Supporting Information

Rec. Nat. Prod. X:X (202X) XX-XX

An Undescribed Zhepiresionol Analogue from *Ailanthus altissima*

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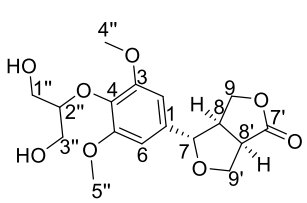
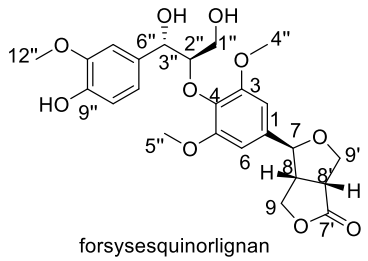


1*



forsysesquinorlignan

Figure S1: Structure of compound **1** and forsysesquinorlignan

Table S1: Comparison of ^{13} CNMR and ^{1}H NMR spectra between compound **1** and forsysesquinorlignan

	1		**forsysesquinorlignan**	
pos	δ_C, type	δ_H (*J* in Hz)	δ_C, type	δ_H (*J* in Hz)
1	137.6, C		137.6, C	
2	104.3, CH	6.75, s	104.1, CH	6.69, s
3	154.8, C		154.3, C	
4	136.7, C		137.0, C	
5	154.8, C		154.3, C	
6	104.3, CH	6.75, s	104.1, CH	6.69, s
7	87.6, CH	4.75, d, *J* = 6.4 Hz	87.5, CH	4.72, d, *J* = 6.0 Hz
8	49.8, CH	3.22, dtd, *J* = 8.9, 6.7, 2.1 Hz	49.8, CH	3.16-3.18, m
9	71.9, CH_2	4.57, dd, *J* = 9.6, 6.8 Hz 4.46, dd, *J* = 9.7, 2.0 Hz	72.0, CH_2	4.57, dd, *J* = 9.5, 7.0 Hz 4.43, dd, *J* = 9.5, 2.0 Hz
7'	180.9, C		181.0, C	
8'	47.6, CH	3.57, td, *J* = 8.7, 3.4 Hz	47.5, CH	3.54-3.56, m
9'	71.3, CH_2	4.34, dd, *J* = 9.2, 8.3 Hz 4.14, dd, *J* = 9.1, 3.4 Hz	71.3, CH_2	4.31, dd, *J* = 9.0, 2.0 Hz 4.12, dd, *J* = 9.0, 3.5 Hz
1"	62.1, CH_2	3.76, dd, *J* = 5.0, 0.9 Hz	61.0, CH_2	3.78, dd, *J* = 12.0, 4.0 Hz 3.37, dd, *J* = 12.0, 3.5 Hz
2"	84.8, CH	4.01, p, *J* = 5.0 Hz	88.5, CH	4.15, overlap
3"	62.1, CH_2	3.76, dd, *J* = 5.0, 0.9 Hz	74.2, CH	4.97, d, *J* = 6.5 Hz
4"	56.7, CH_3	3.88, s	56.7, CH_3	3.87, s
5"	56.7, CH_3	3.88, s	56.7, CH_3	3.87, s
6"			133.5, C	
7"			111.4, CH	6.97, d, *J* = 2.0 Hz
8"			148.6, C	
9"			147.0, C	
10"			115.7, CH	6.84, d, *J* = 8.0 Hz
11"			120.6, CH	6.72, d, *J* = 8.0, 2.0 Hz
12"			56.3, CH_3	3.82, s

Reference:

J. Cao, S.Y. Shao, X. Zhang, X. Yuan, Z.M. Feng, J.S. Jiang, Y.N. Yang, and P.C. Zhang (2020) Two new lignans from the fruits of Forsythia suspensa, *J. Asian Nat. Prod. Res.* 22, 418−424.

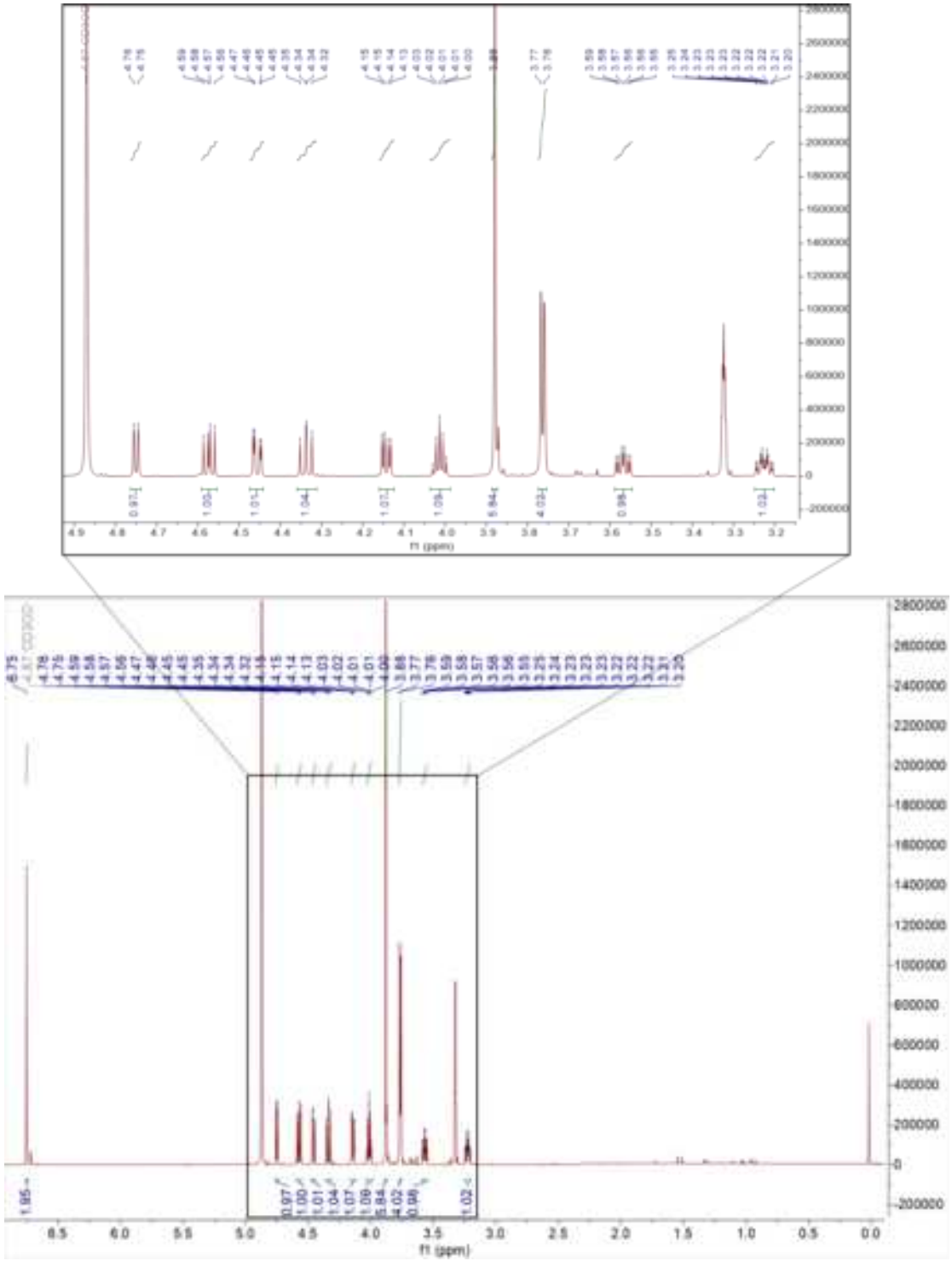


Figure S2: ^{1}H NMR Spectrum of **1** in CD_3OD (700 MHz)

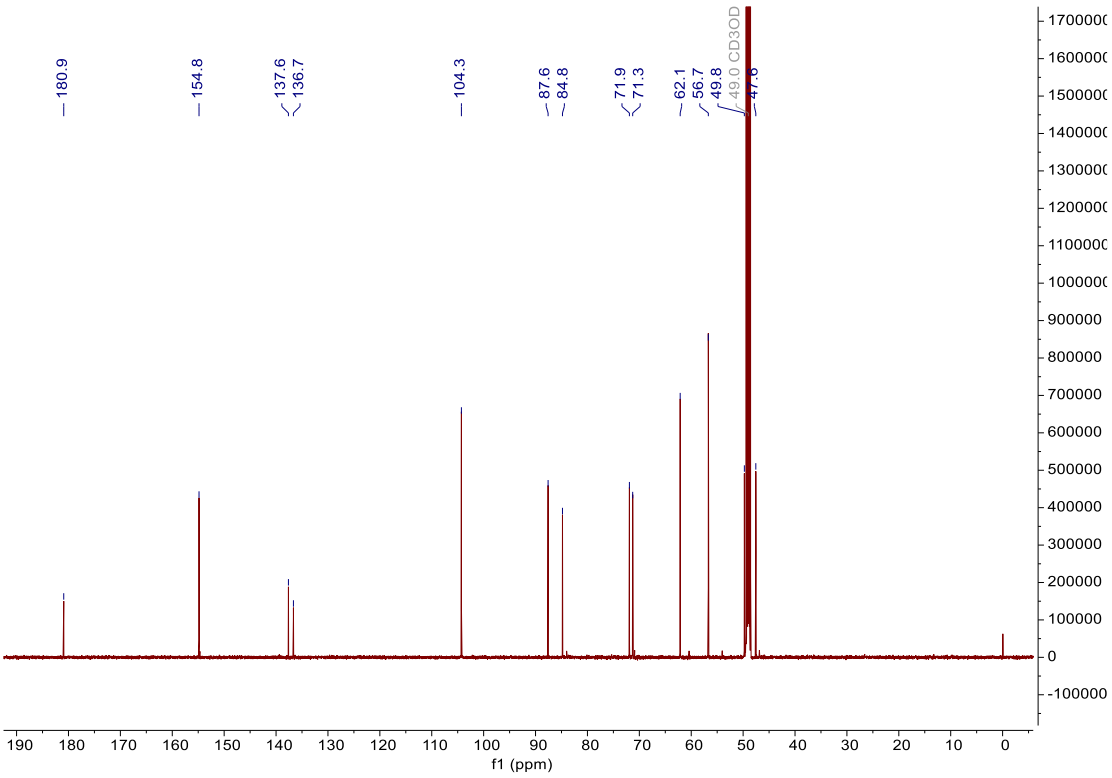


Figure S3: ^{13}C NMR Spectrum of **1** in CD_3OD (175 MHz)

