

Supporting Information

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A New Lignan with Potential Anti-inflammatory Activity from *Notopterygium incisum*

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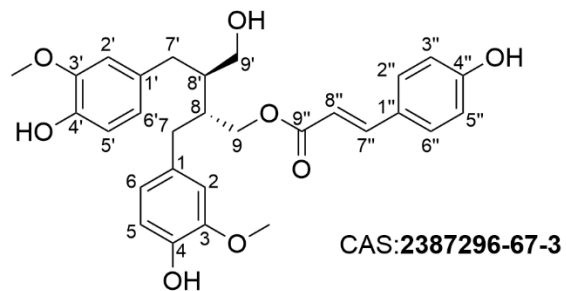
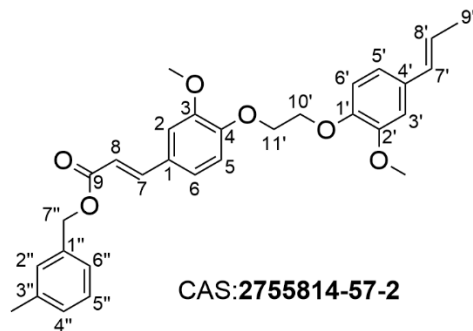
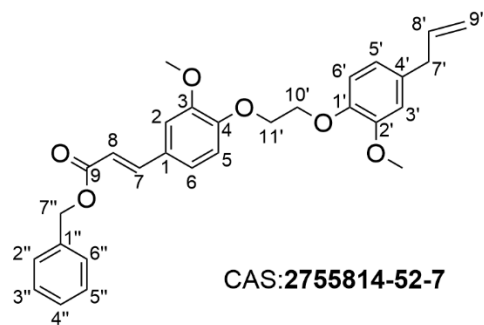
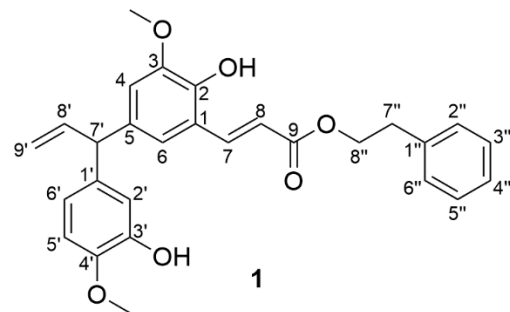
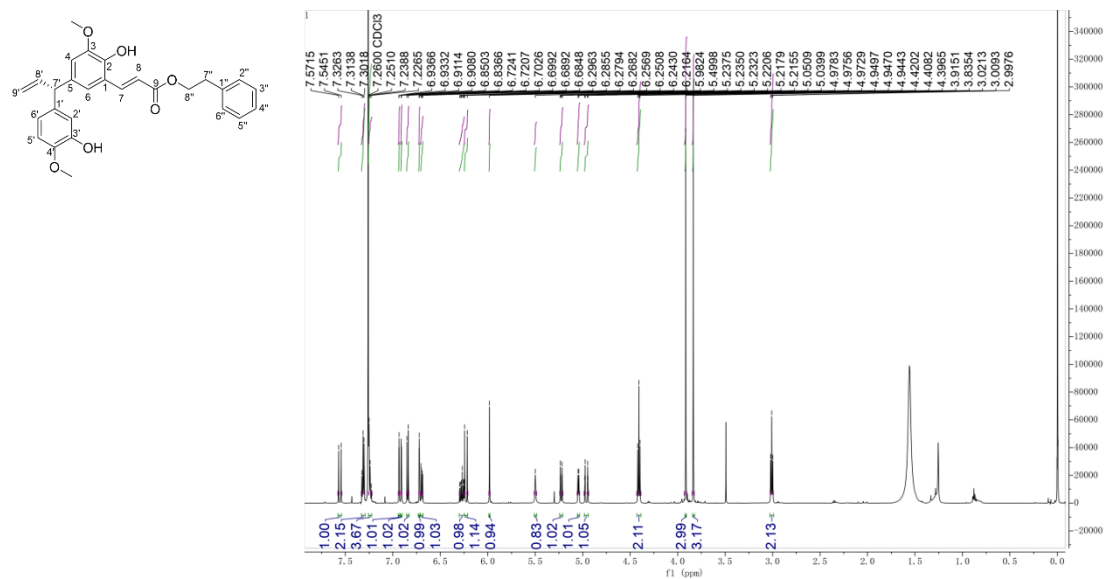


Figure S1: The structures of compound **1** and structurally similar compounds

Table S1: The NMR data of compound **1**, **2755814-52-7**, **2755814-57-2** and **2387296-67-3** (δ in ppm, J in Hz)

Compound 1			2755814-52-7			2755814-57-2			2387296-67-3		
δ_C	δ_H	$J(\text{Hz})$	δ_C	δ_H	$J(\text{Hz})$	δ_C	δ_H	$J(\text{Hz})$	δ_C	δ_H	$J(\text{Hz})$
1	126.3	-	1	127.7	-	1	127.7	-	1	132.3	-
2	146.8	-	2	111.2	7.32 (d, 6.5)	2	111.1	7.36 (s)	2	112.1	6.72 (d, 2.4)
3	145.4	-	3	150.6	-	3	150.6	-	3	147.3	-
4	107.4	6.94 (d, 2.0)	4	149.6	-	4	149.5	-	4	144.7	-
5	129.6	-	5	116.1	7.02 (d, 8.5)	5	116.0	7.02 (d, 8.0)	5	114.5	6.70 (d, 8.4)
6	123.5	6.91 (d, 2.0)	6	123.6	6.67, (dd, 8.0, 2.0)	6	123.6	7.23 (d, 8.5)	6	121.2	6.63 (dd, 8.4, 1.8)
7	145.6	7.56 (d, 15.8)	7	145.6	7.61 (d, 15.5)	7	145.5	7.61 (d, 15.5)	7	34.7	2.68 (dd, 13.8, 7.8) 2.72 (dd, 13.8, 7.8)
8	115.4	6.23 (d, 15.8)	8	115.9	6.61 (d, 16.0)	8	113.7	6.62 (d, 16.5)	8	43.3	2.33 (m)
9	167.3	-	9	166.9	-	9	166.9	-	9	64.2	4.36 (dd, 11.4, 6.0) 4.12 (dd, 11.4, 6.0)
1'	134.1	-	1'	146.6	-	1'	147.4	-	1'	132.4	-
2'	111.3	6.2 (d, 2.0)	2'	149.4	-	2'	149.5	-	2'	112.4	6.74 (d, 2.4)
3'	146.5	-	3'	113.2	6.76 (d, 2.5)	3'	109.6	6.98 (d, 2.0)	3'	147.3	-
4'	144.3	-	4'	133.3	-	4'	131.5	-	4'	144.7	-
5'	121.3	6.70 (dd, 8.0, 2.0)	5'	120.8	6.66 (dd, 8.0, 2.0)	5'	119.1	6.82 (d, 8.0)	5'	114.5	6.72 (d, 8.4)
6'	114.3	6.85 (d, 8.0)	6'	113.1	6.90 (d, 8.5)	6'	113.2	6.90 (d, 8.0)	6'	121.2	6.63 (dd, 8.4, 1.8)
7'	47.3	5.05 (d, 6.6)	7'	40.0	3.26 (d, 6.5)	7'	131.1	6.30 (d, 16.0)	7'	34.3	2.68 (dd, 13.8, 7.8) 2.72 (dd, 13.8, 7.8)
8'	139.7	6.27 (ddd, 17.0, 10.1, 6.6)	8'	138.5	5.94-5.88, (m)	8'	123.9	6.18-6.11 (m)	8'	39.8	2.01 (m)

9'	116.6	5.23 (dt, 10.1, 1.6), 4.96 (dt, 17.0, 1.6)	9'	114.0	5.05-4.98, (m)	9'	18.7	1.78 (d, 6.5)	9'	61.2	3.60 (dd, 11.4, 5.4) 3.69 (dd, 11.4, 5.4)
			10'	67.6	4.22, (t, 3.0)	10'	67.5	4.24 (t, 3.5)			
			11'	67.7	4.28, (t, 3.0)	11'	67.7	4.28 (t, 3.5)			
1"	138.1	-	1"	136.9	-	1"	136.8	-	1"	126.1	-
2", 6"	128.7	7.32 (t, 7.3)	2", 6"	128.7	7.40-7.35 (m)	2"	129.2	7.42 (s)	2"	130.1	7.55 (d, 8.4)
3", 5"	129.1	7.26-7.20 (m)	3", 5"	129.0	7.40-7.35 (m)	3"	138.2	-	3"	115.8	6.89 (d, 8.4)
4"	126.7	7.26-7.20 (m)	4"	128.6	7.40-7.35 (m)	4"	128.9	7.42 (s)	4"	160.6	-
						5"	129.2	7.42 (s)	5"	115.8	6.89 (d, 8.4)
						6"	125.8	7.42 (s)	6"	130.1	7.55 (d, 8.4)
7"	35.9	3.01 (t, 7.2)	7"	65.9	5.18, (s)	7"	66.0	5.17 (s)	7"	144.4	7.60 (d, 16.0)
8"	64.9	4.41 (t, 7.2)							8"	114.9	6.39 (d, 16.0)
									9"	167.6	-
3-OMe	56.1	3.84 (s)	3-OMe	56.1	3.77 (s)	3-OMe	56.1	3.77 (s)	3-OMe	55.1	3.77 (s)
4'-OMe	56.3	3.91 (s)	4'-OMe	55.9	3.69 (s)	4'-OMe	55.9	3.73 (s)	4'-OMe	55.1	3.76 (s)
2-OH	-	5.99 (s)									
3'-OH	-	5.50 (s)									



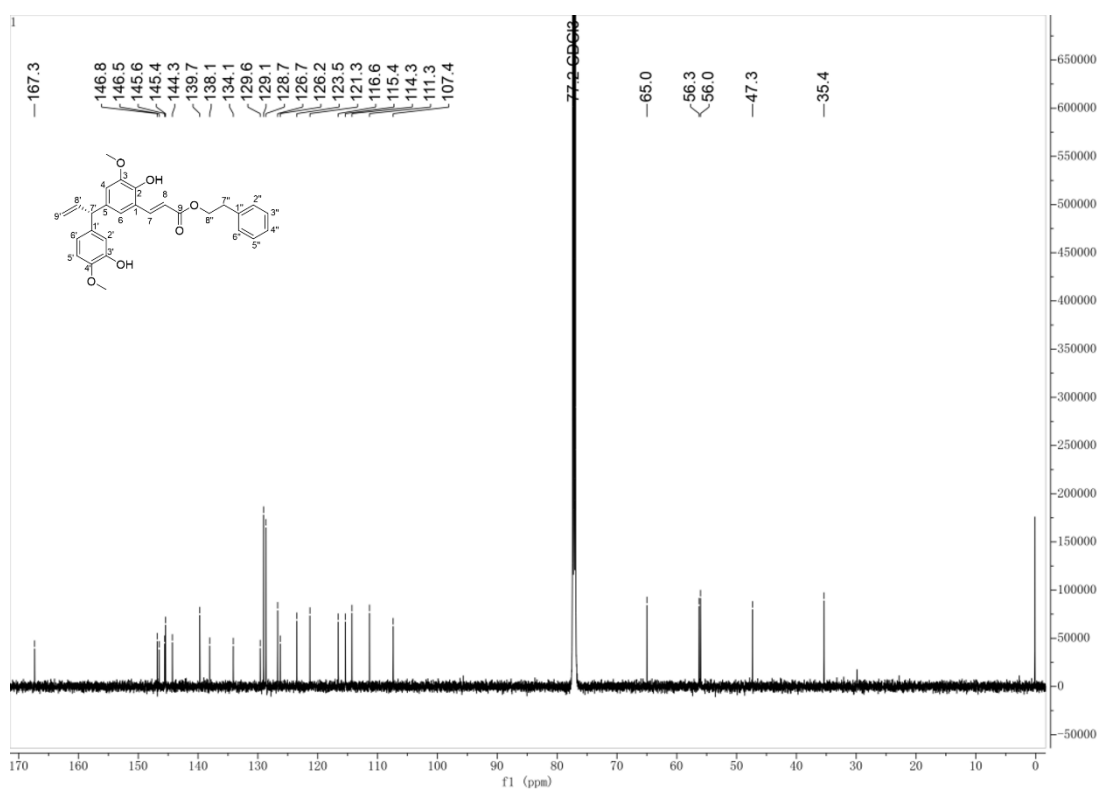


Figure S4: ^{13}C NMR Spectrum of **1** in CDCl_3 (150 MHz)

