Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Fusaresters A–E, new *γ*-pyrone-containing polyketides from fungus *Fusarium* sp. Hungcl and structure revision of fusariumin D

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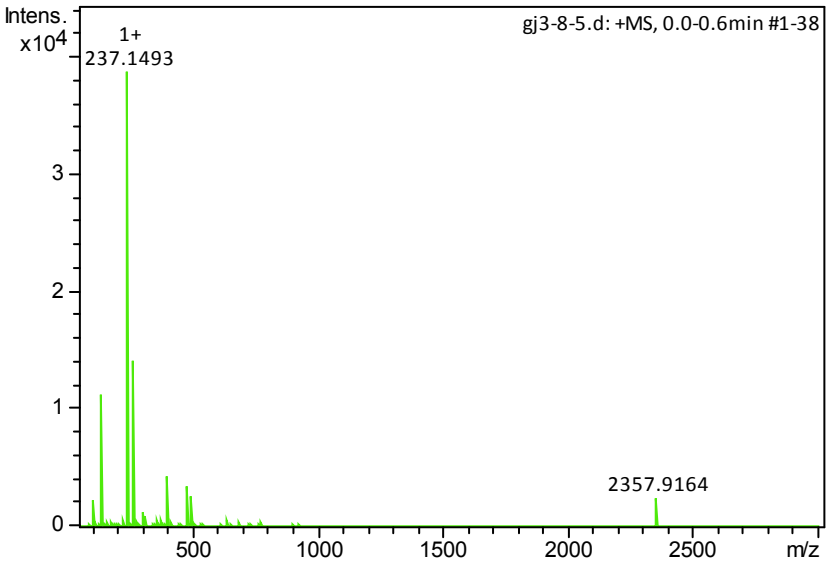

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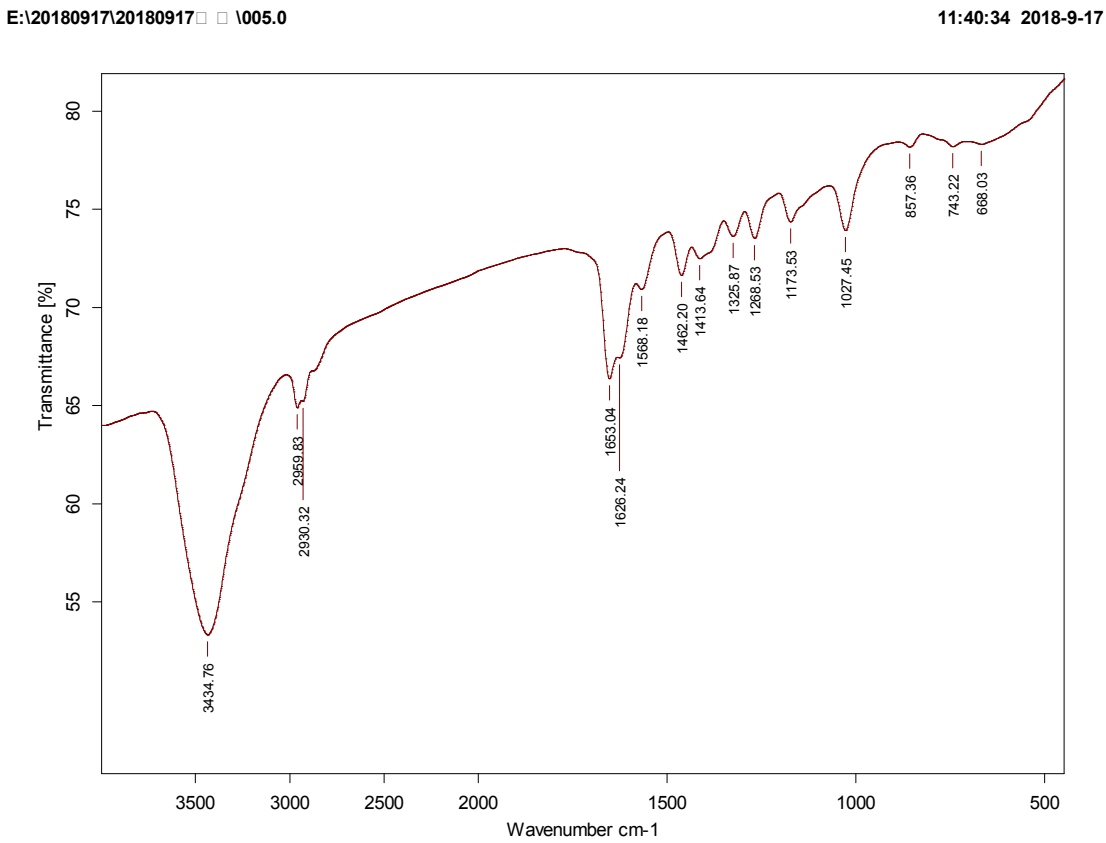

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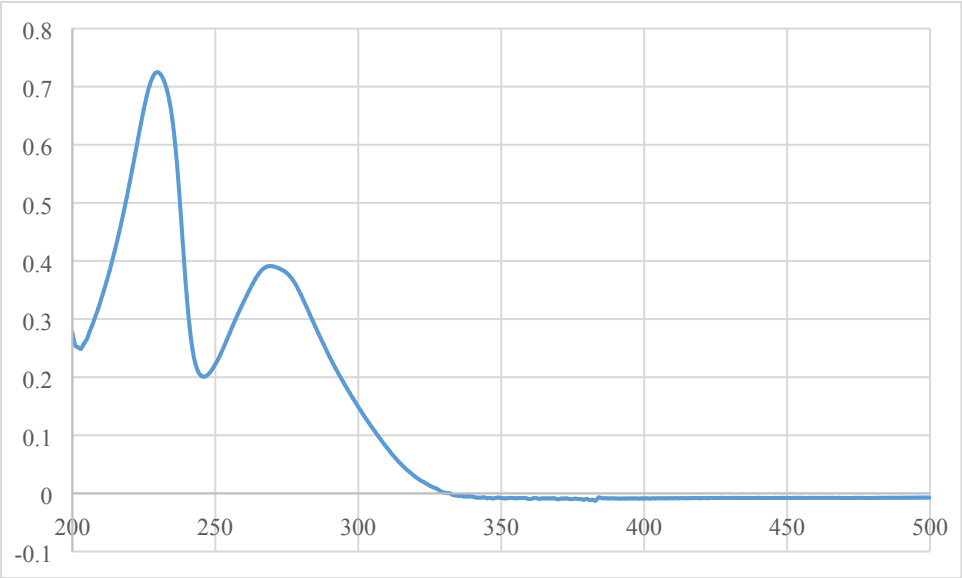

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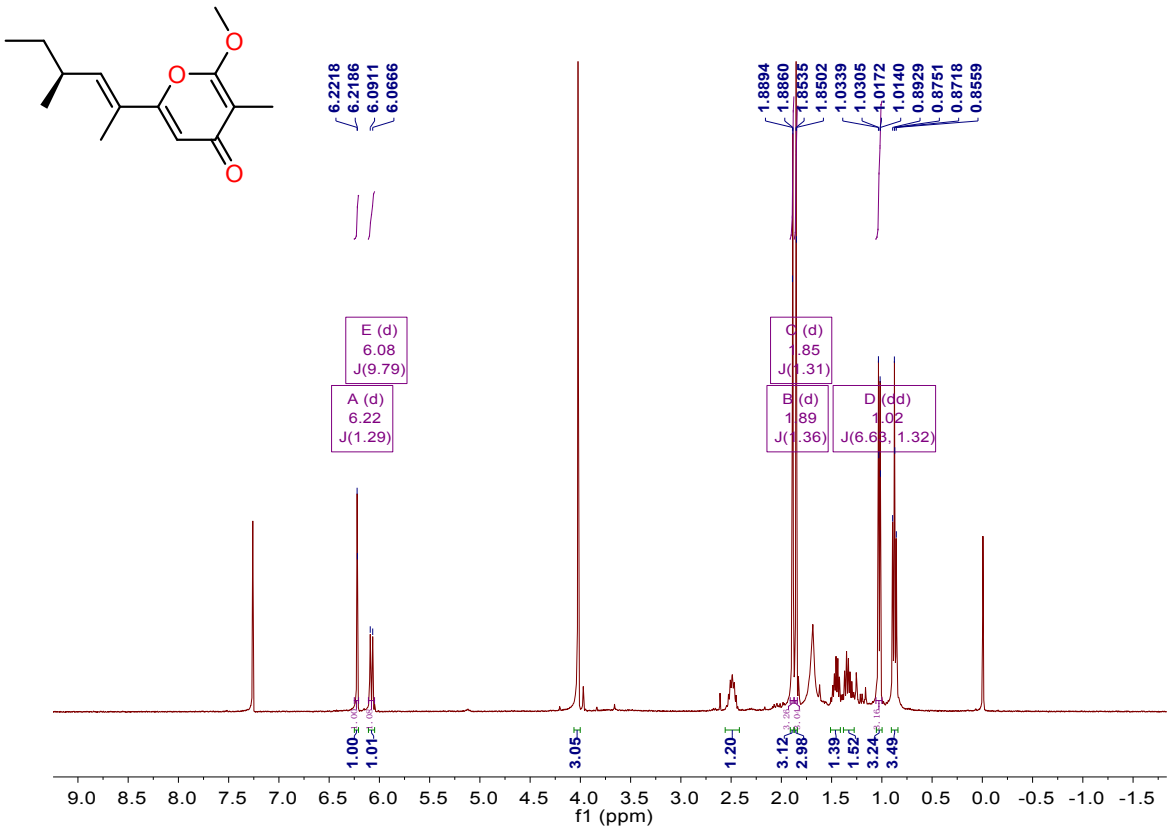

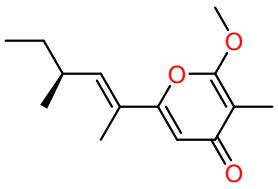

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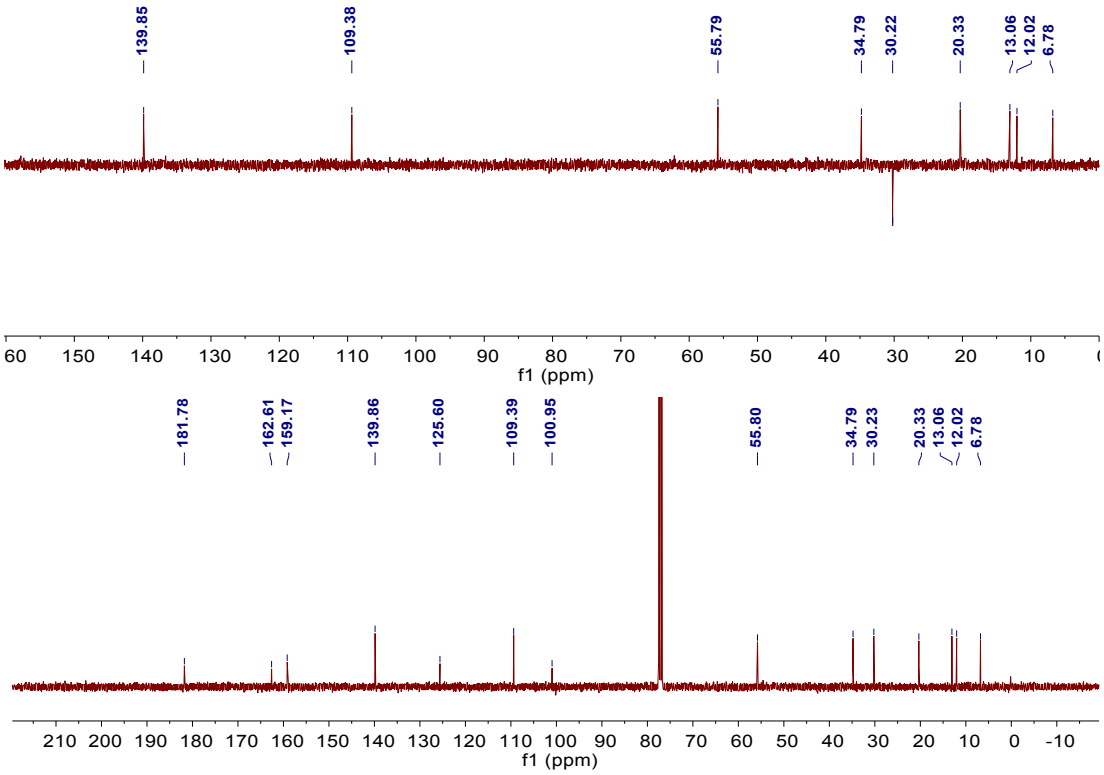

