Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Discovery of New Polycyclic Polyprenylated Acylphloroglucinols with Diverse Architectures as Potent Cyclooxygenase-2 Inhibitors

Shuangshuang Xie,[a,‡] Changxing Qi,[a,‡] Yulin Duan,[a] Qianqian Xu,[a] Yaping Liu,[a] Yingying Huang,[a] Xu Yin,[b] Weiguang Sun,[a,*] Yuan Zhou,[a,*] and Yonghui Zhang[a,*]

[a]Hubei Key Laboratory of Natural Medicinal Chemistry and Resource Evaluation, School of Pharmacy, Tongji Medical College, Huazhong University of Science and Technology, Wuhan 430030, People's Republic of China

[b]Department of Natural Medicines, School of Pharmaceutical Sciences, Peking University Health Science Center, Beijing, 100191, People's Republic of China

Tel.: (86) 27-83692892

E-mail: zhangyh@mails.tjmu.edu.cn (Y. Zhang),
yuan2273@163.com (Y. Zhou),
weiguang_s@hust.edu.cn (W. Sun)

Contents of Supporting Information

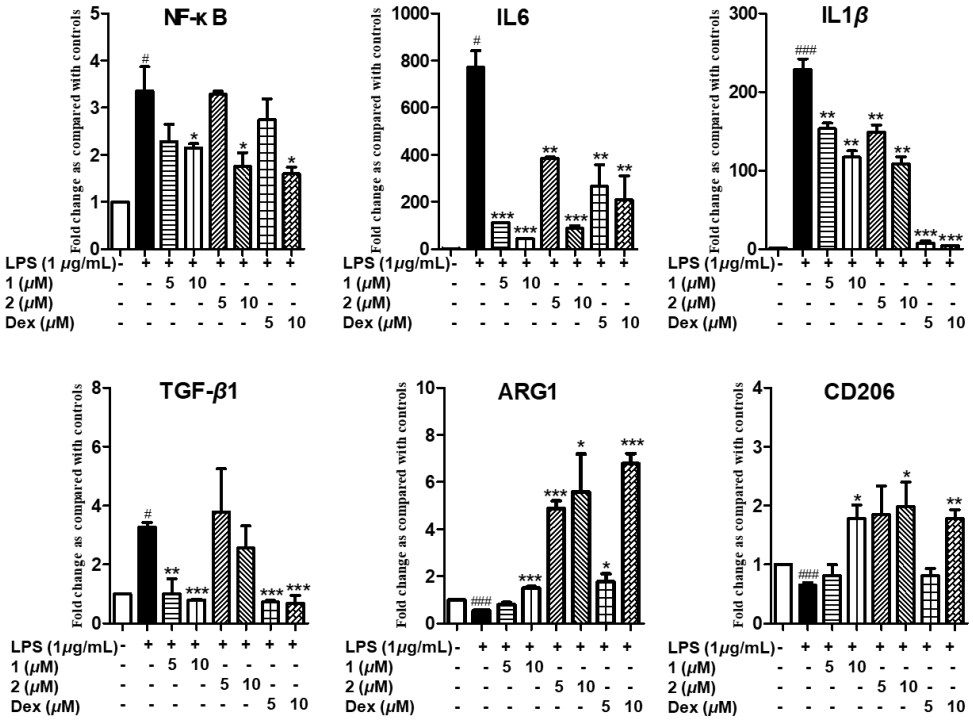


Figure S1. Effect of **1** and **2** on the transcription level of proinflammatory cytokines NF-κB, IL6, IL1β, TGF-β1, and anti-inflammatory M2 macrophage markers ARG1, CD206 of RAW264.7. Dexamethasone (Dex) was used as positive control. Mean ± SEM of four replicates are shown; $^{\#}$indicates $0.01 < p < 0.05$, $^{\#\#}$indicates $0.001 < p \leq 0.01$, and $^{\#\#\#}$indicates $p < 0.001$, compared to control; *indicates $0.01 < p < 0.05$, **indicates $0.001 < p \leq 0.01$, and *** indicates $p < 0.001$, compared to model.

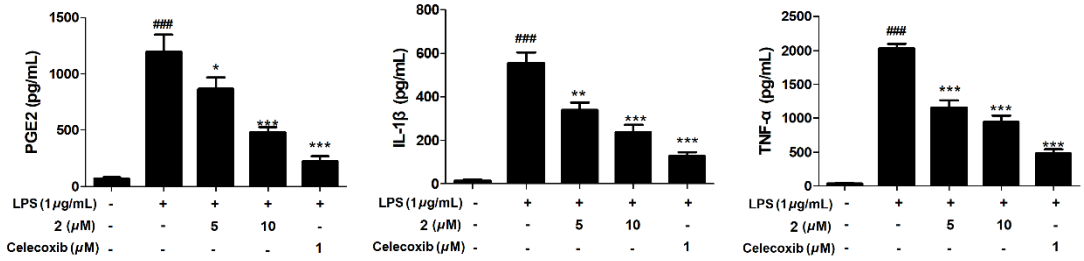


Figure S2. Effect of **2** on the PGE2, IL-1β, and TNF-α production in RAW264.7 cells stimulated with LPS; Celecoxib was used as positive control. $^{\#\#\#}$indicates $p < 0.001$, compared with control group; *indicates $p < 0.05$, **indicates $p < 0.01$, and ***indicates $p < 0.001$, compared with model group.

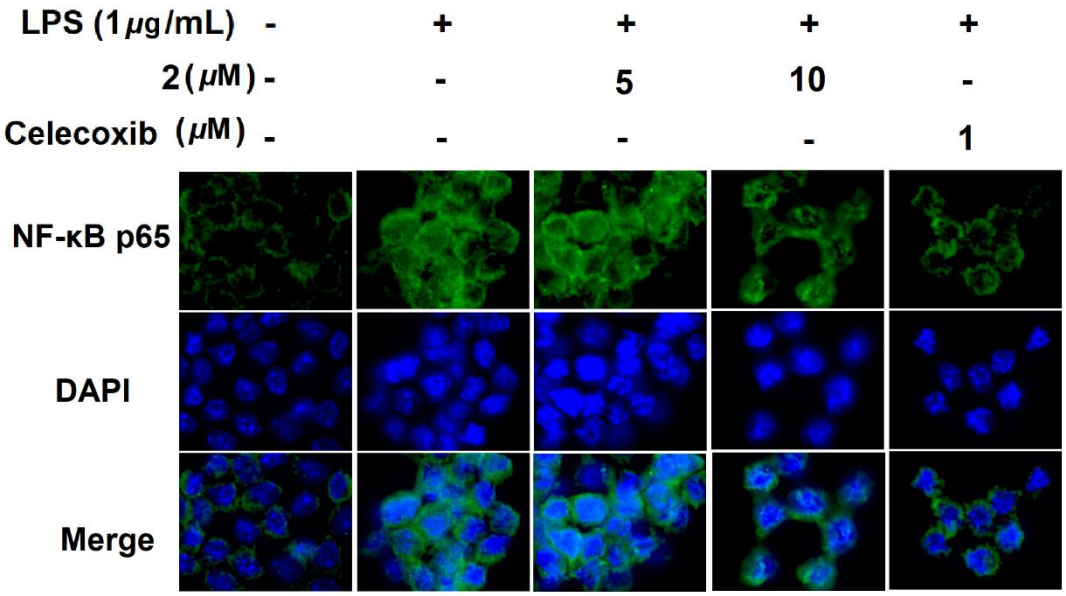
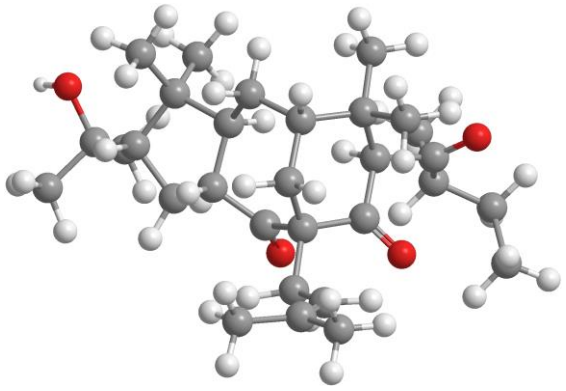


Figure S3. Effect of **2** (5 and 10 μM) or Celecoxib (1 μM) on the NF-κB activation level in RAW264.7 cells stimulated with LPS.

Table S1. Important thermodynamic parameters (a.u.) and Boltzmann distribution of the optimized compound **2** at B3LYP/6-31G(d) level in methanol.

Conformation	**Internal Energy**	**%**
1	-1472.63	20.62%
2	-1472.63	18.94%
3	-1472.63	17.22%
4	-1472.63	12.27%
5	-1472.63	7.62%
6	-1472.63	7.46%
7	-1472.63	5.09%
8	-1472.63	4.35%
9	-1472.63	2.23%
10	-1472.63	1.02%



Conformation 1

Table S2. Optimized coordinates of compound **2** at B3LYP/6-31G(d) level in methanol.

Conformation 1							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-2.262	0.962	0.283	H	-1.476	-0.986	0.004
C	0.124	1.011	-0.328	H	1.834	1.113	0.952
C	0.287	3.9	0.649	H	-0.831	-0.166	3.644
C	1.133	4.468	-0.229	H	0.472	-1.501	0.222
C	-3.579	-1.118	-0.134	H	4.001	-0.179	0.54
C	2.453	0.135	-0.88	H	3.272	4.78	-0.15
C	0.586	-0.909	2.288	H	2.329	6.264	-0.09
C	-0.67	1.325	2.143	H	2.424	5.224	1.347
C	-2.323	-0.546	0.545	H	0.854	5.46	-2.123
C	1.415	0.429	0.203	H	1.878	4.033	-2.201
C	-0.754	-0.164	2.548	H	0.125	3.842	-2.067
C	1.175	-0.963	0.871	H	-3.069	-0.429	3.981
C	3.446	-0.803	-0.175	H	-4.203	-0.702	2.642
C	-0.919	1.62	0.642	H	-3.36	0.841	2.785

C	-2.098	-0.834	2.073	H	-1.806	-2.575	3.35
C	2.558	-1.747	0.736	H	-1.33	-2.858	1.667
C	2.351	5.22	0.255	H	-3.044	-2.797	2.103
C	0.974	4.441	-1.73	H	3.159	-3.728	0.024
C	-3.254	-0.241	2.916	H	1.733	-3.077	-0.813
C	-2.064	-2.357	2.307	H	1.582	-3.682	0.837
C	2.247	-3.139	0.153	H	4.253	-2.422	1.895
C	3.283	-1.953	2.082	H	2.715	-2.601	2.759
C	-4.85	-0.703	-3.813	H	3.468	-1.004	2.6
C	-3.127	-2.652	-2.032	H	-4.693	-1.688	-4.265
C	5.55	-0.277	-1.468	H	-5.807	-0.319	-4.187
C	4.037	-2.04	-2.403	H	-4.06	-0.036	-4.178
C	-0.987	3.15	0.353	H	-3.906	-3.353	-1.713
C	-4.861	-0.765	-2.282	H	-2.185	-2.95	-1.556
C	-3.519	-1.204	-1.662	H	-2.993	-2.751	-3.113
C	4.548	-1.391	-1.105	H	6.367	-0.688	-2.075
O	-3.223	1.589	-0.126	H	5.984	0.158	-0.562
O	-0.15	0.986	-1.521	H	5.08	0.524	-2.049
O	-4.554	-1.522	0.478	H	4.889	-2.444	-2.965
O	5.246	-2.38	-0.317	H	3.345	-2.861	-2.209
H	0.528	4.007	1.707	H	3.539	-1.311	-3.05
H	1.958	-0.359	-1.723	H	-1.294	3.277	-0.687
H	2.919	1.048	-1.266	H	-1.8	3.556	0.969
H	1.318	-0.417	2.941	H	-5.11	0.226	-1.883
H	0.497	-1.932	2.669	H	-5.648	-1.447	-1.937
H	-1.414	1.899	2.708	H	-2.726	-0.534	-2.017
H	0.302	1.73	2.443	H	5.98	-2.71	-0.861

Conformation 2

Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-2.276	1.236	-0.01	H	-1.625	-0.778	-0.053
C	0.152	1.04	-0.442	H	1.771	1.127	0.949
C	0.504	3.968	0.294	H	-1.149	0.29	3.532
C	1.432	4.407	-0.573	H	0.274	-1.445	0.335
C	-3.751	-0.817	-0.256	H	3.849	-0.319	0.817
C	2.437	-0.049	-0.744	H	3.586	4.546	-0.409
C	0.283	-0.679	2.35	H	2.771	6.103	-0.481
C	-0.773	1.626	1.928	H	2.714	5.15	1.017
C	-2.476	-0.235	0.373	H	1.328	5.298	-2.533
C	1.352	0.411	0.229	H	2.223	3.786	-2.477
C	-1.003	0.189	2.448	H	0.455	3.757	-2.42
C	0.965	-0.899	0.99	H	-3.408	0.202	3.747

C	3.312	-0.973	0.116	H	-4.487	-0.065	2.363
C	-0.9	1.807	0.396	H	-3.522	1.404	2.453
C	-2.366	-0.411	1.941	H	-2.305	-2.067	3.356
C	2.297	-1.777	1.03	H	-1.75	-2.518	1.735
C	2.688	5.085	-0.075	H	-3.477	-2.288	2.054
C	1.338	4.299	-2.076	H	2.81	-3.847	0.534
C	-3.515	0.33	2.664	H	1.501	-3.182	-0.467
C	-2.475	-1.909	2.285	H	1.184	-3.631	1.21
C	1.935	-3.193	0.539	H	3.854	-2.452	2.368
C	2.907	-1.91	2.441	H	2.249	-2.461	3.122
C	-2.669	-2.078	-3.78	H	3.119	-0.933	2.892
C	-4.839	-2.67	-1.584	H	-3.509	-2.687	-4.129
C	5.534	-0.685	-1.047	H	-2.294	-1.51	-4.638
C	3.989	-2.444	-1.939	H	-1.872	-2.758	-3.455
C	-0.815	3.307	-0.017	H	-5.65	-2.033	-1.952
C	-3.078	-1.127	-2.649	H	-5.176	-3.131	-0.649
C	-3.561	-1.855	-1.363	H	-4.671	-3.47	-2.311
C	4.442	-1.705	-0.667	H	6.369	-1.194	-1.545
O	-3.128	1.905	-0.561	H	5.922	-0.188	-0.152
O	-0.031	0.942	-1.649	H	5.159	0.08	-1.735
O	-4.861	-0.446	0.085	H	4.856	-2.935	-2.4
O	5.017	-2.652	0.259	H	3.244	-3.211	-1.725
H	0.706	4.124	1.354	H	3.575	-1.754	-2.681
H	1.968	-0.59	-1.572	H	-1.055	3.371	-1.08
H	2.99	0.792	-1.175	H	-1.62	3.831	0.515
H	1.007	-0.191	3.014	H	-2.225	-0.481	-2.41
H	0.08	-1.655	2.804	H	-3.883	-0.463	-2.993
H	-1.502	2.301	2.391	H	-2.75	-2.528	-1.045
H	0.207	1.98	2.264	H	5.762	-3.079	-0.197

Conformation 3

Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	2.102	0.09	-0.376	H	0.594	1.457	0.201
C	-0.135	-0.666	-1.029	H	-1.486	-1.968	0.006
C	2.991	-2.95	-0.808	H	0.832	-0.932	3.099
C	3.167	-4.238	-0.468	H	-1.367	1.024	0.52
C	2.435	2.503	0.207	H	-4.012	-1.635	0.071
C	-2.672	-0.666	-1.257	H	4.494	-5.165	0.968
C	-0.932	-0.335	2.136	H	4.879	-5.54	-0.707
C	1.039	-1.612	1.099	H	5.278	-3.938	-0.05
C	1.619	1.237	0.521	H	2.365	-6.115	-1.161
C	-1.465	-0.932	-0.358	H	1.999	-5.755	0.52

C	0.612	-0.519	2.105	H	1.11	-4.929	-0.769
C	-1.694	0.03	0.852	H	2.85	0.014	3.583
C	-3.845	-0.603	-0.267	H	3.598	1.24	2.537
C	1.183	-1.142	-0.369	H	3.411	-0.417	1.963
C	1.533	0.754	2.014	H	0.818	1.543	3.915
C	-3.278	0.142	1.012	H	0.022	2.278	2.514
C	4.529	-4.737	-0.043	H	1.683	2.729	2.927
C	2.094	-5.301	-0.475	H	-4.708	1.783	1.227
C	2.934	0.374	2.551	H	-3.277	2.213	0.266
C	0.977	1.894	2.889	H	-3.144	2.06	2.018
C	-3.63	1.637	1.128	H	-4.913	-0.524	2.257
C	-3.821	-0.571	2.268	H	-3.468	-0.1	3.192
C	4.176	3.127	-2.39	H	-3.535	-1.629	2.297
C	0.877	4.267	-0.592	H	3.71	2.534	-3.185
C	-5.725	-1.343	-1.781	H	4.977	3.723	-2.842
C	-5.167	1.098	-1.752	H	4.629	2.428	-1.68
C	1.73	-2.282	-1.291	H	1.276	5.006	0.112
C	3.149	4.034	-1.704	H	0.035	3.759	-0.109
C	1.987	3.283	-1.033	H	0.487	4.801	-1.465
C	-5.204	-0.187	-0.905	H	-6.71	-1.091	-2.192
O	3.137	0.153	-1.014	H	-5.827	-2.258	-1.188
O	-0.06	-0.055	-2.088	H	-5.059	-1.548	-2.626
O	3.351	2.9	0.908	H	-6.174	1.309	-2.133
O	-6.121	-0.01	0.197	H	-4.838	1.964	-1.177
H	3.857	-2.293	-0.756	H	-4.51	0.987	-2.621
H	-2.526	0.289	-1.773	H	0.929	-3.016	-1.424
H	-2.795	-1.435	-2.026	H	1.91	-1.83	-2.273
H	-1.323	-1.293	2.498	H	3.645	4.651	-0.945
H	-1.185	0.396	2.912	H	2.724	4.725	-2.443
H	2.005	-2.027	1.397	H	1.546	2.572	-1.744
H	0.337	-2.453	1.145	H	-6.99	0.193	-0.187

Conformation 4

Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-2.28	0.572	-0.295	H	-1.246	-1.229	0.127
C	0.097	0.671	-0.924	H	1.757	1.43	0.186
C	-0.078	3.704	-1.061	H	-0.82	0.891	3.219
C	0.053	4.918	-0.5	H	0.766	-1.425	0.496
C	-3.314	-1.68	0.072	H	4.076	0.378	0.187
C	2.517	-0.082	-1.171	H	2.063	5.176	-1.285
C	0.713	-0.112	2.204	H	1.119	6.677	-1.168
C	-0.787	1.756	1.283	H	1.782	5.951	0.29

C	-2.163	-0.744	0.481	H	-1.917	5.026	0.446
C	1.435	0.472	-0.247	H	-0.614	5.833	1.333
C	-0.711	0.511	2.194	H	-1.27	6.576	-0.119
C	1.359	-0.591	0.894	H	-0.957	-2.366	2.36
C	3.614	-0.542	-0.197	H	-1.521	-1.551	3.828
C	-1.029	1.464	-0.219	H	-2.681	-2.349	2.757
C	-1.957	-0.434	2.009	H	-4.08	-0.349	2.509
C	2.844	-1.164	1.04	H	-3.029	0.512	3.653
C	1.325	5.714	-0.681	H	-3.418	1.229	2.085
C	-1.001	5.61	0.329	H	3.699	-3.19	1.212
C	-1.764	-1.755	2.779	H	2.084	-3.007	1.894
C	-3.197	0.285	2.594	H	2.287	-3.096	0.142
C	2.731	-2.702	1.062	H	3.589	0.374	2.43
C	3.537	-0.718	2.345	H	3.024	-1.103	3.232
C	-5.23	-1.48	-2.461	H	4.564	-1.095	2.374
C	-2.328	-3.693	-1.005	H	-5.481	-0.8	-1.64
C	5.95	-1.597	0.076	H	-4.634	-0.914	-3.187
C	4.439	-2.504	-1.728	H	-6.163	-1.778	-2.952
C	-1.267	2.78	-1.022	H	-1.362	-3.498	-0.527
C	-4.468	-2.71	-1.958	H	-2.897	-4.371	-0.359
C	-3.129	-2.395	-1.27	H	-2.132	-4.206	-1.953
C	4.806	-1.265	-0.894	H	6.255	-0.705	0.633
O	-3.302	0.905	-0.866	H	5.682	-2.381	0.791
O	-0.142	0.195	-2.027	H	6.82	-1.956	-0.488
O	-4.29	-1.89	0.772	H	5.319	-2.828	-2.298
O	5.288	-0.243	-1.805	H	3.643	-2.281	-2.443
H	0.768	3.334	-1.643	H	4.126	-3.347	-1.109
H	2.882	0.653	-1.892	H	-1.535	2.487	-2.044
H	2.101	-0.921	-1.74	H	-2.148	3.268	-0.597
H	1.358	0.664	2.633	H	-4.263	-3.38	-2.803
H	0.728	-0.938	2.923	H	-5.093	-3.274	-1.255
H	-1.607	2.401	1.618	H	-2.522	-1.751	-1.921
H	0.121	2.359	1.395	H	6.039	-0.627	-2.288