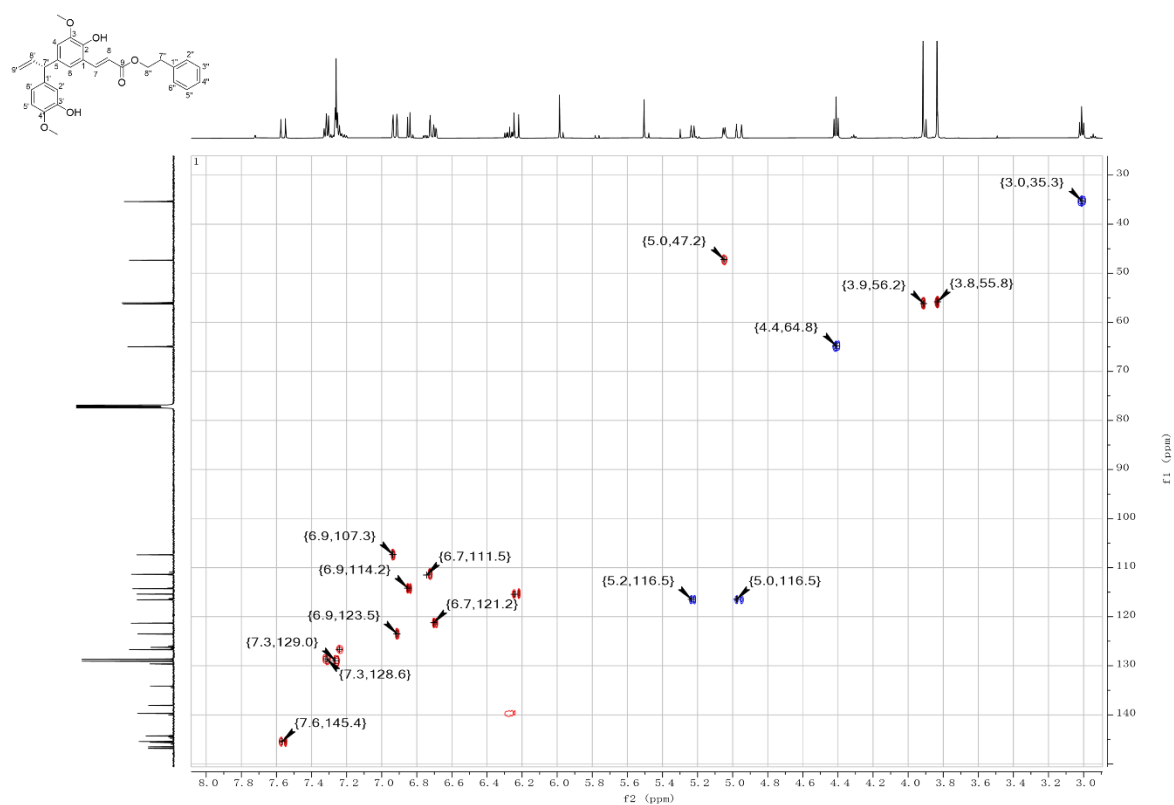


Figure S5: HSQC Spectrum of **1** in CDCl_3

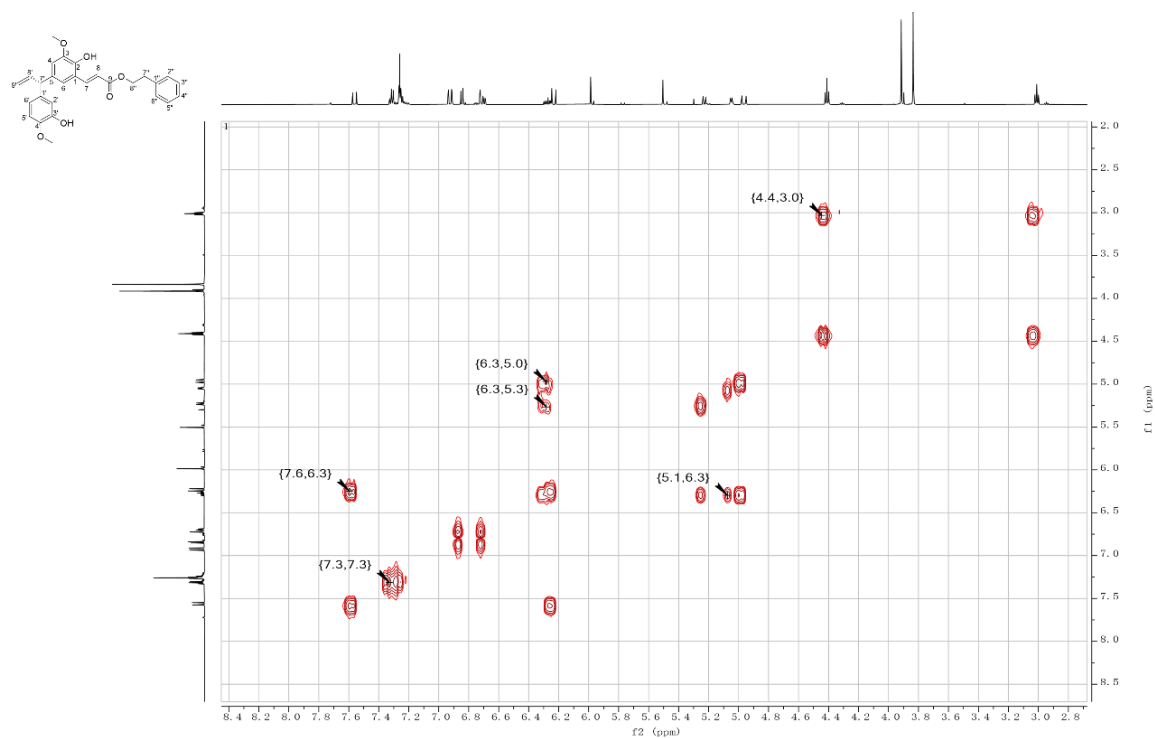


Figure S6: ^1H - ^1H COSY Spectrum of **1** in CDCl_3

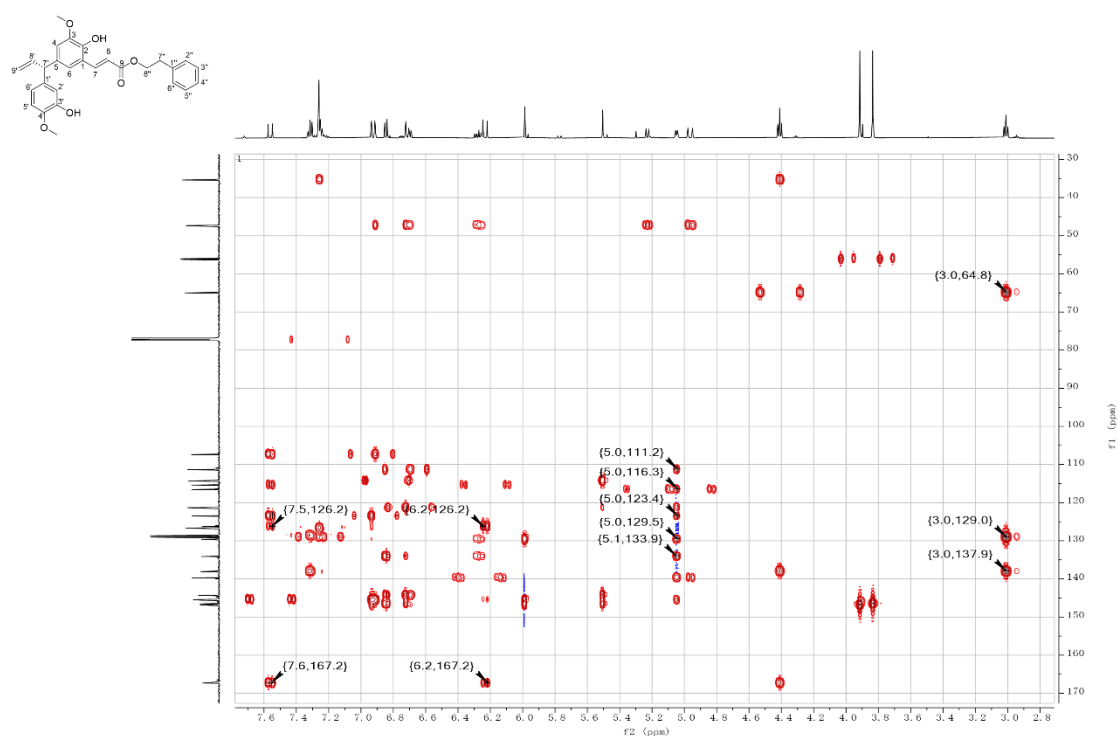


Figure S7: HMBC Spectrum of **1** in CDCl_3

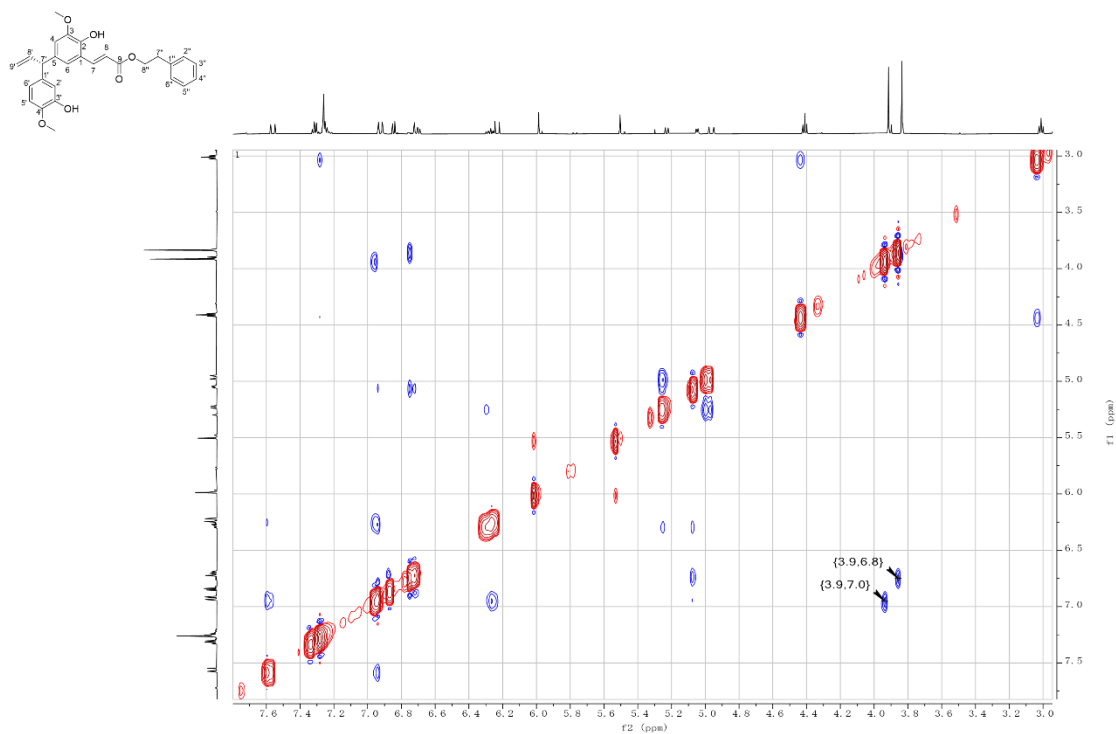


Figure S8: NOESY Spectrum of **1** in CDCl_3

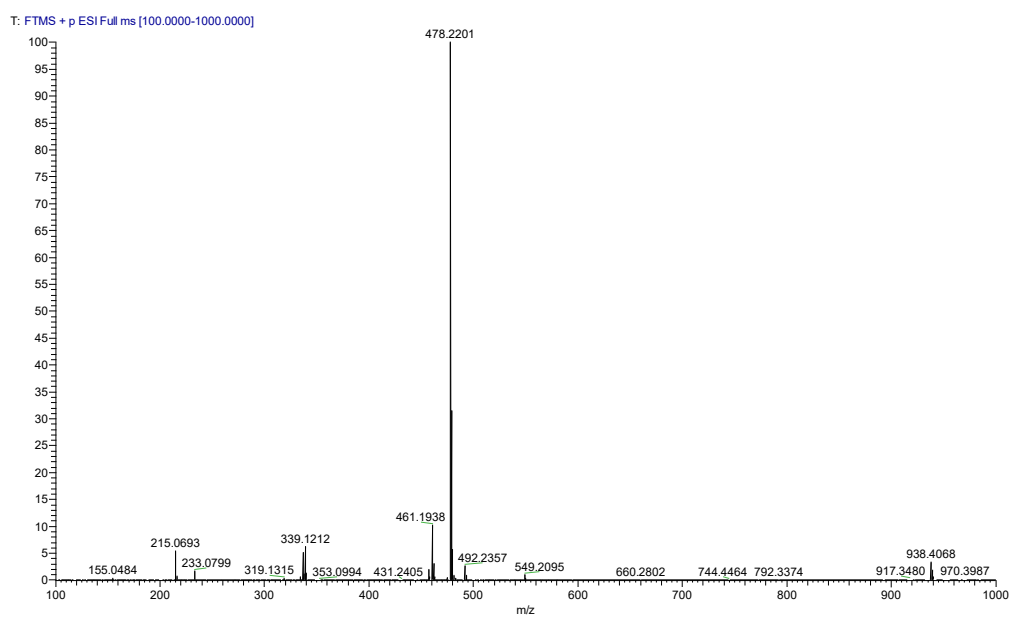


Figure S9: HRESIMS Spectrum of **1**

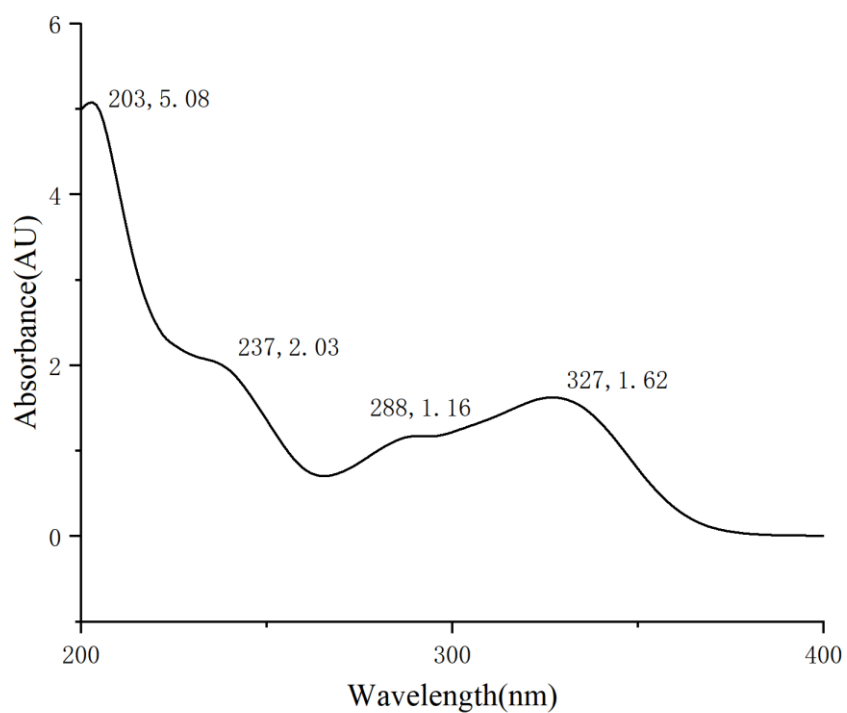


Figure S10: UV spectrum of compound **1**

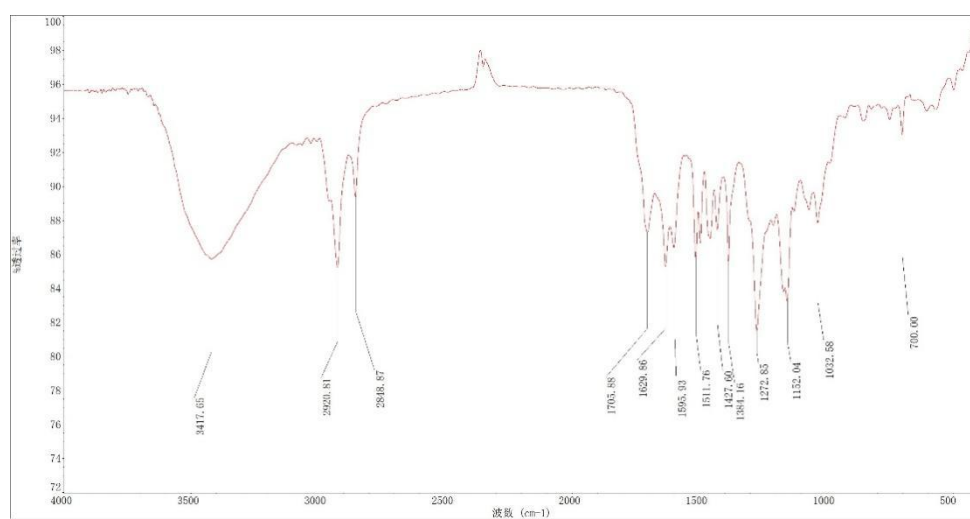


Figure S11: IR spectrum of compound **1**

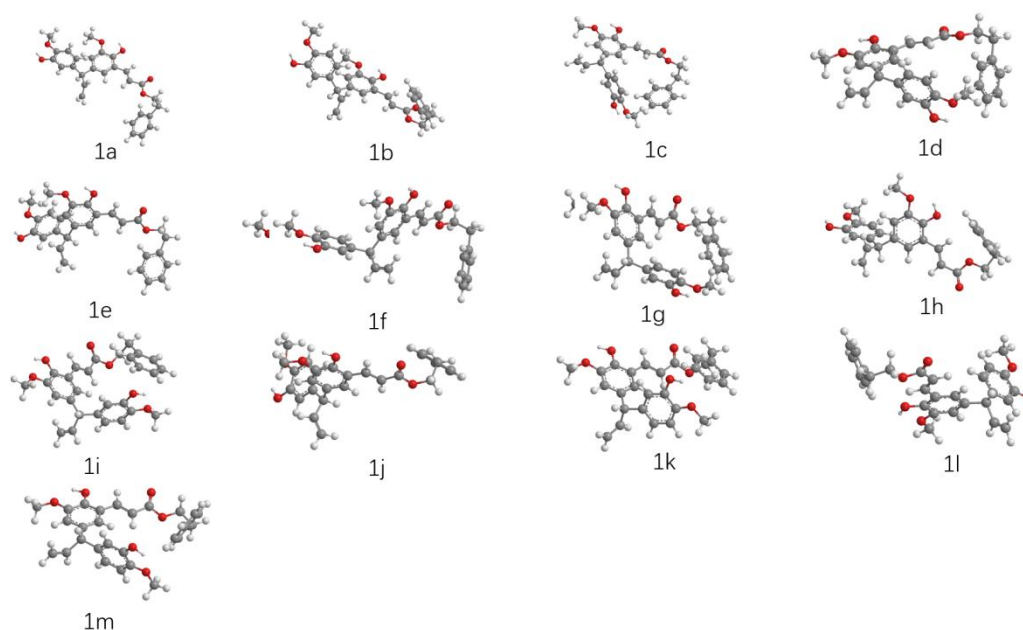


Figure S12: Most stable conformers of 7'S-1 calculated at the CAM-B3LYP/DGTZVP level

Table S2: Energies and atomic Cartesian coordinates of geometry-optimized conformers of 7'S-1 at wb97xd/dgdzvp in methanol

	Conformer 1			Conformer 2			Conformer 3			Conformer 4		
Gibbs free energy (hartrees)	-1534.361793			-1534.361681			-1534.361156			-1534.361154		
ΔG (kcal/mol)				0.07			0.4			0.401		
Population Proportion	16.63%			14.77%			8.47%			8.45%		
Element	X	Y	Z	X	Y	Z	X	Y	Z	X	Y	Z
C	-1.307391	-2.263157	-0.060618	1.429732	-1.305883	2.167284	-3.768439	2.709092	0.014506	-3.953259	2.592840	0.396317
C	-0.742399	-3.299968	-0.679090	1.217671	-1.612408	3.447034	-4.705310	3.436267	-0.593843	-4.972026	3.335149	-0.037254
C	-2.121996	-1.194472	-0.750098	2.366800	-0.221768	1.690299	-2.755265	1.845341	-0.702218	-3.024174	1.808500	-0.503164
C	-3.548369	-1.232128	-0.214012	3.478004	-0.853880	0.860032	-1.359598	2.406016	-0.471414	-1.616148	2.377709	-0.426296
C	-1.503553	0.196972	-0.636396	1.654919	0.897433	0.934217	-2.878654	0.367785	-0.324279	-3.081509	0.306317	-0.211500
C	-4.570335	-1.797911	-0.983223	4.753905	-1.019883	1.408473	-0.797537	2.411329	0.814377	-0.917204	2.396100	0.790586
C	-5.867322	-1.867353	-0.494656	5.765713	-1.623021	0.674776	0.452122	2.964229	1.034116	0.363506	2.916837	0.860659
C	-6.166798	-1.370528	0.785626	5.515456	-2.078400	-0.631262	1.175783	3.528292	-0.034261	0.979606	3.437982	-0.293811
C	-5.155327	-0.808549	1.557074	4.248585	-1.918558	-1.182277	0.635725	3.510066	-1.312056	0.299011	3.418125	-1.502526
C	-3.853096	-0.742135	1.054485	3.237667	-1.307881	-0.435353	-0.631647	2.951380	-1.522370	-0.997107	2.889350	-1.560810
C	-2.261104	1.308060	-1.057169	2.436796	1.870312	0.280045	-4.120139	-0.158934	0.070802	-4.312921	-0.288668	0.119353
C	-1.724143	2.579544	-1.003586	1.832512	2.916350	-0.389477	-4.244640	-1.504967	0.377006	-4.392345	-1.652354	0.344436

C	-0.411106	2.778441	-0.526676	0.425688	3.020909	-0.425228	-3.131512	-2.360606	0.288042	-3.242782	-2.460184	0.242193
C	0.353753	1.690043	-0.108383	-0.363487	2.068696	0.218953	-1.896216	-1.856996	-0.120625	-2.016448	-1.887930	-0.095869
C	-0.216713	0.400246	-0.176983	0.278741	1.011412	0.899920	-1.791621	-0.486052	-0.419503	-1.961195	-0.498360	-0.320201
O	-2.348648	3.731818	-1.376424	2.469776	3.916217	-1.060898	-5.386062	-2.132260	0.780293	-5.518330	-2.345310	0.676574
C	-3.689031	3.644317	-1.848970	3.892279	3.885278	-1.115912	-6.566863	-1.350415	0.925559	-6.732631	-1.618289	0.830404
O	0.094200	4.038045	-0.475674	-0.146893	4.054024	-1.095493	-3.267974	-3.678792	0.589978	-3.339330	-3.796192	0.469753
C	1.713374	1.934190	0.374644	-1.818854	2.209211	0.159074	-0.742044	-2.757592	-0.182654	-0.827977	-2.741347	-0.171960
C	2.562501	1.023502	0.877778	-2.729062	1.373389	0.684963	0.390615	-2.521014	-0.861633	0.365995	-2.377241	-0.664519
C	3.916533	1.425188	1.304717	-4.169960	1.649981	0.528874	1.545185	-3.432472	-0.750690	1.524461	-3.289431	-0.614424
O	4.374361	2.555920	1.260217	-4.655224	2.613099	-0.042987	1.585097	-4.465733	-0.102727	1.532015	-4.425339	-0.168375
