

Supporting Information

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Vilmorinine G, a new quassinoid from *Ailanthus altissima*

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Abstract: A new quassinoid, vilmorinine G (**1**), along with two known congeners (**2** and **3**), was isolated from the root bark of *Ailanthus altissima* (Mill.) Swingle. The structure of compound **1** was elucidated through comprehensive spectroscopic analyses, including 1D and 2D NMR, HRESIMS, and further confirmed by X-ray crystallography.

Keywords: Quassinoid; *Ailanthus altissima*; absolute configuration

Table of Contents	Page
Figure S1: ¹ H NMR Spectrum of 1 in DMSO- <i>d</i> ₆ (600 MHz)	3
Figure S2: ¹³ C NMR Spectrum of 1 in DMSO- <i>d</i> ₆ (150 MHz)	3
Figure S3: HSQC Spectrum of 1 in DMSO- <i>d</i> ₆	4
Figure S4: ¹ H- ¹ H COSY Spectrum of 1 in DMSO- <i>d</i> ₆	4
Figure S5: HMBC Spectrum of 1 in DMSO- <i>d</i> ₆	5
Figure S6: NOESY Spectrum of 1 in DMSO- <i>d</i> ₆	5
Figure S7: HRESIMS Spectrum of 1	6
Figure S8: UV spectrum of compound 1	6
Figure S9: IR spectrum of compound 1	7
Figure S10: Most stable conformers of 1 <i>S</i> , 2 <i>S</i> , 5 <i>S</i> , 7 <i>R</i> , 8 <i>S</i> , 9 <i>R</i> , 10 <i>S</i> , 14 <i>S</i> , 15 <i>R</i> - 1 at the CAM-B3LYP/DGDZVP level	7
Table S1: Energies and atomic Cartesian coordinates of geometry-optimized conformers of 1 <i>S</i> , 2 <i>S</i> , 5 <i>S</i> , 7 <i>R</i> , 8 <i>S</i> , 9 <i>R</i> , 10 <i>S</i> , 14 <i>S</i> , 15 <i>R</i> - 1 at ωb97xd/dgdzvp in methanol	7
Figure S11: Most stable conformers of 1 <i>R</i> , 2 <i>R</i> , 5 <i>R</i> , 7 <i>S</i> , 8 <i>R</i> , 9 <i>S</i> , 10 <i>R</i> , 14 <i>R</i> , 15 <i>S</i> - 1 at the CAM-B3LYP/DGDZVP level	12
Table S2: Energies and atomic Cartesian coordinates of geometry-optimized conformers of 1 <i>R</i> , 2 <i>R</i> , 5 <i>R</i> , 7 <i>S</i> , 8 <i>R</i> , 9 <i>S</i> , 10 <i>R</i> , 14 <i>R</i> , 15 <i>S</i> - 1 at ωb97xd/dgdzvp in methanol	12

Figure S12: SciFinder search results for compound 1 (similarity >95%).	17
Figure S13: Structure of compound 1 and vilmorinine B.	17
Table S3: Comparison of NMR data between compound 1 and vilmorinine B.	18

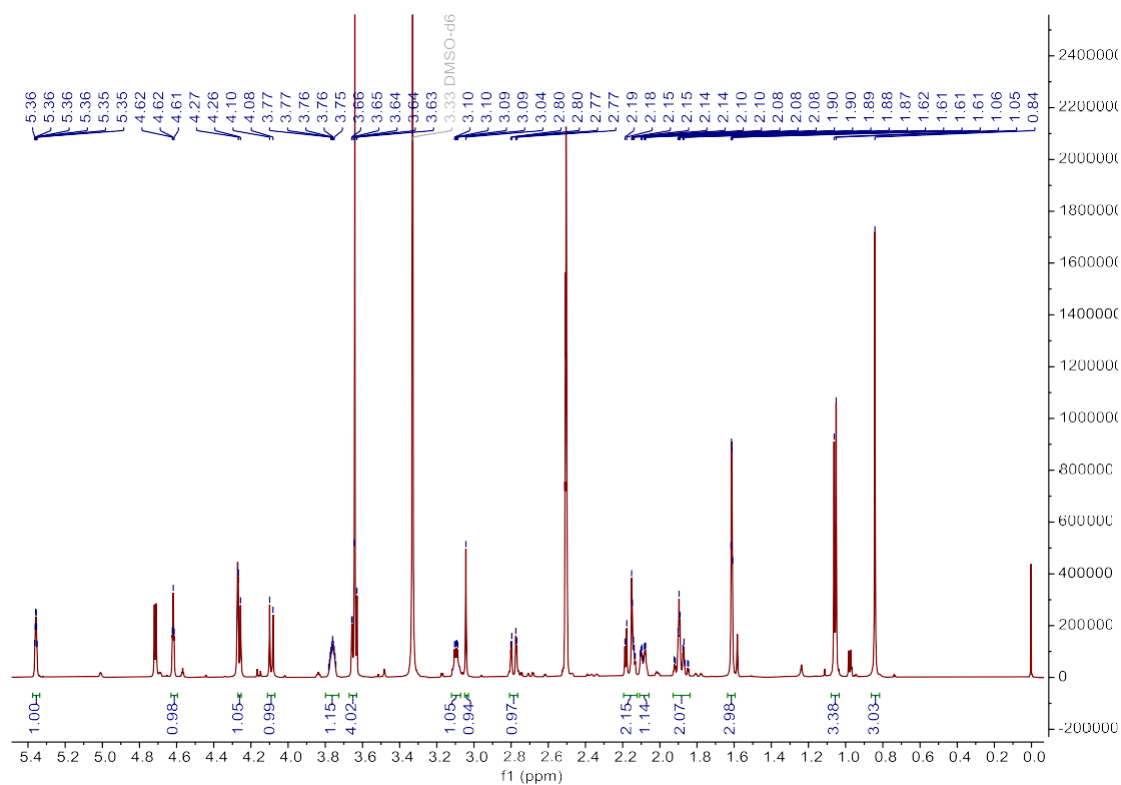


Figure S1 ¹H NMR Spectrum of **1** in DMSO-*d*₆ (600 MHz)

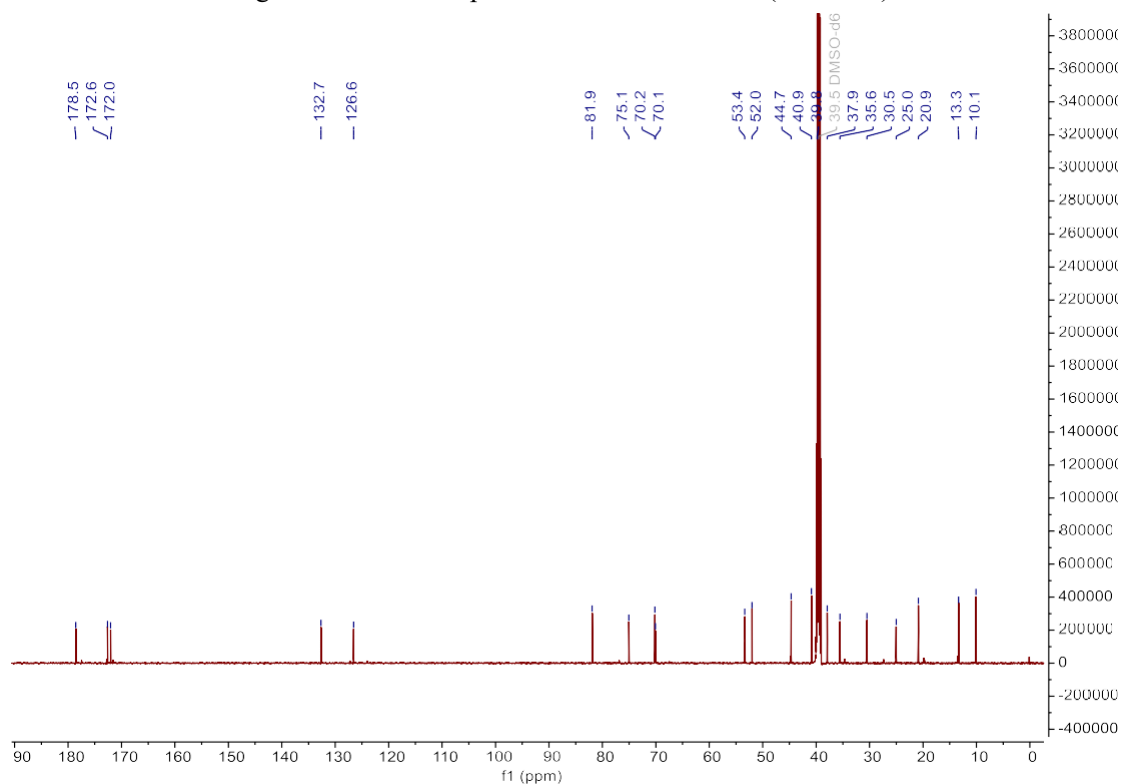


Figure S2 ¹³C NMR Spectrum of **1** in DMSO-*d*₆ (150 MHz)