Conformation 5

Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-2.332	0.77	-0.466	H	-1.422	-1.054	0.106
C	0.09	0.708	-0.958	H	1.728	1.432	0.206
C	0.111	3.712	-1.266	H	-1.029	1.192	3.112
C	0.308	4.942	-0.762	H	0.559	-1.343	0.604
C	-3.525	-1.412	0.051	H	3.985	0.251	0.388
C	2.473	-0.187	-1.03	H	2.365	5.008	-1.46

C	0.5	0.064	2.235	H	1.534	6.578	-1.469
C	-0.857	1.949	1.139	H	2.073	5.888	0.056
C	-2.328	-0.507	0.383	H	-1.694	5.256	0.063
C	1.376	0.472	-0.195	H	-0.377	5.989	0.992
C	-0.887	0.753	2.115	H	-0.886	6.719	-0.525
C	1.18	-0.524	0.99	H	-1.276	-2.107	2.368
C	3.488	-0.658	0.023	H	-1.867	-1.22	3.784
C	-1.031	1.591	-0.357	H	-3.013	-1.998	2.688
C	-2.167	-0.141	1.914	H	-4.306	0.065	2.329
C	2.619	-1.17	1.246	H	-3.249	0.9	3.486
C	1.644	5.631	-0.922	H	-3.547	1.589	1.883
C	-0.726	5.755	-0.023	H	3.343	-3.23	1.564
C	-2.069	-1.444	2.73	H	1.71	-2.92	2.15
C	-3.392	0.652	2.428	H	1.993	-3.111	0.418
C	2.414	-2.695	1.339	H	3.376	0.396	2.599
C	3.269	-0.694	2.563	H	2.692	-1.007	3.44
C	-2.366	-3.543	-2.999	H	4.27	-1.122	2.665
C	-4.376	-3.704	-0.588	H	-1.478	-3.991	-2.536
C	5.738	-1.832	0.479	H	-3.123	-4.327	-3.101
C	4.27	-2.746	-1.357	H	-2.088	-3.219	-4.008
C	-1.143	2.877	-1.233	H	-4.619	-3.901	0.461
C	-2.875	-2.352	-2.18	H	-5.278	-3.315	-1.072
C	-3.22	-2.706	-0.705	H	-4.115	-4.657	-1.058
C	4.667	-1.487	-0.569	H	6.614	-2.267	-0.018
O	-3.281	1.123	-1.139	H	6.064	-0.93	1.008
O	-0.104	0.202	-2.056	H	5.387	-2.561	1.216
O	-4.668	-1.102	0.346	H	5.16	-3.159	-1.848
O	5.259	-0.546	-1.503	H	3.539	-2.514	-2.137
H	0.952	3.251	-1.787	H	3.86	-3.53	-0.717
H	2.918	0.49	-1.763	H	-1.389	2.55	-2.25
H	2.041	-1.028	-1.582	H	-2.003	3.448	-0.873
H	1.162	0.834	2.649	H	-3.771	-1.929	-2.653
H	0.439	-0.714	3.003	H	-2.113	-1.564	-2.202
H	-1.663	2.645	1.395	H	-2.315	-3.141	-0.254
H	0.071	2.516	1.273	H	6.008	-1	-1.923

Conformation 6

Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	2.122	-0.299	-0.292	H	0.785	1.237	0.292
C	-0.215	-0.814	-0.911	H	-1.596	-1.984	0.206
C	0.54	-3.716	-1.329	H	0.829	-1.192	3.191
C	0.647	-4.977	-0.876	H	-1.205	0.992	0.667

C	2.734	2.064	0.274	H	-4.716	-0.049	-0.313
C	-2.775	-0.672	-1.086	H	-1.292	-5.54	-1.681
C	-0.888	-0.424	2.264	H	-0.08	-6.839	-1.701
C	0.933	-1.878	1.187	H	-0.843	-6.383	-0.183
C	1.781	0.899	0.6	H	2.621	-4.799	0.051
C	-1.543	-0.967	-0.2	H	1.501	-5.895	0.875
C	0.629	-0.755	2.203	H	2.255	-6.391	-0.634
C	-1.627	0.035	0.997	H	0.307	2.086	2.608
C	-3.691	0.338	-0.327	H	1.052	1.288	4.004
C	1.066	-1.418	-0.288	H	2.008	2.384	2.995
C	1.664	0.428	2.098	H	3.768	0.72	2.608
C	-3.165	0.288	1.16	H	2.921	-0.442	3.65
C	-0.455	-5.979	-1.129	H	3.427	-0.908	2.021
C	1.824	-5.528	-0.109	H	-4.506	1.729	2.104
C	1.228	1.619	2.973	H	-3.071	1.333	3.061
C	3.029	-0.082	2.62	H	-2.946	2.423	1.672
C	-3.435	1.519	2.043	H	-3.698	-1.859	1.293
C	-3.866	-0.919	1.832	H	-3.531	-1.06	2.865
C	4.605	2.425	-2.281	H	-4.947	-0.745	1.861
C	1.392	3.955	-0.621	H	4.104	1.836	-3.059
C	-2.537	2.502	-1.243	H	5.465	2.926	-2.743
C	-4.465	1.449	-2.467	H	4.983	1.726	-1.529
C	1.534	-2.591	-1.205	H	0.486	3.555	-0.151
C	3.651	3.452	-1.663	H	1.849	4.667	0.076
C	2.401	2.846	-1.002	H	1.086	4.502	-1.519
C	-3.836	1.696	-1.079	H	-2.732	3.404	-1.837
O	3.176	-0.383	-0.897	H	-2.139	2.823	-0.277
O	-0.098	-0.193	-1.961	H	-1.765	1.925	-1.762
O	3.663	2.393	0.991	H	-4.699	2.412	-2.939
O	-4.789	2.46	-0.31	H	-5.397	0.883	-2.368
H	-0.369	-3.464	-1.878	H	-3.799	0.909	-3.146
H	-3.312	-1.601	-1.298	H	1.726	-2.164	-2.197
H	-2.442	-0.278	-2.047	H	2.498	-2.94	-0.825
H	-1.364	-1.348	2.616	H	3.315	4.15	-2.441
H	-1.055	0.312	3.057	H	4.182	4.05	-0.913
H	1.879	-2.362	1.454	H	1.905	2.163	-1.704
H	0.175	-2.665	1.258	H	-4.937	3.292	-0.788

Conformation 7

Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	1.494	1.669	-0.493	H	-0.476	1.402	0.234
C	0.625	-0.61	-0.92	H	0.922	-2.337	0.284

C	3.43	-1.587	-1.451	H	1.745	0.296	3.079
C	4.57	-2.168	-1.041	H	-1.34	-0.371	0.771
C	-0.133	3.507	0.151	H	-2.405	-3.94	0.058
C	-0.895	-2.681	-0.885	H	3.921	-4.137	-1.694
C	0.12	-0.782	2.308	H	5.667	-3.848	-1.848
C	2.26	-0.103	1.06	H	4.971	-4.145	-0.26
C	0.355	2.08	0.449	H	5.564	-0.376	-0.275
C	0.074	-1.763	-0.105	H	5.927	-1.868	0.605
C	1.212	0.307	2.118	H	6.645	-1.592	-0.976
C	-0.74	-1.223	1.115	H	-1.335	1.599	2.577
C	-2.184	-2.87	-0.028	H	-0.195	1.876	3.905
C	1.861	0.173	-0.411	H	-0.649	3.21	2.84
C	0.769	1.808	1.951	H	1.688	3.763	2.308
C	-1.765	-2.372	1.411	H	2.233	2.482	3.409
C	4.784	-3.653	-1.225	H	2.841	2.558	1.749
C	5.726	-1.449	-0.39	H	-3.634	-2.673	2.498
C	-0.427	2.138	2.866	H	-2.47	-1.628	3.325
C	1.954	2.708	2.373	H	-3.412	-1.012	1.958
C	-2.888	-1.89	2.345	H	-0.231	-3.967	1.529
C	-1.076	-3.574	2.106	H	-0.709	-3.312	3.103
C	-2.683	3.139	-2.773	H	-1.799	-4.389	2.228
C	-2.068	5.051	-0.352	H	-3.357	2.422	-2.29
C	-3.456	-0.783	-0.964	H	-3.197	4.105	-2.821
C	-3.675	-3.031	-2.069	H	-2.517	2.802	-3.802
C	3.044	-0.132	-1.382	H	-1.437	5.793	-0.852
C	-1.349	3.232	-2.022	H	-3.077	5.118	-0.77
C	-1.497	3.641	-0.529	H	-2.125	5.321	0.707
C	-3.457	-2.302	-0.727	H	-4.361	-0.492	-1.513
O	2.081	2.453	-1.213	H	-3.449	-0.23	-0.022
O	0.112	-0.248	-1.972	H	-2.593	-0.467	-1.559
O	0.546	4.487	0.409	H	-2.91	-2.793	-2.813
O	-4.558	-2.658	0.136	H	-4.644	-2.736	-2.492
H	2.685	-2.236	-1.916	H	-3.688	-4.116	-1.917
H	-0.416	-3.643	-1.087	H	2.737	0.21	-2.377
H	-1.112	-2.23	-1.854	H	3.885	0.498	-1.082
H	0.66	-1.663	2.677	H	-0.693	3.961	-2.516
H	-0.54	-0.477	3.127	H	-0.842	2.263	-2.091
H	3.192	0.443	1.243	H	-2.172	2.912	-0.056
H	2.517	-1.161	1.178	H	-5.371	-2.355	-0.303

Conformation 8

Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**

C	1.816	-1.553	-0.186	H	1.448	0.508	0.13
C	-0.581	-0.981	-0.452	H	-2.101	-1.123	1.029
C	-1.298	-3.915	-0.199	H	0.941	-1.082	3.516
C	-2.296	-4.079	-1.085	H	-0.338	1.332	0.715
C	3.551	0.301	-0.179	H	-4.061	1.935	0.329
C	-2.781	0.345	-0.44	H	-3.633	-4.897	0.42
C	-0.388	0.24	2.578	H	-4.443	-3.955	-0.85
C	0.343	-2.074	1.739	H	-3.855	-5.574	-1.207
C	2.227	-0.205	0.417	H	-1.276	-3.276	-2.847
C	-1.673	-0.346	0.385	H	-2.364	-4.641	-3.165
C	0.776	-0.785	2.472	H	-3.03	-3.05	-2.827
C	-1.069	0.766	1.304	H	1.851	1.887	2.173
C	-2.993	1.781	0.132	H	2.399	1.103	3.665
C	0.389	-2.002	0.192	H	3.542	1.393	2.35
C	2.19	-0.284	1.997	H	4.258	-0.956	2.255
C	-2.273	1.744	1.537	H	3.187	-1.33	3.621
C	-3.622	-4.657	-0.647	H	3.116	-2.289	2.134
C	-2.22	-3.739	-2.554	H	-2.626	3.79	2.208
C	2.508	1.108	2.574	H	-1.376	2.928	3.12
C	3.251	-1.276	2.528	H	-1.028	3.564	1.504
C	-1.795	3.086	2.118	H	-3.671	0.169	2.225
C	-3.295	1.15	2.537	H	-2.868	1.044	3.539
C	2.574	2.123	-3.481	H	-4.158	1.821	2.62
C	4.825	2.181	-1.286	H	1.865	2.839	-3.049
C	-1.197	2.948	-1.371	H	3.472	2.675	-3.776
C	-3.584	2.745	-2.134	H	2.123	1.715	-4.392
C	0.091	-3.388	-0.457	H	4.741	3.076	-1.909
C	2.888	0.994	-2.492	H	5.22	2.485	-0.311
C	3.466	1.491	-1.136	H	5.556	1.507	-1.745
C	-2.661	2.895	-0.907	H	-1.078	3.726	-2.136
O	2.556	-2.228	-0.875	H	-0.522	3.189	-0.546
O	-0.411	-0.695	-1.63	H	-0.879	1.999	-1.814
O	4.615	-0.242	0.066	H	-3.447	3.603	-2.804
O	-3.012	4.138	-0.262	H	-4.634	2.722	-1.822
H	-1.496	-4.215	0.83	H	-3.375	1.842	-2.716
H	-3.706	-0.237	-0.384	H	0.296	-3.303	-1.526
H	-2.487	0.364	-1.491	H	0.83	-4.093	-0.055
H	-1.152	-0.261	3.185	H	3.608	0.296	-2.939
H	-0.048	1.092	3.176	H	1.971	0.421	-2.315
H	0.997	-2.901	2.039	H	2.741	2.202	-0.714
H	-0.66	-2.361	2.07	H	-2.853	4.847	-0.907

Conformation 9

Atom	X	Y	Z	Atom	X	Y	Z
C	2.224	0.244	-0.734	H	1.09	-1.207	0.329
C	-0.087	0.956	-0.255	H	-1.796	0.942	-1.558
C	1.625	3.4	-0.711	H	0.452	-1.873	-3.352
C	1.001	4.562	-0.458	H	-1.041	-1.388	0.241
C	3.132	-1.675	0.582	H	-4.246	0.452	-0.676
C	-2.523	0.918	0.487	H	1.769	6.454	0.26
C	-1.041	-1.69	-1.895	H	0.699	5.641	1.394
C	0.644	0.103	-2.607	H	2.357	5.045	1.169
C	1.976	-1.21	-0.319	H	-1.032	5.275	-0.51
C	-1.503	0.533	-0.581	H	0.031	6.061	-1.668
C	0.415	-1.404	-2.359	H	-0.561	4.424	-1.989
C	-1.603	-1.023	-0.629	H	2.555	-2.737	-3.435
C	-3.737	0.018	0.196	H	3.677	-2.611	-2.065
C	1.001	0.94	-1.348	H	3.14	-1.155	-2.907
C	1.617	-2.068	-1.586	H	0.905	-4.084	-2.007
C	-3.129	-1.361	-0.315	H	0.476	-3.516	-0.384
C	1.489	5.466	0.651	H	2.139	-4.007	-0.74
C	-0.2	5.092	-1.204	H	-4.125	-2.914	0.897
C	2.823	-2.142	-2.555	H	-2.685	-2.23	1.652
C	1.261	-3.502	-1.149	H	-2.531	-3.355	0.286
C	-3.123	-2.526	0.697	H	-4.97	-1.953	-1.312
C	-3.915	-1.81	-1.566	H	-3.544	-2.76	-1.965
C	4.74	0.1	3.677	H	-3.873	-1.066	-2.37
C	2.562	-2.06	2.968	H	4.452	-0.529	4.526
C	-6.071	-0.762	0.966	H	5.776	0.419	3.843
C	-5.241	1.506	1.593	H	4.109	0.998	3.696
C	1.315	2.404	-1.796	H	3.177	-2.966	3.016
C	4.616	-0.64	2.342	H	1.548	-2.353	2.672
C	3.173	-1.045	1.977	H	2.498	-1.63	3.972
C	-4.812	0.049	1.32	H	-6.806	-0.677	1.777
O	3.327	0.757	-0.665	H	-5.854	-1.822	0.824
O	0.241	1.266	0.884	H	-6.543	-0.38	0.053
O	3.949	-2.519	0.254	H	-6.046	1.524	2.339
O	-4.205	-0.48	2.515	H	-4.408	2.097	1.982
H	2.481	3.141	-0.092	H	-5.62	1.992	0.686
H	-2.113	0.707	1.48	H	2.184	2.326	-2.464
H	-2.765	1.985	0.451	H	0.479	2.741	-2.416
H	-1.668	-1.385	-2.741	H	5.002	-0.001	1.539
H	-1.176	-2.774	-1.806	H	5.241	-1.541	2.35

H	1.464	0.238	-3.32	H	2.54	-0.148	1.973
H	-0.239	0.536	-3.092	H	-4.857	-0.391	3.229

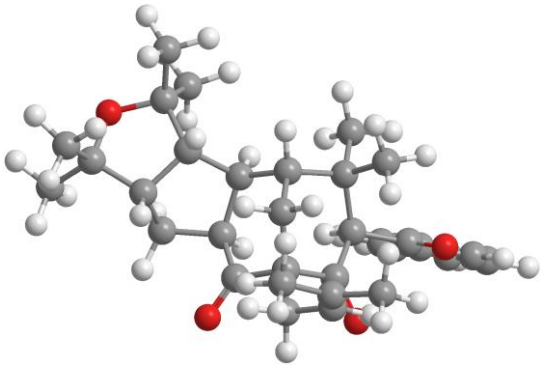
Conformation 10

Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-2.458	0.432	-0.563	H	-1.294	-1.252	-0.023
C	-0.046	0.8	-0.987	H	1.422	1.687	0.286
C	-0.544	3.788	-1.136	H	-1.326	0.89	3.071
C	-0.592	5.007	-0.574	H	0.671	-1.249	0.479
C	-3.316	-1.918	-0.204	H	3.817	0.845	0.508
C	2.449	0.288	-1.014	H	0.334	6.871	-1.16
C	0.367	0.031	2.185	H	0.939	6.219	0.357
C	-1.221	1.758	1.139	H	1.44	5.481	-1.179
C	-2.283	-0.866	0.238	H	-1.512	5.837	1.189
C	1.235	0.712	-0.186	H	-2.11	6.515	-0.318
C	-1.101	0.524	2.06	H	-2.64	4.904	0.193
C	1.157	-0.375	0.932	H	-3.501	0.35	3.32
C	3.487	-0.098	0.051	H	-4.395	-0.625	2.135
C	-1.313	1.45	-0.376	H	-3.848	0.993	1.709
C	-2.239	-0.527	1.782	H	-1.872	-1.592	3.645
C	2.666	-0.822	1.197	H	-1.105	-2.359	2.245
C	0.598	5.936	-0.648	H	-2.854	-2.497	2.488
C	-1.783	5.58	0.156	H	3.716	-2.736	1.353
C	-3.578	0.086	2.259	H	2.334	-2.775	0.237
C	-1.998	-1.821	2.58	H	2.057	-2.752	1.979
C	2.703	-2.362	1.182	H	4.274	-0.624	2.624
C	3.218	-0.352	2.559	H	2.692	-0.82	3.399
C	-1.553	-5.162	-1.493	H	3.148	0.735	2.68
C	-2.528	-2.33	-2.583	H	-1.243	-4.948	-2.521
C	5.606	0.373	-1.237	H	-0.778	-5.787	-1.037
C	4.6	-1.906	-1.481	H	-2.477	-5.752	-1.536
C	-1.626	2.741	-1.194	H	-1.638	-1.696	-2.514
C	-1.756	-3.88	-0.676	H	-3.354	-1.714	-2.953
C	-2.885	-2.974	-1.228	H	-2.33	-3.107	-3.328
C	4.794	-0.723	-0.517	H	6.565	-0.035	-1.582
O	-3.435	0.658	-1.251	H	5.814	1.206	-0.557
O	-0.12	0.355	-2.125	H	5.08	0.762	-2.115
O	-4.459	-1.918	0.225	H	5.583	-2.275	-1.801
O	5.553	-1.16	0.632	H	4.067	-2.736	-1.016
H	0.385	3.514	-1.64	H	4.058	-1.607	-2.384
H	2.172	-0.566	-1.64	H	-1.778	2.431	-2.234
H	2.792	1.084	-1.683	H	-2.585	3.13	-0.842

H	0.903	0.858	2.668	H	-1.992	-4.158	0.359
H	0.401	-0.796	2.903	H	-0.811	-3.322	-0.642
H	-2.122	2.321	1.405	H	-3.779	-3.595	-1.364
H	-0.387	2.444	1.321	H	6.395	-1.513	0.3

Table S3. Important thermodynamic parameters (a.u.) and Boltzmann distribution of the optimized compound **4** at B3LYP/6-31G(d) level in methanol.

Conformation	**Internal Energy**	**%**
1	-1545.3	35.65%
2	-1545.3	27.07%
3	-1545.3	13.45%
4	-1545.3	7.05%
5	-1545.3	4.29%
6	-1545.3	3.70%
7	-1545.3	3.25%
8	-1545.3	3.22%
9	-1545.29	1.44%



Conformation 1

Table S4. Optimized coordinates of compound **4** at B3LYP/6-31G(d) level in methanol.