O	4.604832	0.363463	1.758060	-4.903530	0.683521	1.107097	2.589127	-2.947542	-1.443380	2.609562	-2.682028	-1.116575
C	5.978967	0.574998	2.131502	-6.334703	0.769859	0.976785	3.878983	-3.539633	-1.207832	3.872549	-3.357168	-0.997035
C	6.899151	0.627187	0.913152	-6.814934	0.294112	-0.393179	4.443066	-3.125352	0.154033	4.958404	-2.320292	-1.254006
C	6.787246	-0.604282	0.046256	-6.351903	-1.105875	-0.718819	4.339527	-1.635818	0.385422	4.909534	-1.187886	-0.253860
C	7.492899	-1.769551	0.365897	-5.201347	-1.318027	-1.485189	5.276104	-0.755769	-0.167095	4.176637	-0.026855	-0.522934
C	7.356042	-2.922627	-0.405989	-4.745803	-2.609880	-1.749040	5.140466	0.622912	-0.007125	4.075241	0.991110	0.424333
C	6.505998	-2.927423	-1.512784	-5.438413	-3.712049	-1.247952	4.060064	1.142945	0.706660	4.711062	0.862920	1.659618
C	5.798550	-1.771057	-1.841607	-6.589064	-3.512321	-0.483854	3.120089	0.275451	1.262797	5.449368	-0.287847	1.937500
C	5.940208	-0.619894	-1.066698	-7.039267	-2.218937	-0.222267	3.264009	-1.102683	1.104299	5.545322	-1.304186	0.986788
O	-6.851578	-2.416207	-1.262336	7.005042	-1.769455	1.224224	0.987478	2.957046	2.288547	1.030419	2.921554	2.049546
O	-7.479004	-1.498167	1.142082	6.595981	-2.649087	-1.241271	2.382389	4.055912	0.326492	2.238618	3.924048	-0.081825
C	-7.870578	-1.021656	2.423928	6.429626	-3.144079	-2.564464	3.228356	4.549740	-0.705930	2.963872	4.411020	-1.205758
H	-1.212351	-2.166571	1.020589	0.924788	-1.876404	1.388243	-3.697136	2.729277	1.101531	-3.751947	2.533375	1.465206
H	-0.188147	-4.051926	-0.125559	0.549990	-2.420915	3.729104	-5.394828	4.054642	-0.027069	-5.599342	3.889817	0.654024
H	-0.816421	-3.429748	-1.756280	1.704598	-1.066167	4.251523	-4.811157	3.437141	-1.676249	-5.209572	3.412388	-1.095778
H	-2.161616	-1.444678	-1.815615	2.829162	0.228499	2.575091	-2.963744	1.920391	-1.774848	-3.374691	1.947180	-1.531592
H	-4.368252	-2.190144	-1.976025	4.976246	-0.678044	2.415508	-1.324283	1.973227	1.657594	-1.355622	1.985940	1.695876
H	-5.365530	-0.416723	2.545646	4.035393	-2.260023	-2.188744	1.179763	3.928147	-2.151006	0.756408	3.809242	-2.403959
H	-3.076620	-0.288604	1.663601	2.256999	-1.178523	-0.883909	-1.044738	2.950899	-2.526530	-1.517350	2.879867	-2.513795
H	-3.272596	1.153950	-1.417258	3.517837	1.783391	0.302398	-4.979742	0.498106	0.140312	-5.198341	0.332049	0.201647
H	0.376833	-0.453701	0.130151	-0.326771	0.273456	1.414238	-0.823602	-0.083280	-0.697831	-1.006956	-0.044164	-0.560556
H	-4.345203	3.226523	-1.080358	4.241852	2.972755	-1.606780	-6.859431	-0.905658	-0.029637	-7.015072	-1.129798	-0.106285
H	-3.993207	4.663642	-2.074670	4.187411	4.752070	-1.702454	-7.340695	-2.037727	1.259358	-7.487985	-2.352435	1.100672
H	-3.742441	3.036244	-2.756134	4.321737	3.957623	-0.113029	-6.424836	-0.566277	1.674412	-6.642185	-0.874391	1.626767
H	-0.586397	4.644973	-0.809599	0.566320	4.597382	-1.468636	-4.185315	-3.824594	0.872994	-4.260486	-3.991240	0.707021
H	2.065145	2.960847	0.316234	-2.194446	3.080965	-0.370252	-0.812212	-3.684050	0.382015	-0.928022	-3.751478	0.216971
H	2.314832	-0.026785	0.986700	-2.467913	0.470376	1.225917	0.534587	-1.636593	-1.472929	0.553295	-1.397501	-1.090589
H	6.060871	1.491842	2.716932	-6.715558	0.122886	1.766819	3.811190	-4.625559	-1.288994	3.958796	-3.781656	0.005384
H	6.220708	-0.279480	2.763304	-6.656305	1.795457	1.163670	4.498342	-3.155489	-2.017630	3.915467	-4.168368	-1.727445
H	6.674444	1.524619	0.332610	-7.908062	0.339337	-0.377481	3.915876	-3.666394	0.942523	5.920762	-2.836775	-1.202699
H	7.919782	0.734674	1.292467	-6.473973	0.996456	-1.156799	5.487451	-3.449706	0.180033	4.849848	-1.935854	-2.271521