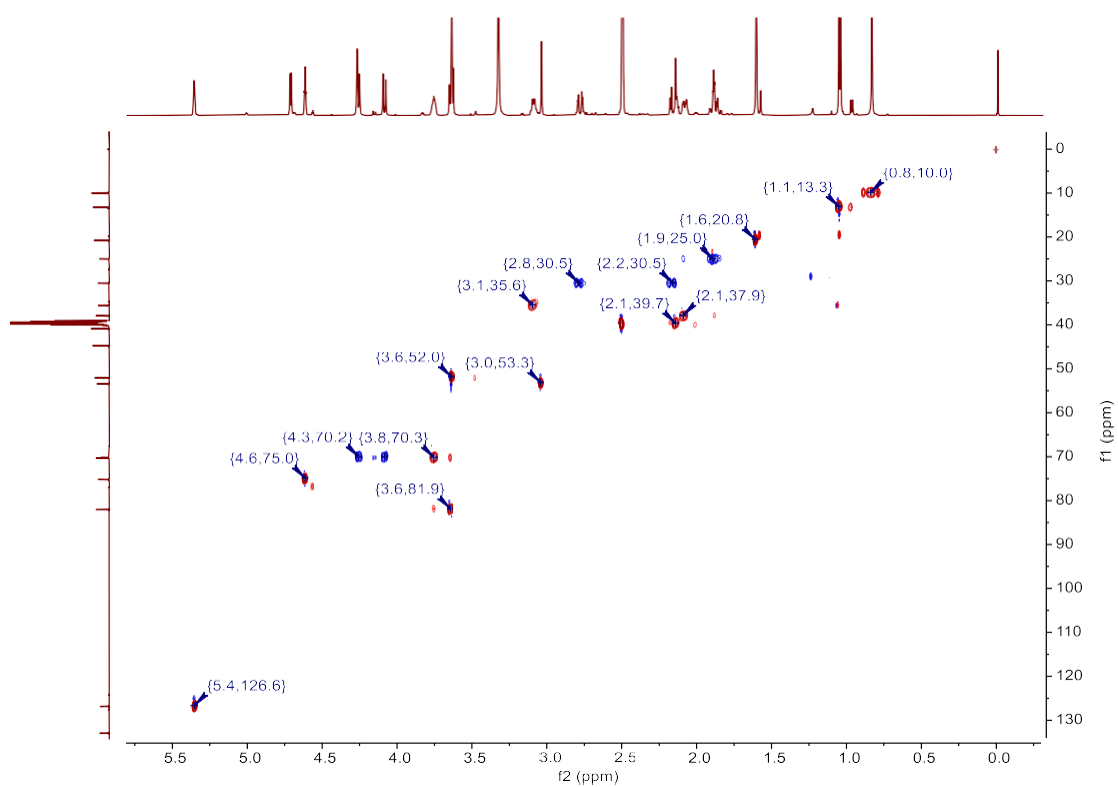


Figure S3: HSQC Spectrum of **1** in DMSO- d_6

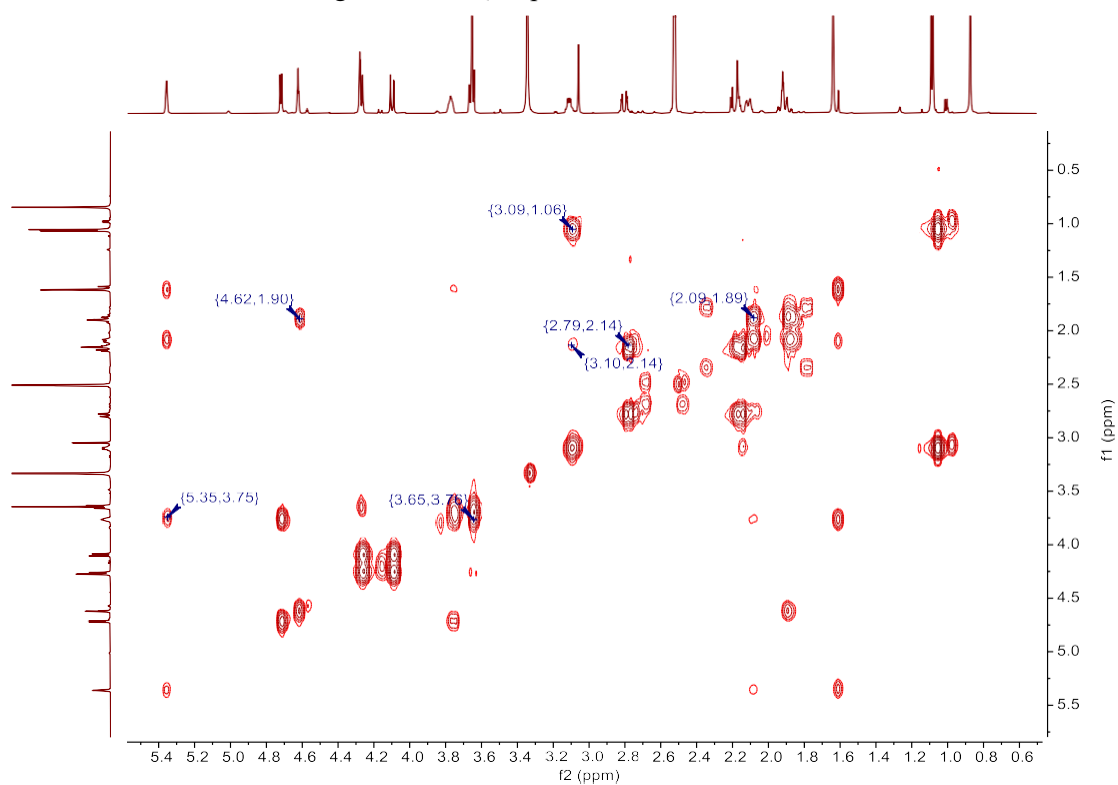


Figure S4: ^1H - ^1H COSY Spectrum of **1** in DMSO- d_6

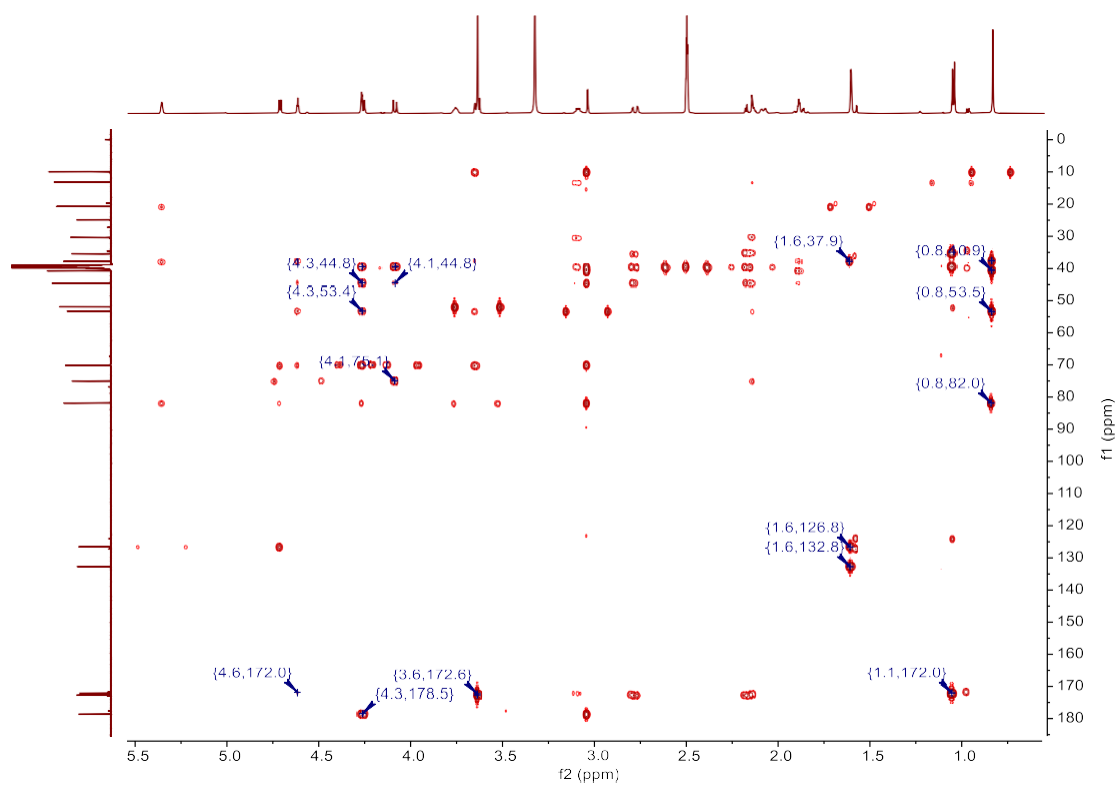


Figure S5: HMBC Spectrum of **1** in DMSO- d_6

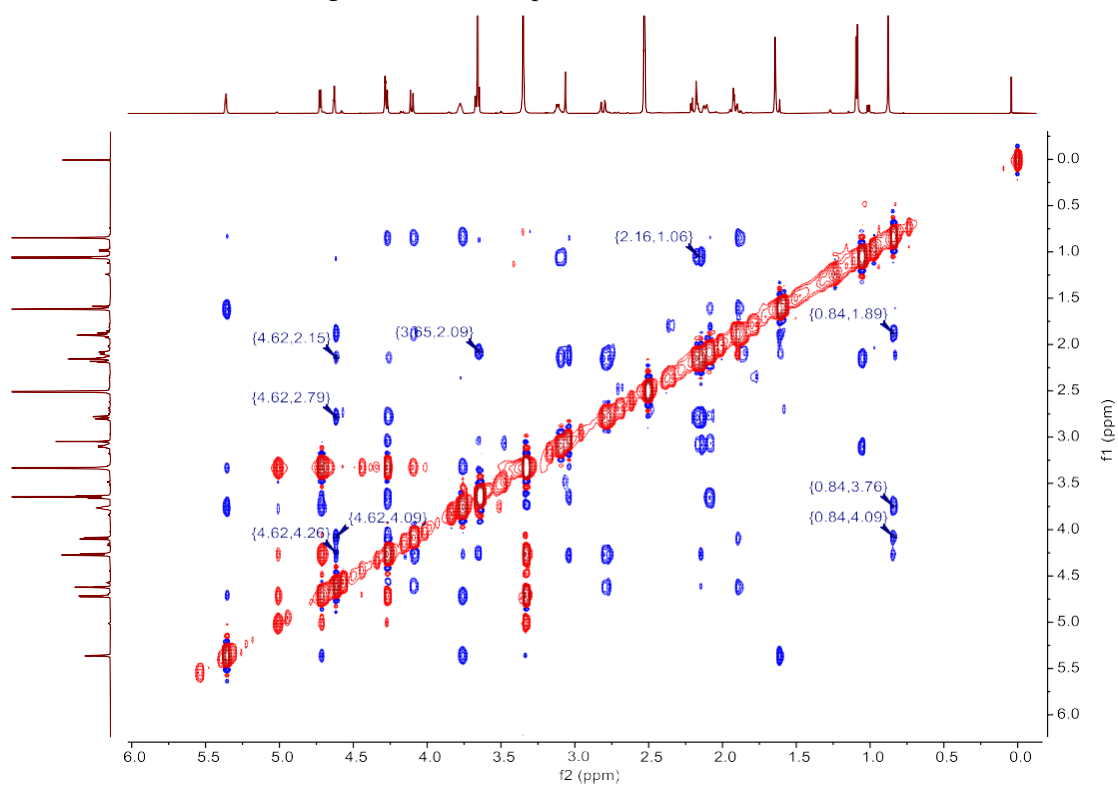


Figure S6: NOESY Spectrum of **1** in DMSO- d_6

AAH27 #1293 RT: 4.94 AV: 1 NL: 7.40E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]