Conformation 1							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-5.531	-3.882	-0.901	H	-2.37	-2.661	-0.904
C	-4.153	-3.817	-1.108	H	-5.993	-0.827	0.527
C	-6.199	-2.804	-0.31	H	-2.054	3.888	-0.421
C	-3.439	-2.679	-0.728	H	2.54	-0.791	-2.803
C	-5.489	-1.671	0.068	H	2.418	-2.21	-1.751
C	-4.098	-1.589	-0.134	H	0.06	2.356	1.282
C	-1.61	1.071	-0.743	H	1.553	1.877	0.514
C	0.679	0.768	-1.694	H	-1.502	-0.994	-0.435
C	-0.985	4.088	-0.48	H	0.231	-1.277	-1.583
C	-3.416	-0.328	0.303	H	3.54	0.542	-1.025
C	-0.526	5.17	0.173	H	0.866	0.198	2.212
C	2.39	-1.115	-1.771	H	0.872	-1.816	0.583
C	0.498	1.598	0.629	H	2.938	0.173	1.234
C	-1.896	-0.155	0.145	H	-2.505	5.697	0.898

C	1.041	-0.639	-1.204	H	-1.181	6.12	2.004
C	3.41	-0.521	-0.785	H	-1.453	7.087	0.56
C	0.385	0.192	1.225	H	1.275	5.685	1.241
C	1.194	-0.803	0.347	H	1.591	4.969	-0.348
C	2.737	-0.697	0.601	H	1.008	6.636	-0.213
C	-0.181	1.667	-0.763	H	-2.658	0.523	2.896
C	-1.112	-0.169	1.506	H	-1.007	0.953	3.366
C	4.788	-1.199	-0.644	H	-1.84	1.846	2.081
C	3.479	-1.928	1.243	H	-0.62	-1.608	3.066
C	-1.473	6.058	0.947	H	-2.263	-1.778	2.44
C	0.914	5.624	0.205	H	-0.9	-2.372	1.492
C	-1.69	0.854	2.514	H	5.488	0.378	0.713
C	-1.227	-1.565	2.154	H	6.1	0.52	-0.942
C	5.844	-0.194	-0.15	H	6.757	-0.724	0.144
C	5.299	-1.901	-1.906	H	4.601	-2.672	-2.242
C	4.038	-1.571	2.63	H	6.263	-2.38	-1.703
C	2.676	-3.231	1.346	H	5.442	-1.181	-2.719
C	-0.208	3.112	-1.324	H	4.638	-2.398	3.026
O	-2.467	1.51	-1.489	H	4.672	-0.68	2.586
O	1.052	1.176	-2.779	H	3.222	-1.372	3.336
O	-4.069	0.579	0.804	H	3.342	-4.03	1.689
O	4.582	-2.226	0.349	H	2.264	-3.533	0.378
H	-6.084	-4.769	-1.198	H	1.855	-3.147	2.067
H	-3.629	-4.651	-1.567	H	-0.646	3.071	-2.327
H	-7.272	-2.851	-0.147	H	0.83	3.431	-1.452

Conformation 2

Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-6.487	-1.988	-1.484	H	-3.146	-1.425	-1.421
C	-5.131	-2.117	-1.788	H	-6.275	0.523	0.805
C	-6.904	-1.036	-0.547	H	2.414	2.853	-1.604
C	-4.19	-1.302	-1.157	H	2.001	-0.904	-2.752
C	-5.967	-0.221	0.078	H	1.62	-2.415	-1.915
C	-4.595	-0.342	-0.214	H	0.404	2.11	1.752
C	-1.538	1.721	-0.246	H	1.724	1.36	0.891
C	0.432	0.776	-1.451	H	-1.926	-0.337	-0.392
C	1.91	3.446	-0.841	H	-0.35	-1.165	-1.538
C	-3.658	0.579	0.509	H	3.251	-0.068	-0.822
C	2.669	4.291	-0.122	H	0.586	-0.278	2.384
C	1.797	-1.344	-1.772	H	0.143	-2.017	0.555
C	0.633	1.356	0.994	H	2.603	-0.672	1.38
C	-2.139	0.437	0.35	H	4.482	3.721	-1.175

C	0.555	-0.715	-1.106	H	4.432	5.422	-0.666
C	2.911	-1.108	-0.74	H	4.73	4.165	0.527
C	0.14	-0.034	1.41	H	2.688	5.007	1.911
C	0.687	-1.085	0.407	H	2.372	6.256	0.715
C	2.215	-1.359	0.622	H	1.091	5.114	1.153
C	0.009	1.789	-0.356	H	-2.742	0.819	3.181
C	-1.407	-0.032	1.666	H	-1.059	0.643	3.702
C	4.124	-2.061	-0.74	H	-1.534	1.965	2.622
C	2.67	-2.811	1.028	H	-2.959	-1.407	2.354
C	4.154	4.398	-0.38	H	-1.825	-2.16	1.232
C	2.163	5.207	0.967	H	-1.332	-1.825	2.901
C	-1.704	0.91	2.857	H	5.108	-0.905	0.847
C	-1.907	-1.439	2.051	H	5.756	-0.612	-0.774
C	5.353	-1.383	-0.107	H	6.138	-2.125	0.074
C	4.503	-2.632	-2.109	H	3.671	-3.185	-2.554
C	3.27	-2.822	2.444	H	5.35	-3.319	-2.007
C	1.609	-3.913	0.925	H	4.797	-1.831	-2.796
C	0.422	3.229	-0.756	H	3.67	-3.814	2.683
O	-2.233	2.629	-0.659	H	4.082	-2.094	2.537
O	0.631	1.155	-2.593	H	2.505	-2.573	3.189
O	-4.106	1.45	1.246	H	2.09	-4.882	1.099
O	3.7	-3.176	0.073	H	1.146	-3.944	-0.066
H	-7.218	-2.626	-1.974	H	0.821	-3.792	1.677
H	-4.803	-2.852	-2.516	H	-0.041	3.913	-0.04
H	-7.958	-0.932	-0.307	H	-0.032	3.444	-1.729

Conformation 3

Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-6.214	-0.85	-2.489	H	-6.209	-1.136	0.903
C	-6.7	-1.077	-1.197	H	-2.982	-0.129	-1.763
C	-4.873	-0.511	-2.679	H	1.467	3.158	-1.527
C	-5.846	-0.965	-0.104	H	1.821	-0.283	-2.78
C	-4.016	-0.403	-1.583	H	1.91	-1.945	-2.188
C	-4.492	-0.63	-0.281	H	0.208	1.712	2.149
C	-1.86	1.172	0.425	H	1.519	1.33	1.06
C	-0.008	0.706	-1.177	H	-1.818	-0.891	-0.091
C	1.096	3.518	-0.567	H	-0.241	-1.355	-1.463
C	-3.637	-0.535	0.948	H	3.041	0.548	-0.823
C	1.903	4.333	0.136	H	0.884	-0.645	2.464
C	1.834	-0.898	-1.876	H	0.603	-2.242	0.488
C	0.472	1.099	1.282	H	2.815	-0.539	1.287
C	-2.126	-0.296	0.775	H	3.339	5.811	-0.523

C	0.546	-0.72	-1.036	H	4.059	4.429	0.293
C	2.963	-0.544	-0.895	H	3.466	4.256	-1.372
C	0.297	-0.398	1.57	H	0.586	4.655	1.854
C	0.927	-1.205	0.401	H	2.317	4.65	2.227
C	2.493	-1.16	0.445	H	1.603	6.039	1.419
C	-0.398	1.532	0.074	H	-1.6	1.089	3.139
C	-1.187	-0.74	1.958	H	-2.481	-0.336	3.671
C	4.354	-1.162	-1.136	H	-0.746	-0.187	4.018
C	3.282	-2.52	0.539	H	-0.611	-2.596	2.941
C	3.26	4.721	-0.403	H	-2.345	-2.468	2.61
C	1.57	4.942	1.476	H	-1.226	-2.847	1.298
C	-1.526	0.005	3.272	H	5.196	-0.092	0.587
C	-1.352	-2.253	2.209	H	5.605	0.621	-0.981
C	5.452	-0.327	-0.451	H	6.397	-0.879	-0.454
C	4.722	-1.385	-2.606	H	3.993	-2.03	-3.104
C	4.004	-2.645	1.89	H	5.705	-1.863	-2.678
C	2.471	-3.796	0.283	H	4.768	-0.431	-3.142
C	-0.292	3.051	-0.215	H	4.623	-3.549	1.911
O	-2.739	2.014	0.464	H	4.651	-1.782	2.075
O	-0.185	1.174	-2.291	H	3.279	-2.708	2.711
O	-4.145	-0.667	2.054	H	1.918	-3.748	-0.66
O	4.271	-2.467	-0.522	H	1.763	-3.999	1.093
H	-6.879	-0.937	-3.344	H	3.161	-4.645	0.223
H	-7.743	-1.34	-1.045	H	-0.686	3.578	0.657
H	-4.492	-0.329	-3.679	H	-0.969	3.276	-1.047

Conformation 4

Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-6.009	-1.447	-2.277	H	-2.878	-0.282	-1.692
C	-4.731	-0.942	-2.525	H	-5.86	-1.609	1.12
C	-6.419	-1.69	-0.963	H	1.083	3.429	-1.834
C	-3.86	-0.684	-1.466	H	2.178	-0.164	-2.856
C	-5.554	-1.428	0.095	H	2.389	1.131	-1.69
C	-4.262	-0.926	-0.141	H	0.251	2.029	2.044
C	-1.853	1.229	0.459	H	1.524	1.75	0.88
C	-0.103	0.871	-1.223	H	-1.573	-0.821	-0.051
C	0.782	3.792	-0.85	H	0.377	-1.11	-1.679
C	-3.391	-0.672	1.054	H	4.217	-0.119	-1.043
C	1.587	4.69	-0.257	H	1.167	-0.226	2.391
C	2.201	0.055	-1.785	H	0.898	-1.894	0.37
C	0.522	1.421	1.176	H	3.039	0.118	1.004
C	-1.927	-0.257	0.822	H	2.832	6.245	-1.1

C	0.846	-0.312	-1.096	H	3.734	4.953	-0.318
C	3.286	-0.694	-1.005	H	2.997	4.673	-1.911
C	0.524	-0.08	1.514	H	2.168	5.102	1.777
C	1.2	-0.845	0.338	H	1.294	6.416	1
C	2.759	-0.78	0.442	H	0.414	4.986	1.566
C	-0.459	1.722	0.016	H	-0.447	0.091	4.004
C	-0.901	-0.563	1.977	H	-2.171	-0.229	3.722
C	3.628	-2.173	-1.388	H	-1.444	1.256	3.123
C	3.521	-2.004	1.013	H	-0.133	-2.314	3.019
C	2.851	5.158	-0.94	H	-0.735	-2.686	1.394
C	1.338	5.322	1.091	H	-1.873	-2.368	2.706
C	-1.266	0.188	3.281	H	5.27	-3.307	-2.257
C	-0.909	-2.073	2.284	H	5.779	-1.81	-1.449
C	5	-2.262	-2.072	H	4.986	-1.738	-3.036
C	2.586	-2.906	-2.245	H	2.912	-3.941	-2.399
C	4.903	-1.57	1.54	H	2.474	-2.442	-3.231
C	2.809	-2.821	2.093	H	1.609	-2.94	-1.757
C	-0.521	3.228	-0.346	H	5.513	-2.454	1.753
O	-2.813	1.972	0.547	H	4.8	-0.991	2.465
O	-0.592	1.145	-2.31	H	5.44	-0.951	0.814
O	-3.849	-0.807	2.181	H	3.441	-3.666	2.39
O	3.688	-2.883	-0.124	H	1.861	-3.226	1.733
H	-6.683	-1.65	-3.105	H	2.62	-2.215	2.985
H	-4.409	-0.746	-3.544	H	-1.288	3.346	-1.119
H	-7.413	-2.083	-0.765	H	-0.882	3.765	0.535

Conformation 5

Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-5.894	-0.461	-2.691	H	-2.809	0.358	-1.545
C	-4.629	0.129	-2.638	H	-5.783	-2.201	0.233
C	-6.314	-1.303	-1.656	H	1.291	3.462	2.136
C	-3.781	-0.124	-1.56	H	2.346	1.242	-2.217
C	-5.47	-1.553	-0.578	H	2.38	1.827	-0.561
C	-4.192	-0.97	-0.516	H	0.112	0.84	2.944
C	-1.901	0.736	1.072	H	1.431	1.143	1.838
C	-0.099	1.225	-0.515	H	-1.5	-0.852	-0.293
C	0.629	3.704	1.304	H	0.601	-0.277	-1.786
C	-3.345	-1.29	0.68	H	4.287	0.526	-0.436
C	1.044	4.664	0.458	H	1.14	-1.301	2.302
C	2.3	0.92	-1.173	H	1.044	-1.888	-0.27
C	0.437	0.688	1.91	H	3.022	-0.335	1.367
C	-1.902	-0.756	0.725	H	3.029	5.227	-0.193

C	0.956	0.186	-0.861	H	2.231	6.439	0.802
C	3.413	-0.049	-0.758	H	2.89	4.975	1.561
C	0.519	-0.805	1.546	H	-0.014	6.214	-0.602
C	1.284	-0.929	0.194	H	0.898	5.125	-1.639
C	2.832	-0.856	0.422	H	-0.632	4.582	-0.941
C	-0.528	1.432	0.955	H	-0.526	-1.828	3.79
C	-0.886	-1.504	1.667	H	-2.221	-2.045	3.307
C	3.908	-1.133	-1.774	H	-1.558	-0.425	3.484
C	3.658	-2.167	0.385	H	-0.033	-3.5	1.847
C	2.37	5.356	0.677	H	-0.568	-3.124	0.2
C	0.27	5.161	-0.739	H	-1.757	-3.488	1.454
C	-1.328	-1.441	3.15	H	5.696	-1.617	-2.918
C	-0.804	-2.989	1.26	H	6.018	-0.684	-1.442
C	5.322	-0.81	-2.278	H	5.321	0.118	-2.863
C	2.992	-1.399	-2.977	H	3.413	-2.216	-3.574
C	4.973	-1.986	1.169	H	2.909	-0.52	-3.626
C	2.963	-3.44	0.873	H	1.99	-1.703	-2.665
C	-0.672	2.941	1.279	H	5.643	-2.83	0.968
O	-2.9	1.318	1.452	H	4.781	-1.948	2.247
O	-0.622	1.885	-1.401	H	5.493	-1.065	0.887
O	-3.806	-1.973	1.586	H	3.648	-4.29	0.781
O	3.949	-2.37	-1.016	H	2.071	-3.667	0.283
H	-6.551	-0.264	-3.533	H	2.676	-3.353	1.927
H	-4.301	0.788	-3.437	H	-1.378	3.373	0.568
H	-7.297	-1.763	-1.692	H	-1.147	3.008	2.266

Conformation 6

Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-6.056	0.21	-2.687	H	-2.899	0.634	-1.527
C	-4.729	0.641	-2.626	H	-6.168	-1.556	0.222
C	-6.579	-0.583	-1.661	H	1.676	2.932	2.221
C	-3.922	0.275	-1.549	H	1.953	0.888	-2.321
C	-5.776	-0.942	-0.583	H	2.061	-0.864	-2.51
C	-4.436	-0.522	-0.513	H	0.122	0.564	2.896
C	-1.876	0.813	1.028	H	1.478	0.669	1.798
C	0.023	1.067	-0.551	H	-1.771	-0.824	-0.325
C	1.085	3.333	1.397	H	-0.127	-0.673	-1.701
C	-3.637	-0.956	0.681	H	3.073	0.795	-0.148
C	1.668	4.278	0.639	H	0.821	-1.701	2.204
C	1.947	-0.059	-1.776	H	0.654	-2.302	-0.273
C	0.424	0.379	1.861	H	2.795	-1.101	1.273
C	-2.126	-0.662	0.698	H	3.735	4.578	0.071

C	0.621	-0.274	-1.004	H	3.102	5.816	1.148
C	3.026	-0.16	-0.687	H	3.508	4.213	1.796
C	0.265	-1.097	1.476	H	1.655	4.915	-1.416
C	0.958	-1.326	0.103	H	0.041	4.567	-0.786
C	2.519	-1.298	0.232	H	0.896	6.052	-0.31
C	-0.407	1.289	0.92	H	-2.599	-1.933	3.276
C	-1.226	-1.573	1.615	H	-0.882	-1.969	3.729
C	4.442	-0.606	-1.105	H	-1.706	-0.428	3.453
C	3.333	-2.561	-0.236	H	-1.209	-3.188	0.112
C	3.077	4.738	0.937	H	-0.652	-3.671	1.723
C	1.016	4.981	-0.526	H	-2.377	-3.414	1.418
C	-1.63	-1.464	3.106	H	5.189	-0.378	0.948
C	-1.374	-3.045	1.185	H	5.635	0.947	-0.139
C	5.489	-0.137	-0.077	H	6.45	-0.625	-0.275
C	4.874	-0.174	-2.509	H	4.184	-0.548	-3.271
C	3.992	-3.266	0.96	H	5.871	-0.57	-2.731
C	2.563	-3.596	-1.067	H	4.918	0.918	-2.582
C	-0.318	2.79	1.298	H	3.23	-3.678	1.633
O	-2.771	1.554	1.392	H	4.627	-4.09	0.618
O	-0.171	1.941	-1.38	H	4.612	-2.571	1.535
O	-4.188	-1.55	1.598	H	3.274	-4.331	-1.46
O	4.37	-2.049	-1.113	H	2.051	-3.139	-1.92
H	-6.681	0.493	-3.529	H	1.825	-4.135	-0.464
H	-4.32	1.262	-3.417	H	-0.809	2.897	2.274
H	-7.611	-0.92	-1.704	H	-0.92	3.358	0.588

Conformation 7

Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-4.55	-4.223	-1.757	H	-5.014	-2.803	1.302
C	-5.114	-3.987	-0.499	H	-2.07	-1.91	-1.707
C	-3.453	-3.47	-2.181	H	-1.034	4.16	0.887
C	-4.582	-3.002	0.327	H	2.511	-0.123	-2.813
C	-2.911	-2.493	-1.347	H	2.875	-1.546	-1.824
C	-3.468	-2.247	-0.082	H	-0.102	2.304	1.605
C	-1.7	0.69	-0.216	H	1.345	2.176	0.632
C	0.446	0.87	-1.474	H	-1.008	-1.289	-0.019
C	-1.608	3.851	0.013	H	0.569	-1.221	-1.368
C	-2.954	-1.201	0.858	H	3.349	1.384	-1.081
C	-2.855	4.34	-0.091	H	1.253	0.396	2.373
C	2.57	-0.495	-1.788	H	1.519	-1.574	0.713
C	0.401	1.669	0.873	H	3.156	0.805	1.211
C	-1.558	-0.591	0.621	H	-3.697	6.228	0.549

C	1.218	-0.39	-1.057	H	-4.32	4.834	1.422
C	3.516	0.317	-0.888	H	-2.688	5.437	1.778
C	0.675	0.276	1.448	H	-4.063	5.004	-1.747
C	1.58	-0.515	0.463	H	-3.411	3.364	-1.964
C	3.078	-0.063	0.548	H	-4.75	3.657	-0.849
C	-0.452	1.581	-0.42	H	-2.123	-0.048	3.49
C	-0.665	-0.406	1.894	H	-0.585	0.812	3.698
C	5.025	0.005	-0.931	H	-1.794	1.39	2.539
C	4.153	-1.113	1.016	H	0.04	-2.5	1.836
C	-3.41	5.257	0.975	H	0.294	-1.675	3.384
C	-3.806	4.068	-1.231	H	-1.325	-2.215	2.919
C	-1.335	0.493	2.964	H	5.464	1.641	0.466
C	-0.395	-1.781	2.537	H	5.825	2.015	-1.226
C	5.848	1.222	-0.47	H	6.891	0.929	-0.31
C	5.547	-0.485	-2.284	H	5.024	-1.389	-2.608
C	4.763	-0.713	2.369	H	6.616	-0.718	-2.213
C	3.692	-2.575	1.086	H	5.419	0.286	-3.051
C	-0.863	2.975	-0.963	H	5.575	-1.397	2.641
O	-2.754	0.952	-0.767	H	5.168	0.303	2.337
O	0.528	1.305	-2.608	H	4.005	-0.752	3.161
O	-3.637	-0.849	1.811	H	4.563	-3.21	1.28
O	5.191	-1.084	0.002	H	3.242	-2.906	0.145
H	-4.966	-4.99	-2.405	H	2.973	-2.738	1.895
H	-5.968	-4.57	-0.167	H	-1.427	2.832	-1.884
H	-3.018	-3.643	-3.162	H	0.069	3.482	-1.248

Conformation 8

Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	4.419	4.86	-0.609	H	1.764	2.815	-1.115
C	3.178	4.413	-1.066	H	5.381	2.078	1.102
C	5.216	4.019	0.176	H	2.792	-3.537	-0.457
C	2.729	3.134	-0.737	H	-2.538	1.375	-2.654
C	4.772	2.742	0.498	H	-2.688	-0.359	-2.81
C	3.519	2.28	0.05	H	0.303	-2.547	1.121
C	1.77	-0.866	-0.747	H	-1.203	-2.403	0.253
C	-0.459	-1.028	-1.856	H	1.159	1.11	-0.419
C	1.799	-3.959	-0.606	H	-0.494	1.044	-1.637
C	3.125	0.888	0.44	H	-4.44	-0.254	-1.314
C	1.54	-5.141	-0.02	H	-1.029	-0.683	2.035
C	-2.537	0.443	-2.084	H	-1.418	1.359	0.465
C	-0.254	-1.89	0.45	H	-3.023	-1.217	0.326
C	1.703	0.367	0.17	H	2.252	-6.012	1.829

