1.294351	-0.64641	0.635809	C	-1.36112	-0.67284	-0.71121
C	2.498819	-0.23177	-0.27547	C	-2.54067	-0.14893	0.181424
C	1.790175	-0.79944	2.091977	C	-1.89821	-0.88061	-2.14327
C	-0.24728	-2.74457	1.15731	C	0.118332	-2.83011	-1.11881
C	3.742709	-1.14784	-0.26846	C	-3.81528	-1.01851	0.26015
C	-1.53588	-2.08902	1.580092	C	1.410986	-2.20161	-1.56935
C	-2.78395	-2.57862	1.476574	C	2.662772	-2.65228	-1.37496
C	-3.95566	-1.81521	2.04848	C	3.843136	-1.93209	-1.98461
C	-3.15972	-3.88929	0.827457	C	3.036938	-3.88303	-0.58388
C	4.792539	-0.65517	-1.22964	C	-4.82296	-0.42634	1.210267
C	6.041167	-0.23829	-0.96848	C	-6.06463	0.012584	0.952182
C	6.946199	0.231282	-2.08281	C	-6.92482	0.584526	2.054219
C	6.669206	-0.19228	0.402945	C	-6.72714	-0.01234	-0.40343
C	-0.01414	1.466977	1.634526	C	0.030459	1.35331	-1.78026
C	1.028043	2.568101	1.847258	C	0.058875	2.860245	-1.48829
C	0.839681	3.629292	0.739391	C	1.157323	3.555904	-2.30061
C	0.92725	3.182144	3.246202	C	-1.33475	3.432032	-1.82607
O	-1.04706	1.445602	2.28943	O	0.197131	0.949199	-2.92448

O	-1.59754	1.383101	-0.70103	O	1.622706	1.263019	0.575921
C	-2.46053	0.968235	-1.79948	C	2.363056	0.91574	1.786108
C	-2.10492	-0.50882	-2.00528	C	1.948749	-0.53402	2.045488
C	-3.90854	1.282925	-1.36932	C	3.855753	1.177719	1.507016
C	-4.90619	0.740456	-2.39428	C	4.707182	0.715743	2.691519
C	-4.08551	2.799201	-1.18428	C	4.091266	2.668752	1.216458
O	-4.1881	0.608784	-0.1425	O	4.273779	0.392544	0.387845
H	-0.75755	-2.68042	-1.3434	H	0.578841	-2.68058	1.392753
H	1.523968	-2.68628	0.022775	H	-1.6761	-2.67877	-0.02682
H	2.138487	-0.11723	-1.30263	H	-2.17165	0.033515	1.194605
H	2.821653	0.770209	0.034189	H	-2.83021	0.835611	-0.20778
H	2.418971	0.046734	2.385424	H	-2.45152	0.001425	-2.48056
H	0.963482	-0.86163	2.804059	H	-1.10509	-1.05391	-2.86821
H	2.394754	-1.70398	2.207143	H	-2.58595	-1.73171	-2.16547
H	-0.44937	-3.72988	0.723902	H	0.311197	-3.79327	-0.63419
H	0.34448	-2.94676	2.059778	H	-0.46936	-3.06959	-2.01411
H	4.148956	-1.2295	0.743396	H	-4.24885	-1.15298	-0.73398
H	3.453959	-2.16639	-0.56494	H	-3.55417	-2.02481	0.618896
H	-1.43249	-1.1253	2.075251	H	1.296889	-1.30651	-2.17858
H	-3.62855	-0.92182	2.587292	H	3.525892	-1.07579	-2.58728
H	-4.64613	-1.49695	1.25892	H	4.532185	-1.57463	-1.20975
H	-4.52644	-2.44233	2.746529	H	4.41823	-2.60391	-2.63601
H	-2.31588	-4.4152	0.37623	H	2.182461	-4.38808	-0.12921
H	-3.62061	-4.56465	1.560494	H	3.552531	-4.6107	-1.2246
H	-3.91263	-3.72807	0.044798	H	3.743053	-3.62754	0.217125
H	4.468658	-0.62787	-2.27155	H	-4.47107	-0.33911	2.239832
H	6.453586	0.181335	-3.05769	H	-6.40819	0.583478	3.017946
H	7.271011	1.267451	-1.91858	H	-7.22209	1.617468	1.828754
H	7.860753	-0.3749	-2.13224	H	-7.85596	0.01294	2.166749
H	5.996026	-0.5134	1.199666	H	-6.08606	-0.40865	-1.19253
H	7.562749	-0.82934	0.44172	H	-7.64162	-0.61967	-0.37703
H	7.006614	0.825616	0.638403	H	-7.03745	0.998472	-0.69905
H	2.022192	2.125921	1.707361	H	0.241398	3.005857	-0.42026
H	1.606024	4.405415	0.831115	H	1.133331	4.637549	-2.13331
H	0.914936	3.188729	-0.25844	H	2.149764	3.190801	-2.01723
H	-0.14178	4.105816	0.82798	H	1.022667	3.362809	-3.368
H	1.663583	3.983069	3.366841	H	-1.3631	4.505983	-1.61543
H	1.104673	2.433695	4.024543	H	-2.12397	2.955699	-1.23511
H	-0.07043	3.596486	3.411224	H	-1.56306	3.284056	-2.88649
H	-2.18864	1.56205	-2.68021	H	2.010795	1.569322	2.59263
H	-2.67276	-1.12083	-1.29833	H	2.537283	-1.19769	1.405319
H	-2.29477	-0.85983	-3.02412	H	2.067695	-0.83708	3.089691
H	-5.92383	0.989342	-2.08126	H	5.760341	0.927423	2.488165

H	-4.83478	-0.3476	-2.47149	H	4.604602	-0.36074	2.850125
H	-4.73342	1.177408	-3.38296	H	4.421726	1.238197	3.609938
H	-5.09673	3.00672	-0.82387	H	5.144915	2.830858	0.973801
H	-3.36952	3.183748	-0.45288	H	3.484515	3.00072	0.369507
H	-3.93358	3.338379	-2.12577	H	3.833209	3.290227	2.08073
H	-3.48906	0.860239	0.48215	H	3.657981	0.588208	-0.33409
H	0.758212	-2.12703	-2.02736	H	-0.93903	-2.06731	2.017589
O	0.145544	0.09166	-2.71135	O	-0.30091	0.180641	2.605423
H	0.071243	-0.48606	-3.4845	H	-0.31742	-0.37999	3.394446
3-c				**3-d**			
C	-0.25266	0.399123	-0.64126	C	0.137474	-0.22689	0.661211
C	0.536906	0.427981	0.446273	C	0.957932	-0.8898	-0.17121
C	0.470211	-0.51753	1.62209	C	0.772562	-1.0651	-1.66116
C	-0.13248	-1.8922	1.27964	C	-0.20624	-0.04388	-2.28855
C	-0.77597	-2.03874	-0.13013	C	-0.71453	1.051603	-1.32102
C	-1.34736	-0.69372	-0.70287	C	-1.13223	0.419369	0.054531
C	-2.54045	-0.1818	0.179059	C	-2.1966	-0.71497	-0.1274
C	-1.87127	-0.91151	-2.13823	C	-1.7299	1.499573	0.977671
C	0.146053	-2.8409	-1.09777	C	0.305886	2.223411	-1.17413
C	-3.81863	-1.04874	0.221147	C	-3.52265	-0.32807	-0.81854
C	1.42919	-2.20243	-1.56167	C	-0.31792	3.595762	-1.16242
C	2.686714	-2.64168	-1.37882	C	-0.08859	4.613872	-0.31853
C	3.854389	-1.9162	-2.00653	C	-0.77082	5.946212	-0.51987
C	3.079496	-3.86581	-0.58667	C	0.844091	4.559871	0.86746
C	-4.82622	-0.48703	1.189835	C	-4.44472	-1.51258	-0.94144
C	-6.05321	-0.00447	0.939339	C	-5.66421	-1.68584	-0.40855
C	-6.91736	0.523843	2.05992	C	-6.43345	-2.9645	-0.64218
C	-6.69464	0.062445	-0.425	C	-6.387	-0.673	0.445452
C	0.019884	1.352772	-1.76817	C	0.592445	0.016008	2.074502
C	0.020155	2.861507	-1.48145	C	0.831398	-1.19367	2.983406
C	1.111514	3.5731	-2.2895	C	1.796908	-0.85468	4.122616
C	-1.38073	3.408859	-1.82931	C	-0.53057	-1.68281	3.522497
O	0.204048	0.949279	-2.90946	O	0.752547	1.155751	2.491007
O	1.593595	1.298973	0.609423	O	2.184436	-1.38709	0.200355
C	2.359323	0.942911	1.803612	C	2.972521	-1.71933	-0.98299
C	1.937838	-0.49979	2.087527	C	2.240319	-1.00465	-2.12301
C	3.850631	1.187696	1.491953	C	4.420009	-1.25853	-0.70959
C	4.718663	0.731712	2.666528	C	5.288569	-1.45894	-1.95305
C	4.095687	2.672043	1.176544	C	5.004934	-2.01907	0.491035
O	4.236605	0.382943	0.377293	O	4.421365	0.146737	-0.44799
H	0.638889	-2.65954	1.395568	H	0.254083	0.428421	-3.16437
H	-1.64544	-2.69399	0.000933	H	-1.61811	1.472041	-1.78017
H	-2.18717	-0.02579	1.202067	H	-1.74879	-1.55629	-0.66506

H	-2.82297	0.810467	-0.19632	H	-2.4368	-1.09887	0.871835
H	-2.43319	-0.03724	-2.48194	H	-2.11113	1.050514	1.901138
H	-1.07116	-1.0777	-2.85708	H	-1.00179	2.256379	1.258127
H	-2.54833	-1.77081	-2.16248	H	-2.56409	2.000115	0.478501
H	0.352119	-3.7976	-0.60624	H	0.934943	2.068144	-0.29403
H	-0.44375	-3.09483	-1.98781	H	0.98823	2.18514	-2.03681
H	-4.24899	-1.14377	-0.77893	H	-4.00847	0.490417	-0.28157
H	-3.56305	-2.06794	0.544096	H	-3.31026	0.052714	-1.82792
H	1.302212	-1.31064	-2.17348	H	-1.01381	3.779097	-1.98392
H	3.524461	-1.06328	-2.60738	H	-1.41878	5.947167	-1.40093
H	4.552659	-1.55353	-1.24251	H	-1.38067	6.213438	0.353422
H	4.423795	-2.58675	-2.66424	H	-0.03435	6.752216	-0.63971
H	2.234684	-4.37314	-0.11695	H	1.162879	3.549398	1.128122
H	3.590361	-4.59391	-1.23075	H	1.741539	5.165752	0.682063
H	3.795129	-3.60121	0.202703	H	0.359446	4.989942	1.752925
H	-4.48756	-0.468	2.227172	H	-4.04191	-2.33529	-1.53514
H	-6.41474	0.458328	3.028804	H	-5.87626	-3.66802	-1.26683
H	-7.19088	1.573635	1.888269	H	-6.66753	-3.46439	0.30729
H	-7.86125	-0.03362	2.128296	H	-7.39627	-2.76391	-1.1311
H	-6.04995	-0.30423	-1.22548	H	-5.80943	0.235403	0.62458
H	-7.62308	-0.52351	-0.44635	H	-7.33686	-0.38046	-0.02142
H	-6.97707	1.095259	-0.66802	H	-6.64398	-1.10518	1.421426
H	0.195387	3.014502	-0.41294	H	1.253348	-1.99276	2.364922
H	1.068643	4.654685	-2.12587	H	1.946166	-1.72552	4.76885
H	2.108321	3.225201	-2.00002	H	2.77318	-0.5448	3.73705
H	0.985612	3.374279	-3.3568	H	1.407892	-0.03221	4.728461
H	-1.42893	4.48291	-1.62274	H	-0.38806	-2.56595	4.153423
H	-2.16645	2.920545	-1.24338	H	-1.21339	-1.9576	2.713115
H	-1.5991	3.253711	-2.89068	H	-1.00915	-0.90727	4.130246
H	2.050401	1.617805	2.615194	H	2.936613	-2.807	-1.11238
H	2.540725	-1.17029	1.468251	H	2.585126	0.032775	-2.17984
H	2.026402	-0.78149	3.138388	H	2.387405	-1.48379	-3.09526
H	5.770198	0.925017	2.438322	H	6.313801	-1.14729	-1.73622
H	4.603018	-0.34021	2.844324	H	4.923466	-0.85468	-2.78737
H	4.459851	1.272257	3.582367	H	5.304521	-2.51013	-2.25765
H	5.146081	2.819158	0.911701	H	6.009881	-1.64559	0.705451
H	3.476735	2.999506	0.336621	H	4.383941	-1.87885	1.380193
H	3.862527	3.308402	2.037231	H	5.06839	-3.09404	0.290643
H	3.61733	0.580589	-0.34102	H	3.824711	0.285595	0.302817
H	-0.88082	-2.08868	2.052098	H	-1.06241	-0.61694	-2.65717
O	-0.37139	0.040374	2.66406	O	0.288205	-2.41802	-1.82837
H	-0.21853	0.994257	2.709795	H	0.206646	-2.57308	-2.78039
3-e				**3-f**			

C	-0.24602	-0.36397	0.699091	C	-0.25592	-0.37015	0.678417
C	0.557364	-0.43748	-0.37839	C	0.533376	-0.44848	-0.40902
C	0.483089	0.451495	-1.59818	C	0.482782	0.46569	-1.61034
C	-0.16057	1.830246	-1.33098	C	-0.11034	1.855895	-1.32053
C	-0.82699	2.031793	0.061345	C	-0.77723	2.052166	0.072981
C	-1.37093	0.700149	0.686963	C	-1.34793	0.727801	0.692212
C	-2.53261	0.109385	-0.18863	C	-2.53434	0.18228	-0.17999
C	-1.93503	0.979202	2.096178	C	-1.88826	0.999827	2.1119
C	0.066691	2.899485	0.998124	C	0.129053	2.897835	1.017551
C	-3.8144	0.958001	-0.34219	C	-3.82	1.036471	-0.25305
C	1.370202	2.314414	1.472512	C	1.435432	2.297239	1.464176
C	2.613308	2.777145	1.255572	C	2.675697	2.773832	1.260648
C	3.80687	2.084224	1.869145	C	3.875569	2.069326	1.848017
C	2.963677	3.99038	0.4272	C	3.01664	4.020773	0.479769
C	-4.80801	0.284954	-1.25227	C	-4.81198	0.445784	-1.22059
C	-6.06329	-0.10695	-0.98463	C	-6.03397	-0.0506	-0.97265
C	-6.90366	-0.78003	-2.04405	C	-6.88104	-0.60902	-2.09172
C	-6.76195	0.070384	0.341269	C	-6.6854	-0.10582	0.387453
C	0.030937	-1.24375	1.880998	C	0.001824	-1.27936	1.843152
C	0.124851	-2.7625	1.671857	C	0.038089	-2.7981	1.614013
C	1.211135	-3.37207	2.565568	C	1.122249	-3.45482	2.476497
C	-1.26082	-3.36697	1.983714	C	-1.35988	-3.35986	1.9497
O	0.135955	-0.77929	3.009992	O	0.141511	-0.83492	2.975778
O	1.630637	-1.27876	-0.48502	O	1.559255	-1.34935	-0.55978
C	2.365202	-0.99395	-1.70525	C	2.34683	-1.02344	-1.73896
C	1.959213	0.445095	-2.03731	C	1.955114	0.422154	-2.05916
C	3.861316	-1.26967	-1.49023	C	3.834665	-1.30092	-1.46337
C	4.599927	-1.13702	-2.83348	C	4.639112	-1.09321	-2.7579
C	4.069346	-2.66738	-0.89094	C	4.025788	-2.72569	-0.92497
O	4.336754	-0.26956	-0.58148	O	4.244681	-0.34577	-0.48025
H	0.591011	2.612948	-1.47724	H	0.672829	2.610104	-1.44313
H	-1.70898	2.660701	-0.11098	H	-1.64938	2.69557	-0.09466
H	-2.14777	-0.1326	-1.18317	H	-2.17603	0.000626	-1.1971
H	-2.8175	-0.85127	0.259464	H	-2.81047	-0.80122	0.222218
H	-2.48052	0.108568	2.473045	H	-2.45298	0.138381	2.482159
H	-1.15872	1.205635	2.824191	H	-1.09723	1.193779	2.833505
H	-2.63657	1.818653	2.056509	H	-2.56701	1.858232	2.093433
H	0.240621	3.844597	0.472202	H	0.30296	3.850877	0.506681
H	-0.53062	3.164454	1.879633	H	-0.45602	3.150741	1.910719
H	-4.25812	1.163757	0.635092	H	-4.2615	1.147927	0.74045
H	-3.55842	1.936668	-0.77425	H	-3.57063	2.051249	-0.59423
H	1.274796	1.435412	2.106859	H	1.345767	1.394512	2.065673
H	3.506634	1.229749	2.480661	H	3.586982	1.171189	2.399373

H	4.485073	1.71887	1.088955	H	4.575757	1.77124	1.058363
H	4.381718	2.775348	2.50084	H	4.424627	2.732447	2.530785
H	2.097782	4.473858	-0.02954	H	2.147298	4.515275	0.042346
H	3.479119	4.741018	1.041323	H	3.527173	4.750666	1.122368
H	3.66191	3.72183	-0.37672	H	3.715912	3.788889	-0.33452
H	-4.43138	0.08648	-2.25747	H	-4.4644	0.414859	-2.25475
H	-6.36298	-0.88548	-2.98859	H	-6.37125	-0.55128	-3.05738
H	-7.22136	-1.78049	-1.72077	H	-7.14071	-1.65996	-1.90591
H	-7.82359	-0.21275	-2.24015	H	-7.83242	-0.06669	-2.17673
H	-6.13663	0.540006	1.102316	H	-6.05271	0.283606	1.186711
H	-7.66486	0.684246	0.223546	H	-7.62306	0.465723	0.392339
H	-7.09738	-0.89877	0.733288	H	-6.95355	-1.13898	0.644914
H	0.358442	-2.95835	0.622488	H	0.243964	-2.98956	0.557775
H	1.23537	-4.46115	2.454266	H	1.108424	-4.54252	2.351173
H	2.200066	-2.98019	2.307233	H	2.117785	-3.09152	2.202556
H	1.020928	-3.13079	3.614592	H	0.961381	-3.22104	3.532009
H	-1.24208	-4.45158	1.834825	H	-1.3818	-4.44257	1.787959
H	-2.03972	-2.95471	1.333724	H	-2.14004	-2.91316	1.324231
H	-1.54088	-3.16846	3.023389	H	-1.60904	-3.16491	2.99772
H	1.996686	-1.67832	-2.47932	H	2.032426	-1.70147	-2.54634
H	2.544075	1.140728	-1.43072	H	2.557462	1.100562	-1.44994
H	2.077604	0.695736	-3.0956	H	2.055612	0.676832	-3.11601
H	5.667661	-1.33598	-2.6914	H	5.699836	-1.29284	-2.57143
H	4.499507	-0.12529	-3.23554	H	4.548749	-0.0629	-3.11146
H	4.225584	-1.84979	-3.57575	H	4.310611	-1.7685	-3.55507
H	5.140295	-2.86751	-0.76545	H	5.08973	-2.91957	-0.74372
H	3.579882	-2.73773	0.081535	H	3.479642	-2.85269	0.010967
H	3.662531	-3.44623	-1.54389	H	3.672857	-3.47495	-1.64118
H	5.219537	-0.53237	-0.29072	H	5.119597	-0.60434	-0.16321
H	-0.91519	1.97968	-2.11099	H	-0.84149	2.03829	-2.11267
O	-0.2855	-0.30572	-2.56724	O	-0.34914	-0.12277	-2.64579
H	-0.30935	0.219722	-3.3799	H	-0.25177	-1.08417	-2.6121
3-g				**3-h**			
C	0.1276	-0.1973	0.66961	C	0.105914	-0.27	0.628731
C	0.950529	-0.87367	-0.15328	C	0.868017	-0.985	-0.21737
C	0.763954	-1.06698	-1.64245	C	0.678998	-1.11885	-1.71144
C	-0.20991	-0.05481	-2.28869	C	-0.2297	-0.04118	-2.33022
C	-0.71735	1.054309	-1.33745	C	-0.64532	1.084794	-1.35422
C	-1.13883	0.440991	0.045428	C	-1.1055	0.483549	0.022711
C	-2.20063	-0.69863	-0.12387	C	-2.25166	-0.56868	-0.16018
C	-1.74978	1.534813	0.943655	C	-1.62528	1.60019	0.949965
C	0.307236	2.223997	-1.20625	C	0.467965	2.168592	-1.21889
C	-3.52658	-0.32586	-0.82339	C	-3.55742	-0.0842	-0.82811

C	-0.31053	3.598813	-1.18703	C	-0.03148	3.582277	-1.06727
C	-0.06945	4.614593	-0.34361	C	0.358633	4.519488	-0.18942
C	-0.74664	5.950672	-0.53742	C	-0.21141	5.9167	-0.25217
C	0.870263	4.552352	0.836399	C	1.373023	4.303227	0.907974
C	-4.43976	-1.51765	-0.94194	C	-4.55138	-1.2076	-0.96379
C	-5.65465	-1.70176	-0.40221	C	-5.76902	-1.32284	-0.41129
C	-6.41372	-2.98745	-0.63066	C	-6.61785	-2.54642	-0.66405
C	-6.38098	-0.69539	0.456434	C	-6.41394	-0.29302	0.483778
C	0.554261	0.047297	2.089441	C	0.538726	-0.11663	2.059687
C	0.851162	-1.16258	2.983778	C	0.719873	-1.37866	2.913223
C	1.815261	-0.79405	4.115219	C	1.729257	-1.14686	4.041506
C	-0.48762	-1.69975	3.534938	C	-0.66121	-1.78924	3.468842
O	0.630052	1.183597	2.538244	O	0.709496	0.991186	2.549937
O	2.160824	-1.39007	0.22178	O	2.009557	-1.66375	0.141239
C	2.956994	-1.7159	-0.94714	C	2.877862	-1.83667	-1.01537
C	2.230498	-1.02031	-2.10644	C	2.147311	-1.13624	-2.17455
C	4.413397	-1.28015	-0.70717	C	4.280149	-1.28458	-0.69043
C	5.287917	-1.7486	-1.8826	C	5.233972	-1.58895	-1.85747
C	4.934121	-1.84702	0.620475	C	4.808669	-1.88419	0.618994
O	4.39246	0.150956	-0.65857	O	4.111801	0.130405	-0.55256
H	0.253977	0.403746	-3.17007	H	0.25513	0.396842	-3.2096
H	-1.61903	1.471151	-1.8041	H	-1.51543	1.57797	-1.80633
H	-1.74997	-1.54689	-0.64796	H	-1.87277	-1.43097	-0.71712
H	-2.4417	-1.0686	0.880525	H	-2.50521	-0.94809	0.837911
H	-2.13877	1.101692	1.871117	H	-2.05909	1.175292	1.861442
H	-1.02779	2.298641	1.218724	H	-0.84301	2.290928	1.2518
H	-2.58058	2.022076	0.425441	H	-2.4068	2.171835	0.441689
H	0.95237	2.065338	-0.33869	H	1.161935	1.900199	-0.41832
H	0.974549	2.183498	-2.08067	H	1.063925	2.141231	-2.14398
H	-4.02023	0.493002	-0.29427	H	-3.98553	0.751152	-0.26833
H	-3.31266	0.049385	-1.83456	H	-3.3319	0.301623	-1.83242
H	-1.01276	3.786915	-2.00219	H	-0.77355	3.878387	-1.81191
H	-1.40051	5.956479	-1.41418	H	-0.92128	6.034195	-1.07583
H	-1.34961	6.218795	0.340412	H	-0.72658	6.175271	0.682641
H	-0.00752	6.75393	-0.66044	H	0.584593	6.662573	-0.3817
H	1.182831	3.538967	1.092889	H	1.591048	3.251011	1.096296
H	1.770841	5.152605	0.647114	H	2.316631	4.81475	0.672496
H	0.393593	4.983383	1.725727	H	1.013464	4.735916	1.849805
H	-4.03286	-2.3375	-1.5369	H	-4.20936	-2.03511	-1.58797
H	-5.85386	-3.68619	-1.25837	H	-6.11605	-3.26275	-1.32028
H	-6.63749	-3.4892	0.320367	H	-6.86301	-3.05935	0.275757
H	-7.38134	-2.79606	-1.11387	H	-7.57649	-2.2751	-1.1265
H	-5.81148	0.219387	0.628631	H	-5.77841	0.572878	0.676391

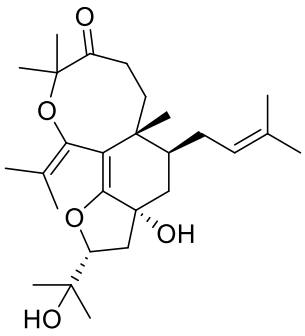
H	-7.33839	-0.41414	-0.00199	H	-7.35204	0.0703	0.043413
H	-6.62399	-1.12845	1.43565	H	-6.6801	-0.7363	1.452373
H	1.295073	-1.94305	2.358666	H	1.073992	-2.18227	2.260524
H	2.00363	-1.66145	4.756322	H	1.826976	-2.04548	4.659321
H	2.774484	-0.4457	3.719709	H	2.717714	-0.89641	3.643666
H	1.401503	0.011002	4.727999	H	1.412176	-0.31676	4.677947
H	-0.31105	-2.58247	4.158156	H	-0.5701	-2.70112	4.067955
H	-1.17031	-1.99035	2.730598	H	-1.38016	-1.98521	2.66736
H	-0.98423	-0.9435	4.152516	H	-1.06951	-1.00151	4.110954
H	2.930686	-2.80514	-1.0703	H	2.97234	-2.91699	-1.18734
H	2.577311	0.013031	-2.19175	H	2.523025	-0.11539	-2.27742
H	2.373573	-1.52581	-3.06609	H	2.249941	-1.66131	-3.12656
H	6.327566	-1.44564	-1.7174	H	6.230295	-1.19024	-1.63748
H	4.953443	-1.29827	-2.82106	H	4.882454	-1.12288	-2.78167
H	5.273864	-2.83826	-1.99072	H	5.338766	-2.6662	-2.02535
H	5.974464	-1.53868	0.779781	H	5.807324	-1.48842	0.838786
H	4.326966	-1.48186	1.450178	H	4.140357	-1.63424	1.444398
H	4.910417	-2.94162	0.623983	H	4.894156	-2.97396	0.554114
H	5.258956	0.449349	-0.35345	H	4.931853	0.495543	-0.19604
H	-1.06656	-0.63088	-2.65183	H	-1.1171	-0.56278	-2.69664
O	0.276335	-2.42254	-1.78763	O	0.058179	-2.39311	-2.00695
H	0.18457	-2.58809	-2.7369	H	0.449903	-3.06101	-1.42677
3-i				**3-j**			
C	0.269249	-0.44747	-0.66594	C	0.27082	-0.43295	-0.63649
C	-0.52217	-0.48265	0.421797	C	-0.49764	-0.48557	0.46665
C	-0.46994	0.477959	1.587961	C	-0.46	0.482204	1.625973
C	0.184133	1.840958	1.260442	C	0.152354	1.856004	1.294827
C	0.801635	1.98823	-0.15814	C	0.762779	2.015668	-0.12608
C	1.369135	0.638191	-0.71917	C	1.344567	0.678994	-0.70543
C	2.547749	0.121487	0.179979	C	2.547422	0.182493	0.173113
C	1.914798	0.853746	-2.14661	C	1.860648	0.907969	-2.14147
C	-0.13687	2.787946	-1.11135	C	-0.18567	2.812517	-1.07119
C	3.807697	1.008897	0.286321	C	3.814345	1.065642	0.214391
C	-1.50247	2.226204	-1.40837	C	-1.52806	2.218569	-1.40911
C	-2.69135	2.835462	-1.24897	C	-2.73707	2.791314	-1.26587
C	-3.9667	2.157784	-1.69646	C	-3.98079	2.095042	-1.771
C	-2.8969	4.223742	-0.68995	C	-2.99485	4.157719	-0.67533
C	4.824703	0.404809	1.218781	C	4.834555	0.512662	1.17484
C	6.083806	0.02228	0.955501	C	6.064962	0.044218	0.914511
C	6.950898	-0.57511	2.038502	C	6.94247	-0.47814	2.027456
C	6.761351	0.138899	-0.38795	C	6.697448	-0.01211	-0.45448
C	-0.01122	-1.38444	-1.80363	C	0.000489	-1.38078	-1.76814
C	-0.06916	-2.8934	-1.52911	C	-0.01569	-2.89145	-1.49584

C	-1.17697	-3.55675	-2.35581	C	-1.13637	-3.57515	-2.28835
C	1.315563	-3.48631	-1.86667	C	1.368844	-3.45491	-1.8807
O	-0.15333	-0.96626	-2.94612	O	-0.17168	-0.96667	-2.90755
O	-1.57648	-1.3382	0.577016	O	-1.50043	-1.40051	0.67156
C	-2.3653	-0.95941	1.734314	C	-2.34899	-0.98612	1.778164
C	-1.95937	0.497221	1.98542	C	-1.94542	0.46982	2.036119
C	-3.85575	-1.24955	1.450466	C	-3.82749	-1.26442	1.417898
C	-4.69097	-0.8857	2.688557	C	-4.72768	-0.83534	2.58772
C	-4.04422	-2.72505	1.085524	C	-4.02185	-2.75005	1.100877
O	-4.31765	-0.52161	0.311195	O	-4.20045	-0.57747	0.22472
H	-0.54633	2.642955	1.413641	H	-0.60276	2.63453	1.444257
H	1.671674	2.646365	-0.04463	H	1.626309	2.681788	-0.01109
H	2.171716	-0.08148	1.186986	H	2.198868	0.01855	1.197138
H	2.85497	-0.85317	-0.22024	H	2.84084	-0.80567	-0.20445
H	2.482112	-0.02092	-2.47939	H	2.437694	0.044767	-2.48763
H	1.123805	1.012972	-2.87676	H	1.053924	1.055877	-2.85674
H	2.590956	1.714514	-2.16398	H	2.520719	1.780655	-2.16745
H	-0.22962	3.789671	-0.67849	H	-0.31562	3.79869	-0.61345
H	0.39068	2.931339	-2.06248	H	0.350764	2.99774	-2.01035
H	4.239546	1.181102	-0.70267	H	4.237908	1.170999	-0.78753
H	3.529222	1.999402	0.6754	H	3.547432	2.080012	0.543549
H	-1.50879	1.238757	-1.86475	H	-1.49572	1.243551	-1.89118
H	-3.80935	1.107069	-1.94905	H	-3.7842	1.062157	-2.06684
H	-4.74312	2.211739	-0.91978	H	-4.77774	2.090594	-1.01344
H	-4.39197	2.664104	-2.57386	H	-4.40102	2.626106	-2.63605
H	-1.97451	4.7079	-0.36481	H	-2.09569	4.652319	-0.3044
H	-3.36546	4.873232	-1.44141	H	-3.45286	4.818116	-1.42378
H	-3.58531	4.202623	0.165533	H	-3.71109	4.095635	0.154834
H	4.464574	0.254643	2.238241	H	4.503258	0.486655	2.214427
H	6.424993	-0.63787	2.995104	H	6.446402	-0.41976	3.00017
H	7.283549	-1.58585	1.766518	H	7.224824	-1.52484	1.851329
H	7.862025	0.01943	2.18941	H	7.881403	0.088301	2.09017
H	6.115728	0.549497	-1.16596	H	6.04318	0.349423	-1.2495
H	7.651288	0.778432	-0.31831	H	7.619371	0.583873	-0.4808
H	7.113976	-0.84356	-0.72819	H	6.989183	-1.0412	-0.70218
H	-0.26117	-3.04924	-0.46453	H	-0.17136	-3.05475	-0.42631
H	-1.18025	-4.63992	-2.19542	H	-1.11405	-4.65834	-2.12975
H	-2.16122	-3.1664	-2.07913	H	-2.11853	-3.20313	-1.98102
H	-1.02697	-3.36059	-3.42068	H	-1.02268	-3.37501	-3.35691
H	1.323112	-4.56347	-1.67062	H	1.405402	-4.53228	-1.68914
H	2.110498	-3.03273	-1.26506	H	2.174928	-2.98625	-1.30583
H	1.552763	-3.32832	-2.92373	H	1.566407	-3.28863	-2.94444
H	-2.03962	-1.5812	2.577701	H	-2.09305	-1.60994	2.647404

H	-2.49986	1.17261	1.313751	H	-2.49909	1.144874	1.374734
H	-2.11175	0.81884	3.019689	H	-2.07881	0.782434	3.073444
H	-5.74251	-1.11754	2.499669	H	-5.76987	-1.05936	2.345251
H	-4.61678	0.182932	2.922087	H	-4.64856	0.240547	2.780783
H	-4.36851	-1.44416	3.573423	H	-4.46926	-1.36077	3.513184
H	-5.10202	-2.92231	0.89249	H	-5.06602	-2.93327	0.834435
H	-3.4751	-2.96513	0.185929	H	-3.39166	-3.04111	0.258761
H	-3.70773	-3.37577	1.898455	H	-3.76669	-3.37247	1.964253
H	-4.3749	0.415052	0.539935	H	-4.20957	0.373005	0.397026
H	0.971913	1.993914	2.005613	H	0.92358	2.026041	2.050425
O	0.270083	-0.21946	2.618591	O	0.338291	-0.06751	2.704185
H	0.284605	0.356921	3.396178	H	0.212717	-1.02631	2.722902
3-k							
C	0.13016	-0.17895	0.676075				
C	0.961872	-0.85098	-0.1416				
C	0.772959	-1.05994	-1.62902				
C	-0.21065	-0.0619	-2.28284				
C	-0.73324	1.04601	-1.33877				
C	-1.14609	0.43539	0.047904				
C	-2.192	-0.72009	-0.11447				
C	-1.77409	1.526602	0.937694				
C	0.274705	2.230923	-1.21385				
C	-3.52143	-0.37017	-0.81938				
C	-0.36149	3.597521	-1.2159				
C	-0.14287	4.6244	-0.37975				
C	-0.83705	5.948706	-0.59305				
C	0.785836	4.587474	0.810064				
C	-4.41718	-1.57548	-0.93445				
C	-5.62972	-1.77494	-0.3949				
C	-6.37046	-3.07189	-0.61971				
C	-6.37059	-0.77627	0.460246				
C	0.557404	0.091236	2.092171				
C	0.877502	-1.10042	3.001524				
C	1.815812	-0.69297	4.141136				
C	-0.45118	-1.67491	3.539632				
O	0.616282	1.23564	2.521863				
O	2.184108	-1.33899	0.233415				
C	2.969491	-1.693	-0.93404				
C	2.241022	-1.0021	-2.09264				
C	4.442685	-1.28668	-0.69759				
C	5.30435	-1.78597	-1.86734				
C	4.943106	-1.86218	0.63034				
O	4.561463	0.133636	-0.56577				

H	0.249455	0.396881	-3.16631				
H	-1.6406	1.446977	-1.80804				
H	-1.72924	-1.56644	-0.631				
H	-2.42991	-1.08539	0.892275				
H	-2.15355	1.094883	1.869643				
H	-1.06518	2.305358	1.204724				
H	-2.61425	1.994399	0.416779				
H	0.91329	2.092374	-0.33801				
H	0.949253	2.188921	-2.08327				
H	-4.02811	0.444102	-0.29566				
H	-3.31047	0.003481	-1.83187				
H	-1.05817	3.767288	-2.03974				
H	-1.48213	5.937411	-1.47621				
H	-1.45235	6.215991	0.276339				
H	-0.108	6.76106	-0.71584				
H	1.112553	3.582197	1.080535				
H	1.67833	5.200605	0.624168				
H	0.293332	5.01948	1.69016				
H	-3.9982	-2.39155	-1.52625				
H	-5.80049	-3.76491	-1.24464				
H	-6.58806	-3.57347	0.332811				
H	-7.3402	-2.89551	-1.10432				
H	-5.81482	0.147579	0.62875				
H	-7.33233	-0.51124	0.001314				
H	-6.60649	-1.20924	1.441205				
H	1.353303	-1.87177	2.38842				
H	2.026483	-1.5504	4.788673				
H	2.766289	-0.31362	3.75387				
H	1.367746	0.099968	4.745572				
H	-0.25512	-2.5476	4.170981				
H	-1.11487	-1.99179	2.729296				
H	-0.9784	-0.93073	4.146494				
H	2.914605	-2.78235	-1.05182				
H	2.55998	0.043049	-2.17165				
H	2.391543	-1.49489	-3.0575				
H	6.34744	-1.50372	-1.69972				
H	4.982705	-1.3478	-2.8202				
H	5.255976	-2.87458	-1.96955				
H	5.995176	-1.60056	0.771083				
H	4.365676	-1.44611	1.457172				
H	4.845225	-2.95208	0.648017				
H	4.58168	0.522255	-1.44979				
H	-1.06022	-0.6491	-2.6448				

O	0.302041	-2.42037	-1.76737				
H	0.186675	-2.58536	-2.71418				



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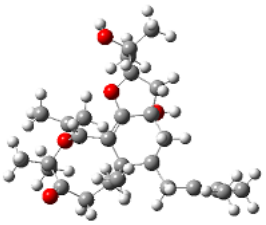

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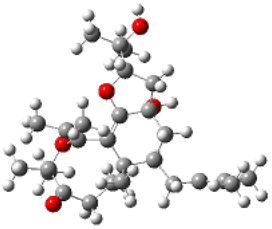

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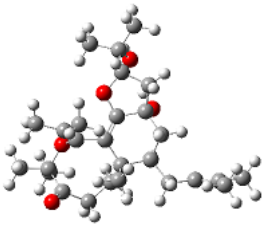

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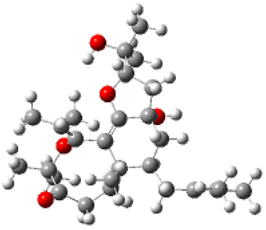

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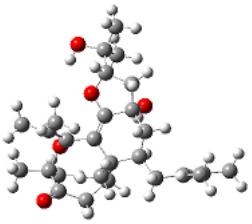

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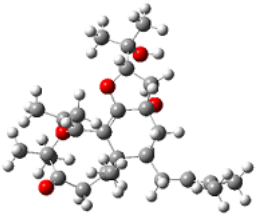

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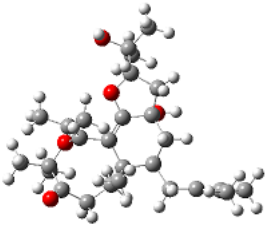

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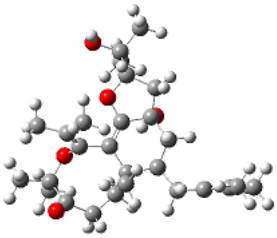


i

j

Figure S6. Optimized geometries of predominant conformers for compound **5** at the B3LYP/6-31G(d,p) level in the gas phase.