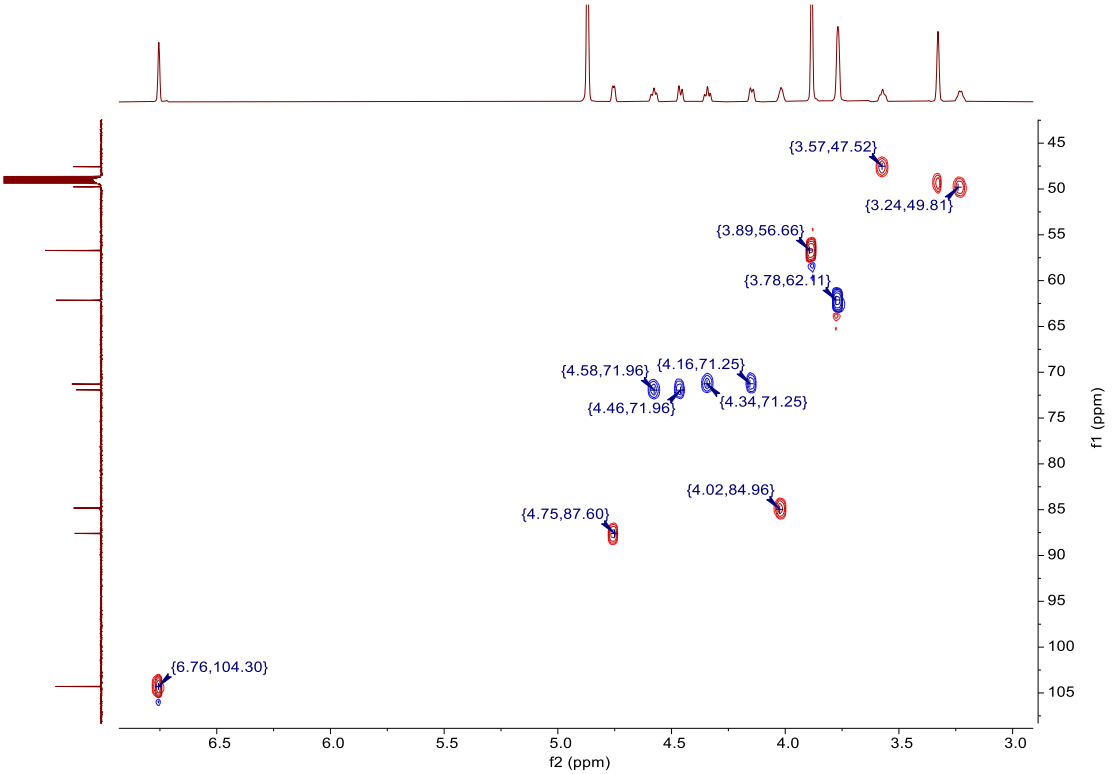


Figure S4: HSQC Spectrum of **1** in CD_3OD

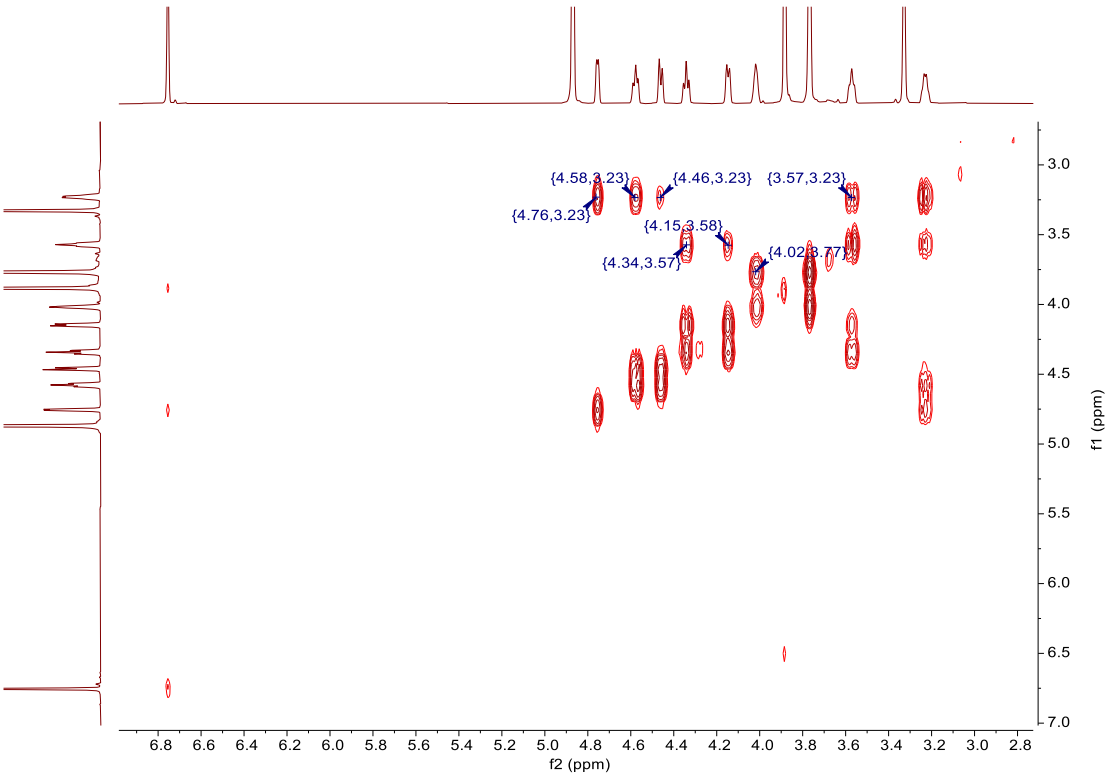


Figure S5: ^{1}H- ^{1}H COSY Spectrum of **1** in CD_3OD

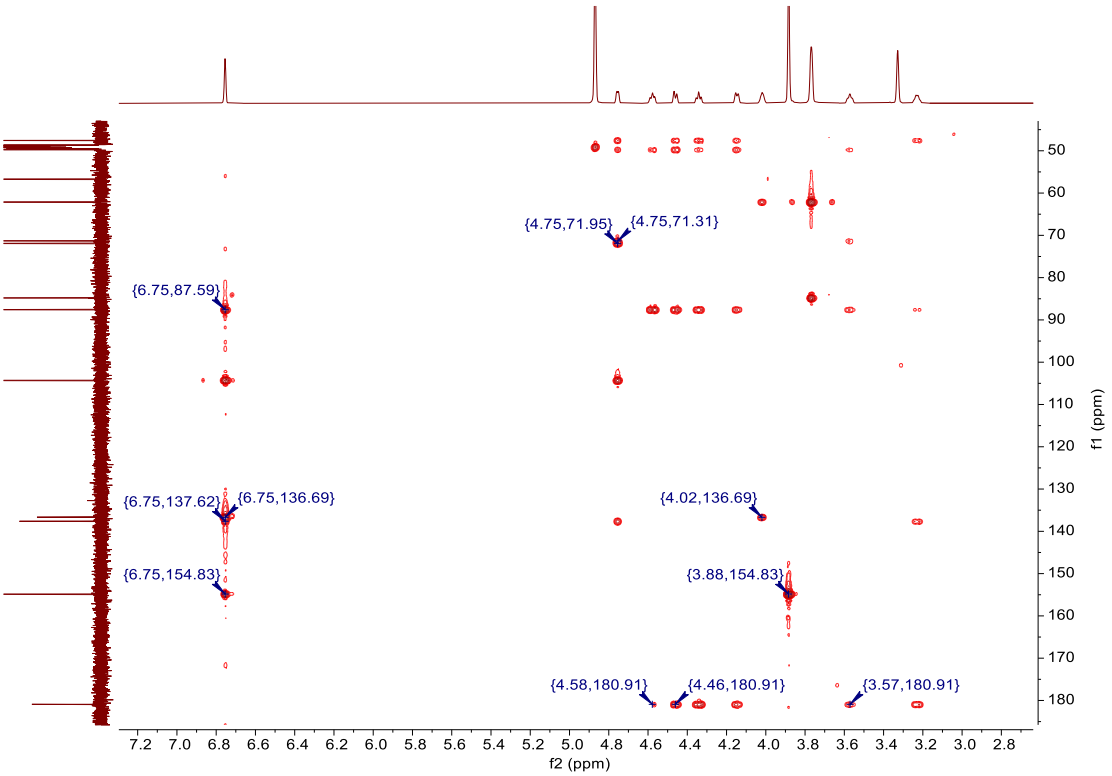


Figure S6: HMBC Spectrum of **1** in CD_3OD

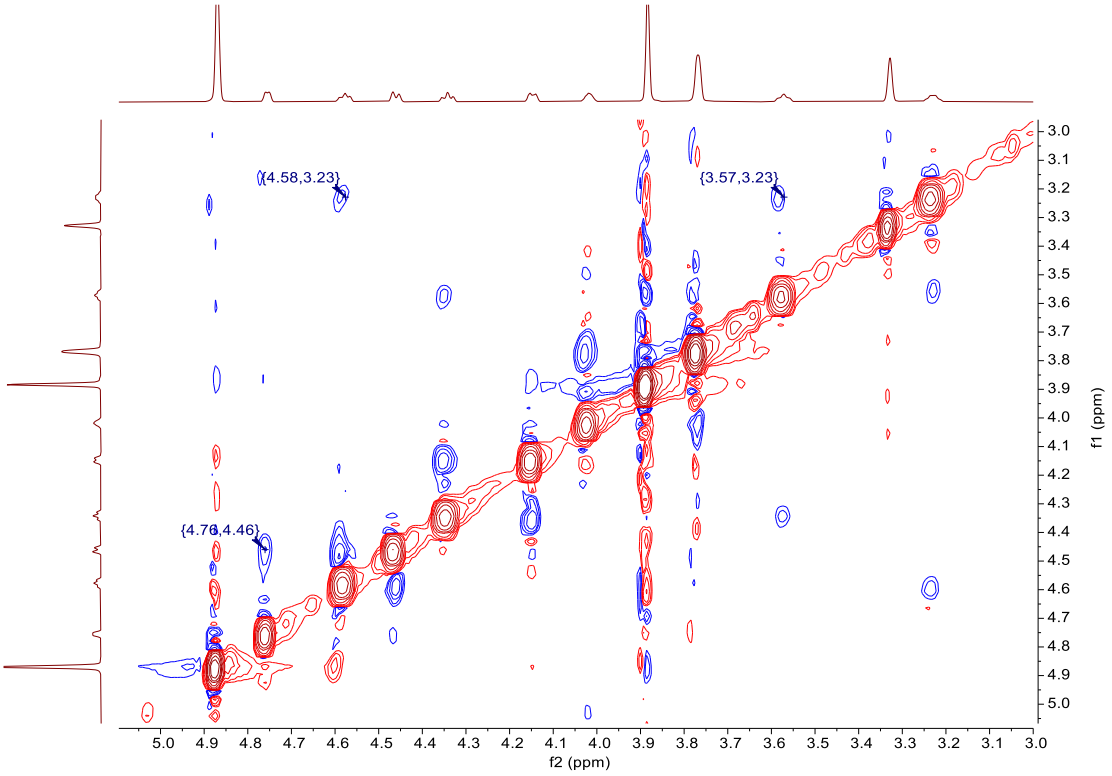


Figure S7: NOESY Spectrum of **1** in CD_3OD