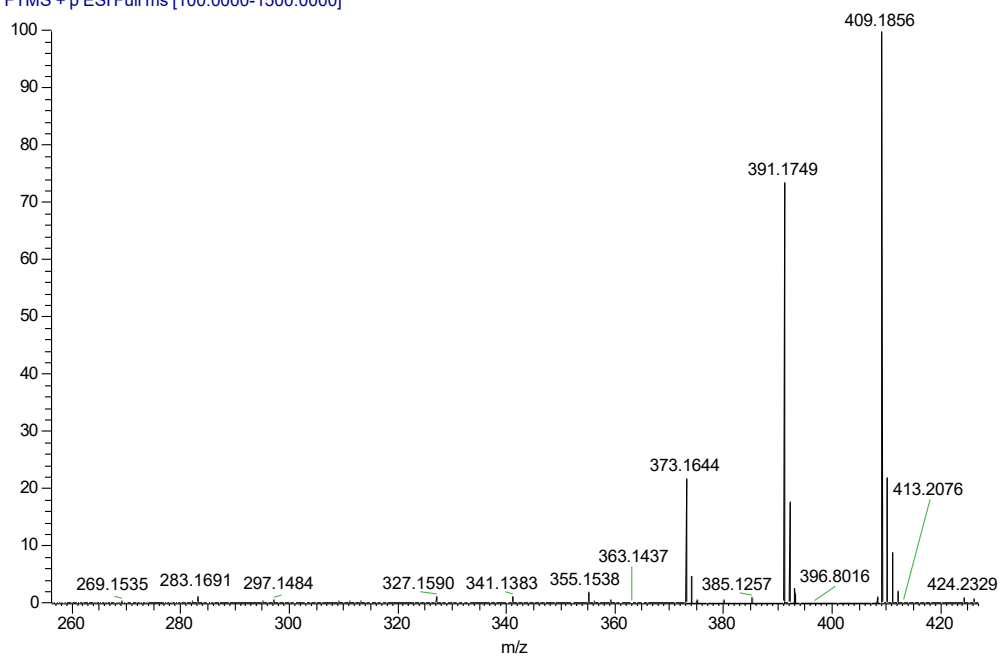


Figure S7: HRESIMS Spectrum of **1**

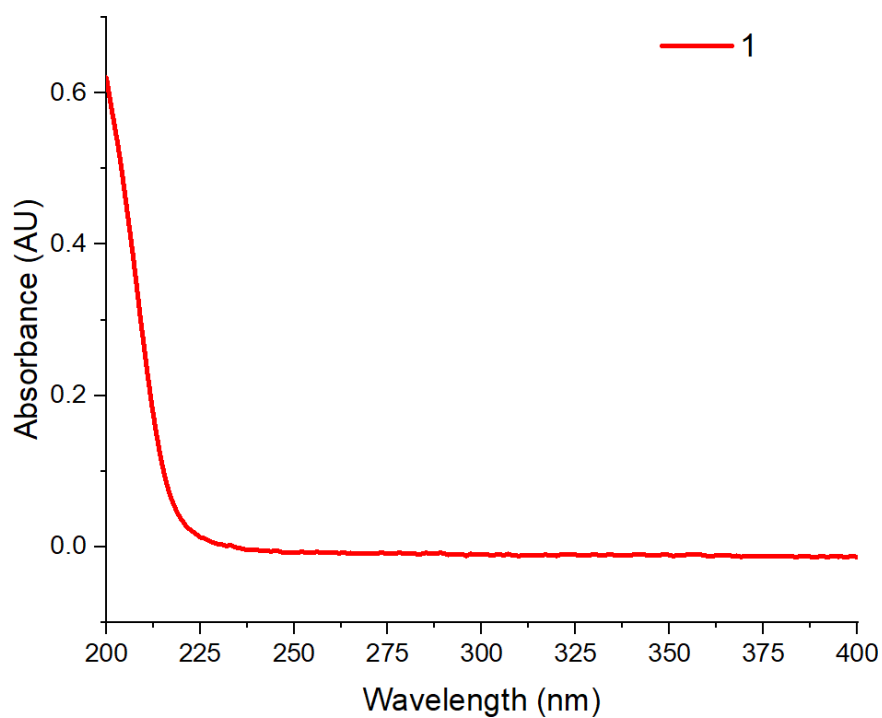


Figure S8: UV spectrum of compound **1**

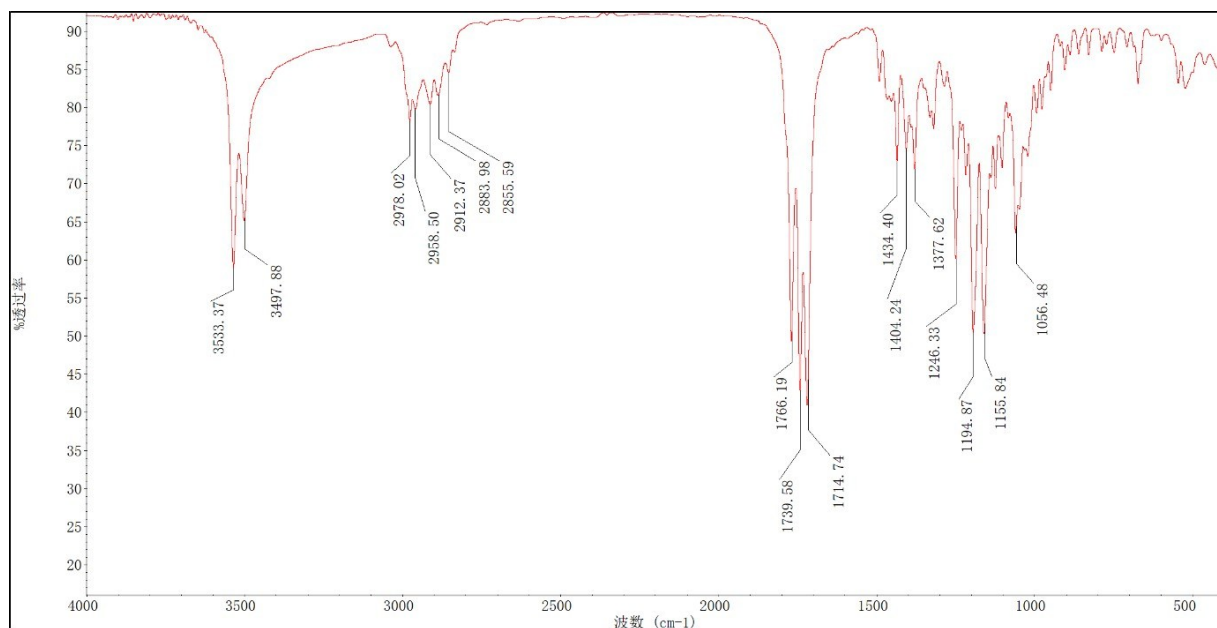


Figure S9: IR spectrum of compound **1**

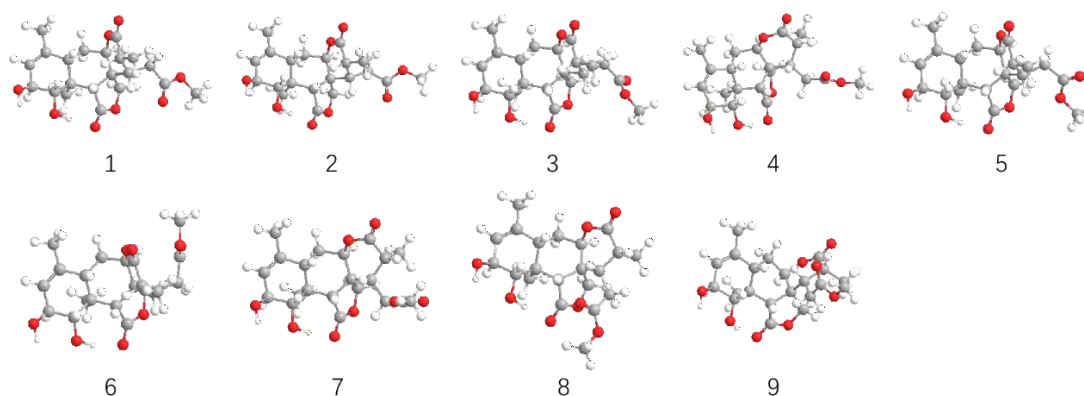


Figure S10: Most stable conformers of 1S, 2S, 5S, 7R, 8S, 9R, 10S, 14S, 15R-1 at the CAM-B3LYP/DGDZVP level

Table S1: Energies and atomic Cartesian coordinates of geometry-optimized conformers of 1S, 2S, 5S, 7R, 8S, 9R, 10S, 14S, 15R-1 at ω b97xd/dgdzvp in methanol

Gibbs free energy												
Conformer 1				Conformer 2			Conformer 3			Conformer 4		
Gibbs free energy (hartrees)												
ΔG (kcal/mol)												
Population Proportion												
Element	X	Y	Z	X	Y	Z	X	Y	Z	X	Y	Z
C	1.820481	0.326812	0.611775	1.858397	-0.165091	0.144447	1.886699	0.377387	0.387134	-1.817105	0.275375	-0.094086
C	1.276079	1.473735	1.480042	1.616857	0.809726	1.307612	1.392046	1.400463	1.422814	-2.607745	1.599083	-0.072190
C	0.992816	2.684680	0.625467	1.231047	2.176588	0.781239	1.001766	2.685738	0.734119	-1.706706	2.673227	-0.638362
O	1.138068	3.833223	0.990184	1.432954	3.211693	1.382548	1.149431	3.792221	1.210234	-2.077371	3.566987	-1.369042