Table S8. Important thermodynamic parameters (a.u.) and Boltzmann distributions of the optimized compound **5** at B3LYP/6-31G(d,p) level in the gas phase

Conformations	E+ZPE	G	%
5-a	-1429.622563	-1429.687595	0
5-b	-1429.625178	-1429.690055	0
5-c	-1429.626598	-1429.691792	0
5-d	-1429.634380	-1429.699077	7.5
5-e	-1429.628324	-1429.693111	0
5-f	-1429.630290	-1429.695098	0.1
5-g	-1429.633130	-1429.697011	0.9
5-h	-1429.622103	-1429.687289	0
5-i	-1429.624657	-1429.689649	0
5-j	-1429.636996	-1429.701441	91.5

E+ZPE, G: total energy with zero point energy (ZPE) and Gibbs free energy in the gas phase at B3LYP/6-31G(d,p) level., %: Boltzmann distributions, using the relative Gibbs free energies as weighting factors

Table S9. Optimized Z-matrixes of compound **5** in the gas phase (Å) at B3LYP/6-31G(d,p) level

5-a				**5-b**			
C	-0.54294	-0.24664	0.22557	C	-0.53928	-0.24684	0.21258
C	-0.11818	1.024323	0.094489	C	-0.129	1.03417	0.104622
C	1.309735	1.47355	-0.08687	C	1.287369	1.49683	-0.11764
C	2.245446	0.417387	0.48681	C	2.2611	0.462365	0.427423
C	1.912301	-0.9369	-0.15497	C	1.9318	-0.91157	-0.17215
C	0.451469	-1.42925	0.168053	C	0.4775	-1.41409	0.172409
C	0.412464	-2.14643	1.539772	C	0.45732	-2.09128	1.56507
C	0.063091	-2.39907	-0.99834	C	0.098677	-2.42634	-0.96083
C	-0.91733	-3.54832	-0.69972	C	-0.85725	-3.58462	-0.62202
C	-2.31494	-3.23115	-0.19068	C	-2.26445	-3.27681	-0.13447
C	-3.19836	-2.21233	-0.95527	C	-3.15525	-2.29409	-0.93696
O	-2.66707	-0.86818	-0.77223	O	-2.63249	-0.94023	-0.80162
C	-2.01874	-0.45353	0.406585	C	-2.01326	-0.4773	0.376593
O	-2.7538	-3.81318	0.785152	O	-2.70349	-3.83864	0.852667
C	-3.14134	-2.43312	-2.47393	C	-3.09229	-2.5696	-2.44659
C	-4.64837	-2.33976	-0.48225	C	-4.60533	-2.42019	-0.46449
C	-2.70406	-0.00324	1.47642	C	-2.72412	-0.00713	1.421369

C	-2.01374	0.488942	2.723635	C	-2.06332	0.517396	2.67142
C	-4.20037	0.167165	1.506447	C	-4.22142	0.156951	1.417226
O	-0.93953	2.116652	0.179338	O	-0.95746	2.118476	0.198415
C	-0.18807	3.302788	0.526434	C	-0.20281	3.313076	0.526761
C	1.294616	2.856085	0.591799	C	1.286365	2.883682	0.536342
C	-0.57297	4.468354	-0.41321	C	-0.62932	4.478517	-0.39249
C	-0.54021	4.083679	-1.89411	C	-0.60895	4.112748	-1.8789
C	0.302576	5.699821	-0.12488	C	0.228475	5.72181	-0.10291
O	-1.92199	4.770024	-0.01463	O	-1.97834	4.746781	0.028812
O	1.533314	1.622881	-1.50652	O	1.528344	1.721219	-1.52797
C	3.013852	-1.97774	0.172261	C	3.045538	-1.93324	0.17699
C	4.315973	-1.6751	-0.52231	C	4.347301	-1.63041	-0.5178
C	5.532312	-1.47595	0.010345	C	5.560862	-1.42442	0.017706
C	6.726128	-1.20294	-0.87411	C	6.755655	-1.15005	-0.8646
C	5.848314	-1.51488	1.485521	C	5.872174	-1.45097	1.49403
H	3.292358	0.677727	0.283045	H	3.286856	0.743598	0.168864
H	2.134704	0.375907	1.577464	H	2.191702	0.430378	1.522319
H	1.938835	-0.7621	-1.23793	H	1.962685	-0.78026	-1.26387
H	0.837029	-1.50852	2.321863	H	0.876071	-1.42305	2.32425
H	-0.61199	-2.38459	1.833306	H	-0.56252	-2.33504	1.870107
H	0.978797	-3.08255	1.53013	H	1.037136	-3.01882	1.580006
H	-0.29957	-1.78741	-1.82889	H	-0.28543	-1.8512	-1.80828
H	0.974697	-2.88838	-1.35949	H	1.017343	-2.9076	-1.31388
H	-1.0509	-4.11442	-1.63274	H	-0.97319	-4.18996	-1.53252
H	-0.49	-4.24554	0.025193	H	-0.41844	-4.24343	0.131194
H	-3.75845	-1.67408	-2.9628	H	-3.71412	-1.83398	-2.96449
H	-3.53412	-3.41951	-2.74007	H	-3.47705	-3.56791	-2.677
H	-2.12657	-2.33832	-2.86275	H	-2.07737	-2.48331	-2.8373
H	-5.04928	-3.31105	-0.78804	H	-4.99351	-3.40617	-0.73755
H	-4.72683	-2.28404	0.601088	H	-4.68836	-2.32836	0.61596
H	-5.25626	-1.55544	-0.94049	H	-5.22083	-1.65982	-0.95178
H	-0.94591	0.270656	2.732426	H	-0.99631	0.298619	2.712335
H	-2.14373	1.574321	2.824547	H	-2.19477	1.6047	2.740691
H	-2.4657	0.030946	3.612923	H	-2.53766	0.081168	3.559883
H	-4.63821	0.103618	0.511967	H	-4.64046	0.062934	0.417155
H	-4.6926	-0.5674	2.156576	H	-4.72428	-0.55849	2.080153
H	-4.43463	1.155906	1.920364	H	-4.46454	1.157178	1.796851
H	-0.53311	3.61087	1.520354	H	-0.51941	3.609172	1.533519
H	1.979022	3.54526	0.092752	H	1.94233	3.556708	-0.01701
H	1.611306	2.773988	1.635977	H	1.651937	2.823483	1.56529
H	-0.81641	4.948766	-2.50999	H	-0.91293	4.978792	-2.47989
H	-1.24912	3.274683	-2.07925	H	-1.30941	3.295514	-2.06368
H	0.448253	3.739572	-2.20484	H	0.384473	3.797101	-2.20469

H	-0.1116	6.568003	-0.64839	H	-0.20412	6.587578	-0.61586
H	0.309112	5.929895	0.945386	H	0.24112	5.943163	0.969069
H	1.33516	5.574225	-0.46436	H	1.25903	5.613985	-0.45314
H	-2.30747	5.331571	-0.69997	H	-2.36773	5.350354	-0.61769
H	2.460216	1.880367	-1.61699	H	1.00996	1.071744	-2.02076
H	2.681663	-2.97358	-0.15199	H	2.725737	-2.94039	-0.12471
H	3.1502	-2.04501	1.255505	H	3.177931	-1.97268	1.261877
H	4.238283	-1.62372	-1.61029	H	4.27247	-1.58366	-1.60594
H	6.455113	-1.18398	-1.93327	H	6.487678	-1.1397	-1.92451
H	7.193458	-0.24111	-0.6238	H	7.213542	-0.18251	-0.61974
H	7.502524	-1.96725	-0.7364	H	7.537158	-1.90761	-0.71831
H	4.972641	-1.68919	2.112709	H	4.996198	-1.62758	2.12025
H	6.57785	-2.30621	1.702481	H	6.607532	-2.23466	1.718981
H	6.311742	-0.57289	1.806798	H	6.326419	-0.5026	1.809243
5-c				**5-d**			
C	-0.53638	-0.25327	0.222046	C	-0.55533	-0.23282	0.258696
C	-0.12618	1.019538	0.076105	C	-0.11128	1.033193	0.167906
C	1.296445	1.488459	-0.10396	C	1.319552	1.483797	-0.02566
C	2.241279	0.445532	0.481631	C	2.249923	0.404752	0.504387
C	1.926298	-0.91662	-0.15274	C	1.891779	-0.92873	-0.16969
C	0.470565	-1.42561	0.169745	C	0.429289	-1.42102	0.153536
C	0.437344	-2.1442	1.540557	C	0.394391	-2.18648	1.498823
C	0.093623	-2.39993	-0.99583	C	0.021467	-2.34771	-1.03971
C	-0.89285	-3.54675	-0.70554	C	-0.98653	-3.48309	-0.77893
C	-2.29622	-3.23119	-0.2112	C	-2.37992	-3.15575	-0.26617
C	-3.17567	-2.21484	-0.98409	C	-3.24205	-2.09665	-1.00097
O	-2.66969	-0.86515	-0.76427	O	-2.70736	-0.76537	-0.74107
C	-2.00887	-0.47495	0.414827	C	-2.03117	-0.42852	0.447172
O	-2.74348	-3.81232	0.761341	O	-2.83527	-3.75873	0.689274
C	-3.0831	-2.41071	-2.50424	C	-3.16125	-2.24607	-2.52714
C	-4.63459	-2.36315	-0.54595	C	-4.70175	-2.22963	-0.55989
C	-2.68337	-0.06548	1.507553	C	-2.69539	-0.04136	1.554673
C	-1.9812	0.407981	2.755572	C	-1.98095	0.370894	2.817363
C	-4.18336	0.058149	1.572146	C	-4.192	0.116069	1.626509
O	-0.96445	2.104093	0.145613	O	-0.92895	2.133514	0.296241
C	-0.22716	3.287148	0.527689	C	-0.15744	3.316478	0.600175
C	1.262854	2.875035	0.568331	C	1.310239	2.838371	0.716168
C	-0.61788	4.461884	-0.3973	C	-0.45482	4.418734	-0.44057
C	-2.10227	4.794708	-0.18945	C	0.149834	5.754818	0.013853
C	-0.32903	4.199767	-1.87775	C	-1.96575	4.547995	-0.66506
O	0.200196	5.53858	0.094214	O	0.181541	4.00899	-1.66953
O	1.518964	1.621315	-1.52418	O	1.639995	1.659559	-1.40631
C	3.03963	-1.94264	0.181373	C	2.982667	-1.99098	0.120839

C	4.338096	-1.62845	-0.51495	C	4.290702	-1.67526	-0.55626
C	5.551736	-1.41099	0.016517	C	5.514224	-1.56177	-0.01595
C	6.741808	-1.12736	-0.86964	C	6.713504	-1.25267	-0.88079
C	5.868077	-1.43649	1.491877	C	5.833261	-1.73186	1.449333
H	3.285367	0.716526	0.27921	H	3.287331	0.667639	0.274971
H	2.127006	0.410055	1.572257	H	2.155286	0.332262	1.59521
H	1.952998	-0.74636	-1.23633	H	1.91247	-0.72361	-1.24694
H	0.855487	-1.50352	2.323772	H	0.833808	-1.58182	2.298822
H	-0.58466	-2.39431	1.833117	H	-0.62997	-2.42557	1.793347
H	1.01365	-3.07419	1.529081	H	0.951215	-3.12721	1.450117
H	-0.25496	-1.79084	-1.83435	H	-0.32081	-1.70418	-1.85477
H	1.0087	-2.89302	-1.34268	H	0.922748	-2.84841	-1.41063
H	-1.01698	-4.11391	-1.6393	H	-1.12831	-4.01811	-1.72915
H	-0.47333	-4.24329	0.024552	H	-0.57647	-4.21046	-0.07404
H	-3.70038	-1.65278	-2.99467	H	-3.76509	-1.46039	-2.99006
H	-3.45658	-3.3979	-2.79421	H	-3.55675	-3.21554	-2.84627
H	-2.06217	-2.2962	-2.87033	H	-2.13979	-2.14178	-2.89467
H	-5.02533	-3.32639	-0.88851	H	-5.11352	-3.1733	-0.93115
H	-4.73574	-2.33933	0.536562	H	-4.7975	-2.23916	0.523337
H	-5.23562	-1.56784	-0.99451	H	-5.28905	-1.40843	-0.97921
H	-0.90447	0.2438	2.726061	H	-0.90899	0.179287	2.779941
H	-2.15974	1.48039	2.909675	H	-2.13103	1.441984	3.008283
H	-2.38409	-0.10759	3.637005	H	-2.39711	-0.16359	3.681262
H	-4.63885	0.021785	0.584021	H	-4.64961	0.124595	0.638609
H	-4.63854	-0.72046	2.197588	H	-4.66582	-0.67199	2.225755
H	-4.44349	1.018634	2.034651	H	-4.42898	1.06617	2.122233
H	-0.55896	3.566236	1.535113	H	-0.52362	3.692147	1.56361
H	1.902623	3.599908	0.061034	H	2.031092	3.525343	0.270027
H	1.600727	2.806824	1.606545	H	1.569327	2.700638	1.770222
H	-2.39838	5.640802	-0.82084	H	-0.04799	6.528893	-0.73513
H	-2.28814	5.065715	0.854384	H	1.23301	5.677283	0.137297
H	-2.73353	3.940408	-0.44772	H	-0.28658	6.088909	0.960723
H	-0.61741	5.076991	-2.4696	H	-2.17168	5.326475	-1.41005
H	0.728271	3.995751	-2.04972	H	-2.38076	3.599596	-1.00893
H	-0.89816	3.340621	-2.23974	H	-2.47787	4.835149	0.258475
H	-0.02821	6.327915	-0.41446	H	-0.20946	4.50241	-2.4014
H	2.420279	1.957224	-1.63435	H	1.087702	2.389229	-1.7396
H	2.719996	-2.94464	-0.13682	H	2.641837	-2.97185	-0.24017
H	3.176733	-2.00158	1.265063	H	3.115495	-2.0997	1.201348
H	4.259585	-1.58365	-1.60311	H	4.210184	-1.52728	-1.63468
H	6.47037	-1.11798	-1.92882	H	6.439853	-1.13871	-1.93313
H	7.196039	-0.15786	-0.62496	H	7.20716	-0.32715	-0.55555
H	7.528392	-1.88042	-0.72761	H	7.468651	-2.04712	-0.80936

H	4.994972	-1.62016	2.119978	H	4.952389	-1.91619	2.066495
H	6.609519	-2.21533	1.71367	H	6.527587	-2.56939	1.599289
H	6.316881	-0.48555	1.807425	H	6.338755	-0.83931	1.840739
5-e				**5-f**			
C	-0.53073	-0.2539	0.224582	C	-0.52743	-0.25091	0.211674
C	-0.12274	1.018696	0.076161	C	-0.12859	1.030622	0.087433
C	1.297054	1.491058	-0.1075	C	1.283394	1.510217	-0.13416
C	2.247709	0.452012	0.474936	C	2.262721	0.486079	0.422912
C	1.932863	-0.91236	-0.15498	C	1.948199	-0.89505	-0.16898
C	0.478909	-1.42394	0.17272	C	0.498075	-1.41041	0.175694
C	0.449685	-2.13954	1.545058	C	0.482634	-2.08815	1.567823
C	0.101712	-2.4011	-0.99034	C	0.127837	-2.42619	-0.95644
C	-0.88372	-3.54801	-0.69705	C	-0.83543	-3.58094	-0.62484
C	-2.28731	-3.23138	-0.20398	C	-2.24659	-3.27201	-0.14887
C	-3.16733	-2.21876	-0.98113	C	-3.1332	-2.29141	-0.95893
O	-2.66282	-0.86742	-0.76168	O	-2.63027	-0.93172	-0.79055
C	-2.00355	-0.47646	0.417368	C	-1.99903	-0.49156	0.388235
O	-2.73357	-3.80752	0.771862	O	-2.69206	-3.83004	0.837384
C	-3.07189	-2.41645	-2.50066	C	-3.03975	-2.54397	-2.47056
C	-4.62655	-2.3674	-0.54485	C	-4.59084	-2.43468	-0.51618
C	-2.67795	-0.06568	1.509831	C	-2.69752	-0.05443	1.455482
C	-1.97627	0.410106	2.757307	C	-2.02282	0.457049	2.703772
C	-4.17821	0.054596	1.575409	C	-4.1987	0.068727	1.487358
O	-0.96096	2.103495	0.143	O	-0.96984	2.109331	0.175119
C	-0.22526	3.297433	0.523824	C	-0.22316	3.311902	0.521893
C	1.263303	2.879347	0.567921	C	1.268339	2.902239	0.515249
C	-0.66594	4.450387	-0.40687	C	-0.70643	4.458089	-0.39427
C	-0.27976	4.238556	-1.87607	C	-0.4306	4.214679	-1.88278
C	-0.13181	5.782737	0.122665	C	-0.10961	5.786192	0.075218
O	-2.09246	4.540187	-0.29756	O	-2.12086	4.580807	-0.18576
O	1.508698	1.629114	-1.52676	O	1.527243	1.733881	-1.54079
C	3.049469	-1.93467	0.179568	C	3.072211	-1.90333	0.186772
C	4.34699	-1.61721	-0.51712	C	4.370094	-1.59227	-0.51174
C	5.559723	-1.39527	0.014702	C	5.579662	-1.35873	0.021503
C	6.749554	-1.11018	-0.87128	C	6.77082	-1.07992	-0.86426
C	5.875448	-1.41785	1.490263	C	5.889654	-1.35621	1.498304
H	3.290181	0.724702	0.266522	H	3.28711	0.774295	0.167135
H	2.138975	0.418073	1.566182	H	2.188341	0.459704	1.517609
H	1.956296	-0.74524	-1.23919	H	1.979833	-0.77159	-1.26181
H	0.86731	-1.49635	2.326519	H	0.896377	-1.41796	2.327979
H	-0.57128	-2.39173	1.839447	H	-0.53507	-2.34141	1.872343
H	1.028271	-3.06805	1.534319	H	1.070162	-3.01077	1.580907
H	-0.24754	-1.79429	-1.83023	H	-0.24281	-1.85297	-1.81133

H	1.017164	-2.89401	-1.33626	H	1.049063	-2.91193	-1.29645
H	-1.00688	-4.11771	-1.62932	H	-0.94461	-4.18631	-1.53614
H	-0.4638	-4.24205	0.035149	H	-0.40431	-4.24018	0.132392
H	-3.68975	-1.66053	-2.99342	H	-3.65995	-1.80778	-2.98961
H	-3.44339	-3.40465	-2.78957	H	-3.41036	-3.54254	-2.72201
H	-2.05068	-2.30109	-2.86567	H	-2.01936	-2.4423	-2.84232
H	-5.01605	-3.33121	-0.88718	H	-4.97152	-3.41398	-0.82218
H	-4.72918	-2.34281	0.537479	H	-4.69341	-2.37149	0.564465
H	-5.22763	-1.57312	-0.99509	H	-5.19951	-1.66343	-0.99515
H	-0.89911	0.248402	2.72788	H	-0.94853	0.274809	2.712822
H	-2.15824	1.481874	2.911299	H	-2.18845	1.536893	2.810588
H	-2.37764	-0.10658	3.638677	H	-2.45952	-0.01927	3.590841
H	-4.63502	0.01539	0.587993	H	-4.63724	-0.00299	0.493612
H	-4.6302	-0.7248	2.20205	H	-4.66513	-0.68644	2.132516
H	-4.44049	1.014641	2.037369	H	-4.46575	1.04491	1.911294
H	-0.57785	3.566118	1.526655	H	-0.54244	3.582896	1.534977
H	1.918643	3.586004	0.051962	H	1.902434	3.586345	-0.0517
H	1.603136	2.809952	1.605534	H	1.650193	2.853639	1.538749
H	-0.73282	5.034346	-2.4738	H	-0.86049	5.038049	-2.46002
H	-0.64133	3.273713	-2.23883	H	-0.89964	3.282383	-2.20921
H	0.80258	4.260889	-2.0285	H	0.636482	4.140327	-2.10318
H	-0.54366	6.600862	-0.47435	H	-0.56171	6.604757	-0.49113
H	-0.43868	5.936597	1.161647	H	-0.32219	5.952948	1.135695
H	0.959811	5.831263	0.065143	H	0.972925	5.817803	-0.078
H	-2.43424	3.65564	-0.49681	H	-2.49667	3.706704	-0.36742
H	2.411871	1.955757	-1.6484	H	1.072294	1.039468	-2.03474
H	2.732505	-2.93777	-0.13755	H	2.762253	-2.91574	-0.10731
H	3.186862	-1.99214	1.263276	H	3.205761	-1.93325	1.271837
H	4.268878	-1.57494	-1.6054	H	4.295697	-1.56428	-1.60053
H	6.478734	-1.10281	-1.93061	H	6.503786	-1.09076	-1.92438
H	7.201721	-0.1395	-0.6275	H	7.21315	-0.10155	-0.63456
H	7.537523	-1.86142	-0.72776	H	7.56381	-1.82271	-0.70505
H	5.002536	-1.60192	2.118534	H	5.016352	-1.5384	2.126659
H	6.617937	-2.19523	1.713475	H	6.638726	-2.12281	1.736206
H	6.322954	-0.46584	1.804395	H	6.326414	-0.39489	1.798492
5-g				**5-h**			
C	-0.57731	-0.21616	0.256515	C	-0.54092	-0.25081	0.219165
C	-0.09028	1.033598	0.162911	C	-0.11903	1.018033	0.068158
C	1.355859	1.438265	0.009256	C	1.308213	1.470081	-0.1096
C	2.2518	0.325482	0.524247	C	2.243683	0.42127	0.478978
C	1.847352	-0.99226	-0.15421	C	1.915251	-0.93954	-0.15139
C	0.369986	-1.4357	0.170209	C	0.455064	-1.43278	0.174022
C	0.306934	-2.18505	1.523047	C	0.415221	-2.14235	1.549318

C	-0.06325	-2.36023	-1.01635	C	0.069586	-2.41035	-0.98651
C	-1.09891	-3.46749	-0.74572	C	-0.91995	-3.55198	-0.68708
C	-2.48444	-3.09469	-0.24342	C	-2.31991	-3.22506	-0.19051
C	-3.312	-2.02161	-0.99718	C	-3.19476	-2.20937	-0.96889
O	-2.72995	-0.70467	-0.76446	O	-2.67108	-0.86329	-0.77073
C	-2.06171	-0.36165	0.425231	C	-2.01624	-0.45853	0.405683
O	-2.9598	-3.67014	0.719167	O	-2.7664	-3.79492	0.789084
C	-3.23849	-2.2024	-2.52025	C	-3.11466	-2.42427	-2.48715
C	-4.77462	-2.09915	-0.55273	C	-4.65186	-2.33873	-0.51896
C	-2.72673	0.072107	1.514988	C	-2.69421	-0.02439	1.486719
C	-2.01588	0.485089	2.77967	C	-1.99537	0.45851	2.732981
C	-4.21683	0.288547	1.560722	C	-4.19234	0.124131	1.535615
O	-0.86946	2.166311	0.241403	O	-0.94463	2.110679	0.123192
C	-0.06875	3.319141	0.595227	C	-0.20373	3.29015	0.501344
C	1.366298	2.773569	0.785743	C	1.285432	2.858437	0.561609
C	-0.25521	4.440786	-0.45971	C	-0.59162	4.480822	-0.40982
C	0.321326	5.759256	0.072239	C	-0.3657	4.200474	-1.89396
C	-1.73472	4.597483	-0.81641	C	0.14943	5.748049	0.048873
O	0.40115	4.096041	-1.70088	O	-2.00395	4.698187	-0.28984
O	1.698964	1.646885	-1.36592	O	1.53435	1.607712	-1.52744
C	2.903379	-2.09033	0.132681	C	3.019554	-1.97441	0.185237
C	4.215856	-1.82089	-0.55586	C	4.320293	-1.67387	-0.51293
C	5.446462	-1.74091	-0.0257	C	5.536404	-1.46605	0.016861
C	6.64768	-1.47733	-0.90278	C	6.728419	-1.19686	-0.87118
C	5.771674	-1.90922	1.438378	C	5.853832	-1.49095	1.492027
H	3.296652	0.555224	0.29245	H	3.290724	0.681494	0.276395
H	2.160967	0.249589	1.614935	H	2.128811	0.389519	1.569635
H	1.873298	-0.78466	-1.23118	H	1.942543	-0.77331	-1.23566
H	0.759796	-1.58509	2.319029	H	0.838181	-1.50031	2.328932
H	-0.72539	-2.39113	1.814652	H	-0.60916	-2.38152	1.842507
H	0.836534	-3.14176	1.486894	H	0.983337	-3.07737	1.544401
H	-0.39165	-1.71483	-1.83545	H	-0.28125	-1.80343	-1.82554
H	0.824624	-2.88538	-1.38524	H	0.981337	-2.90802	-1.33558
H	-1.25032	-4.01056	-1.68972	H	-1.04914	-4.12358	-1.61733
H	-0.71031	-4.1958	-0.02977	H	-0.50147	-4.2462	0.045837
H	-3.8184	-1.40738	-2.99743	H	-3.72684	-1.66527	-2.98211
H	-3.66481	-3.16509	-2.81947	H	-3.50076	-3.4108	-2.76243
H	-2.21518	-2.13721	-2.89179	H	-2.09504	-2.32504	-2.86143
H	-5.2147	-3.03773	-0.90369	H	-5.0515	-3.3045	-0.84358
H	-4.87017	-2.08288	0.530452	H	-4.74615	-2.29697	0.563664
H	-5.33716	-1.27002	-0.98976	H	-5.2499	-1.54639	-0.97642
H	-0.95443	0.238766	2.770328	H	-0.92168	0.272818	2.717794
H	-2.11565	1.567439	2.937516	H	-2.15512	1.53694	2.865802

H	-2.47487	-0.00289	3.649236	H	-2.4169	-0.03273	3.61959
H	-4.66061	0.286913	0.566646	H	-4.63881	0.077102	0.544033
H	-4.72916	-0.46216	2.175846	H	-4.66662	-0.63355	2.172449
H	-4.42187	1.261422	2.025531	H	-4.43973	1.098492	1.975526
H	-0.47245	3.698868	1.542234	H	-0.54203	3.559449	1.514347
H	2.150863	3.436768	0.412823	H	1.954133	3.552889	0.047848
H	1.555866	2.59625	1.848667	H	1.615352	2.78939	1.602526
H	0.21686	6.539595	-0.6868	H	-0.70922	5.05934	-2.47723
H	1.38454	5.666728	0.324114	H	-0.93622	3.320332	-2.19371
H	-0.20522	6.086525	0.973624	H	0.686861	4.014913	-2.11432
H	-1.85622	5.411785	-1.53565	H	-0.24209	6.606457	-0.50302
H	-2.11448	3.674024	-1.25517	H	-0.00918	5.934015	1.118909
H	-2.32756	4.823512	0.075047	H	1.228292	5.692288	-0.12497
H	1.33788	4.324932	-1.62216	H	-2.20829	4.835967	0.645608
H	1.034095	2.252988	-1.73956	H	2.455932	1.882451	-1.64001
H	2.527098	-3.06028	-0.22192	H	2.690399	-2.97414	-0.12998
H	3.04004	-2.19936	1.212744	H	3.156614	-2.03154	1.269033
H	4.13178	-1.68008	-1.63497	H	4.241418	-1.63223	-1.60121
H	6.368833	-1.36121	-1.95351	H	6.456238	-1.18812	-1.93016
H	7.175174	-0.56693	-0.5881	H	7.192721	-0.23126	-0.6299
H	7.376431	-2.2961	-0.83258	H	7.50752	-1.95729	-0.72752
H	4.890878	-2.0652	2.063449	H	4.979312	-1.66288	2.121518
H	6.44396	-2.76434	1.588958	H	6.586338	-2.27778	1.715189
H	6.304467	-1.02824	1.81967	H	6.314252	-0.54456	1.804598
5-i				**5-j**			
C	-0.53727	-0.24964	0.213007	C	-0.54608	-0.22392	0.305296
C	-0.13245	1.031767	0.096762	C	-0.10669	1.04498	0.260784
C	1.282217	1.499108	-0.12517	C	1.321728	1.50916	0.063516
C	2.257694	0.471102	0.42969	C	2.256618	0.415957	0.556195
C	1.936091	-0.90493	-0.169	C	1.901263	-0.89515	-0.16259
C	0.483552	-1.41349	0.174282	C	0.440848	-1.40445	0.144819
C	0.464233	-2.09259	1.565849	C	0.411625	-2.22943	1.454615
C	0.108756	-2.4257	-0.96007	C	0.030272	-2.28041	-1.08453
C	-0.84946	-3.58373	-0.62598	C	-0.9932	-3.41306	-0.87515
C	-2.25862	-3.27726	-0.14303	C	-2.38822	-3.09485	-0.35991
C	-3.14796	-2.29483	-0.9475	C	-3.2363	-1.99649	-1.05319
O	-2.63295	-0.9388	-0.79666	O	-2.70822	-0.68202	-0.70105
C	-2.01018	-0.48544	0.381399	C	-2.02002	-0.43008	0.50118
O	-2.69976	-3.83848	0.843521	O	-2.85603	-3.73398	0.565277
C	-3.07227	-2.55836	-2.45843	C	-3.12725	-2.05693	-2.58343
C	-4.60138	-2.42835	-0.48773	C	-4.70449	-2.14743	-0.64819
C	-2.71617	-0.03123	1.436368	C	-2.66997	-0.12231	1.640913
C	-2.04883	0.485801	2.686145	C	-1.93892	0.215241	2.916169

C	-4.21526	0.115001	1.447556	C	-4.16724	0.00634	1.746444
O	-0.96708	2.114141	0.180994	O	-0.93433	2.136339	0.466327
C	-0.2197	3.309081	0.51271	C	-0.14746	3.339006	0.674183
C	1.274055	2.890117	0.522781	C	1.302787	2.837734	0.841134
C	-0.65543	4.482372	-0.3999	C	-0.48444	4.310618	-0.49434
C	-0.52829	4.164124	-1.8882	C	0.500055	5.473218	-0.59361
C	0.12803	5.750565	-0.02305	C	-1.92295	4.821536	-0.32504
O	-2.0556	4.717895	-0.19269	O	-0.39381	3.598313	-1.74613
O	1.530607	1.709689	-1.53557	O	1.645458	1.731184	-1.31076
C	3.053788	-1.92151	0.181562	C	2.997036	-1.96269	0.087369
C	4.354069	-1.61317	-0.51369	C	4.300685	-1.61992	-0.58512
C	5.567832	-1.40655	0.021063	C	5.524159	-1.50834	-0.04424
C	6.760868	-1.12622	-0.86176	C	6.719032	-1.16836	-0.90357
C	5.881181	-1.43833	1.496865	C	5.847387	-1.70973	1.416154
H	3.283329	0.755578	0.174266	H	3.292361	0.689354	0.332045
H	2.183736	0.442746	1.524439	H	2.165079	0.30746	1.644151
H	1.967183	-0.77122	-1.26	H	1.919393	-0.65138	-1.23169
H	0.880693	-1.42457	2.326539	H	0.852895	-1.66178	2.28016
H	-0.55479	-2.34112	1.869918	H	-0.61106	-2.48517	1.740798
H	1.047491	-3.01795	1.579106	H	0.971086	-3.1648	1.358842
H	-0.27006	-1.8504	-1.80977	H	-0.29602	-1.60319	-1.87849
H	1.028864	-2.90755	-1.30842	H	0.928879	-2.77799	-1.46607
H	-0.96207	-4.18771	-1.53779	H	-1.13308	-3.90851	-1.84692
H	-0.41344	-4.24363	0.127907	H	-0.59513	-4.17179	-0.19706
H	-3.69283	-1.82114	-2.97549	H	-3.72569	-1.24772	-3.01163
H	-3.45175	-3.55626	-2.69912	H	-3.51419	-3.0069	-2.96539
H	-2.05493	-2.46559	-2.84104	H	-2.10016	-1.93053	-2.92734
H	-4.98683	-3.41093	-0.7766	H	-5.11801	-3.05804	-1.09287
H	-4.69269	-2.35069	0.593096	H	-4.81946	-2.23227	0.429824
H	-5.21347	-1.66214	-0.97017	H	-5.27667	-1.29265	-1.01864
H	-0.97803	0.284561	2.711705	H	-0.86482	0.045655	2.84767
H	-2.19658	1.570056	2.774679	H	-2.10299	1.268333	3.180141
H	-2.50531	0.030319	3.574292	H	-2.33025	-0.38326	3.748934
H	-4.64111	0.034233	0.449238	H	-4.63976	0.094264	0.769324
H	-4.70344	-0.61924	2.100819	H	-4.61884	-0.84046	2.278855
H	-4.46973	1.104453	1.847777	H	-4.41154	0.903986	2.328216
H	-0.52516	3.588205	1.532638	H	-0.50713	3.797737	1.602088
H	1.920624	3.566251	-0.03819	H	2.063744	3.525662	0.470875
H	1.64456	2.839412	1.550563	H	1.493353	2.658834	1.904424
H	-0.84419	5.032759	-2.4726	H	0.149593	6.194807	-1.33644
H	-1.1825	3.325752	-2.1362	H	1.488649	5.125816	-0.90254
H	0.495993	3.898137	-2.15421	H	0.59483	5.98772	0.367945
H	-0.30272	6.602764	-0.55511	H	-2.21366	5.40683	-1.20159

H	0.059844	5.954412	1.053456	H	-2.61923	3.984593	-0.21257
H	1.187744	5.68284	-0.28498	H	-2.01371	5.4571	0.561843
H	-2.18591	4.944144	0.738852	H	-1.07047	2.903631	-1.70498
H	0.957031	1.109139	-2.02894	H	1.032959	2.408414	-1.65716
H	2.738438	-2.93026	-0.11968	H	2.657369	-2.93205	-0.30427
H	3.186609	-1.96008	1.266486	H	3.135681	-2.10656	1.162999
H	4.277623	-1.56243	-1.6015	H	4.216534	-1.44691	-1.65946
H	6.491344	-1.11194	-1.92121	H	6.442683	-1.0324	-1.95255
H	7.217234	-0.15883	-0.61354	H	7.204739	-0.24628	-0.55744
H	7.544021	-1.88289	-0.71974	H	7.481248	-1.95746	-0.8515
H	5.0062	-1.61813	2.123618	H	4.969242	-1.91441	2.030801
H	6.617484	-2.22225	1.71789	H	6.548109	-2.54529	1.545531
H	6.33515	-0.4908	1.815022	H	6.347214	-0.82268	1.826717

NMR calculation details of 2.