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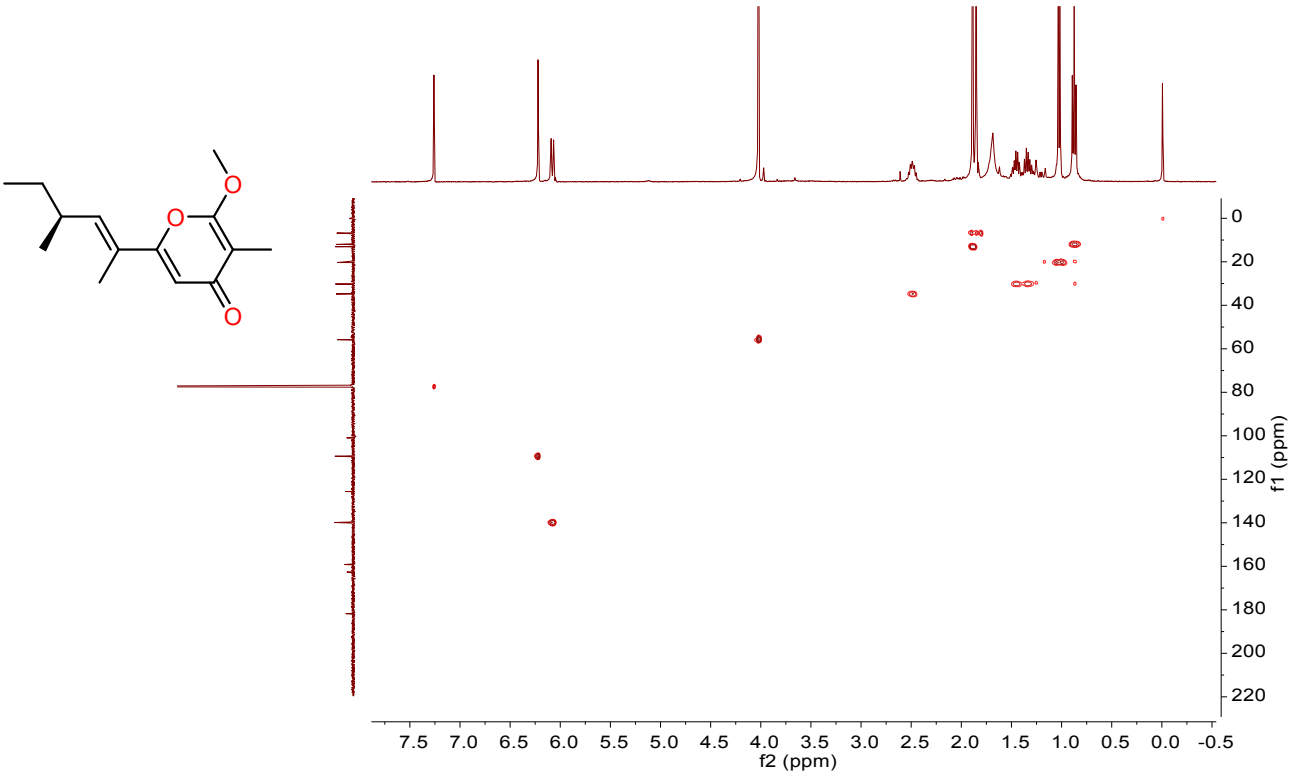

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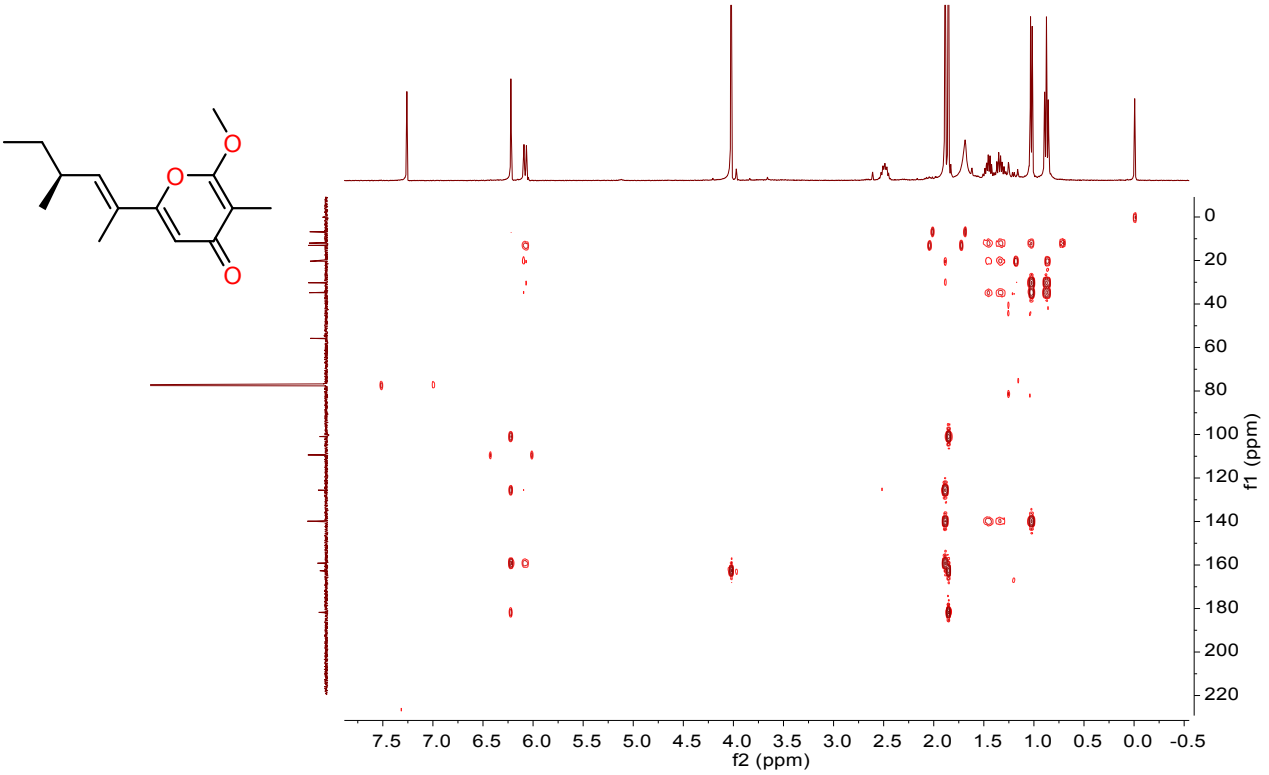

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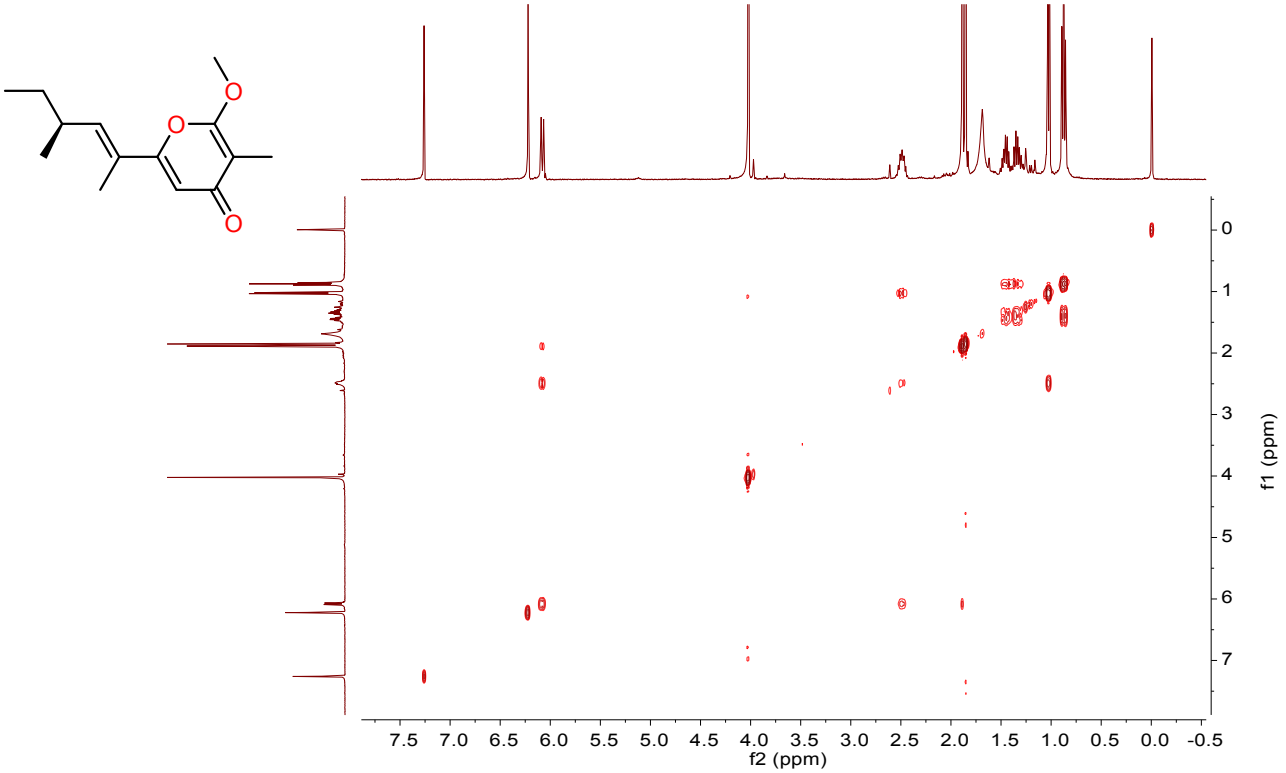

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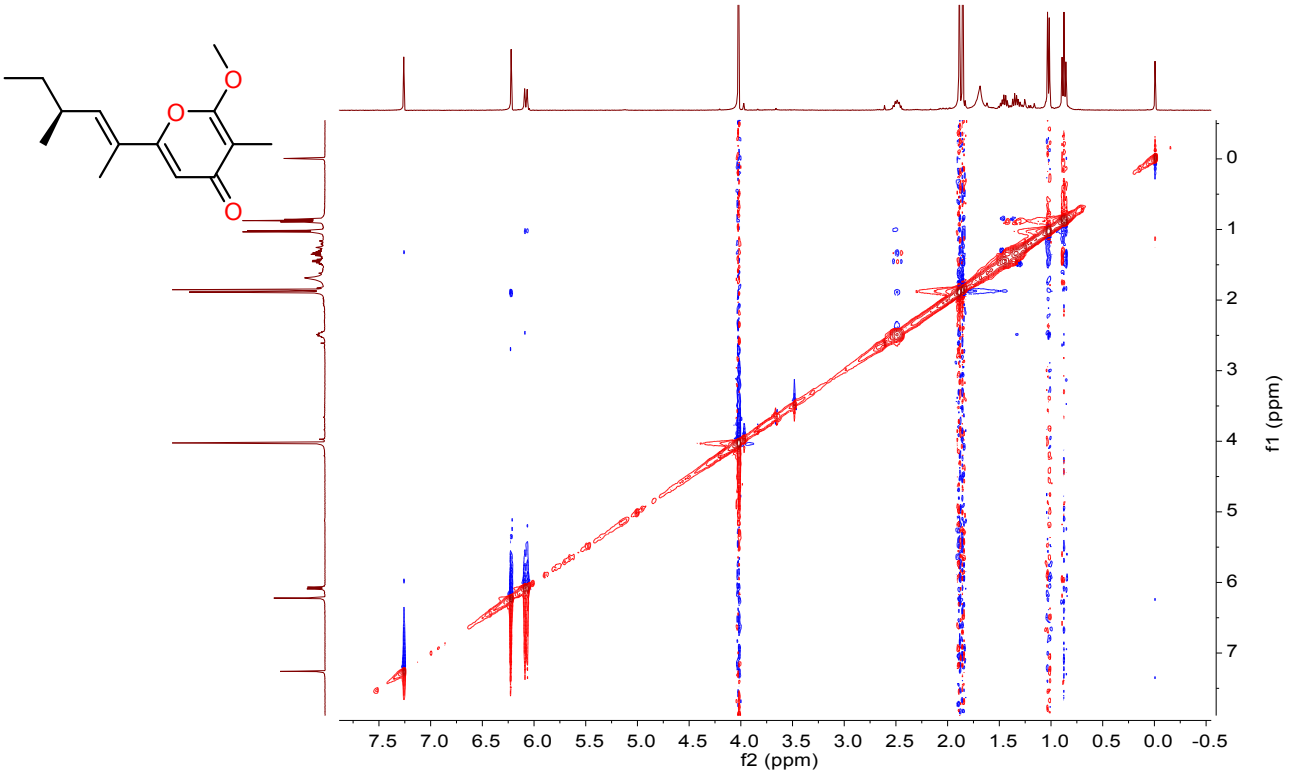

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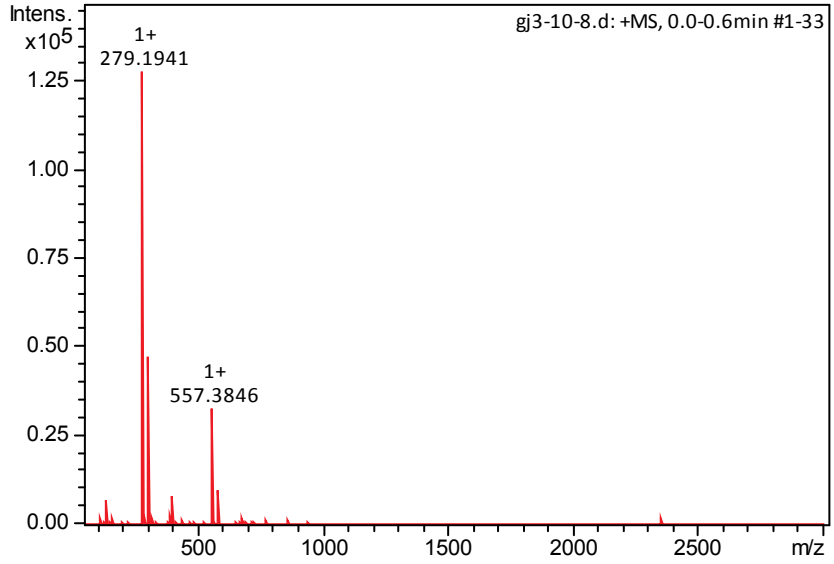