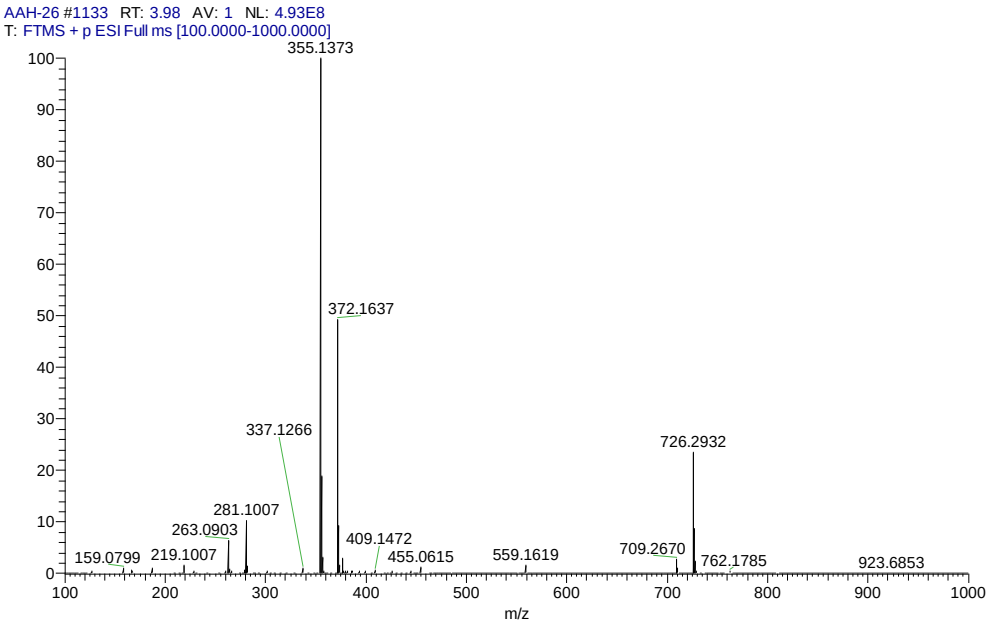


Figure S8: HRESIMS Spectrum of **1**

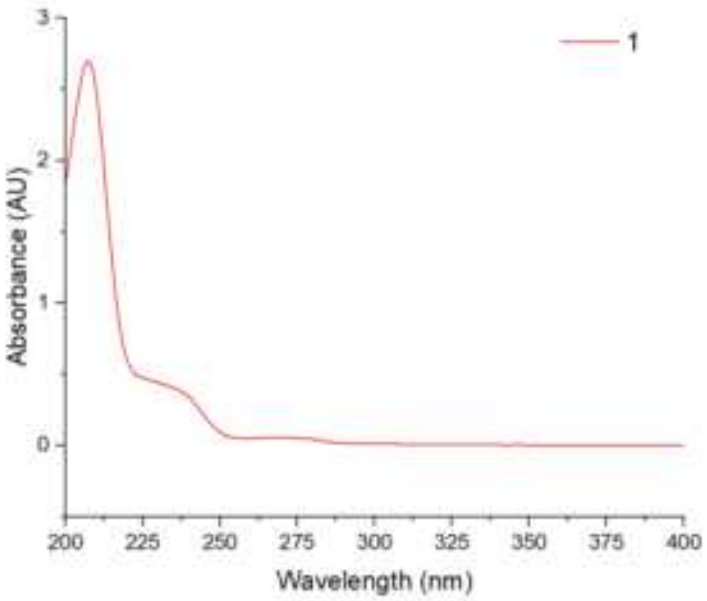


Figure S9: UV spectrum of compound **1**

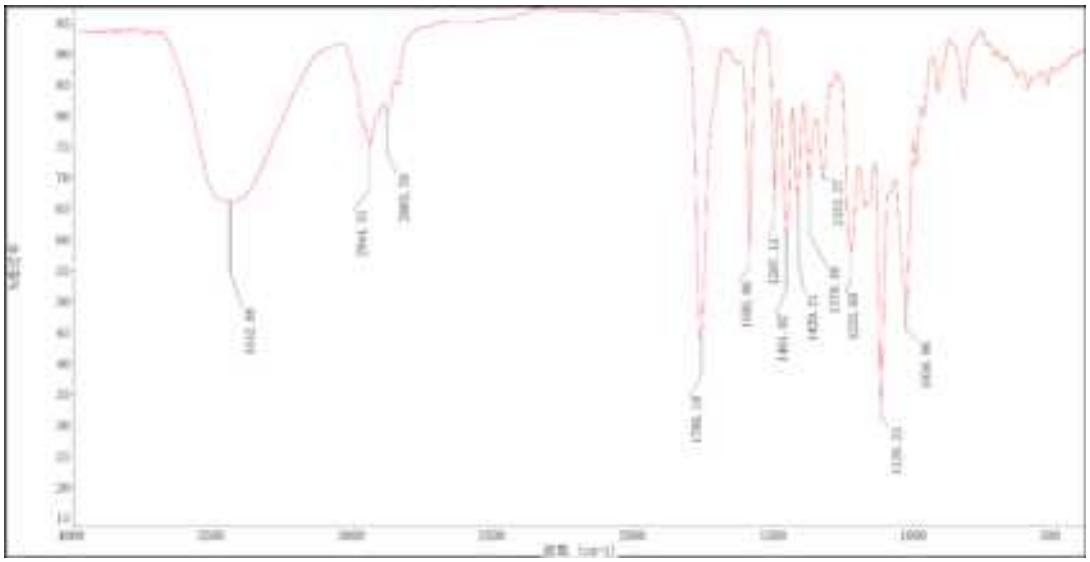


Figure S10: IR spectrum of compound **1**

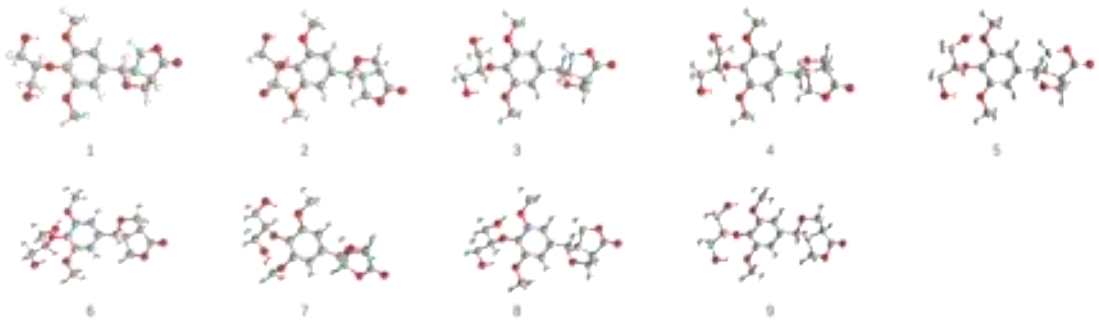


Figure S11: Most stable conformers of 7*R*, 8*S*, 8"*S* -**1** at the CAM-B3LYP/DGDZVP level