O	0.518186	2.469321	-0.611057	0.611055	2.254264	-0.406973	0.420914	2.588019	-0.471728	-0.396024	2.559209	-0.354851
C	0.344743	1.183035	-1.263194	0.278262	1.154474	-1.296844	0.235073	1.377245	-1.252613	0.000677	1.787052	0.803631
C	0.734929	-0.054839	-0.431996	0.581396	-0.239883	-0.736686	0.726381	0.072140	-0.599044	-0.525788	0.330319	0.779334
C	-0.405225	-0.822333	0.301935	-0.565035	-0.939192	0.055983	-0.327626	-0.809774	0.134496	0.459198	-0.772685	0.286431
C	-1.871650	-0.675773	-0.230108	-2.049782	-0.549233	-0.279152	-1.835488	-0.666234	-0.267284	2.000454	-0.479886	0.315450
C	-2.049906	0.811792	-0.625212	-2.077409	0.985036	-0.486969	-2.091589	0.846420	-0.484514	2.177980	0.988073	-0.145594
C	-3.500830	1.201405	-0.862459	-3.485765	1.557975	-0.529248	-3.568503	1.198487	-0.574518	3.616095	1.345875	-0.486391
C	-3.770738	2.453605	-1.653394	-3.679425	2.904686	-1.173026	-3.940235	2.511320	-1.210609	3.984115	2.805322	-0.528317
C	-4.498423	0.504633	-0.311821	-4.499906	0.925086	0.066433	-4.496968	0.409127	-0.028036	4.500090	0.402519	-0.821206
C	-4.308335	-0.745766	0.487479	-4.385009	-0.415307	0.721328	-4.204502	-0.906573	0.621495	4.205458	-1.063586	-0.804123
C	-2.862311	-0.946744	0.929208	-2.938027	-0.838786	0.957169	-2.722152	-1.095537	0.927941	2.710778	-1.362356	-0.741485
O	-2.830010	-2.259760	1.466518	-3.023910	-2.201799	1.343448	-2.606614	-2.455423	1.316949	2.637673	-2.763224	-0.526009
O	-5.169222	-0.687862	1.624195	-5.096061	-0.374258	1.958264	-4.973223	-0.995803	1.820606	4.777400	-1.651308	-1.972185
C	-1.092806	1.169078	-1.763069	-1.181423	1.377450	-1.663055	-1.236017	1.362123	-1.641921	1.511699	1.924956	0.860589
C	-2.168081	-1.632073	-1.400592	-2.599259	-1.311943	-1.499546	-2.195965	-1.505731	-1.507406	2.613050	-0.734890	1.705893
H	-1.738653	1.419788	0.239187	-1.623155	1.442470	0.405092	-1.737421	1.371417	0.416701	1.624480	1.106072	-1.089949
H	-0.423585	-0.559081	1.360880	-0.435760	-0.806862	1.130246	-0.272066	-0.656882	1.213696	0.207482	-1.057427	-0.738565
H	1.020534	1.245353	-2.120324	0.909007	1.320888	-2.174403	0.837867	1.559681	-2.146096	-0.426235	2.295344	1.671832
C	3.180154	0.674877	-0.014008	3.127372	0.247587	-0.626282	3.180486	0.856654	-0.318398	-2.719118	-0.937460	0.165333
H	1.983616	-0.529735	1.272802	2.041703	-1.158798	0.565315	2.123587	-0.537201	0.938962	-1.472132	0.173760	-1.127978
C	0.101996	-2.254353	0.229623	-0.286770	-2.402018	-0.240903	0.218849	-2.205622	-0.125132	0.093289	-1.942295	1.185022
C	1.230674	-1.143215	-1.403130	0.770661	-1.242187	-1.893684	1.174165	-0.887447	-1.717202	-0.765466	-0.107718	2.238807
O	1.013932	-2.396116	-0.736720	0.441911	-2.533129	-1.352928	1.061544	-2.209460	-1.162945	-0.567075	-1.531098	2.272103
O	-0.231624	-3.188250	0.930060	-0.647682	-3.367819	0.400243	-0.027577	-3.218950	0.496371	0.327181	-3.119686	0.998558
C	4.130531	-0.501382	-0.086769	4.377242	-0.420114	-0.093084	4.204691	-0.237314	-0.518151	-3.801821	-1.084595	-0.883017
O	5.112774	-0.273813	-0.961384	5.456768	0.340226	-0.287750	4.572189	-0.778814	0.645310	-4.901618	-1.643179	-0.374403
O	4.039984	-1.514724	0.578437	4.411192	-1.523599	0.415309	4.652541	-0.583803	-1.594787	-3.681380	-0.772122	-2.051877
C	6.113239	-1.301702	-1.074169	6.712088	-0.223349	0.131483	5.531367	-1.848246	0.578063	-5.971151	-1.895956	-1.303116
C	2.127532	1.811251	2.701748	2.778273	0.903690	2.298504	2.342801	1.628080	2.595286	-3.254975	2.025217	1.254722
H	0.292831	1.173817	1.858844	0.746394	0.478030	1.881630	0.455347	1.026256	1.849916	-3.411739	1.514216	-0.805623
H	-3.181713	3.293152	-1.269713	-2.970468	3.636244	-0.771564	-3.356134	3.332863	-0.782910	3.266181	3.372934	-1.129389
H	-3.505038	2.327321	-2.707281	-3.518416	2.858268	-2.254340	-3.747119	2.503798	-2.287575	3.987931	3.246917	0.472802
H	-4.826258	2.725919	-1.602420	-4.689924	3.277724	-0.997960	-4.998538	2.730556	-1.059590	4.976390	2.943913	-0.960905
H	-5.529709	0.821879	-0.450054	-5.493739	1.367239	0.072971	-5.545943	0.695609	-0.057264	5.513038	0.676639	-1.107796
H	-4.595449	-1.614678	-0.122184	-4.852450	-1.174021	0.077092	-4.512850	-1.720440	-0.050529	4.674481	-1.519885	0.079662
H	-2.652998	-0.215488	1.725123	-2.548603	-0.240452	1.794921	-2.472931	-0.444008	1.779573	2.280446	-1.116206	-1.724033
H	-1.914038	-2.553377	1.614100	-2.143547	-2.615605	1.359654	-1.673028	-2.724708	1.368968	1.736429	-3.030785	-0.274470
H	-5.041416	-1.515401	2.109887	-5.029619	-1.259154	2.344945	-4.784524	-1.863419	2.206062	4.580115	-2.598078	-1.928571
H	-1.194208	0.479377	-2.604137	-1.435428	0.823568	-2.569851	-1.380999	0.764184	-2.544430	1.867920	1.739164	1.875775
H	-1.291490	2.165688	-2.157182	-1.283244	2.434954	-1.907353	-1.495381	2.387078	-1.906906	1.730727	2.970569	0.644240
H	-1.370759	-1.661480	-2.143950	-1.912955	-1.324160	-2.346442	-1.463285	-1.424584	-2.310860	2.000819	-0.347614	2.521800
H	-2.310175	-2.650364	-1.031222	-2.815295	-2.349638	-1.234684	-2.274875	-2.562044	-1.239951	2.742131	-1.806749	1.873436
H	-3.078872	-1.335346	-1.924737	-3.526741	-0.857319	-1.853065	-3.156188	-1.192355	-1.922331	3.593668	-0.262099	1.792463

H	3.096014	1.123529	-1.006368	3.088327	-0.040388	-1.679404	2.984016	1.306995	-1.291636	-2.149972	-1.869690	0.096939
H	3.702207	1.418489	0.594517	3.280261	1.328968	-0.629674	3.672121	1.622060	0.286013	-3.180422	-0.928006	1.153203
H	0.669424	-1.150746	-2.340139	0.110195	-1.039605	-2.738557	0.531416	-0.827308	-2.598017	-0.054708	0.349387	2.931387
H	2.288129	-1.082436	-1.650249	1.787506	-1.314122	-2.269465	2.204075	-0.755599	-2.041758	-1.772187	0.087018	2.604229
H	6.816330	-0.940797	-1.819917	7.460633	0.527811	-0.105661	5.690545	-2.159803	1.606781	-6.763593	-2.351275	-0.715393
H	6.613688	-1.447623	-0.116868	6.695921	-0.420660	1.203453	5.133316	-2.672907	-0.013344	-6.313508	-0.960703	-1.746048
H	5.657138	-2.236436	-1.400338	6.911962	-1.146673	-0.412389	6.462739	-1.491515	0.138451	-5.637415	-2.576545	-2.086455
H	3.083711	2.263208	2.432214	2.495400	1.513778	3.156233	3.269758	2.118565	2.292947	-3.845179	2.929638	1.096307
H	1.601638	2.516548	3.345600	3.039017	-0.095225	2.653935	1.868961	2.255892	3.350141	-3.933052	1.247544	1.611999
H	2.322451	0.901259	3.273312	3.664878	1.357938	1.849512	2.593443	0.668110	3.051731	-2.534567	2.236910	2.046145
Conformer 5				Conformer 6			Conformer 7			Conformer 8		
Gibbs free												
energy	-1418.247939			-1418.247827			-1418.247508			-1418.247052		
(hartrees)												
ΔG												
(kcal/mol)	1.062			1.132			1.332			1.618		
Population												
Proportion	5.01%			4.45%			3.18%			1.96%		
Element	X	Y	Z	X	Y	Z	X	Y	Z	X	Y	Z
C	1.907949	0.318922	0.313160	1.704773	-1.138905	0.689068	-1.877224	0.089220	0.037033	-2.060762	0.731030	-0.419798
C	1.458333	1.363002	1.344862	1.675268	-0.032638	1.760420	-2.760211	1.352472	0.040714	-2.686878	2.136573	-0.520372
C	1.018337	2.625746	0.639606	1.891706	1.346828	1.183122	-1.955048	2.473467	-0.578146	-1.617957	3.091594	-1.000388
O	1.128254	3.740795	1.106152	2.351015	2.278603	1.810569	-2.411816	3.317011	-1.319455	-1.806958	3.992452	-1.790034
O	0.444529	2.501720	-0.567760	1.517972	1.567476	-0.086391	-0.632636	2.462198	-0.332222	-0.368691	2.853961	-0.562840
C	0.261620	1.278254	-1.331780	0.881827	0.619012	-0.982575	-0.144431	1.752661	0.831511	-0.193517	2.077666	0.646047
C	0.720989	-0.010048	-0.630994	0.661504	-0.796487	-0.416912	-0.565365	0.262431	0.863205	-0.856706	0.679615	0.578605
C	-0.356205	-0.813449	0.158595	-0.751899	-1.123218	0.160926	0.477017	-0.783206	0.363519	0.067895	-0.520250	0.206441
C	-1.861097	-0.651408	-0.254729	-1.980714	-0.278377	-0.319746	1.993406	-0.383865	0.331276	1.616891	-0.379957	0.411751
C	-2.079847	0.850876	-0.563079	-1.494195	1.189127	-0.414570	2.050539	1.079549	-0.173143	1.989994	1.055530	-0.032429
C	-3.547571	1.231111	-0.684352	-2.629118	2.190357	-0.563446	3.447113	1.526409	-0.575771	3.485727	1.264740	-0.208877
C	-3.885970	2.507904	-1.406506	-2.294402	3.556669	-1.099475	3.709934	3.006038	-0.670047	4.000047	2.679861	-0.214589
C	-4.496220	0.500929	-0.092171	-3.863788	1.895108	-0.148312	4.383114	0.637505	-0.918288	4.302663	0.233528	-0.439167
C	-4.237023	-0.777455	0.640541	-4.270757	0.561998	0.395767	4.193557	-0.844634	-0.853093	3.862355	-1.195927	-0.451360
C	-2.760197	-0.985223	0.961922	-3.077100	-0.309456	0.774012	2.726751	-1.244371	-0.727987	2.347847	-1.342604	-0.557507
O	-2.681579	-2.321504	1.433133	-3.635297	-1.586133	1.043780	2.758797	-2.640332	-0.474169	2.108335	-2.726183	-0.351383
O	-5.008765	-0.772094	1.841089	-5.105970	0.776745	1.533128	4.764167	-1.423170	-2.026456	4.500142	-1.854048	-1.545591
C	-1.203358	1.277665	-1.741258	-0.389575	1.304402	-1.464209	1.354343	1.996556	0.831723	1.306354	2.068934	0.884022
C	-2.242978	-1.552850	-1.443975	-2.563851	-0.790934	-1.650111	2.670065	-0.557803	1.704429	2.044542	-0.674903	1.862050
H	-1.719855	1.420090	0.308474	-1.028108	1.443247	0.550669	1.457687	1.131340	-1.099562	1.561589	1.210854	-1.034712
H	-0.295496	-0.599643	1.226394	-0.741315	-1.069728	1.251176	0.212837	-1.111100	-0.645243	-0.093007	-0.796541	-0.837526
H	0.884255	1.432118	-2.217036	1.584694	0.545362	-1.814536	-0.578730	2.253356	1.700797	-0.667340	2.647846	1.449209
C	3.180044	0.813028	-0.429974	3.127684	-1.514040	0.211102	-2.681175	-1.181798	0.370837	-3.158824	-0.327314	-0.226650
H	2.159402	-0.594323	0.859985	1.359209	-2.048599	1.191570	-1.555181	-0.023774	-1.003022	-1.635768	0.541573	-1.410432