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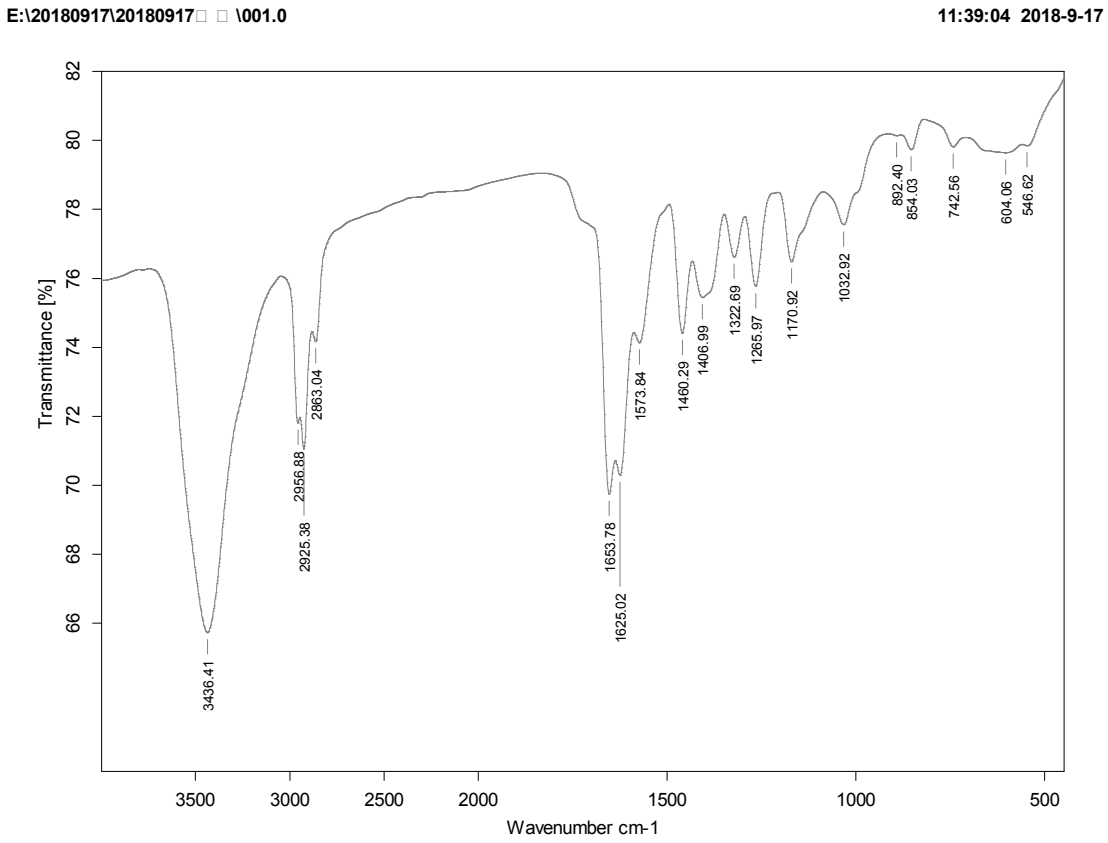

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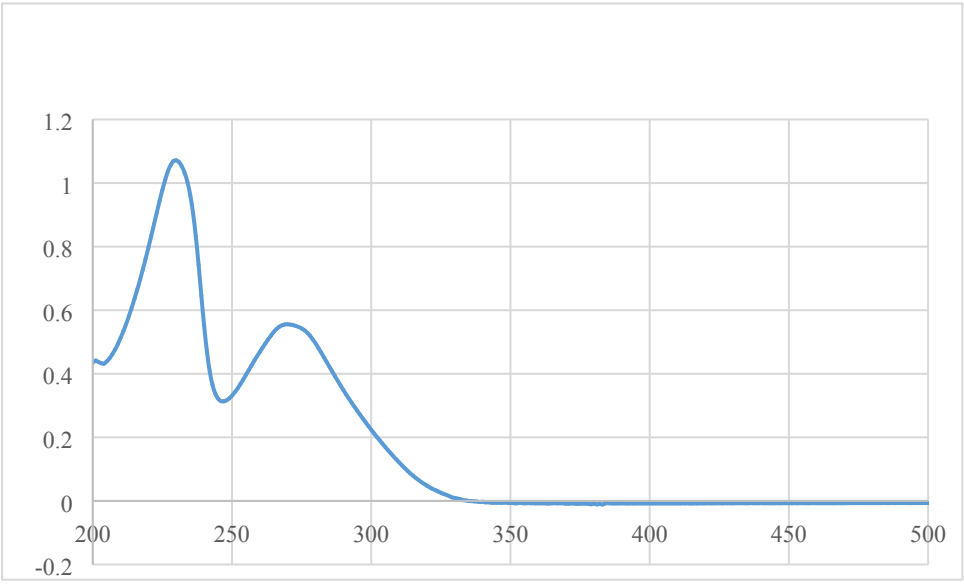

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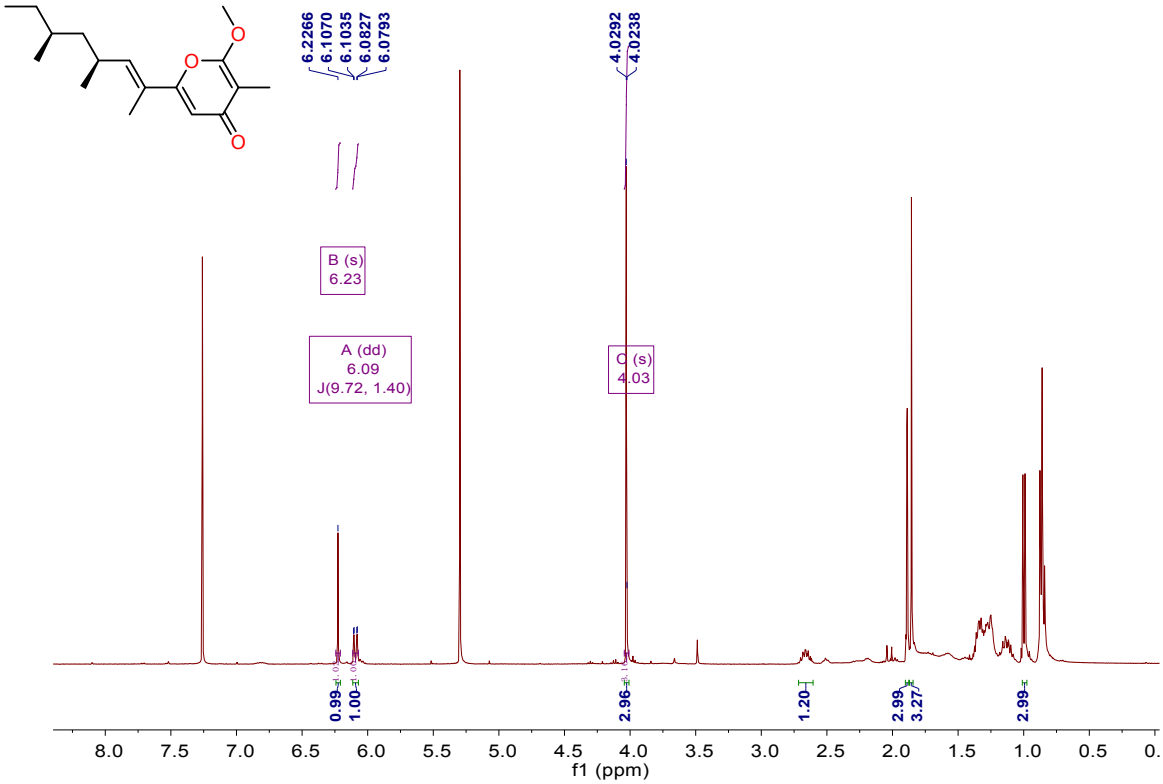

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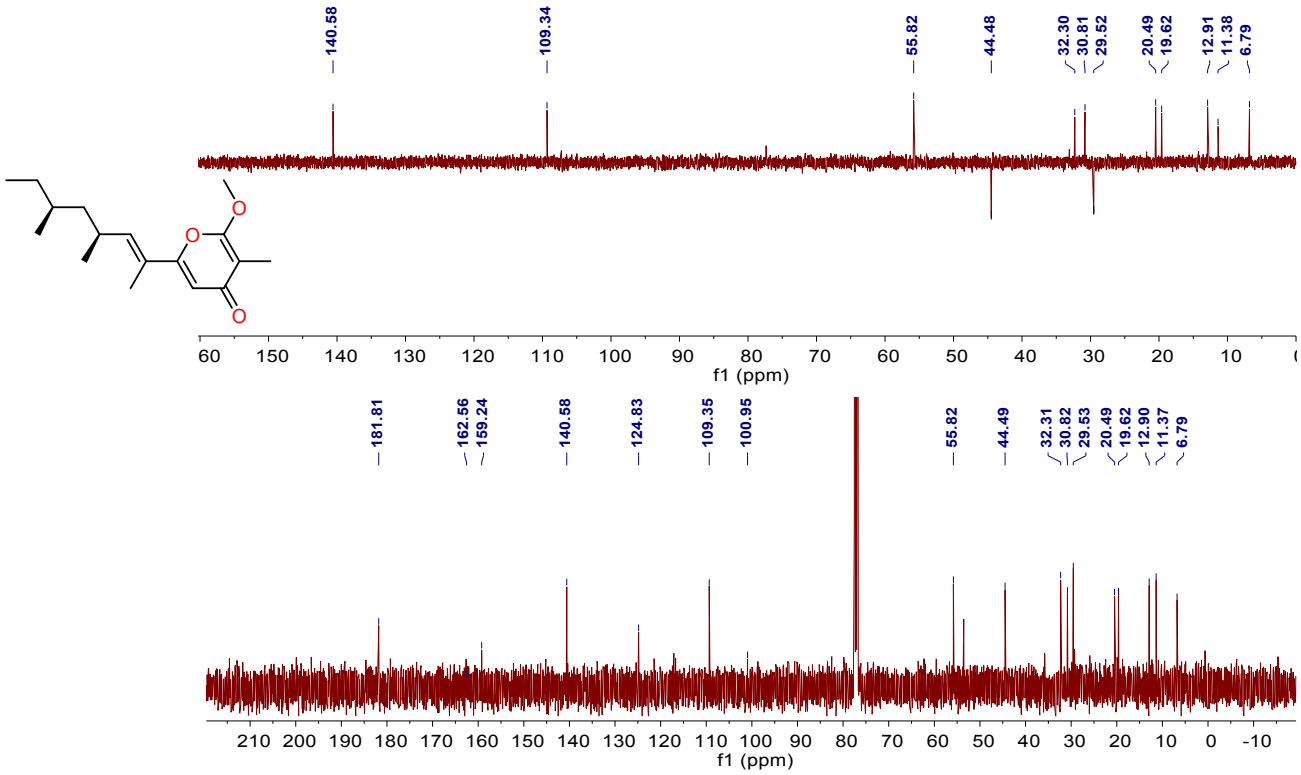

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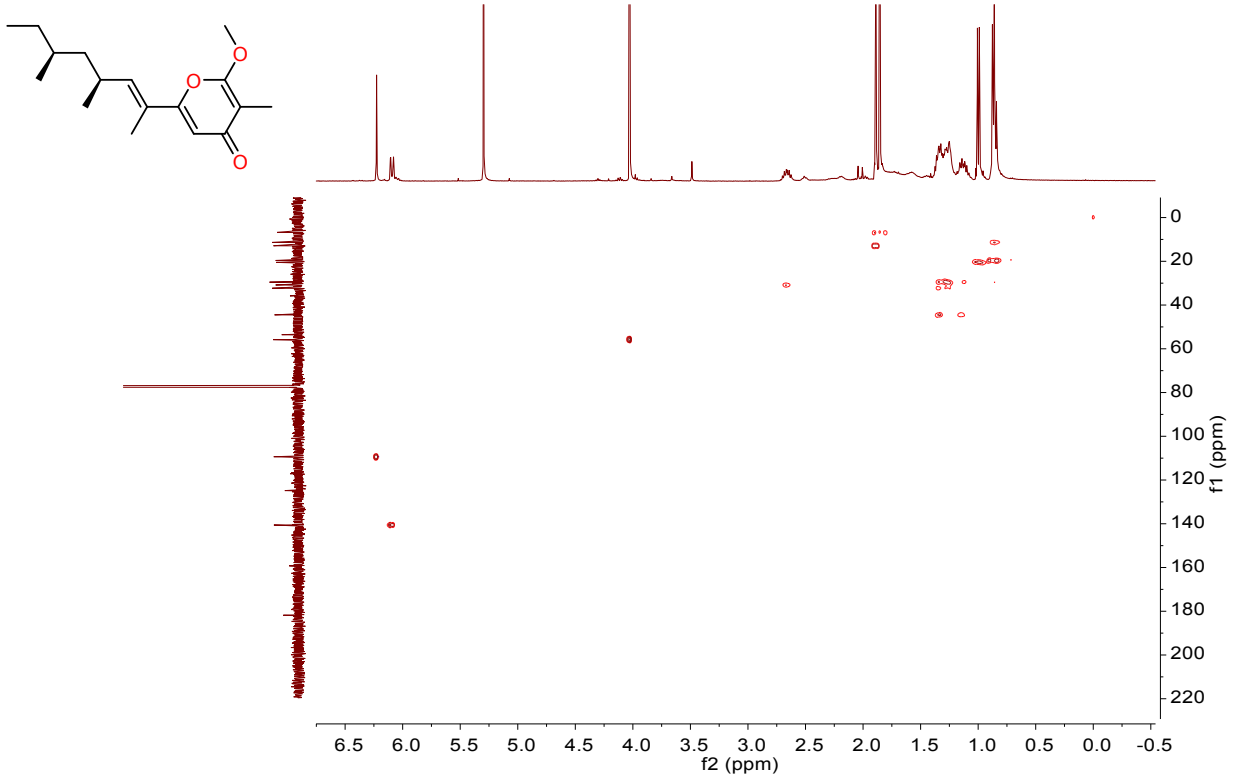