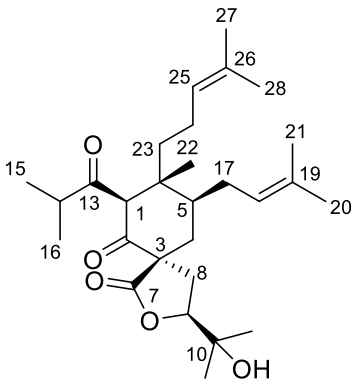
For the calculations of ^{13}C NMR chemical shifts, B3LYP/6-31G(d,p) method was used to optimize the selected conformations. For all optimized structures, vibrational spectra were calculated to ensure that no imaginary frequencies for energy minimum were obtained. NMR calculations were performed at the levels of mPW1PW91/6-31G(d,p) with the gauge-independent atomic orbital (GIAO) method.[2] The solvent effect was considered by using methanol in the calculations to resemble the experimental condition. The polarized continuum model (PCM) of Tomasiet al. was used.[3] The calculated ^{13}C NMR chemical shifts were analyzed by subtracting the isotopic shifts for TMS calculated with the same methods.[2] Different conformers for structure **2** were considered. The ^{13}C NMR chemical shifts in each compound were considered as the average values of the same atoms in the different conformers. The average values were obtained by the Boltzmann distributions, using the relative Gibbs free energies as weighting factors.[4] The differences $\Delta\delta$ were determined by subtracting the experimental chemical shifts δexptl from the calculated chemical shifts δcalcd.

References

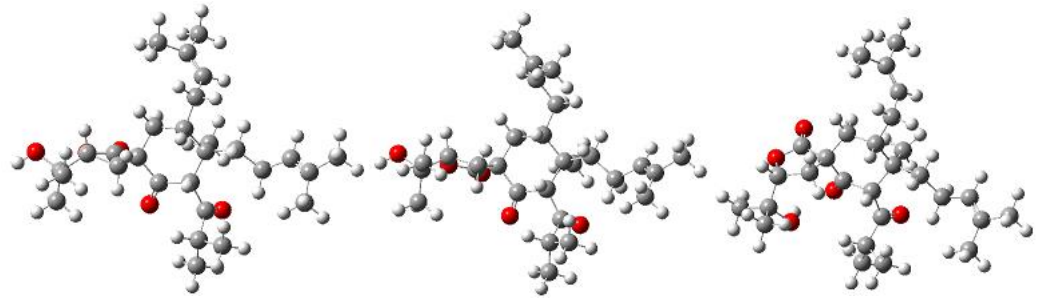
(2) (a) Ditchfield, R. *Mol. Phys.* **1974**, *27*, 789.(b) Rohlfing, C. M.; Allen, L. C.; Ditchfield, R. *Chem. Phys.* **1984**, *87*, 9.(c) Wolinski, K.; Hinton, J. F.; Pulay, P. *J. Am. Chem. Soc.* **1990**, *112*, 8251.

(3) (a) Miertus, S.; Scrocc, E.; Tomasi, J. *J. Chem. Phys.* **1981**, *55*, 117. (b) Miertus, S.; Tomasi, J. *J. Chem. Phys.* **1982**, *65*, 239. (c) Cossi, M.; Barone, V.; Cammi, R.; Tomasi, J. *Chem. Phys. Lett.* **1996**, *255*, 327.

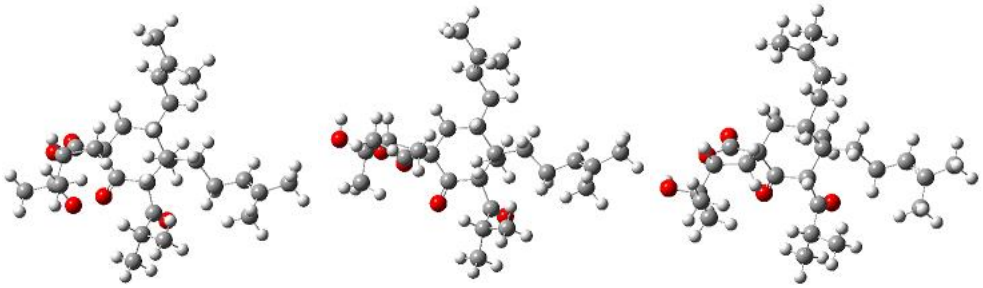
(4) Tähtinen, P.; Bagno, A.; Klika, K. D.; Pihlaja, K. *J. Am. Chem. Soc.* **2003**, *125*, 4609−4618.



2B



a **b** **c**



d **e** **f**

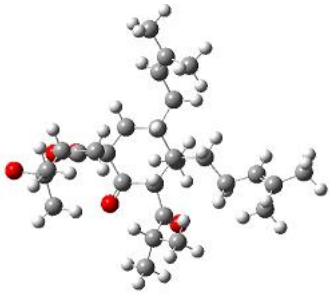


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Figure S7. Optimized geometries of predominant conformers for compound **2B** at the mPW1PW91/6-31G(d,p) level in the gas phase.

Table S10. Important thermodynamic parameters (a.u.) and Boltzmann distributions of the optimized compound **2B** at mPW1PW91/6-31G(d,p) level in the gas phase

Conformations	E+ZPE	G	%
2B-a	-1468.961823	-1469.034629	0.0
2B-b	-1468.964935	-1469.037813	0.0
2B-c	-1468.972271	-1469.044284	4.8
2B-d	-1468.975831	-1469.047082	92.7
2B-e	-1468.964244	-1469.037174	0.0
2B-f	-1468.966009	-1469.038400	0.0
2B-g	-1468.969854	-1469.043655	2.5

E+ZPE, G: total energy with zero point energy (ZPE) and Gibbs free energy in the gas phase at mPW1PW91/6-31G(d,p) level., %: Boltzmann distributions, using the relative Gibbs free energies as weighting factors

Table S11. Optimized Z-matrixes of compound **2B** in the gas phase (Å) at mPW1PW91/6-31G(d,p) level

2B-a				**2B-b**			
C	-0.80443	-1.05751	-0.75902	C	-0.7877	-1.38067	-0.74902
C	-1.81188	-0.0186	-0.25267	C	-1.80563	-0.24028	-0.72286
C	-1.18829	1.367063	0.03619	C	-1.20263	1.091939	-1.21862
C	0.224715	1.30556	0.63002	C	0.21184	1.389117	-0.69711
C	1.214757	0.48663	-0.29087	C	1.230094	0.226079	-1.03105
C	0.649395	-0.97986	-0.26087	C	0.65418	-1.05336	-0.32053
C	2.624703	0.591057	0.360104	C	2.607543	0.644972	-0.43291
C	1.239227	1.000486	-1.74798	C	1.345054	-0.00024	-2.55374
C	3.837467	-0.1569	-0.23859	C	3.820791	-0.31192	-0.46912
C	5.122942	0.382063	0.335396	C	5.091516	0.442111	-0.1705
C	6.045975	-0.24542	1.080283	C	5.946638	0.289357	0.852298
C	7.279158	0.484895	1.557265	C	7.177428	1.157916	0.963825
C	5.976717	-1.69113	1.506735	C	5.799698	-0.72476	1.959987
C	0.651577	2.734138	1.099295	C	0.64492	2.803768	-1.18582
C	0.82571	3.807913	0.055578	C	-0.31051	3.909363	-0.80022
C	0.013375	4.842182	-0.21931	C	-0.2387	4.71075	0.275129
C	0.37856	5.843514	-1.2893	C	-1.27121	5.787355	0.508134
C	-1.29777	5.126011	0.471768	C	0.841869	4.639775	1.326287
C	1.394009	-2.11067	-1.00755	C	1.41513	-2.39521	-0.42413
C	1.224333	-3.52214	-0.42974	C	1.20053	-3.38334	0.731045
O	2.069049	-1.91427	-1.99786	O	2.132602	-2.67522	-1.36307
C	1.161993	-4.5623	-1.55212	C	1.153847	-4.82198	0.206697
C	2.381176	-3.80873	0.550246	C	2.318281	-3.19451	1.777358
O	-1.18447	-1.97924	-1.45735	O	-1.13242	-2.51956	-1.00247
C	-2.93199	0.170549	-1.2947	C	-3.01264	-0.57822	-1.61838

O	-4.14772	0.039619	-0.70405	O	-4.16957	-0.42975	-0.92209
C	-4.03036	-0.15498	0.722192	C	-3.93374	0.096208	0.401801
C	-2.57978	-0.61982	0.952416	C	-2.44117	-0.15994	0.688785
O	-2.79703	0.461078	-2.45313	O	-2.98576	-0.86742	-2.78426
C	-5.1434	-1.09776	1.21643	C	-4.93988	-0.51567	1.394638
C	-5.25696	-2.36546	0.361368	C	-5.01513	-2.04293	1.280827
C	-4.91984	-1.43126	2.70104	C	-4.59612	-0.06735	2.825037
O	-6.33335	-0.30864	1.086907	O	-6.19053	0.06859	1.008442
H	-1.16984	1.94723	-0.89016	H	-1.1949	1.073635	-2.31345
H	-1.84889	1.910357	0.722638	H	-1.87343	1.907076	-0.92818
H	0.166475	0.732078	1.56932	H	0.162695	1.449682	0.401454
H	0.600709	-1.28173	0.798816	H	0.581341	-0.80899	0.752839
H	2.88635	1.654958	0.353453	H	2.916689	1.546412	-0.97124
H	2.544363	0.316699	1.422041	H	2.455004	0.960704	0.609465
H	0.253215	0.947272	-2.22079	H	0.38835	-0.29016	-2.99992
H	1.568497	2.039864	-1.79578	H	1.685533	0.910251	-3.05669
H	1.907803	0.388464	-2.35199	H	2.048922	-0.80214	-2.77168
H	3.757207	-1.23139	-0.0707	H	3.688218	-1.13845	0.229913
H	3.851138	-0.02514	-1.3265	H	3.90275	-0.76916	-1.46143
H	5.30665	1.433796	0.106125	H	5.3284	1.220712	-0.89852
H	7.292506	1.525992	1.223429	H	7.244481	1.877737	0.143557
H	7.344683	0.477781	2.653637	H	7.183816	1.716654	1.909381
H	8.192984	-0.00122	1.190334	H	8.092203	0.550299	0.958083
H	5.067861	-2.1963	1.176679	H	4.900141	-1.33575	1.871753
H	6.833904	-2.25265	1.112336	H	6.663407	-1.4023	1.980504
H	6.031435	-1.77416	2.600279	H	5.775758	-0.22734	2.938672
H	1.582355	2.649386	1.670338	H	0.73528	2.789741	-2.27888
H	-0.10561	3.045796	1.826957	H	1.638063	3.034469	-0.79876
H	1.748195	3.750048	-0.52062	H	-1.14361	4.074679	-1.48264
H	1.330107	5.601022	-1.76981	H	-2.03252	5.799252	-0.27637
H	-0.3941	5.887199	-2.06789	H	-1.77696	5.650202	1.473151
H	0.455198	6.856129	-0.87154	H	-0.80333	6.780077	0.543679
H	-1.51467	4.441311	1.293567	H	1.576871	3.854428	1.140718
H	-1.306	6.147151	0.873913	H	1.378223	5.595169	1.39515
H	-2.13061	5.067747	-0.24088	H	0.404572	4.461767	2.317465
H	0.284876	-3.54497	0.135011	H	0.243227	-3.14397	1.208974
H	1.071694	-5.57067	-1.13567	H	1.030098	-5.52739	1.034644
H	0.302205	-4.37341	-2.19956	H	0.319643	-4.94763	-0.48774
H	2.065763	-4.51612	-2.16521	H	2.078064	-5.06365	-0.32449
H	2.249535	-4.79335	1.009791	H	2.156928	-3.86859	2.624444
H	2.43622	-3.07055	1.358491	H	2.352806	-2.17192	2.169844
H	3.339845	-3.80817	0.021667	H	3.295115	-3.42713	1.341435
H	-4.209	0.818415	1.195161	H	-4.14389	1.171845	0.362004

H	-2.19107	-0.28448	1.916793	H	-2.00555	0.627463	1.308059
H	-2.52819	-1.71198	0.922247	H	-2.31918	-1.11196	1.214636
H	-5.47195	-2.1013	-0.67528	H	-5.30587	-2.3303	0.269169
H	-6.06874	-2.99659	0.741629	H	-5.75912	-2.43009	1.986777
H	-4.34248	-2.96597	0.384479	H	-4.06217	-2.52503	1.519797
H	-5.77885	-1.99313	3.082536	H	-5.3815	-0.40087	3.511459
H	-4.83206	-0.5149	3.292942	H	-4.54431	1.024224	2.883773
H	-4.02744	-2.044	2.862121	H	-3.64923	-0.48622	3.179693
H	-7.0907	-0.89222	1.227945	H	-6.89152	-0.39062	1.489924
2B-c				**2B-d**			
C	-1.122	-0.38121	-0.76069	C	-1.29	-0.58813	-0.93341
C	-1.87478	0.652059	0.086904	C	-1.90863	0.768237	-0.57833
C	-0.99185	1.902884	0.249966	C	-0.94951	1.880817	-1.03808
C	0.450954	1.604913	0.684258	C	0.510791	1.69607	-0.5928
C	1.207609	0.63169	-0.30816	C	1.129471	0.318211	-1.06393
C	0.324475	-0.67785	-0.34871	C	0.167181	-0.80329	-0.51064
C	2.603085	0.343966	0.320821	C	2.537797	0.202597	-0.40538
C	1.360256	1.221384	-1.72638	C	1.232955	0.253706	-2.60184
C	3.606637	-0.59734	-0.38254	C	3.420949	-1.04505	-0.63479
C	4.982348	-0.44073	0.213076	C	4.839362	-0.77356	-0.20268
C	5.732911	-1.34775	0.85696	C	5.558741	-1.37163	0.759336
C	7.102702	-0.98431	1.379684	C	6.983666	-0.95157	1.032251
C	5.327213	-2.77733	1.118541	C	5.062715	-2.49259	1.639237
C	1.143991	2.952819	1.071634	C	1.319017	2.956725	-1.0235
C	1.183275	4.048999	0.036812	C	0.82834	4.239946	-0.39332
C	0.481241	5.194242	0.013295	C	1.282418	4.819025	0.730101
C	0.679329	6.193467	-1.10176	C	0.691971	6.116361	1.227617
C	-0.54112	5.613009	1.04119	C	2.395953	4.268573	1.587131
C	0.7563	-1.88591	-1.21382	C	0.463264	-2.29131	-0.81411
C	0.220947	-3.24774	-0.75412	C	-0.11501	-3.2987	0.187771
O	1.462951	-1.78451	-2.19649	O	1.099863	-2.65631	-1.78195
C	-0.07089	-4.14843	-1.95856	C	-0.54695	-4.58315	-0.52707
C	1.251052	-3.89231	0.198096	C	0.940385	-3.58516	1.277188
O	-1.65255	-0.95315	-1.69785	O	-1.92784	-1.45667	-1.50444
C	-3.18042	1.012787	-0.63644	C	-3.25386	0.893497	-1.30821
O	-4.23284	0.383265	-0.0508	O	-4.27985	0.676776	-0.44403
C	-3.86509	-0.31823	1.162404	C	-3.83859	0.538921	0.929388
C	-2.37357	0.019295	1.412125	C	-2.31641	0.826495	0.916381
O	-3.30922	1.749683	-1.57686	O	-3.42865	1.156705	-2.4676
C	-4.18908	-1.82689	1.023282	C	-4.24617	-0.84991	1.481907
C	-4.06615	-2.50522	2.391567	C	-4.03253	-0.88142	2.998509
C	-5.5994	-2.02673	0.449587	C	-5.71062	-1.15938	1.139414
O	-3.2219	-2.47096	0.189599	O	-3.39103	-1.86763	0.953463

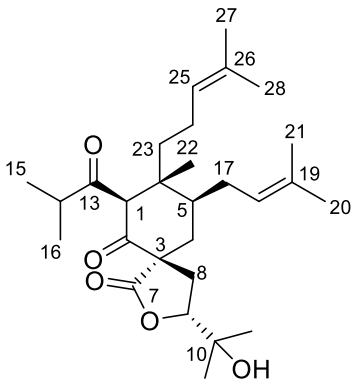
H	-1.00308	2.453022	-0.69496	H	-1.01096	1.941383	-2.13002
H	-1.46417	2.562643	0.987536	H	-1.32693	2.83473	-0.65565
H	0.398708	1.048927	1.633876	H	0.528209	1.681857	0.50795
H	0.267339	-1.04021	0.689249	H	0.171803	-0.69488	0.585211
H	3.105754	1.312497	0.413806	H	3.122768	1.056884	-0.76031
H	2.459206	-0.01169	1.351256	H	2.428713	0.350684	0.67864
H	0.416131	1.616283	-2.11354	H	0.26224	0.409084	-3.08345
H	2.086163	2.037777	-1.73039	H	1.915415	1.02409	-2.97343
H	1.702444	0.455324	-2.42072	H	1.595607	-0.7206	-2.92499
H	3.274854	-1.63436	-0.32927	H	3.016418	-1.91354	-0.11408
H	3.650272	-0.3535	-1.45036	H	3.417747	-1.30717	-1.69898
H	5.40719	0.558741	0.098576	H	5.33048	0.026195	-0.76107
H	7.358483	0.05734	1.167249	H	7.305157	-0.14102	0.372639
H	7.165351	-1.13581	2.465717	H	7.105322	-0.61483	2.070565
H	7.877806	-1.62187	0.933787	H	7.676077	-1.79332	0.897741
H	4.328551	-3.01735	0.75084	H	4.021196	-2.75912	1.454092
H	6.03383	-3.47247	0.646378	H	5.670074	-3.39586	1.4948
H	5.353139	-2.9955	2.194385	H	5.159422	-2.22304	2.699207
H	2.165845	2.748442	1.408282	H	1.259936	3.059199	-2.11367
H	0.616066	3.310025	1.962164	H	2.375258	2.819858	-0.78706
H	1.891796	3.900973	-0.77537	H	0.020703	4.748292	-0.91911
H	1.418647	5.852222	-1.83115	H	-0.10704	6.479747	0.575781
H	-0.26237	6.380218	-1.63416	H	0.281422	6.002469	2.239756
H	1.010602	7.163468	-0.70786	H	1.459757	6.89862	1.292884
H	-0.63048	4.918062	1.878233	H	2.804456	3.326978	1.216167
H	-0.29139	6.600239	1.450658	H	3.220515	4.989686	1.660397
H	-1.53255	5.711264	0.580216	H	2.044652	4.099293	2.613386
H	-0.70708	-3.08439	-0.19407	H	-0.98765	-2.84515	0.671559
H	-0.42941	-5.12731	-1.62521	H	-0.94067	-5.30668	0.193607
H	-0.83488	-3.6987	-2.59811	H	-1.32508	-4.36923	-1.2644
H	0.831029	-4.28996	-2.55976	H	0.299514	-5.03434	-1.05147
H	0.863544	-4.84084	0.582552	H	0.527349	-4.26534	2.028498
H	1.48022	-3.25543	1.06017	H	1.26096	-2.675	1.796749
H	2.186756	-4.09881	-0.33171	H	1.825725	-4.05962	0.841404
H	-4.50029	0.098161	1.951425	H	-4.37953	1.305887	1.493671
H	-2.27711	0.746207	2.223906	H	-2.11127	1.825793	1.31087
H	-1.81656	-0.87455	1.695546	H	-1.78021	0.105544	1.53444
H	-3.06449	-2.38354	2.814042	H	-2.99245	-0.67244	3.264736
H	-4.25059	-3.57642	2.278527	H	-4.27775	-1.878	3.374055
H	-4.79536	-2.10028	3.099389	H	-4.67484	-0.15303	3.502126
H	-5.8104	-3.09666	0.373983	H	-5.97883	-2.13716	1.54805
H	-5.6832	-1.57998	-0.54402	H	-5.86205	-1.17516	0.057463
H	-6.36005	-1.5658	1.088461	H	-6.38698	-0.40814	1.560502

H	-3.24767	-2.0722	-0.69446	H	-3.48487	-1.89253	-0.01176
2B-e				**2B-f**			
C	-0.788	-1.37759	-0.77559	C	-1.02563	-0.60763	-0.77806
C	-1.80612	-0.2375	-0.73257	C	-1.84216	0.483174	-0.07104
C	-1.2029	1.09253	-1.23368	C	-0.99997	1.752524	0.171207
C	0.210948	1.391631	-0.71114	C	0.412444	1.465576	0.697106
C	1.231472	0.229188	-1.04028	C	1.234467	0.534741	-0.28149
C	0.651483	-1.05297	-0.33708	C	0.425035	-0.81813	-0.31145
C	2.604007	0.646693	-0.42969	C	2.646131	0.355447	0.349537
C	1.358054	0.007635	-2.56265	C	1.337195	1.109402	-1.71115
C	3.817916	-0.30953	-0.45935	C	3.703548	-0.55947	-0.30844
C	5.085236	0.443665	-0.1444	C	5.065637	-0.29573	0.280996
C	5.931181	0.284635	0.885059	C	5.861402	-1.12387	0.97494
C	7.159987	1.153641	1.013873	C	7.205525	-0.65758	1.482146
C	5.775514	-0.73744	1.984203	C	5.533775	-2.55769	1.312172
C	0.643337	2.805562	-1.20257	C	1.065783	2.800161	1.183303
C	-0.30997	3.912343	-0.81493	C	1.338792	3.878364	0.16522
C	-0.23545	4.712774	0.260977	C	0.654011	5.014043	-0.05009
C	-1.26478	5.7922	0.495259	C	1.107858	5.996088	-1.10382
C	0.846109	4.638712	1.310877	C	-0.58744	5.436605	0.696587
C	1.412484	-2.39476	-0.44298	C	0.945376	-2.01451	-1.1408
C	1.185819	-3.39039	0.703209	C	0.508636	-3.40347	-0.65552
O	2.139353	-2.66855	-1.37646	O	1.649976	-1.88733	-2.12146
C	1.140562	-4.82534	0.168582	C	0.225722	-4.32722	-1.8445
C	2.295479	-3.21104	1.75988	C	1.603386	-3.97912	0.266859
O	-1.12857	-2.51163	-1.05343	O	-1.53453	-1.32295	-1.6211
C	-3.0236	-0.5711	-1.61503	C	-3.04995	0.837024	-0.95334
O	-4.17343	-0.43681	-0.90063	O	-4.20855	0.46141	-0.35316
C	-3.9238	0.084296	0.419575	C	-4.00931	-0.0593	0.983331
C	-2.42342	-0.15651	0.687241	C	-2.47769	-0.12283	1.213014
O	-3.01272	-0.84558	-2.78419	O	-3.02253	1.401882	-2.01353
C	-4.92329	-0.53007	1.426604	C	-4.81378	-1.37359	1.10878
C	-4.9218	-2.05937	1.390837	C	-4.30894	-2.47562	0.165705
C	-4.6246	0.007239	2.835299	C	-4.8212	-1.8401	2.565713
O	-6.25048	-0.15978	1.042294	O	-6.17575	-1.06195	0.802217
H	-1.195	1.069163	-2.32843	H	-0.94818	2.318754	-0.76234
H	-1.87359	1.909411	-0.94708	H	-1.5354	2.388502	0.886316
H	0.160083	1.454785	0.387156	H	0.304566	0.878832	1.623725
H	0.574326	-0.81283	0.736866	H	0.352765	-1.16497	0.73206
H	2.91748	1.5502	-0.96205	H	3.090501	1.355843	0.394691
H	2.442631	0.958365	0.612582	H	2.525981	0.041126	1.396577
H	0.404059	-0.27803	-3.01734	H	0.352501	1.281023	-2.15739
H	1.705098	0.918803	-3.05978	H	1.868136	2.062768	-1.71586

H	2.06123	-0.79562	-2.77762	H	1.860781	0.410513	-2.36199
H	3.679154	-1.13965	0.234149	H	3.43162	-1.61026	-0.20429
H	3.90932	-0.76162	-1.45321	H	3.739367	-0.36547	-1.38655
H	5.328031	1.227395	-0.86493	H	5.435148	0.718127	0.113643
H	7.23389	1.879343	0.199404	H	7.402506	0.385	1.218228
H	7.157122	1.705627	1.9634	H	7.270638	-0.75075	2.574549
H	8.075356	0.54693	1.012246	H	8.01789	-1.27151	1.070872
H	4.87797	-1.34938	1.883228	H	4.555566	-2.87521	0.948039
H	6.640179	-1.41362	2.007991	H	6.285101	-3.23633	0.887407
H	5.741596	-0.24699	2.966092	H	5.557259	-2.71394	2.398829
H	0.730082	2.790517	-2.29583	H	2.002229	2.563765	1.699662
H	1.637908	3.036006	-0.81907	H	0.39881	3.18807	1.960937
H	-1.14298	4.080392	-1.49692	H	2.227661	3.726318	-0.44493
H	-2.02682	5.806473	-0.2886	H	2.00546	5.651487	-1.62414
H	-1.76945	5.657001	1.461195	H	0.322607	6.161414	-1.85296
H	-0.79418	6.78362	0.530017	H	1.325285	6.977047	-0.66097
H	1.578255	3.850959	1.12452	H	-0.8614	4.758148	1.506664
H	1.385606	5.592379	1.378688	H	-0.45415	6.437511	1.126629
H	0.409647	4.46242	2.302729	H	-1.44417	5.504938	0.013778
H	0.225159	-3.15253	1.175223	H	-0.4077	-3.28625	-0.06399
H	1.008758	-5.53599	0.990722	H	-0.05573	-5.32594	-1.49579
H	0.31173	-4.94479	-0.53332	H	-0.58825	-3.92738	-2.45415
H	2.068635	-5.06518	-0.35669	H	1.112868	-4.41385	-2.47708
H	2.126043	-3.8909	2.600712	H	1.291098	-4.95113	0.661198
H	2.328742	-2.19135	2.160033	H	1.813783	-3.32637	1.121678
H	3.275339	-3.44237	1.330094	H	2.534415	-4.12305	-0.29054
H	-4.12249	1.166349	0.378297	H	-4.47577	0.664707	1.659628
H	-1.98691	0.638637	1.29592	H	-2.19535	0.452241	2.098279
H	-2.28788	-1.10344	1.218115	H	-2.15566	-1.15271	1.38635
H	-5.14475	-2.40994	0.38177	H	-4.24575	-2.11779	-0.86537
H	-5.69531	-2.43102	2.06746	H	-5.01028	-3.31311	0.202009
H	-3.9614	-2.47607	1.706267	H	-3.32056	-2.85012	0.449193
H	-5.39782	-0.34423	3.523045	H	-5.46412	-2.719	2.660331
H	-4.63357	1.104565	2.849584	H	-5.22208	-1.05806	3.217471
H	-3.65216	-0.32552	3.211401	H	-3.81829	-2.10969	2.910136
H	-6.31343	0.805511	1.05398	H	-6.18259	-0.67551	-0.08592
2B-g							
C	-1.07656	-0.92985	-0.89064				
C	-1.87754	0.358501	-0.6795				
C	-1.05418	1.581207	-1.12867				
C	0.39752	1.599272	-0.62414				
C	1.201125	0.300944	-1.03589				
C	0.39217	-0.91113	-0.43664				

C	2.610929	0.409302	-0.37841				
C	1.321867	0.180416	-2.5695				
C	3.652316	-0.72208	-0.53779				
C	5.020984	-0.2353	-0.13547				
C	5.818628	-0.67171	0.851412				
C	7.170083	-0.03925	1.086349				
C	5.488208	-1.7996	1.79774				
C	1.057696	2.943788	-1.05347				
C	0.336882	4.171616	-0.54631				
C	0.598532	4.865428	0.573399				
C	-0.20991	6.088534	0.933434				
C	1.6914	4.524921	1.556833				
C	0.898682	-2.35495	-0.65991				
C	0.472251	-3.3857	0.394967				
O	1.582986	-2.67794	-1.60947				
C	0.173349	-4.73734	-0.26108				
C	1.579715	-3.50263	1.462722				
O	-1.59639	-1.93663	-1.33455				
C	-3.16485	0.288296	-1.51622				
O	-4.25619	0.229142	-0.71034				
C	-3.92963	0.356291	0.69506				
C	-2.38374	0.420434	0.789099				
O	-3.24561	0.319276	-2.71453				
C	-4.65572	-0.77743	1.455791				
C	-4.16739	-2.17647	1.051901				
C	-4.53339	-0.55369	2.964314				
O	-6.05011	-0.65098	1.163643				
H	-1.07264	1.613028	-2.22306				
H	-1.56778	2.484476	-0.78378				
H	0.372222	1.610216	0.476734				
H	0.359022	-0.74872	0.653197				
H	3.078467	1.309501	-0.7893				
H	2.482666	0.607783	0.695669				
H	0.343034	0.140864	-3.05811				
H	1.865902	1.035414	-2.98245				
H	1.847941	-0.73244	-2.84399				
H	3.36824	-1.60181	0.040439				
H	3.683358	-1.04923	-1.58345				
H	5.395676	0.591633	-0.74223				
H	7.368756	0.77316	0.382057				
H	7.246132	0.365675	2.104442				
H	7.975516	-0.77916	0.987417				
H	4.504811	-2.23851	1.622803				

H	6.23208	-2.60285	1.715186				
H	5.52363	-1.45332	2.839183				
H	1.091328	2.98914	-2.14862				
H	2.094073	2.968432	-0.71453				
H	-0.4796	4.53289	-1.17082				
H	-0.98814	6.296498	0.194273				
H	-0.69178	5.971386	1.91318				
H	0.432376	6.97575	1.010141				
H	2.267613	3.640926	1.277561				
H	2.390668	5.364403	1.663428				
H	1.270289	4.348007	2.555174				
H	-0.43587	-3.01565	0.886269				
H	-0.10228	-5.47836	0.496037				
H	-0.64976	-4.64315	-0.97364				
H	1.051282	-5.09909	-0.80242				
H	1.274255	-4.20282	2.246398				
H	1.798642	-2.54221	1.942909				
H	2.504343	-3.87938	1.013967				
H	-4.38063	1.298578	1.02297				
H	-2.06335	1.347226	1.271338				
H	-1.99816	-0.4041	1.394017				
H	-4.20534	-2.31313	-0.03217				
H	-4.8175	-2.9207	1.518825				
H	-3.14125	-2.37273	1.377588				
H	-5.1259	-1.30679	3.490194				
H	-4.92088	0.431809	3.239294				
H	-3.49631	-0.63468	3.303579				
H	-6.1393	-0.69192	0.199996				



2D

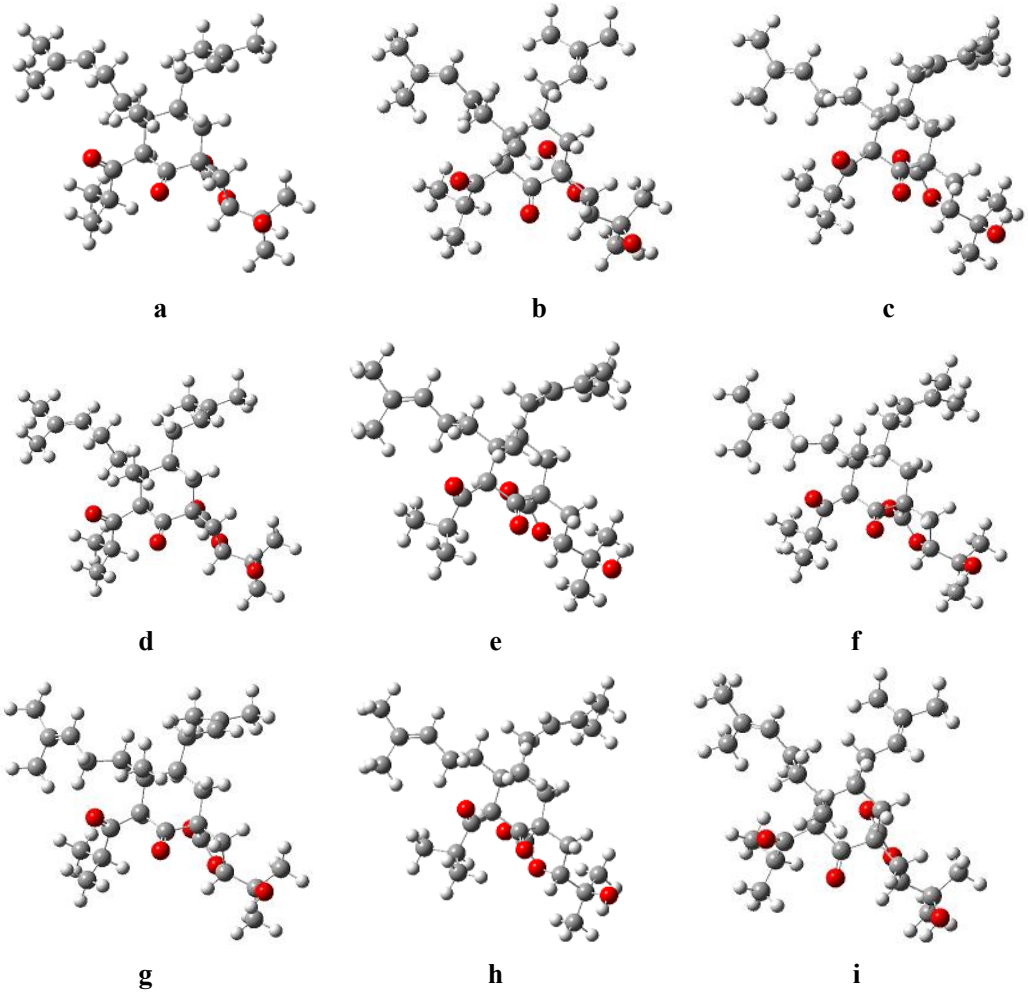


Figure S8. Optimized geometries of predominant conformers for compound **2D** at the mPW1PW91/6-31G(d,p) level in the gas phase.