Table S2: Energies and atomic Cartesian coordinates of geometry-optimized conformers of 7*R*, 8*S*, 8"*S* -

1 at ωb97xd/dgdzvp in methanol

	Conformer 1			Conformer 2			Conformer 3			Conformer 4		
Gibbs free energy (hartrees)	-1262.251209			-1262.250763			-1262.250645			-1262.250208		
ΔG (kcal/mol)	0			0.28			0.354			0.628		
Population Proportion	35.42%			22.09%			19.49%			12.27%		
Element	**X**	**Y**	**Z**	**X**	**Y**	**Z**	**X**	**Y**	**Z**	**X**	**Y**	**Z**
C	-4.152864	-1.514546	1.064396	-4.305274	1.497109	-0.709706	-4.142597	-1.388899	1.243450	-4.304281	1.410990	-0.855174
C	-4.531685	-0.826359	-0.263378	-4.404739	0.761457	0.643062	-4.528164	-0.871220	-0.158004	-4.410342	0.806237	0.559591
C	-3.235578	-0.198318	-0.766206	-3.022069	0.156226	0.865477	-3.238059	-0.297412	-0.735504	-3.026627	0.233556	0.849500
C	-2.398388	-0.123766	0.526605	-2.441258	0.155295	-0.563225	-2.396642	-0.065576	0.535942	-2.443030	0.082222	-0.569952
O	-2.751866	-1.305406	1.230449	-2.954977	1.345535	-1.141750	-2.742577	-1.154914	1.378618	-2.956553	1.203450	-1.273222
C	-5.457363	0.364815	-0.097605	-5.319714	-0.448866	0.618639	-5.465112	0.322338	-0.135938	-5.317128	-0.407859	0.644887
O	-4.923151	1.460520	-0.668412	-4.660111	-1.547719	1.029859	-4.939896	1.347826	-0.831698	-4.657174	-1.452929	1.177724
C	-3.676060	1.147096	-1.329971	-3.314213	-1.222338	1.446143	-3.688822	0.970602	-1.450921	-3.317687	-1.076382	1.571777
H	-2.723354	-0.804734	-1.512701	-2.392804	0.751240	1.526770	-2.724224	-0.983549	-1.408208	-2.400953	0.897217	1.445716
H	-4.989200	-1.518555	-0.971124	-4.731119	1.420914	1.447881	-4.979554	-1.648789	-0.775088	-4.748060	1.535975	1.296299
C	-0.911668	-0.063943	0.290739	-0.935487	0.141989	-0.608304	-0.910637	-0.031160	0.289859	-0.937012	0.066655	-0.612574
C	-0.261314	1.166153	0.364399	-0.225953	1.319929	-0.372056	-0.263609	1.199374	0.206187	-0.272861	-1.156414	-0.686216
C	1.100853	1.241335	0.062144	1.167288	1.282180	-0.342668	1.100446	1.242710	-0.099862	1.123395	-1.182473	-0.644258
C	1.805424	0.083371	-0.286178	1.843622	0.067216	-0.525025	1.805718	0.053115	-0.302445	1.842667	0.012542	-0.527284
C	1.139154	-1.146588	-0.362975	1.123209	-1.104088	-0.775588	1.140763	-1.179403	-0.226236	1.164692	1.237152	-0.479644
C	-0.223899	-1.220744	-0.075099	-0.273926	-1.065236	-0.820802	-0.219886	-1.223983	0.072664	-0.229937	1.264486	-0.514818
O	1.907406	-2.206286	-0.733396	1.869640	-2.223691	-0.974751	1.920909	-2.264730	-0.465289	1.955410	2.341511	-0.404276
O	1.839143	2.380572	0.079093	1.970956	2.358790	-0.146297	1.827518	2.386149	-0.219424	1.882937	-2.305253	-0.720005
O	3.135249	0.168990	-0.604450	3.213484	0.048011	-0.522690	3.135757	0.085605	-0.629063	3.212382	-0.018583	-0.527842
O	-6.527946	0.397167	0.466690	-6.480053	-0.492497	0.276033	-6.537146	0.411186	0.419553	-6.471723	-0.495329	0.291605
C	1.303038	-3.496957	-0.759598	1.189798	-3.465617	-1.139908	1.324617	-3.554687	-0.368405	1.323237	3.610926	-0.259822
C	1.198682	3.592432	0.466509	1.356142	3.621256	0.092659	1.184394	3.626213	0.064303	1.219555	-3.563834	-0.788545
C	4.053086	0.192370	0.513046	3.840353	0.003963	0.779689	4.058836	-0.158434	0.457087	3.836231	-0.317432	0.742027
C	4.367630	-1.232500	0.959618	3.930474	-1.439757	1.265673	5.281675	-0.773408	-0.197295	5.151911	-0.983639	0.385628
C	5.254600	0.974442	0.016241	5.181014	0.689190	0.593151	4.331842	1.140388	1.210484	3.976624	0.958749	1.566739
O	4.782617	-2.056801	-0.114154	4.522108	-2.297224	0.306882	4.976294	-2.029564	-0.786491	4.940071	-2.217850	-0.285179
O	4.908433	2.320088	-0.279857	5.017545	2.057068	0.246145	4.712027	2.196618	0.347589	4.602053	2.003542	0.844550
H	-4.327290	-2.589266	1.041673	-4.507440	2.563474	-0.620857	-4.312251	-2.458890	1.354076	-4.492872	2.483597	-0.864763
H	-4.705824	-1.082036	1.904915	-4.992059	1.065048	-1.445288	-4.695622	-0.858562	2.025902	-4.998268	0.921860	-1.546715
H	-2.707781	0.758304	1.108601	-2.828294	-0.717768	-1.111280	-2.707678	0.878939	1.008623	-2.827178	-0.845104	-1.022564
H	-3.867530	1.100863	-2.402177	-3.291293	-1.222996	2.536022	-3.877427	0.800459	-2.511005	-3.307199	-0.959603	2.655584

H	-2.982279	1.961747	-1.122128	-2.657823	-2.007548	1.070676	-3.002052	1.809347	-1.336521	-2.653467	-1.893491	1.290090
H	-0.815770	2.050714	0.656018	-0.770335	2.244957	-0.226499	-0.821378	2.111173	0.385871	-0.843219	-2.072501	-0.788105
H	-0.761743	-2.159602	-0.124508	-0.847482	-1.961648	-1.025779	-0.753546	-2.164221	0.140000	-0.778078	2.197654	-0.474951
H	2.094190	-4.187659	-1.042834	1.969423	-4.218718	-1.230373	2.122355	-4.264617	-0.575116	2.130713	4.335531	-0.180937
H	0.917094	-3.767997	0.226526	0.565874	-3.688569	-0.270309	0.931338	-3.729463	0.636610	0.708823	3.844051	-1.133246
H	0.500613	-3.538323	-1.500748	0.581191	-3.461777	-2.047872	0.527964	-3.674720	-1.107563	0.713508	3.642943	0.646998
H	1.968165	4.359862	0.421562	2.173349	4.324471	0.237035	1.950075	4.389480	-0.055424	2.008672	-4.312124	-0.810614
H	0.389198	3.846566	-0.223256	0.753496	3.932463	-0.764830	0.369422	3.814920	-0.639474	0.590112	-3.722911	0.091251
H	0.812534	3.522518	1.486948	0.736936	3.590885	0.993245	0.807221	3.645650	1.090140	0.617888	-3.641614	-1.698110
H	3.593132	0.735723	1.346538	3.238900	0.584143	1.489167	3.619055	-0.887453	1.147472	3.212093	-1.031949	1.291159
H	5.179002	-1.211145	1.690883	4.545878	-1.479831	2.167426	5.679217	-0.077120	-0.945518	5.747334	-0.300158	-0.231621
H	3.484185	-1.656067	1.453185	2.925497	-1.791168	1.530686	6.051440	-0.944519	0.558248	5.710531	-1.199325	1.298871
H	6.021526	0.997545	0.793295	5.741842	0.653773	1.529522	3.439377	1.414150	1.786730	2.984081	1.269991	1.915613
H	5.670718	0.474534	-0.866733	5.754886	0.156823	-0.174913	5.149321	0.982687	1.917830	4.589775	0.754092	2.447462
H	4.005989	-2.137656	-0.690985	3.901001	-2.316410	-0.439000	4.061125	-1.977860	-1.105680	4.136964	-2.114604	-0.820376
H	3.998260	2.310156	-0.616606	4.212126	2.118155	-0.292082	3.928388	2.379733	-0.195428	3.984440	2.227588	0.129831