C	-1.18	0.232	-1.358	H	2.834	-6.828	0.384
C	-3.634	0.415	-0.998	H	3.528	-5.26	0.848
C	-0.51	-0.518	1.084	H	0.392	-6.884	-0.562
C	-1.473	0.304	0.179	H	-0.179	-6.071	0.888
C	-2.965	-0.123	0.291	H	-0.526	-5.375	-0.703
C	0.512	-1.755	-0.888	H	0.88	-1.023	3.299
C	0.851	0.161	1.475	H	2.418	-0.217	2.96
C	-4.287	1.773	-0.567	H	1.977	-1.659	2.061
C	-3.843	0.484	1.416	H	0.006	1.413	3.046
C	2.6	-5.838	0.801	H	0.139	2.256	1.492
C	0.234	-5.893	-0.114	H	1.579	1.965	2.469
C	1.577	-0.742	2.501	H	-6.207	2.794	-0.69
C	0.626	1.529	2.15	H	-6.333	1.024	-0.697
C	-5.74	1.872	-1.054	H	-5.781	1.88	-2.15
C	-3.529	3.042	-0.98	H	-3.973	3.902	-0.468
C	-5.064	-0.42	1.677	H	-3.597	3.223	-2.058
C	-3.165	0.805	2.75	H	-2.471	2.998	-0.703
C	0.892	-3.136	-1.483	H	-5.782	0.101	2.319
O	2.761	-1.09	-1.419	H	-4.76	-1.345	2.181
O	-0.635	-1.449	-2.985	H	-5.573	-0.695	0.748
O	3.932	0.157	1	H	-3.884	1.306	3.407
O	-4.277	1.755	0.883	H	-2.312	1.474	2.615
H	4.765	5.858	-0.863	H	-2.828	-0.105	3.257
H	2.558	5.059	-1.68	H	-0.039	-3.664	-1.703
H	6.183	4.363	0.534	H	1.382	-2.958	-2.446

Conformation 9

Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-6.156	-1.072	-2.394	H	-6.117	-1.184	1.008
C	-6.622	-1.256	-1.089	H	-2.958	-0.158	-1.734
C	-4.834	-0.678	-2.612	H	1.324	3.273	-1.748
C	-5.769	-1.047	-0.01	H	2.471	1.082	-1.501
C	-3.975	-0.474	-1.532	H	2.64	-0.46	-2.312
C	-4.433	-0.658	-0.216	H	0.309	1.847	2.092
C	-1.845	1.283	0.43	H	1.563	1.452	0.944
C	-0.062	0.796	-1.198	H	-1.752	-0.788	-0.056
C	1.043	3.624	-0.754	H	0.535	-1.094	-1.828
C	-3.577	-0.456	0.998	H	3.447	0.331	0.483
C	1.915	4.428	-0.121	H	0.979	-0.501	2.398
C	2.353	0.003	-1.366	H	0.245	-2.021	0.252
C	0.527	1.23	1.215	H	2.579	-1.595	1.598
C	-2.075	-0.186	0.803	H	3.297	5.901	-0.895

C	0.864	-0.4	-1.052	H	4.076	4.51	-0.153
C	3.218	-0.505	-0.186	H	3.338	4.351	-1.761
C	0.353	-0.266	1.528	H	1.743	6.128	1.193
C	0.874	-1.133	0.331	H	0.75	4.752	1.703
C	2.351	-1.564	0.528	H	2.506	4.726	1.929
C	-0.394	1.65	0.046	H	-2.364	-0.081	3.712
C	-1.118	-0.574	1.99	H	-0.621	0.101	4.001
C	4.521	-1.27	-0.519	H	-1.511	1.319	3.078
C	2.833	-2.929	-0.085	H	-1.168	-2.728	1.478
C	3.222	4.811	-0.775	H	-0.533	-2.359	3.089
C	1.702	5.032	1.246	H	-2.271	-2.251	2.771
C	-1.423	0.245	3.268	H	4.983	-1.498	1.618
C	-1.282	-2.067	2.343	H	5.919	-0.234	0.803
C	5.486	-1.234	0.683	H	6.303	-1.945	0.522
C	5.267	-0.814	-1.775	H	4.653	-0.926	-2.672
C	3.1	-3.959	1.025	H	6.172	-1.416	-1.91
C	1.926	-3.562	-1.149	H	5.57	0.236	-1.687
C	-0.312	3.164	-0.286	H	3.516	-4.88	0.601
O	-2.739	2.108	0.463	H	3.809	-3.57	1.762
O	-0.542	1.086	-2.285	H	2.17	-4.213	1.547
O	-4.074	-0.522	2.115	H	2.424	-4.45	-1.555
O	4.083	-2.626	-0.757	H	1.739	-2.881	-1.983
H	-6.82	-1.235	-3.238	H	0.966	-3.882	-0.73
H	-7.65	-1.563	-0.915	H	-0.644	3.713	0.598
H	-4.469	-0.528	-3.624	H	-1.05	3.362	-1.072

Figure S4. ^{1}H NMR spectrum of soniiglucinol A (**1**) in $CDCl_3$.

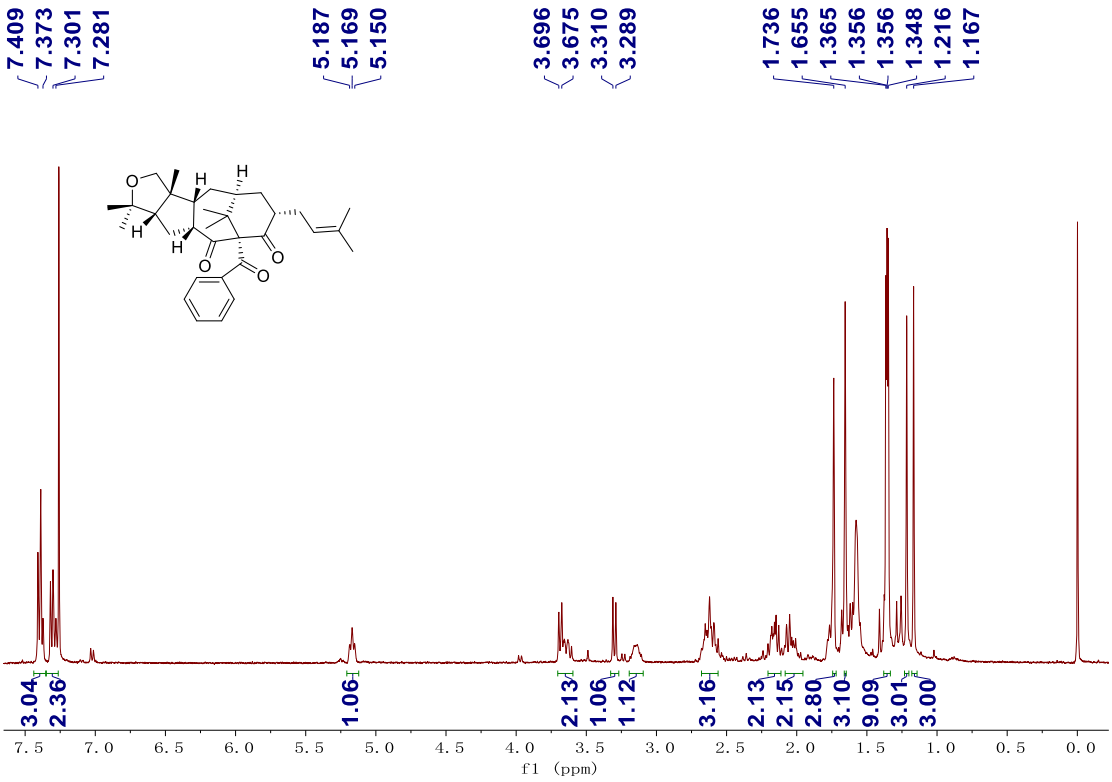


Figure S5. ^{13}C and DEPT NMR spectra of soniiglucinol A (**1**) in $CDCl_3$.

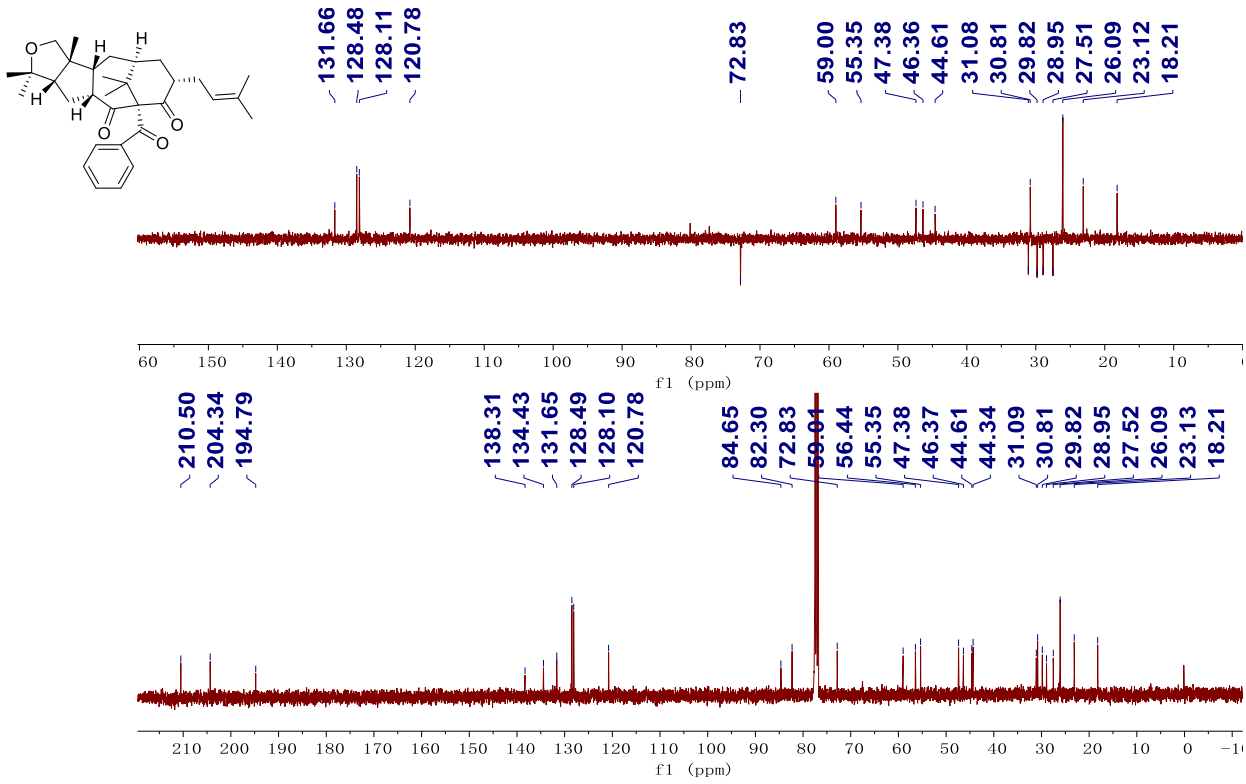


Figure S6. HSQC spectrum of soniiglucinol A (**1**) in $CDCl_3$.

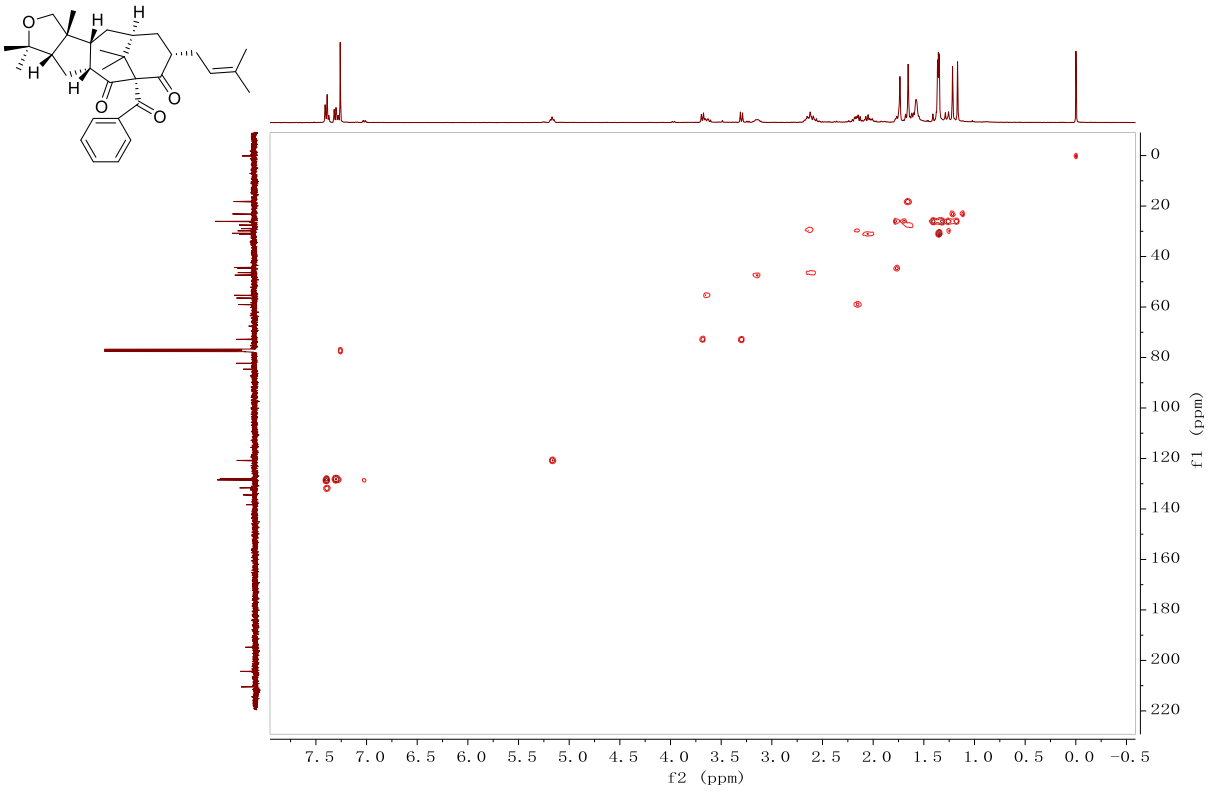


Figure S7. HMBC spectrum of soniiglucinol A (**1**) in $CDCl_3$.

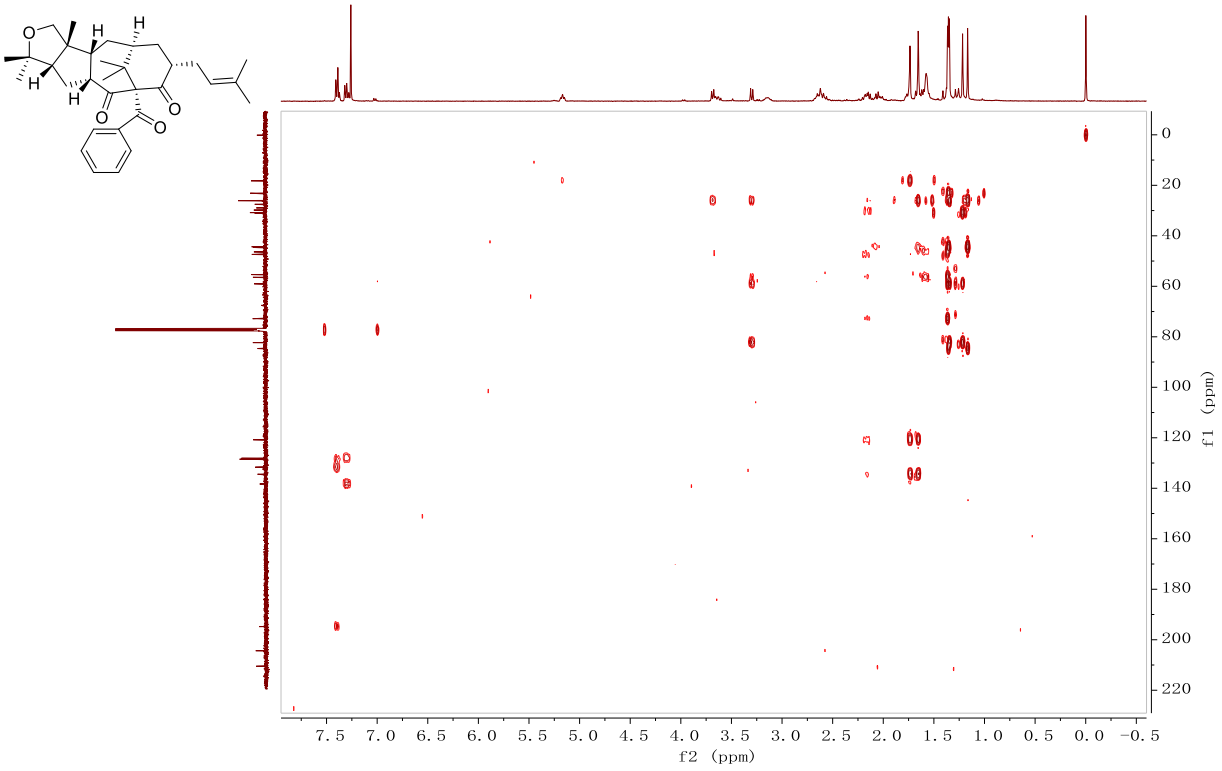


Figure S8. ^{1}H–^{1}H COSY spectrum of soniiglucinol A (**1**) in $CDCl_3$.

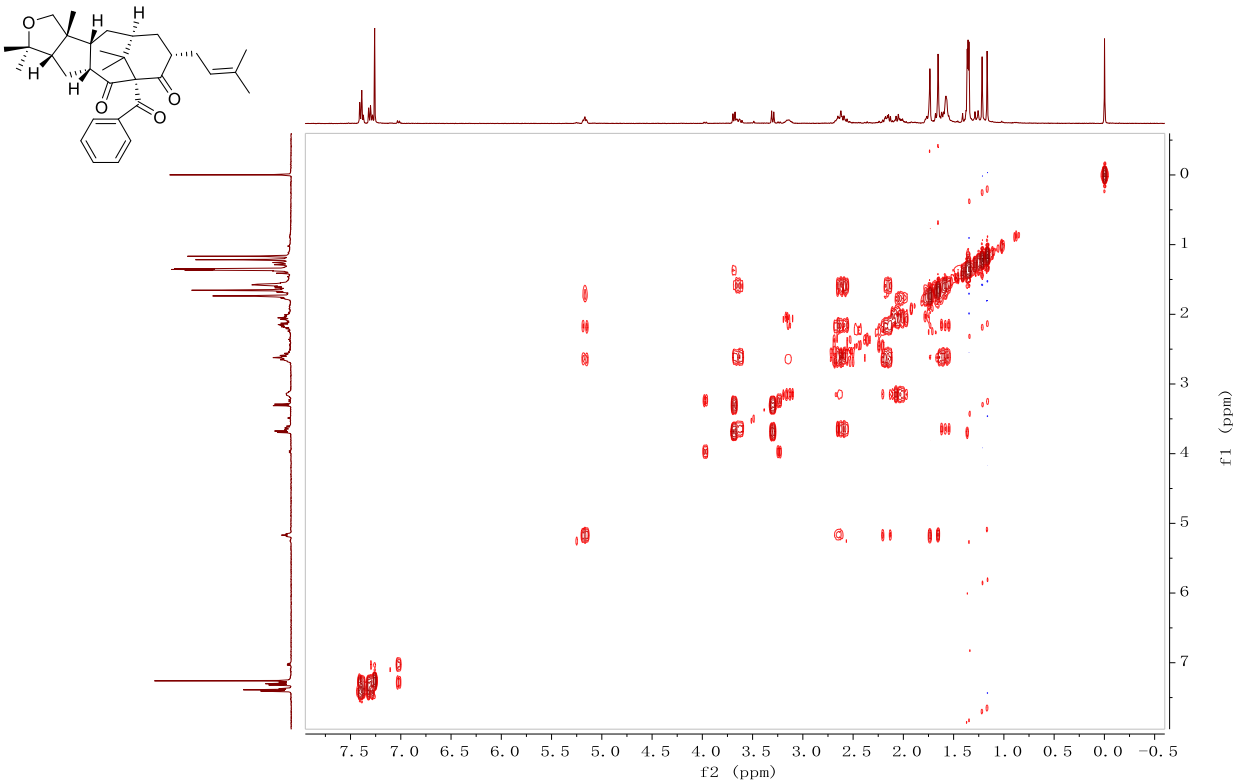


Figure S9. NOESY spectrum of soniiglucinol A (**1**) in $CDCl_3$.

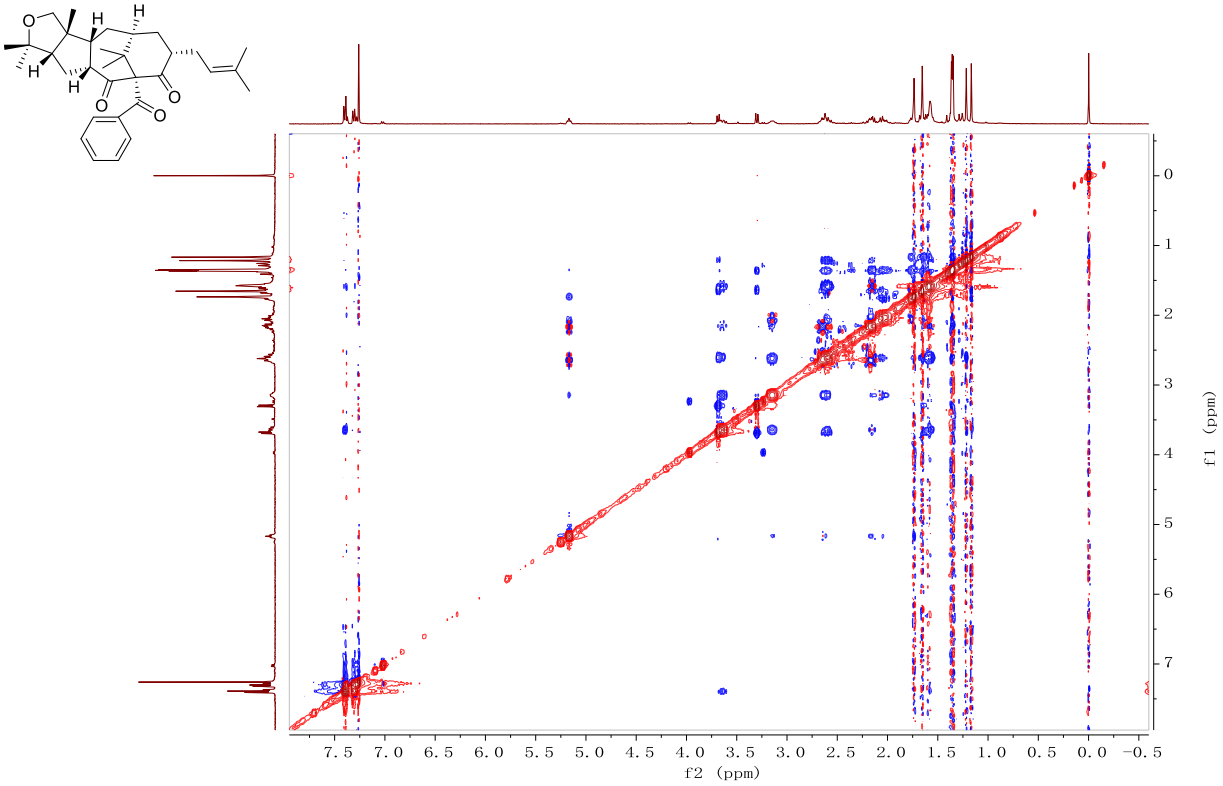


Figure S10. HRESIMS spectrum of soniiglucinol A (**1**).