C	0.137760	-2.239064	-0.021491	-0.881344	-2.597374	-0.193778	0.220289	-1.950863	1.301826	-0.510810	-1.632903	1.064816
C	1.134943	-1.050784	-1.691296	0.719924	-1.786901	-1.593746	-0.721223	-0.149531	2.340517	-1.284173	0.296705	2.007937
O	0.952549	-2.336190	-1.074392	-0.036618	-2.935625	-1.173036	-0.432139	-1.556150	2.399819	-1.251798	-1.139500	2.063391
O	-0.130860	-3.203683	0.665836	-1.624605	-3.412470	0.313713	0.528958	-3.113974	1.136515	-0.370278	-2.830997	0.920934
C	4.407093	-0.016566	-0.134719	3.840994	-0.470707	-0.613680	-3.910372	-1.312028	-0.500141	-2.844454	-1.675723	-0.841424
O	4.193722	-1.310083	-0.399432	4.427697	0.450700	0.154176	-3.587694	-1.418842	-1.792277	-3.467269	-2.662366	-0.197531
O	5.461933	0.423182	0.277213	3.865358	-0.448252	-1.830548	-5.053423	-1.312667	-0.086743	-2.142837	-1.845004	-1.821004
C	5.290627	-2.206264	-0.153083	5.029054	1.565166	-0.527482	-4.684072	-1.511031	-2.718474	-3.251274	-3.988494	-0.711751
C	2.489402	1.635385	2.438200	2.590065	-0.284514	2.959009	-3.410346	1.763452	1.370327	-3.433194	2.666807	0.713458
H	0.555885	1.000887	1.847299	0.652667	0.008072	2.153410	-3.574201	1.192706	-0.670729	-3.408720	2.108331	-1.339750
H	-3.287064	3.342616	-1.027614	-1.442443	3.988851	-0.564288	2.933013	3.504834	-1.258717	3.414406	3.306085	-0.895677
H	-3.685181	2.426735	-2.479054	-2.023677	3.516209	-2.158841	3.718414	3.475972	0.318044	3.935001	3.134417	0.778609
H	-4.940286	2.759046	-1.279007	-3.143138	4.234499	-0.994056	4.674040	3.200234	-1.143068	5.043599	2.713408	-0.532283
H	-5.538081	0.809122	-0.145002	-4.656473	2.636935	-0.216270	5.363458	0.973327	-1.249153	5.363625	0.401582	-0.610897
H	-4.565294	-1.624185	0.020563	-4.851991	0.020995	-0.364818	4.724495	-1.242385	0.023864	4.181069	-1.684179	0.481012
H	-2.494910	-0.290213	1.773251	-2.641657	0.106294	1.695511	2.246330	-1.056011	-1.700025	2.057071	-1.066053	-1.582136
H	-1.755534	-2.611704	1.504697	-2.938465	-2.260623	1.123548	1.887557	-2.962168	-0.183274	1.161619	-2.897008	-0.203815
H	-4.841720	-1.618241	2.280552	-5.372038	-0.098493	1.849589	4.637953	-2.380014	-1.951004	4.202260	-2.774923	-1.524007
H	-1.352929	0.631532	-2.609348	-0.703339	0.886544	-2.423578	1.756121	1.865364	1.838409	1.518976	1.866504	1.935881
H	-1.434440	2.291812	-2.067020	-0.122745	2.343944	-1.654629	1.491988	3.048249	0.580555	1.651172	3.084792	0.690773
H	-1.509860	-1.535319	-2.250821	-1.801834	-1.017301	-2.396275	2.061057	-0.192271	2.532674	1.387127	-0.219328	2.604009
H	-2.346982	-2.589853	-1.116221	-3.141837	-1.702964	-1.483628	2.879941	-1.613224	1.893287	2.048001	-1.751961	2.045268
H	-3.195994	-1.241047	-1.876155	-3.230163	-0.048430	-2.093959	3.617520	-0.015981	1.743298	3.051255	-0.298870	2.056617
H	3.048673	0.800187	-1.514580	3.729091	-1.732410	1.094294	-2.072506	-2.071877	0.192069	-3.460553	-0.469157	0.810693
H	3.426417	1.843098	-0.173699	3.088960	-2.430105	-0.376263	-3.019656	-1.206248	1.406011	-4.057979	0.010618	-0.753294
H	0.514218	-1.006546	-2.588453	0.256997	-1.380412	-2.495406	-0.013851	0.369902	2.991104	-0.596996	0.680951	2.765234
H	2.179062	-0.994585	-1.989357	1.719983	-2.122156	-1.853098	-1.722601	-0.006657	2.742733	-2.292687	0.610288	2.272935
H	4.921083	-3.194585	-0.412610	5.420995	2.206663	0.256963	-4.227718	-1.580626	-3.702117	-3.825854	-4.646671	-0.065525
H	6.142253	-1.940008	-0.779095	5.831912	1.220329	-1.178936	-5.279856	-2.399587	-2.509980	-3.605506	-4.057782	-1.740363
H	5.576589	-2.169574	0.898119	4.274068	2.093720	-1.110709	-5.309118	-0.620380	-2.650241	-2.190372	-4.234851	-0.663122
H	3.407939	2.070714	2.039430	3.641262	-0.151344	2.698857	-4.068622	2.618021	1.204131	-3.901011	3.623800	0.475160
H	2.086127	2.324753	3.179970	2.354054	0.409532	3.765612	-4.020705	0.944806	1.756979	-4.225067	1.971231	0.999157
H	2.742252	0.697993	2.938829	2.442642	-1.302322	3.328201	-2.690020	2.046646	2.139224	-2.789481	2.821509	1.580607

Conformer 9

Gibbs free

energy -1418.246487

(hartrees)

ΔG

1.973

(kcal/mol)

Population

1.08%

Proportion

Element	X	Y	Z
C	1.606384	-0.031135	-0.080191
C	2.790821	-0.973614	-0.411080
C	2.397394	-2.423740	-0.640077
O	3.157337	-3.217668	-1.155850

O	1.218603	-2.883799	-0.187796
C	0.122170	-2.009736	0.146683
C	0.573065	-0.720303	0.843191
C	-0.695259	0.113433	1.199869
C	-1.983235	-0.110556	0.336875
C	-1.494197	-0.440576	-1.089922
C	-2.584837	-0.348636	-2.144744
C	-2.299797	-0.985350	-3.478857
C	-3.704465	0.347102	-1.923763
C	-4.018011	1.032968	-0.628055
C	-2.766067	1.214029	0.225863
O	-3.158703	1.805839	1.457726
O	-4.600007	2.301983	-0.921441
C	-0.731900	-1.775707	-1.110613
C	-2.897010	-1.230669	0.884634
H	-0.784032	0.348579	-1.367405
H	-0.453975	1.178670	1.148766
H	-0.437069	-2.610970	0.863366
C	2.076406	1.347636	0.392628
H	1.108794	0.144697	-1.035133
C	-0.914273	-0.168574	2.674295
C	1.144816	-1.046413	2.241598
O	0.067820	-0.908494	3.184094
O	-1.848276	0.203019	3.358772
C	2.922633	2.051414	-0.646214
O	3.802567	2.880802	-0.081523
O	2.801218	1.911357	-1.848102
C	4.618029	3.650225	-0.983263
C	3.975359	-0.970619	0.576449
H	3.192898	-0.648918	-1.373488
H	-1.346622	-0.625751	-3.880597
H	-2.223490	-2.073604	-3.400017
H	-3.084498	-0.752370	-4.200490
H	-4.455600	0.438231	-2.705371
H	-4.746794	0.440242	-0.056852
H	-2.122954	1.938258	-0.293401
H	-2.859777	1.263838	2.210917
H	-4.792667	2.718138	-0.068669
H	-1.424953	-2.614552	-1.208317
H	-0.081254	-1.806430	-1.988138
H	-2.339348	-2.086262	1.267655
H	-3.524866	-0.872804	1.702247
H	-3.555505	-1.603849	0.098195

H	1.219365	2.010102	0.543989
H	2.617829	1.325404	1.338338
H	1.520579	-2.065292	2.329384
H	1.923876	-0.349870	2.550361
H	5.259045	4.256122	-0.348693
H	5.216289	2.987021	-1.608029
H	3.991402	4.284907	-1.609966
H	4.769713	-1.605710	0.183370
H	4.384526	0.034313	0.690557
H	3.708245	-1.345339	1.565942

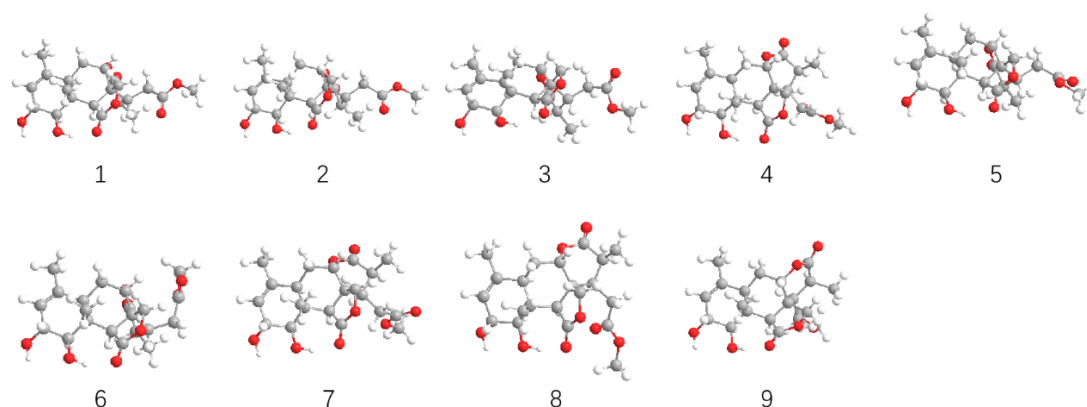


Figure S11: Most stable conformers of 1*R*, 2*R*, 5*R*, 7*S*, 8*R*, 9*S*, 10*R*, 14*R*, 15*S*-1 at the CAM-B3LYP/DGDZVP level

Table S2: Energies and atomic Cartesian coordinates of geometry-optimized conformers of 1*R*, 2*R*, 5*R*, 7*S*, 8*R*, 9*S*, 10*R*, 14*R*, 15*S*-1 at ω b97xd/dgdzvp in methanol