	Conformer 5			Conformer 6			Conformer 7			Conformer 8		
Gibbs free energy (hartrees)	-1262.248812			-1262.248537			-1262.248504			-1262.248491		
ΔG (kcal/mol)	1.504			1.677			1.697			1.706		
Population Proportion	2.8%			2.09%			2.02%			1.99%		
Element	**X**	**Y**	**Z**	**X**	**Y**	**Z**	**X**	**Y**	**Z**	**X**	**Y**	**Z**
C	-4.225037	1.600664	-0.681805	-4.307073	1.279573	-0.968462	4.291942	1.485929	0.725929	-4.074706	-1.425321	1.261316
C	-4.349485	0.815800	0.640283	-4.407402	0.763132	0.481687	4.420238	0.758735	-0.628859	-4.477055	-0.939771	-0.146648
C	-2.985670	0.162707	0.841876	-3.010349	0.249403	0.815998	3.052660	0.126485	-0.868823	-3.203300	-0.343521	-0.737742
C	-2.405387	0.191783	-0.586707	-2.408712	0.032583	-0.587343	2.458542	0.104216	0.554022	-2.365470	-0.068070	0.527540
O	-2.882456	1.415427	-1.125542	-2.947986	1.095594	-1.359040	2.941664	1.301144	1.145679	-2.681369	-1.150325	1.390050
C	-5.298360	-0.366413	0.568088	-5.281128	-0.467983	0.637192	5.359110	-0.433153	-0.600305	-5.443464	0.230451	-0.141213
O	-4.672764	-1.497183	0.944390	-4.595502	-1.460835	1.233613	4.726815	-1.542529	-1.025524	-4.946879	1.255851	-0.857878
C	-3.319857	-1.224808	1.376401	-3.269807	-1.024172	1.611847	3.378820	-1.242490	-1.454083	-3.688640	0.899155	-1.474633
H	-2.338994	0.716101	1.522249	-2.410528	0.965040	1.377601	2.418147	0.712059	-1.533545	-2.673233	-1.028266	-1.399225
H	-4.659333	1.452142	1.469936	-4.770876	1.528668	1.168078	4.741668	1.428207	-1.427342	-4.910783	-1.738029	-0.749860
C	-0.900887	0.136408	-0.633413	-0.903160	0.061057	-0.621435	0.953890	0.061913	0.587227	-0.881850	-0.001205	0.275469
C	-0.155741	1.282338	-0.361021	-0.196242	-1.137067	-0.669188	0.298345	-1.141031	0.814341	-0.152967	-1.177537	0.110016
C	1.235482	1.207089	-0.339066	1.199901	-1.117067	-0.631213	-1.093630	-1.190517	0.756702	1.203544	-1.106708	-0.200852
C	1.888749	-0.018125	-0.551344	1.890127	0.098566	-0.529454	-1.843844	-0.047466	0.484301	1.843078	0.136910	-0.332255
C	1.124216	-1.156423	-0.835652	1.160492	1.297038	-0.503229	-1.170435	1.175274	0.290982	1.091307	1.308186	-0.177824
C	-0.269736	-1.078537	-0.883046	-0.232310	1.280089	-0.545027	0.219452	1.223222	0.327417	-0.269010	1.240070	0.132472
O	1.830264	-2.303835	-1.049892	1.906594	2.436248	-0.423725	-1.969331	2.253827	0.079865	1.779490	2.476130	-0.330229

O	2.051952	2.273475	-0.128641	1.978775	-2.228631	-0.708189	-1.726341	-2.402092	0.927867	1.994164	-2.192891	-0.409138
O	3.257101	-0.082618	-0.588786	3.259760	0.130204	-0.565254	-3.211954	-0.094132	0.499945	3.160993	0.209815	-0.700560
O	-6.457332	-0.364608	0.218268	-6.431024	-0.608431	0.285514	6.516051	-0.455098	-0.244339	-6.515063	0.302596	0.417433
C	1.110592	-3.479289	-1.423837	1.227340	3.691165	-0.479668	-1.353985	3.510160	-0.198264	1.048447	3.701799	-0.278213
C	1.458591	3.538463	0.156948	1.344072	-3.505312	-0.740677	-2.338309	-2.576298	2.215543	1.427560	-3.490275	-0.237177
C	3.979627	-0.051591	0.668087	3.986115	-0.247822	0.631336	-3.911015	-0.114976	-0.771863	4.171231	-0.073781	0.300584
C	4.392230	-1.461423	1.075587	5.178116	-1.072926	0.169940	-4.329230	-1.538295	-1.123880	5.251707	-0.888335	-0.395111
C	5.200846	0.827254	0.442646	4.444047	0.994664	1.386668	-5.123905	0.788228	-0.605887	4.743721	1.225130	0.856635
O	3.295028	-2.299274	1.387362	4.809811	-2.327090	-0.375411	-3.243256	-2.386757	-1.443616	4.817798	-2.182025	-0.774779
O	4.876544	2.190912	0.240081	3.374233	1.755674	1.915346	-4.780197	2.152197	-0.443436	3.805293	1.980330	1.599325
H	-4.385625	2.669524	-0.548577	-4.534618	2.341450	-1.049639	4.469871	2.557115	0.643193	-4.214084	-2.497884	1.388189
H	-4.929977	1.226137	-1.431477	-4.974369	0.721167	-1.633414	4.982090	1.066801	1.465734	-4.640754	-0.899029	2.037093
H	-2.817805	-0.651074	-1.162802	-2.762057	-0.930300	-0.987450	2.856248	-0.764961	1.100330	-2.698820	0.876806	0.984000
H	-3.302195	-1.260878	2.465768	-3.270112	-0.844441	2.687039	3.367081	-1.237334	-2.544088	-3.876233	0.704346	-2.530666
H	-2.685018	-2.016654	0.978586	-2.581105	-1.837136	1.381821	2.734723	-2.042805	-1.089641	-3.023681	1.757608	-1.378663
H	-0.672082	2.218594	-0.189060	-0.733435	-2.074206	-0.756937	0.843801	-2.053746	1.033886	-0.656690	-2.130039	0.218756
H	-0.864892	-1.954159	-1.113371	-0.808146	2.196971	-0.521294	0.750627	2.154762	0.173008	-0.849155	2.144113	0.275155
H	1.864817	-4.248935	-1.570212	2.007967	4.447441	-0.442135	-2.171427	4.208157	-0.364377	1.777653	4.485011	-0.471802
H	0.422425	-3.788177	-0.632761	0.668254	3.786579	-1.413529	-0.752968	3.845999	0.650445	0.274189	3.722902	-1.049029
H	0.565377	-3.318508	-2.356984	0.557462	3.814661	0.375059	-0.735966	3.449567	-1.097560	0.603281	3.853693	0.708323
H	2.288567	4.223406	0.315767	2.151117	-4.234444	-0.756610	-2.782801	-3.569996	2.209609	2.238687	-4.191751	-0.419522
H	0.854354	3.885164	-0.685068	0.731510	-3.658099	0.151394	-1.577600	-2.514944	2.998123	1.054377	-3.619752	0.781689
H	0.849023	3.486854	1.062494	0.734433	-3.616152	-1.640889	-3.111451	-1.822738	2.379356	0.624623	-3.664167	-0.957890
H	3.335828	0.384286	1.439297	3.332317	-0.850539	1.270461	-3.248073	0.280787	-1.548610	3.718509	-0.656314	1.109802
H	5.007651	-1.899947	0.280029	5.743057	-0.483993	-0.564923	-4.922328	-1.950060	-0.297462	5.598387	-0.325607	-1.272162
H	5.002338	-1.397355	1.979307	5.833416	-1.269310	1.021598	-4.966216	-1.501453	-2.010719	6.099812	-1.015678	0.281601
H	5.850284	0.775087	1.319492	5.052680	0.679373	2.237075	-5.752350	0.716972	-1.496242	5.558700	0.980332	1.541395
H	5.758099	0.431567	-0.416966	5.072249	1.605989	0.726675	-5.708421	0.431336	0.252721	5.159071	1.816919	0.031179
H	2.826018	-2.482796	0.556075	3.940618	-2.216112	-0.794654	-2.753202	-2.565390	-0.621168	3.866861	-2.124448	-0.964910
H	4.009288	2.220269	-0.196609	2.911187	2.164058	1.164635	-3.934592	2.184539	0.033863	3.150091	2.326807	0.970521

Conformer 9

Gibbs free energy (hartrees)	-1262.248411		
ΔG (kcal/mol)	1.756		
Population Proportion	1.83%		
Element	**X**	**Y**	**Z**
C	-4.156825	1.544056	-0.942346
C	-4.526340	0.724972	0.311371
C	-3.216812	0.089975	0.768691

C	-2.366484	0.159388	-0.516245
O	-2.749715	1.387728	-1.115040
C	-5.415259	-0.471419	0.025052
O	-4.854402	-1.599874	0.498057
C	-3.623094	-1.314143	1.200170
H	-2.728707	0.638567	1.573815
H	-5.010364	1.334839	1.074951
C	-0.881355	0.124564	-0.266923
C	-0.217455	1.279566	0.140719
C	1.143698	1.221546	0.436057
C	1.844798	0.010100	0.338178
C	1.154680	-1.147302	-0.047910
C	-0.202771	-1.086718	-0.370070
O	1.893375	-2.288078	-0.076180
O	1.886451	2.298967	0.821267
O	3.162929	-0.051798	0.708001
O	-6.479386	-0.481324	-0.552036
C	1.271510	-3.492371	-0.519623
C	1.214550	3.543020	1.021438
C	4.164723	-0.171219	-0.333541
C	4.793400	1.187614	-0.620656
C	5.206234	-1.153641	0.181141
O	3.888447	2.115512	-1.188789
O	4.715520	-2.477395	0.295992
H	-4.359792	2.607048	-0.820529
H	-4.692435	1.178451	-1.824756
H	-2.642155	-0.675796	-1.178549
H	-3.825268	-1.373140	2.269777
H	-2.904551	-2.086657	0.925817
H	-0.771170	2.207596	0.209836
H	-0.734517	-1.973994	-0.693226
H	2.046949	-4.254308	-0.483365
H	0.450213	-3.775169	0.143806
H	0.909491	-3.388766	-1.545482
H	1.981323	4.238686	1.354357
H	0.771541	3.905276	0.090387
H	0.446140	3.447449	1.792334
H	3.691717	-0.560520	-1.241203
H	5.232965	1.583232	0.303657
H	5.597639	1.051759	-1.347139
H	6.051629	-1.179682	-0.510260
H	5.572056	-0.793178	1.151827