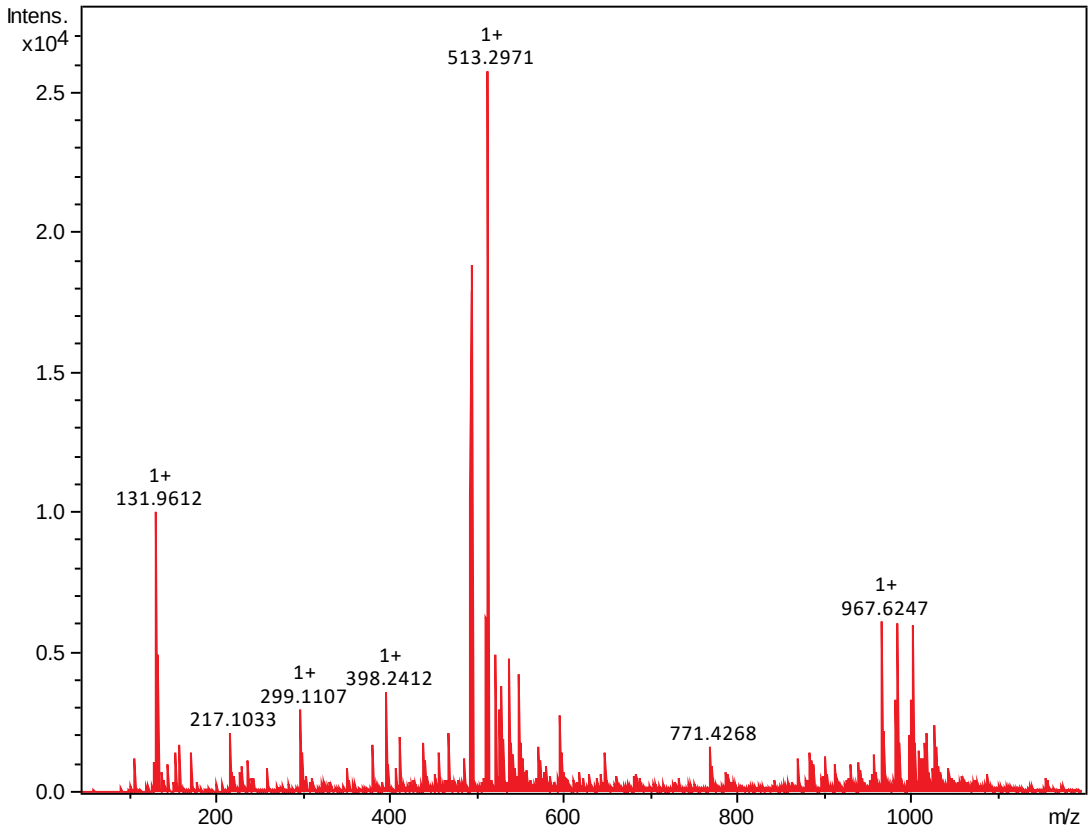


Figure S11. UV spectrum of soniiglucinol A (**1**).

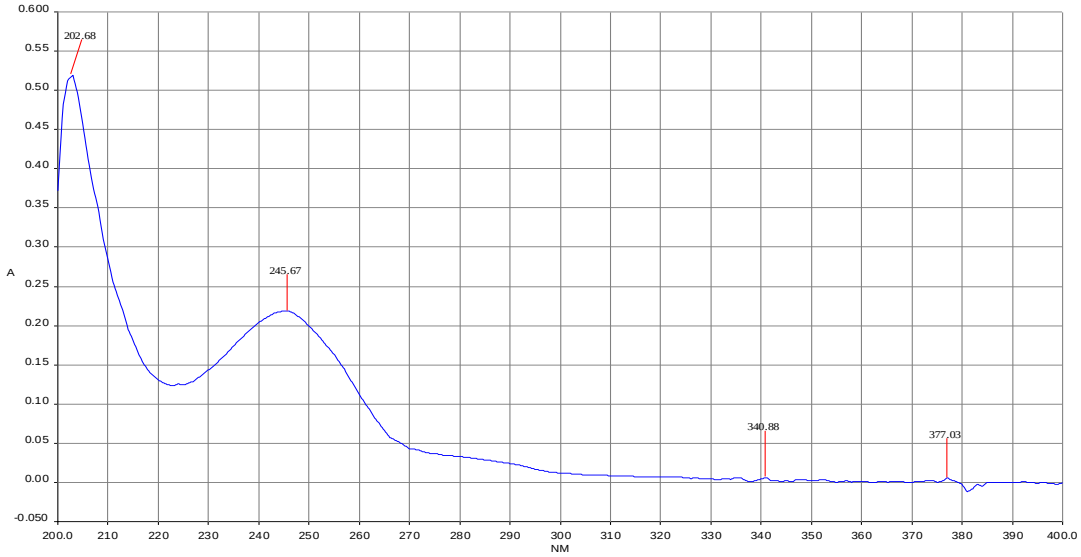


Figure S12. IR spectrum of soniiglucinol A (**1**).

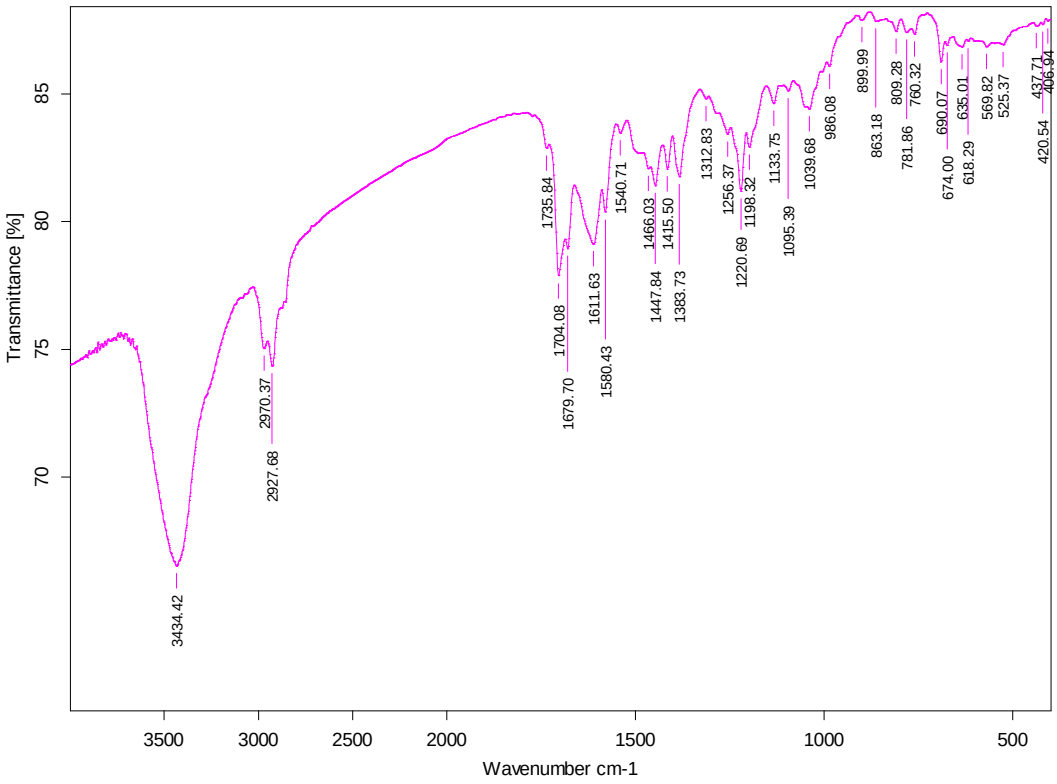
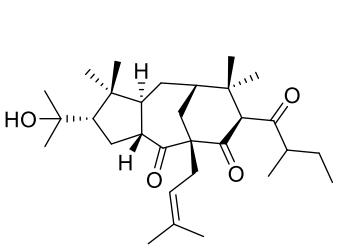


Figure S13. ^{1}H NMR spectrum of soniiglucinol B (**2**) in $CDCl_3$.



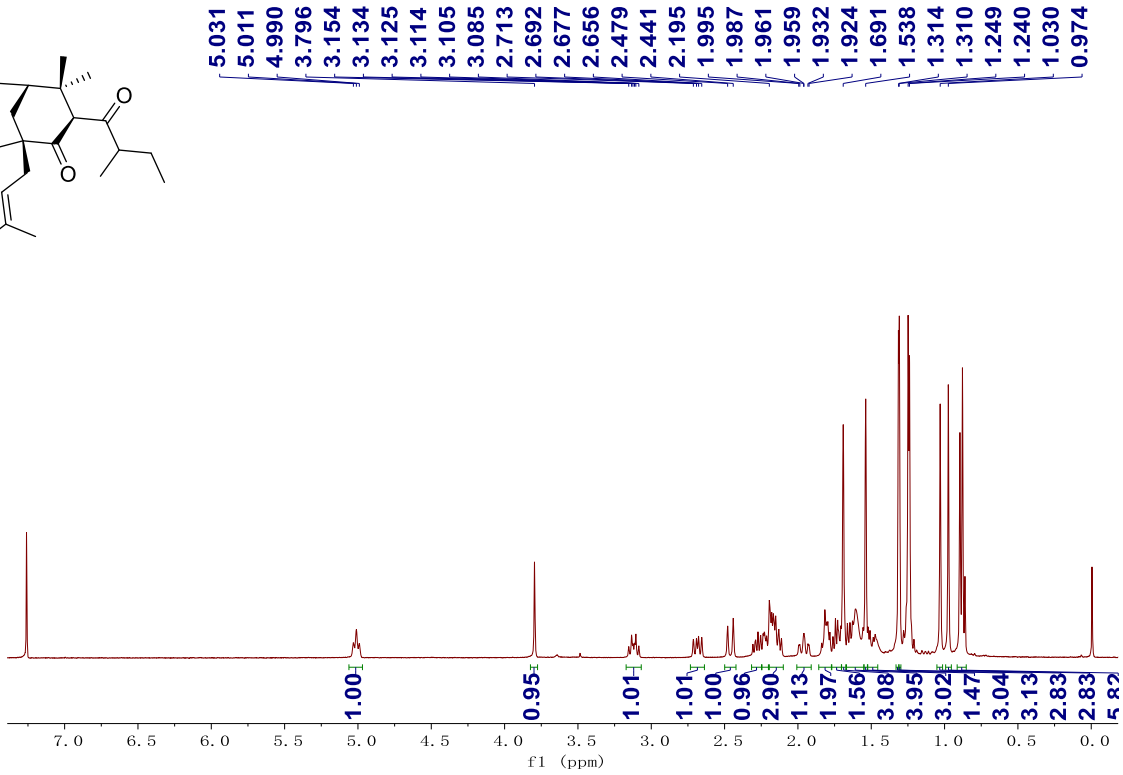


Figure S14. ^{13}C and DEPT NMR spectra of soniiglucinol B (**2**) in $CDCl_3$.

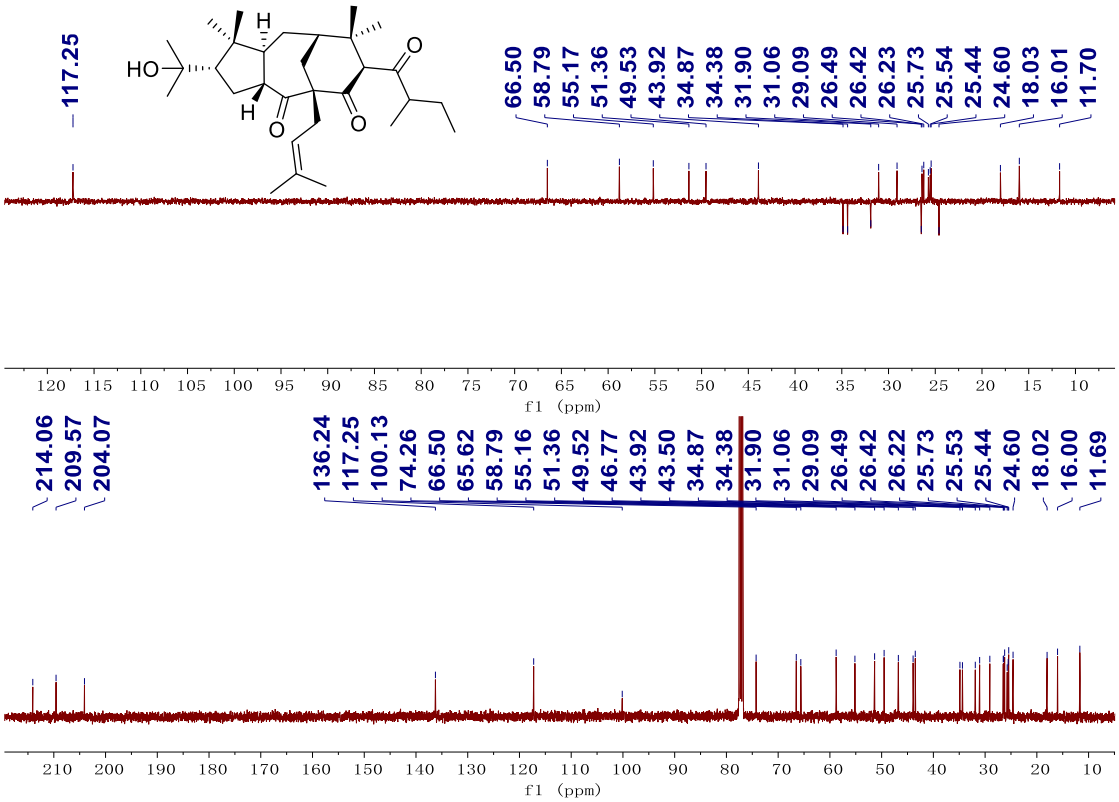


Figure S15. HSQC spectrum of soniiglucinol B (**2**) in $CDCl_3$.

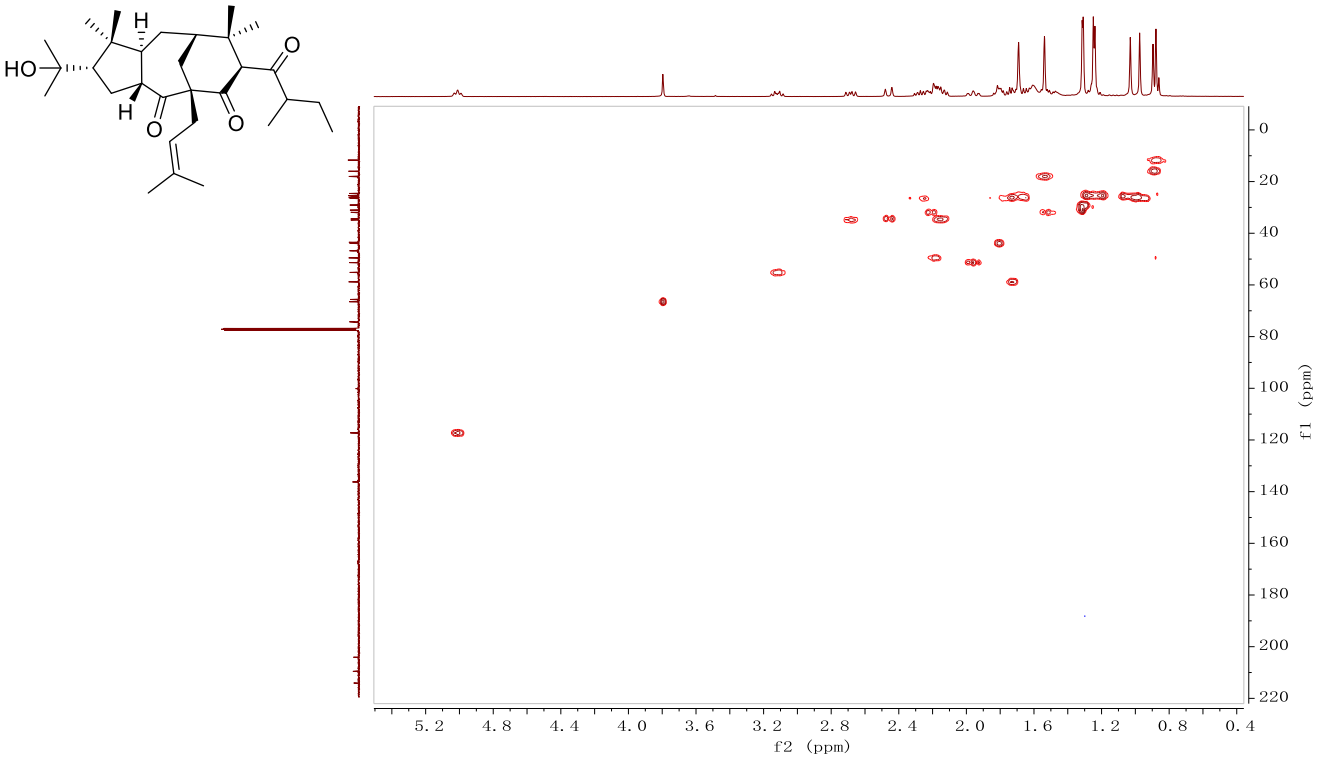


Figure S16. HMBC spectrum of soniiglucinol B (**2**) in $CDCl_3$.

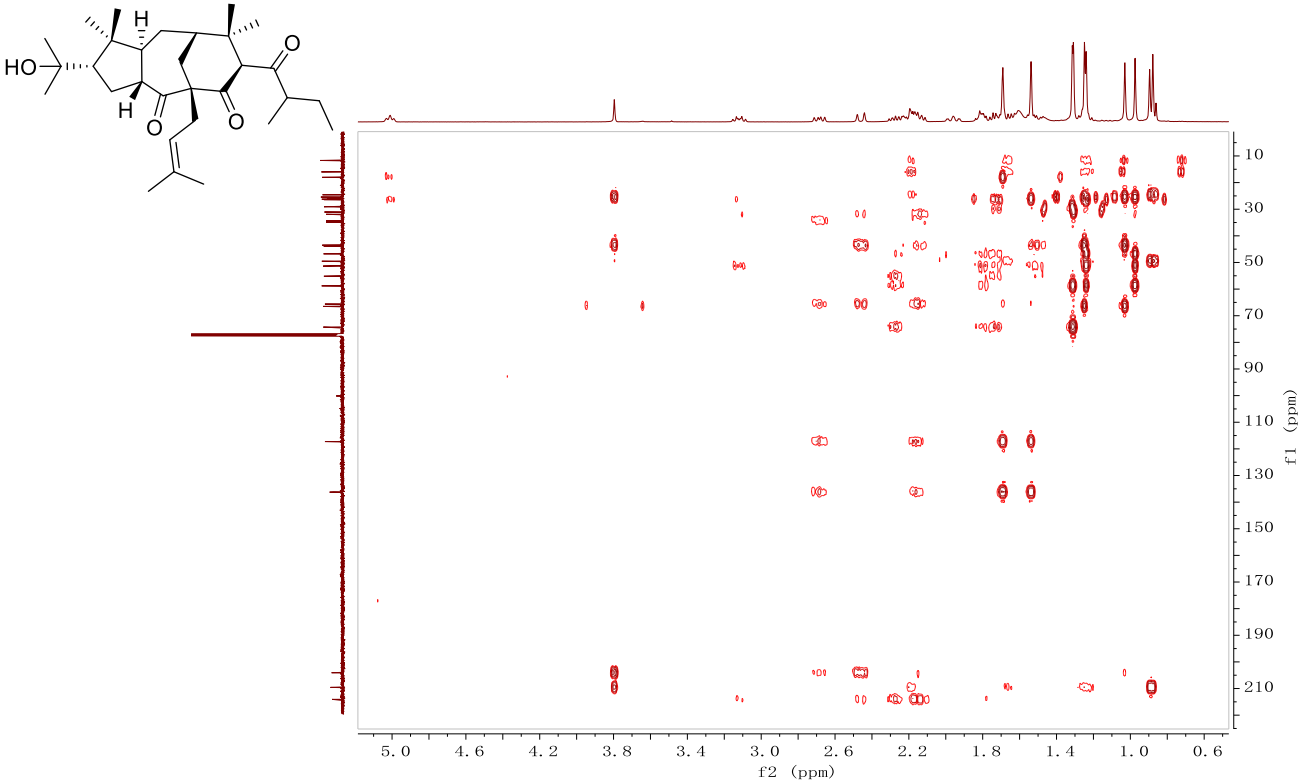


Figure S17. ^{1}H–^{1}H COSY spectrum of soniiglucinol B (**2**) in $CDCl_3$.