H	8.158214	-1.774322	1.225644	-4.657069	-0.465244	-1.882848	6.119047	-1.152096	-0.727763	3.672722	0.077150	-1.479815
H	7.914493	-3.816235	-0.145295	-3.851295	-2.754999	-2.346662	5.878280	1.291881	-0.439367	3.499561	1.884174	0.200080
H	6.399087	-3.823593	-2.115618	-5.087181	-4.718130	-1.453831	3.950237	2.215292	0.831571	4.632442	1.653891	2.398948
H	5.136959	-1.764144	-2.702175	-7.137409	-4.364125	-0.093828	2.276941	0.673189	1.820641	5.950719	-0.395085	2.894362
H	5.387335	0.277420	-1.332653	-7.937288	-2.072403	0.372645	2.529509	-1.771411	1.546381	6.119841	-2.198903	1.213290
H	-7.679558	-2.373710	-0.758154	7.571446	-2.204822	0.567655	1.848549	3.402554	2.247550	1.897822	3.331372	1.904537
H	-8.937401	-1.218152	2.503933	7.394784	-3.552763	-2.855330	4.142172	4.876208	-0.214070	3.936078	4.716009	-0.825086
H	-7.339978	-1.555178	3.217764	5.674160	-3.934513	-2.593444	3.461674	3.760909	-1.427269	3.094006	3.624879	-1.955366
H	-7.689095	0.053298	2.513223	6.151791	-2.339042	-3.250863	2.765610	5.398486	-1.217440	2.458257	5.271685	-1.652533
	Conformer 5			Conformer 6			Conformer 7			Conformer 8		
Gibbs free energy (hartrees)	-1534.361105			-1534.360971			-1534.360967			-1534.360925		
ΔG (kcal/mol)	0.432			0.516			0.518			0.545		
Population Proportion	8.02%			6.96%			6.93%			6.63%		
Element	X	Y	Z	X	Y	Z	X	Y	Z	X	Y	Z
C	2.141497	-1.580682	-2.223593	1.973022	-1.750815	-2.200800	-3.132510	2.369075	1.992832	-2.949711	-0.156904	2.922902
C	1.457393	-2.608831	-2.724894	1.505087	-1.062614	-3.242502	-3.477134	1.470569	2.915733	-2.831974	-0.886296	4.032127
C	2.131507	-1.174556	-0.768182	2.033003	-1.287886	-0.760259	-2.764054	2.089253	0.550048	-2.779228	-0.696744	1.521944
C	3.511529	-1.247606	-0.114448	3.429025	-1.440516	-0.167727	-1.365374	2.594957	0.220786	-4.040622	-0.561059	0.668475
C	1.510641	0.209960	-0.642885	1.487656	0.116781	-0.556122	-2.959668	0.629878	0.161458	-1.575043	-0.028304	0.873481
C	4.564621	-1.949040	-0.711733	4.577578	-1.302634	-0.956492	-0.327934	2.525614	1.158585	-5.288475	-0.307516	1.248456
C	5.801968	-2.037317	-0.088389	5.839903	-1.383156	-0.386889	0.957320	2.924871	0.823074	-6.431632	-0.225308	0.465053
C	6.012441	-1.427024	1.158617	5.980316	-1.609257	0.993285	1.230236	3.417759	-0.464691	-6.352148	-0.403503	-0.925598
C	4.969434	-0.733977	1.763459	4.844835	-1.752862	1.782729	0.206341	3.490919	-1.402142	-5.117234	-0.663112	-1.510171
C	3.729904	-0.647116	1.125450	3.577921	-1.667663	1.198451	-1.083834	3.080198	-1.054107	-3.972416	-0.738400	-0.713364
C	2.225698	1.339587	-1.084256	2.275515	1.239918	-0.867550	-4.237353	0.196029	-0.233703	-1.644562	1.328613	0.504596
C	1.655418	2.595852	-1.004466	1.760761	2.514130	-0.714729	-4.452282	-1.130042	-0.571900	-0.546524	1.951243	-0.057986
C	0.354300	2.755005	-0.482213	0.444901	2.699015	-0.243647	-3.391980	-2.056365	-0.522603	0.649828	1.232889	-0.265401
C	-0.366958	1.645149	-0.040036	-0.348713	1.595614	0.074388	-2.122125	-1.643002	-0.122122	0.734029	-0.112890	0.093862
C	0.237293	0.373292	-0.133186	0.198583	0.306749	-0.093865	-1.927370	-0.289368	0.212854	-0.400262	-0.725333	0.667570
O	2.234649	3.767169	-1.389545	2.415143	3.680024	-0.978538	-5.634429	-1.674450	-0.977099	-0.479022	3.250347	-0.462611
C	3.553888	3.718066	-1.923387	3.755118	3.602057	-1.453983	-6.770525	-0.821111	-1.065461	-1.639529	4.060860	-0.307626
O	-0.184321	3.999689	-0.409767	-0.037245	3.959984	-0.093220	-3.615229	-3.354334	-0.857675	1.715106	1.864927	-0.823706
C	-1.712905	1.853954	0.495501	-1.709707	1.828951	0.559615	-1.020073	-2.608501	-0.105246	1.993600	-0.818910	-0.147097
C	-2.542048	0.912606	0.974574	-2.572431	0.902112	1.006453	0.124251	-2.458879	0.579539	2.267193	-2.100724	0.149193
C	-3.884056	1.283389	1.463799	-3.925725	1.295672	1.444022	1.231040	-3.422642	0.432671	3.582771	-2.715029	-0.111370
O	-4.343081	2.413714	1.504061	-4.371945	2.431811	1.452269	1.228706	-4.416350	-0.275380	3.886416	-3.837619	0.263567
O	-4.559398	0.193522	1.866611	-4.627151	0.220094	1.840696	2.284122	-3.037399	1.173650	4.414579	-1.918579	-0.793924

C	-5.923168	0.377908	2.289571	-6.000467	0.427752	2.219645	3.538569	-3.703684	0.946133	5.758370	-2.384308	-0.999012
C	-6.875460	0.511367	1.102476	-6.915395	0.548097	1.002302	4.211034	-3.188963	-0.327298	6.526231	-1.252223	-1.666685
C	-6.787372	-0.657503	0.150357	-6.817132	-0.643550	0.079887	4.346431	-1.684211	-0.339261	6.569573	-0.005484	-0.813447
C	-7.490597	-1.840369	0.403779	-5.969349	-0.618549	-1.032297	3.360340	-0.883921	-0.926985	5.625729	1.012847	-0.983388
C	-7.376520	-2.936757	-0.450114	-5.842348	-1.734104	-1.860075	3.450612	0.507013	-0.889188	5.631837	2.137825	-0.159323
C	-6.551904	-2.866265	-1.573767	-6.565156	-2.895117	-1.585582	4.538308	1.120248	-0.267562	6.587228	2.261270	0.849845
C	-5.846706	-1.691809	-1.836740	-7.415617	-2.930801	-0.479643	5.530168	0.332829	0.317802	7.535488	1.253080	1.026466
C	-5.965563	-0.597540	-0.979904	-7.537850	-1.813264	0.345117	5.430911	-1.057844	0.283835	7.524162	0.129638	0.200168
O	6.814710	-2.722229	-0.693784	6.945915	-1.243730	-1.172233	1.954079	2.836539	1.748345	-7.635374	0.028885	1.054679
O	7.273155	-1.589773	1.658438	7.275533	-1.669570	1.421773	2.531288	3.785526	-0.660210	-7.548558	-0.296112	-1.575860
C	7.569636	-1.004072	2.920425	7.509227	-1.889892	2.807685	2.916837	4.214330	-1.960813	-7.556946	-0.471590	-2.987419
H	2.740340	-0.960938	-2.890563	2.345207	-2.761711	-2.362270	-3.097943	3.422349	2.268028	-3.162833	0.908702	3.003929
H	1.483752	-2.839181	-3.785690	1.491555	-1.502392	-4.235168	-3.724688	1.781098	3.926320	-2.941940	-0.438245	5.015081
H	0.850224	-3.251569	-2.091678	1.121548	-0.050731	-3.142581	-3.523627	0.407091	2.696731	-2.622188	-1.952657	3.992555
H	1.480351	-1.875638	-0.235694	1.382325	-1.967979	-0.198400	-3.457793	2.680358	-0.059489	-2.555883	-1.765395	1.606469
H	4.438636	-2.440717	-1.671390	4.503137	-1.126633	-2.026015	-0.507475	2.145765	2.160313	-5.392222	-0.172382	2.320606
H	5.106896	-0.256034	2.726639	4.929935	-1.932076	2.848329	0.395336	3.866886	-2.401074	-5.030358	-0.805841	-2.581250
H	2.930056	-0.095024	1.609352	2.698964	-1.774776	1.827586	-1.872874	3.136788	-1.798357	-3.016137	-0.933927	-1.188745
H	3.231900	1.215784	-1.470630	3.287974	1.097793	-1.228672	-5.052105	0.911595	-0.271768	-2.571042	1.873887	0.650919
H	-0.309514	-0.501748	0.203669	-0.410594	-0.562397	0.134150	-0.931019	0.043820	0.481525	-0.353468	-1.771738	0.952290
H	3.581945	3.113150	-2.833834	3.798338	3.071245	-2.409021	-6.601858	-0.022847	-1.793519	-1.919004	4.141234	0.746421
H	3.818791	4.745886	-2.159707	4.083128	4.629564	-1.592295	-7.592025	-1.450967	-1.398635	-1.371323	5.042778	-0.690184
H	4.256269	3.317881	-1.187004	4.398943	3.106371	-0.722115	-7.010741	-0.391228	-0.089077	-2.475169	3.657097	-0.885918
H	0.467734	4.627002	-0.762418	0.658406	4.578860	-0.369091	-4.544441	-3.436402	-1.127096	1.457544	2.785006	-0.997344
H	-2.072277	2.879559	0.499296	-2.049194	2.861369	0.555149	-1.140751	-3.505423	-0.707917	2.780983	-0.230083	-0.607914
H	-2.288607	-0.141107	1.015307	-2.335650	-0.154789	1.063248	0.309822	-1.611889	1.231461	1.555390	-2.766042	0.625698
H	-6.148539	-0.517456	2.868578	-6.253337	-0.453434	2.808989	4.135678	-3.463818	1.825459	6.196476	-2.647856	-0.033458
H	-5.988735	1.253096	2.937491	-6.074788	1.316311	2.848117	3.383117	-4.782240	0.896984	5.738911	-3.275146	-1.630473
H	-7.885574	0.590984	1.515271	-7.935909	0.651752	1.383035	5.194887	-3.663672	-0.384825	7.538379	-1.617350	-1.861533
H	-6.666317	1.446762	0.578848	-6.676689	1.468253	0.464508	3.638924	-3.525873	-1.195043	6.067274	-1.035783	-2.634863
H	-8.136464	-1.903560	1.275943	-5.404698	0.282921	-1.256110	2.512656	-1.351630	-1.421547	4.876573	0.923021	-1.765291
H	-7.933021	-3.844807	-0.240080	-5.180222	-1.695723	-2.719407	2.672107	1.110664	-1.346464	4.889831	2.916578	-0.304984
H	-6.462988	-3.718101	-2.240423	-6.469783	-3.763458	-2.229665	4.615228	2.202736	-0.248819	6.594304	3.136394	1.491794
H	-5.204793	-1.626364	-2.709663	-7.985814	-3.828226	-0.260846	6.382296	0.801419	0.800186	8.285312	1.342142	1.806331
H	-5.415021	0.314765	-1.194905	-8.203651	-1.849327	1.203754	6.207291	-1.663400	0.744624	8.266400	-0.651310	0.345238
H	7.592041	-2.674508	-0.114995	7.726985	-1.330559	-0.603082	2.779544	3.121455	1.325930	-8.309665	0.047207	0.357364
H	8.607904	-1.251864	3.129685	8.589769	-1.897919	2.932008	3.984659	4.415275	-1.906176	-8.591782	-0.348295	-3.298996
H	7.453620	0.082977	2.883590	7.077818	-1.084671	3.409255	2.729645	3.431639	-2.702012	-6.935053	0.282284	-3.478746
H	6.929639	-1.419557	3.704095	7.097653	-2.852297	3.125118	2.387409	5.128601	-2.243910	-7.210565	-1.473022	-3.258646