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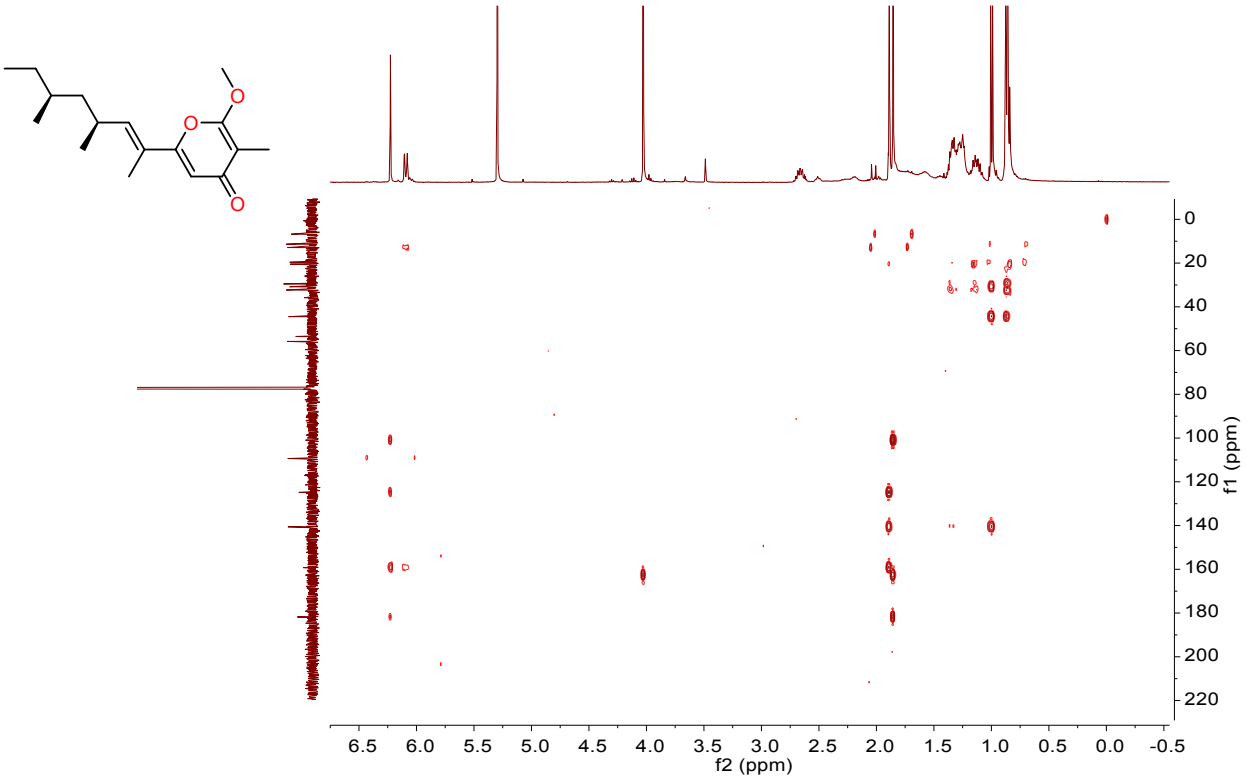

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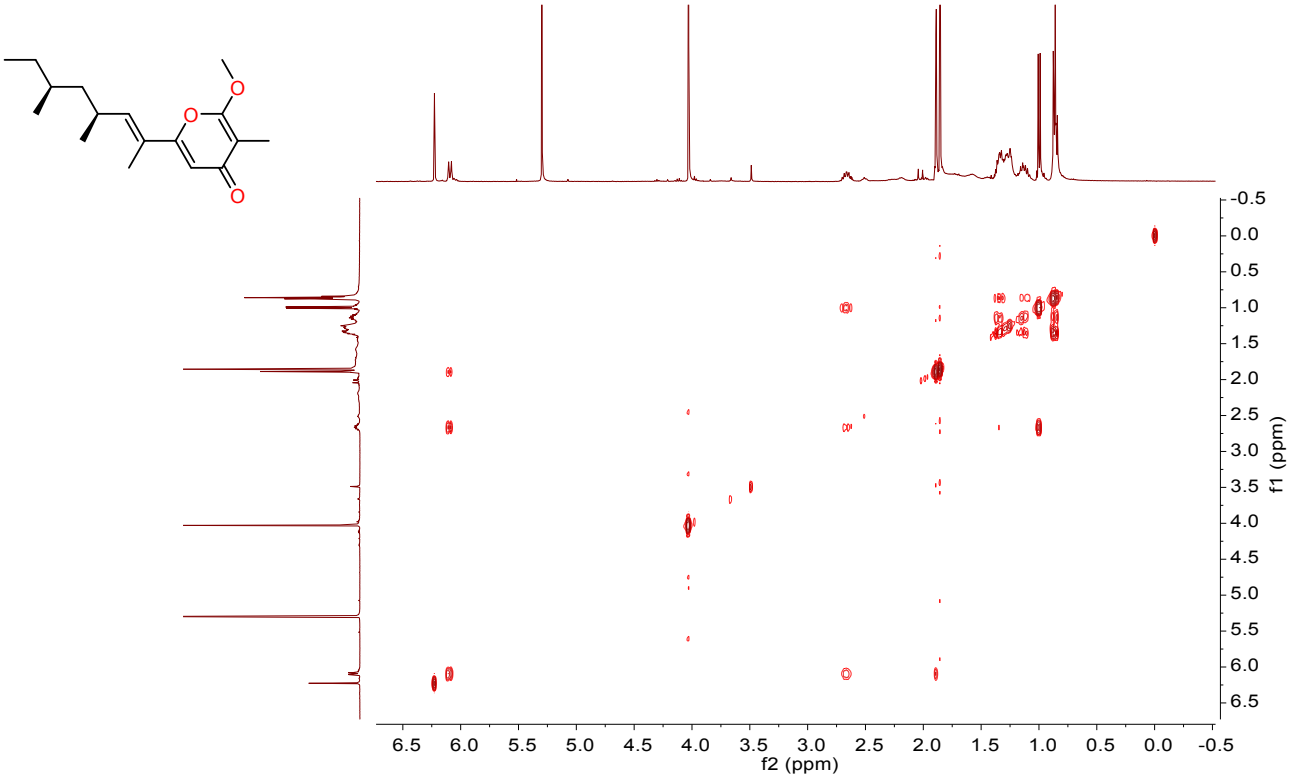

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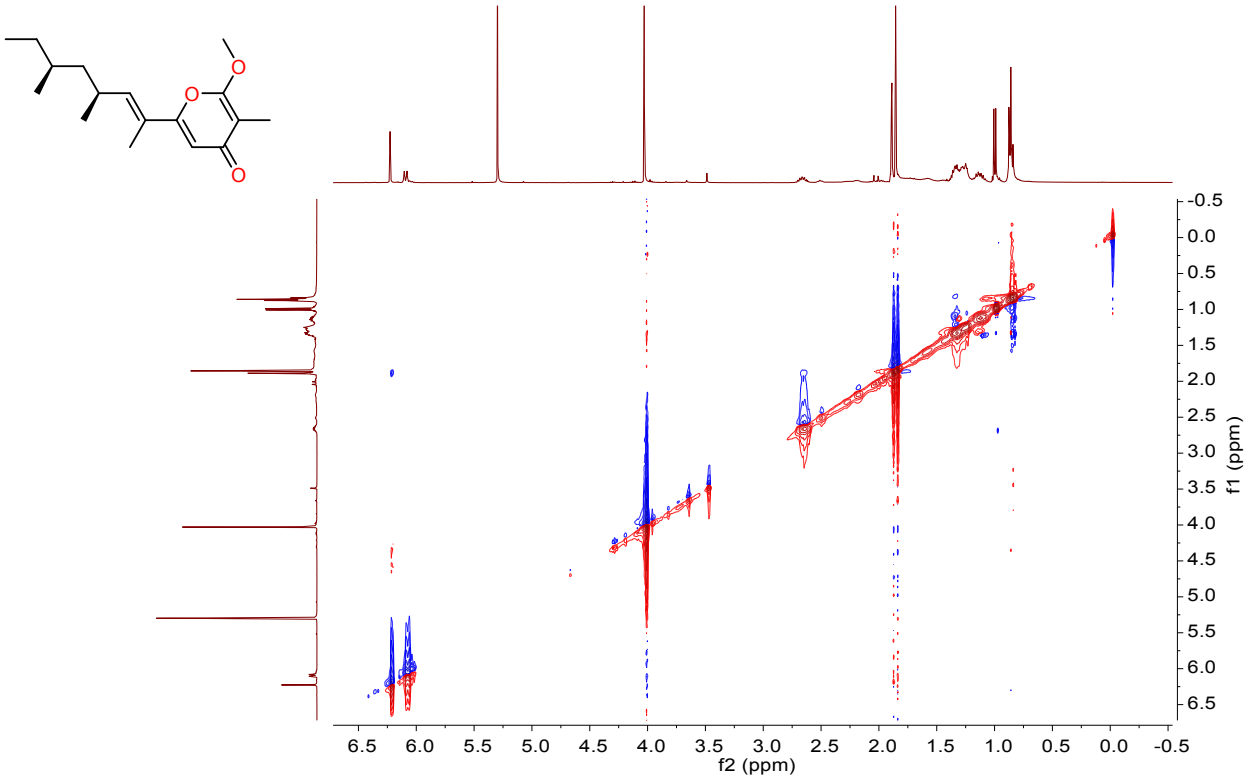

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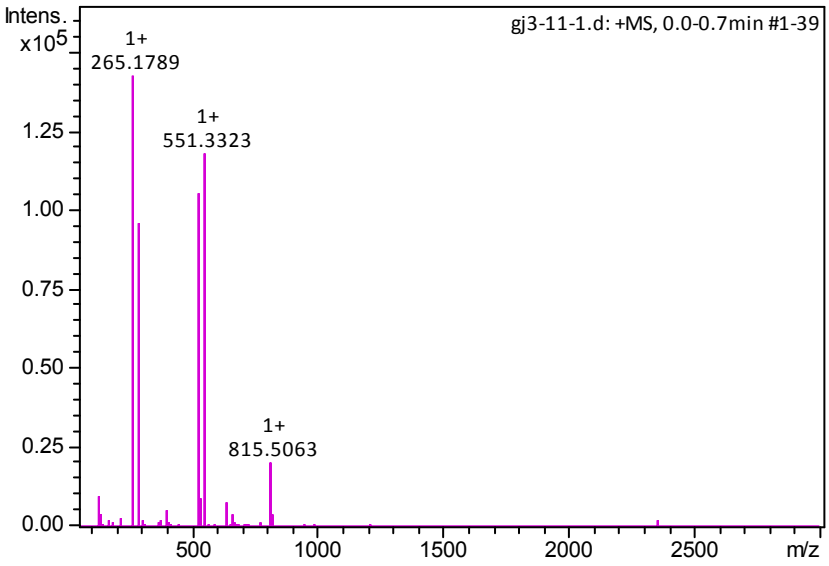

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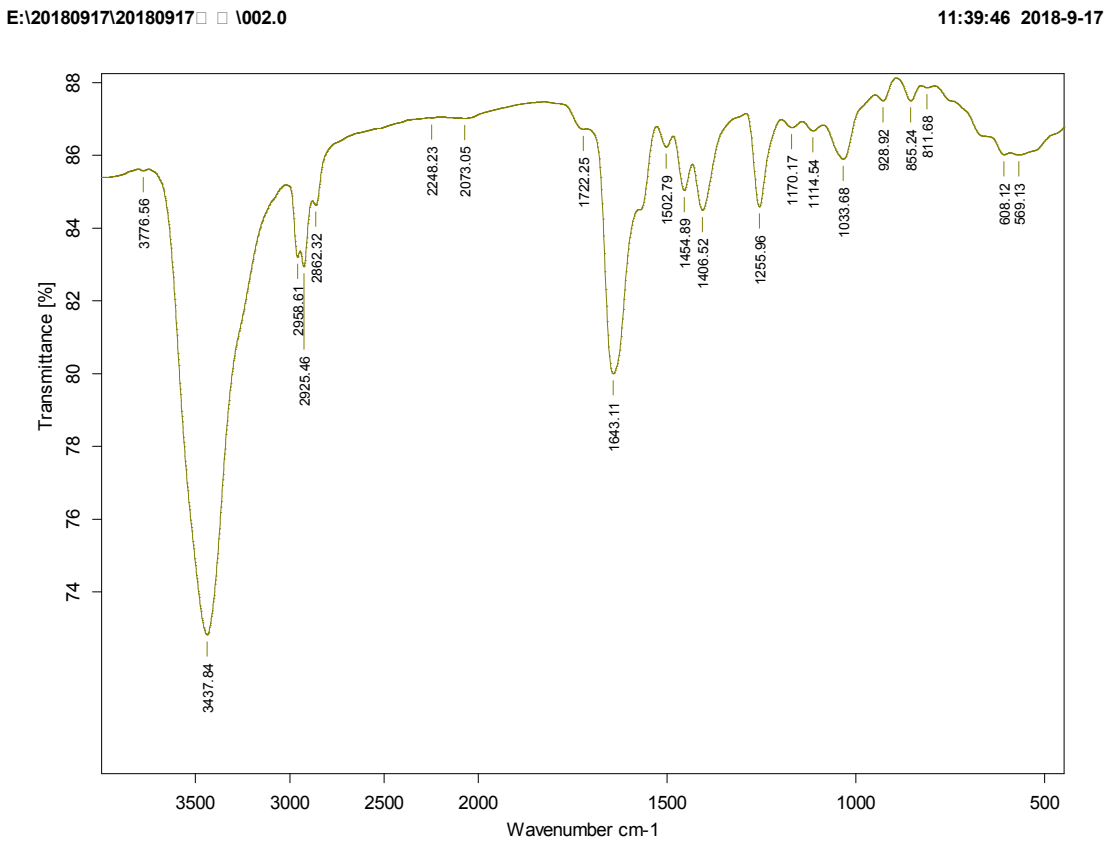