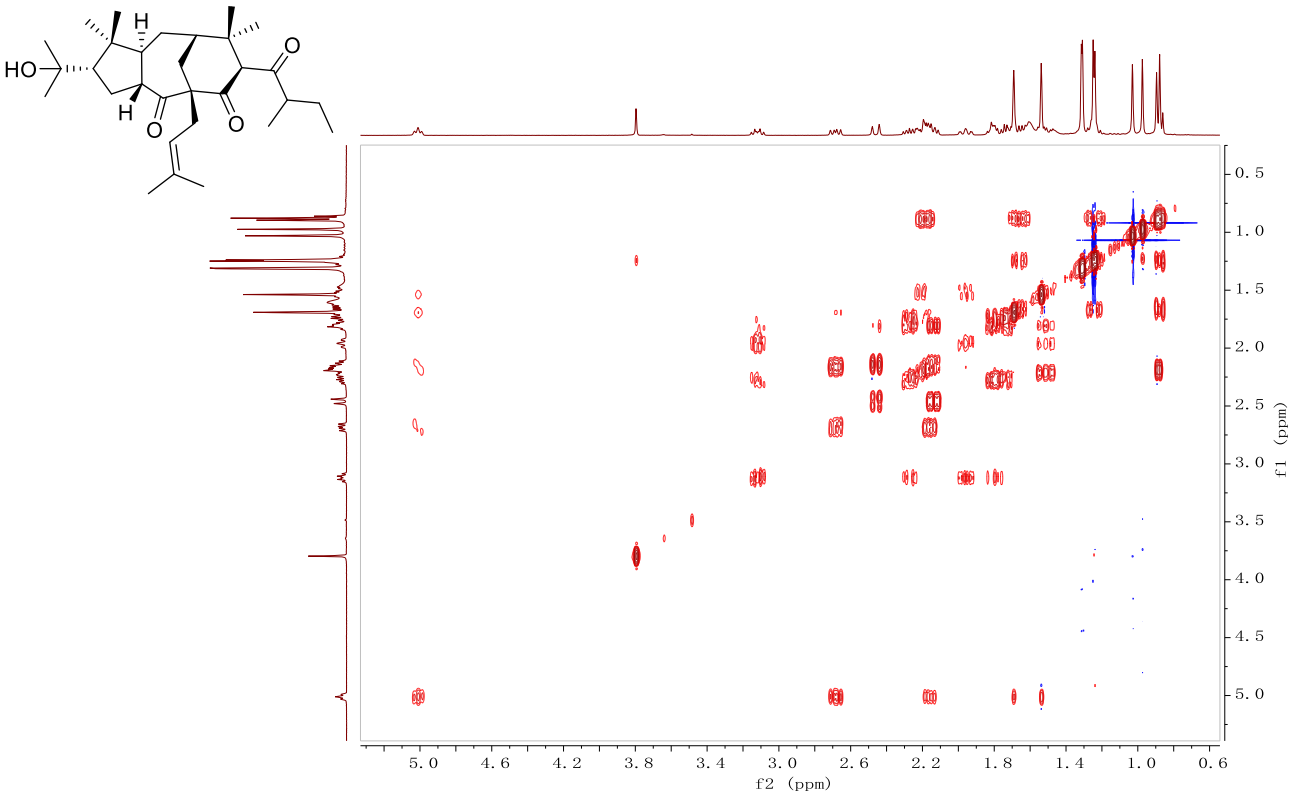


Figure S18. NOESY spectrum of soniiglucinol B (**2**) in $CDCl_3$.

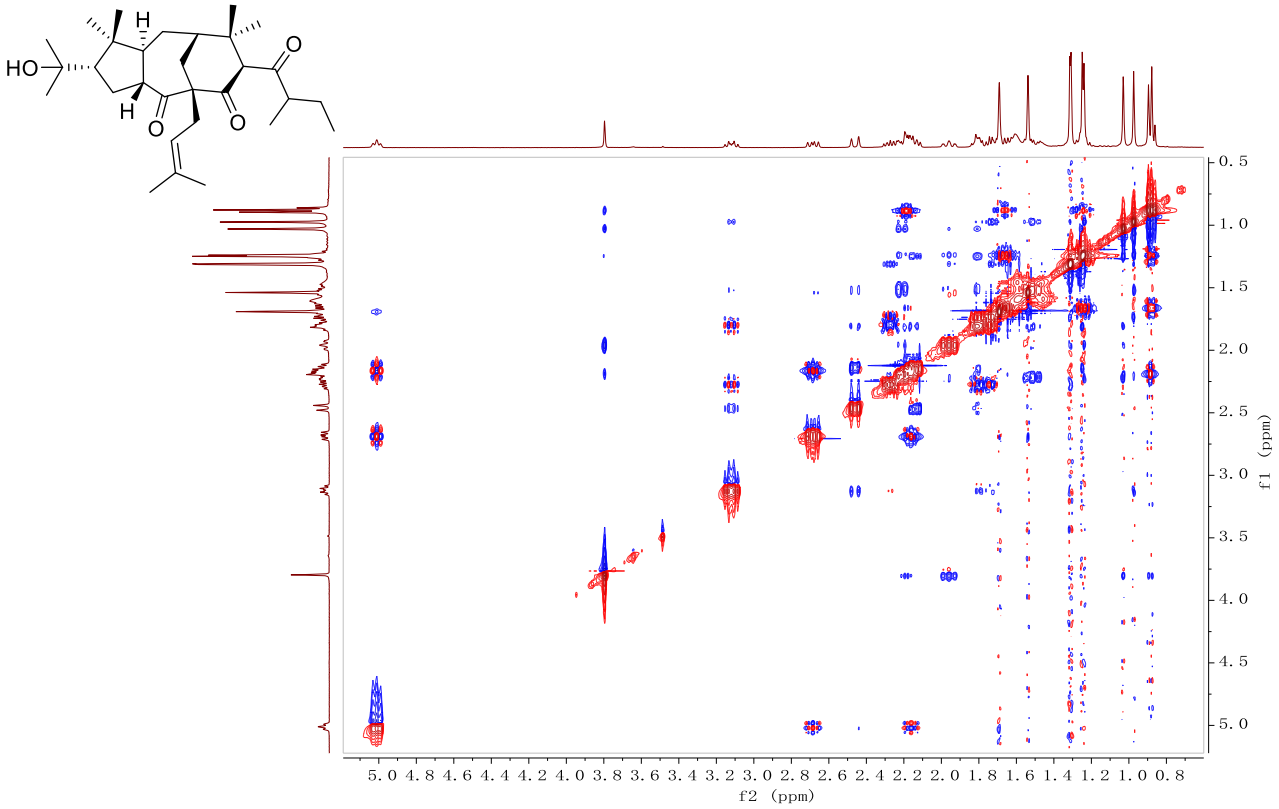


Figure S19. HRMSESI spectrum of soniiglucinol B (**2**) in $CDCl_3$.

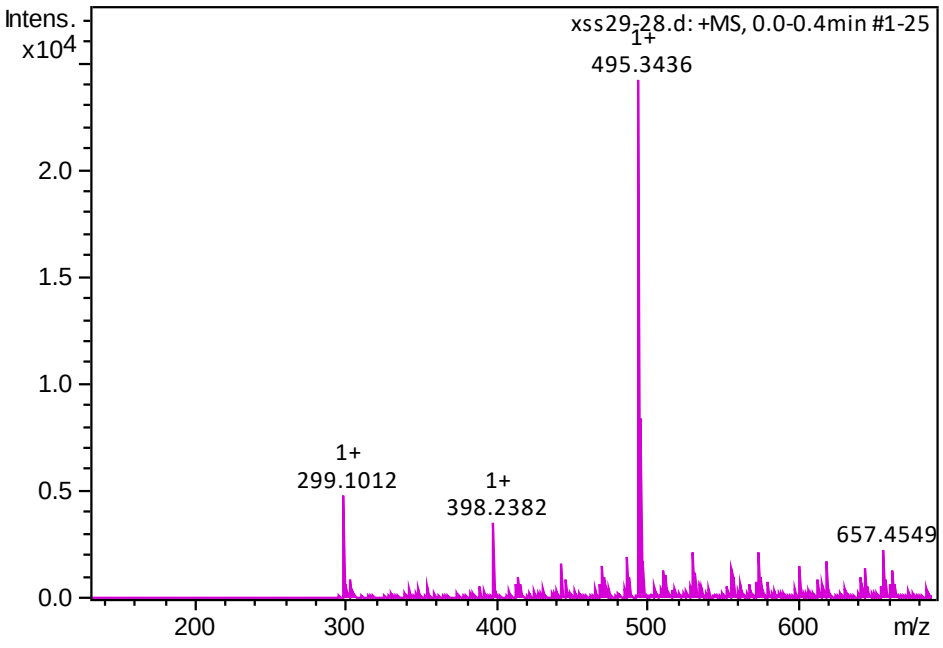


Figure S20. IR spectrum of soniiglucinol B (**2**) in $CDCl_3$.

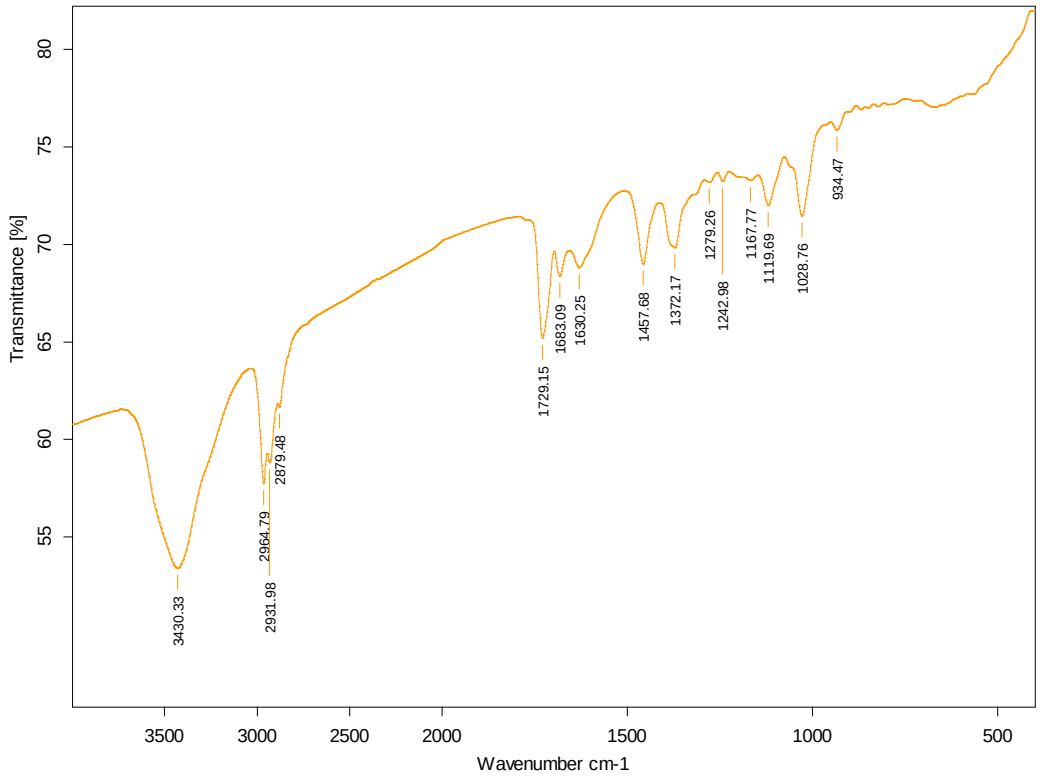


Figure S21. UV spectrum of soniiglucinol B (**2**) in $CDCl_3$.

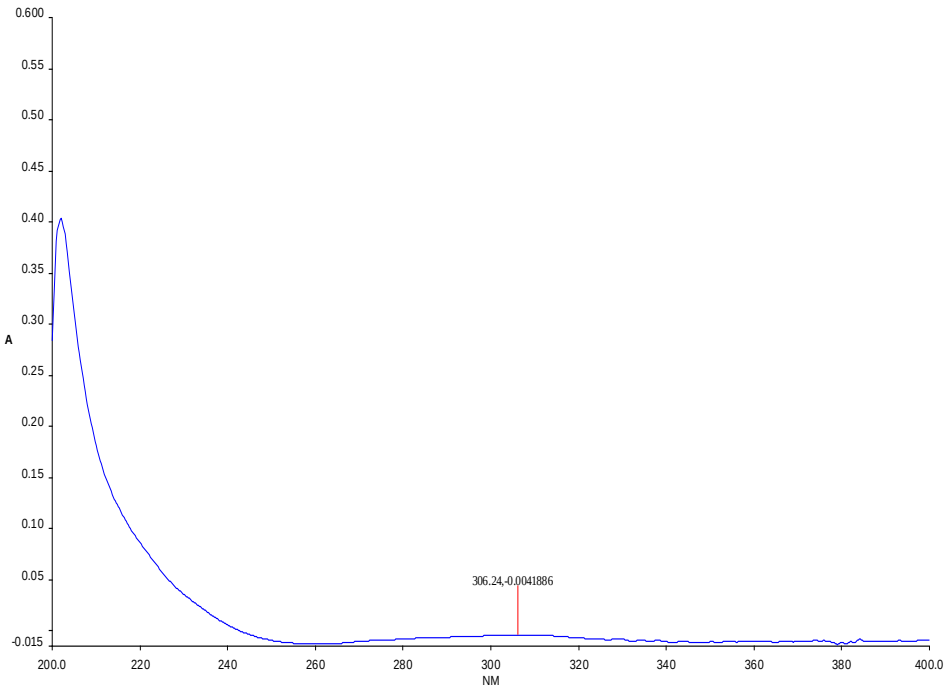


Figure S22. ^{1}H NMR spectrum of soniiglucinol C (**3**) in $CDCl_3$.

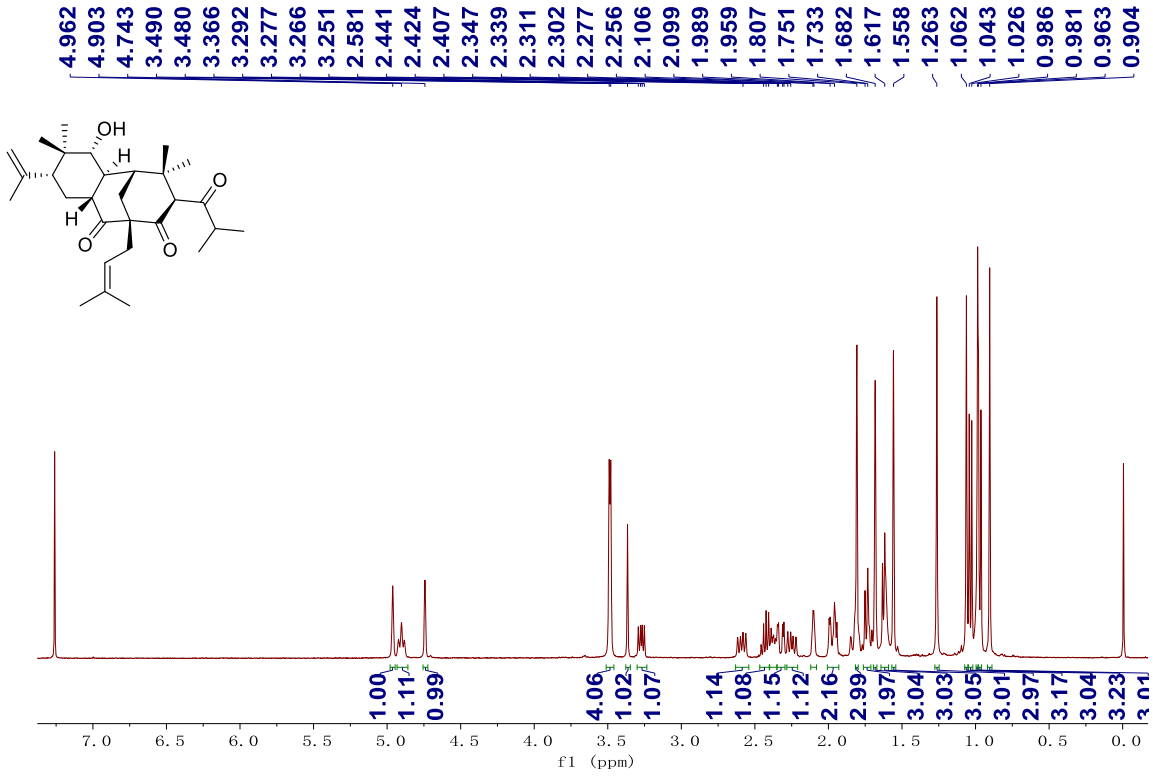


Figure S23. ^{13}C and DEPT NMR spectra of soniiglucinol C (**3**) in $CDCl_3$.

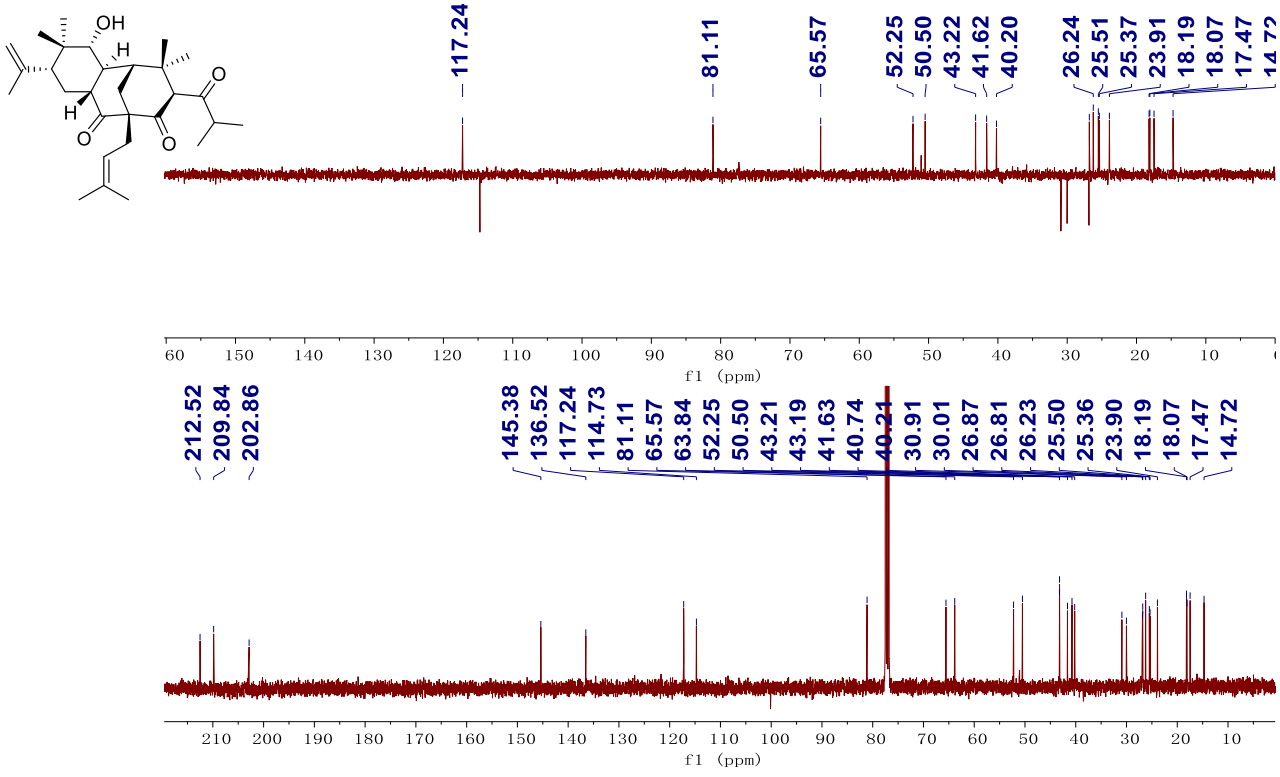


Figure S24. HSQC spectrum of soniiglucinol C (**3**) in $CDCl_3$.