H	3.248738	2.356132	-0.497653
H	3.767837	-2.418016	0.500474

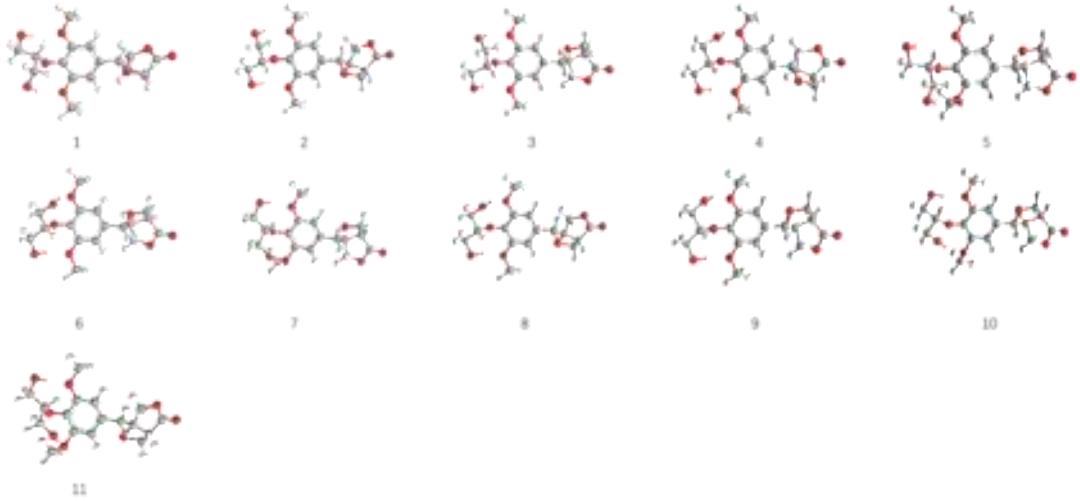


Figure S12: Most stable conformers of 7*S*, 8*R*, 8"*R* -**1**at the CAM-B3LYP/DGDZVP level

Table S3: Energies and atomic Cartesian coordinates of geometry-optimized conformers of 7*S*, 8*R*, 8"*R* -**1** at ωb97xd/dgdzvp in methanol

	Conformer 1			Conformer 2			Conformer 3			Conformer 4		
Gibbs free energy (hartrees)	-1262.251209			-1262.250645			-1262.250208			-1262.248812		
ΔG (kcal/mol)	0			0.354			0.628			1.504		
Population Proportion	42.99%			23.65%			14.89%			3.39%		
Element	**X**	**Y**	**Z**	**X**	**Y**	**Z**	**X**	**Y**	**Z**	**X**	**Y**	**Z**
C	4.152864	-1.514546	1.064396	4.142597	-1.388899	1.243450	4.304281	1.410990	-0.855174	4.225037	1.600664	-0.681805
C	4.531685	-0.826359	-0.263378	4.528164	-0.871220	-0.158004	4.410342	0.806237	0.559591	4.349485	0.815800	0.640283
C	3.235578	-0.198318	-0.766206	3.238059	-0.297412	-0.735504	3.026627	0.233556	0.849500	2.985670	0.162707	0.841876
C	2.398388	-0.123766	0.526605	2.396642	-0.065576	0.535942	2.443030	0.082222	-0.569952	2.405387	0.191783	-0.586707
O	2.751866	-1.305406	1.230449	2.742577	-1.154914	1.378618	2.956553	1.203450	-1.273222	2.882456	1.415427	-1.125542
C	5.457363	0.364815	-0.097605	5.465112	0.322338	-0.135938	5.317128	-0.407859	0.644887	5.298360	-0.366413	0.568088
O	4.923151	1.460520	-0.668412	4.939896	1.347826	-0.831698	4.657174	-1.452929	1.177724	4.672764	-1.497183	0.944390
C	3.676060	1.147096	-1.329971	3.688822	0.970602	-1.450921	3.317687	-1.076382	1.571777	3.319857	-1.224808	1.376401
H	2.723354	-0.804734	-1.512701	2.724224	-0.983549	-1.408208	2.400953	0.897217	1.445716	2.338994	0.716101	1.522249
H	4.989200	-1.518555	-0.971124	4.979554	-1.648789	-0.775088	4.748060	1.535975	1.296299	4.659333	1.452142	1.469936
C	0.911668	-0.063943	0.290739	0.910637	-0.031160	0.289859	0.937012	0.066655	-0.612574	0.900887	0.136408	-0.633413
C	0.223899	-1.220744	-0.075099	0.219886	-1.223983	0.072664	0.272861	-1.156414	-0.686216	0.155741	1.282338	-0.361021

C	-1.139154	-1.146588	-0.362975	-1.140763	-1.179403	-0.226236	-1.123395	-1.182473	-0.644258	-1.235482	1.207089	-0.339066
C	-1.805424	0.083371	-0.286178	-1.805718	0.053115	-0.302445	-1.842667	0.012542	-0.527284	-1.888749	-0.018125	-0.551344
C	-1.100853	1.241335	0.062144	-1.100446	1.242710	-0.099862	-1.164692	1.237152	-0.479644	-1.124216	-1.156423	-0.835652
C	0.261314	1.166153	0.364399	0.263609	1.199374	0.206187	0.229937	1.264486	-0.514818	0.269736	-1.078537	-0.883046
O	-1.839143	2.380572	0.079093	-1.827518	2.386149	-0.219424	-1.955410	2.341511	-0.404276	-1.830264	-2.303835	-1.049892
O	-1.907406	-2.206286	-0.733396	-1.920909	-2.264730	-0.465289	-1.882937	-2.305253	-0.720005	-2.051952	2.273475	-0.128641
O	-3.135249	0.168990	-0.604450	-3.135757	0.085605	-0.629063	-3.212382	-0.018583	-0.527842	-3.257101	-0.082618	-0.588786
O	6.527946	0.397167	0.466690	6.537146	0.411186	0.419553	6.471723	-0.495329	0.291605	6.457332	-0.364608	0.218268
C	-1.198682	3.592432	0.466509	-1.184394	3.626213	0.064303	-1.323237	3.610926	-0.259822	-1.110592	-3.479289	-1.423837
C	-1.303038	-3.496957	-0.759598	-1.324617	-3.554687	-0.368405	-1.219555	-3.563834	-0.788545	-1.458591	3.538463	0.156948
C	-4.053086	0.192370	0.513046	-4.058836	-0.158434	0.457087	-3.836231	-0.317432	0.742027	-3.979627	-0.051591	0.668087
C	-5.254600	0.974442	0.016241	-4.331842	1.140388	1.210484	-3.976624	0.958749	1.566739	-5.200846	0.827254	0.442646
C	-4.367630	-1.232500	0.959618	-5.281675	-0.773408	-0.197295	-5.151911	-0.983639	0.385628	-4.392230	-1.461423	1.075587
O	-4.908433	2.320088	-0.279857	-4.712027	2.196618	0.347589	-4.602053	2.003542	0.844550	-4.876544	2.190912	0.240081
O	-4.782617	-2.056801	-0.114154	-4.976294	-2.029564	-0.786491	-4.940071	-2.217850	-0.285179	-3.295028	-2.299274	1.387362
H	4.705824	-1.082036	1.904915	4.695622	-0.858562	2.025902	4.998268	0.921860	-1.546715	4.929977	1.226137	-1.431477
H	4.327290	-2.589266	1.041673	4.312251	-2.458890	1.354076	4.492872	2.483597	-0.864763	4.385625	2.669524	-0.548577
H	2.707781	0.758304	1.108601	2.707678	0.878939	1.008623	2.827178	-0.845104	-1.022564	2.817805	-0.651074	-1.162802
H	3.867530	1.100863	-2.402177	3.877427	0.800459	-2.511005	3.307199	-0.959603	2.655584	3.302195	-1.260878	2.465768
H	2.982279	1.961747	-1.122128	3.002052	1.809347	-1.336521	2.653467	-1.893491	1.290090	2.685018	-2.016654	0.978586
H	0.761743	-2.159602	-0.124508	0.753546	-2.164221	0.140000	0.843219	-2.072501	-0.788105	0.672082	2.218594	-0.189060
H	0.815770	2.050714	0.656018	0.821378	2.111173	0.385871	0.778078	2.197654	-0.474951	0.864892	-1.954159	-1.113371
H	-1.968165	4.359862	0.421562	-1.950075	4.389480	-0.055424	-2.130713	4.335531	-0.180937	-1.864817	-4.248935	-1.570212
H	-0.812534	3.522518	1.486948	-0.807221	3.645650	1.090140	-0.713508	3.642943	0.646998	-0.565377	-3.318508	-2.356984
H	-0.389198	3.846566	-0.223256	-0.369422	3.814920	-0.639474	-0.708823	3.844051	-1.133246	-0.422425	-3.788177	-0.632761
H	-2.094190	-4.187659	-1.042834	-2.122355	-4.264617	-0.575117	-2.008672	-4.312124	-0.810614	-2.288567	4.223406	0.315767
H	-0.500613	-3.538323	-1.500748	-0.527964	-3.674720	-1.107563	-0.617888	-3.641614	-1.698110	-0.849023	3.486854	1.062494
H	-0.917094	-3.767997	0.226526	-0.931338	-3.729463	0.636610	-0.590112	-3.722911	0.091251	-0.854354	3.885164	-0.685068
H	-3.593132	0.735723	1.346538	-3.619055	-0.887453	1.147472	-3.212093	-1.031949	1.291159	-3.335828	0.384286	1.439297
H	-5.670718	0.474534	-0.866733	-5.149321	0.982687	1.917830	-4.589775	0.754092	2.447462	-5.758099	0.431567	-0.416966
H	-6.021526	0.997545	0.793295	-3.439377	1.414150	1.786730	-2.984081	1.269990	1.915613	-5.850284	0.775087	1.319492
H	-3.484185	-1.656067	1.453185	-6.051440	-0.944519	0.558248	-5.710531	-1.199325	1.298871	-5.002338	-1.397355	1.979307
H	-5.179002	-1.211145	1.690883	-5.679217	-0.077120	-0.945518	-5.747334	-0.300158	-0.231621	-5.007651	-1.899947	0.280029
H	-3.998260	2.310156	-0.616606	-3.928388	2.379733	-0.195428	-3.984440	2.227588	0.129831	-4.009288	2.220269	-0.196609
H	-4.005989	-2.137656	-0.690985	-4.061125	-1.977860	-1.105680	-4.136964	-2.114604	-0.820376	-2.826018	-2.482796	0.556075