Table S12. Important thermodynamic parameters (a.u.) and Boltzmann distributions of the optimized compound **2D** at mPW1PW91/6-31G(d,p) level in the gas phase

Conformations	E+ZPE	G	%
2D-a	-1468.977978	-1469.050829	2.7
2D-b	-1468.981122	-1469.053382	40.7

2D-c	-1468.972796	-1469.045745	0
2D-d	-1468.977359	-1469.049858	1
2D-e	-1468.977457	-1469.049469	0.6
2D-f	-1468.973568	-1469.046564	0
2D-g	-1468.976692	-1469.049767	0.9
2D-h	-1468.978285	-1469.050120	1.3
2D-i	-1468.981384	-1469.053628	52.8

E+ZPE, G: total energy with zero point energy (ZPE) and Gibbs free energy in the gas phase at mPW1PW91/6-31G(d,p) level., %: Boltzmann distributions, using the relative Gibbs free energies as weighting factors

Table S13. Optimized Z-matrixes of compound **2D** in the gas phase (Å) at mPW1PW91/6-31G(d,p) level.

2D-a				**2D-b**			
C	0.970306	-1.2562	0.549229	C	1.021412	-1.18797	0.808719
C	1.834885	0.015365	0.431139	C	1.787765	0.100044	0.445346
C	1.03136	1.248347	0.912406	C	1.035281	1.333829	1.002643
C	-0.42589	1.330028	0.425305	C	-0.49238	1.334846	0.81026
C	-1.24167	0.019534	0.717919	C	-1.16193	0.009379	1.324391
C	-0.45065	-1.14308	0.008558	C	-0.47732	-1.16485	0.526116
C	-2.64906	0.111897	0.030323	C	-2.69736	0.011784	1.072213
C	-1.34392	-0.27079	2.231504	C	-0.94791	-0.19312	2.842382
C	-3.86252	0.486854	0.910812	C	-3.19295	0.19423	-0.37809
C	-5.11422	0.64793	0.08649	C	-4.68671	0.387386	-0.4245
C	-6.13312	-0.21578	-0.04405	C	-5.61996	-0.35561	-1.03837
C	-7.31798	0.11223	-0.9206	C	-7.08072	0.019343	-0.95373
C	-6.21266	-1.55735	0.643095	C	-5.34374	-1.59482	-1.85292
C	-1.09459	2.622593	0.9704	C	-1.09995	2.626124	1.429432
C	-0.35822	3.895879	0.625231	C	-0.47729	3.908597	0.930173
C	-0.57429	4.706975	-0.42268	C	-0.92077	4.713407	-0.04884
C	0.254584	5.952641	-0.62332	C	-0.16676	5.968405	-0.41765
C	-1.6248	4.476168	-1.48051	C	-2.16754	4.470764	-0.86246
C	-1.08469	-2.54666	0.023392	C	-1.02362	-2.59194	0.713762
C	-0.55932	-3.53767	-1.0216	C	-0.58538	-3.63165	-0.32744
O	-1.98843	-2.85931	0.775893	O	-1.79133	-2.90027	1.605719
C	-0.3726	-4.92789	-0.40289	C	-0.19446	-4.94475	0.362773
C	-1.5569	-3.56345	-2.19891	C	-1.739	-3.83997	-1.32969
O	1.409621	-2.27974	1.042914	O	1.589343	-2.1497	1.29471
C	2.242216	0.127877	-1.05448	C	1.897248	0.131415	-1.09432
O	3.519506	-0.28809	-1.21505	O	3.137604	-0.25128	-1.47622
C	4.105023	-0.72307	0.044539	C	3.96729	-0.59499	-0.33023
C	3.191172	-0.14934	1.133517	C	3.259655	0.027414	0.878622

O	1.565725	0.501827	-1.98215	O	1.040128	0.42569	-1.89249
C	5.588233	-0.29994	0.069577	C	5.414346	-0.14482	-0.61623
C	6.372083	-1.09908	-0.98073	C	6.001625	-0.98688	-1.75733
C	5.78156	1.206981	-0.14417	C	5.52179	1.351281	-0.93857
O	5.99758	-0.67847	1.391033	O	6.081442	-0.44381	0.617734
H	1.059053	1.246681	2.009463	H	1.277515	1.404928	2.070515
H	1.565312	2.148573	0.592795	H	1.454875	2.227945	0.531666
H	-0.3885	1.433628	-0.66568	H	-0.66646	1.38953	-0.2694
H	-0.34155	-0.84966	-1.047	H	-0.56994	-0.92517	-0.54358
H	-2.57764	0.821671	-0.8047	H	-3.10645	-0.92193	1.464733
H	-2.89599	-0.85011	-0.4242	H	-3.1325	0.805636	1.691009
H	-0.35658	-0.40327	2.685774	H	0.110358	-0.21465	3.121597
H	-1.83975	0.544049	2.764424	H	-1.42306	0.610491	3.412601
H	-1.90422	-1.18923	2.404141	H	-1.39032	-1.13929	3.156358
H	-3.99956	-0.27919	1.677783	H	-2.71679	1.075162	-0.83012
H	-3.67418	1.425188	1.446655	H	-2.88988	-0.65874	-0.99286
H	-5.17219	1.577347	-0.48272	H	-5.03801	1.25743	0.13385
H	-7.22054	1.095475	-1.38918	H	-7.23734	0.923842	-0.35972
H	-7.44075	-0.63437	-1.71656	H	-7.50368	0.190665	-1.95269
H	-8.25148	0.102605	-0.34199	H	-7.67035	-0.79009	-0.50304
H	-5.3096	-1.81382	1.199191	H	-4.28797	-1.86761	-1.88345
H	-7.0634	-1.59062	1.336864	H	-5.89963	-2.45164	-1.45061
H	-6.38468	-2.35306	-0.09303	H	-5.68644	-1.46215	-2.88761
H	-1.17541	2.556105	2.062767	H	-0.98339	2.590791	2.520174
H	-2.11717	2.673599	0.589873	H	-2.17551	2.637059	1.238275
H	0.438012	4.180984	1.312871	H	0.441657	4.209427	1.433465
H	1.002265	6.078621	0.164587	H	0.728273	6.102174	0.19606
H	0.777553	5.927612	-1.58845	H	0.141766	5.948135	-1.4712
H	-0.37885	6.84955	-0.63781	H	-0.79866	6.858371	-0.29724
H	-2.23514	3.590352	-1.29624	H	-2.7188	3.580474	-0.55518
H	-2.296	5.341528	-1.55611	H	-2.84775	5.32986	-0.7955
H	-1.15738	4.358523	-2.46658	H	-1.91705	4.356777	-1.92508
H	0.405001	-3.17543	-1.39643	H	0.279551	-3.24052	-0.87521
H	-0.04613	-5.64497	-1.16284	H	0.077402	-5.70068	-0.3809
H	0.377703	-4.89748	0.391535	H	0.657242	-4.79018	1.030002
H	-1.31369	-5.27934	0.028404	H	-1.03126	-5.32293	0.956071
H	-1.20072	-4.24211	-2.98005	H	-1.45862	-4.5897	-2.07602
H	-1.68594	-2.57384	-2.65096	H	-1.98878	-2.91759	-1.86518
H	-2.53643	-3.9129	-1.85852	H	-2.63623	-4.1894	-0.80992
H	4.058885	-1.81664	0.060406	H	3.960078	-1.68618	-0.24182
H	3.549459	0.825749	1.473529	H	3.634524	1.03464	1.07854
H	3.135511	-0.81842	1.991631	H	3.399266	-0.58116	1.771463
H	7.433934	-0.82805	-0.95468	H	7.041734	-0.69876	-1.94957

H	6.287047	-2.17127	-0.78104	H	5.983252	-2.04819	-1.49256
H	5.997578	-0.89931	-1.98843	H	5.436052	-0.84639	-2.68251
H	6.849646	1.449989	-0.11417	H	6.568554	1.613029	-1.12942
H	5.288988	1.788653	0.639292	H	5.174469	1.965393	-0.10385
H	5.392603	1.522051	-1.11578	H	4.943961	1.607639	-1.83032
H	6.946817	-0.51128	1.463083	H	7.02273	-0.26287	0.493701
2D-c				**2D-d**			
C	-0.75653	-0.92111	-0.76008	C	0.973875	-1.24258	0.557682
C	-1.74776	-0.02799	0.006925	C	1.8336	0.031432	0.428779
C	-1.16224	1.396523	0.114369	C	1.026166	1.259294	0.917311
C	0.31831	1.481538	0.521137	C	-0.43212	1.33519	0.431436
C	1.275871	0.617272	-0.39363	C	-1.2427	0.020736	0.720933
C	0.703937	-0.85536	-0.30944	C	-0.44511	-1.13894	0.012716
C	2.694582	0.695767	0.246102	C	-2.64836	0.107482	0.028763
C	1.31278	1.102987	-1.85764	C	-1.34817	-0.2706	2.234021
C	3.894839	-0.03316	-0.39981	C	-3.86704	0.472651	0.906102
C	5.192866	0.482179	0.167306	C	-5.1169	0.627507	0.077765
C	6.126847	-0.17482	0.871967	C	-6.12948	-0.24277	-0.05821
C	7.372392	0.533278	1.350315	C	-7.31348	0.079318	-0.93807
C	6.057833	-1.6338	1.250401	C	-6.2024	-1.5864	0.625626
C	0.67403	2.988849	0.743674	C	-1.10571	2.623765	0.97993
C	0.374326	3.956653	-0.37376	C	-0.37703	3.901213	0.633335
C	-0.53166	4.948923	-0.39226	C	-0.59689	4.708324	-0.4169
C	-0.65593	5.853055	-1.5962	C	0.2238	5.959017	-0.6195
C	-1.48264	5.283919	0.730848	C	-1.64436	4.467758	-1.4755
C	1.410002	-2.00379	-1.0603	C	-1.07213	-2.54605	0.028805
C	1.185098	-3.40571	-0.47797	C	-0.53336	-3.5385	-1.00768
O	2.093188	-1.84081	-2.05176	O	-1.98028	-2.85948	0.775471
C	1.079539	-4.44807	-1.59522	C	-0.34544	-4.92562	-0.38227
C	2.334966	-3.72886	0.49933	C	-1.52076	-3.57349	-2.19344
O	-1.12952	-1.64388	-1.66697	O	1.414145	-2.25636	1.070214
C	-1.97316	-0.68161	1.388653	C	2.233259	0.15009	-1.05936
O	-3.15532	-1.33588	1.401054	O	3.51013	-0.25918	-1.22732
C	-3.83629	-1.24621	0.113652	C	4.103926	-0.70708	0.027251
C	-3.15248	-0.08013	-0.6126	C	3.194847	-0.13154	1.12169
O	-1.2368	-0.65827	2.345703	O	1.548434	0.526935	-1.97972
C	-5.36194	-1.14523	0.347778	C	5.597782	-0.3071	0.056994
C	-5.88094	-2.46305	0.926133	C	6.365619	-1.11111	-0.994
C	-5.75081	0.032095	1.249213	C	5.817691	1.196658	-0.14496
O	-5.97159	-1.02442	-0.94477	O	6.116024	-0.73492	1.324188
H	-1.31276	1.890803	-0.85165	H	1.054472	1.253204	2.014484
H	-1.76138	1.962747	0.837135	H	1.554811	2.163551	0.599927
H	0.394073	1.028729	1.516416	H	-0.39498	1.441544	-0.65913

H	0.6908	-1.1161	0.759012	H	-0.33702	-0.84565	-1.04284
H	2.962876	1.757251	0.271678	H	-2.57796	0.820329	-0.80368
H	2.624064	0.385476	1.29764	H	-2.88802	-0.85435	-0.42988
H	0.30907	1.267146	-2.26311	H	-0.36159	-0.3961	2.692021
H	1.858872	2.046633	-1.93692	H	-1.85192	0.540617	2.764916
H	1.806	0.367738	-2.49234	H	-1.90263	-1.19291	2.404655
H	3.815048	-1.11247	-0.27002	H	-4.00186	-0.29601	1.670842
H	3.887806	0.137065	-1.48281	H	-3.68641	1.410966	1.444719
H	5.376971	1.540705	-0.02832	H	-5.17915	1.557904	-0.48935
H	7.385088	1.58506	1.051651	H	-7.22126	1.064418	-1.40377
H	7.457729	0.488707	2.444397	H	-7.42821	-0.66606	-1.73635
H	8.276852	0.055589	0.950436	H	-8.24887	0.061617	-0.36276
H	5.138267	-2.12197	0.9244	H	-5.29932	-1.83862	1.183646
H	6.9024	-2.18661	0.818165	H	-7.05485	-1.62657	1.316895
H	6.135756	-1.75381	2.338961	H	-6.36742	-2.38141	-0.11282
H	1.733939	3.074857	1.005915	H	-1.18324	2.555879	2.072431
H	0.133363	3.2918	1.646015	H	-2.12967	2.669442	0.602468
H	0.994368	3.853627	-1.26192	H	0.415962	4.193461	1.3218
H	0.044737	5.577775	-2.389	H	0.969031	6.092683	0.169466
H	-1.67157	5.821334	-2.01269	H	0.748728	5.934721	-1.58355
H	-0.4673	6.900039	-1.32394	H	-0.41589	6.85134	-0.63793
H	-1.3865	4.626449	1.596483	H	-2.24953	3.578754	-1.28952
H	-1.3246	6.314599	1.074288	H	-2.32075	5.328707	-1.55456
H	-2.52303	5.232831	0.383704	H	-1.17475	4.350166	-2.4605
H	0.250335	-3.3927	0.096071	H	0.43244	-3.17335	-1.37598
H	0.946328	-5.44939	-1.17371	H	-0.00999	-5.64382	-1.13714
H	0.23002	-4.22808	-2.2471	H	0.398593	-4.88959	0.417832
H	1.984952	-4.44309	-2.20758	H	-1.28834	-5.27964	0.042891
H	2.170666	-4.70662	0.962571	H	-1.15451	-4.2536	-2.96856
H	2.41539	-2.99043	1.304469	H	-1.65048	-2.58636	-2.65066
H	3.290891	-3.76222	-0.03341	H	-2.50151	-3.92625	-1.86008
H	-3.63658	-2.17945	-0.42212	H	4.044993	-1.79994	0.038899
H	-3.66359	0.868553	-0.41539	H	3.54496	0.851648	1.45396
H	-3.11615	-0.24949	-1.68918	H	3.136359	-0.8001	1.981243
H	-6.96191	-2.40547	1.078374	H	7.425556	-0.84503	-0.96845
H	-5.67747	-3.28313	0.231414	H	6.27747	-2.18118	-0.78499
H	-5.39673	-2.68276	1.880878	H	5.971814	-0.91465	-1.9943
H	-6.83676	0.049368	1.374128	H	6.88873	1.413656	-0.112
H	-5.44998	0.994925	0.819827	H	5.333731	1.792118	0.638183
H	-5.28557	-0.05582	2.234189	H	5.422583	1.526248	-1.10906
H	-5.83953	-0.11898	-1.25655	H	5.817519	-0.10966	1.998327
2D-e				**2D-f**			
C	0.768206	-0.90377	0.871814	C	-0.78266	-0.92076	-0.72333

C	1.671116	0.000331	0.005712	C	-1.76053	0.004901	0.021935
C	1.057075	1.418492	-0.09372	C	-1.1492	1.41708	0.143234
C	-0.46266	1.468586	-0.32682	C	0.330881	1.465801	0.555564
C	-1.2633	0.609839	0.716699	C	1.267839	0.596677	-0.37516
C	-0.71951	-0.86236	0.54105	C	0.681778	-0.86903	-0.28023
C	-2.79217	0.666649	0.437038	C	2.698305	0.669937	0.237249
C	-1.0469	1.060202	2.180166	C	1.281147	1.075015	-1.84225
C	-3.29323	0.206918	-0.94885	C	3.879657	-0.08192	-0.41715
C	-4.7502	0.540752	-1.1418	C	5.192627	0.429565	0.1181
C	-5.79188	-0.28534	-1.32174	C	6.133398	-0.22528	0.815708
C	-7.18869	0.263489	-1.49268	C	7.394165	0.478204	1.259802
C	-5.70475	-1.79026	-1.37653	C	6.057717	-1.67751	1.218131
C	-0.90813	2.950189	-0.53752	C	0.721204	2.957767	0.815203
C	-0.59287	3.952358	0.544727	C	0.519668	3.95029	-0.30222
C	0.323504	4.934949	0.526576	C	-0.3886	4.937395	-0.38305
C	0.465916	5.875806	1.69981	C	-0.40942	5.866023	-1.5744
C	1.270608	5.220912	-0.61318	C	-1.44257	5.240058	0.653967
C	-1.42012	-1.99981	1.305681	C	1.370704	-2.02898	-1.0287
C	-1.09405	-3.42878	0.84903	C	1.148624	-3.42355	-0.42763
O	-2.22318	-1.80752	2.199084	O	2.037593	-1.87971	-2.03338
C	-0.82332	-4.32679	2.063562	C	1.034813	-4.47945	-1.53106
C	-2.27287	-3.95711	0.006616	C	2.30363	-3.73669	0.546828
O	1.231002	-1.592	1.763745	O	-1.17085	-1.66827	-1.60433
C	1.787792	-0.68034	-1.37614	C	-2.01792	-0.64665	1.399577
O	2.974524	-1.31813	-1.47768	O	-3.20885	-1.28836	1.389717
C	3.764841	-1.18516	-0.25827	C	-3.86495	-1.17947	0.092167
C	3.125003	-0.01442	0.500334	C	-3.1581	-0.01867	-0.61537
O	0.970605	-0.68679	-2.26558	O	-1.29962	-0.63514	2.370103
C	5.261228	-1.05997	-0.62979	C	-5.39303	-1.06208	0.295938
C	5.757918	-2.38271	-1.21619	C	-5.93857	-2.35913	0.906447
C	5.542356	0.098742	-1.5933	C	-5.78754	0.143338	1.149446
O	5.979242	-0.88952	0.600124	O	-5.96885	-0.83385	-0.99797
H	1.310788	1.956781	0.825777	H	-1.28703	1.924732	-0.81758
H	1.561256	1.952663	-0.90748	H	-1.73994	1.98554	0.87057
H	-0.63619	0.991047	-1.29687	H	0.394295	0.991946	1.542101
H	-0.79136	-1.10949	-0.52837	H	0.669175	-1.12556	0.78944
H	-3.30145	0.077463	1.203087	H	2.976574	1.729299	0.239602
H	-3.11496	1.702701	0.597569	H	2.643756	0.378092	1.295112
H	0.011083	1.134222	2.450208	H	0.270858	1.22937	-2.23483
H	-1.49895	2.037838	2.358983	H	1.817823	2.022012	-1.93695
H	-1.51464	0.344529	2.857661	H	1.769623	0.338065	-2.47887
H	-2.71885	0.704352	-1.74234	H	3.791443	-1.15802	-0.26739
H	-3.1193	-0.86582	-1.07644	H	3.855107	0.069982	-1.5026

H	-4.96657	1.610558	-1.11852	H	5.38284	1.483102	-0.09757
H	-7.20756	1.355778	-1.44698	H	7.410724	1.525165	0.944839
H	-7.6191	-0.04441	-2.455	H	7.499808	0.449523	2.352639
H	-7.86202	-0.12146	-0.71527	H	8.286556	-0.01392	0.850383
H	-4.69261	-2.17146	-1.2342	H	5.129049	-2.16239	0.913727
H	-6.34331	-2.24065	-0.60554	H	6.890764	-2.24442	0.781833
H	-6.07298	-2.16484	-2.34071	H	6.151224	-1.78136	2.307162
H	-1.98883	2.964585	-0.72035	H	1.766317	3.003051	1.139374
H	-0.4519	3.271365	-1.47982	H	0.139283	3.266717	1.689659
H	-1.21315	3.888571	1.436714	H	1.221336	3.872275	-1.1305
H	-0.23038	5.632649	2.506799	H	0.3635	5.611391	-2.30449
H	1.484571	5.847499	2.109035	H	-1.38202	5.83586	-2.08327
H	0.284735	6.915323	1.395738	H	-0.25547	6.908283	-1.2647
H	1.138877	4.554859	-1.46751	H	-1.40272	4.581024	1.52283
H	1.144327	6.251816	-0.96858	H	-1.34426	6.273131	1.011985
H	2.313504	5.137088	-0.27991	H	-2.44711	5.160536	0.218014
H	-0.20134	-3.40268	0.213489	H	0.217313	-3.40145	0.151705
H	-0.63211	-5.35555	1.742145	H	0.902278	-5.47542	-1.09669
H	0.045504	-3.96901	2.621715	H	0.182108	-4.26552	-2.18084
H	-1.68688	-4.3249	2.734114	H	1.936505	-4.48365	-2.14887
H	-2.07467	-4.9837	-0.31678	H	2.139139	-4.70713	1.025243
H	-2.43816	-3.35348	-0.8925	H	2.391968	-2.98705	1.340676
H	-3.19344	-3.95327	0.598022	H	3.256104	-3.78121	0.008718
H	3.633219	-2.10907	0.313496	H	-3.65698	-2.1155	-0.44149
H	3.599368	0.937503	0.23837	H	-3.66796	0.928119	-0.41875
H	3.186297	-0.15938	1.579401	H	-3.11771	-0.17399	-1.69311
H	6.819519	-2.30686	-1.46575	H	-7.02603	-2.2994	1.003847
H	5.636289	-3.18624	-0.48399	H	-5.69658	-3.22019	0.270751
H	5.196637	-2.6406	-2.11777	H	-5.50366	-2.54299	1.892544
H	6.613729	0.13942	-1.80711	H	-6.87218	0.152813	1.283735
H	5.250489	1.066496	-1.16886	H	-5.50789	1.081593	0.66386
H	5.001669	-0.03101	-2.5341	H	-5.31068	0.09475	2.131156
H	5.85582	0.022151	0.896988	H	-5.89119	-1.65194	-1.5087
2D-g				**2D-h**			
C	0.94644	-1.15691	0.729981	C	0.786657	-0.89809	0.8516
C	1.842337	0.059723	0.445245	C	1.678221	0.024039	-0.00675
C	1.147823	1.329869	0.981677	C	1.045844	1.433298	-0.11449
C	-0.34681	1.482536	0.646021	C	-0.47424	1.461505	-0.34627
C	-1.21259	0.218511	1.037261	C	-1.25889	0.599404	0.706269
C	-0.52436	-1.01753	0.334954	C	-0.70382	-0.86779	0.529113
C	-2.63877	0.451076	0.451176	C	-2.79044	0.645058	0.440926
C	-1.27067	0.02775	2.566572	C	-1.03107	1.053305	2.167101
C	-3.76362	-0.58758	0.668501	C	-3.30022	0.178639	-0.9396

C	-5.10978	0.019868	0.366439	C	-4.75988	0.505731	-1.1232
C	-5.99239	-0.31343	-0.58772	C	-5.79905	-0.32477	-1.29716
C	-7.30288	0.425792	-0.72004	C	-7.19926	0.217989	-1.45952
C	-5.79876	-1.41991	-1.59501	C	-5.70571	-1.82929	-1.35335
C	-0.84487	2.823478	1.262881	C	-0.94311	2.933854	-0.56939
C	-0.10354	4.043079	0.762993	C	-0.67415	3.945327	0.516574
C	-0.41401	4.802817	-0.29954	C	0.240003	4.930048	0.528294
C	0.428036	5.999204	-0.67079	C	0.333653	5.879027	1.699822
C	-1.5916	4.556411	-1.20982	C	1.232442	5.208665	-0.57403
C	-1.12413	-2.42871	0.505083	C	-1.39116	-2.01068	1.296963
C	-0.80598	-3.41977	-0.62305	C	-1.06491	-3.43691	0.831196
O	-1.79384	-2.76327	1.461977	O	-2.18417	-1.82528	2.200773
C	-0.61125	-4.83335	-0.06627	C	-0.78707	-4.34055	2.039757
C	-1.93992	-3.36832	-1.66844	C	-2.24657	-3.9633	-0.00844
O	1.397204	-2.17336	1.228949	O	1.260676	-1.59982	1.727802
C	2.06945	0.100463	-1.08212	C	1.809361	-0.66129	-1.38496
O	3.290793	-0.40294	-1.37725	O	3.001736	-1.29432	-1.47332
C	3.998794	-0.82878	-0.17629	C	3.780844	-1.14036	-0.25035
C	3.26668	-0.1427	0.981714	C	3.130293	0.031452	0.492859
O	1.308196	0.486594	-1.93588	O	1.000698	-0.67916	-2.28167
C	5.50835	-0.53487	-0.33596	C	5.279189	-1.00803	-0.60824
C	6.09155	-1.39956	-1.4606	C	5.787026	-2.31908	-1.22103
C	5.802764	0.94427	-0.58573	C	5.565058	0.169	-1.54099
O	6.128574	-0.85382	0.917561	O	5.974929	-0.72061	0.612899
H	1.285068	1.336542	2.070672	H	1.293582	1.980333	0.801406
H	1.686605	2.202064	0.598865	H	1.543208	1.967979	-0.93185
H	-0.41924	1.584856	-0.44288	H	-0.64255	0.973839	-1.31241
H	-0.51271	-0.78532	-0.74033	H	-0.7773	-1.11669	-0.53995
H	-3.00635	1.387921	0.881547	H	-3.28952	0.05464	1.212808
H	-2.54543	0.639746	-0.62725	H	-3.11789	1.679658	0.601486
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2D-i							
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H	5.943799	-2.03957	-1.53182				
H	5.441294	-0.79837	-2.6864				
H	6.60983	1.589773	-1.11671				
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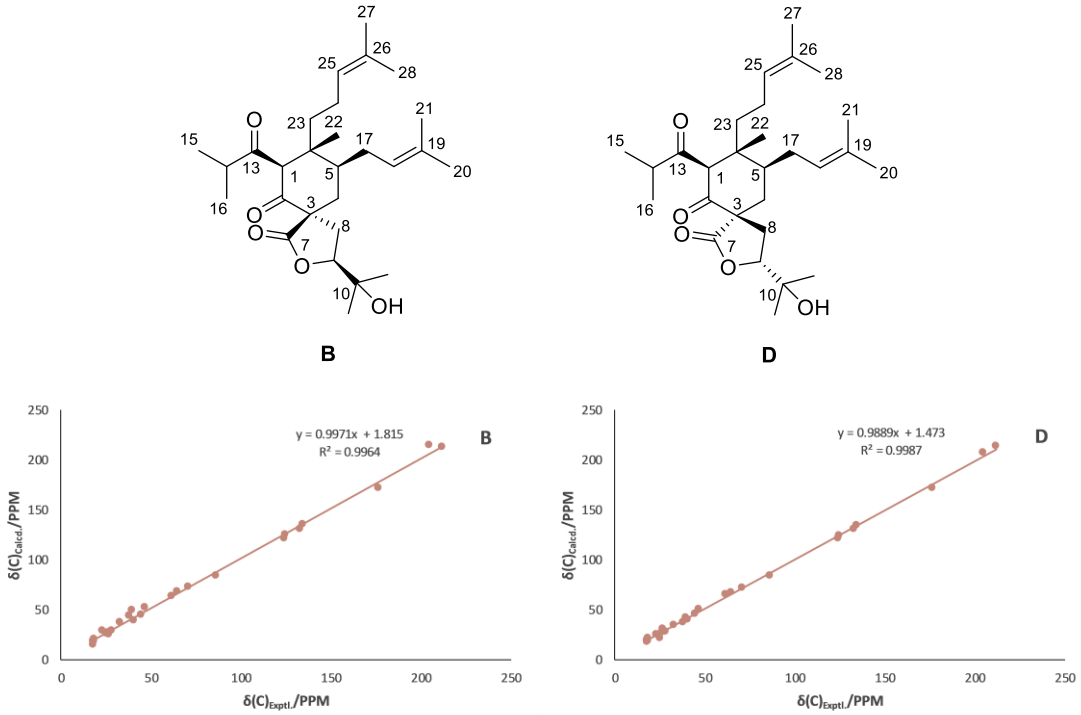
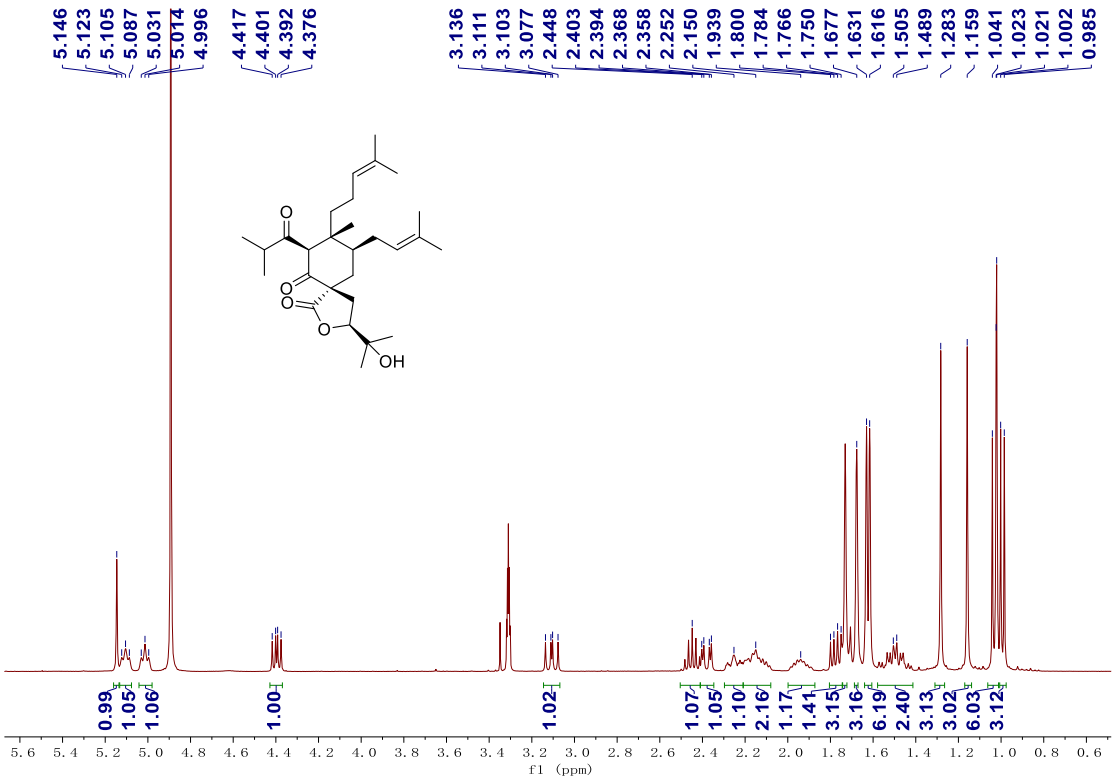


Figure S9. Linear correlation between experimental and calculated ^{13}C NMR chemical shifts of **2**.