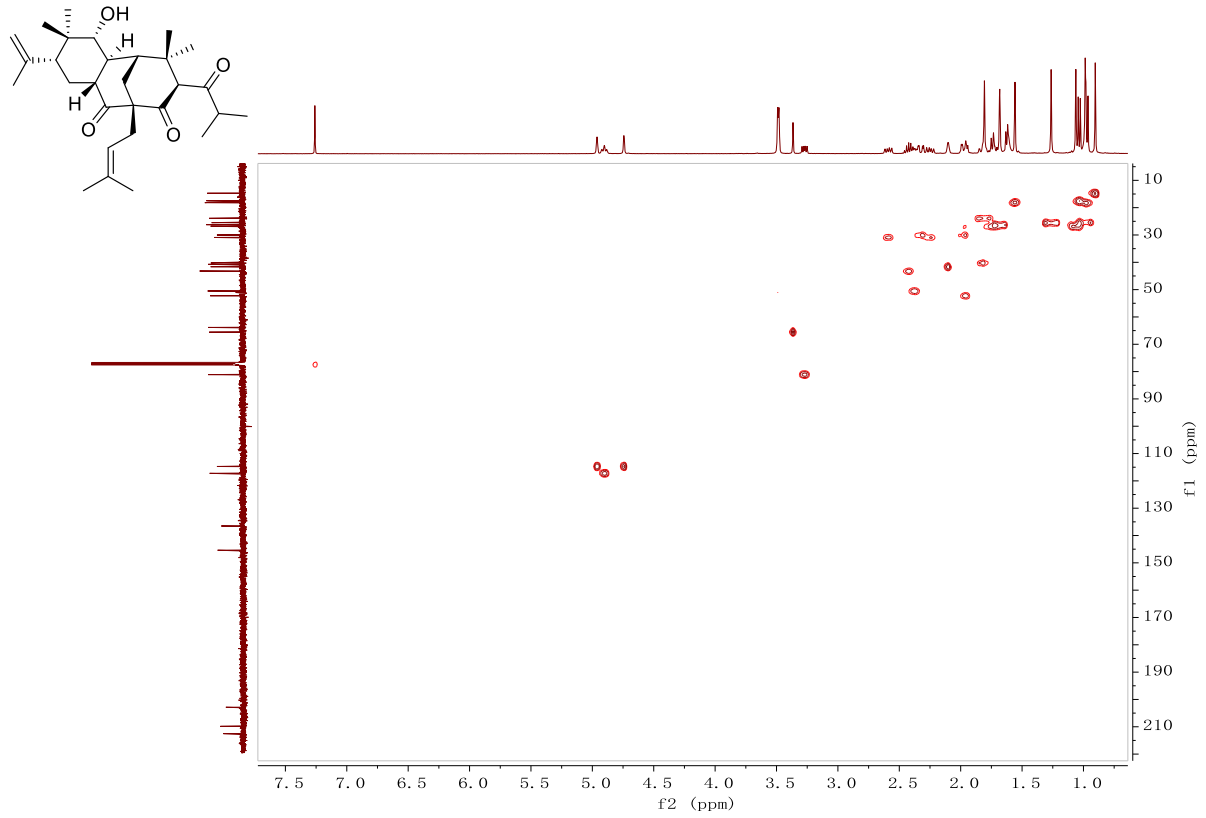


Figure S25. HMBC spectrum of soniiglucinol C (**3**) in $CDCl_3$.

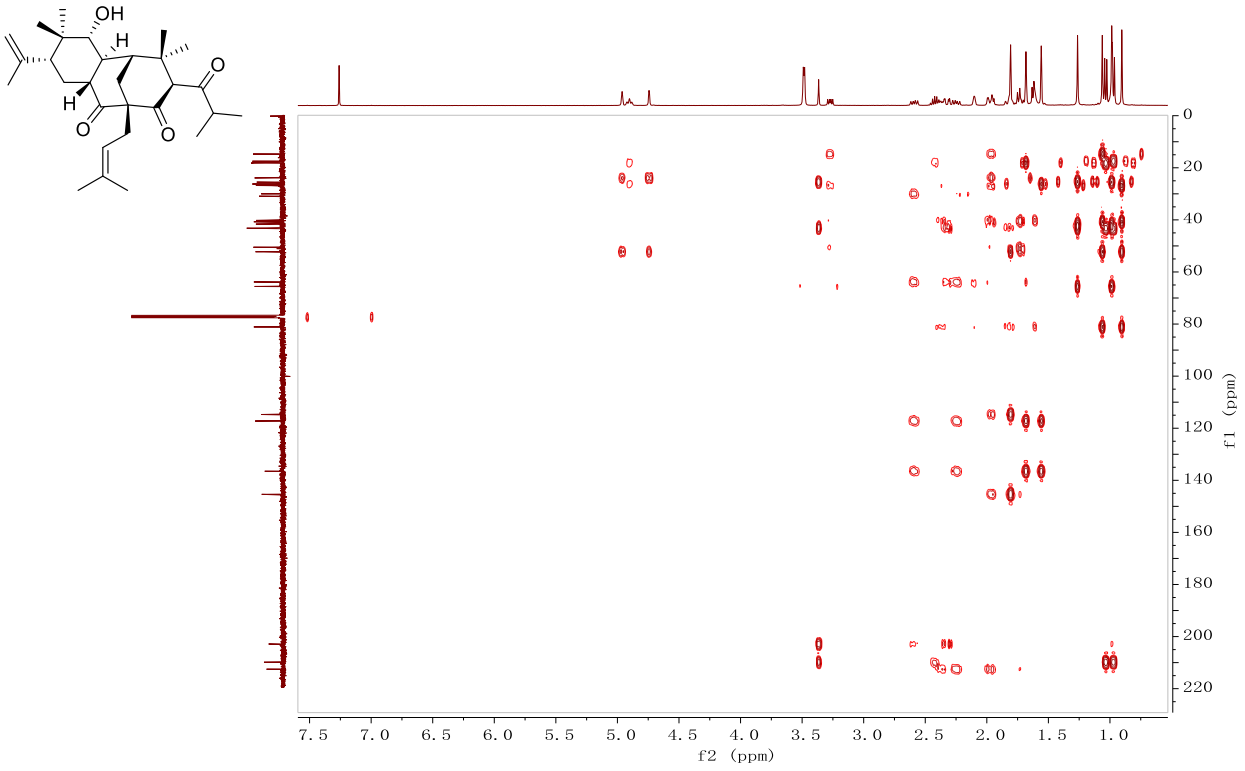


Figure S26. $^{1}H–^{1}H$ COSY spectrum of soniiglucinol C (**3**) in $CDCl_3$.

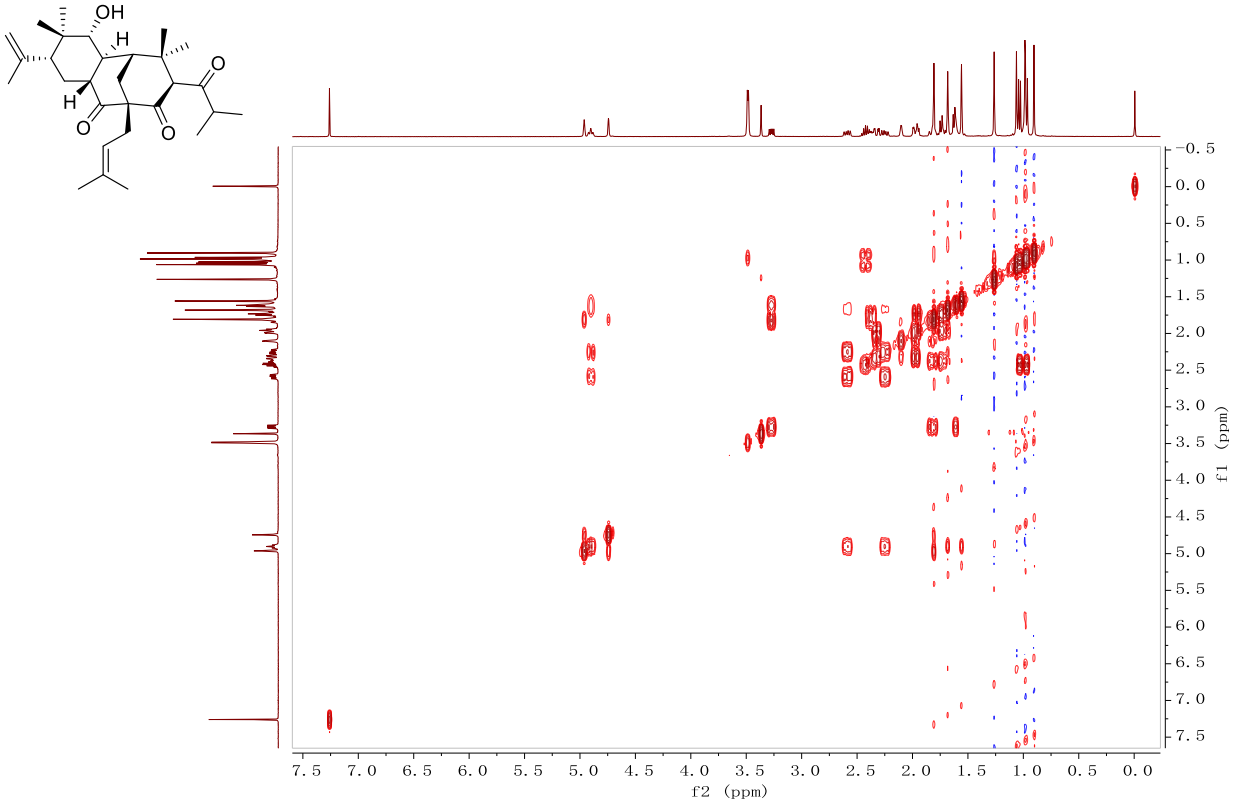


Figure S27. NOESY spectrum of soniiglucinol C (**3**) in $CDCl_3$.

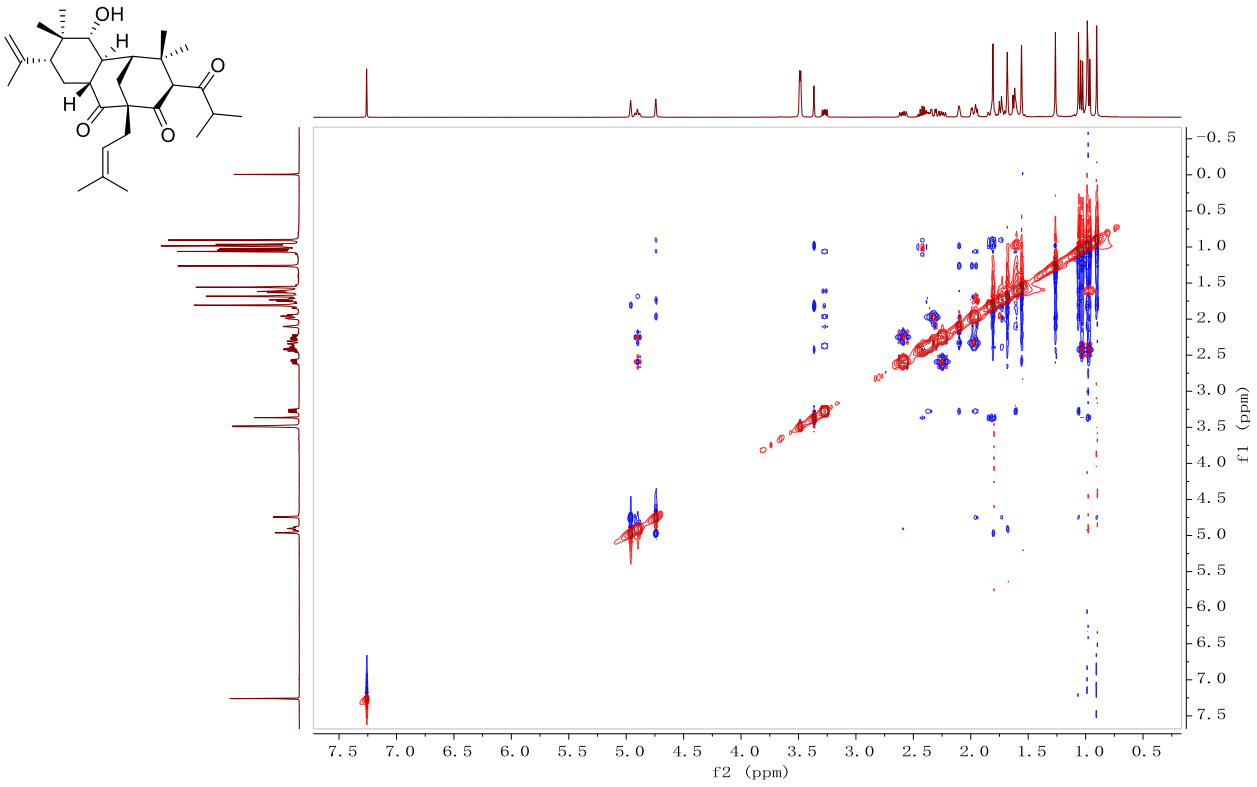


Figure S28. HRESIMS spectrum of soniiglucinol C (**3**).

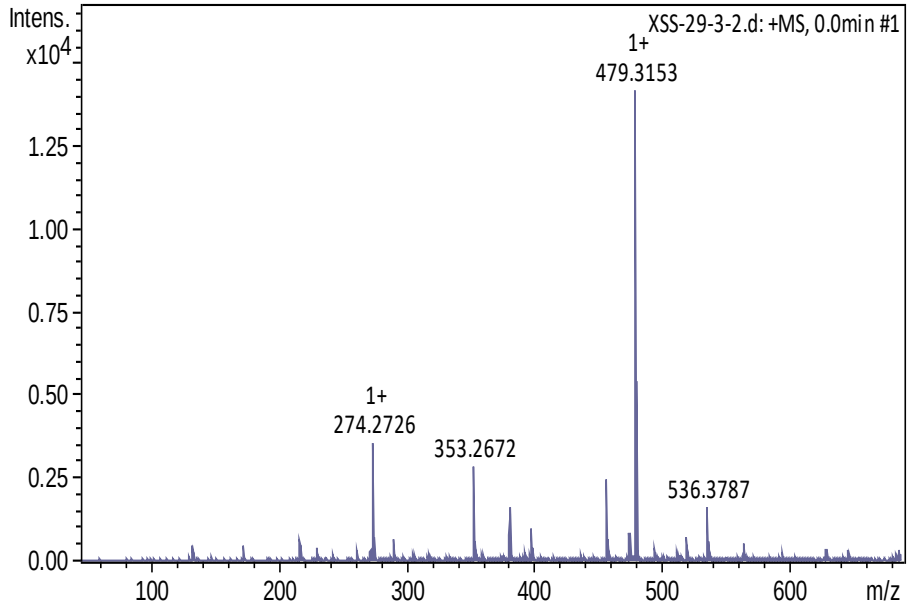


Figure S29. UV spectrum of soniiglucinol C (**3**).

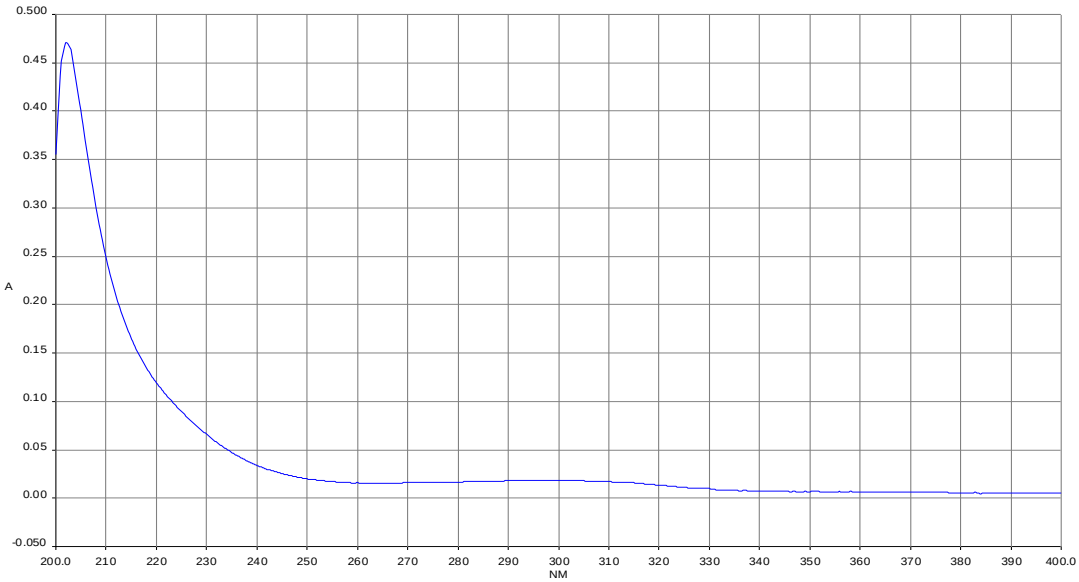


Figure S30. IR spectrum of soniiglucinol C (**3**).

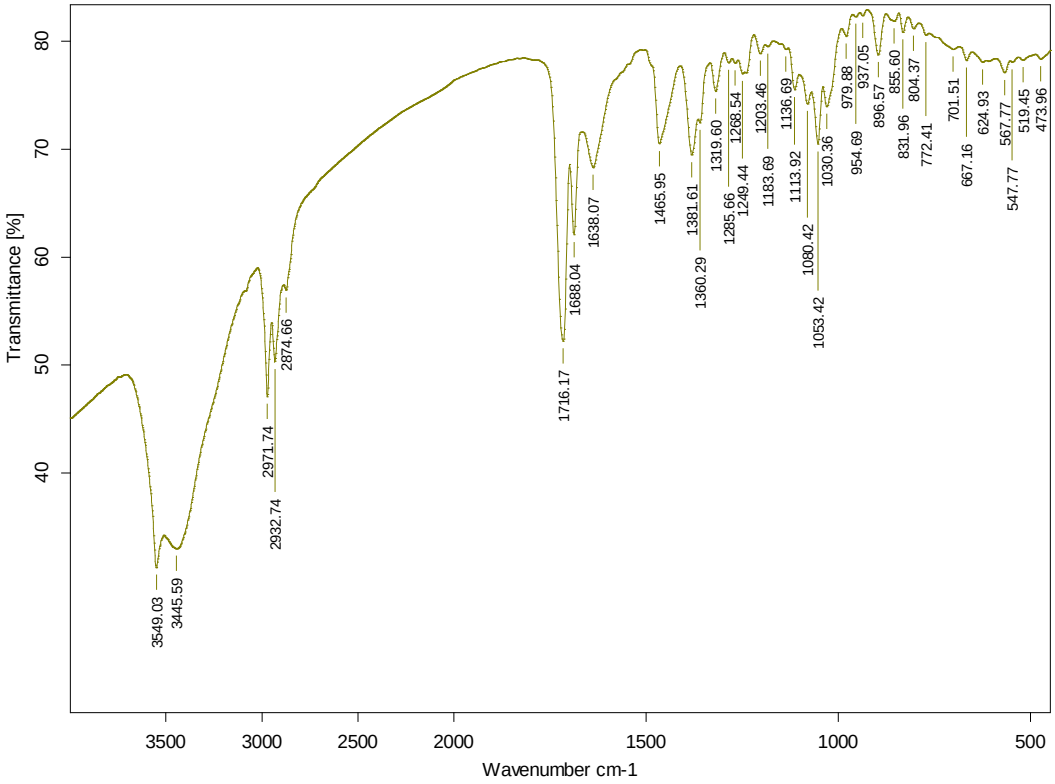


Figure S31. ^{1}H NMR spectrum of soniiglucinol D (**4**) in $CDCl_3$.

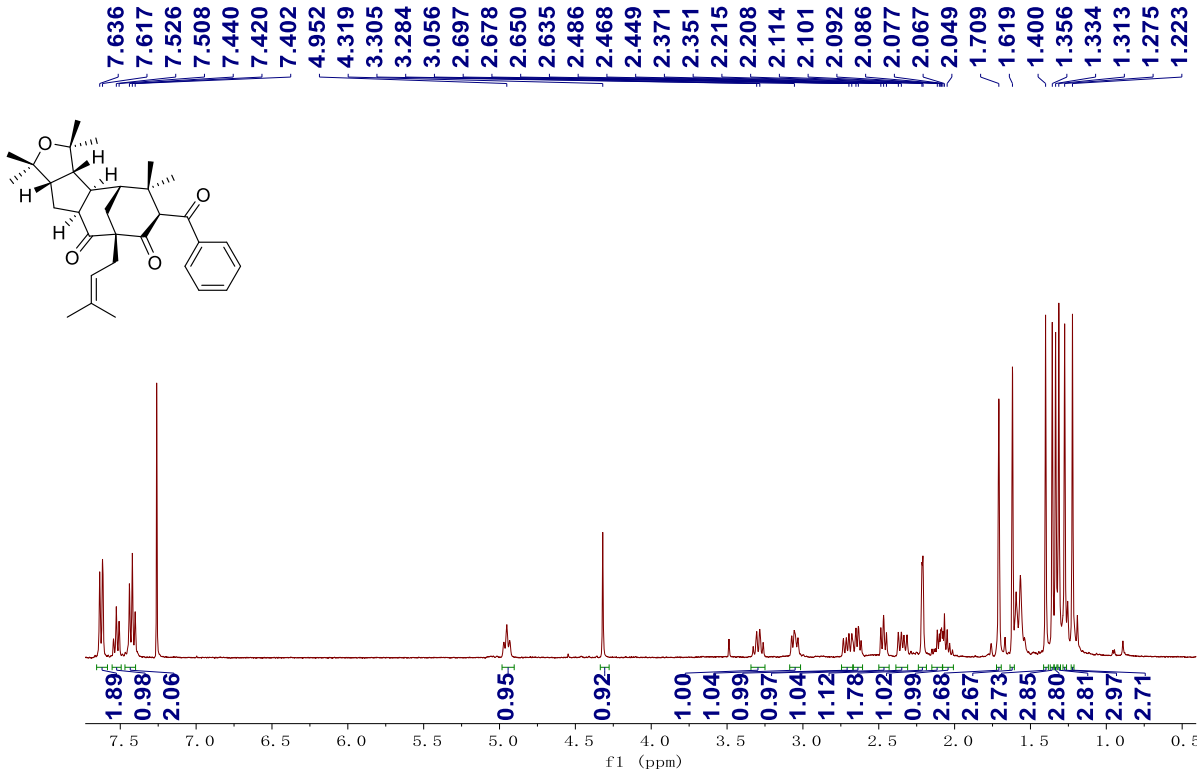


Figure S32. ^{13}C and DEPT NMR spectra of soniiglucinol D (**4**) in $CDCl_3$.