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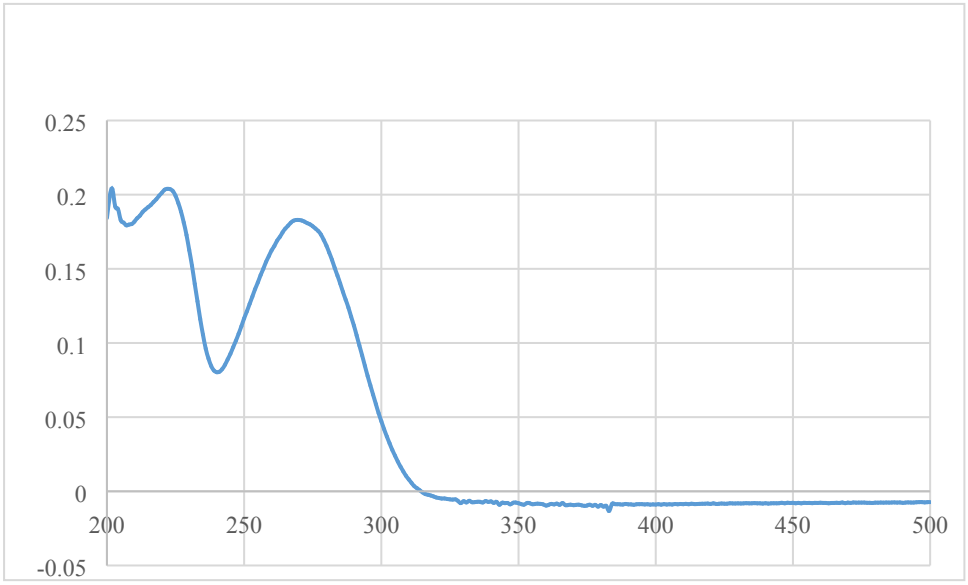

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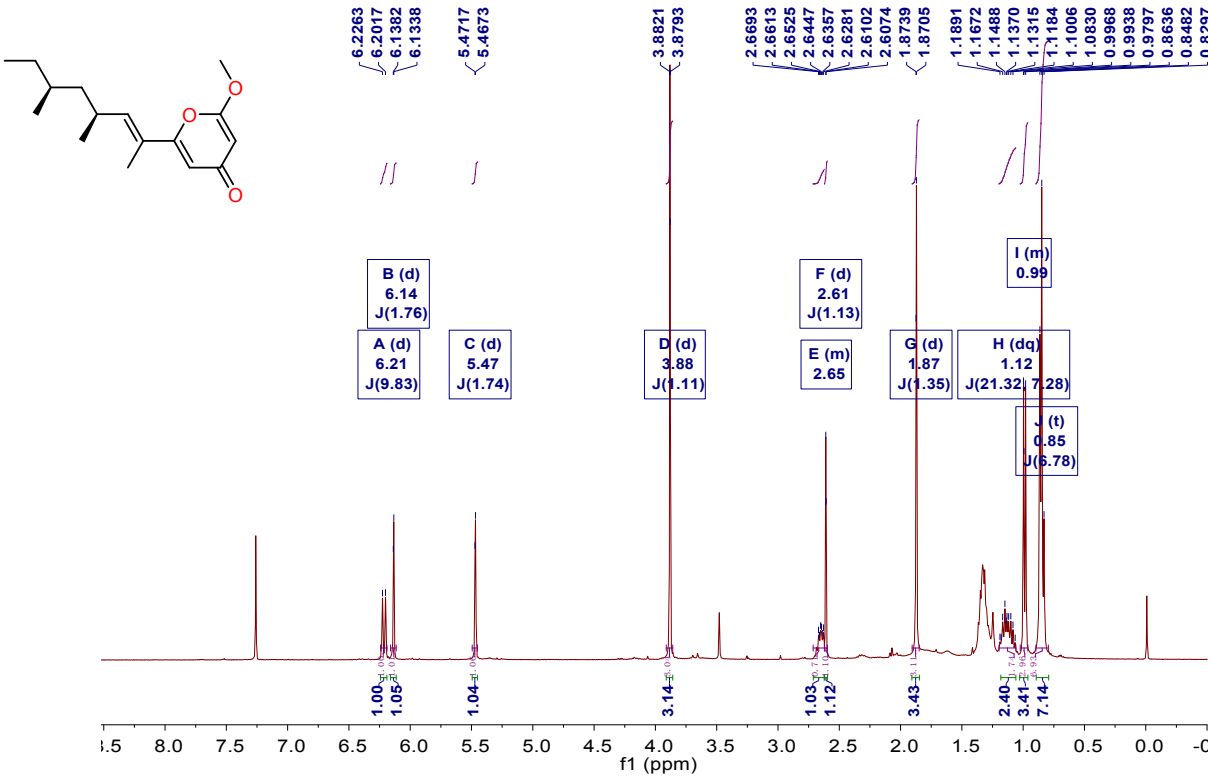

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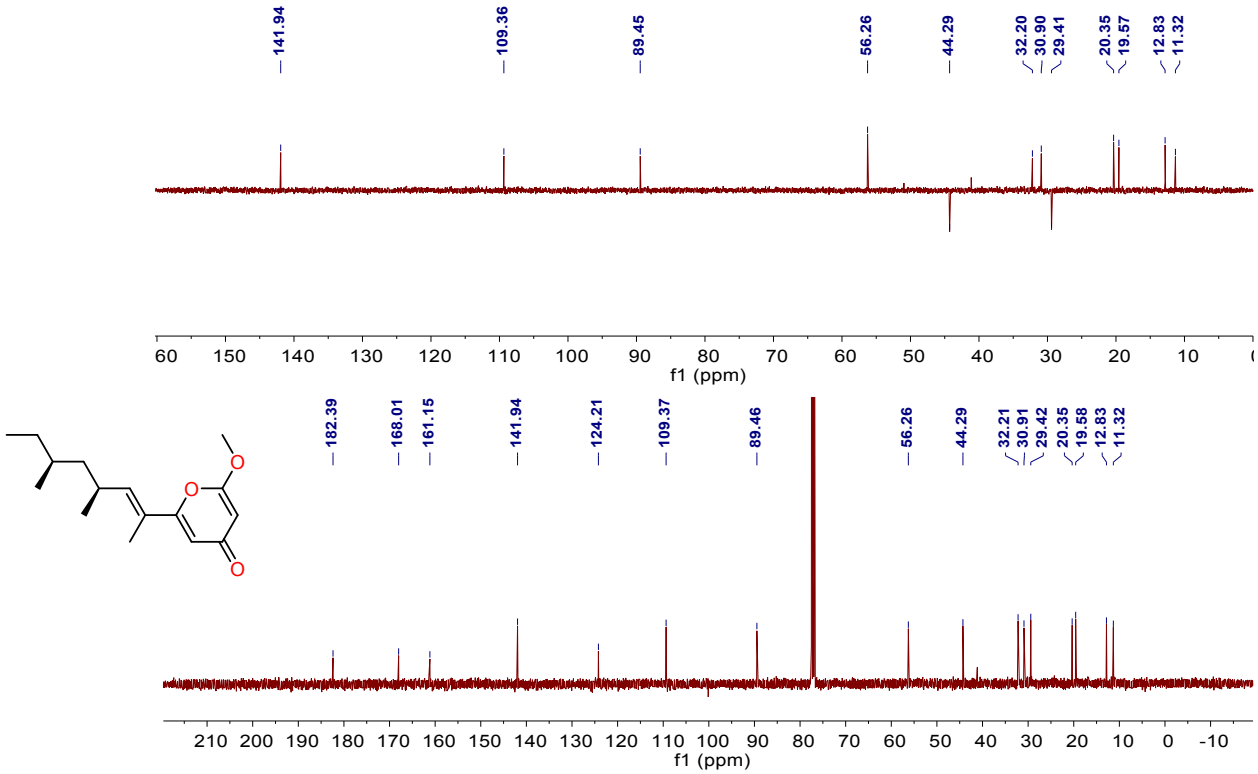

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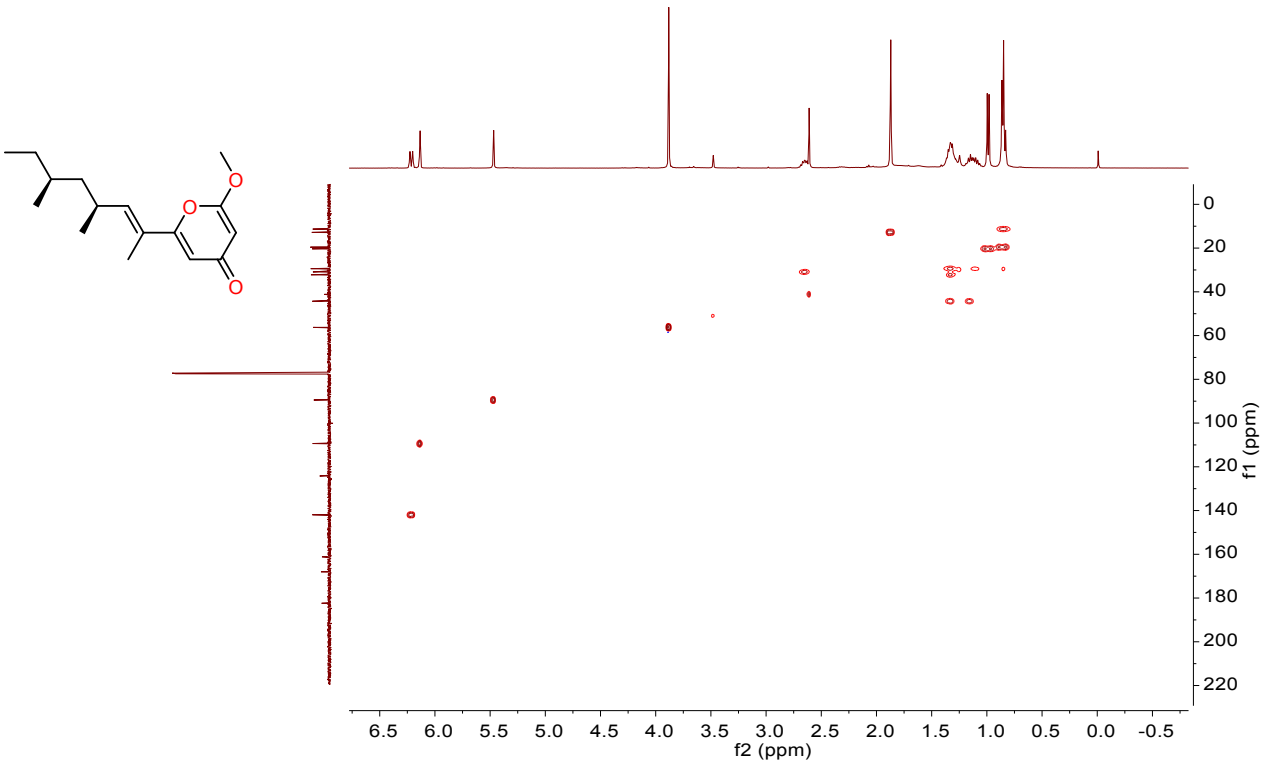

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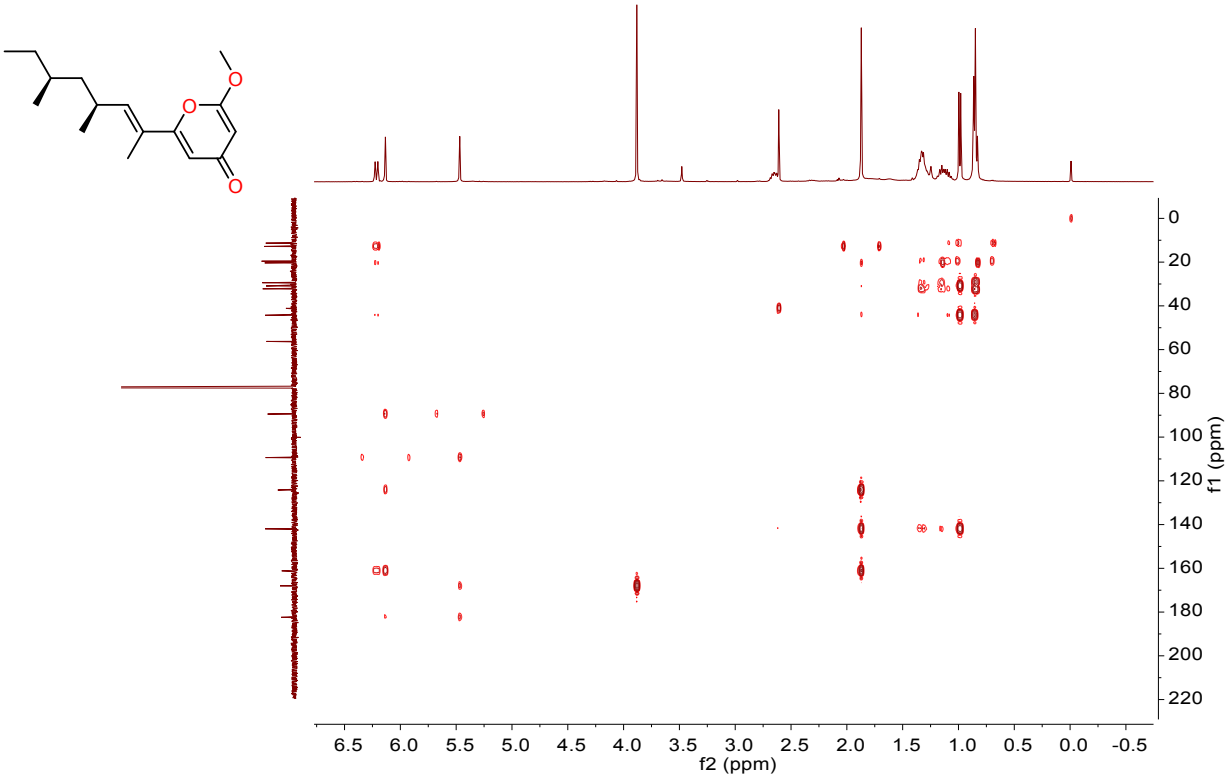