IR, 2R, 3R, 4S, 5R, 6S, 7R, 8R, 9S, 10R, 11R, 12S, 13R, 14S, 15S, 16R, 17R, 18R, 19R, 20R, 21R, 22R, 23R, 24R, 25R, 26R, 27R, 28R, 29R, 30R, 31R, 32R, 33R, 34R, 35R, 36R, 37R, 38R, 39R, 40R, 41R, 42R, 43R, 44R, 45R, 46R, 47R, 48R, 49R, 50R, 51R, 52R, 53R, 54R, 55R, 56R, 57R, 58R, 59R, 60R, 61R, 62R, 63R, 64R, 65R, 66R, 67R, 68R, 69R, 70R, 71R, 72R, 73R, 74R, 75R, 76R, 77R, 78R, 79R, 80R, 81R, 82R, 83R, 84R, 85R, 86R, 87R, 88R, 89R, 90R, 91R, 92R, 93R, 94R, 95R, 96R, 97R, 98R, 99R, 100R, 101R, 102R, 103R, 104R, 105R, 106R, 107R, 108R, 109R, 110R, 111R, 112R, 113R, 114R, 115R, 116R, 117R, 118R, 119R, 120R, 121R, 122R, 123R, 124R, 125R, 126R, 127R, 128R, 129R, 130R, 131R, 132R, 133R, 134R, 135R, 136R, 137R, 138R, 139R, 140R, 141R, 142R, 143R, 144R, 145R, 146R, 147R, 148R, 149R, 150R, 151R, 152R, 153R, 154R, 155R, 156R, 157R, 158R, 159R, 160R, 161R, 162R, 163R, 164R, 165R, 166R, 167R, 168R, 169R, 170R, 171R, 172R, 173R, 174R, 175R, 176R, 177R, 178R, 179R, 180R, 181R, 182R, 183R, 184R, 185R, 186R, 187R, 188R, 189R, 190R, 191R, 192R, 193R, 194R, 195R, 196R, 197R, 198R, 199R, 200R, 201R, 202R, 203R, 204R, 205R, 206R, 207R, 208R, 209R, 210R, 211R, 212R, 213R, 214R, 215R, 216R, 217R, 218R, 219R, 220R, 221R, 222R, 223R, 224R, 225R, 226R, 227R, 228R, 229R, 230R, 231R, 232R, 233R, 234R, 235R, 236R, 237R, 238R, 239R, 240R, 241R, 242R, 243R, 244R, 245R, 246R, 247R, 248R, 249R, 250R, 251R, 252R, 253R, 254R, 255R, 256R, 257R, 258R, 259R, 260R, 261R, 262R, 263R, 264R, 265R, 266R, 267R, 268R, 269R, 270R, 271R, 272R, 273R, 274R, 275R, 276R, 277R, 278R, 279R, 280R, 281R, 282R, 283R, 284R, 285R, 286R, 287R, 288R, 289R, 290R, 291R, 292R, 293R, 294R, 295R, 296R, 297R, 298R, 299R, 300R, 301R, 302R, 303R, 304R, 305R, 306R, 307R, 308R, 309R, 310R, 311R, 312R, 313R, 314R, 315R, 316R, 317R, 318R, 319R, 320R, 321R, 322R, 323R, 324R, 325R, 326R, 327R, 328R, 329R, 330R, 331R, 332R, 333R, 334R, 335R, 336R, 337R, 338R, 339R, 340R, 341R, 342R, 343R, 344R, 345R, 346R, 347R, 348R, 349R, 350R, 351R, 352R, 353R, 354R, 355R, 356R, 357R, 358R, 359R, 360R, 361R, 362R, 363R, 364R, 365R, 366R, 367R, 368R, 369R, 370R, 371R, 372R, 373R, 374R, 375R, 376R, 377R, 378R, 379R, 380R, 381R, 382R, 383R, 384R, 385R, 386R, 387R, 388R, 389R, 390R, 391R, 392R, 393R, 394R, 395R, 396R, 397R, 398R, 399R, 400R, 401R, 402R, 403R, 404R, 405R, 406R, 407R, 408R, 409R, 410R, 411R, 412R, 413R, 414R, 415R, 416R, 417R, 418R, 419R, 420R, 421R, 422R, 423R, 424R, 425R, 426R, 427R, 428R, 429R, 430R, 431R, 432R, 433R, 434R, 435R, 436R, 437R, 438R, 439R, 440R, 441R, 442R, 443R, 444R, 445R, 446R, 447R, 448R, 449R, 450R, 451R, 452R, 453R, 454R, 455R, 456R, 457R, 458R, 459R, 460R, 461R, 462R, 463R, 464R, 465R, 466R, 467R, 468R, 469R, 470R, 471R, 472R, 473R, 474R, 475R, 476R, 477R, 478R, 479R, 480R, 481R, 482R, 483R, 484R, 485R, 486R, 487R, 488R, 489R, 490R, 491R, 492R, 493R, 494R, 495R, 496R, 497R, 498R, 499R, 500R, 501R, 502R, 503R, 504R, 505R, 506R, 507R, 508R, 509R, 510R, 511R, 512R, 513R, 514R, 515R, 516R, 517R, 518R, 519R, 520R, 521R, 522R, 523R, 524R, 525R, 526R, 527R, 528R, 529R, 530R, 531R, 532R, 533R, 534R, 535R, 536R, 537R, 538R, 539R, 540R, 541R, 542R, 543R, 544R, 545R, 546R, 547R, 548R, 549R, 550R, 551R, 552R, 553R, 554R, 555R, 556R, 557R, 558R, 559R, 560R, 561R, 562R, 563R, 564R, 565R, 566R, 567R, 568R, 569R, 570R, 571R, 572R, 573R, 574R, 575R, 576R, 577R, 578R, 579R, 580R, 581R, 582R, 583R, 584R, 585R, 586R, 587R, 588R, 589R, 590R, 591R, 592R, 593R, 594R, 595R, 596R, 597R, 598R, 599R, 600R, 601R, 602R, 603R, 604R, 605R, 606R, 607R, 608R, 609R, 610R, 611R, 612R, 613R, 614R, 615R, 616R, 617R, 618R, 619R, 620R, 621R, 622R, 623R, 624R, 625R, 626R, 627R, 628R, 629R, 630R, 631R, 632R, 633R, 634R, 635R, 636R, 637R, 638R, 639R, 640R, 641R, 642R, 643R, 644R, 645R, 646R, 647R, 648R, 649R, 650R, 651R, 652R, 653R, 654R, 655R, 656R, 657R, 658R, 659R, 660R, 661R, 662R, 663R, 664R, 665R, 666R, 667R, 668R, 669R, 670R, 671R, 672R, 673R, 674R, 675R, 676R, 677R, 678R, 679R, 680R, 681R, 682R, 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849R, 850R, 851R, 852R, 853R, 854R, 855R, 856R, 857R, 858R, 859R, 860R, 861R, 862R, 863R, 864R, 865R, 866R, 867R, 868R, 869R, 870R, 871R, 872R, 873R, 874R, 875R, 876R, 877R, 878R, 879R, 880R, 881R, 882R, 883R, 884R, 885R, 886R, 887R, 888R, 889R, 890R, 891R, 892R, 893R, 894R, 895R, 896R, 897R, 898R, 899R, 900R, 901R, 902R, 903R, 904R, 905R, 906R, 907R, 908R, 909R, 910R, 911R, 912R, 913R, 914R, 915R, 916R, 917R, 918R, 919R, 920R, 921R, 922R, 923R, 924R, 925R, 926R, 927R, 928R, 929R, 930R, 931R, 932R, 933R, 934R, 935R, 936R, 937R, 938R, 939R, 940R, 941R, 942R, 943R, 944R, 945R, 946R, 947R, 948R, 949R, 950R, 951R, 952R, 953R, 954R, 955R, 956R, 957R, 958R, 959R, 960R, 961R, 962R, 963R, 964R, 965R, 966R, 967R, 968R, 969R, 970R, 971R, 972R, 973R, 974R, 975R, 976R, 977R, 978R, 979R, 980R, 981R, 982R, 983R, 984R, 985R, 986R, 987R, 988R, 989R, 990R, 991R, 992R, 993R, 994R, 995R, 996R, 997R, 998R, 999R, 1000R, 1001R, 1002R, 1003R, 1004R, 1005R, 1006R, 1007R, 1008R, 1009R, 1010R, 1011R, 1012R, 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1871R, 1872R, 1873R, 1874R, 1875R, 1876R, 1877R, 1878R, 1879R, 1880R, 1881R, 1882R, 1883R, 1884R, 1885R, 1886R, 1887R, 1888R, 1889R, 1890R, 1891R, 1892R, 1893R, 1894R, 1895R, 1896R, 1897R, 1898R, 1899R, 1900R, 1901R, 1902R, 1903R, 1904R, 1905R, 1906R, 1907R, 1908R, 1909R, 1910R, 1911R, 1912R, 1913R, 1914R, 1915R, 1916R, 1917R, 1918R, 1919R, 1920R, 1921R, 1922R, 1923R, 1924R, 1925R, 1926R,												
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C	2.049906	0.811792	-0.625212	2.077409	0.985036	-0.486969	2.091589	0.846420	-0.484514	-2.177980	0.988073	-0.145594
C	3.500830	1.201405	-0.862459	3.485765	1.557975	-0.529248	3.568503	1.198487	-0.574518	-3.616095	1.345875	-0.486391
C	3.770738	2.453605	-1.653394	3.679425	2.904686	-1.173026	3.940235	2.511320	-1.210609	-3.984115	2.805322	-0.528317
C	4.498423	0.504633	-0.311821	4.499906	0.925086	0.066433	4.496968	0.409127	-0.028036	-4.500090	0.402519	-0.821206
C	4.308335	-0.745766	0.487479	4.385009	-0.415307	0.721328	4.204502	-0.906573	0.621495	-4.205458	-1.063586	-0.804123
C	2.862311	-0.946744	0.929208	2.938027	-0.838786	0.957169	2.722152	-1.095537	0.927941	-2.710778	-1.362356	-0.741485
O	2.830010	-2.259760	1.466518	3.023910	-2.201799	1.343448	2.606614	-2.455423	1.316949	-2.637673	-2.763224	-0.526009
O	5.169222	-0.687862	1.624195	5.096061	-0.374258	1.958264	4.973223	-0.995803	1.820606	-4.777400	-1.651308	-1.972185
C	1.092806	1.169078	-1.763069	1.181423	1.377450	-1.663055	1.236017	1.362123	-1.641921	-1.511699	1.924956	0.860589
C	2.168081	-1.632073	-1.400592	2.599259	-1.311943	-1.499546	2.195965	-1.505731	-1.507406	-2.613050	-0.734890	1.705893
H	1.738653	1.419788	0.239187	1.623155	1.442470	0.405092	1.737421	1.371417	0.416701	-1.624480	1.106072	-1.089949
H	0.423585	-0.559081	1.360880	0.435760	-0.806862	1.130246	0.272066	-0.656882	1.213696	-0.207482	-1.057427	-0.738565
H	-1.020534	1.245353	-2.120324	-0.909007	1.320888	-2.174403	-0.837867	1.559681	-2.146096	0.426235	2.295344	1.671832
C	-3.180154	0.674877	-0.014008	-3.127372	0.247587	-0.626282	-3.180486	0.856654	-0.318398	2.719118	-0.937460	0.165333
H	-1.983616	-0.529735	1.272802	-2.041703	-1.158798	0.565315	-2.123587	-0.537201	0.938962	1.472132	0.173760	-1.127978
C	-0.101996	-2.254353	0.229623	0.286770	-2.402018	-0.240903	-0.218849	-2.205622	-0.125132	-0.093289	-1.942295	1.185022
C	-1.230674	-1.143215	-1.403130	-0.770661	-1.242187	-1.893684	-1.174165	-0.887447	-1.717202	0.765466	-0.107718	2.238807
O	-1.013932	-2.396116	-0.736720	-0.441911	-2.533129	-1.352928	-1.061544	-2.209460	-1.162945	0.567075	-1.531098	2.272103
O	0.231624	-3.188250	0.930060	0.647682	-3.367819	0.400243	0.027577	-3.218950	0.496371	-0.327181	-3.119686	0.998558
C	-4.130531	-0.501382	-0.086769	-4.377242	-0.420114	-0.093084	-4.204691	-0.237314	-0.518151	3.801821	-1.084595	-0.883017
O	-5.112774	-0.273813	-0.961384	-5.456768	0.340226	-0.287750	-4.572189	-0.778814	0.645310	4.901618	-1.643179	-0.374403
O	-4.039984	-1.514724	0.578437	-4.411192	-1.523599	0.415309	-4.652541	-0.583803	-1.594787	3.681380	-0.772122	-2.051877
C	-6.113239	-1.301702	-1.074169	-6.712088	-0.223349	0.131483	-5.531367	-1.848246	0.578063	5.971151	-1.895956	-1.303116
C	-2.127532	1.811251	2.701748	-2.778273	0.903690	2.298504	-2.342801	1.628080	2.595286	3.254975	2.025217	1.254722
H	-0.292831	1.173817	1.858844	-0.746394	0.478030	1.881630	-0.455347	1.026256	1.849916	3.411739	1.514216	-0.805623
H	3.181713	3.293152	-1.269713	2.970468	3.636244	-0.771564	3.356134	3.332863	-0.782910	-3.266181	3.372934	-1.129389
H	4.826258	2.725919	-1.602420	4.689924	3.277724	-0.997960	4.998538	2.730556	-1.059590	-4.976390	2.943913	-0.960905
H	3.505038	2.327321	-2.707281	3.518416	2.858268	-2.254340	3.747119	2.503798	-2.287575	-3.987931	3.246917	0.472802
H	5.529709	0.821879	-0.450054	5.493739	1.367239	0.072971	5.545943	0.695609	-0.057264	-5.513038	0.676639	-1.107796
H	4.595449	-1.614678	-0.122184	4.852450	-1.174021	0.077092	4.512850	-1.720440	-0.050529	-4.674481	-1.519885	0.079662
H	2.652998	-0.215488	1.725123	2.548603	-0.240452	1.794921	2.472931	-0.444008	1.779573	-2.280446	-1.116206	-1.724033
H	1.914038	-2.553377	1.614100	2.143547	-2.615605	1.359654	1.673028	-2.724708	1.368968	-1.736429	-3.030785	-0.274470
H	5.041416	-1.515401	2.109887	5.029619	-1.259154	2.344945	4.784524	-1.863419	2.206062	-4.580115	-2.598078	-1.928571
H	1.291490	2.165688	-2.157182	1.283244	2.434954	-1.907353	1.495381	2.387078	-1.906906	-1.730727	2.970569	0.644240
H	1.194208	0.479377	-2.604137	1.435428	0.823568	-2.569851	1.380999	0.764184	-2.544430	-1.867920	1.739164	1.875775
H	1.370759	-1.661480	-2.143950	1.912955	-1.324160	-2.346442	1.463285	-1.424584	-2.310860	-2.000819	-0.347614	2.521800
H	3.078872	-1.335346	-1.924737	3.526741	-0.857319	-1.853065	3.156188	-1.192355	-1.922331	-3.593668	-0.262099	1.792463
H	2.310175	-2.650364	-1.031222	2.815295	-2.349638	-1.234684	2.274875	-2.562044	-1.239951	-2.742131	-1.806749	1.873436
H	-3.096014	1.123529	-1.006368	-3.088327	-0.040388	-1.679404	-2.984016	1.306995	-1.291636	2.149972	-1.869690	0.096939
H	-3.702207	1.418489	0.594517	-3.280261	1.328968	-0.629674	-3.672121	1.622060	0.286013	3.180422	-0.928006	1.153203
H	-2.288129	-1.082436	-1.650249	-1.787506	-1.314122	-2.269465	-2.204075	-0.755599	-2.041758	1.772187	0.087018	2.604229
H	-0.669424	-1.150746	-2.340139	-0.110195	-1.039605	-2.738557	-0.531416	-0.827308	-2.598017	0.054708	0.349387	2.931387
H	-6.816330	-0.940797	-1.819917	-7.460633	0.527811	-0.105661	-5.690545	-2.159803	1.606781	6.763593	-2.351275	-0.715393