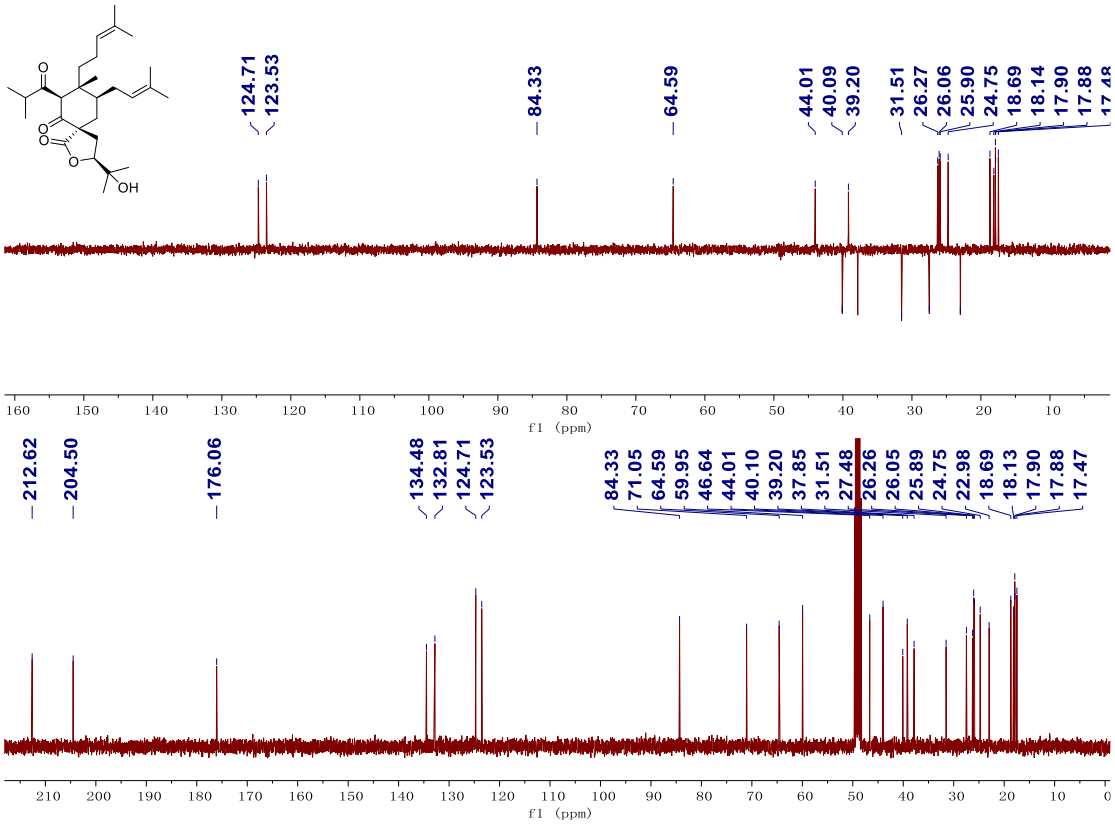
Table S14. Deviations between the calculated and experimental ^{13}C NMR chemical shifts for **2**.

no.	B				D			
	Exptl.	**Scal.calc.**	**Δδ**	**|Δδ|**	**Exptl.**	**Scal.calc.**	**Δδ**	**|Δδ|**
1	64.2	67.8	3.6	3.6	64.2	66.8	2.6	2.6
2	204.6	215.0	10.4	10.4	204.6	207.0	2.4	2.4
3	61.3	63.4	2.1	2.1	61.3	65.1	3.8	3.8
4	40.1	38.9	-1.2	1.2	40.1	39.8	-0.3	0.3
5	39.1	49.3	10.2	10.2	39.1	41.7	2.6	2.6
6	46.7	52.3	5.6	5.6	46.7	50.6	3.9	3.9
7	176.3	171.8	-4.5	4.5	176.3	171.6	-4.7	4.7
8	32.4	37.1	4.7	4.7	32.4	34.8	2.4	2.4
9	85.9	83.9	-2.0	2.0	85.9	84.1	-1.8	1.8
10	70.8	73.2	2.4	2.4	70.8	72.1	1.3	1.3
11	26.5	25.4	-1.1	1.1	26.5	30.4	3.9	3.9
12	24.8	26.5	1.7	1.7	24.8	21.2	-3.6	3.6
13	211.9	212.9	1.0	1.0	211.9	213.6	1.7	1.7
14	44.2	45.1	0.9	0.9	44.2	45.7	1.5	1.5
15	18.5	20.3	1.8	1.8	18.5	21.8	3.3	3.3
16	18.0	18.7	0.7	0.7	18.0	19.6	1.6	1.6
17	27.9	28.9	1.0	1.0	27.9	28.2	0.3	0.3
18	123.7	121.6	-2.1	2.1	123.7	121.4	-2.3	2.3
19	134.1	135.0	0.9	0.9	134.1	134.3	0.2	0.2
20	25.9	26.7	0.8	0.8	25.9	26.9	1.0	1.0
21	18.1	18.5	0.4	0.4	18.1	18.5	0.4	0.4
22	17.6	14.7	-2.9	2.9	17.6	18.2	0.6	0.6
23	37.8	43.5	5.7	5.7	37.8	36.9	-0.9	0.9
24	23.0	28.7	5.7	5.7	23.0	25.0	2.0	2.0
25	124.7	125.2	0.5	0.5	124.7	123.8	-0.9	0.9
26	132.9	130.6	-2.3	2.3	132.9	130.7	-2.2	2.2
27	26.1	26.8	0.7	0.7	26.1	26.9	0.8	0.8
28	17.9	18.6	0.7	0.7	17.9	18.7	0.8	0.8
			AveDev	2.8			AveDev	1.9
			MaxDev	10.4			MaxDev	4.7

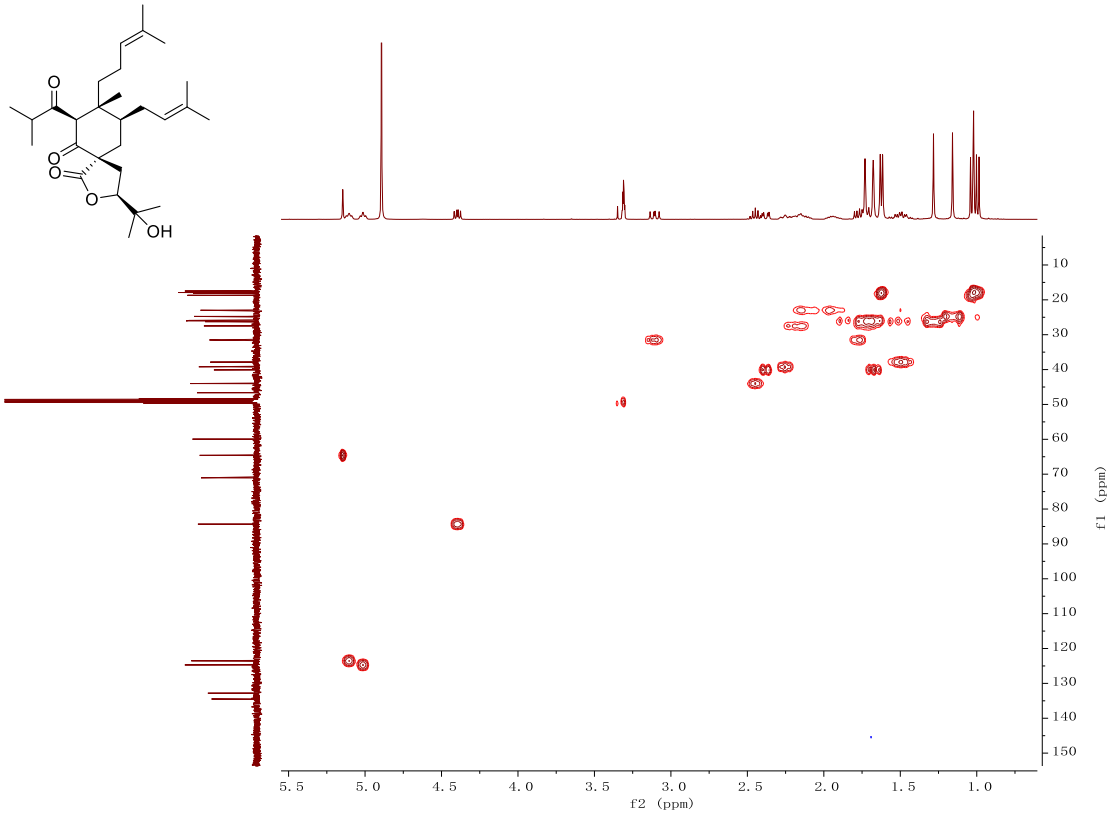
S10. ^{1}H NMR (400MHz, MeOD) spectrum of compound **1**



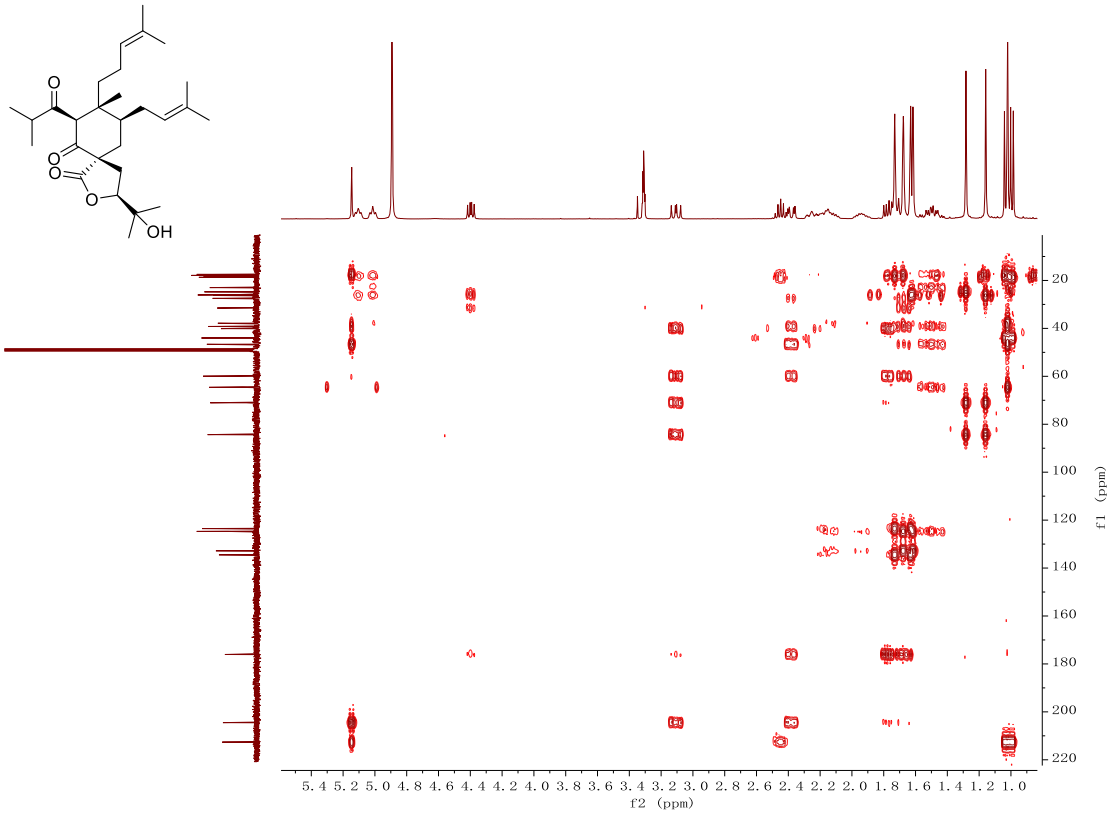
S11. ^{13}C NMR (100MHz, MeOD) spectrum of compound **1**



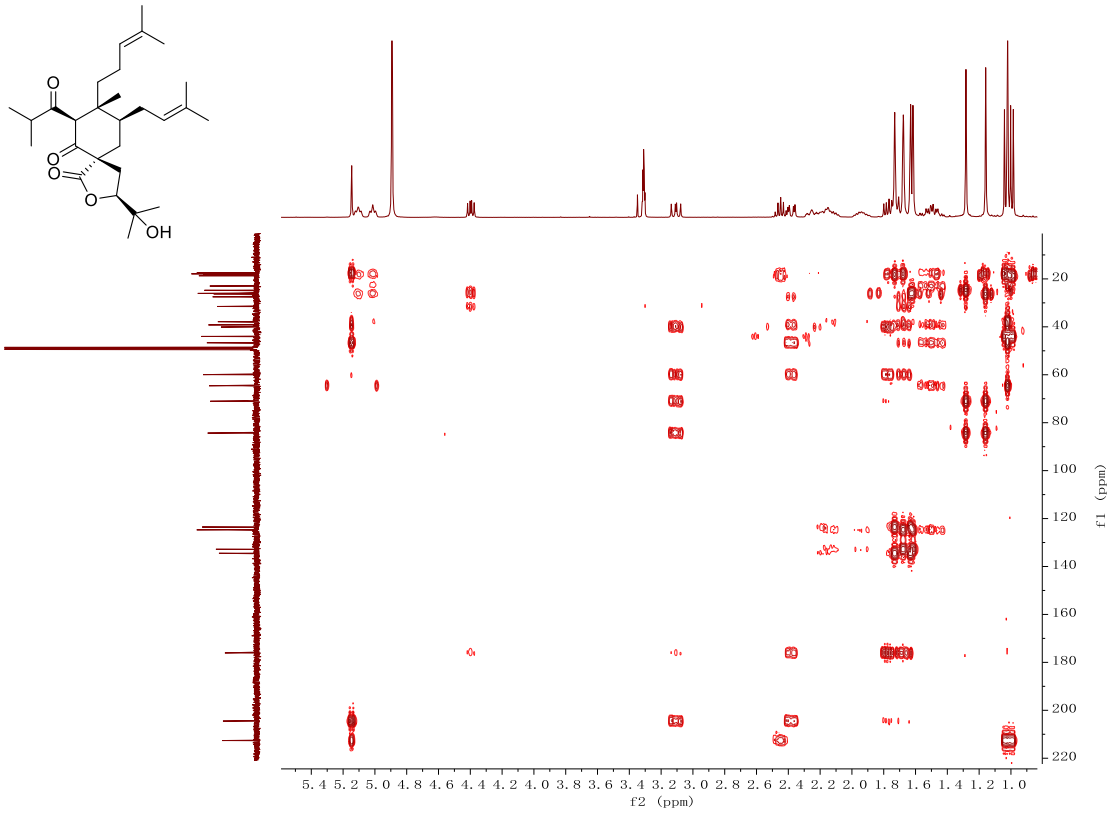
S12. HSQC spectrum of compound **1** in methanol-d_4



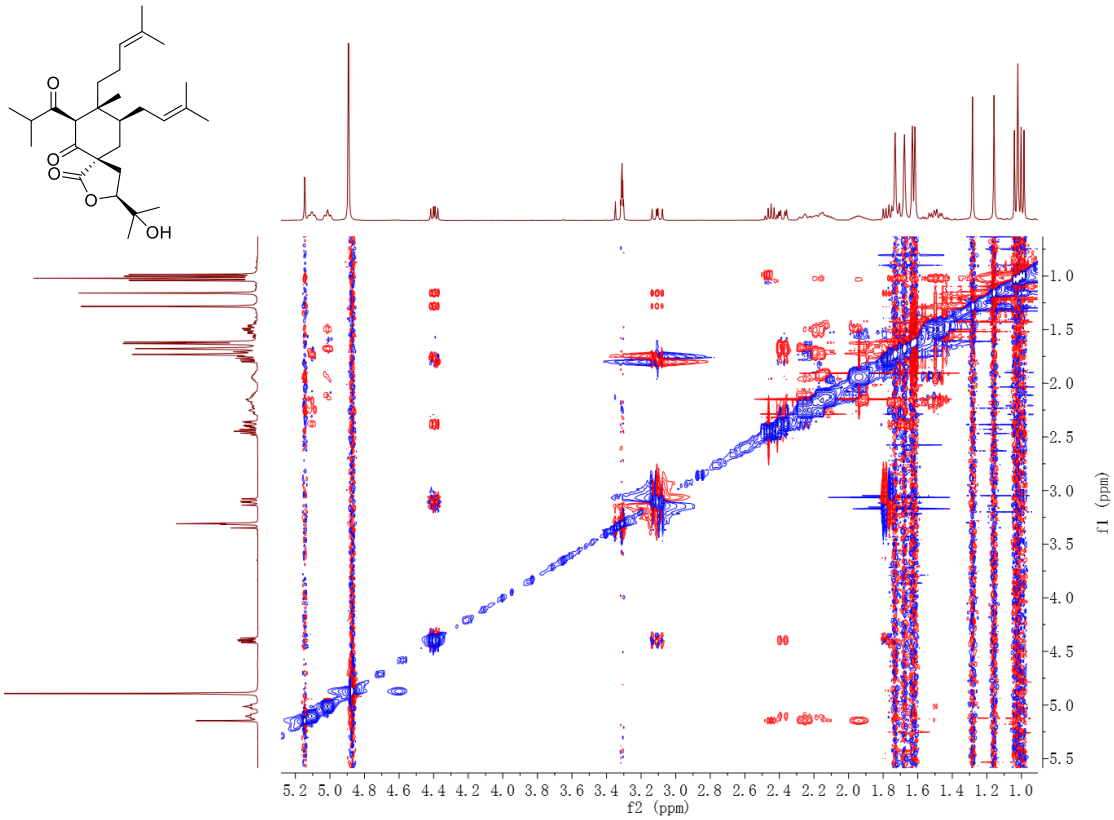
S13. HMBC spectrum of compound **1** in methanol-d_4



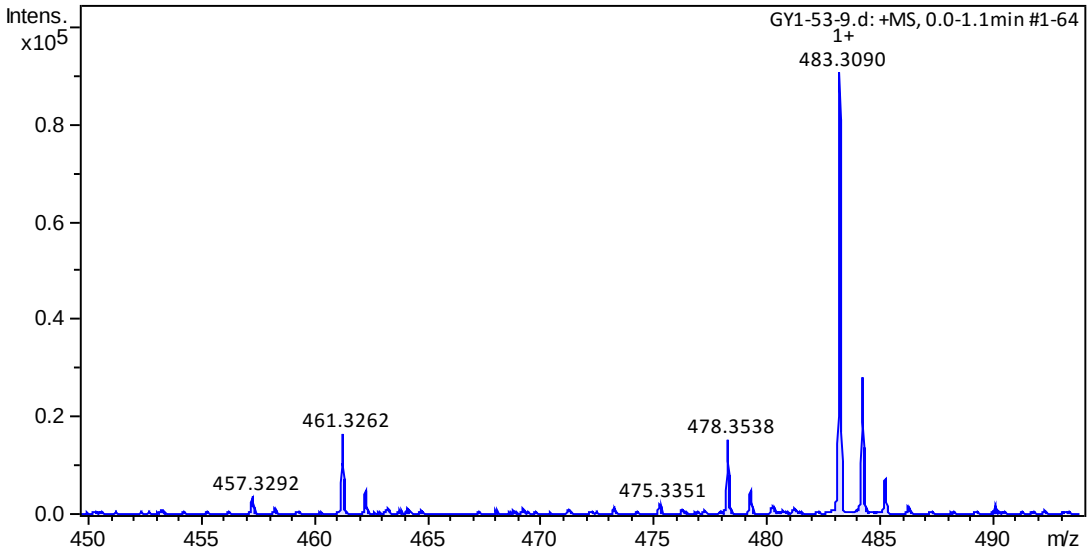
S14. ^{1}H–^{1}H COSY spectrum of compound **1** in methanol-d_4



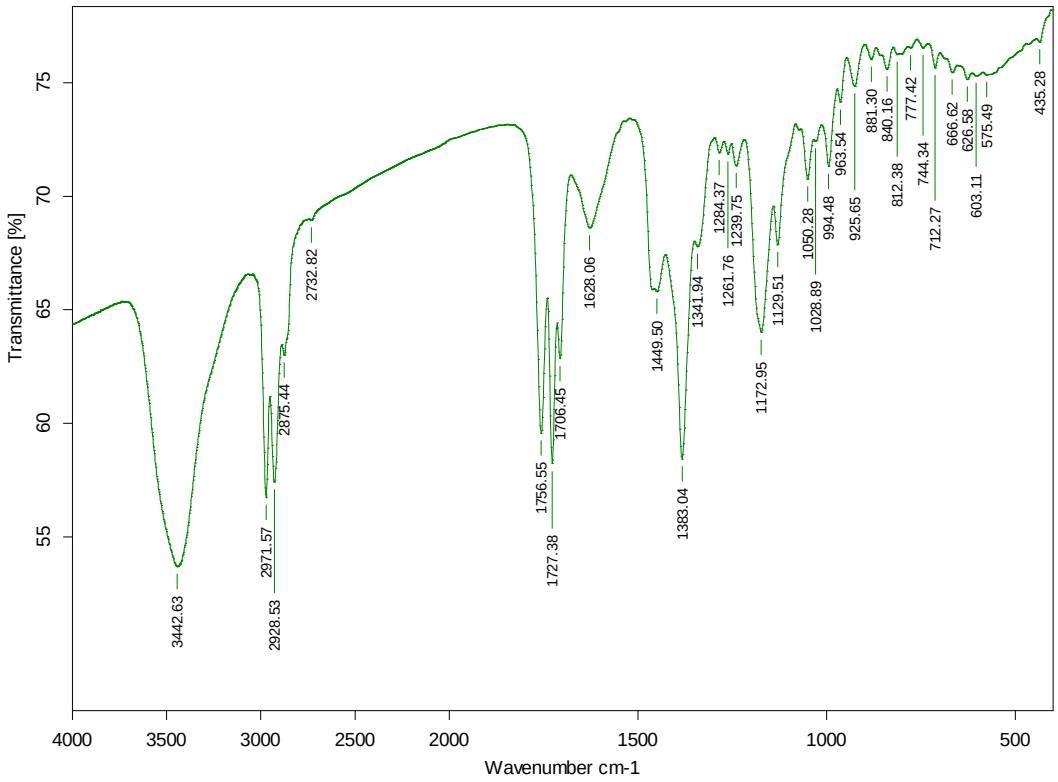
S15. NOESY spectrum of compound **1** in methanol-d_4



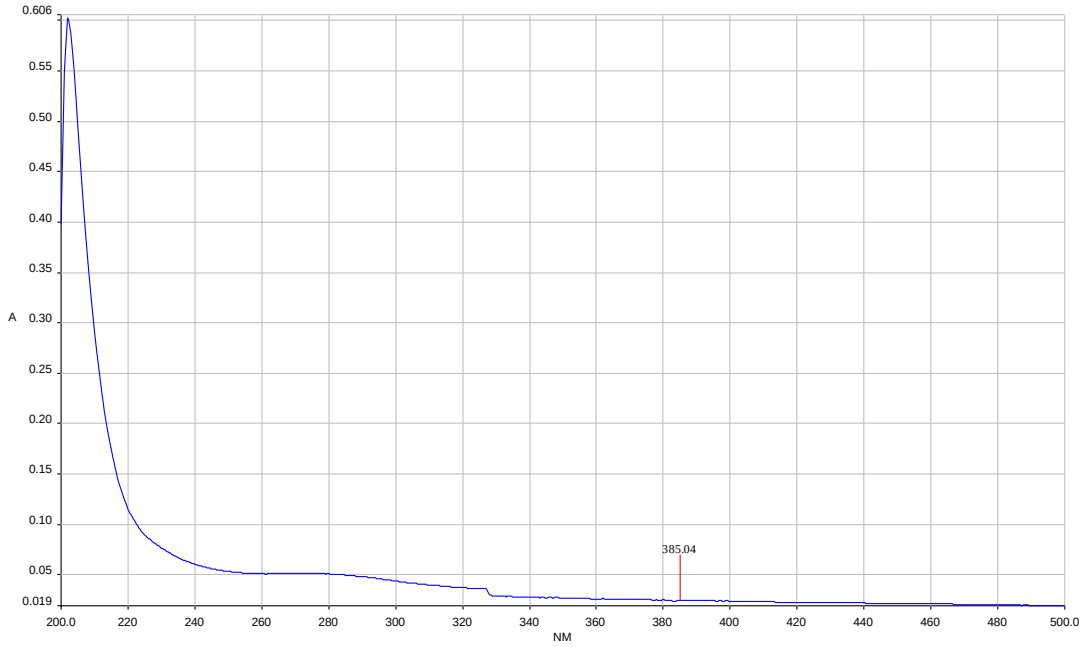
S16. HREIMS spectrum of compound **1**



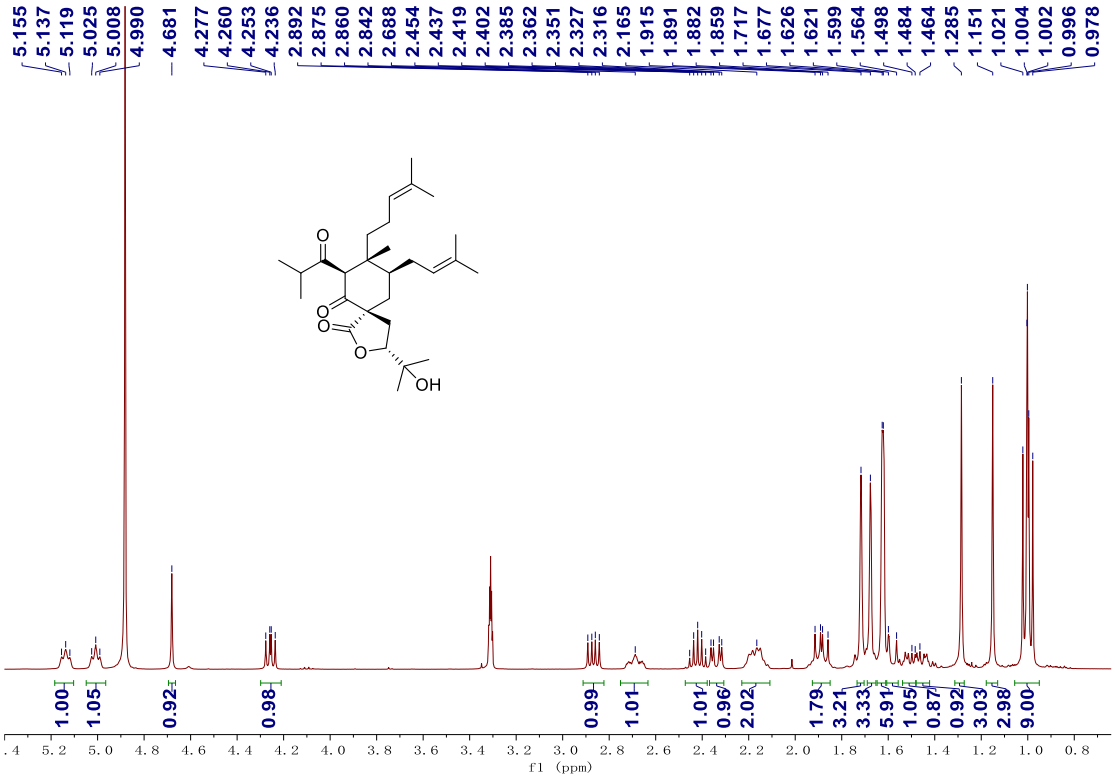
S17. IR spectrum of compound **1**



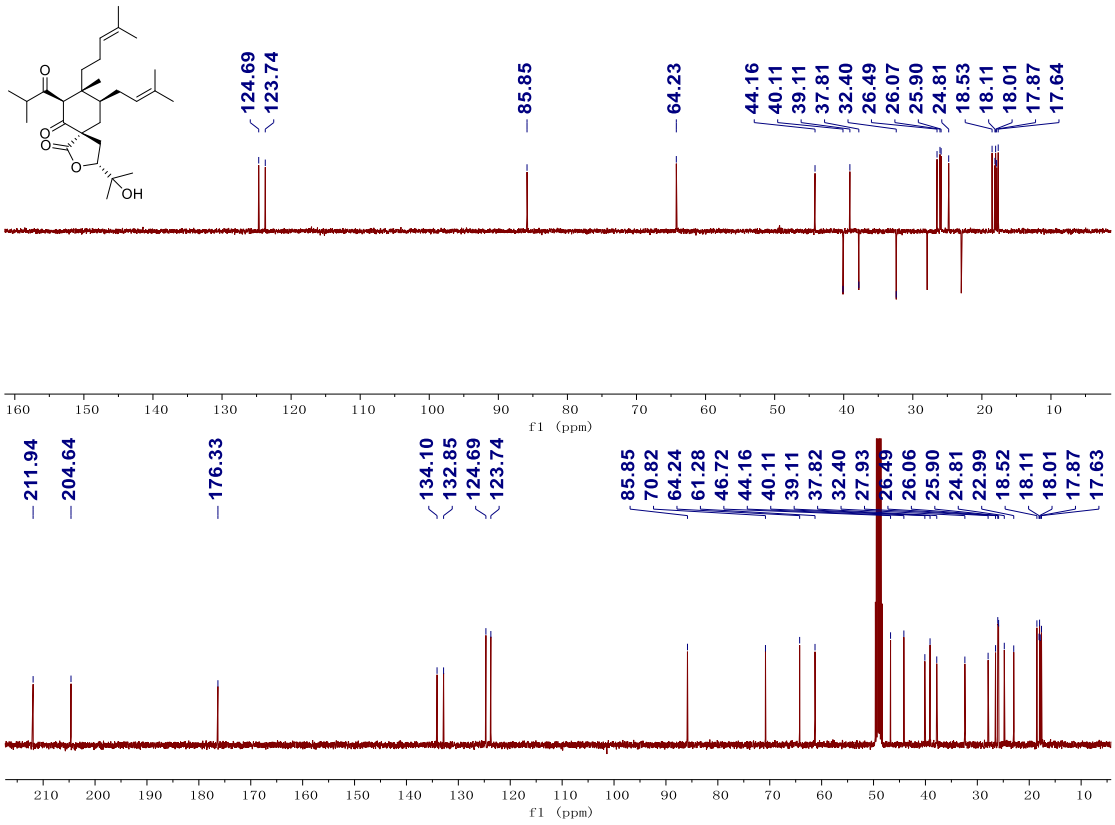
S18. UV spectrum of compound **1**



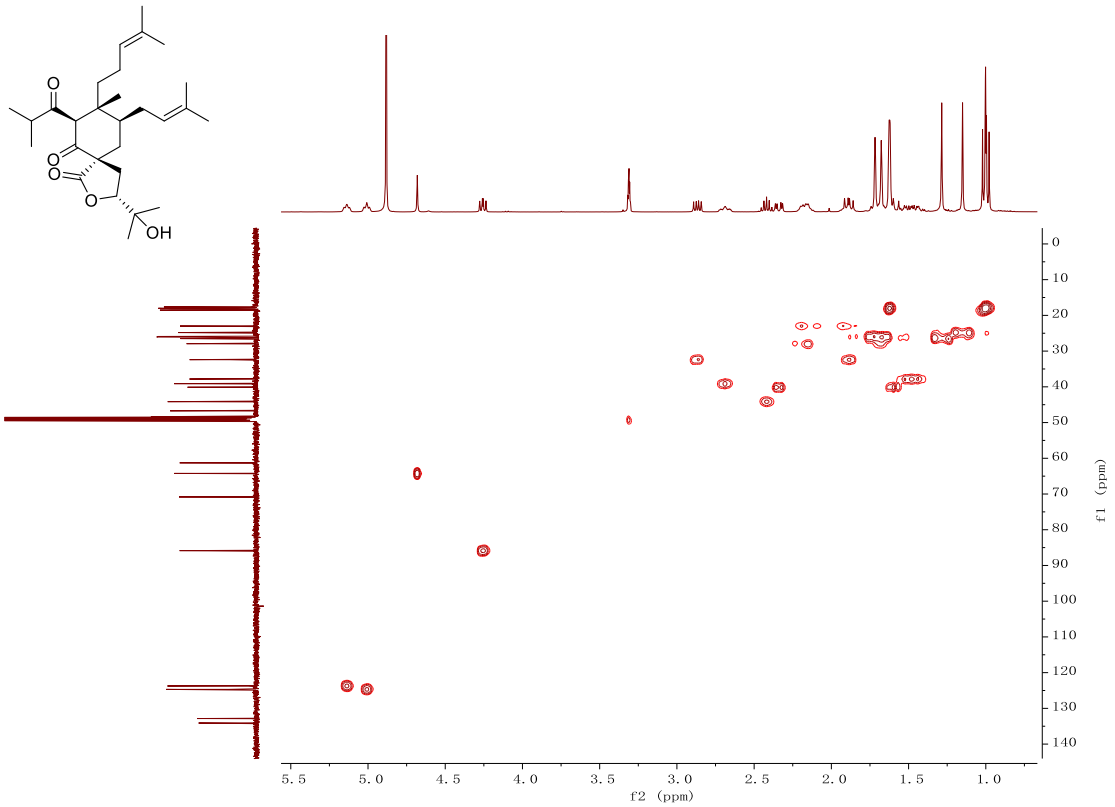
S19. ^{1}H NMR (400MHz, MeOD) spectrum of compound **2**