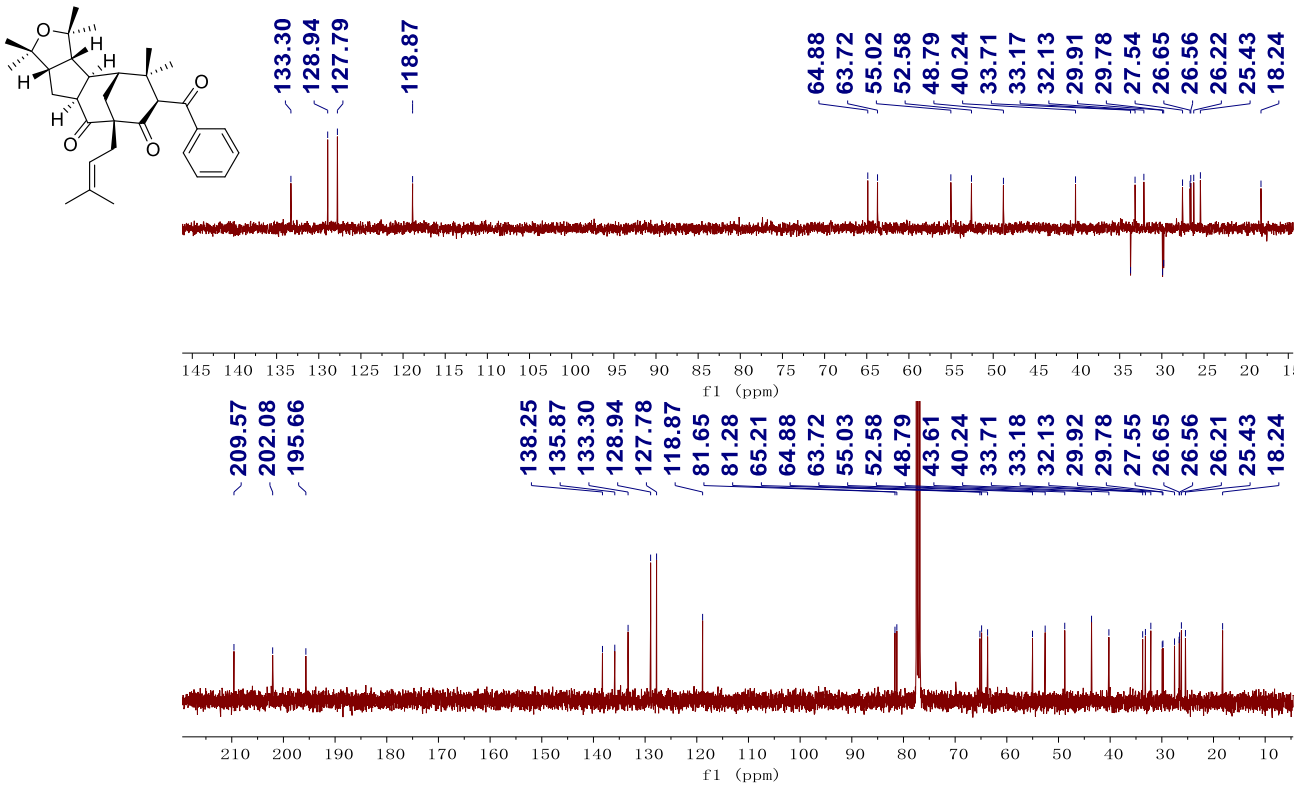


Figure S33. HSQC spectrum of soniiglucinol D (**4**) in $CDCl_3$.

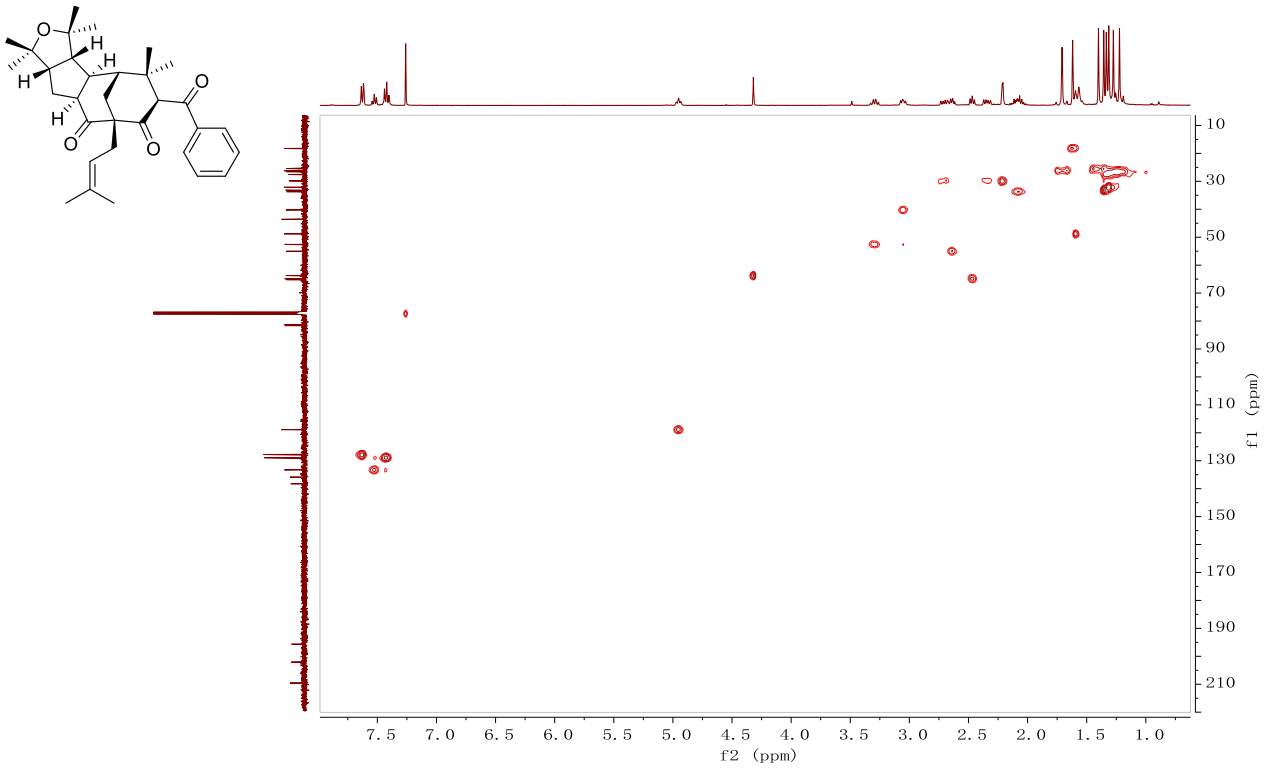


Figure S34. HMBC spectrum of soniiglucinol D (**4**) in $CDCl_3$.

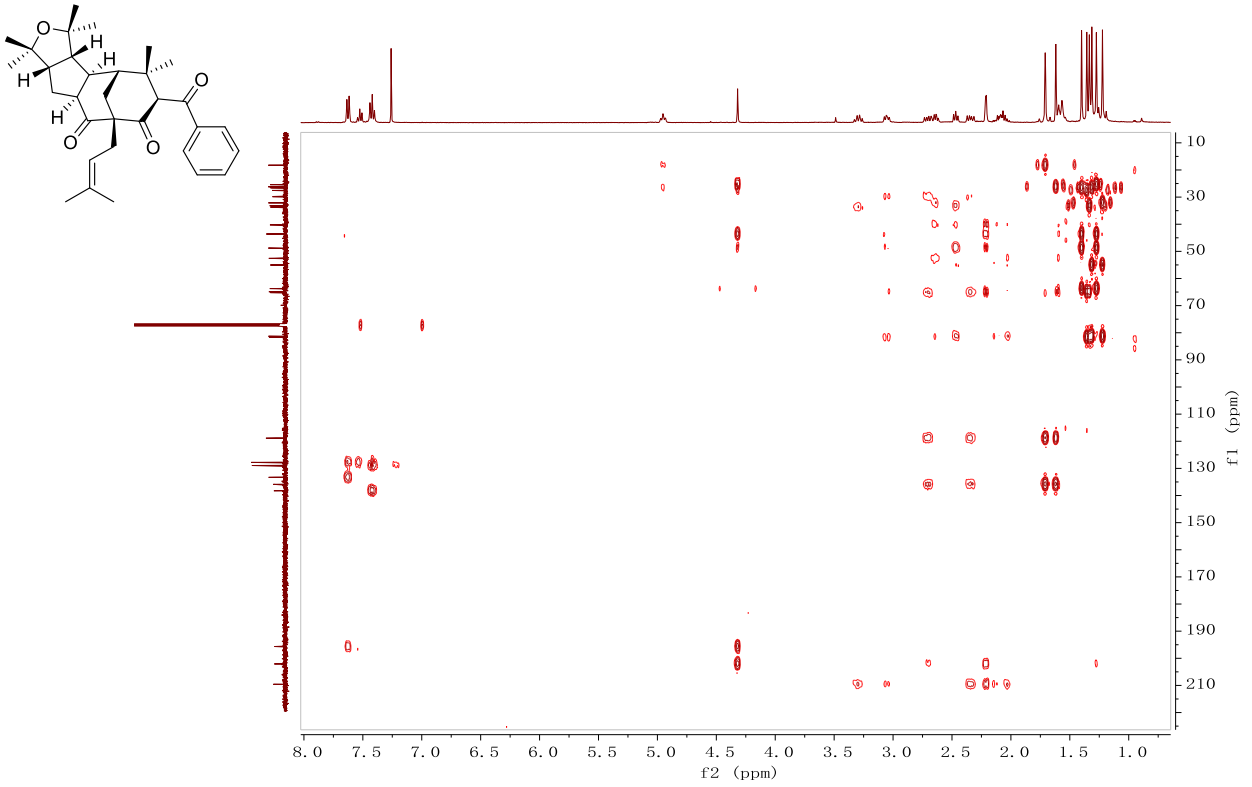


Figure S35. ^1H–^1H COSY spectrum of soniiglucinol D (**4**) in $CDCl_3$.

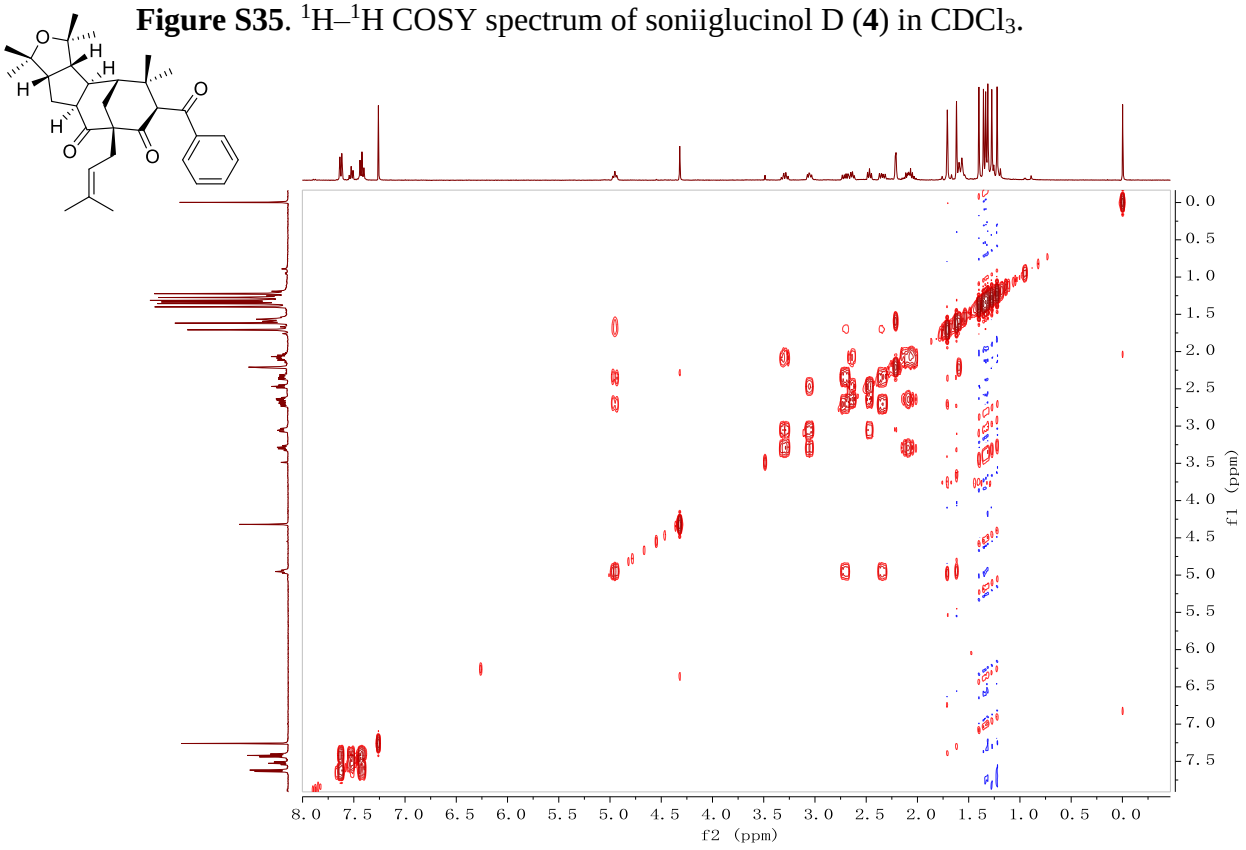


Figure S36. NOESY spectrum of soniiglucinol D (**4**) in $CDCl_3$.

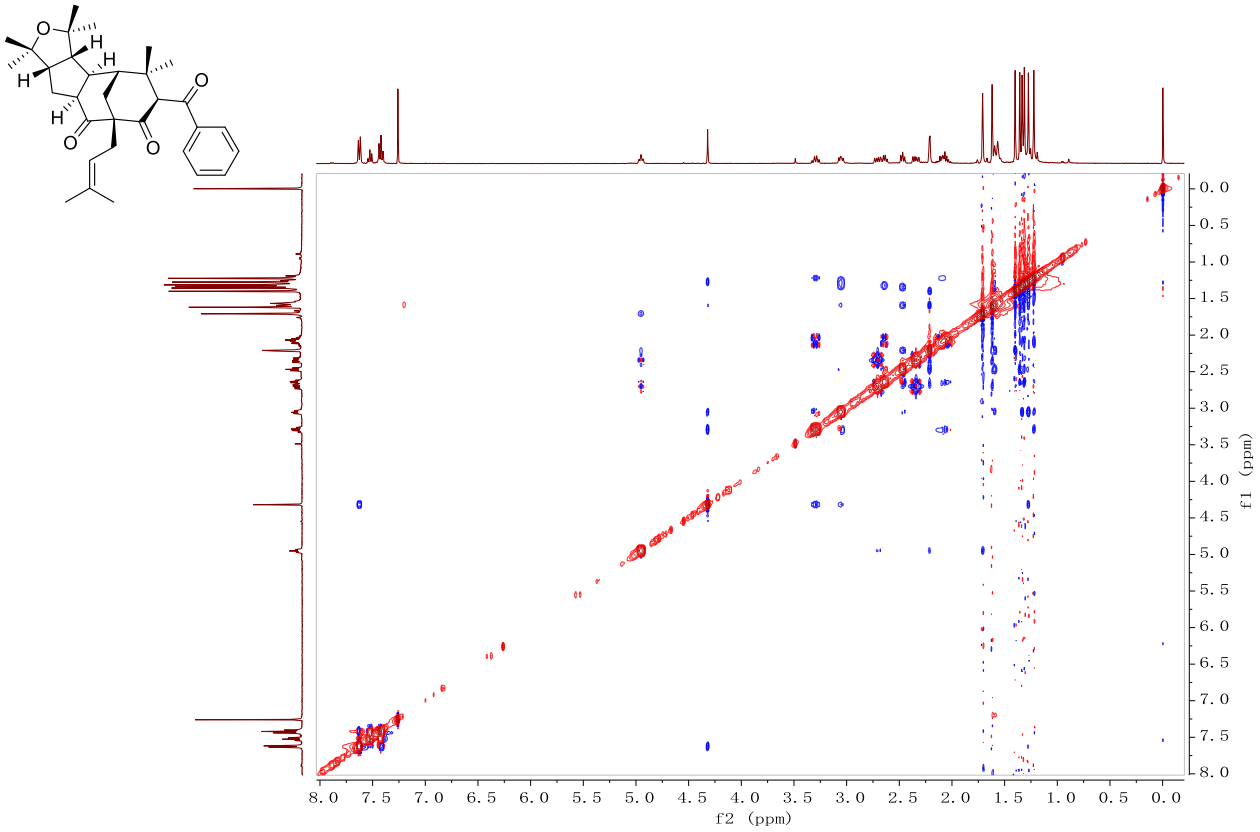


Figure S37. HRESIMS spectrum of soniiglucinol D (**4**).

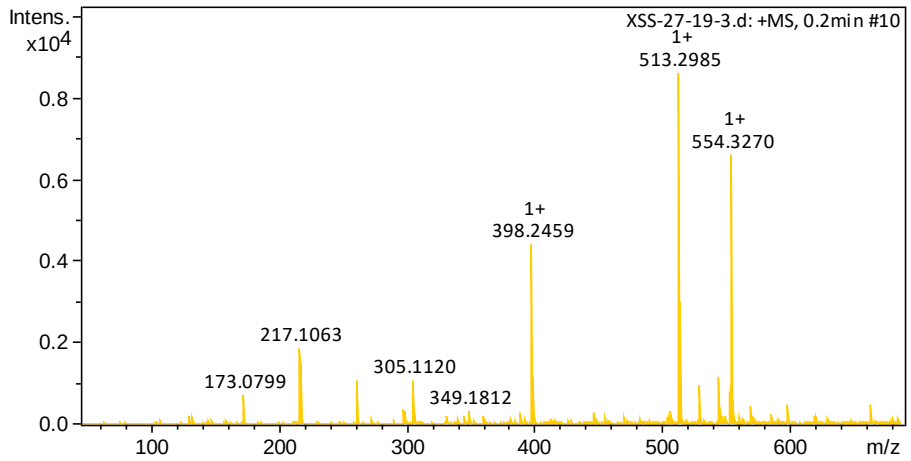


Figure S38. UV spectrum of soniiglucinol D (**4**).

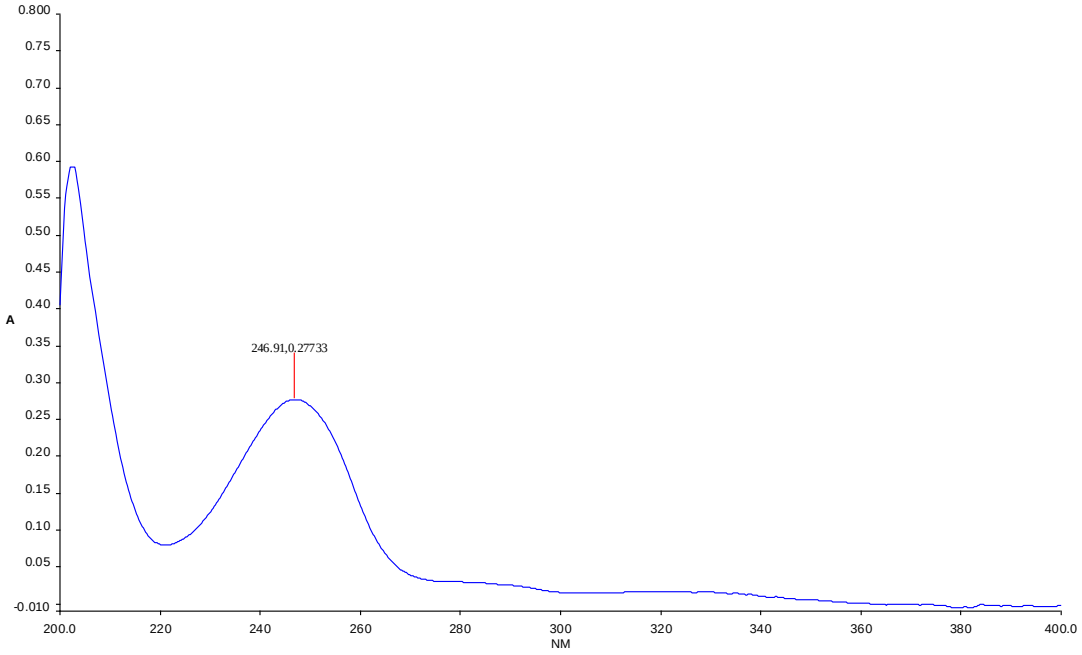


Figure S39. IR spectrum of soniiglucinol D (**4**).