H	-5.657138	-2.236436	-1.400338	-6.911962	-1.146673	-0.412389	-6.462739	-1.491514	0.138451	5.637415	-2.576545	-2.086455
H	-6.613688	-1.447623	-0.116868	-6.695921	-0.420660	1.203453	-5.133316	-2.672907	-0.013344	6.313508	-0.960703	-1.746048
H	-1.601638	2.516548	3.345600	-2.495400	1.513778	3.156233	-1.868961	2.255892	3.350141	3.845179	2.929638	1.096307
H	-2.322451	0.901259	3.273312	-3.039017	-0.095225	2.653935	-2.593443	0.668110	3.051731	3.933052	1.247544	1.611999
H	-3.083711	2.263208	2.432214	-3.664878	1.357938	1.849512	-3.269758	2.118565	2.292947	2.534567	2.236910	2.046145
Conformer 5				Conformer 6			Conformer 7			Conformer 8		
Gibbs free												
energy	-1418.247939			-1418.247827			-1418.247508			-1418.247052		
(hartrees)												
ΔG												
(kcal/mol)	1.062			1.132			1.332			1.618		
Population	5.01%			4.45%			3.18%			1.96%		
Proportion												
Element	X	Y	Z	X	Y	Z	X	Y	Z	X	Y	Z
C	-1.907949	0.318922	0.313160	-1.704773	-1.138905	0.689068	1.877224	0.089220	0.037033	2.060762	0.731030	-0.419798
C	-1.458333	1.363002	1.344862	-1.675268	-0.032638	1.760420	2.760211	1.352472	0.040714	2.686878	2.136573	-0.520372
C	-1.018337	2.625746	0.639606	-1.891706	1.346828	1.183122	1.955048	2.473467	-0.578146	1.617957	3.091594	-1.000388
O	-1.128254	3.740795	1.106152	-2.351015	2.278603	1.810569	2.411816	3.317011	-1.319455	1.806958	3.992452	-1.790034
O	-0.444529	2.501720	-0.567760	-1.517972	1.567476	-0.086391	0.632636	2.462198	-0.332222	0.368691	2.853961	-0.562840
C	-0.261620	1.278254	-1.331780	-0.881827	0.619012	-0.982575	0.144431	1.752661	0.831511	0.193517	2.077666	0.646047
C	-0.720989	-0.010048	-0.630994	-0.661504	-0.796487	-0.416912	0.565365	0.262431	0.863205	0.856706	0.679615	0.578605
C	0.356205	-0.813449	0.158595	0.751899	-1.123218	0.160926	-0.477017	-0.783206	0.363519	-0.067895	-0.520250	0.206441
C	1.861097	-0.651408	-0.254729	1.980714	-0.278377	-0.319746	-1.993406	-0.383865	0.331276	-1.616891	-0.379957	0.411751
C	2.079847	0.850876	-0.563079	1.494195	1.189127	-0.414570	-2.050539	1.079549	-0.173143	-1.989994	1.055530	-0.032429
C	3.547571	1.231111	-0.684352	2.629118	2.190357	-0.563446	-3.447113	1.526409	-0.575772	-3.485727	1.264740	-0.208877
C	3.885970	2.507904	-1.406506	2.294402	3.556669	-1.099475	-3.709934	3.006038	-0.670047	-4.000047	2.679861	-0.214589
C	4.496220	0.500929	-0.092171	3.863788	1.895108	-0.148312	-4.383114	0.637505	-0.918288	-4.302663	0.233528	-0.439167
C	4.237023	-0.777455	0.640541	4.270757	0.561998	0.395767	-4.193557	-0.844634	-0.853093	-3.862355	-1.195927	-0.451360
C	2.760197	-0.985223	0.961922	3.077100	-0.309456	0.774012	-2.726751	-1.244371	-0.727987	-2.347847	-1.342604	-0.557507
O	2.681579	-2.321504	1.433133	3.635297	-1.586133	1.043780	-2.758797	-2.640332	-0.474169	-2.108335	-2.726183	-0.351383
O	5.008765	-0.772094	1.841089	5.105970	0.776745	1.533128	-4.764167	-1.423170	-2.026456	-4.500142	-1.854048	-1.545591
C	1.203358	1.277665	-1.741258	0.389575	1.304402	-1.464209	-1.354343	1.996556	0.831723	-1.306354	2.068934	0.884022
C	2.242978	-1.552850	-1.443975	2.563851	-0.790934	-1.650111	-2.670065	-0.557803	1.704429	-2.044542	-0.674903	1.862050
H	1.719855	1.420090	0.308474	1.028108	1.443247	0.550669	-1.457687	1.131340	-1.099562	-1.561589	1.210854	-1.034712
H	0.295496	-0.599643	1.226394	0.741315	-1.069728	1.251176	-0.212837	-1.111100	-0.645243	0.093007	-0.796541	-0.837526
H	-0.884255	1.432118	-2.217036	-1.584694	0.545362	-1.814536	0.578730	2.253356	1.700797	0.667340	2.647846	1.449209
C	-3.180044	0.813028	-0.429974	-3.127684	-1.514040	0.211102	2.681175	-1.181798	0.370837	3.158824	-0.327314	-0.226650
H	-2.159402	-0.594323	0.859985	-1.359209	-2.048599	1.191570	1.555181	-0.023774	-1.003022	1.635768	0.541573	-1.410432
C	-0.137760	-2.239064	-0.021491	0.881344	-2.597374	-0.193778	-0.220289	-1.950863	1.301826	0.510810	-1.632903	1.064816
C	-1.134943	-1.050784	-1.691296	-0.719924	-1.786901	-1.593746	0.721223	-0.149531	2.340517	1.284173	0.296705	2.007937
O	-0.952549	-2.336190	-1.074392	0.036618	-2.935625	-1.173036	0.432139	-1.556150	2.399819	1.251798	-1.139500	2.063391
O	0.130860	-3.203683	0.665836	1.624605	-3.412470	0.313713	-0.528958	-3.113974	1.136515	0.370278	-2.830997	0.920934
C	-4.407093	-0.016566	-0.134719	-3.840994	-0.470707	-0.613680	3.910372	-1.312028	-0.500141	2.844454	-1.675723	-0.841424