	Conformer 5	Conformer 6	Conformer 7	Conformer 8
Gibbs free energy (hartrees)	-1262.248709	-1262.248537	-1262.248504	-1262.248491
ΔG (kcal/mol)	1.569	1.677	1.697	1.706
Population	3.04%	2.54%	2.45%	2.42%

Proportion

Element	X	Y	Z	X	Y	Z	X	Y	Z	X	Y	Z
C	-4.327705	1.455818	0.775704	4.307073	1.279573	-0.968462	-4.291942	1.485929	0.725929	4.074705	-1.425320	1.261318
C	-4.470544	0.708185	-0.566741	4.407402	0.763132	0.481687	-4.420238	0.758735	-0.628859	4.477055	-0.939771	-0.146647
C	-3.093251	0.108333	-0.832491	3.010349	0.249403	0.815998	-3.052660	0.126485	-0.868823	3.203300	-0.343522	-0.737741
C	-2.464173	0.120500	0.575267	2.408712	0.032583	-0.587343	-2.458542	0.104216	0.554022	2.365469	-0.068070	0.527540
O	-2.962263	1.314218	1.161540	2.947986	1.095594	-1.359040	-2.941664	1.301144	1.145679	2.681368	-1.150324	1.390051
C	-5.376994	-0.507037	-0.500314	5.281128	-0.467983	0.637192	-5.359110	-0.433153	-0.600305	5.443464	0.230451	-0.141213
O	-4.726012	-1.605593	-0.925696	4.595502	-1.460835	1.233613	-4.726815	-1.542529	-1.025524	4.946880	1.255850	-0.857879
C	-3.397443	-1.276297	-1.391918	3.269807	-1.024172	1.611847	-3.378820	-1.242490	-1.454083	3.688640	0.899154	-1.474633
H	-2.490671	0.701346	-1.519970	2.410528	0.965040	1.377601	-2.418147	0.712059	-1.533545	2.673233	-1.028267	-1.399224
H	-4.828705	1.359086	-1.364989	4.770876	1.528668	1.168078	-4.741668	1.428207	-1.427342	4.910783	-1.738030	-0.749857
C	-0.958491	0.112042	0.572083	0.903160	0.061057	-0.621435	-0.953890	0.061913	0.587227	0.881849	-0.001206	0.275469
C	-0.273644	-1.073380	0.806549	0.196242	-1.137067	-0.669188	-0.298345	-1.141031	0.814341	0.152967	-1.177537	0.110016
C	1.117818	-1.092830	0.711732	-1.199901	-1.117067	-0.631213	1.093630	-1.190517	0.756702	-1.203544	-1.106708	-0.200851
C	1.829894	0.063108	0.402677	-1.890127	0.098566	-0.529454	1.843844	-0.047466	0.484301	-1.843079	0.136910	-0.332254
C	1.132610	1.269517	0.191754	-1.160492	1.297038	-0.503229	1.170435	1.175274	0.290982	-1.091307	1.308185	-0.177824
C	-0.257780	1.284134	0.266129	0.232310	1.280089	-0.545027	-0.219452	1.223222	0.327417	0.269010	1.240070	0.132472
O	1.908176	2.348805	-0.070933	-1.906594	2.436248	-0.423725	1.969331	2.253827	0.079865	-1.779491	2.476129	-0.330228
O	1.800720	-2.274658	0.905854	-1.978775	-2.228631	-0.708189	1.726341	-2.402092	0.927867	-1.994165	-2.192891	-0.409137
O	3.197365	0.024236	0.365151	-3.259760	0.130204	-0.565254	3.211954	-0.094132	0.499945	-3.160994	0.209815	-0.700559
O	-6.524298	-0.554065	-0.116657	6.431024	-0.608431	0.285514	-6.516051	-0.455098	-0.244339	6.515063	0.302596	0.417433
C	1.260126	3.591773	-0.317929	-1.227340	3.691165	-0.479668	1.353985	3.510160	-0.198264	-1.048446	3.701798	-0.278218
C	2.275759	-2.443315	2.250328	-1.344072	-3.505312	-0.740677	2.338309	-2.576298	2.215543	-1.427560	-3.490275	-0.237178
C	3.800223	0.074742	-0.948625	-3.986115	-0.247822	0.631336	3.911015	-0.114976	-0.771863	-4.171231	-0.073780	0.300585
C	5.270110	0.341747	-0.680241	-4.444047	0.994664	1.386668	5.123905	0.788228	-0.605887	-4.743719	1.225131	0.856637
C	3.539557	-1.213161	-1.722677	-5.178116	-1.072926	0.169940	4.329230	-1.538295	-1.123880	-5.251708	-0.888333	-0.395110
O	5.456643	1.570067	0.007641	-3.374233	1.755674	1.915346	4.780197	2.152197	-0.443437	-3.805291	1.980330	1.599327
O	3.964770	-2.376088	-1.036134	-4.809811	-2.327090	-0.375411	3.243256	-2.386757	-1.443616	-4.817800	-2.182023	-0.774778
H	-4.986166	1.026702	1.538389	4.974369	0.721167	-1.633414	-4.982090	1.066801	1.465734	4.640753	-0.899026	2.037094
H	-4.538224	2.520415	0.685099	4.534618	2.341450	-1.049639	-4.469871	2.557115	0.643193	4.214084	-2.497882	1.388193
H	-2.828677	-0.749332	1.143295	2.762057	-0.930300	-0.987450	-2.856248	-0.764961	1.100330	2.698819	0.876806	0.984000
H	-3.413089	-1.285494	-2.481872	3.270112	-0.844441	2.687039	-3.367081	-1.237334	-2.544088	3.876233	0.704344	-2.530666
H	-2.723515	-2.054679	-1.033697	2.581105	-1.837136	1.381821	-2.734723	-2.042805	-1.089641	3.023682	1.757607	-1.378664
H	-0.796076	-1.991228	1.058781	0.733435	-2.074206	-0.756937	-0.843801	-2.053746	1.033886	0.656689	-2.130039	0.218757
H	-0.816165	2.198153	0.102479	0.808146	2.196971	-0.521294	-0.750627	2.154762	0.173008	0.849155	2.144113	0.275155
H	2.056548	4.306840	-0.511381	-2.007967	4.447441	-0.442135	2.171427	4.208157	-0.364377	-1.777651	4.485010	-0.471807
H	0.606690	3.528018	-1.192634	-0.557462	3.814661	0.375059	0.735966	3.449567	-1.097560	-0.603275	3.853693	0.708315
H	0.683959	3.914921	0.553727	-0.668254	3.786579	-1.413529	0.752968	3.845999	0.650445	-0.274190	3.722898	-1.049038
H	2.779100	-3.408418	2.280485	-2.151117	-4.234444	-0.756610	2.782801	-3.569996	2.209609	-2.238686	-4.191751	-0.419526
H	2.979700	-1.648277	2.509414	-0.734433	-3.616152	-1.640889	3.111451	-1.822738	2.379356	-0.624623	-3.664165	-0.957891
H	1.434812	-2.442504	2.948892	-0.731510	-3.658099	0.151394	1.577601	-2.514944	2.998123	-1.054378	-3.619754	0.781688

H	3.375417	0.917921	-1.504381	-3.332317	-0.850539	1.270461	3.248073	0.280787	-1.548610	-3.718509	-0.656315	1.109802
H	5.694021	-0.494724	-0.112226	-5.072249	1.605989	0.726675	5.708421	0.431336	0.252721	-5.159068	1.816921	0.031180
H	5.803412	0.422286	-1.628787	-5.052680	0.679373	2.237075	5.752350	0.716972	-1.496242	-5.558699	0.980334	1.541396
H	2.472079	-1.276060	-1.969845	-5.833416	-1.269310	1.021598	4.966216	-1.501453	-2.010719	-6.099813	-1.015674	0.281601
H	4.089880	-1.168568	-2.665682	-5.743057	-0.483993	-0.564923	4.922328	-1.950060	-0.297462	-5.598387	-0.325604	-1.272161
H	4.825596	1.571901	0.742006	-2.911187	2.164058	1.164635	3.934592	2.184539	0.033863	-3.150088	2.326809	0.970525
H	3.354905	-2.484698	-0.285860	-3.940618	-2.216112	-0.794654	2.753202	-2.565390	-0.621168	-3.866863	-2.124448	-0.964910