	Conformer 9			Conformer 10			Conformer 11			Conformer 12		
Gibbs free energy (hartrees)	-1534.36089			-1534.360832			-1534.360655			-1534.360401		
ΔG (kcal/mol)	0.567			0.603			0.714			0.873		
Population Proportion	6.39%			6.01%			4.98%			3.81%		
Element	X	Y	Z	X	Y	Z	X	Y	Z	X	Y	Z
C	-3.501210	2.485774	1.665568	-2.950482	0.611171	2.840241	-3.182970	2.102049	1.956872	-3.477270	2.563061	-1.201841
C	-4.024954	1.679704	2.589538	-2.568652	0.385512	4.097052	-4.236775	2.821966	2.341800	-3.561320	3.890366	-1.115015
C	-2.826240	2.068215	0.375259	-2.327251	-0.039341	1.626907	-2.731819	1.942812	0.523866	-2.949634	1.665762	-0.106488
C	-1.382597	2.551271	0.316651	-3.322091	-0.873858	0.819069	-1.343472	2.516841	0.256872	-3.986776	0.661854	0.397870
C	-2.948720	0.575957	0.096045	-1.650779	1.028812	0.779544	-2.841871	0.467598	0.148340	-1.678427	0.982696	-0.591151
C	-0.796835	2.801127	-0.932500	-4.524086	-1.314838	1.384513	-0.794231	2.387176	-1.028968	-5.350907	0.833371	0.137213
C	0.531467	3.181136	-1.027740	-5.401303	-2.107950	0.657927	0.445434	2.922736	-1.328329	-6.286514	-0.063176	0.634984
C	1.310180	3.328615	0.135909	-5.090579	-2.485706	-0.658600	1.175967	3.611865	-0.340724	-5.875668	-1.155393	1.416301
C	0.741226	3.074454	1.375988	-3.895431	-2.058601	-1.226387	0.647627	3.737118	0.934787	-4.522781	-1.330280	1.686370
C	-0.602284	2.688949	1.460217	-3.021358	-1.257108	-0.487750	-0.610790	3.191866	1.226208	-3.589084	-0.425005	1.176364
C	-4.171210	0.074081	-0.387833	-2.434685	1.963318	0.076049	-4.050782	-0.018354	-0.376488	-1.755978	-0.018232	-1.578226
C	-4.321944	-1.279213	-0.633977	-1.827569	2.948504	-0.679153	-4.185945	-1.361885	-0.686956	-0.603687	-0.619659	-2.047723
C	-3.248549	-2.166288	-0.411537	-0.420366	3.026325	-0.748974	-3.113477	-2.250027	-0.475784	0.656118	-0.235660	-1.542111
C	-2.031153	-1.683885	0.067033	0.370210	2.108983	-0.055929	-1.911293	-1.783223	0.057065	0.749158	0.751821	-0.560550
C	-1.905682	-0.302647	0.317263	-0.273935	1.112304	0.707917	-1.797233	-0.414147	0.363554	-0.441374	1.352997	-0.100220
O	-5.445944	-1.890805	-1.103356	-2.462108	3.906871	-1.410384	-5.294293	-1.958113	-1.209932	-0.535861	-1.598280	-2.993132
C	-6.585837	-1.081703	-1.373173	-3.885928	3.899613	-1.432447	-6.433842	-1.145247	-1.469932	-1.755665	-2.072384	-3.554378
O	-3.410063	-3.490755	-0.666924	0.153521	4.001788	-1.499730	-3.258237	-3.564654	-0.788373	1.774660	-0.844368	-2.015539
C	-0.908372	-2.608699	0.234721	1.825763	2.216995	-0.164246	-0.793448	-2.715071	0.224636	2.076648	1.112041	-0.059135
C	0.236795	-2.336504	0.880121	2.736446	1.471639	0.482397	0.296426	-2.493781	0.975142	2.353841	1.978198	0.930146
C	1.365151	-3.284764	0.851134	4.177153	1.689970	0.248883	1.438010	-3.427247	0.945769	3.729447	2.255333	1.385087
O	1.359087	-4.395285	0.345444	4.661318	2.517146	-0.506913	1.487352	-4.484336	0.338187	3.988318	2.938291	2.364697
O	2.446979	-2.736871	1.432219	4.911083	0.840910	0.988209	2.462924	-2.929491	1.657676	4.666977	1.678174	0.623418
C	3.712462	-3.389326	1.226938	6.339335	0.871216	0.809401	3.757244	-3.529851	1.473421	6.033093	1.792762	1.054269
C	4.247332	-3.124771	-0.181389	6.771921	0.115023	-0.445399	4.348684	-3.177989	0.104678	6.872640	0.943048	0.110859
C	4.295656	-1.652360	-0.517926	6.285543	-1.314591	-0.459823	4.215036	-1.706937	-0.214762	6.474999	-0.514711	0.141850
C	3.215383	-1.029113	-1.153478	6.976702	-2.310833	0.238660	3.157914	-1.247538	-1.008065	6.976737	-1.368987	1.129537
C	3.234976	0.338920	-1.424013	6.506134	-3.623025	0.264863	2.981496	0.114846	-1.249507	6.571818	-2.702057	1.194599
C	4.346433	1.103937	-1.070205	5.331171	-3.959085	-0.409137	3.870003	1.040384	-0.702570	5.654214	-3.200862	0.269339
C	5.428826	0.494713	-0.435672	4.634441	-2.974360	-1.109425	4.932386	0.593685	0.084452	5.148617	-2.358043	-0.720815
C	5.399879	-0.872170	-0.159648	5.110207	-1.663208	-1.132968	5.100778	-0.769238	0.326825	5.558071	-1.026482	-0.782221
O	1.088155	3.410128	-2.251542	-6.569398	-2.520561	1.229320	0.963875	2.777072	-2.581663	-7.610302	0.122406	0.362158

O	2.592309	3.732808	-0.097319	-6.039706	-3.263096	-1.258905	2.375189	4.102479	-0.772752	-6.896121	-1.958148	1.840495
C	3.486792	3.775478	1.008188	-5.802547	-3.690786	-2.594719	3.214785	4.742565	0.181786	-6.566678	-3.085661	2.642719
H	-3.538847	3.562695	1.823379	-3.751934	1.323129	2.644501	-2.607853	1.550970	2.700434	-3.784151	2.066975	-2.122298
H	-4.486894	2.088027	3.483349	-3.038485	0.900632	4.929489	-4.530786	2.876453	3.385667	-3.927136	4.487037	-1.945202
H	-4.011669	0.597858	2.487054	-1.775453	-0.320108	4.332952	-4.837650	3.378587	1.626366	-3.267445	4.421396	-0.212604
H	-3.363290	2.588830	-0.427294	-1.546004	-0.718776	1.983629	-3.436297	2.496561	-0.106154	-2.676718	2.305465	0.739338
H	-1.372113	2.688489	-1.847505	-4.796040	-1.049413	2.401486	-1.330826	1.855996	-1.810214	-5.708090	1.669698	-0.455735
H	1.324477	3.174392	2.284058	-3.632642	-2.337908	-2.240294	1.192991	4.259062	1.712515	-4.181027	-2.164804	2.287976
H	-1.030095	2.488321	2.437187	-2.096497	-0.928131	-0.951212	-1.007555	3.316909	2.227750	-2.536678	-0.582306	1.391573
H	-4.993469	0.760286	-0.561808	-3.516314	1.890633	0.117998	-4.873694	0.669807	-0.539476	-2.727186	-0.322044	-1.954437
H	-0.952545	0.085857	0.657605	0.325158	0.384602	1.246072	-0.852739	-0.032659	0.737838	-0.387203	2.128549	0.657334
H	-6.362702	-0.340629	-2.145703	-4.290703	4.050164	-0.427987	-6.198519	-0.368242	-2.202463	-2.284510	-1.266829	-4.071094
H	-7.356385	-1.760693	-1.730618	-4.178865	4.728913	-2.071866	-7.190161	-1.812587	-1.876366	-1.476071	-2.842702	-4.269129
H	-6.930854	-0.581149	-0.464209	-4.262843	2.962165	-1.850683	-6.804727	-0.689246	-0.547840	-2.396729	-2.504250	-2.780915
H	-4.306987	-3.618944	-1.016335	-0.559285	4.523469	-1.903439	-4.144675	-3.684481	-1.166181	1.499527	-1.495288	-2.681636
H	-1.007092	-3.586269	-0.230535	2.200096	2.981505	-0.839898	-0.848167	-3.649341	-0.328631	2.912309	0.611964	-0.539474
H	0.418854	-1.394723	1.386253	2.475733	0.687108	1.184387	0.425240	-1.599185	1.574684	1.588967	2.509075	1.486554
H	4.366965	-2.951914	1.980354	6.680560	1.906749	0.773494	4.359852	-3.107582	2.276751	6.336247	2.841300	1.017157
H	3.612854	-4.459939	1.411190	6.732946	0.392294	1.705735	3.689465	-4.611089	1.603627	6.113315	1.440058	2.085163
H	5.248829	-3.562015	-0.230517	6.413136	0.649782	-1.327601	5.400914	-3.476391	0.124627	6.779701	1.341841	-0.902630
H	3.627061	-3.658528	-0.905226	7.865317	0.145396	-0.471720	3.856922	-3.774944	-0.665932	7.917324	1.060665	0.411610
H	2.350025	-1.619448	-1.444697	7.893619	-2.058090	0.765261	2.462528	-1.962169	-1.441545	7.691405	-0.988612	1.855107
H	2.386520	0.806594	-1.915466	7.057577	-4.383673	0.808618	2.152939	0.455840	-1.863984	6.973768	-3.351258	1.966189
H	4.367272	2.166192	-1.288942	4.964188	-4.980327	-0.391295	3.736166	2.100638	-0.892364	5.337815	-4.237926	0.318429
H	6.297377	1.083729	-0.157679	3.720876	-3.226393	-1.638795	5.630738	1.307937	0.509799	4.433751	-2.735477	-1.445220
H	6.247741	-1.339055	0.335245	4.561982	-0.903097	-1.683593	5.929128	-1.107681	0.944313	5.158121	-0.376086	-1.555281
H	2.009886	3.679757	-2.112690	-7.044060	-3.059384	0.576732	1.820681	3.231549	-2.605842	-8.104271	-0.595055	0.789613
H	4.453575	4.065845	0.602037	-6.666802	-4.288191	-2.876382	4.120311	5.019276	-0.353759	-7.509432	-3.579059	2.868479
H	3.163456	4.517580	1.743978	-5.714625	-2.834298	-3.269410	2.736643	5.641251	0.581508	-5.914431	-3.775016	2.098851
H	3.569285	2.791106	1.478463	-4.899136	-4.304570	-2.653928	3.465938	4.059346	0.998684	-6.084534	-2.775009	3.574045
Conformer 13												
Gibbs free energy (hartrees)	-1534.359774											
ΔG (kcal/mol)	1.267											
Population Proportion	1.96%											
Element	X	Y	Z									
C	-3.930694	2.679622	0.342112									
C	-4.825607	3.502677	-0.204536									

C	-2.880232	1.921302	-0.437920									
C	-1.486028	2.395047	-0.055639									
C	-3.053555	0.406186	-0.293541									
C	-0.618818	2.876857	-1.041093									
C	0.664385	3.295130	-0.714743									
C	1.106017	3.239499	0.617183									
C	0.252163	2.757850	1.603588									
C	-1.036662	2.340453	1.263783									
C	-4.346636	-0.146969	-0.331827									
C	-4.522369	-1.519543	-0.273902									
C	-3.409386	-2.377458	-0.173772									
C	-2.122660	-1.844132	-0.126012									
C	-1.967942	-0.446340	-0.197693									
O	-5.716652	-2.176431	-0.302275									
C	-6.906435	-1.401524	-0.405193									
O	-3.597889	-3.721532	-0.103629									
C	-0.969855	-2.743730	-0.023017									
C	0.250024	-2.377066	0.398190									
C	1.384205	-3.320712	0.398649									
O	1.359536	-4.482663	0.026846									
O	2.487039	-2.711494	0.857019									
C	3.725613	-3.437475	0.797278									
C	4.834631	-2.457391	1.156395									
C	4.896059	-1.285397	0.203575									
C	5.600703	-1.380760	-1.001037									
C	5.612744	-0.320816	-1.907977									
C	4.915789	0.853405	-1.621792									
C	4.211286	0.960874	-0.422214									
C	4.204389	-0.101253	0.481118									
O	1.494909	3.756233	-1.692805									
O	2.385445	3.683060	0.801645									
C	2.933536	3.615108	2.113360									
H	-3.935386	2.525321	1.420217									
H	-5.552090	4.030615	0.405854									
H	-4.859023	3.675198	-1.277837									
H	-3.029771	2.159173	-1.496562									
H	-0.929384	2.925923	-2.080879									
H	0.575553	2.702153	2.636670									
H	-1.680561	1.950375	2.045891									
H	-5.203871	0.512316	-0.413749									
H	-0.965881	-0.033332	-0.203090									

H	-6.916163	-0.824598	-1.334063									
H	-7.727632	-2.114432	-0.410180									
H	-7.008807	-0.730207	0.451980									
H	-4.551575	-3.891859	-0.168483									
H	-1.123324	-3.780631	-0.311990									
H	0.469249	-1.371378	0.741711									
H	3.689632	-4.271435	1.501741									
H	3.857440	-3.835106	-0.211657									
H	4.680123	-2.107302	2.180373									
H	5.776407	-3.012684	1.141842									
H	6.145214	-2.292643	-1.233199									
H	6.166867	-0.411971	-2.836985									
H	4.922808	1.678772	-2.326792									
H	3.667529	1.871456	-0.188150									
H	3.647827	-0.013956	1.410176									
H	2.331449	4.016552	-1.275869									
H	3.954868	3.979944	2.030143									
H	2.371905	4.250696	2.803862									
H	2.942214	2.584615	2.480117									

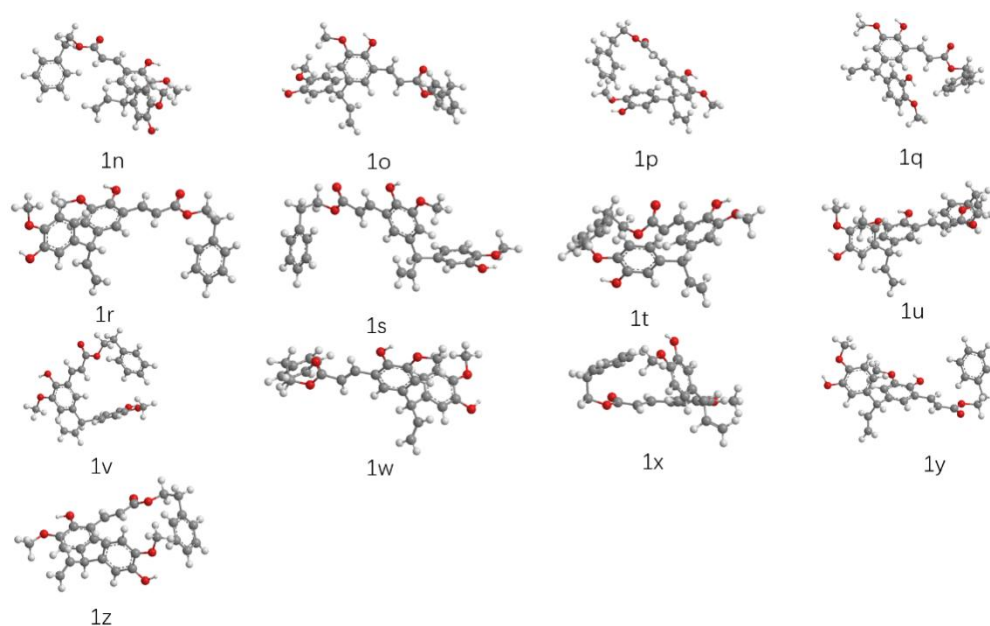


Figure S13: Most stable conformers of 7'R-1 calculated at the CAM-B3LYP/DGTZVP level

Table S3: Energies and atomic Cartesian coordinates of geometry-optimized conformers of 7'R-1 at wb97xd/dgdzvp in methanol