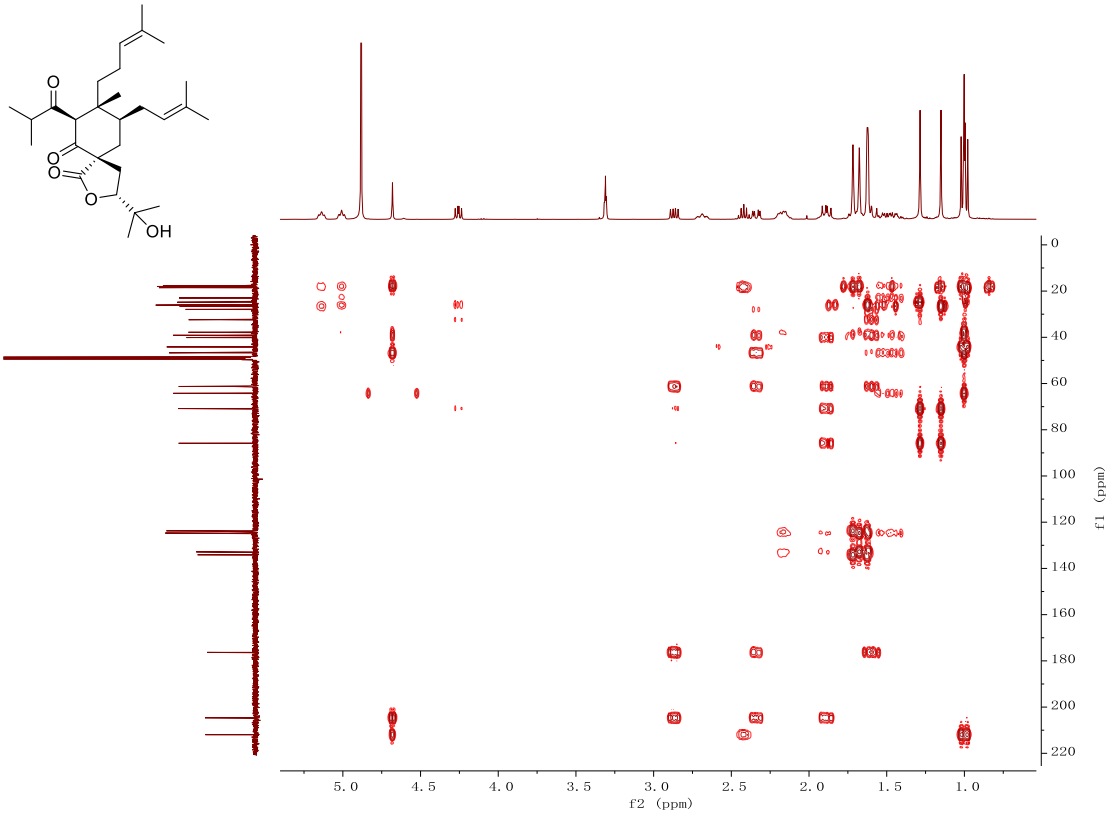
S20. ^{13}C NMR (100MHz, MeOD) spectrum of compound **2**



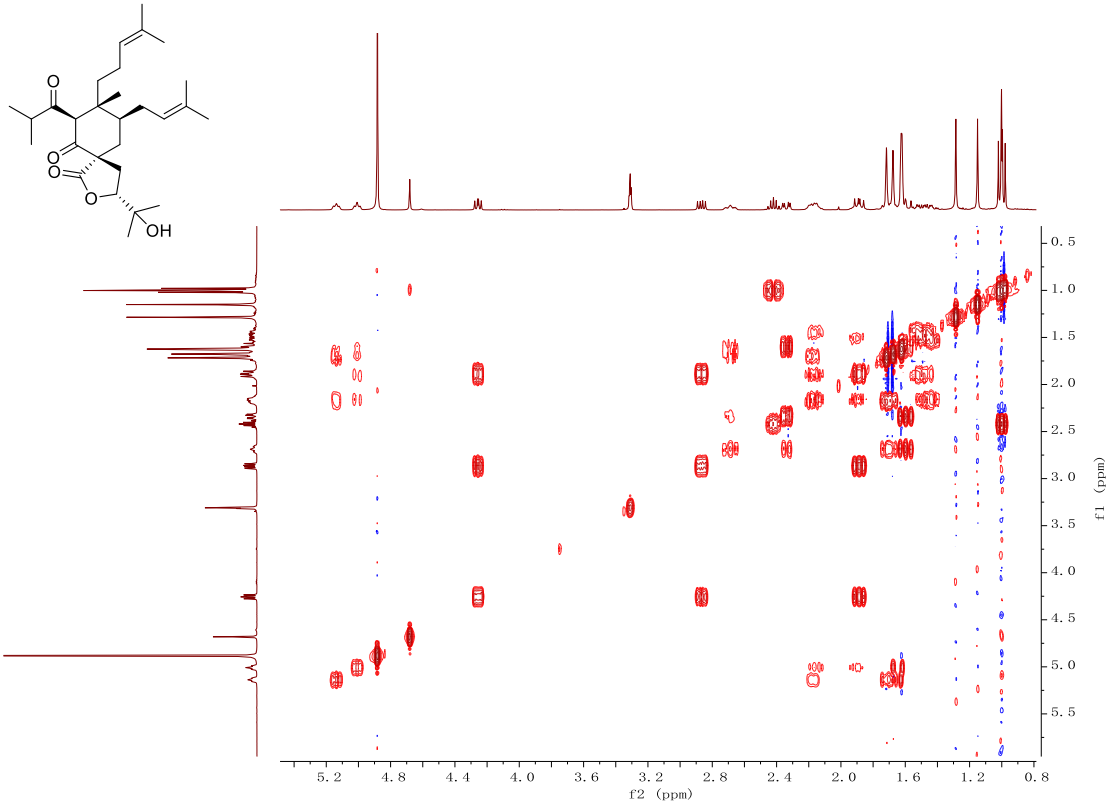
S21. HSQC spectrum of compound **2** in methanol-d_4



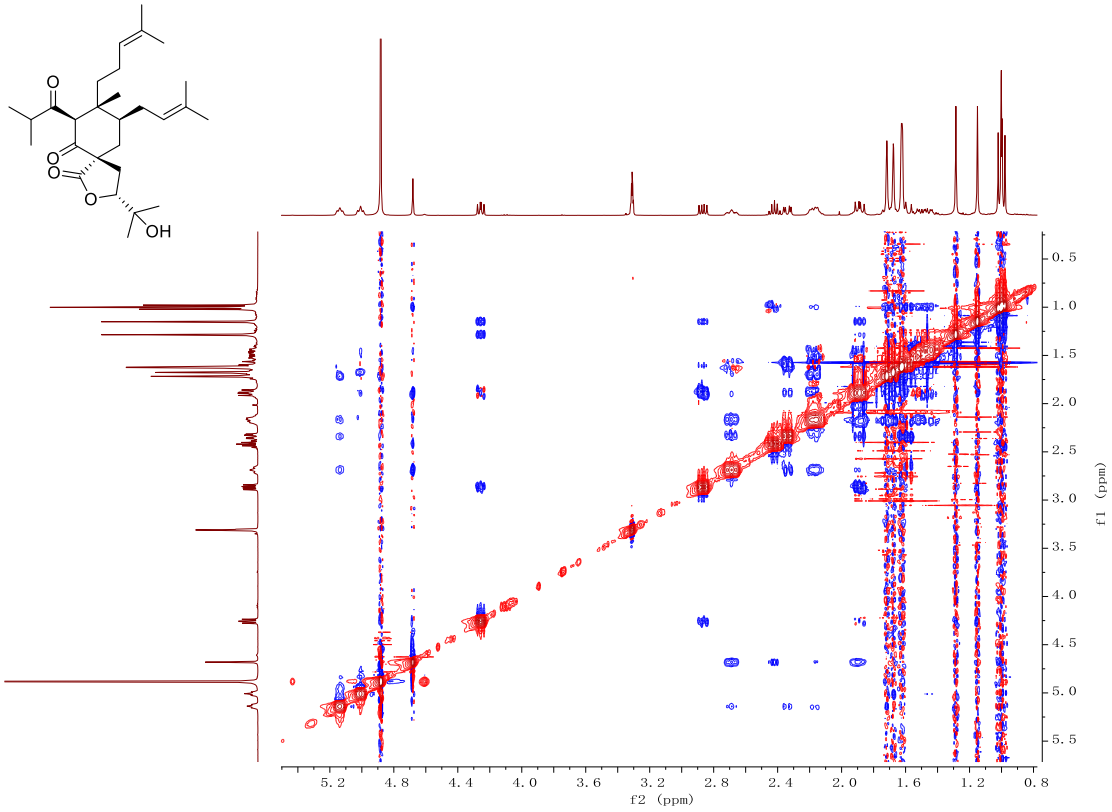
S22. HMBC spectrum of compound **2** in methanol-d_4



S23. ^{1}H–^{1}H COSY spectrum of compound **2** in methanol-d_4



S24. NOESY spectrum of compound **2** in methanol-d_4



S25. HREIMS spectrum of compound **2**

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\test\GY 1-48-16 APCI poss_000001.d	Acquisition Date	10/21/2016 5:27:16 PM
Method	20160104_P	Operator	
Sample Name	Sample	Instrument	solariX
Comment			

Acquisition Parameter

Polarity	Positive	n/a	n/a	No. of Laser Shots	200
n/a	n/a	No. of Cell Fills	1	Laser Power	20.0 lp
Broadband Low Mass	147.5 m/z	n/a	n/a	n/a	n/a
Broadband High Mass	3000.0 m/z	n/a	n/a	n/a	n/a
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Pulse Program	basic	n/a	n/a	Calibration Date	Mon Jan 4 08:26:07 2016
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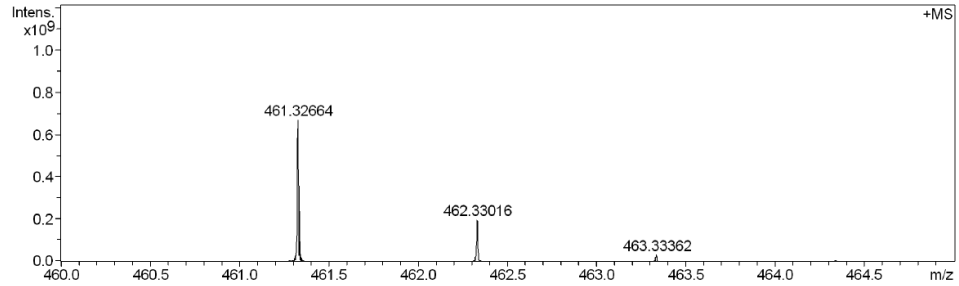
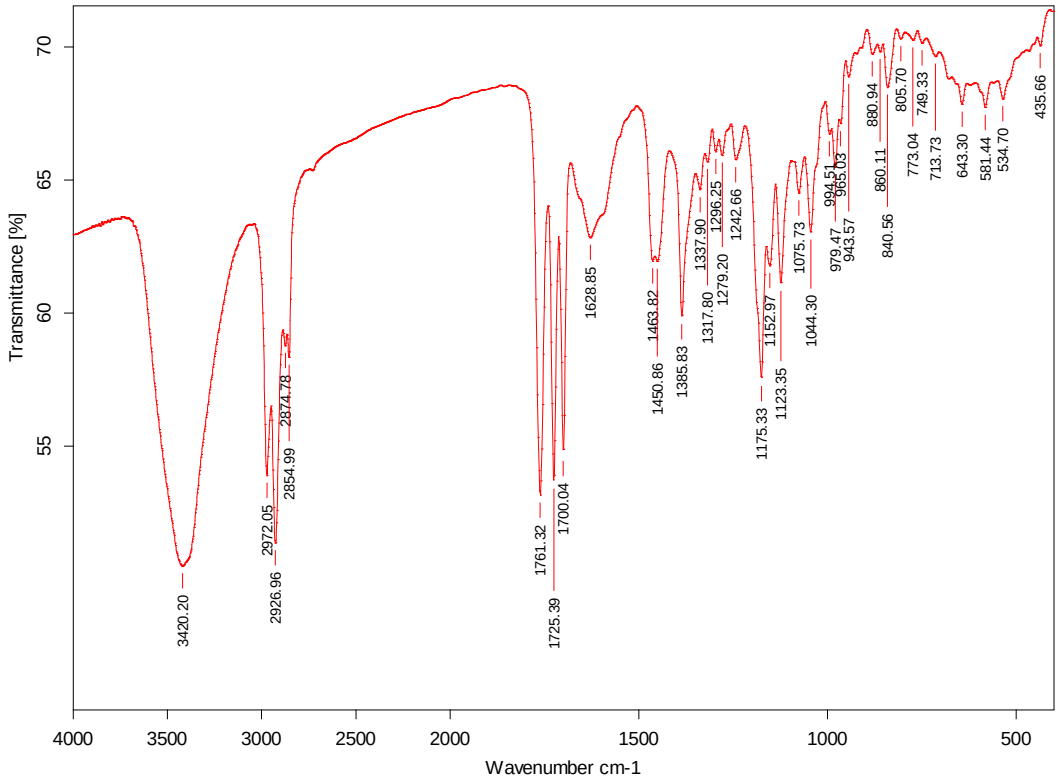
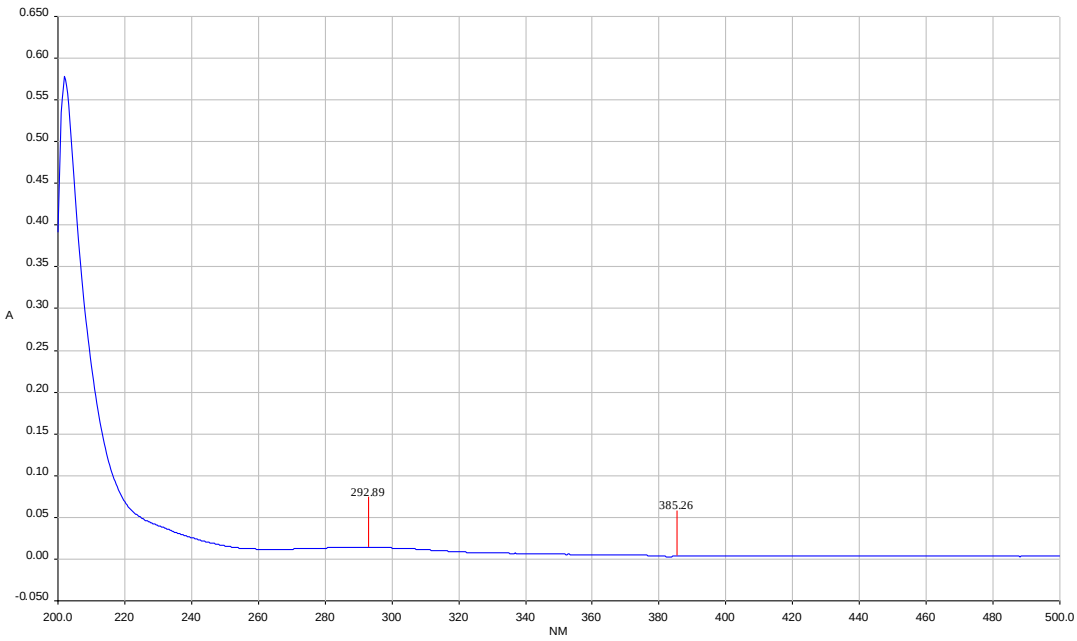


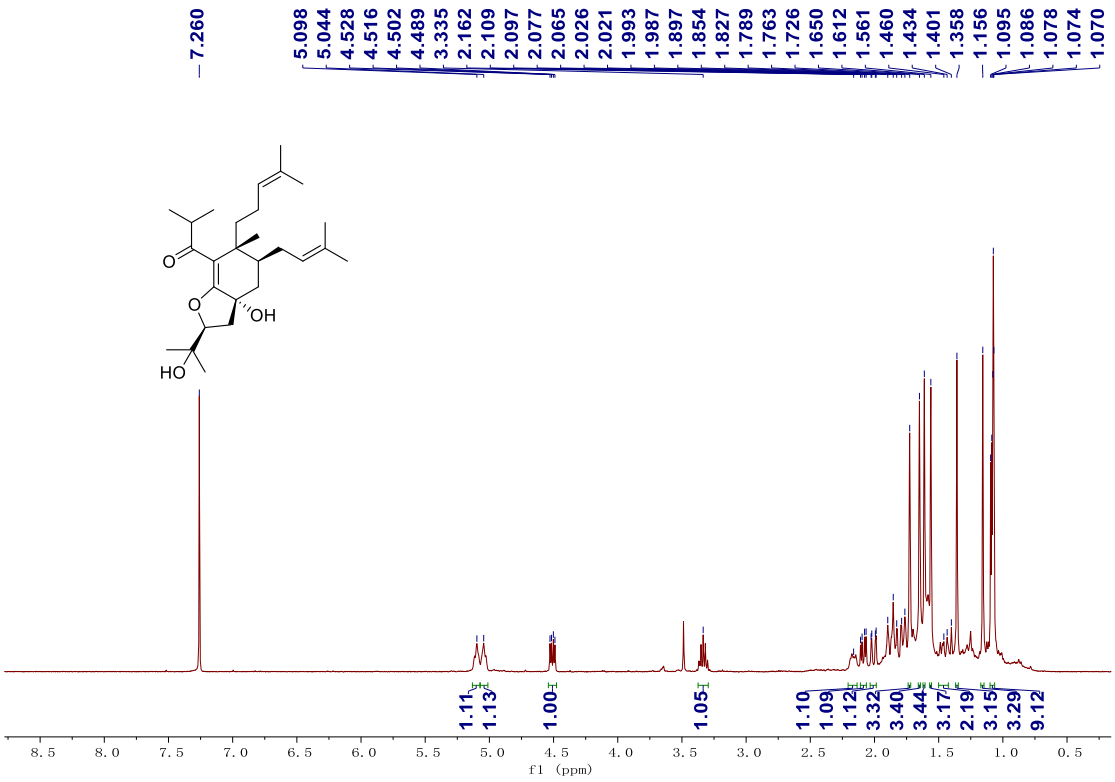
S26. IR spectrum of compound **2**



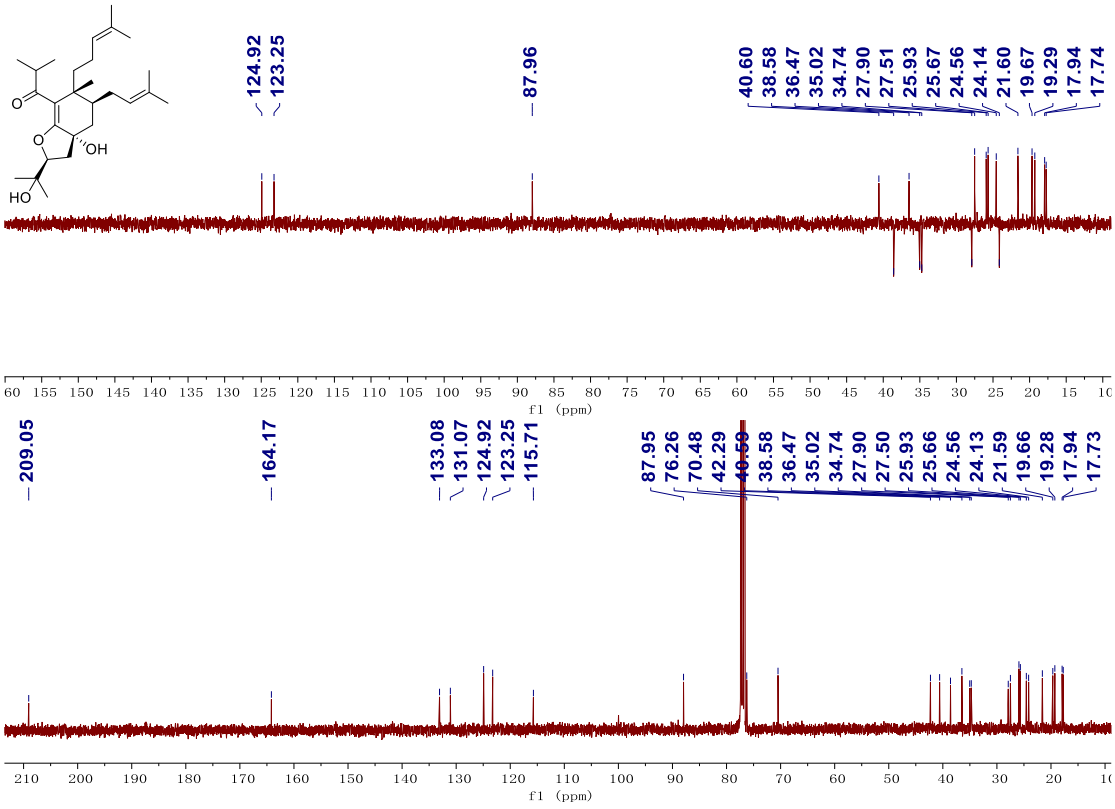
S27. UV spectrum of compound **2**



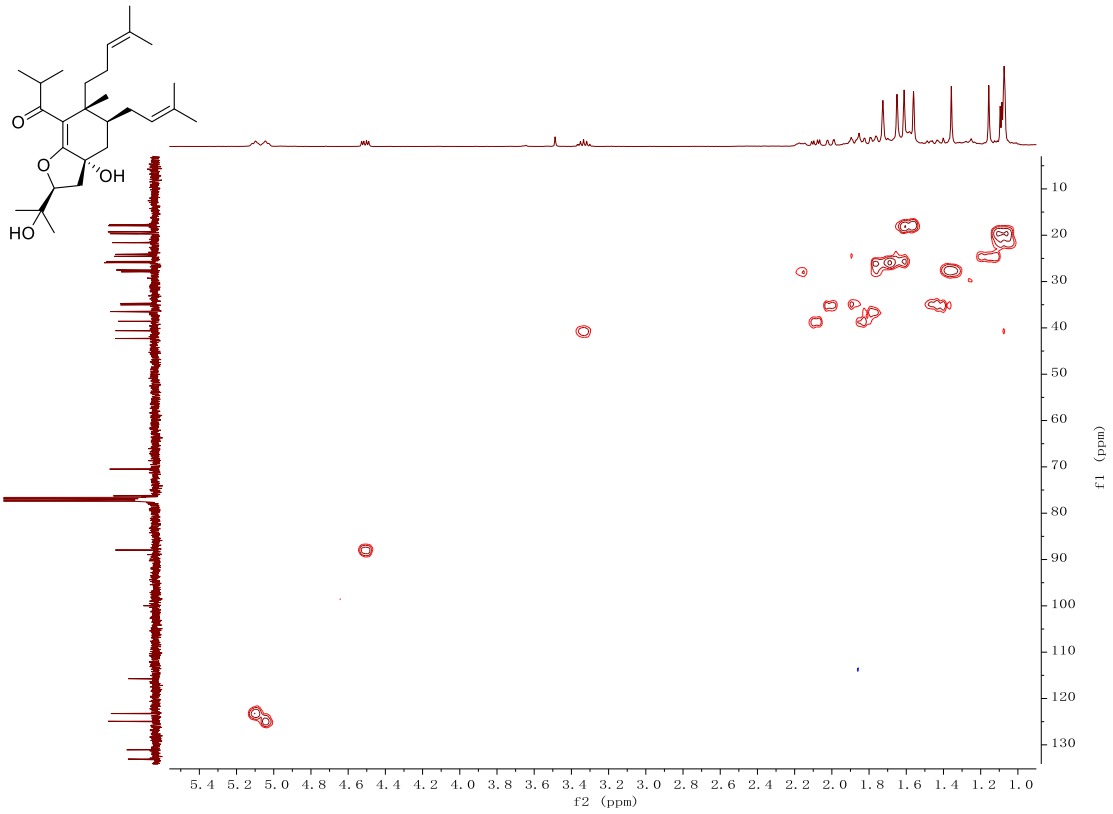
S28. ^{1}H NMR (400MHz, $CDCl_3$) spectrum of compound **3**



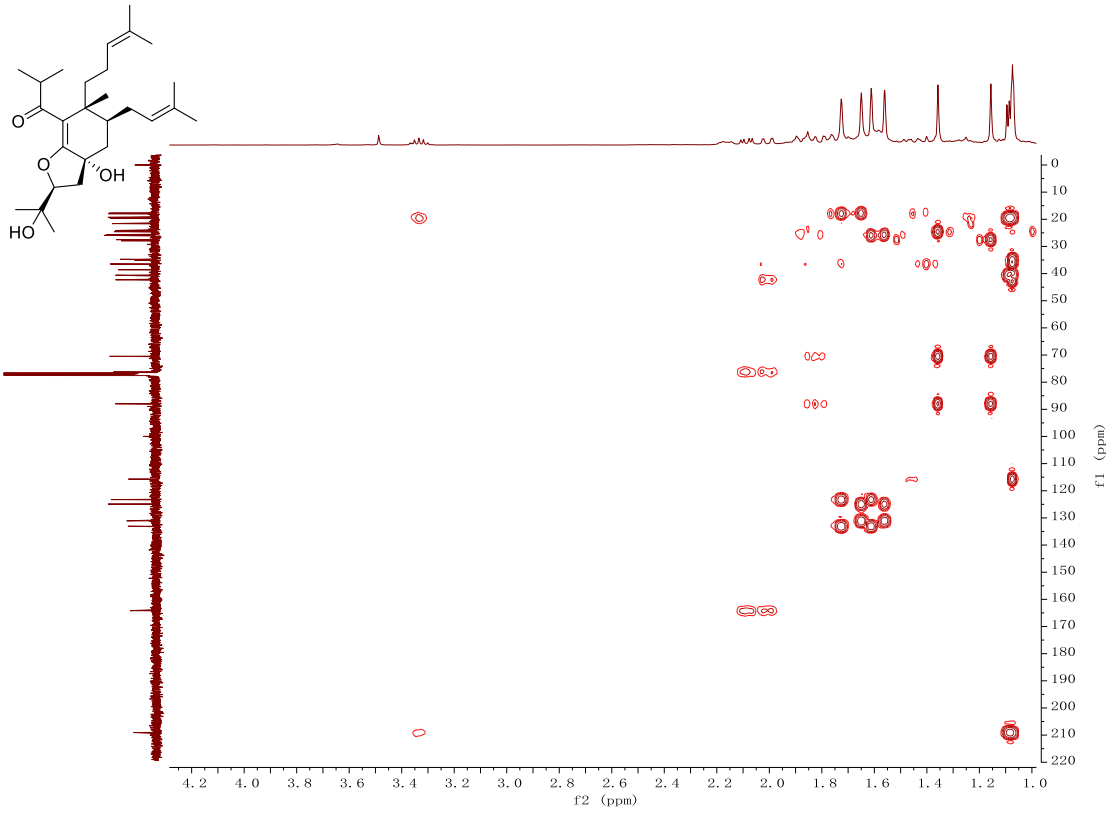
S29. ^{13}C NMR (100MHz, $CDCl_3$) spectrum of compound **3**



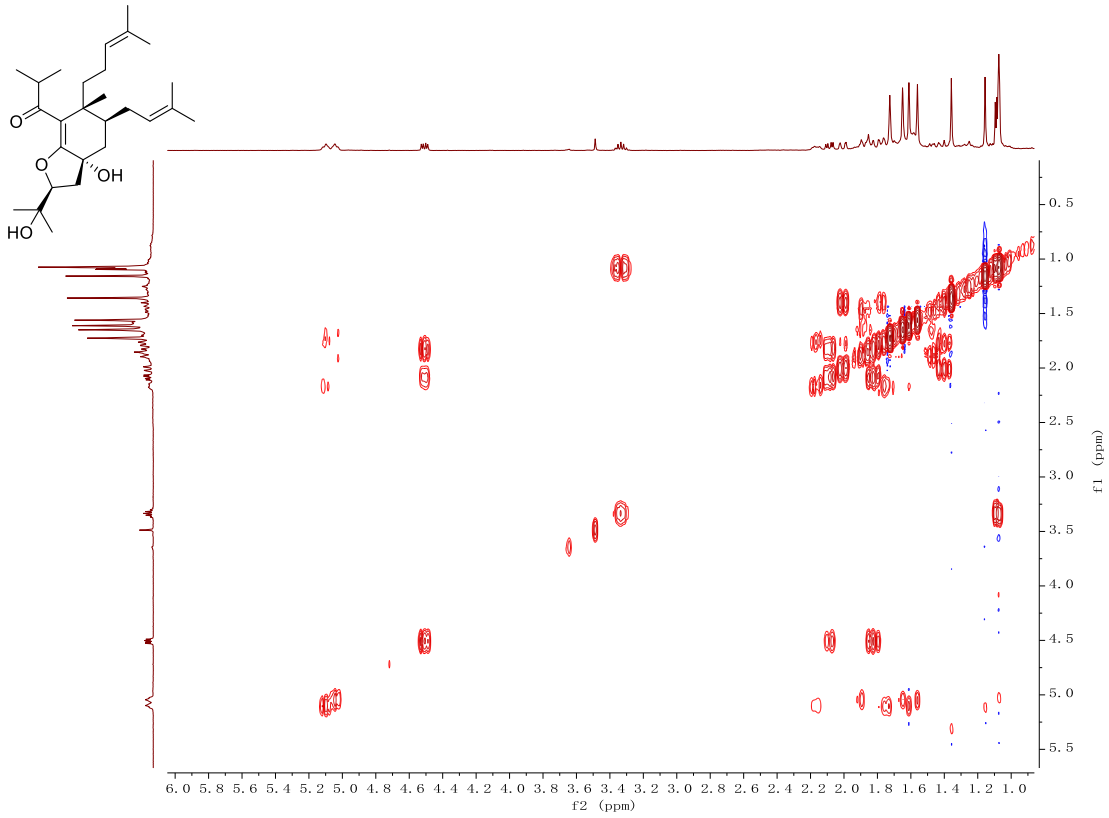
S30. HSQC spectrum of compound **3** in $CDCl_3$



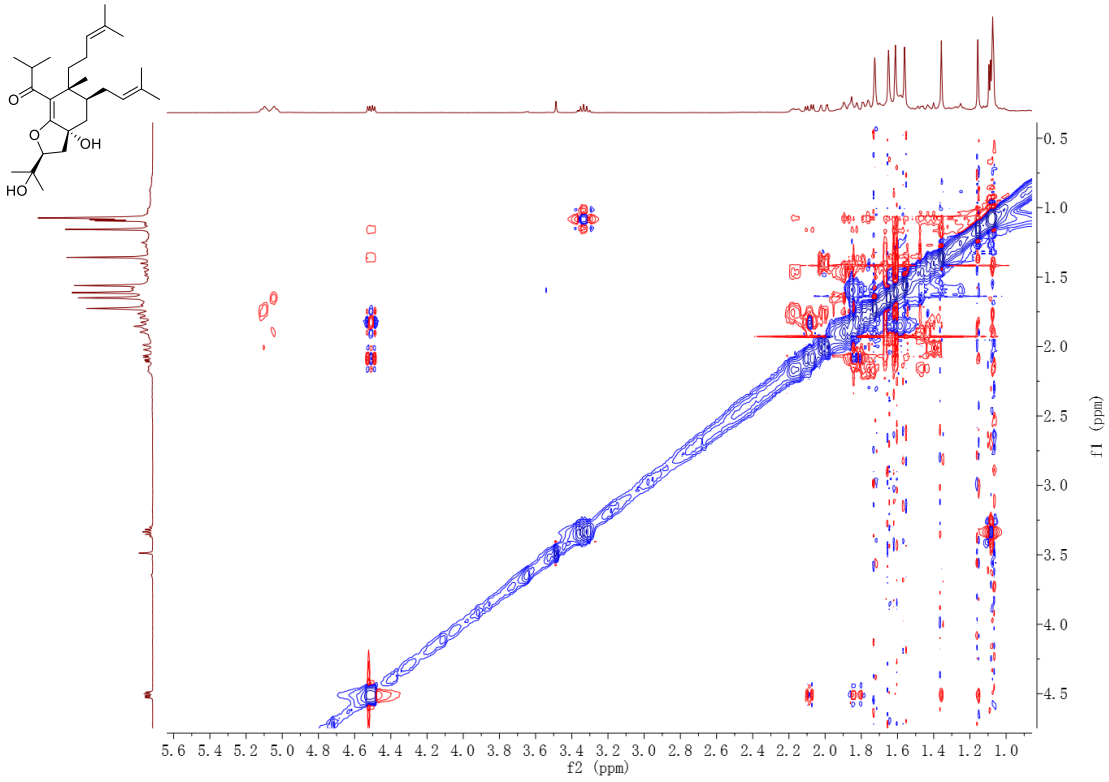
S31. HMBC spectrum of compound **3** in $CDCl_3$



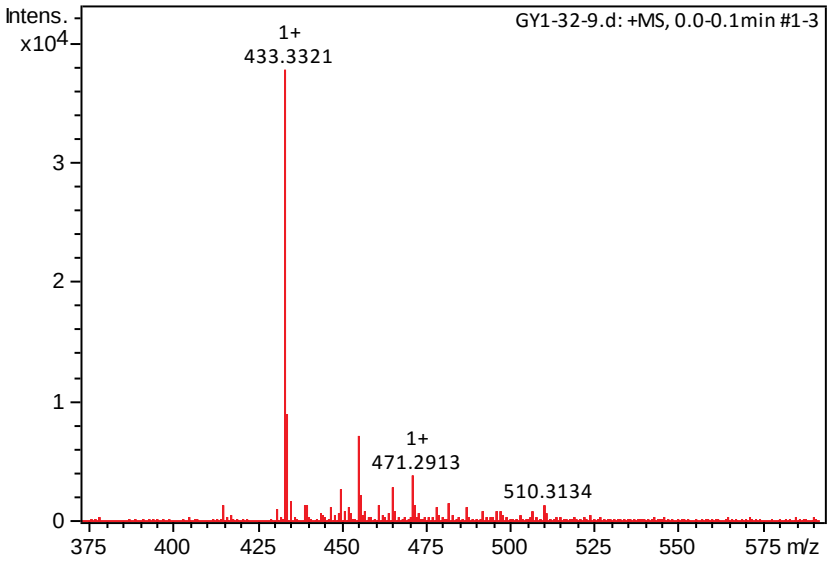
S32. $^{1}H–^{1}H$ COSY spectrum of compound **3** in $CDCl_3$