	Conformer 9			Conformer 10			Conformer 11		
Gibbs free energy (hartrees)	-1262.248411			-1262.247842			-1262.247822		
ΔG (kcal/mol)	1.756			2.113			2.125		
Population Proportion	2.22%			1.22%			1.19%		
Element	**X**	**Y**	**Z**	**X**	**Y**	**Z**	**X**	**Y**	**Z**
C	4.156825	1.544056	-0.942346	4.124922	1.430854	-1.218761	-4.348646	-1.413876	-0.831825
C	4.526340	0.724972	0.311371	4.522171	0.875258	0.164877	-4.453964	-0.781697	0.571528
C	3.216812	0.089975	0.768691	3.246354	0.249546	0.720403	-3.061675	-0.229815	0.861401
C	2.366484	0.159388	-0.516245	2.410267	0.044049	-0.559029	-2.460537	-0.125493	-0.555054
O	2.749715	1.387728	-1.115040	2.730023	1.171815	-1.361138	-2.990553	-1.252378	-1.235918
C	5.415259	-0.471419	0.025052	5.489448	-0.292423	0.103497	-5.338930	0.449815	0.627479
O	4.854402	-1.599874	0.498057	4.989344	-1.354834	0.761303	-4.661811	1.494786	1.138752
C	3.623094	-1.314143	1.200170	3.728104	-1.032001	1.390305	-3.332009	1.102647	1.549771
H	2.728707	0.638567	1.573815	2.717350	0.898341	1.417995	-2.455864	-0.891671	1.479569
H	5.010364	1.334839	1.074951	4.952827	1.642447	0.809134	-4.809711	-1.492224	1.318336
C	0.881355	0.124564	-0.266923	0.925698	-0.032664	-0.319601	-0.955070	-0.146703	-0.580724
C	0.217455	1.279566	0.140719	0.283093	-1.263416	-0.323374	-0.254189	1.055421	-0.694326
C	-1.143698	1.221546	0.436057	-1.079770	-1.331949	-0.037558	1.139368	1.062632	-0.641100
C	-1.844798	0.010100	0.338178	-1.814691	-0.181616	0.244794	1.844061	-0.140533	-0.460336
C	-1.154680	-1.147302	-0.047910	-1.149120	1.060588	0.265049	1.124210	-1.334763	-0.373208
C	0.202771	-1.086718	-0.370070	0.209702	1.131856	-0.023693	-0.265328	-1.344987	-0.428589
O	-1.893375	-2.288078	-0.076180	-1.922867	2.131014	0.583507	1.794447	-2.521372	-0.170873
O	-1.886451	2.298967	0.821267	-1.713580	-2.553456	-0.098538	1.905149	2.177789	-0.766651
O	-3.162929	-0.051798	0.708001	-3.139257	-0.267894	0.579659	3.213124	-0.154650	-0.464198
O	6.479386	-0.481324	-0.552036	6.564463	-0.334166	-0.451746	-6.490616	0.550181	0.268145
C	-1.271510	-3.492371	-0.519623	-1.330788	3.428246	0.557437	2.416758	-3.059523	-1.347852
C	-1.214550	3.543020	1.021438	-2.007188	-3.134219	1.181606	1.254500	3.442672	-0.870894
C	-4.164723	-0.171219	-0.333541	-4.125486	0.084509	-0.425424	3.904423	0.235321	0.750916
C	-5.206234	-1.153641	0.181141	-4.684734	-1.172303	-1.082988	4.354772	-0.999511	1.523613
C	-4.793400	1.187614	-0.620656	-5.217147	0.855298	0.301687	5.095675	1.074132	0.313337
O	-4.715520	-2.477395	0.295992	-3.752120	-1.845453	-1.906530	3.286569	-1.739334	2.083014

O	-3.888447	2.115512	-1.188789	-4.777770	2.109552	0.790464	4.719792	2.312919	-0.260586
H	4.692435	1.178451	-1.824756	4.688163	0.938095	-2.018297	-5.019398	-0.916291	-1.540186
H	4.359792	2.607048	-0.820529	4.271772	2.507218	-1.294207	-4.568200	-2.480536	-0.826309
H	2.642155	-0.675796	-1.178549	2.741734	-0.875569	-1.065383	-2.819270	0.798621	-1.034967
H	3.825268	-1.373140	2.269777	3.910580	-0.895290	2.456285	-3.329750	1.012215	2.636097
H	2.904551	-2.086657	0.925817	3.063400	-1.883402	1.244077	-2.650325	1.899619	1.252531
H	0.771170	2.207596	0.209836	0.813058	-2.181439	-0.557967	-0.802967	1.978962	-0.840341
H	0.734517	-1.973994	-0.693226	0.731859	2.081291	-0.021181	-0.792494	-2.289426	-0.346969
H	-2.046949	-4.254308	-0.483365	-2.130395	4.122010	0.807047	2.896878	-3.987374	-1.041802
H	-0.909491	-3.388766	-1.545482	-0.532686	3.507211	1.299873	1.656973	-3.267408	-2.105752
H	-0.450213	-3.775169	0.143806	-0.943740	3.658649	-0.438202	3.162906	-2.365512	-1.740428
H	-1.981323	4.238686	1.354357	-2.491128	-4.088208	0.979681	0.628769	3.631168	0.005091
H	-0.446140	3.447449	1.792334	-1.078817	-3.299064	1.734770	2.051850	4.181113	-0.914336
H	-0.771541	3.905276	0.090387	-2.678361	-2.488816	1.752164	0.654688	3.498944	-1.782674
H	-3.691717	-0.560520	-1.241203	-3.652166	0.720385	-1.181021	3.226890	0.834018	1.368914
H	-5.572056	-0.793178	1.151827	-5.076098	-1.838132	-0.303374	4.968226	-1.627931	0.865569
H	-6.051629	-1.179682	-0.510260	-5.517203	-0.882842	-1.728518	4.979412	-0.675104	2.359165
H	-5.597639	1.051759	-1.347139	-6.043353	1.047359	-0.386346	5.720019	1.296184	1.181509
H	-5.232965	1.583232	0.303657	-5.595583	0.231382	1.122537	5.694156	0.485366	-0.394711
H	-3.767837	-2.418016	0.500474	-3.086752	-2.257085	-1.326672	2.811791	-2.174217	1.352201
H	-3.248738	2.356132	-0.497653	-3.839705	2.017885	1.025717	3.875927	2.176002	-0.722003

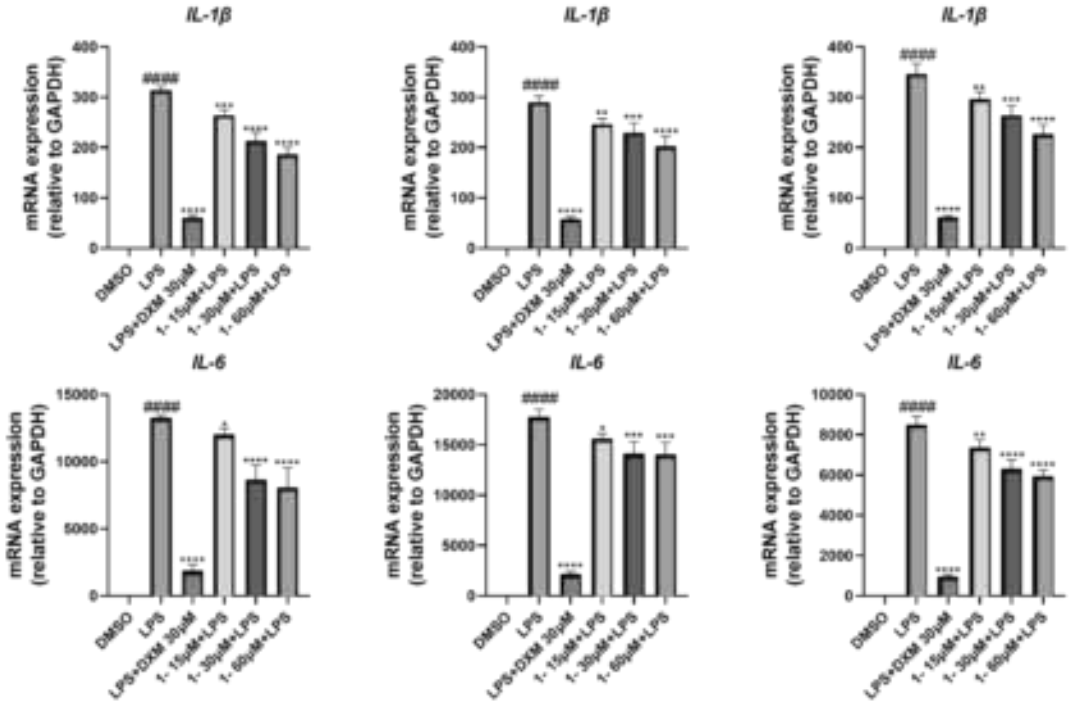


Figure S12: The results of quantitative real-time PCR (RT-PCR) of compound 1. Data are expressed as the mean ± SD.