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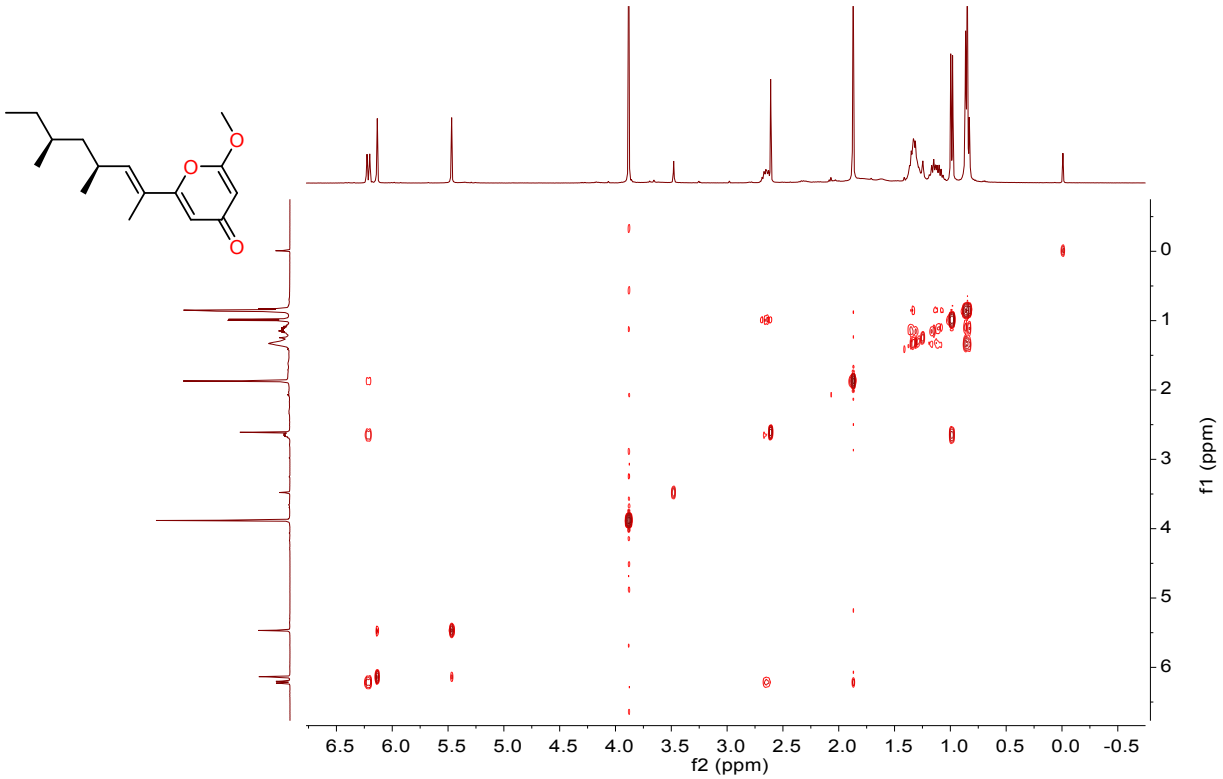

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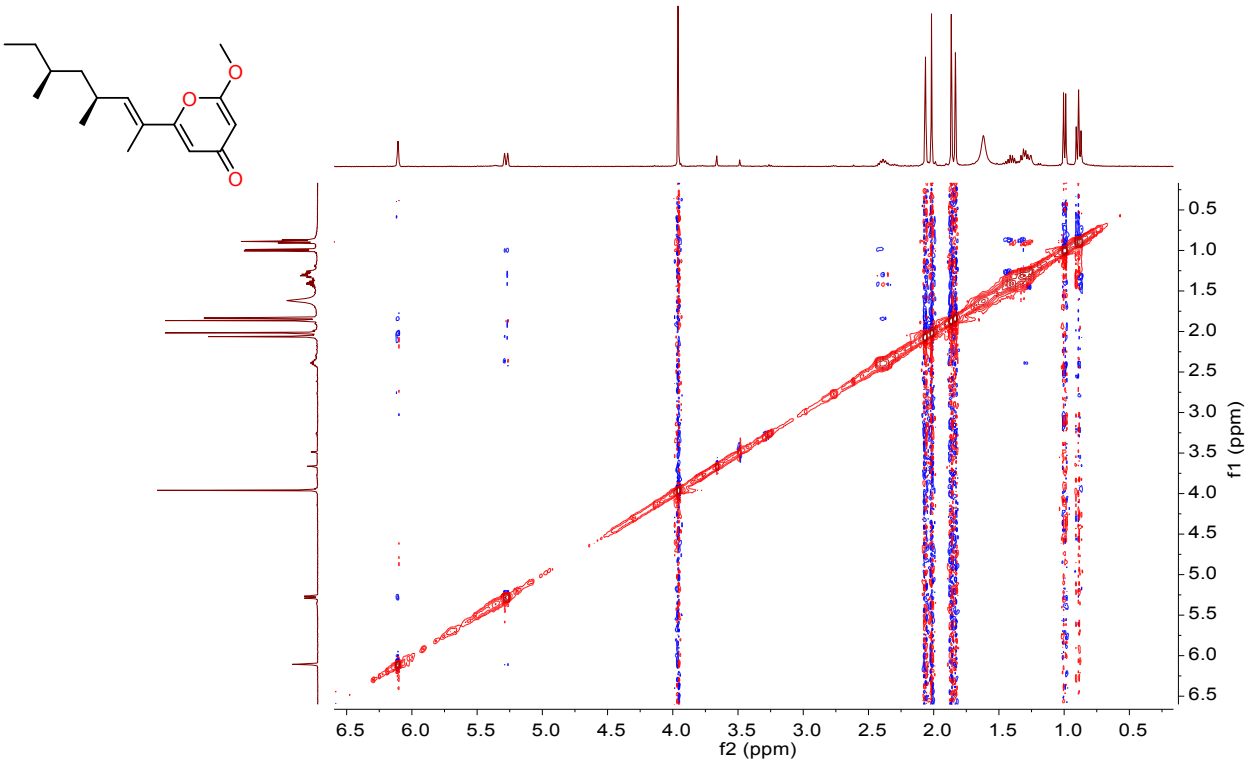

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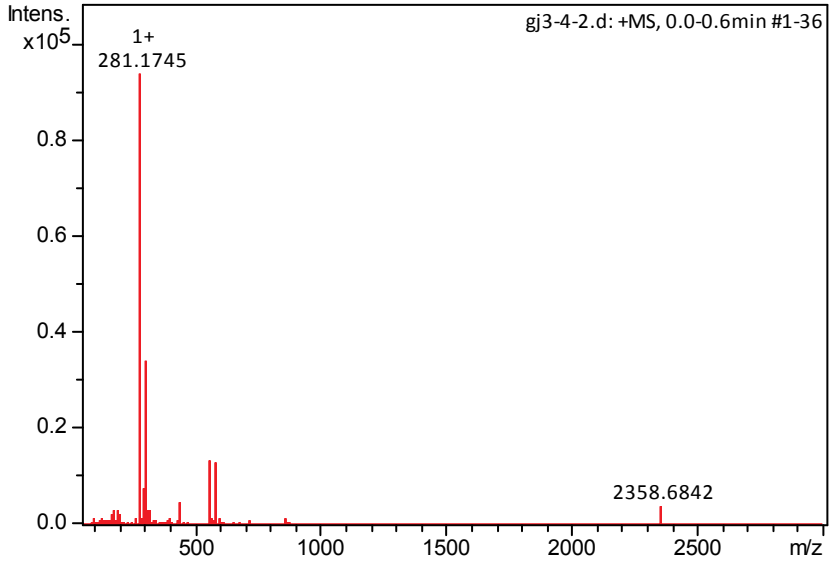