O	-4.193722	-1.310083	-0.399432	-4.427697	0.450700	0.154176	3.587694	-1.418842	-1.792277	3.467269	-2.662366	-0.197531
O	-5.461933	0.423182	0.277213	-3.865358	-0.448252	-1.830548	5.053423	-1.312667	-0.086743	2.142837	-1.845004	-1.821004
C	-5.290627	-2.206264	-0.153083	-5.029054	1.565166	-0.527482	4.684072	-1.511031	-2.718474	3.251274	-3.988494	-0.711751
C	-2.489402	1.635385	2.438200	-2.590065	-0.284514	2.959009	3.410346	1.763452	1.370327	3.433194	2.666807	0.713458
H	-0.555885	1.000887	1.847299	-0.652667	0.008072	2.153410	3.574201	1.192706	-0.670729	3.408720	2.108331	-1.339750
H	3.287064	3.342616	-1.027614	1.442443	3.988851	-0.564288	-2.933013	3.504834	-1.258717	-3.414406	3.306085	-0.895677
H	4.940286	2.759046	-1.279007	3.143138	4.234499	-0.994056	-4.674040	3.200234	-1.143068	-5.043599	2.713408	-0.532283
H	3.685181	2.426735	-2.479054	2.023677	3.516209	-2.158841	-3.718414	3.475972	0.318044	-3.935001	3.134417	0.778609
H	5.538081	0.809122	-0.145002	4.656473	2.636935	-0.216270	-5.363458	0.973327	-1.249153	-5.363625	0.401582	-0.610897
H	4.565294	-1.624185	0.020563	4.851991	0.020995	-0.364818	-4.724495	-1.242385	0.023864	-4.181069	-1.684179	0.481012
H	2.494910	-0.290213	1.773251	2.641657	0.106294	1.695511	-2.246330	-1.056011	-1.700025	-2.057071	-1.066053	-1.582136
H	1.755534	-2.611704	1.504697	2.938465	-2.260623	1.123548	-1.887557	-2.962168	-0.183274	-1.161619	-2.897008	-0.203815
H	4.841720	-1.618241	2.280552	5.372038	-0.098493	1.849589	-4.637953	-2.380014	-1.951004	-4.202260	-2.774923	-1.524007
H	1.434440	2.291812	-2.067020	0.122745	2.343944	-1.654629	-1.491988	3.048249	0.580555	-1.651172	3.084792	0.690773
H	1.352929	0.631532	-2.609348	0.703339	0.886544	-2.423578	-1.756121	1.865364	1.838409	-1.518976	1.866504	1.935881
H	1.509860	-1.535319	-2.250821	1.801834	-1.017301	-2.396275	-2.061057	-0.192271	2.532674	-1.387127	-0.219328	2.604009
H	3.195994	-1.241047	-1.876155	3.230163	-0.048430	-2.093959	-3.617520	-0.015981	1.743298	-3.051255	-0.298870	2.056617
H	2.346982	-2.589853	-1.116221	3.141837	-1.702964	-1.483628	-2.879941	-1.613224	1.893287	-2.048001	-1.751961	2.045268
H	-3.048673	0.800187	-1.514580	-3.729091	-1.732410	1.094294	2.072506	-2.071877	0.192069	3.460553	-0.469157	0.810693
H	-3.426417	1.843098	-0.173699	-3.088960	-2.430105	-0.376263	3.019656	-1.206248	1.406011	4.057979	0.010618	-0.753294
H	-2.179062	-0.994585	-1.989357	-1.719983	-2.122156	-1.853098	1.722601	-0.006657	2.742733	2.292687	0.610288	2.272935
H	-0.514218	-1.006546	-2.588453	-0.256997	-1.380412	-2.495406	0.013851	0.369902	2.991104	0.596996	0.680951	2.765234
H	-4.921083	-3.194585	-0.412610	-5.831912	1.220329	-1.178936	4.227718	-1.580626	-3.702117	3.825854	-4.646671	-0.065525
H	-5.576589	-2.169574	0.898119	-5.420995	2.206663	0.256963	5.309118	-0.620380	-2.650241	2.190372	-4.234851	-0.663122
H	-6.142253	-1.940008	-0.779095	-4.274068	2.093720	-1.110709	5.279856	-2.399587	-2.509980	3.605506	-4.057782	-1.740363
H	-2.086127	2.324753	3.179970	-2.354054	0.409532	3.765612	4.068622	2.618021	1.204131	3.901011	3.623800	0.475160
H	-2.742252	0.697993	2.938829	-2.442642	-1.302322	3.328201	4.020705	0.944806	1.756979	4.225067	1.971231	0.999157
H	-3.407939	2.070714	2.039430	-3.641262	-0.151344	2.698857	2.690020	2.046646	2.139224	2.789481	2.821509	1.580607

Conformer 9

Gibbs free

energy -1418.246487

(hartrees)

ΔG

1.973

(kcal/mol)

Population

1.08%

Proportion

Element	X	Y	Z
C	-1.606384	-0.031135	-0.080191
C	-2.790821	-0.973614	-0.411080
C	-2.397394	-2.423740	-0.640077
O	-3.157337	-3.217668	-1.155850
O	-1.218603	-2.883799	-0.187796
C	-0.122170	-2.009736	0.146683
C	-0.573065	-0.720303	0.843191
C	0.695259	0.113433	1.199869
C	1.983235	-0.110556	0.336875

C	1.494197	-0.440576	-1.089922
C	2.584837	-0.348636	-2.144744
C	2.299797	-0.985350	-3.478857
C	3.704465	0.347102	-1.923763
C	4.018011	1.032968	-0.628055
C	2.766067	1.214029	0.225863
O	3.158703	1.805839	1.457726
O	4.600007	2.301983	-0.921441
C	0.731900	-1.775707	-1.110613
C	2.897010	-1.230669	0.884634
H	0.784032	0.348579	-1.367405
H	0.453975	1.178670	1.148766
H	0.437069	-2.610970	0.863366
C	-2.076406	1.347636	0.392628
H	-1.108794	0.144697	-1.035133
C	0.914273	-0.168574	2.674295
C	-1.144816	-1.046413	2.241598
O	-0.067820	-0.908494	3.184094
O	1.848276	0.203019	3.358772
C	-2.922633	2.051414	-0.646214
O	-3.802567	2.880802	-0.081523
O	-2.801218	1.911357	-1.848102
C	-4.618029	3.650225	-0.983263
C	-3.975359	-0.970619	0.576449
H	-3.192898	-0.648918	-1.373488
H	1.346622	-0.625751	-3.880597
H	3.084498	-0.752370	-4.200490
H	2.223490	-2.073604	-3.400017
H	4.455600	0.438231	-2.705371
H	4.746794	0.440242	-0.056852
H	2.122954	1.938258	-0.293401
H	2.859777	1.263838	2.210917
H	4.792667	2.718138	-0.068669
H	0.081254	-1.806430	-1.988138
H	1.424953	-2.614552	-1.208317
H	2.339348	-2.086262	1.267655
H	3.555505	-1.603849	0.098195
H	3.524866	-0.872804	1.702247
H	-1.219365	2.010102	0.543989
H	-2.617829	1.325404	1.338338
H	-1.923876	-0.349870	2.550361
H	-1.520579	-2.065292	2.329384
H	-5.259045	4.256122	-0.348693

H	-3.991402	4.284907	-1.609966
H	-5.216289	2.987021	-1.608029
H	-4.769713	-1.605710	0.183370
H	-4.384526	0.034313	0.690557
H	-3.708245	-1.345339	1.565942

Figure S12: SciFinder search results for compound **1** (similarity >95%).

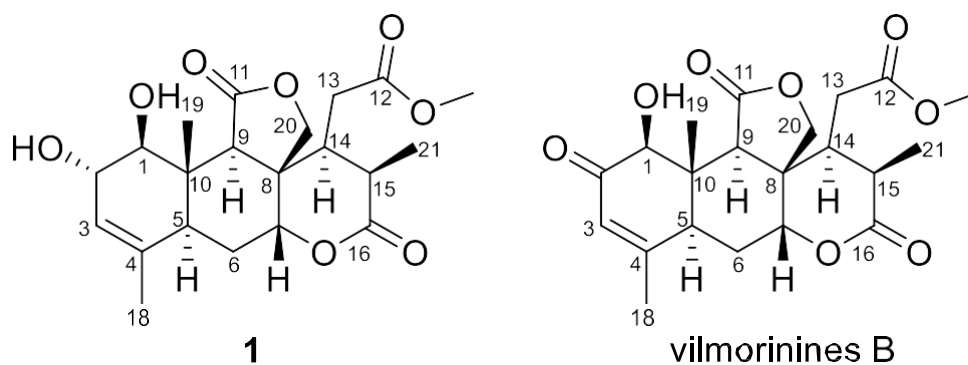


Figure S13: Structure of compound **1** and vilmorinine B.

Table S3: Comparison of NMR data between compound **1** and vilmorinine B.

pos	1^a		vilmorinine B^b [1]	
	δ_C , type	δ_H (J in Hz)	δ_C , type	δ_H (J in Hz)
1	81.9, CH	3.65, overlap	84.65, CH	4.73, s
2	70.2, CH	3.76, m	197.49, C	
3	126.6, CH	5.36, td (2.8, 1.5)	126.88, CH	6.15, br, s
4	132.7, C		160.30, C	
5	37.9, CH	2.09, m	40.87, CH	3.01, br, d (12.5) 2.35, ddd (15.6, 2.4, 2.4)
6	25.0, CH ₂	1.89, m	25.97, CH ₂	2.09, ddd (15.6, 12.5, 2.4)
7	75.1, CH	4.62, t (2.9)	75.64, CH	4.90, br, s
8	44.7, C		45.73, C	
9	53.4, CH	3.04, s	54.25, CH	3.62, s
10	40.9, C		44.99, C	
11	178.6, C		172.72, C	
12	172.6, C		175.51, C	
13	30.5, CH ₂	2.78, m 2.17, m	31.34, CH ₂	2.99, dd (17.1. 4.5) 2.67, dd (17.1. 5.6) 2.81, ddd (5.6. 4.5, 4.3) 3.42, dq (6.5.
14	39.8, CH	2.14, overlap	40.57, CH	
15	35.6, CH	3.10, dd (6.9,	36.90, CH 3.7)	
16	172.0, C			172.23, C
18	20.9, CH ₃		1.61, s	22.15, CH ₃
19	10.1, CH ₃		0.84, s	10.70, CH ₃
20	70.1, CH ₂		4.26, d (7.2) 4.09, d (10.9)	69.41, CH ₂
21	13.3, CH ₃		1.06, d (6.7)	13.70, CH ₃
OCH ₃	52.0, CH ₃		3.64, s	54.25, CH ₃

^a: Measurements were performed on dimethyl sulfoxide-*d*₆, at 600 MHz.

^b: Measurements were performed on pyridine-*d*₅, at 400 MHz.

Reference:

- [1] K. Takeya, H. Kobata, A. Ozeki, H. Morita, H. Itokawa (1998). Quassinoids from *Ailanthus vilmoriniana*, *Phytochemistry*. 1998, 48 (3): 565–568.