	Conformer 1			Conformer 2			Conformer 3			Conformer 4		
Gibbs free energy (hartrees)	-1534.361793			-1534.361681			-1534.361158			-1534.361152		
ΔG (kcal/mol)				0.07			0.398			0.402		
Population Proportion	16.61%			14.75%			8.48%			8.42%		
Element	X	Y	Z	X	Y	Z	X	Y	Z	X	Y	Z
C	1.307390	-2.263157	-0.060618	-1.429732	-1.305883	2.167284	3.768579	2.708881	0.014730	3.953142	2.592666	0.396527
C	0.742398	-3.299968	-0.679090	-1.217671	-1.612408	3.447034	4.705498	3.436043	-0.593562	4.971901	3.335084	-0.036878
C	2.121996	-1.194471	-0.750098	-2.366800	-0.221768	1.690299	2.755384	1.845210	-0.702060	3.024142	1.808416	-0.503127
C	3.548369	-1.232128	-0.214012	-3.478004	-0.853880	0.860032	1.359739	2.405941	-0.471263	1.616111	2.377621	-0.426374
C	1.503553	0.196972	-0.636396	-1.654919	0.897432	0.934217	2.878694	0.367632	-0.324184	3.081454	0.306211	-0.211559
C	4.570335	-1.797910	-0.983223	-4.753905	-1.019883	1.408473	0.797645	2.411211	0.814514	0.917051	2.395996	0.790439
C	5.867322	-1.867353	-0.494656	-5.765713	-1.623022	0.674776	-0.451989	2.964169	1.034252	-0.363644	2.916795	0.860407
C	6.166798	-1.370528	0.785626	-5.515456	-2.078400	-0.631262	-1.175590	3.528334	-0.034111	-0.979596	3.438041	-0.294096
C	5.155327	-0.808549	1.557074	-4.248585	-1.918558	-1.182277	-0.635500	3.510152	-1.311893	-0.298905	3.418151	-1.502759
C	3.853096	-0.742135	1.054485	-3.237667	-1.307881	-0.435353	0.631847	2.951407	-1.522206	0.997186	2.889302	-1.560937
C	2.261104	1.308060	-1.057169	-2.436796	1.870312	0.280046	4.120144	-0.159162	0.070906	4.312909	-0.288809	0.119106
C	1.724143	2.579544	-1.003586	-1.832512	2.916350	-0.389477	4.244573	-1.505214	0.377058	4.392340	-1.652496	0.344151
C	0.411106	2.778441	-0.526676	-0.425688	3.020909	-0.425228	3.131406	-2.360795	0.288033	3.242742	-2.460304	0.242058
C	-0.353753	1.690043	-0.108383	0.363487	2.068696	0.218953	1.896143	-1.857110	-0.120642	2.016377	-1.888022	-0.095832
C	0.216713	0.400246	-0.176983	-0.278741	1.011412	0.899920	1.791621	-0.486148	-0.419467	1.961115	-0.498440	-0.320126
O	2.348648	3.731818	-1.376424	-2.469776	3.916217	-1.060898	5.385956	-2.132578	0.780346	5.518362	-2.345473	0.676108
C	3.689031	3.644317	-1.848970	-3.892279	3.885278	-1.115912	6.566789	-1.350793	0.925671	6.732658	-1.618439	0.829912
O	-0.094200	4.038045	-0.475674	0.146893	4.054024	-1.095493	3.267797	-3.678999	0.589921	3.339298	-3.796319	0.469566
C	-1.713374	1.934190	0.374644	1.818854	2.209211	0.159074	0.741930	-2.757648	-0.182730	0.827885	-2.741420	-0.171791
C	-2.562501	1.023502	0.877778	2.729062	1.373389	0.684963	-0.390702	-2.520996	-0.861730	-0.366100	-2.377346	-0.664348
C	-3.916533	1.425188	1.304717	4.169960	1.649981	0.528874	-1.545317	-3.432401	-0.750839	-1.524571	-3.289528	-0.614124
O	-4.374361	2.555920	1.260217	4.655224	2.613099	-0.042987	-1.585298	-4.465675	-0.102903	-1.532103	-4.425412	-0.168015
O	-4.604832	0.363463	1.758060	4.903530	0.683521	1.107097	-2.589214	-2.947412	-1.443558	-2.609706	-2.682141	-1.116220
C	-5.978967	0.574998	2.131502	6.334703	0.769859	0.976785	-3.879106	-3.539446	-1.208053	-3.872690	-3.357254	-0.996593
C	-6.899150	0.627187	0.913152	6.814934	0.294112	-0.393179	-4.443200	-3.125165	0.153808	-4.958578	-2.320411	-1.253614
C	-6.787245	-0.604282	0.046257	6.351903	-1.105875	-0.718819	-4.339594	-1.635640	0.385227	-4.909577	-1.187841	-0.253658
C	-5.940208	-0.619894	-1.066698	5.201347	-1.318027	-1.485189	-5.276096	-0.755533	-0.167324	-4.176747	-0.026839	-0.523081
C	-5.798550	-1.771057	-1.841607	4.745803	-2.609880	-1.749040	-5.140394	0.623138	-0.007326	-4.075160	0.991282	0.423990
C	-6.505998	-2.927423	-1.512784	5.438413	-3.712049	-1.247952	-4.060002	1.143103	0.706523	-4.710715	0.863290	1.659439
C	-7.356042	-2.922627	-0.405989	6.589064	-3.512321	-0.483854	-3.120102	0.275551	1.262697	-5.448970	-0.287422	1.937654

C	-7.492899	-1.769551	0.365897	7.039267	-2.218937	-0.222267	-3.264086	-1.102574	1.104170	-5.545124	-1.303922	0.987127
O	6.851578	-2.416207	-1.262336	-7.005042	-1.769455	1.224224	-0.987378	2.956941	2.288669	-1.030670	2.921494	2.049233
O	7.479004	-1.498167	1.142082	-6.595981	-2.649087	-1.241271	-2.382177	4.055999	0.326641	-2.238586	3.924202	-0.082195
C	7.870578	-1.021656	2.423928	-6.429626	-3.144079	-2.564464	-3.228078	4.549958	-0.705772	-2.963693	4.411368	-1.206138
H	1.212351	-2.166571	1.020589	-0.924788	-1.876404	1.388243	3.697249	2.729020	1.101754	3.751782	2.533031	1.465397
H	0.188147	-4.051926	-0.125560	-0.549990	-2.420915	3.729104	5.395028	4.054361	-0.026743	5.599158	3.889668	0.654521
H	0.816421	-3.429748	-1.756280	-1.704598	-1.066167	4.251523	4.811372	3.436963	-1.675966	5.209502	3.412494	-1.095377
H	2.161616	-1.444678	-1.815615	-2.829162	0.228499	2.575091	2.963891	1.920298	-1.774681	3.374783	1.947189	-1.531500
H	4.368252	-2.190144	-1.976025	-4.976246	-0.678044	2.415508	1.324345	1.973032	1.657720	1.355367	1.985805	1.695764
H	5.365530	-0.416723	2.545646	-4.035393	-2.260023	-2.188744	-1.179493	3.928311	-2.150834	-0.756190	3.809327	-2.404224
H	3.076619	-0.288604	1.663601	-2.256999	-1.178524	-0.883909	1.044964	2.950961	-2.526355	1.517517	2.879828	-2.513875
H	3.272596	1.153951	-1.417258	-3.517837	1.783391	0.302398	4.979777	0.497833	0.140464	5.198352	0.331888	0.201284
H	-0.376833	-0.453701	0.130151	0.326771	0.273456	1.414238	0.823627	-0.083317	-0.697798	1.006848	-0.044225	-0.560343
H	4.345203	3.226523	-1.080358	-4.241852	2.972755	-1.606780	6.859401	-0.906012	-0.029501	7.015050	-1.129905	-0.106768
H	3.742441	3.036244	-2.756134	-4.321737	3.957623	-0.113029	6.424780	-0.566679	1.674552	6.642233	-0.874574	1.626307
H	3.993207	4.663642	-2.074670	-4.187411	4.752070	-1.702454	7.340581	-2.038155	1.259461	7.488039	-2.352581	1.100116
H	0.586397	4.644973	-0.809599	-0.566320	4.597382	-1.468636	4.185125	-3.824856	0.872950	4.260470	-3.991383	0.706760
H	-2.065145	2.960847	0.316234	2.194446	3.080965	-0.370253	0.812039	-3.684128	0.381912	0.927923	-3.751522	0.217216
H	-2.314832	-0.026785	0.986700	2.467913	0.470376	1.225917	-0.534617	-1.636549	-1.473003	-0.553395	-1.397646	-1.090512
H	-6.220708	-0.279480	2.763304	6.656305	1.795457	1.163670	-4.498425	-3.155254	-2.017858	-3.915638	-4.168524	-1.726922
H	-6.060871	1.491842	2.716932	6.715558	0.122886	1.766819	-3.811363	-4.625373	-1.289236	-3.958918	-3.781645	0.005870
H	-7.919782	0.734674	1.292467	6.473974	0.996456	-1.156799	-5.487601	-3.449469	0.179778	-4.850166	-1.936134	-2.271204
H	-6.674444	1.524619	0.332610	7.908062	0.339337	-0.377481	-3.916053	-3.666247	0.942299	-5.920920	-2.836909	-1.202098
H	-5.387335	0.277420	-1.332653	4.657069	-0.465244	-1.882848	-6.119032	-1.151807	-0.728043	-3.673038	0.077006	-1.480087
H	-5.136959	-1.764144	-2.702175	3.851295	-2.754999	-2.346662	-5.878150	1.292153	-0.439597	-3.499554	1.884324	0.199459
H	-6.399087	-3.823593	-2.115618	5.087180	-4.718130	-1.453831	-3.950125	2.215443	0.831457	-4.631924	1.654389	2.398616
H	-7.914493	-3.816235	-0.145295	7.137409	-4.364125	-0.093828	-2.276963	0.673238	1.820592	-5.950129	-0.394506	2.894634
H	-8.158214	-1.774322	1.225645	7.937288	-2.072403	0.372645	-2.529645	-1.771347	1.546278	-6.119618	-2.198587	1.213898
H	7.679558	-2.373710	-0.758154	-7.571446	-2.204822	0.567655	-1.848424	3.402498	2.247674	-1.898041	3.331364	1.904183
H	8.937401	-1.218152	2.503933	-7.394784	-3.552763	-2.855330	-4.141886	4.876457	-0.213916	-3.935887	4.716453	-0.825513
H	7.689095	0.053298	2.513223	-6.151792	-2.339042	-3.250863	-2.765257	5.398705	-1.217211	-2.457929	5.272000	-1.652806
H	7.339978	-1.555178	3.217764	-5.674160	-3.934513	-2.593444	-3.461433	3.761192	-1.427171	-3.093887	3.625311	-1.955824
	Conformer 5			Conformer 6			Conformer 7			Conformer 8		
Gibbs free energy (hartrees)	-1534.361105			-1534.360971			-1534.360967			-1534.360925		
ΔG (kcal/mol)	0.432			0.516			0.518			0.545		
Population Proportion	8.01%			6.95%			6.92%			6.62%		
Element	X	Y	Z	X	Y	Z	X	Y	Z	X	Y	Z