Figure S29. IR Spectrum of **4**

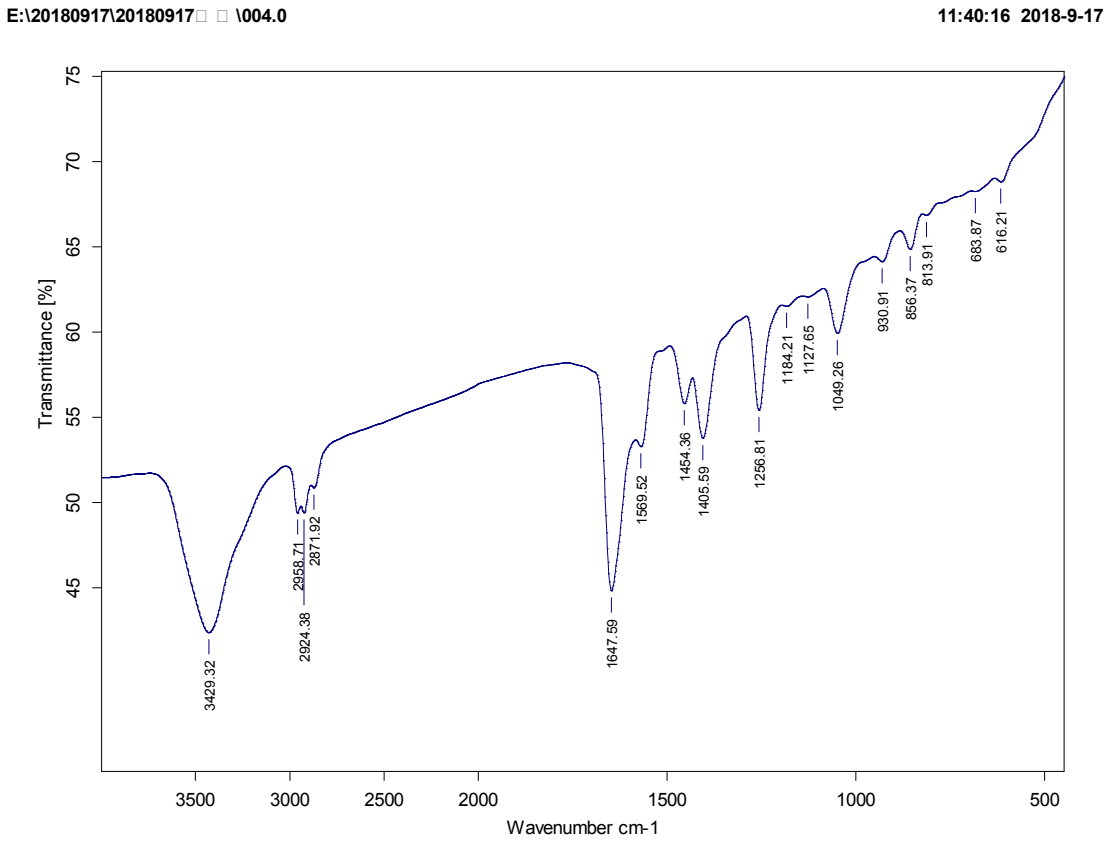


Figure S30. UV Spectrum of **4**

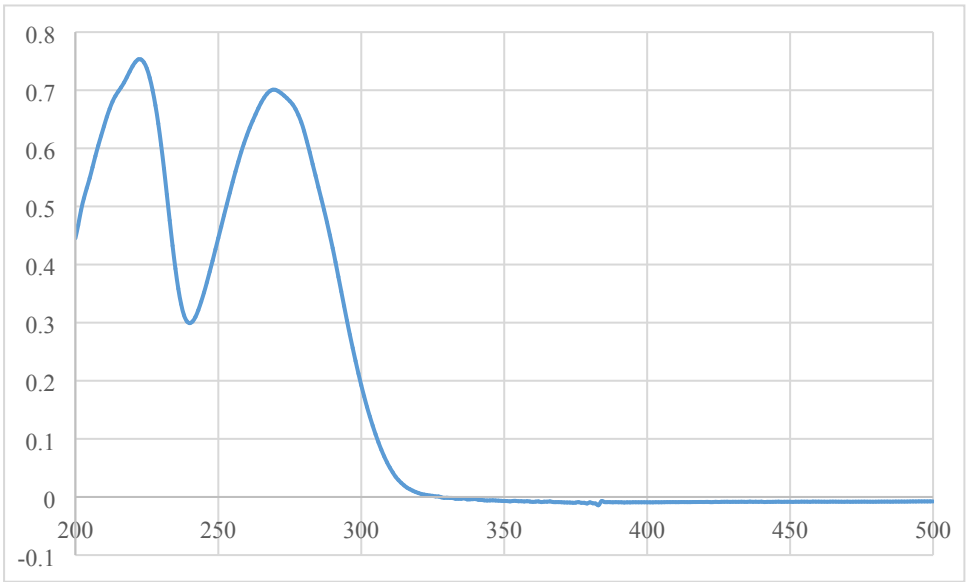


Figure S31. ^{1}H NMR Spectrum of **4** in $CDCl_3$

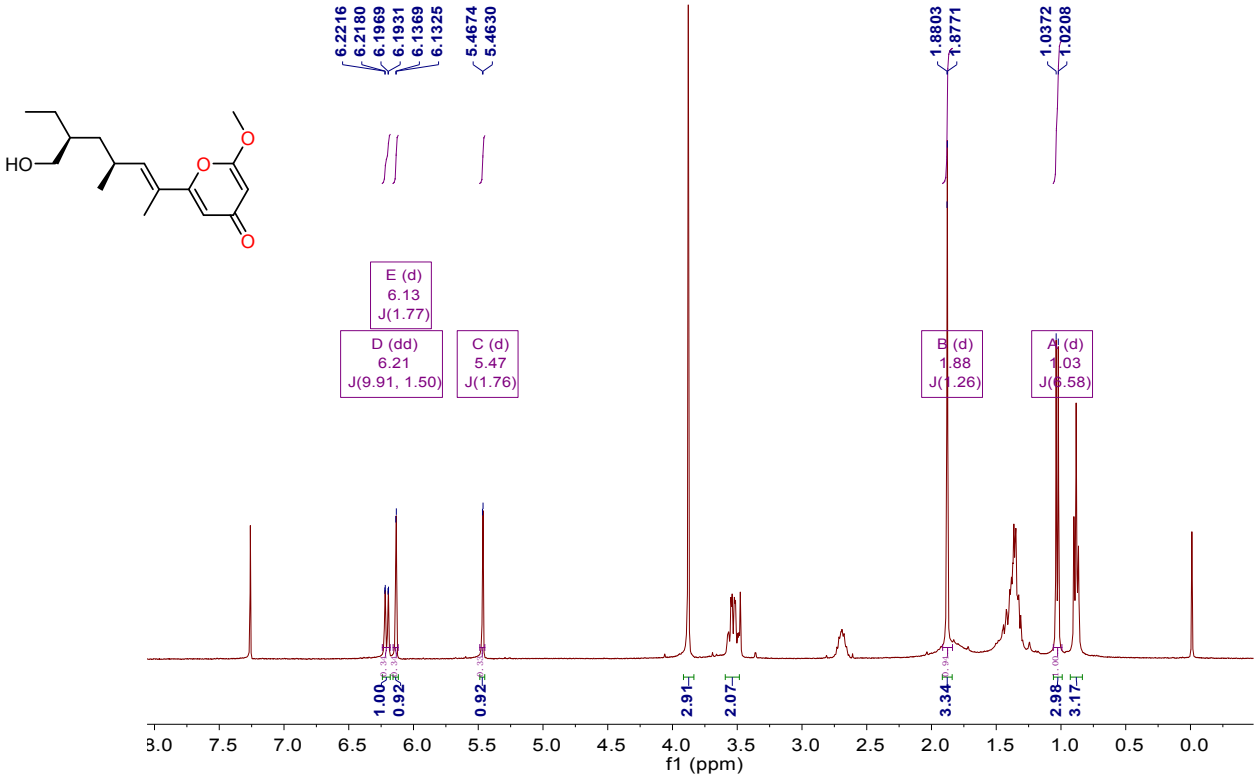


Figure S32. ^{13}C NMR and DEPT Spectrum of **4** in $CDCl_3$

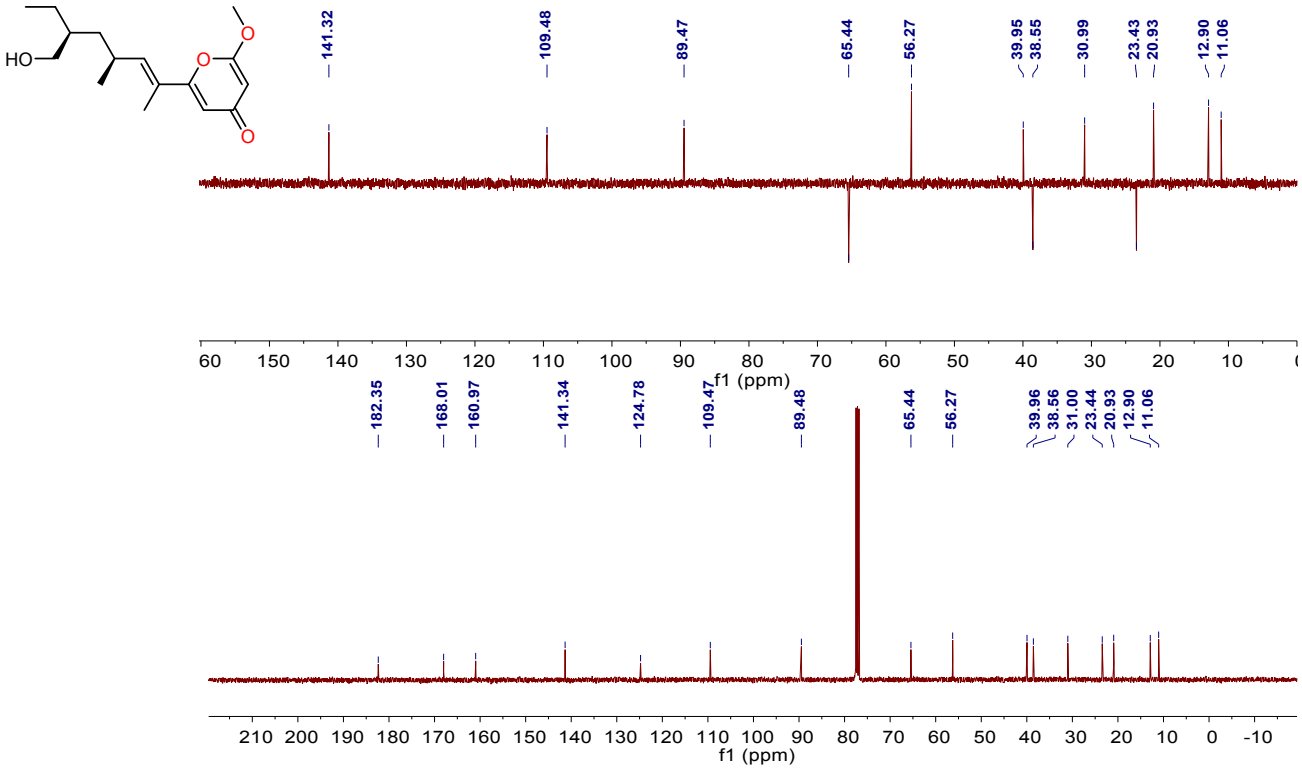


Figure S33. HSQC Spectrum of **4** in $CDCl_3$

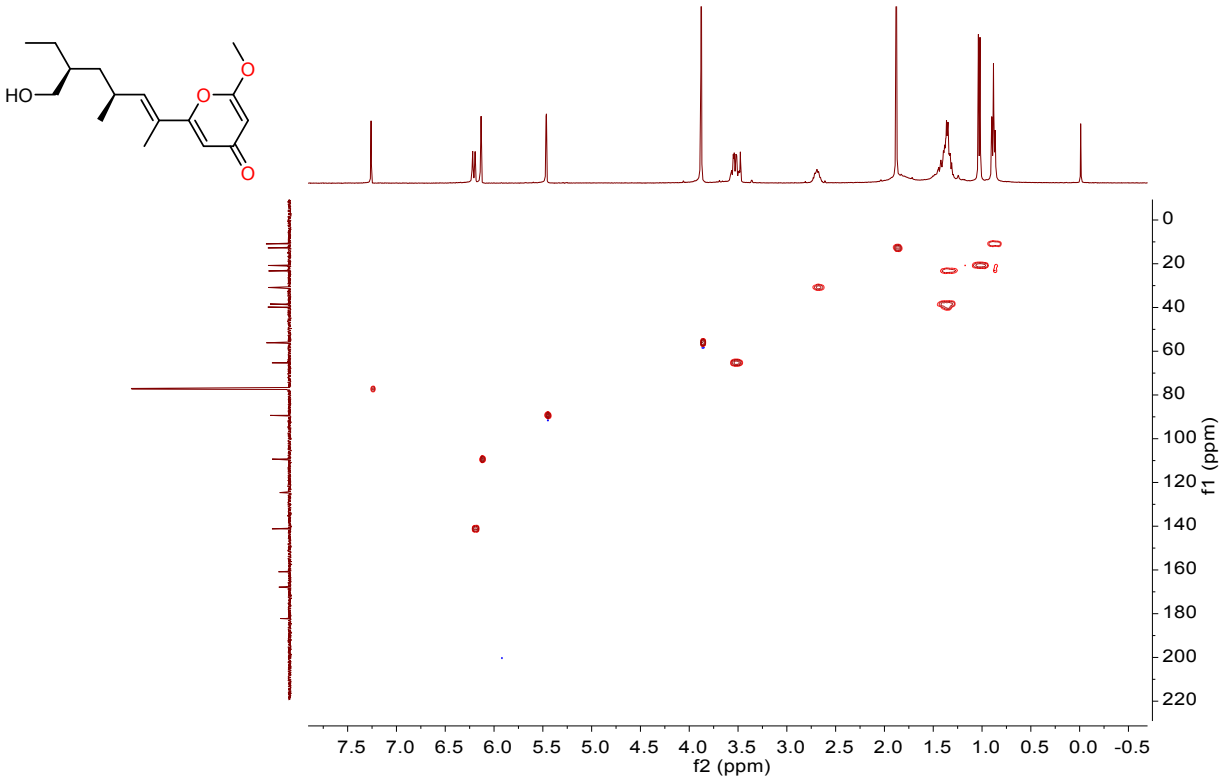


Figure S34. HMBC Spectrum of **4** in $CDCl_3$

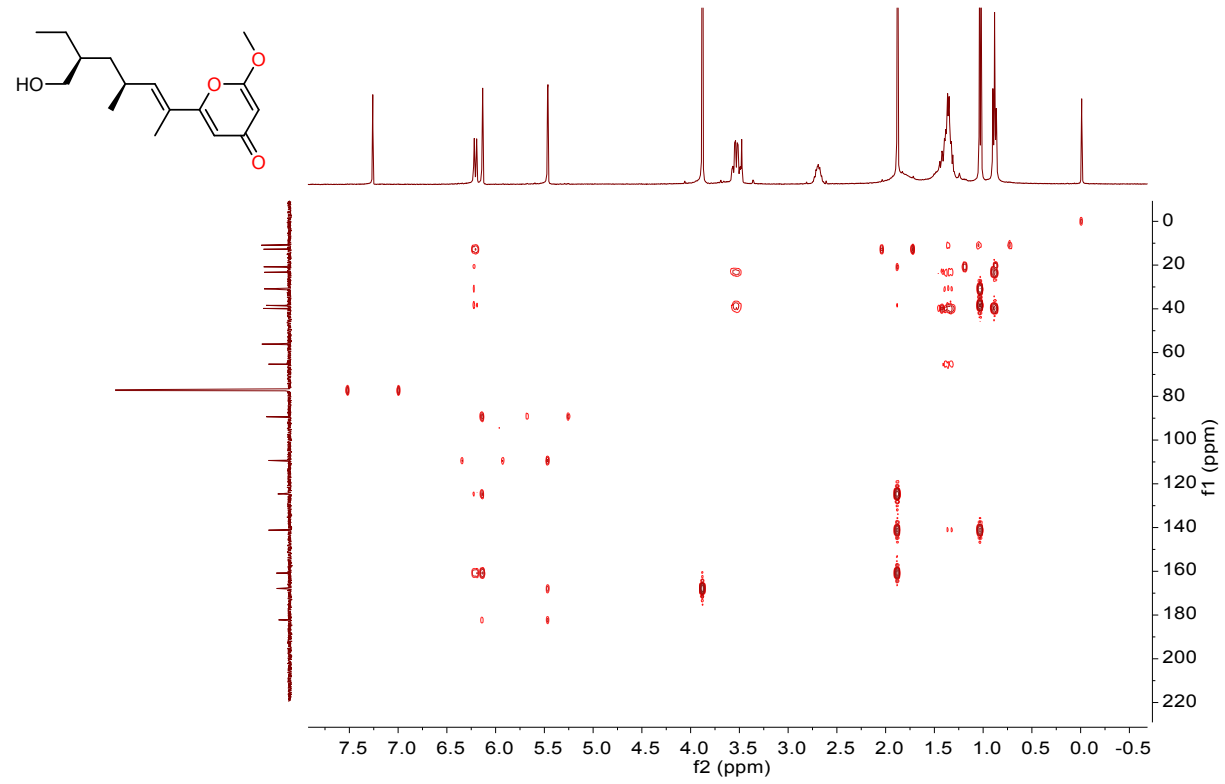