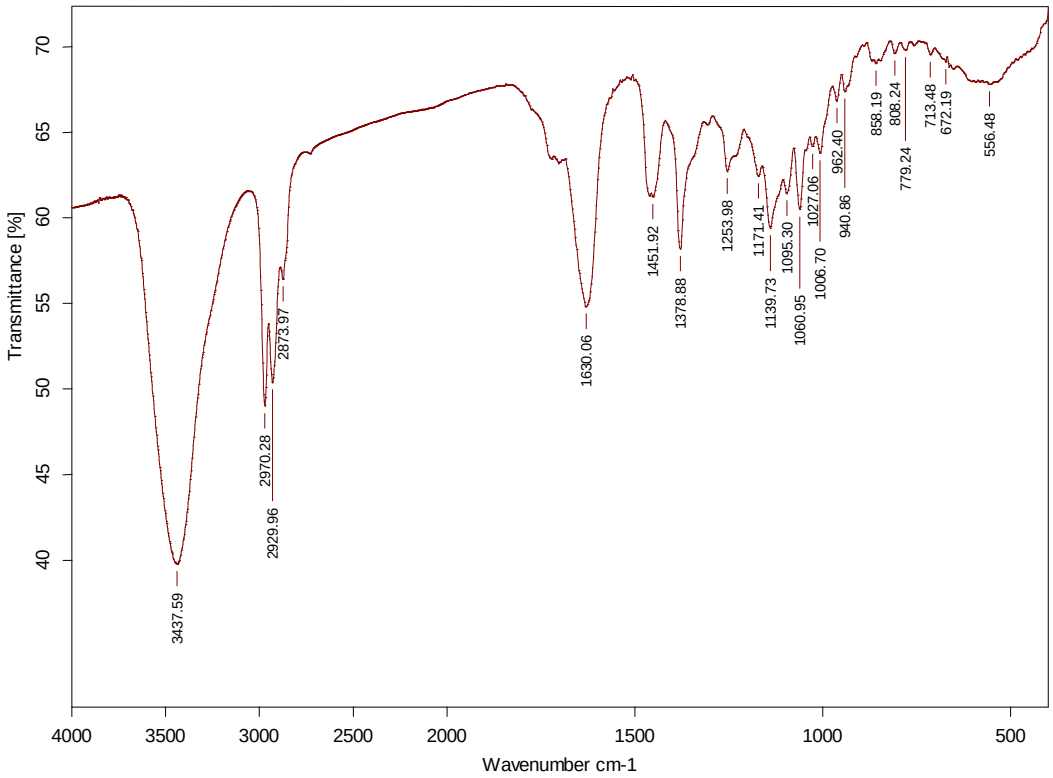
S33. NOESY spectrum of compound **3** in $CDCl_3$



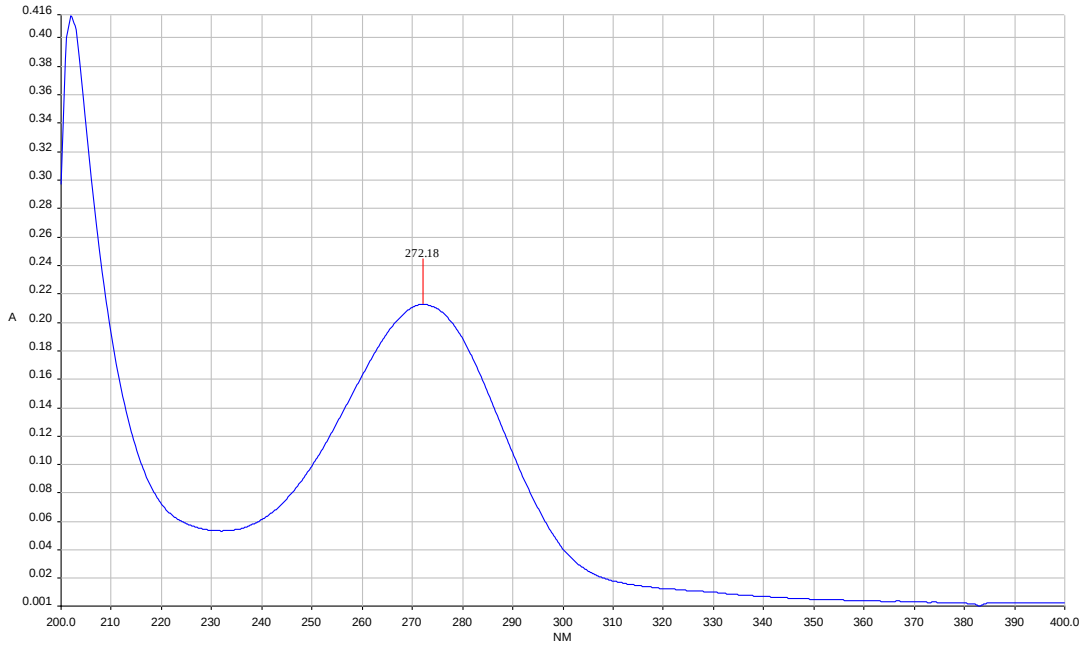
S34. HREIMS spectrum of compound **3**



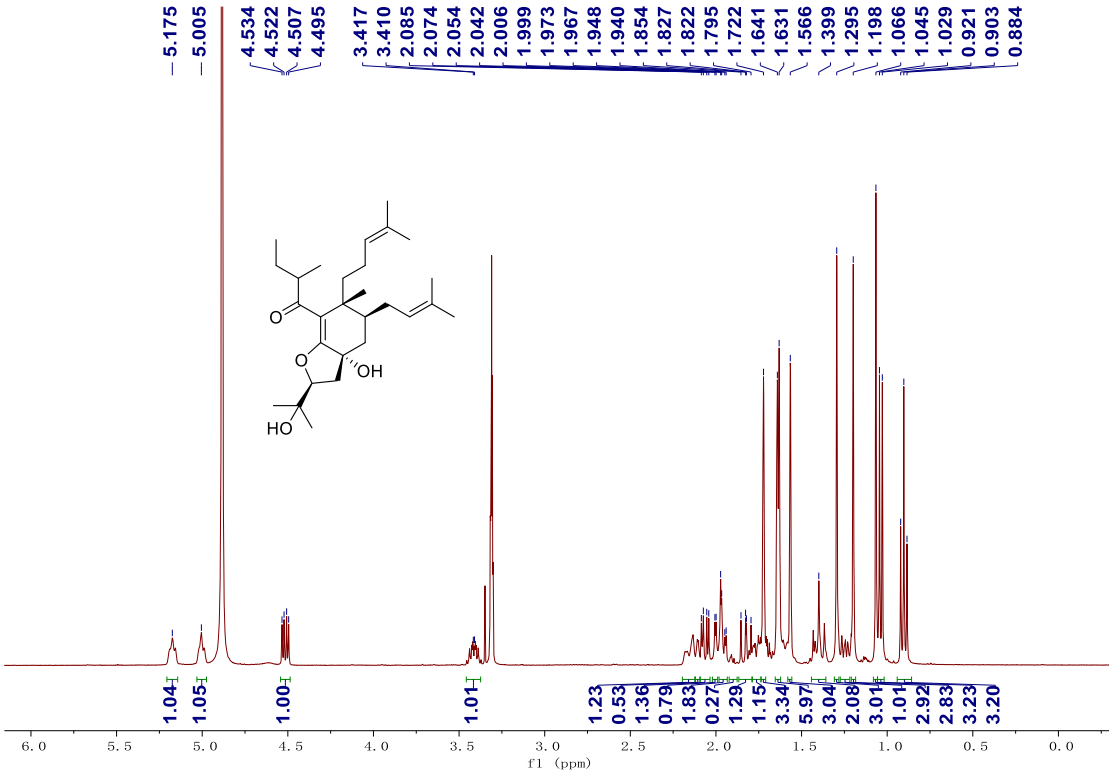
S35. IR spectrum of compound **3**



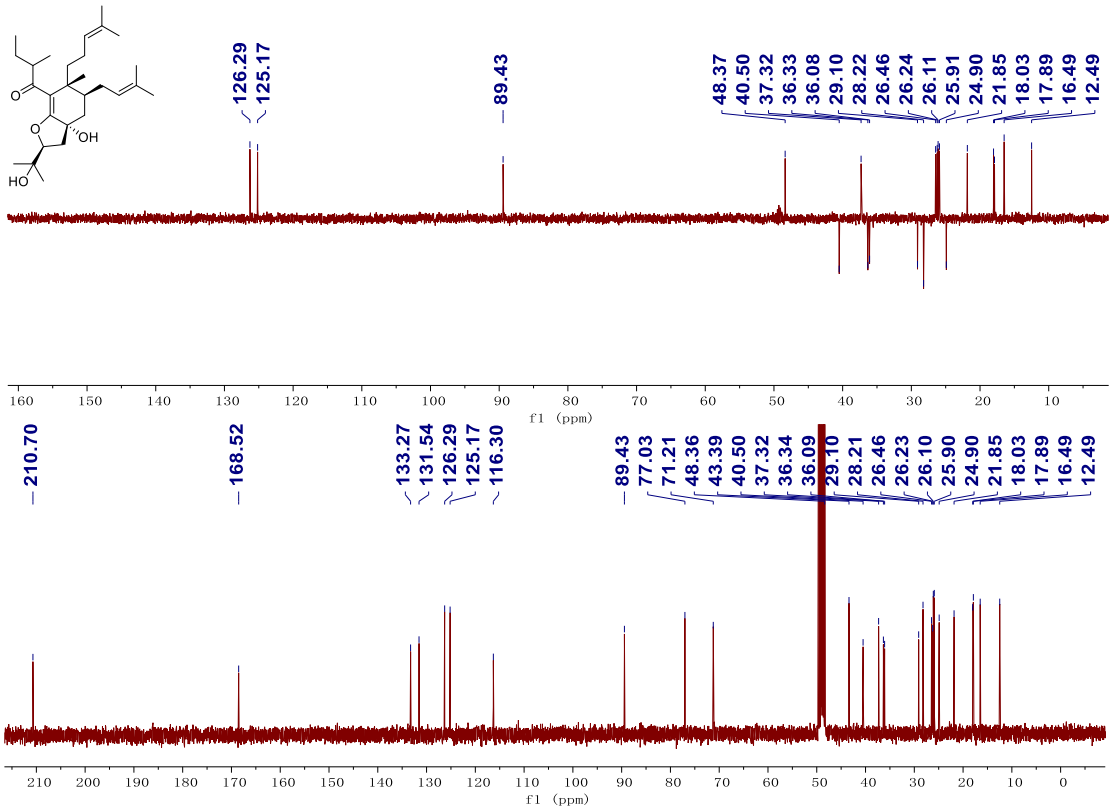
S36. UV spectrum of compound **3**



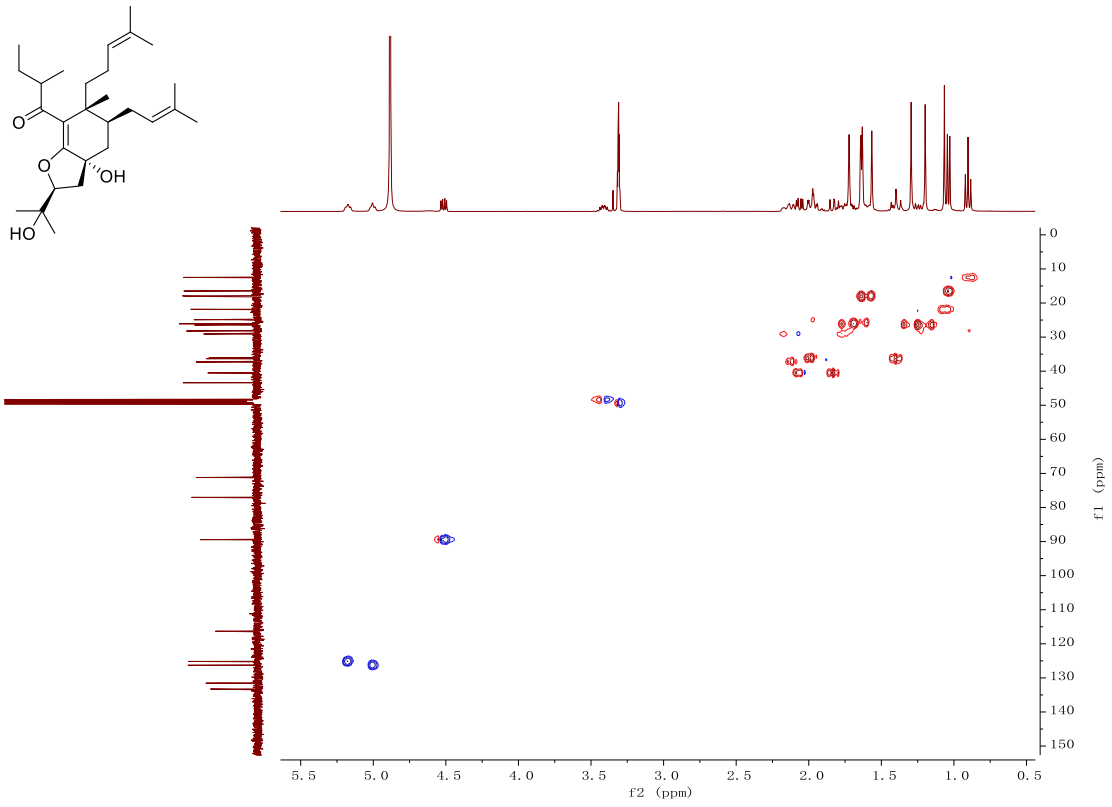
S37. ^{1}H NMR (400MHz, MeOD) spectrum of compound **4**



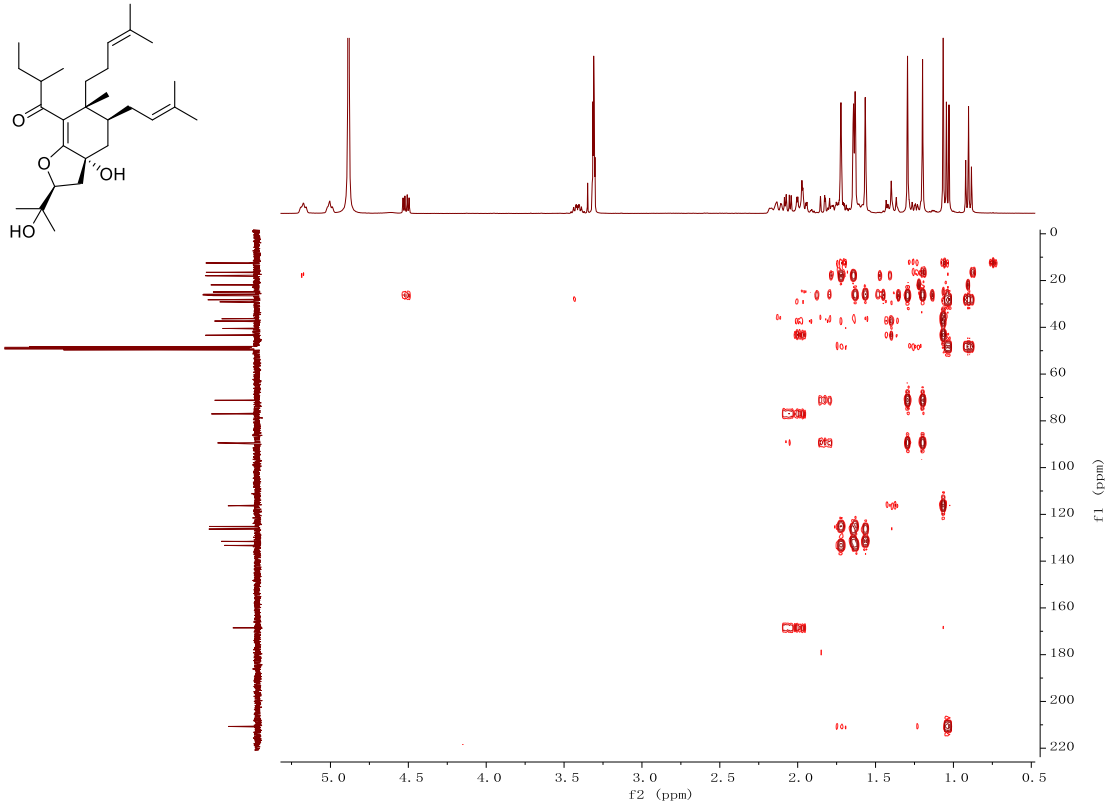
S38. ^{13}C NMR (100MHz, MeOD) spectrum of compound **4**



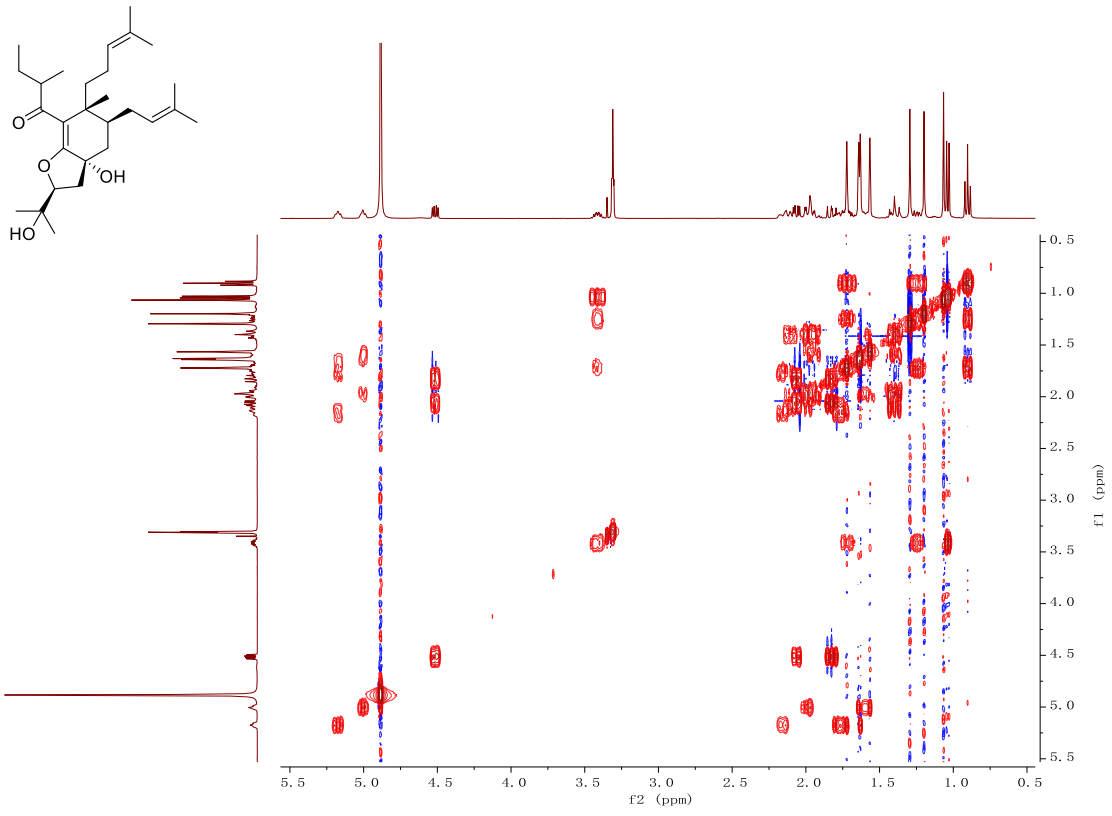
S39. HSQC spectrum of compound **4** in methanol-d_4



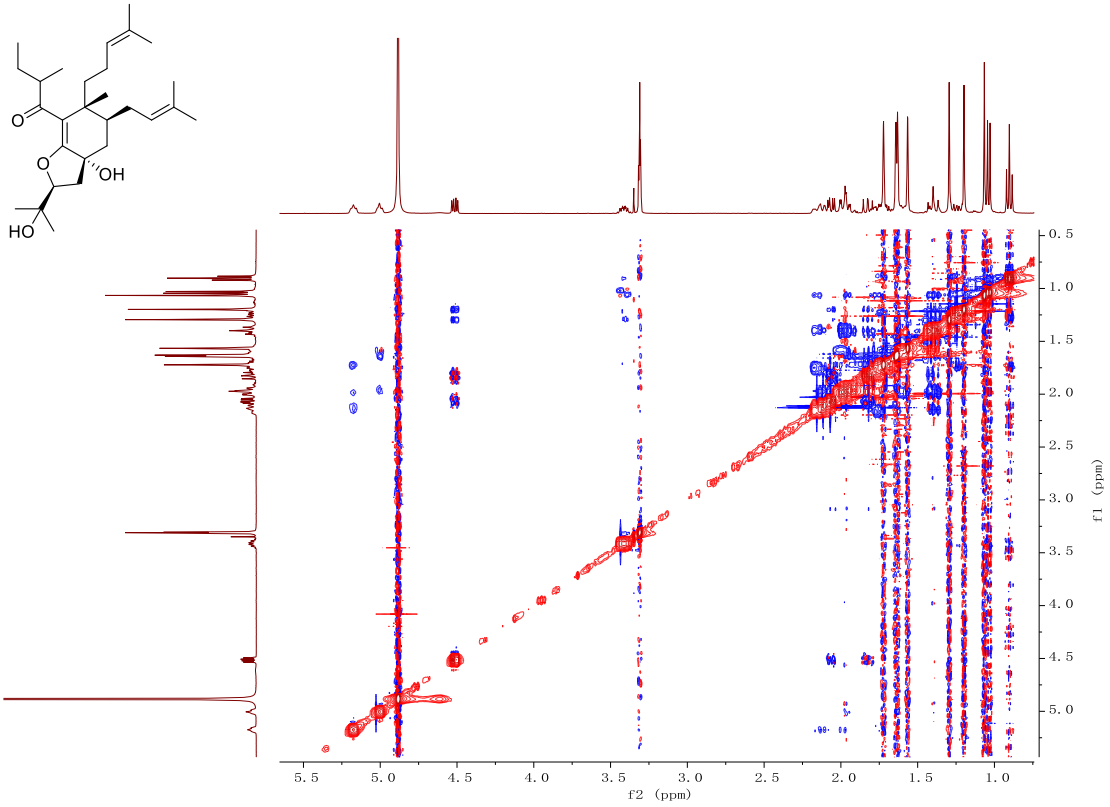
S40. HMBC spectrum of compound **4** in methanol-d_4



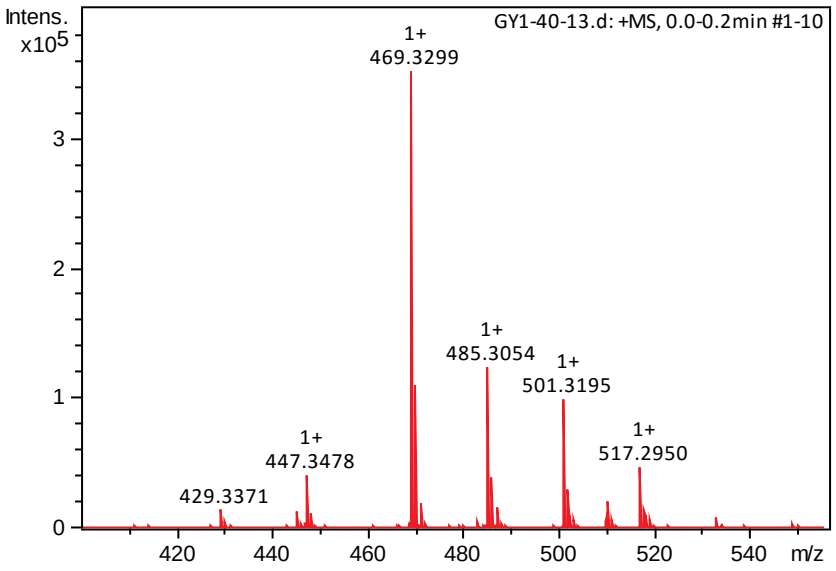
S41. ^{1}H–^{1}H COSY spectrum of compound **4** in methanol-d_4



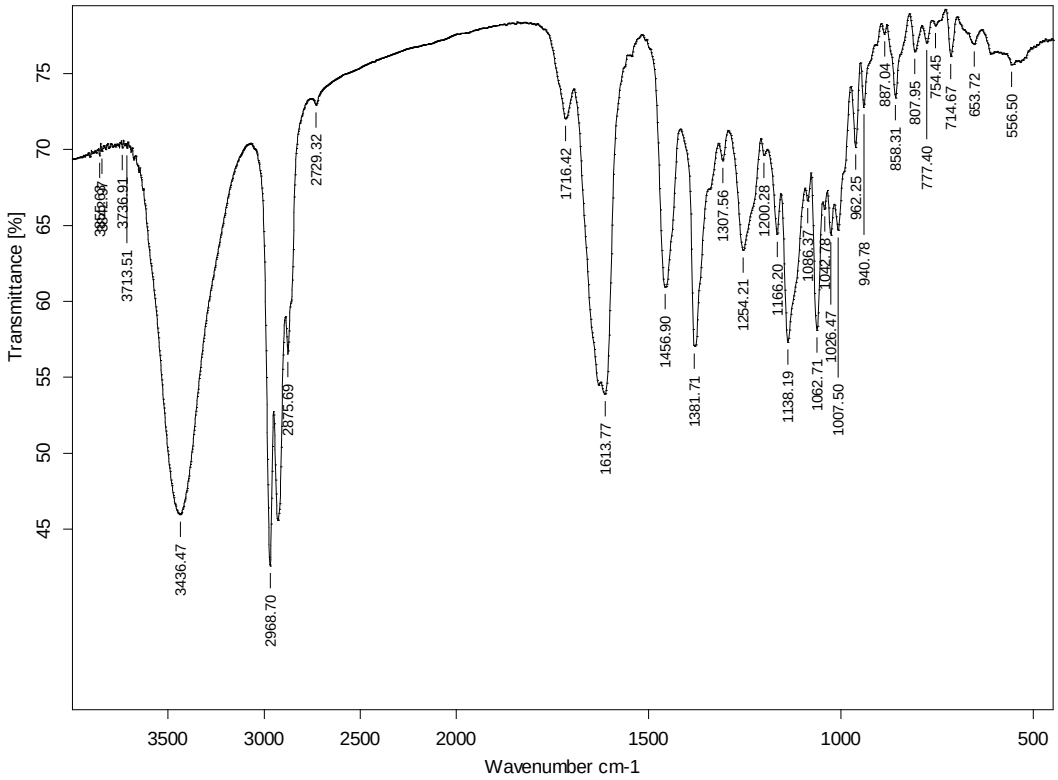
S42. NOESY spectrum of compound **4** in methanol-d_4



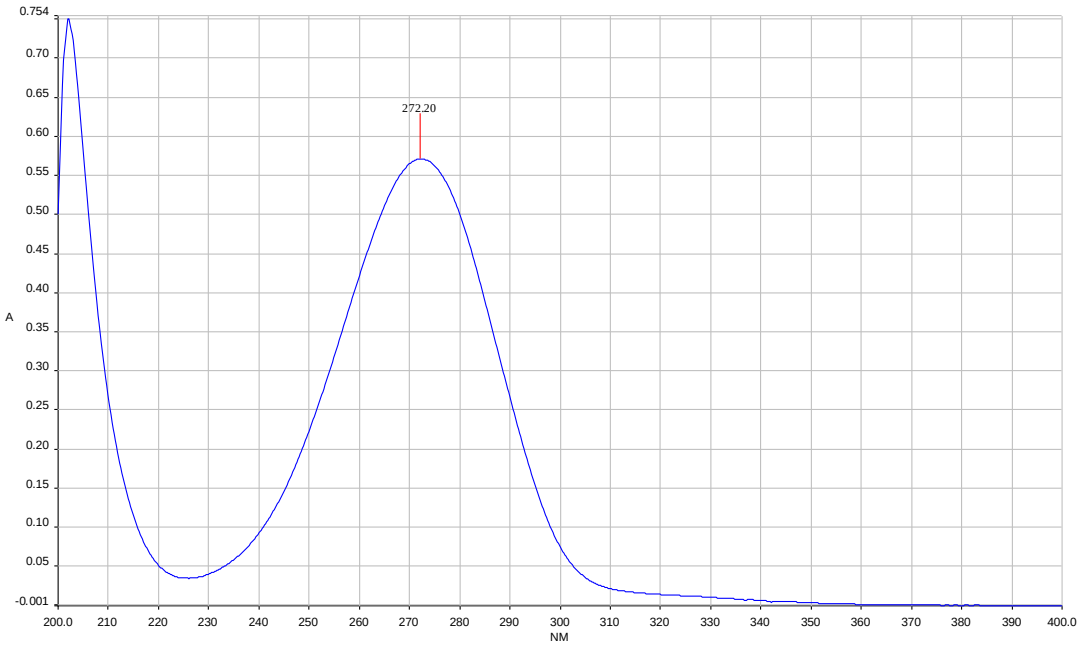
S43. HREIMS spectrum of compound **4**



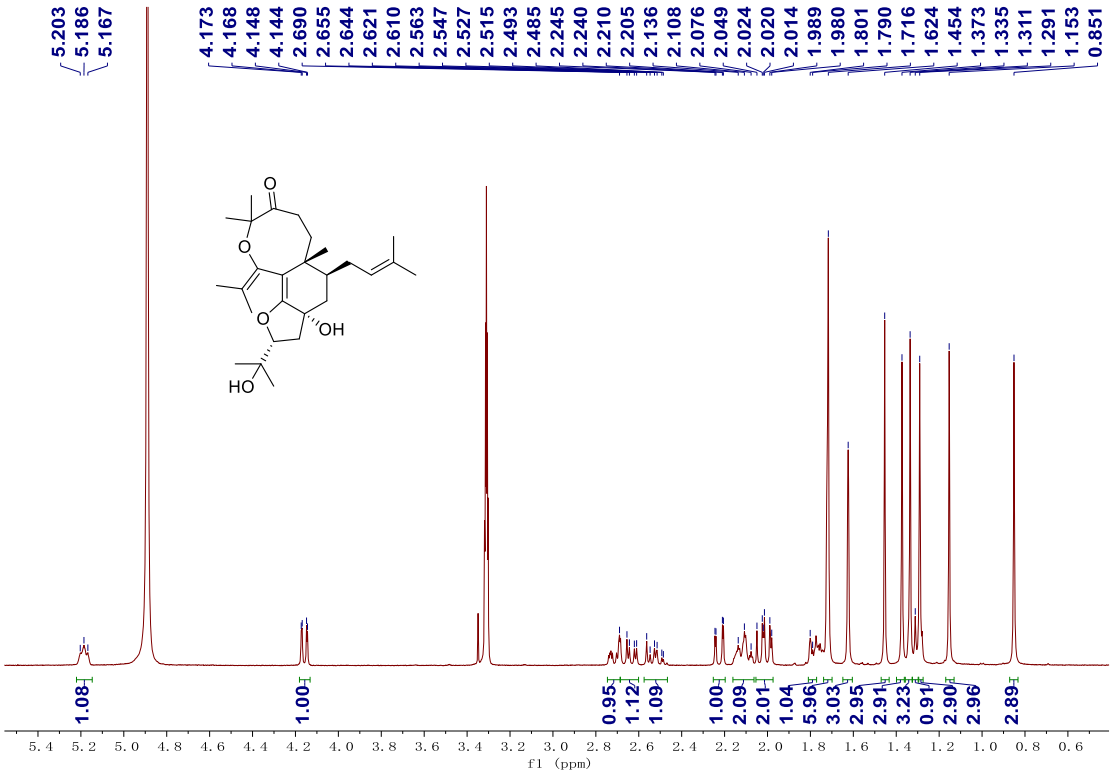
S44. IR spectrum of compound **4**



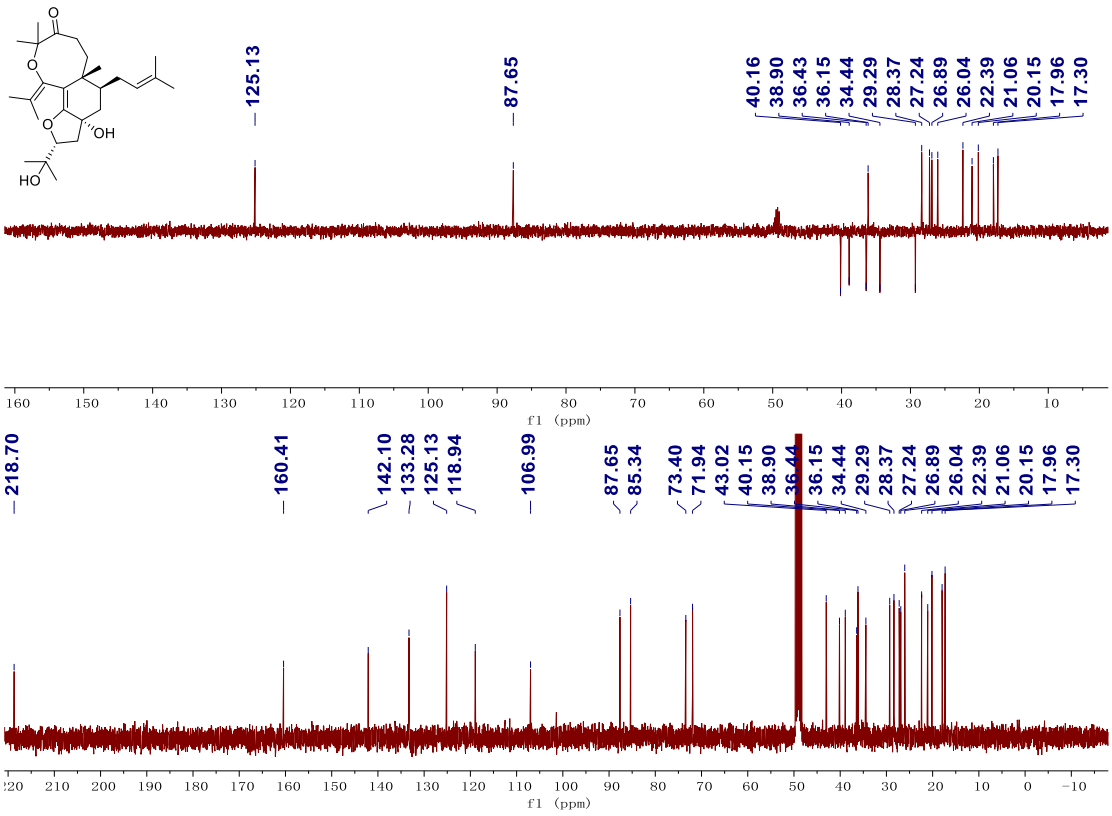
S45. UV spectrum of compound **4**



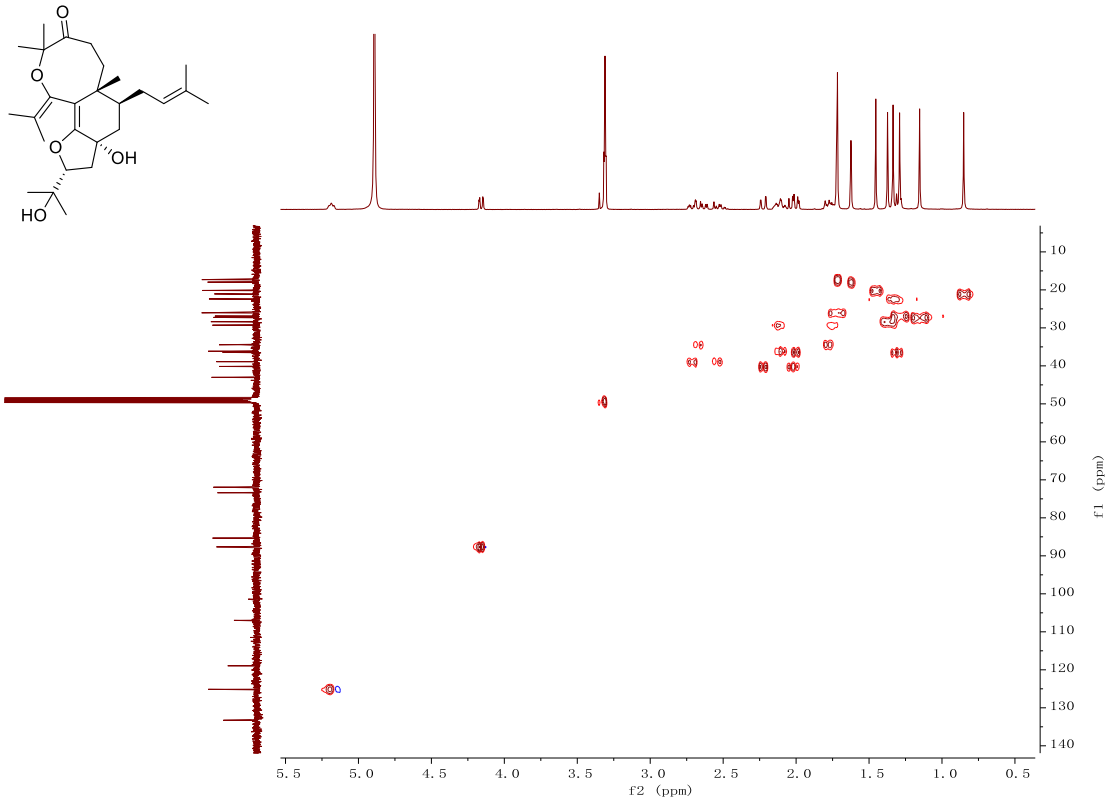
S46. ^{1}H NMR (400MHz, MeOD) spectrum of compound **5**