C	-2.141497	-1.580682	-2.223593	-1.973022	-1.750815	-2.200800	3.132510	2.369075	1.992832	2.949711	-0.156904	2.922902
C	-1.457393	-2.608831	-2.724894	-1.505087	-1.062614	-3.242502	3.477134	1.470569	2.915733	2.831974	-0.886296	4.032127
C	-2.131507	-1.174557	-0.768182	-2.033003	-1.287886	-0.760258	2.764054	2.089253	0.550048	2.779228	-0.696744	1.521944
C	-3.511529	-1.247606	-0.114448	-3.429025	-1.440516	-0.167727	1.365374	2.594957	0.220786	4.040622	-0.561059	0.668475
C	-1.510641	0.209960	-0.642885	-1.487656	0.116781	-0.556122	2.959668	0.629878	0.161458	1.575043	-0.028304	0.873481
C	-4.564621	-1.949040	-0.711733	-4.577578	-1.302634	-0.956492	0.327934	2.525614	1.158585	5.288475	-0.307516	1.248456
C	-5.801968	-2.037317	-0.088389	-5.839903	-1.383156	-0.386889	-0.957320	2.924871	0.823074	6.431632	-0.225308	0.465053
C	-6.012441	-1.427024	1.158617	-5.980316	-1.609257	0.993285	-1.230236	3.417759	-0.464691	6.352148	-0.403503	-0.925598
C	-4.969434	-0.733977	1.763459	-4.844835	-1.752862	1.782729	-0.206341	3.490919	-1.402142	5.117235	-0.663112	-1.510171
C	-3.729904	-0.647116	1.125450	-3.577921	-1.667663	1.198451	1.083834	3.080198	-1.054107	3.972417	-0.738400	-0.713364
C	-2.225698	1.339587	-1.084256	-2.275515	1.239918	-0.867550	4.237353	0.196029	-0.233703	1.644562	1.328613	0.504596
C	-1.655418	2.595852	-1.004466	-1.760761	2.514130	-0.714729	4.452282	-1.130042	-0.571900	0.546524	1.951243	-0.057986
C	-0.354300	2.755005	-0.482213	-0.444901	2.699015	-0.243647	3.391980	-2.056365	-0.522604	-0.649828	1.232889	-0.265401
C	0.366958	1.645149	-0.040035	0.348713	1.595614	0.074388	2.122125	-1.643002	-0.122122	-0.734029	-0.112890	0.093862
C	-0.237293	0.373292	-0.133186	-0.198583	0.306749	-0.093865	1.927370	-0.289368	0.212854	0.400262	-0.725333	0.667569
O	-2.234649	3.767169	-1.389545	-2.415143	3.680024	-0.978538	5.634429	-1.674450	-0.977099	0.479022	3.250347	-0.462611
C	-3.553888	3.718066	-1.923387	-3.755118	3.602057	-1.453983	6.770525	-0.821111	-1.065461	1.639529	4.060860	-0.307626
O	0.184321	3.999689	-0.409767	0.037245	3.959984	-0.093220	3.615229	-3.354334	-0.857675	-1.715106	1.864927	-0.823706
C	1.712905	1.853954	0.495501	1.709707	1.828951	0.559615	1.020073	-2.608501	-0.105246	-1.993600	-0.818910	-0.147097
C	2.542048	0.912606	0.974574	2.572431	0.902112	1.006453	-0.124251	-2.458879	0.579539	-2.267193	-2.100724	0.149193
C	3.884056	1.283389	1.463799	3.925725	1.295672	1.444022	-1.231040	-3.422642	0.432671	-3.582771	-2.715029	-0.111370
O	4.343081	2.413714	1.504061	4.371945	2.431810	1.452269	-1.228706	-4.416350	-0.275380	-3.886416	-3.837619	0.263567
O	4.559398	0.193522	1.866611	4.627151	0.220094	1.840696	-2.284122	-3.037399	1.173650	-4.414579	-1.918579	-0.793924
C	5.923168	0.377908	2.289571	6.000468	0.427752	2.219645	-3.538569	-3.703684	0.946133	-5.758370	-2.384308	-0.999012
C	6.875460	0.511367	1.102476	6.915395	0.548097	1.002302	-4.211034	-3.188963	-0.327298	-6.526231	-1.252223	-1.666685
C	6.787372	-0.657503	0.150357	6.817132	-0.643549	0.079887	-4.346431	-1.684211	-0.339261	-6.569573	-0.005483	-0.813447
C	5.965563	-0.597540	-0.979904	5.969349	-0.618549	-1.032297	-3.360340	-0.883921	-0.926985	-5.625729	1.012847	-0.983388
C	5.846706	-1.691809	-1.836740	5.842348	-1.734104	-1.860075	-3.450612	0.507013	-0.889188	-5.631837	2.137825	-0.159323
C	6.551905	-2.866265	-1.573767	6.565156	-2.895117	-1.585582	-4.538308	1.120248	-0.267562	-6.587228	2.261270	0.849845
C	7.376520	-2.936757	-0.450114	7.415617	-2.930801	-0.479644	-5.530168	0.332829	0.317802	-7.535488	1.253080	1.026466
C	7.490597	-1.840369	0.403779	7.537851	-1.813264	0.345117	-5.430911	-1.057844	0.283835	-7.524162	0.129638	0.200168
O	-6.814710	-2.722229	-0.693784	-6.945915	-1.243730	-1.172233	-1.954079	2.836539	1.748345	7.635374	0.028885	1.054679
O	-7.273155	-1.589773	1.658438	-7.275533	-1.669570	1.421773	-2.531288	3.785526	-0.660210	7.548558	-0.296112	-1.575859
C	-7.569636	-1.004072	2.920425	-7.509227	-1.889892	2.807685	-2.916837	4.214330	-1.960813	7.556946	-0.471590	-2.987419
H	-2.740340	-0.960938	-2.890563	-2.345207	-2.761711	-2.362270	3.097943	3.422349	2.268028	3.162833	0.908702	3.003929
H	-1.483752	-2.839181	-3.785690	-1.491555	-1.502392	-4.235168	3.724688	1.781098	3.926320	2.941939	-0.438245	5.015081
H	-0.850223	-3.251569	-2.091678	-1.121548	-0.050731	-3.142581	3.523627	0.407091	2.696731	2.622188	-1.952657	3.992555
H	-1.480351	-1.875638	-0.235694	-1.382325	-1.967979	-0.198400	3.457793	2.680358	-0.059489	2.555883	-1.765395	1.606469
H	-4.438636	-2.440718	-1.671390	-4.503137	-1.126632	-2.026015	0.507475	2.145765	2.160313	5.392222	-0.172382	2.320606
H	-5.106896	-0.256034	2.726639	-4.929935	-1.932076	2.848329	-0.395336	3.866886	-2.401074	5.030358	-0.805841	-2.581250
H	-2.930056	-0.095024	1.609352	-2.698964	-1.774776	1.827586	1.872874	3.136788	-1.798357	3.016137	-0.933927	-1.188745

H	-3.231900	1.215784	-1.470630	-3.287974	1.097793	-1.228672	5.052105	0.911595	-0.271768	2.571042	1.873887	0.650919
H	0.309514	-0.501748	0.203669	0.410594	-0.562397	0.134150	0.931019	0.043820	0.481525	0.353468	-1.771738	0.952290
H	-3.581945	3.113149	-2.833834	-3.798338	3.071245	-2.409021	6.601858	-0.022847	-1.793519	1.919004	4.141234	0.746420
H	-4.256269	3.317881	-1.187004	-4.398943	3.106371	-0.722115	7.010741	-0.391228	-0.089077	2.475169	3.657097	-0.885918
H	-3.818791	4.745886	-2.159707	-4.083128	4.629564	-1.592295	7.592025	-1.450966	-1.398635	1.371323	5.042778	-0.690185
H	-0.467734	4.627002	-0.762418	-0.658406	4.578860	-0.369091	4.544441	-3.436402	-1.127096	-1.457544	2.785006	-0.997345
H	2.072277	2.879559	0.499296	2.049194	2.861369	0.555150	1.140751	-3.505423	-0.707917	-2.780983	-0.230083	-0.607914
H	2.288607	-0.141107	1.015307	2.335650	-0.154789	1.063248	-0.309822	-1.611889	1.231461	-1.555390	-2.766043	0.625698
H	5.988735	1.253096	2.937491	6.074788	1.316311	2.848117	-3.383117	-4.782240	0.896984	-5.738911	-3.275146	-1.630473
H	6.148539	-0.517456	2.868578	6.253337	-0.453434	2.808989	-4.135678	-3.463818	1.825459	-6.196476	-2.647856	-0.033458
H	6.666317	1.446762	0.578848	6.676689	1.468253	0.464508	-3.638924	-3.525873	-1.195043	-6.067274	-1.035783	-2.634863
H	7.885574	0.590984	1.515270	7.935909	0.651753	1.383035	-5.194887	-3.663672	-0.384825	-7.538379	-1.617349	-1.861533
H	5.415021	0.314765	-1.194905	5.404698	0.282921	-1.256110	-2.512656	-1.351630	-1.421547	-4.876573	0.923021	-1.765291
H	5.204793	-1.626364	-2.709663	5.180222	-1.695723	-2.719407	-2.672107	1.110664	-1.346464	-4.889831	2.916578	-0.304984
H	6.462989	-3.718101	-2.240423	6.469784	-3.763458	-2.229666	-4.615228	2.202736	-0.248819	-6.594304	3.136394	1.491794
H	7.933021	-3.844807	-0.240080	7.985814	-3.828226	-0.260846	-6.382296	0.801419	0.800186	-8.285312	1.342142	1.806331
H	8.136464	-1.903560	1.275943	8.203651	-1.849327	1.203754	-6.207291	-1.663400	0.744624	-8.266400	-0.651310	0.345238
H	-7.592041	-2.674508	-0.114995	-7.726985	-1.330559	-0.603082	-2.779544	3.121455	1.325930	8.309665	0.047208	0.357364
H	-8.607905	-1.251864	3.129685	-8.589769	-1.897919	2.932008	-3.984659	4.415275	-1.906176	8.591783	-0.348294	-3.298996
H	-6.929640	-1.419557	3.704095	-7.097653	-2.852297	3.125118	-2.387409	5.128601	-2.243910	7.210565	-1.473022	-3.258646
H	-7.453620	0.082977	2.883590	-7.077818	-1.084671	3.409255	-2.729645	3.431639	-2.702012	6.935053	0.282284	-3.478745
	Conformer 9			Conformer 10			Conformer 11			Conformer 12		
Gibbs free energy (hartrees)	-1534.360901			-1534.360839			-1534.36065			-1534.360401		
ΔG (kcal/mol)	0.56			0.599			0.717			0.873		
Population Proportion	6.46%			6.05%			4.95%			3.8%		
Element	X	Y	Z	X	Y	Z	X	Y	Z	X	Y	Z
C	3.501307	2.485344	1.666160	-2.950710	-0.611700	2.839975	3.182717	2.102364	1.956587	3.477248	-2.561734	1.204720
C	4.024862	1.679132	2.590113	-2.568992	-0.386336	4.096870	4.236518	2.822282	2.341520	3.561321	-3.889126	1.119257
C	2.826383	2.067982	0.375761	-2.327339	0.039041	1.626838	2.731601	1.943065	0.523575	2.949654	-1.665564	0.108422
C	1.382779	2.551146	0.317164	-3.322058	0.873776	0.819082	1.343206	2.516990	0.256583	3.986805	-0.662149	-0.396898
C	2.948760	0.575750	0.096363	-1.650847	-1.028970	0.779313	2.841790	0.467850	0.148107	1.678402	-0.982034	0.592312
C	0.797098	2.801278	-0.931975	-4.524033	1.314797	1.384530	0.793803	2.387034	-1.029157	5.350927	-0.833395	-0.136013
C	-0.531180	3.181361	-1.027214	-5.401131	2.108100	0.658010	-0.445916	2.922500	-1.328473	6.286548	0.062660	-0.634642
C	-1.309953	3.328638	0.136424	-5.090319	2.485984	-0.658457	-1.176341	3.611822	-0.340924	5.875726	1.154092	-1.417068
C	-0.741071	3.074232	1.376484	-3.895182	2.058848	-1.226242	-0.647826	3.737388	0.934484	4.522850	1.328699	-1.687368
C	0.602422	2.688661	1.460713	-3.021223	1.257174	-0.487670	0.610638	3.192225	1.225861	3.589137	0.423928	-1.176494
C	4.171275	0.073827	-0.387409	-2.434732	-1.963305	0.075571	4.050730	-0.017997	-0.376754	1.755872	0.019898	1.578376

C	4.321921	-1.279444	-0.633721	-1.827591	-2.948357	-0.679784	4.186033	-1.361527	-0.687151	0.603540	0.621776	2.047191
C	3.248409	-2.166453	-0.411560	-0.420388	-3.026218	-0.749513	3.113676	-2.249781	-0.475879	-0.656227	0.237237	1.541893
C	2.030984	-1.684002	0.066882	0.370166	-2.109038	-0.056232	1.911462	-1.783087	0.056993	-0.749185	-0.751240	0.561327
C	1.905602	-0.302784	0.317279	-0.274002	-1.112487	0.707760	1.797262	-0.414006	0.363418	0.441388	-1.352857	0.101680
O	5.445928	-1.891071	-1.103030	-2.462109	-3.906551	-1.411265	5.294421	-1.957661	-1.210144	0.535634	1.601354	2.991604
C	6.586043	-1.082082	-1.372237	-3.885928	-3.899277	-1.433357	6.433893	-1.144703	-1.470187	1.755394	2.076062	3.552435
O	3.409841	-3.490900	-0.667096	0.153532	-4.001548	-1.500419	3.258573	-3.564405	-0.788413	-1.774810	0.846402	2.014634
C	0.908091	-2.608735	0.234285	1.825724	-2.217071	-0.164457	0.793731	-2.715067	0.224644	-2.076635	-1.112000	0.060198
C	-0.237131	-2.336520	0.879581	2.736356	-1.471792	0.482346	-0.296185	-2.493843	0.975106	-2.353746	-1.979134	-0.928250
C	-1.365573	-3.284669	0.850367	4.177081	-1.690082	0.248940	-1.437648	-3.427460	0.945833	-3.729319	-2.256774	-1.382985
O	-1.359577	-4.395104	0.344485	4.661333	-2.517168	-0.506896	-1.486932	-4.484509	0.338178	-3.988114	-2.940718	-2.361926
O	-2.447378	-2.736789	1.431508	4.910926	-0.841083	0.988424	-2.462534	-2.929896	1.657912	-4.666909	-1.678889	-0.621940
C	-3.712904	-3.389103	1.226054	6.339200	-0.871360	0.809779	-3.756803	-3.530391	1.473763	-6.032998	-1.793956	-1.052748
C	-4.247640	-3.124374	-0.182291	6.771911	-0.115130	-0.444957	-4.348456	-3.178479	0.105124	-6.872622	-0.943309	-0.110247
C	-4.295774	-1.651936	-0.518726	6.285486	1.314468	-0.459419	-4.214847	-1.707417	-0.214297	-6.475020	0.514430	-0.142697
C	-3.215398	-1.028778	-1.154194	6.976489	2.310713	0.239213	-3.158008	-1.248036	-1.007982	-6.976730	1.367688	-1.131276
C	-3.234829	0.339268	-1.424670	6.505858	3.622883	0.265390	-2.981620	0.114352	-1.249438	-6.571843	2.700703	-1.197670
C	-4.346217	1.104395	-1.070881	5.330991	3.958917	-0.408790	-3.869878	1.039906	-0.702134	-5.654300	3.200472	-0.272870
C	-5.428703	0.495263	-0.436420	4.634425	2.974192	-1.109236	-4.931982	0.593225	0.085280	-5.148731	2.358671	0.718165
C	-5.399921	-0.871637	-0.160458	5.110253	1.663062	-1.132753	-5.100340	-0.769697	0.327667	-5.558153	1.027163	0.780901
O	-1.087787	3.410630	-2.251003	-6.569205	2.520769	1.229412	-0.964521	2.776549	-2.581705	7.610326	-0.122639	-0.361575
O	-2.592064	3.732885	-0.096797	-6.039353	3.263537	-1.258705	-2.375650	4.102274	-0.772893	6.896191	1.956429	-1.842024
C	-3.486584	3.775348	1.008685	-5.802034	3.691491	-2.594407	-3.215207	4.742418	0.181639	6.566771	3.083149	-2.645371
H	3.539044	3.562246	1.824077	-3.752171	-1.323582	2.643997	2.607569	1.551313	2.700147	3.784075	-2.064702	2.124684
H	4.486753	2.087323	3.484010	-3.038925	-0.901620	4.929150	4.530507	2.876791	3.385391	3.927103	-4.484942	1.950072
H	4.011460	0.597296	2.487538	-1.775780	0.319192	4.333001	4.837415	3.378877	1.626083	3.267500	-4.421083	0.217375
H	3.363498	2.588658	-0.426708	-1.546083	0.718356	1.983768	3.436040	2.496863	-0.106448	2.676803	-2.306136	-0.736767
H	1.372428	2.688799	-1.846966	-4.796059	1.049268	2.401456	1.330298	1.855690	-1.810359	5.708091	-1.669126	0.457787
H	-1.324360	3.174024	2.284546	-3.632318	2.338268	-2.240098	-1.193093	4.259498	1.712167	4.181114	2.162619	-2.289822
H	1.030173	2.487839	2.437670	-2.096370	0.928167	-0.951127	1.007533	3.317498	2.227322	2.536739	0.581007	-1.391904
H	4.993624	0.759982	-0.561161	-3.516364	-1.890597	0.117459	4.873557	0.670248	-0.539822	2.727050	0.324112	1.954339
H	0.952448	0.085764	0.657516	0.325083	-0.384908	1.246093	0.852743	-0.032601	0.737719	0.387279	-2.129181	-0.655088
H	6.363316	-0.340805	-2.144690	-4.290722	-4.050008	-0.428933	6.198500	-0.367757	-2.202758	2.284233	1.271048	4.070001
H	6.930790	-0.581778	-0.463033	-4.262820	-2.961747	-1.851426	6.804736	-0.688620	-0.548118	2.396490	2.507156	2.778568
H	7.356624	-1.761109	-1.729542	-4.178857	-4.728454	-2.072939	7.190273	-1.811993	-1.876587	1.475740	2.847100	4.266384
H	4.306811	-3.619129	-1.016372	-0.559258	-4.523138	-1.904274	4.145015	-3.684153	-1.166233	-1.499733	1.498001	2.680089
H	1.006784	-3.586254	-0.231086	2.200099	-2.981507	-0.840168	0.848576	-3.649379	-0.328539	-2.912340	-0.611484	0.540005
H	-0.419155	-1.394794	1.385826	2.475578	-0.687334	1.184393	-0.425125	-1.599210	1.574565	-1.588823	-2.510525	-1.484101
H	-3.613418	-4.459744	1.410214	6.732702	-0.392457	1.706172	-3.688884	-4.611633	1.603865	-6.113175	-1.442302	-2.084004
H	-4.367428	-2.951699	1.979457	6.680441	-1.906885	0.773880	-4.359360	-3.108272	2.277211	-6.336123	-2.842465	-1.014588
H	-3.627377	-3.658148	-0.906122	7.865311	-0.145474	-0.471146	-3.856803	-3.775402	-0.665579	-7.917286	-1.061261	-0.410936

H	-5.249183	-3.561502	-0.231522	6.413245	-0.649881	-1.327211	-5.400683	-3.476882	0.125206	-6.779728	-1.341070	0.903651
H	-2.350091	-1.619193	-1.445400	7.893329	2.057989	0.765957	-2.462824	-1.962680	-1.441762	-7.691351	0.986559	-1.856497
H	-2.386303	0.806855	-1.916083	7.057178	4.383534	0.809267	-2.153275	0.455332	-1.864209	-6.973771	3.349110	-1.969939
H	-4.366939	2.166660	-1.289583	4.963959	4.980141	-0.390966	-3.736086	2.100159	-0.891958	-5.337926	4.237493	-0.322996
H	-6.297202	1.084361	-0.158440	3.720938	3.226207	-1.638750	-5.630142	1.307492	0.510915	-4.433912	2.736859	1.442222
H	-6.247859	-1.338450	0.334374	4.562151	0.902954	-1.683502	-5.928469	-1.108125	0.945460	-5.158225	0.377562	1.554641
H	-2.009475	3.680410	-2.112159	-7.043764	3.059759	0.576887	-1.821348	3.230986	-2.605871	8.104308	0.594399	-0.789723
H	-4.453371	4.065723	0.602549	-6.666211	4.289032	-2.876020	-4.120838	5.018919	-0.353837	7.509530	3.576334	-2.871576
H	-3.569042	2.790908	1.478816	-4.898562	4.305205	-2.653401	-3.466171	4.059319	0.998696	6.084671	2.771577	-3.576412
H	-3.163303	4.517364	1.744588	-5.714127	2.835139	-3.269271	-2.737129	5.641237	0.581140	5.914495	3.773032	-2.102209
Conformer 13												
Gibbs free energy (hartrees)	-1534.359777											
ΔG (kcal/mol)	1.265											
Population Proportion	1.96%											
Element	X	Y	Z									
C	3.930664	2.679679	0.342097									
C	4.825564	3.502735	-0.204569									
C	2.880205	1.921343	-0.437920									
C	1.485995	2.395081	-0.055653									
C	3.053559	0.406229	-0.293534									
C	0.618775	2.876852	-1.041115									
C	-0.664437	3.295105	-0.714773									
C	-1.106070	3.239495	0.617151									
C	-0.252199	2.757900	1.603568									
C	1.036634	2.340523	1.263771									
C	4.346656	-0.146890	-0.331816									
C	4.522430	-1.519458	-0.273875									
C	3.409474	-2.377402	-0.173730									
C	2.122732	-1.844114	-0.125982									
C	1.967973	-0.446329	-0.197678									
O	5.716728	-2.176321	-0.302238									
C	6.906497	-1.401395	-0.405187									
O	3.598017	-3.721467	-0.103564									
C	0.969950	-2.743736	-0.022990									
C	-0.249950	-2.377084	0.398165									
C	-1.384110	-3.320749	0.398626									
O	-1.359415	-4.482709	0.026869									

O	-2.486964	-2.711525	0.856940									
C	-3.725520	-3.437545	0.797222									
C	-4.834547	-2.457490	1.156370									
C	-4.896018	-1.285486	0.203559									
C	-5.600603	-1.380913	-1.001085									
C	-5.612719	-0.320968	-1.908016									
C	-4.915905	0.853328	-1.621792									
C	-4.211471	0.960866	-0.422184									
C	-4.204492	-0.101272	0.481140									
O	-1.494970	3.756164	-1.692845									
O	-2.385505	3.683043	0.801595									
C	-2.933614	3.615106	2.113305									
H	3.935370	2.525391	1.420204									
H	5.552051	4.030686	0.405805									
H	4.858969	3.675242	-1.277873									
H	3.029752	2.159206	-1.496562									
H	0.929340	2.925903	-2.080903									
H	-0.575573	2.702229	2.636656									
H	1.680545	1.950488	2.045890									
H	5.203868	0.512423	-0.413742									
H	0.965899	-0.033353	-0.203080									
H	6.916209	-0.824499	-1.334075									
H	7.008859	-0.730053	0.451967									
H	7.727706	-2.114290	-0.410155									
H	4.551707	-3.891770	-0.168412									
H	1.123453	-3.780643	-0.311926									
H	-0.469198	-1.371385	0.741641									
H	-3.857348	-3.835164	-0.211716									
H	-3.689495	-4.271514	1.501671									
H	-5.776316	-3.012794	1.141835									
H	-4.680022	-2.107407	2.180347									
H	-6.145011	-2.292850	-1.233278									
H	-6.166790	-0.412176	-2.837050									
H	-4.922986	1.678701	-2.326785									
H	-3.667824	1.871505	-0.188090									
H	-3.647983	-0.013923	1.410225									
H	-2.331496	4.016522	-1.275910									
H	-3.954951	3.979922	2.030063									
H	-2.942279	2.584622	2.480081									
H	-2.372004	4.250720	2.803799									

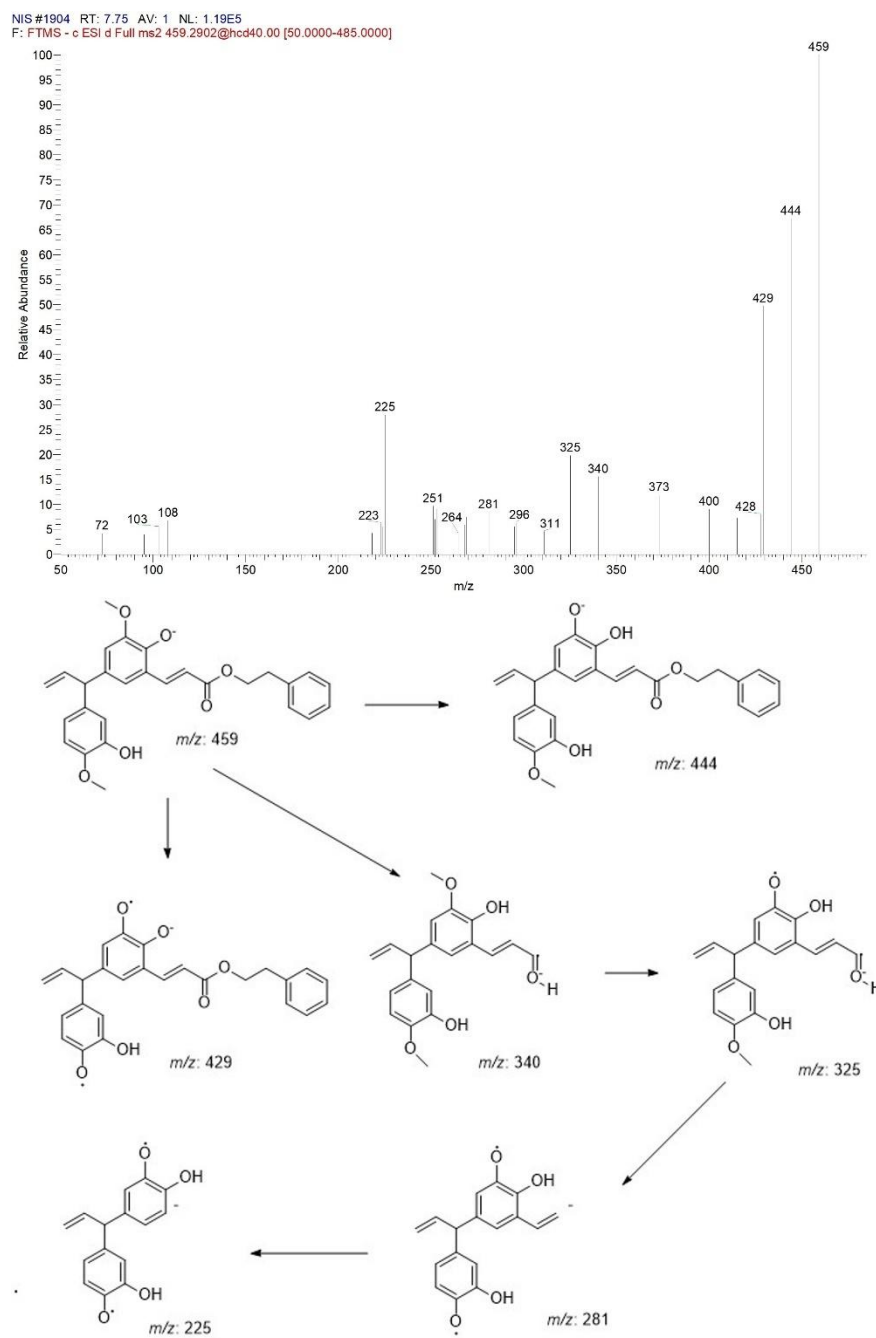


Figure S14: MS/MS spectrum and proposed fragmentation pathway of compound **1**

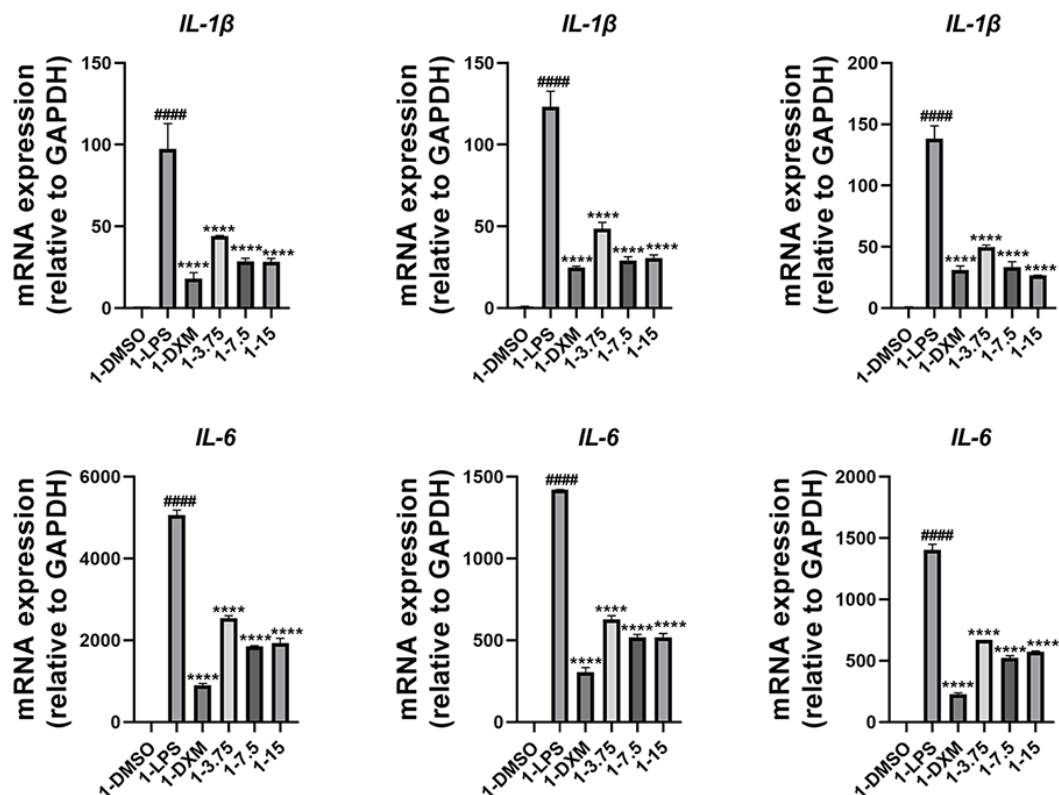


Figure S15: The results of quantitative real-time PCR (RT-PCR) of compound 1. Data are expressed as the mean $\pm$ SD. ####p<0.0001, compared with the normal control group. ****p<0.0001, compared with the LPS group