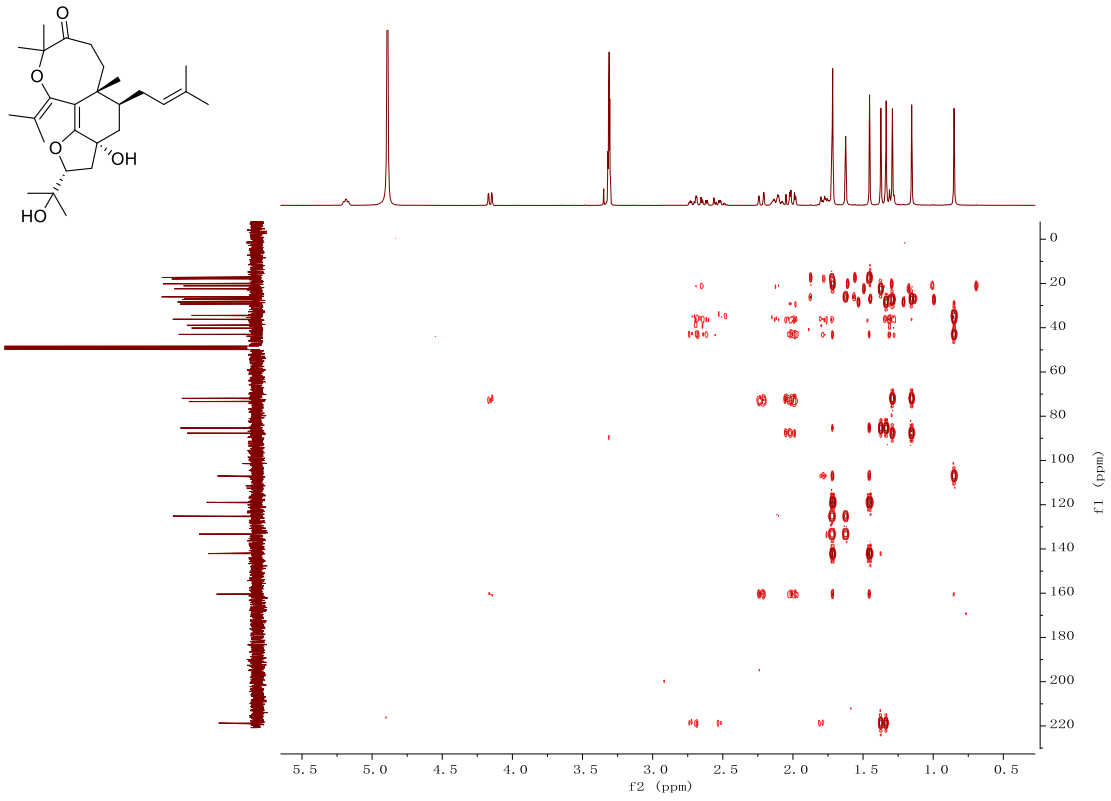
S47. ^{13}C NMR (100MHz, MeOD) spectrum of compound **5**



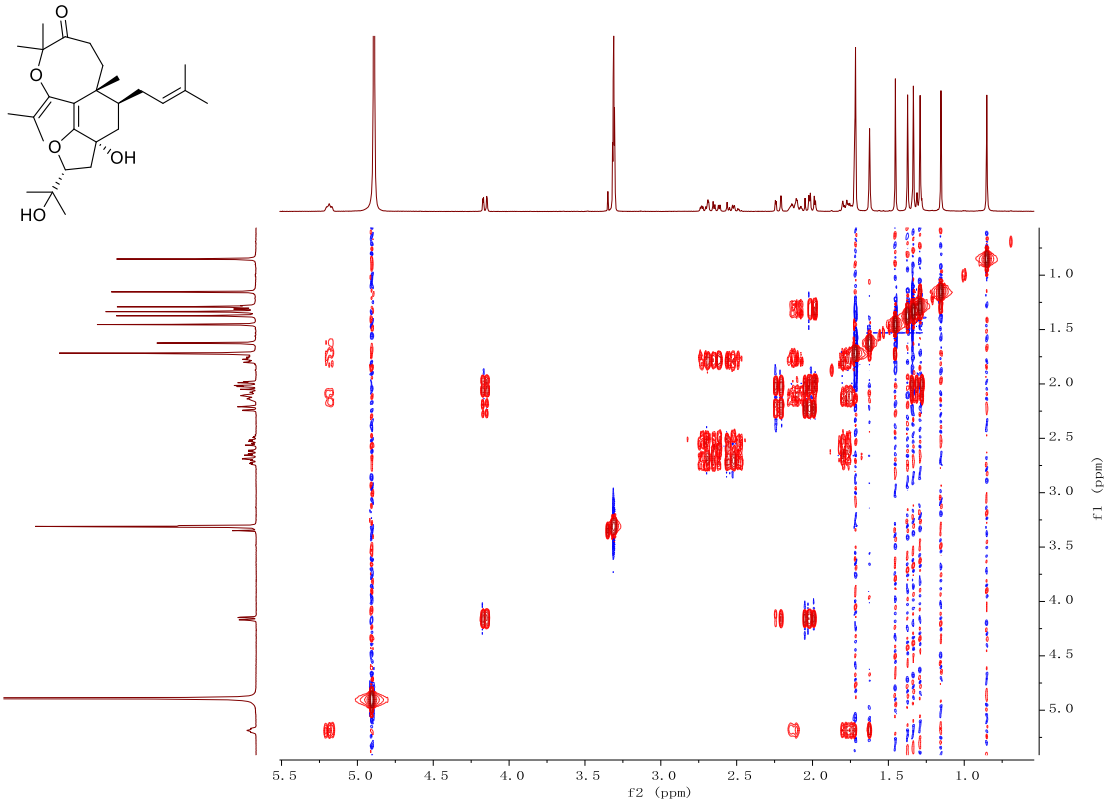
S48. HSQC spectrum of compound **5** in methanol-d_4



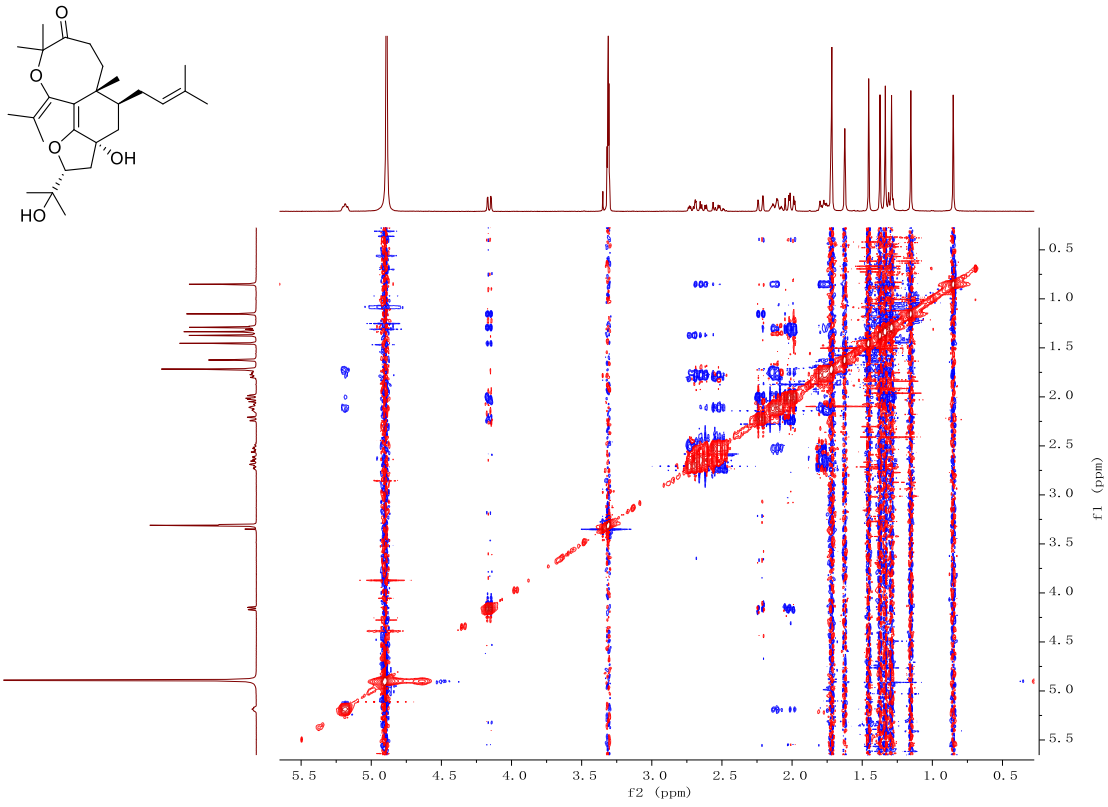
S49. HMBC spectrum of compound **5** in methanol-d_4



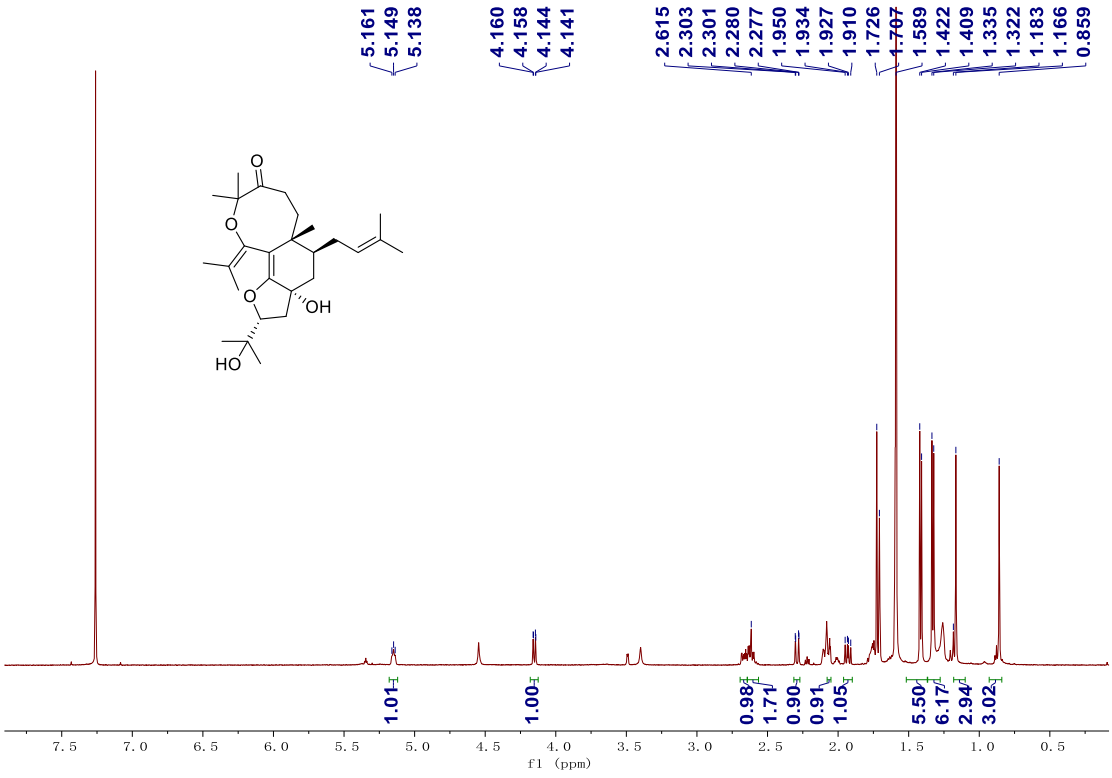
S50. ^{1}H–^{1}H COSY spectrum of compound **5** in methanol-d_4



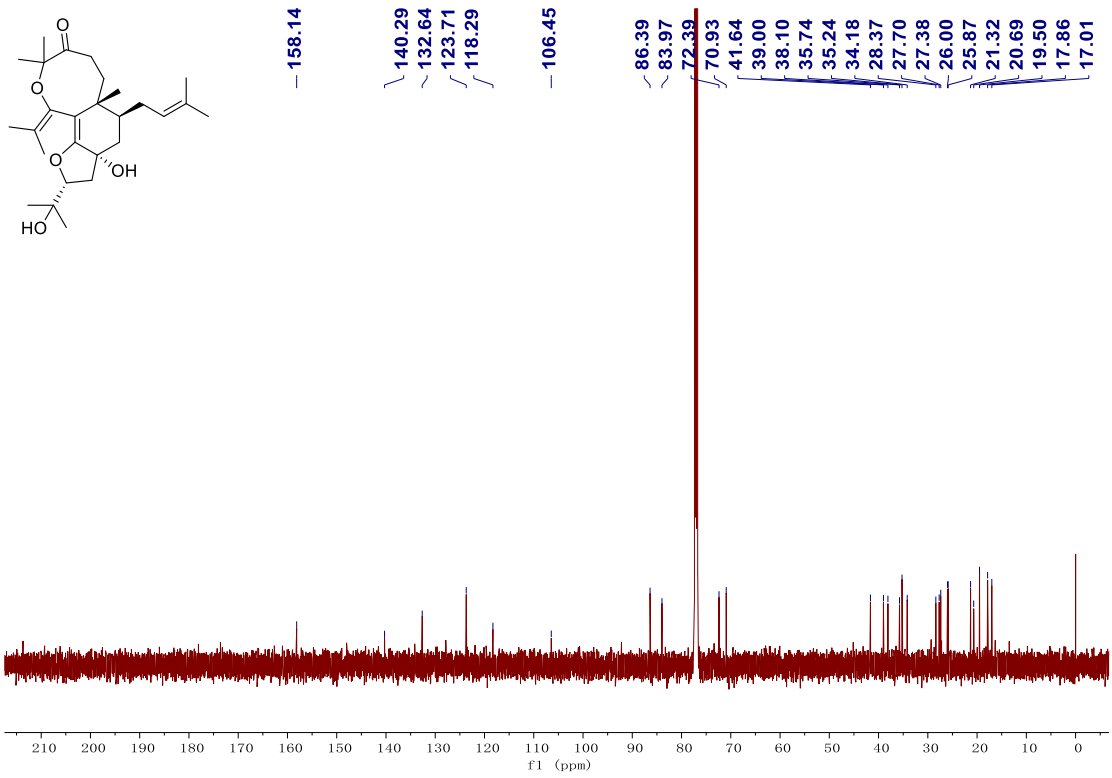
S51. NOESY spectrum of compound **5** in methanol-d_4



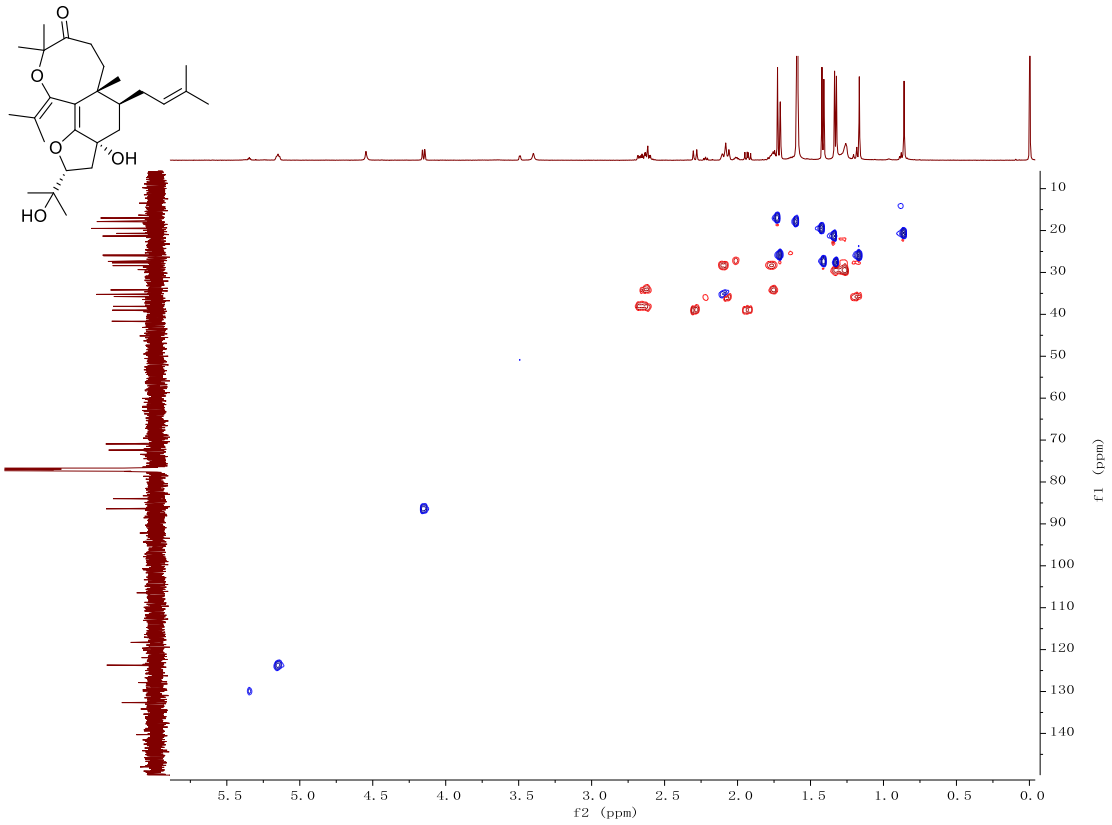
S52. ^{1}H NMR (600MHz, $CDCl_3$) spectrum of compound **5**



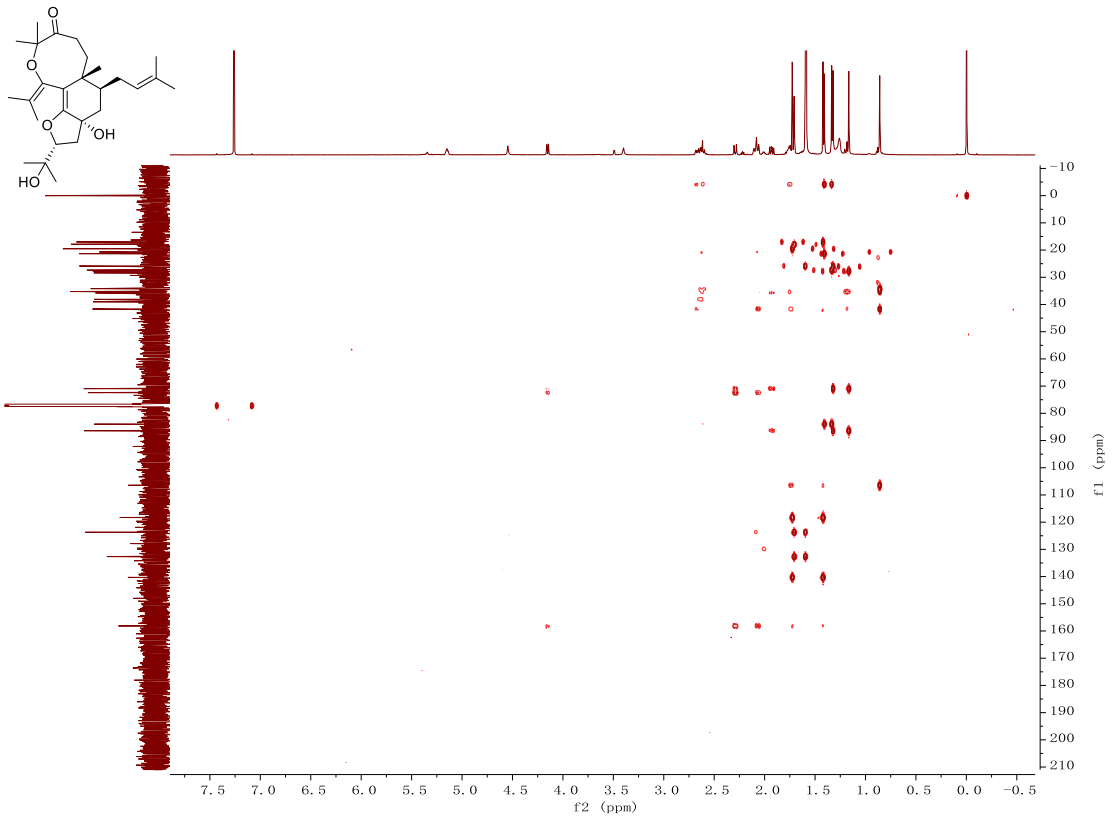
S53. ^{13}C NMR (100MHz, $CDCl_3$) spectrum of compound **5**



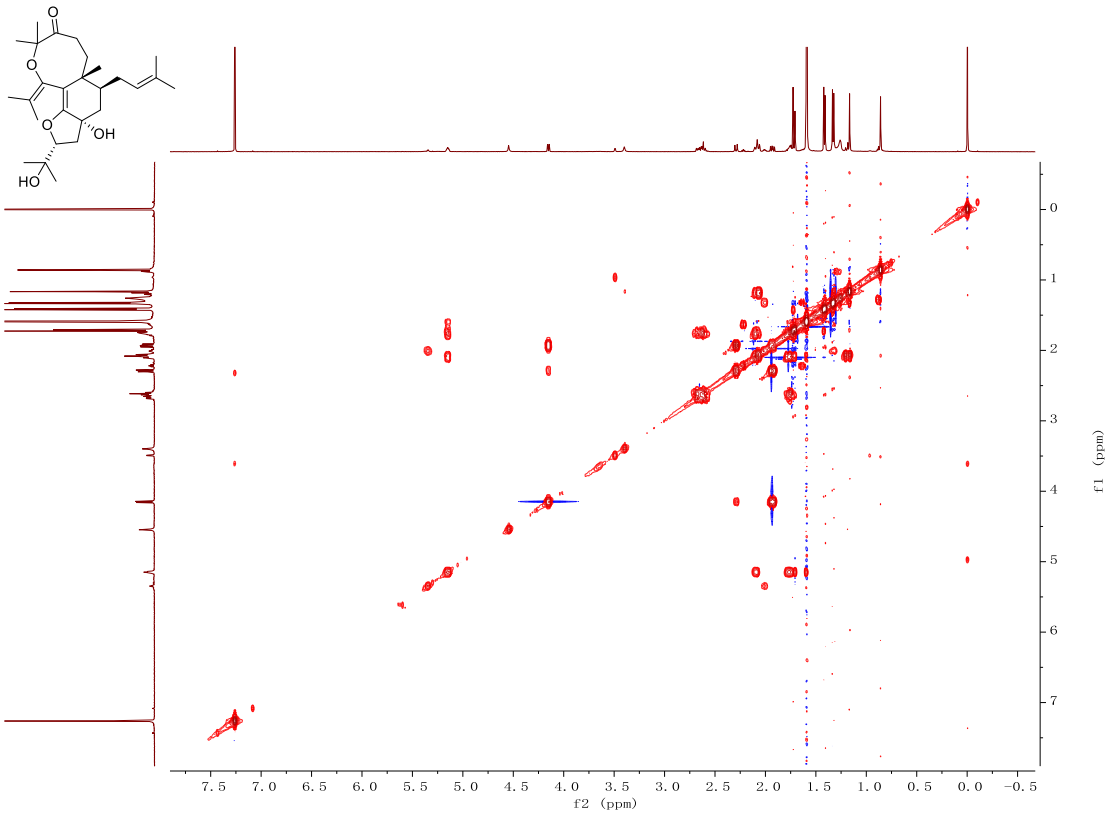
S54. HSQC spectrum of compound **5** in $CDCl_3$



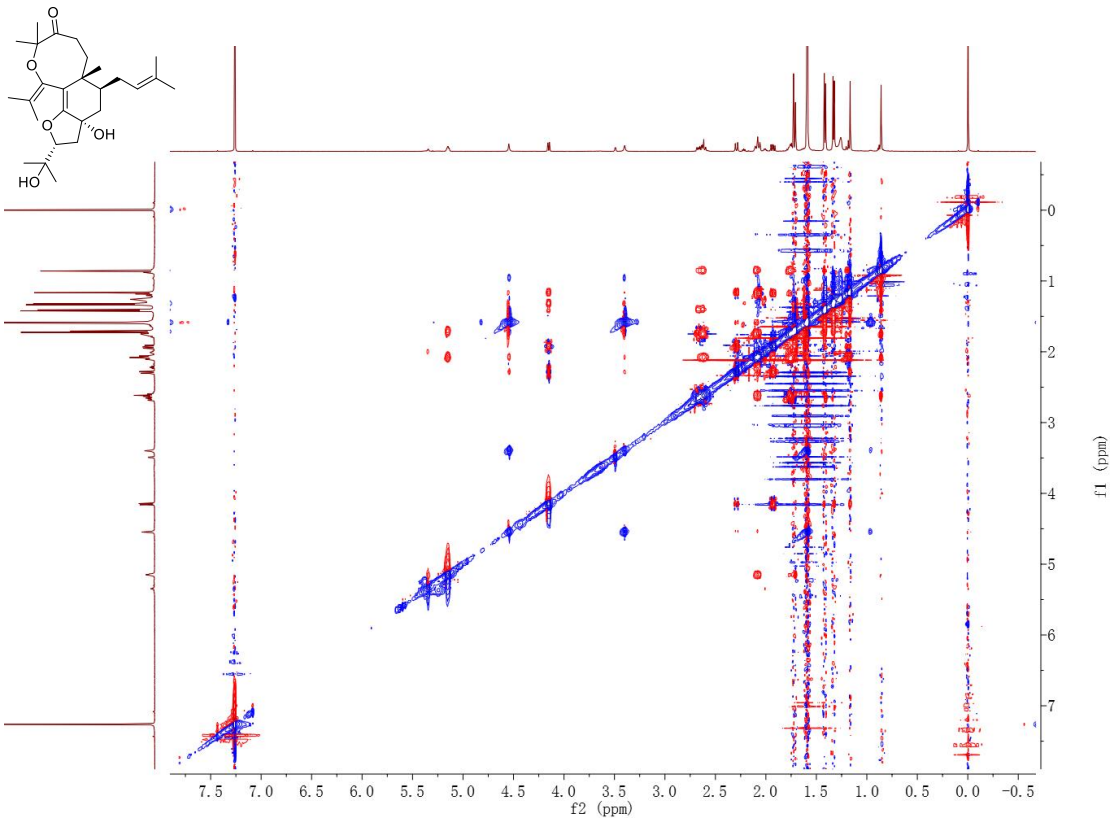
S55. HMBC spectrum of compound **5** in $CDCl_3$



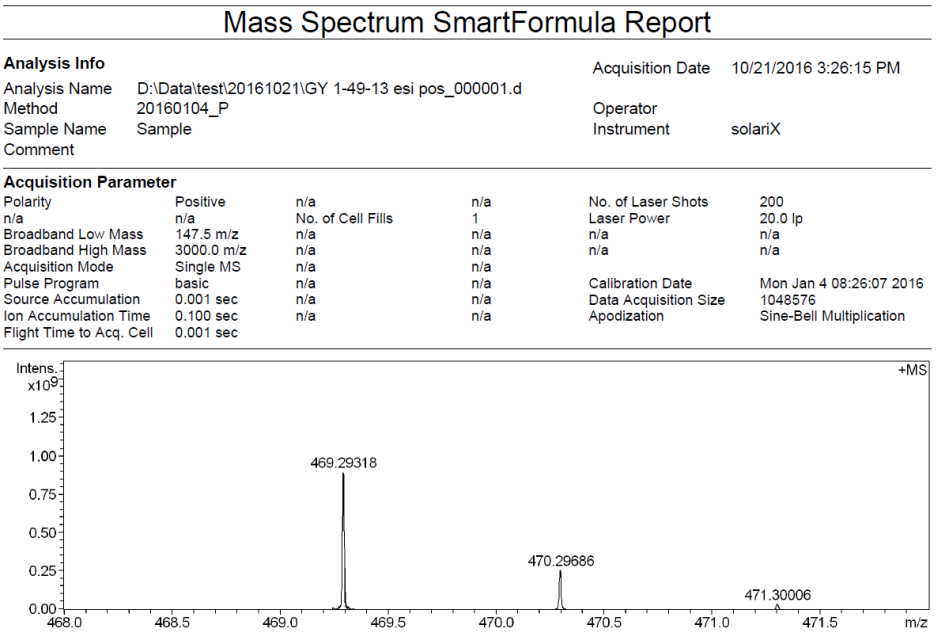
S56. ^{1}H–^{1}H COSY spectrum of compound **5** in $CDCl_3$



S57. NOESY spectrum of compound **5** in $CDCl_3$



S58. HREIMS spectrum of compound **5**



Mass Spectrum SmartFormula Report

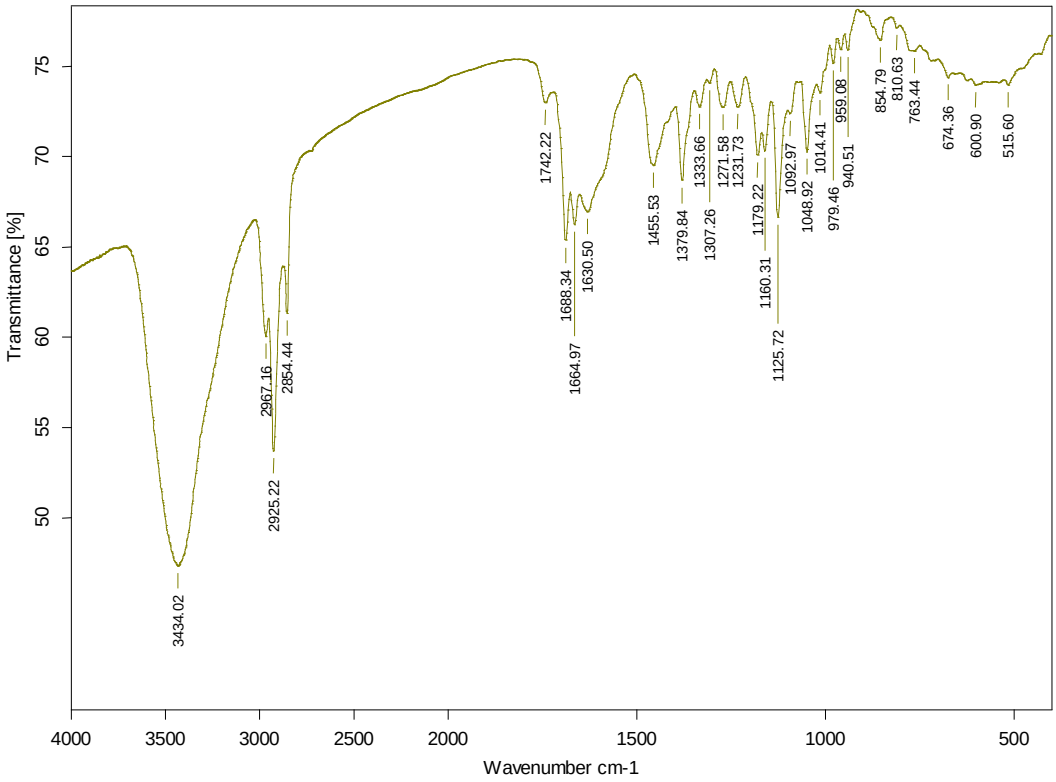
Analysis Info

Analysis Name	D:\Data\test\20161021\GY 1-49-13 esi pos_000001.d	Acquisition Date	10/21/2016 3:26:15 PM
Method	20160104_P	Operator	
Sample Name	Sample	Instrument	solariX
Comment			

Acquisition Parameter

Polarity	Positive	n/a	n/a	No. of Laser Shots	200
n/a	n/a	No. of Cell Fills	1	Laser Power	20.0 lp
Broadband Low Mass	147.5 m/z	n/a	n/a	n/a	n/a
Broadband High Mass	3000.0 m/z	n/a	n/a	n/a	n/a
Acquisition Mode	Single MS	n/a	n/a		
Pulse Program	basic	n/a	n/a	Calibration Date	Mon Jan 4 08:26:07 2016
Source Accumulation	0.001 sec	n/a	n/a	Data Acquisition Size	1048576
Ion Accumulation Time	0.100 sec	n/a	n/a	Apodization	Sine-Bell Multiplication
Flight Time to Acq. Cell	0.001 sec				

S59. IR spectrum of compound **5**



S60. UV spectrum of compound **5**