Figure S35. $^{1}H–^{1}H$ COSY Spectrum of **4** in $CDCl_3$

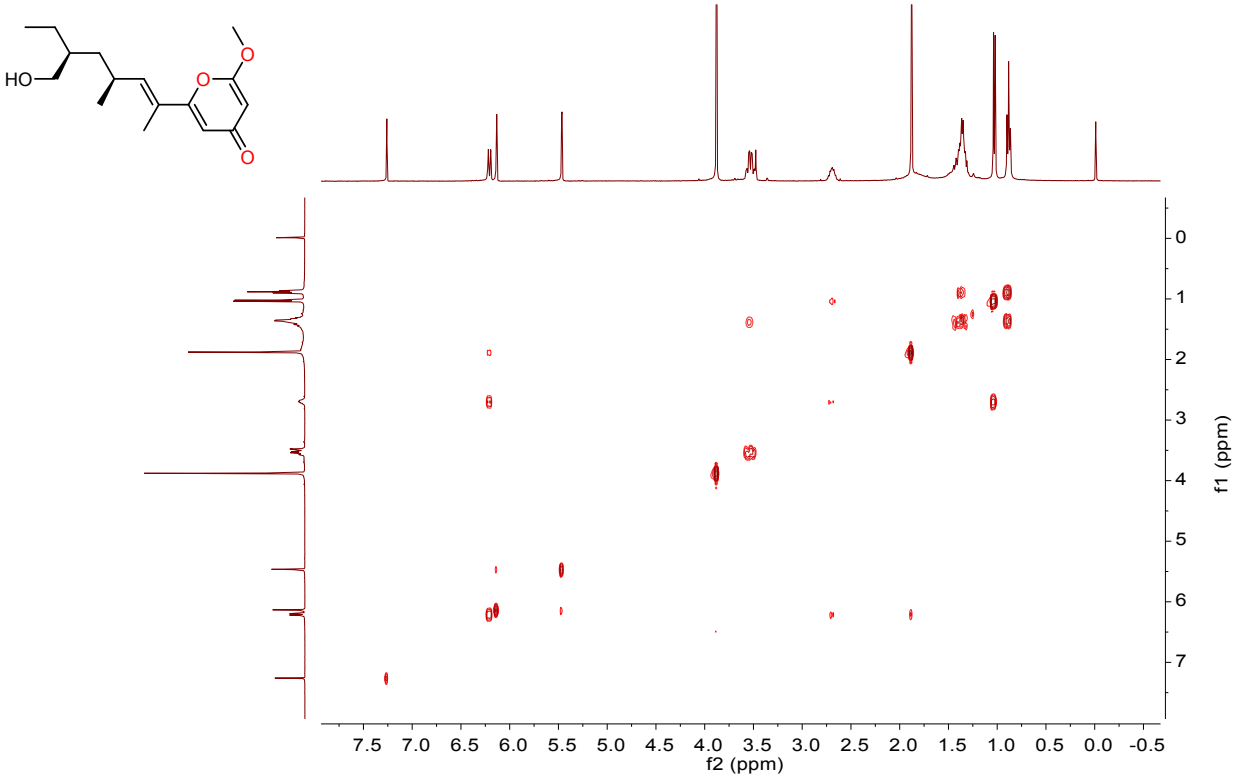


Figure S36. NOESY Spectrum of **4** in $CDCl_3$

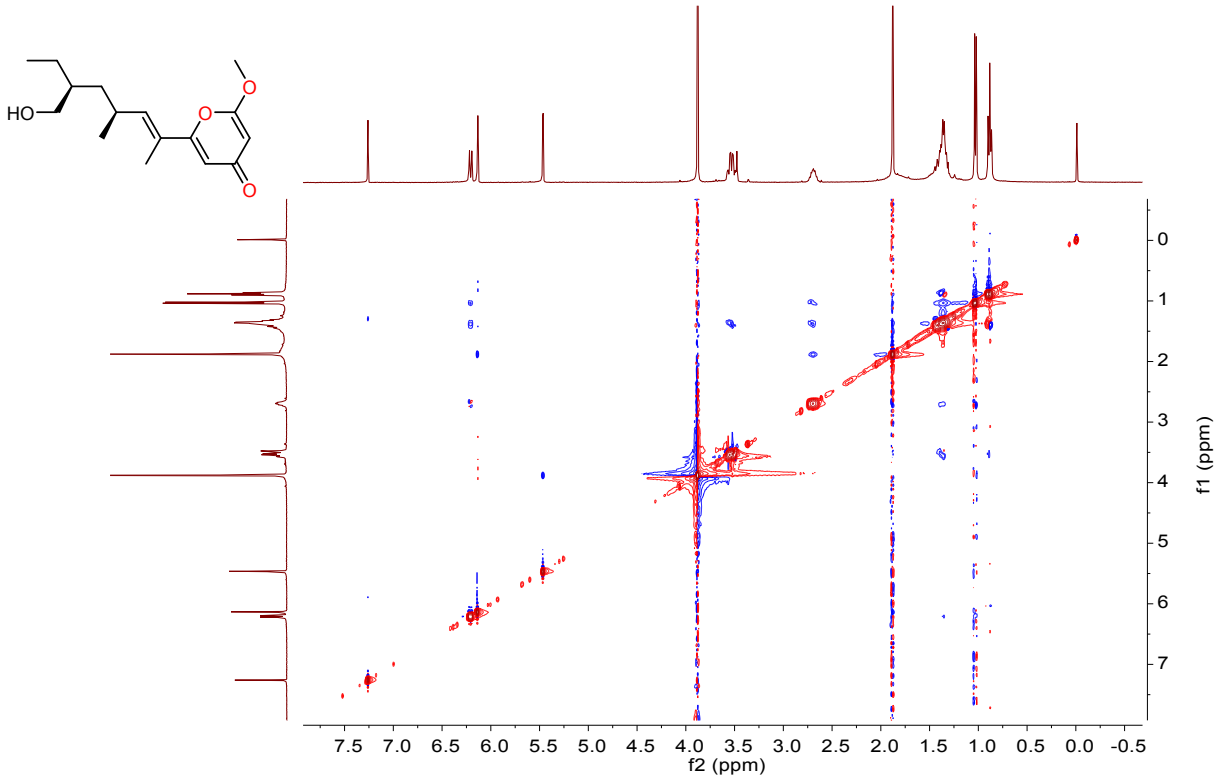


Figure S37. (+)-HRESIMS Spectrum of **5**

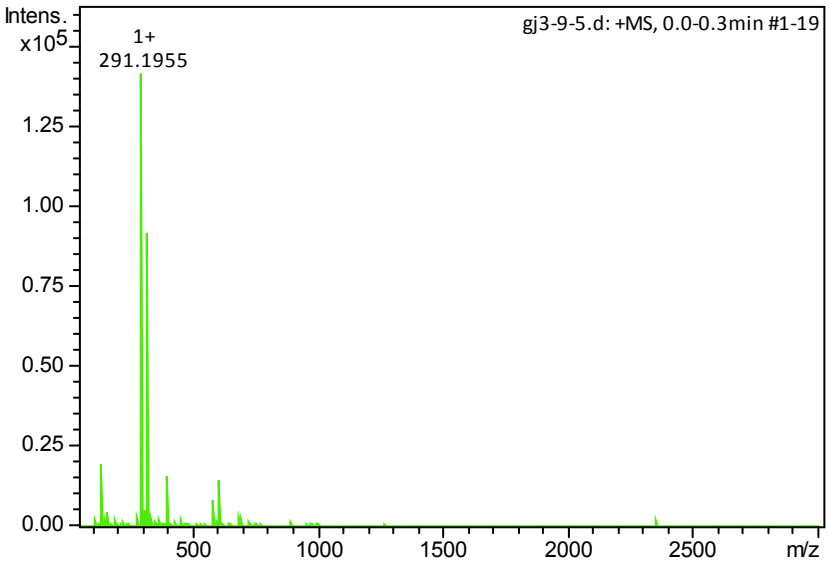


Figure S38. IR Spectrum of **5**

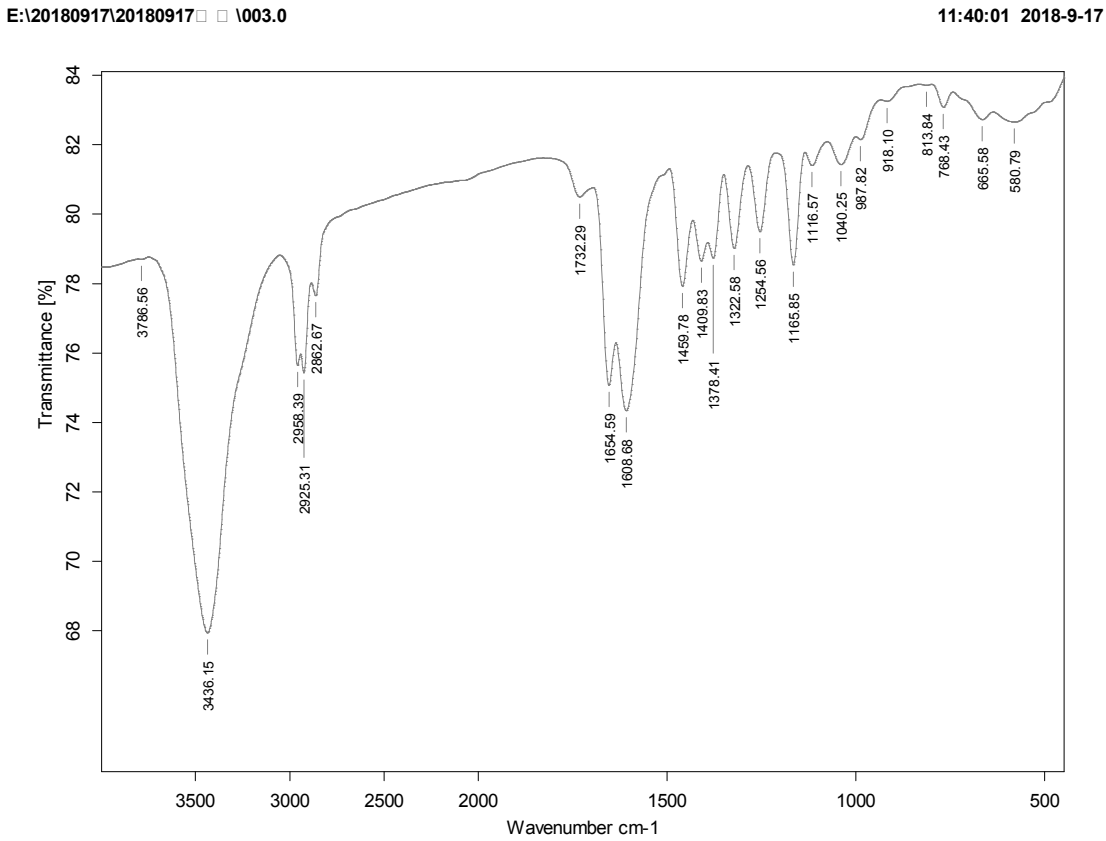


Figure S39. UV Spectrum of **5**

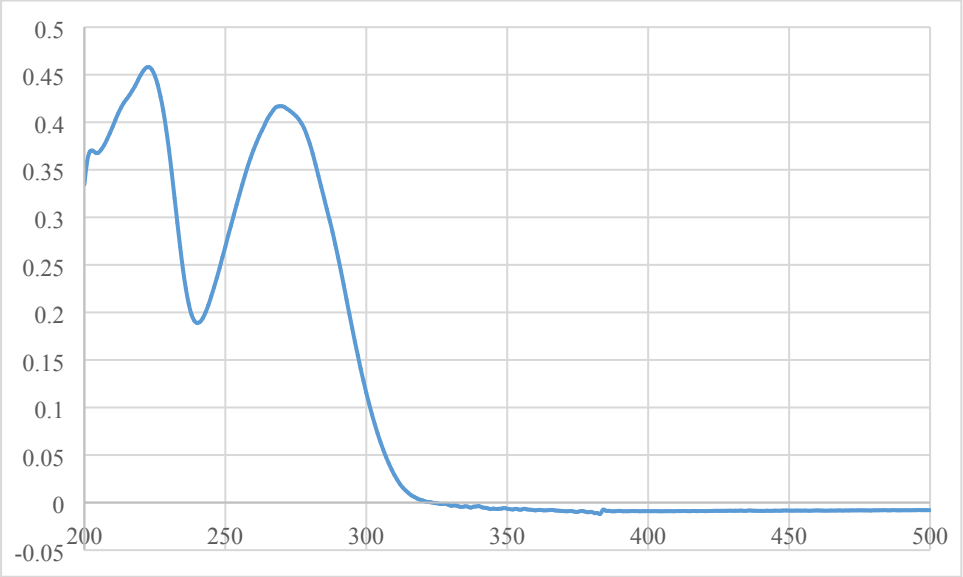


Figure S40. ^{1}H NMR Spectrum of **5** in $CDCl_3$

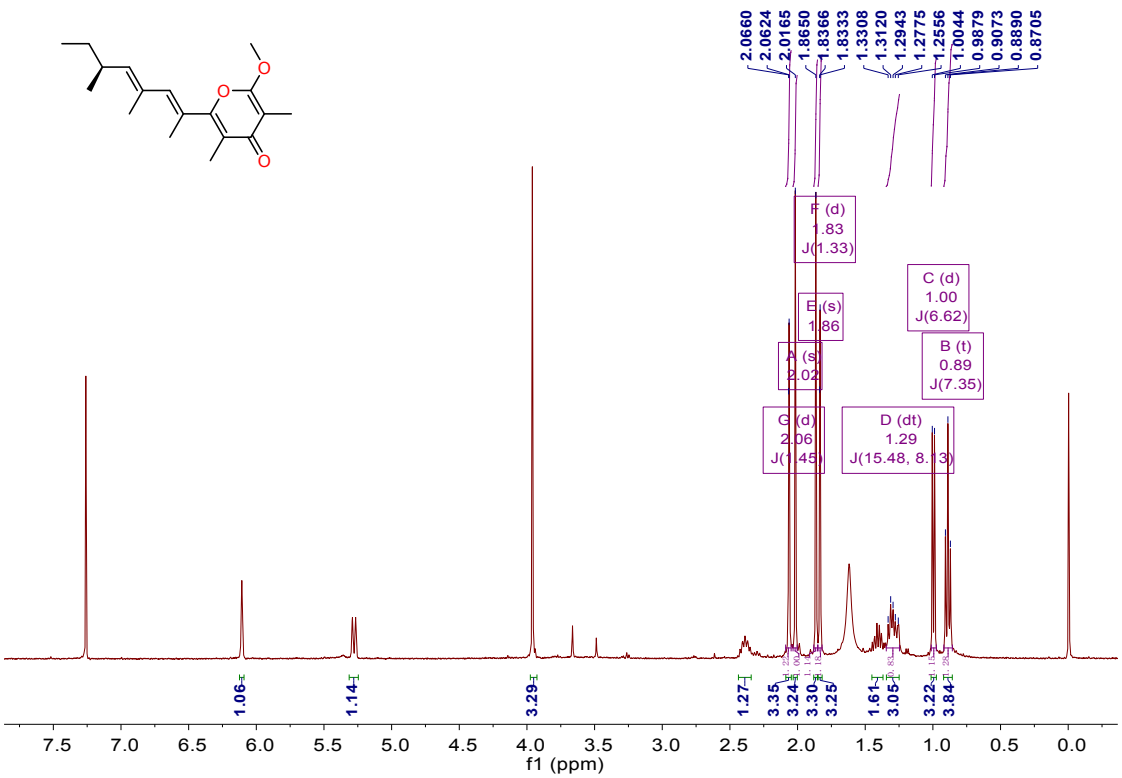


Figure S41. ^{13}C NMR and DEPT Spectrum of **5** in $CDCl_3$

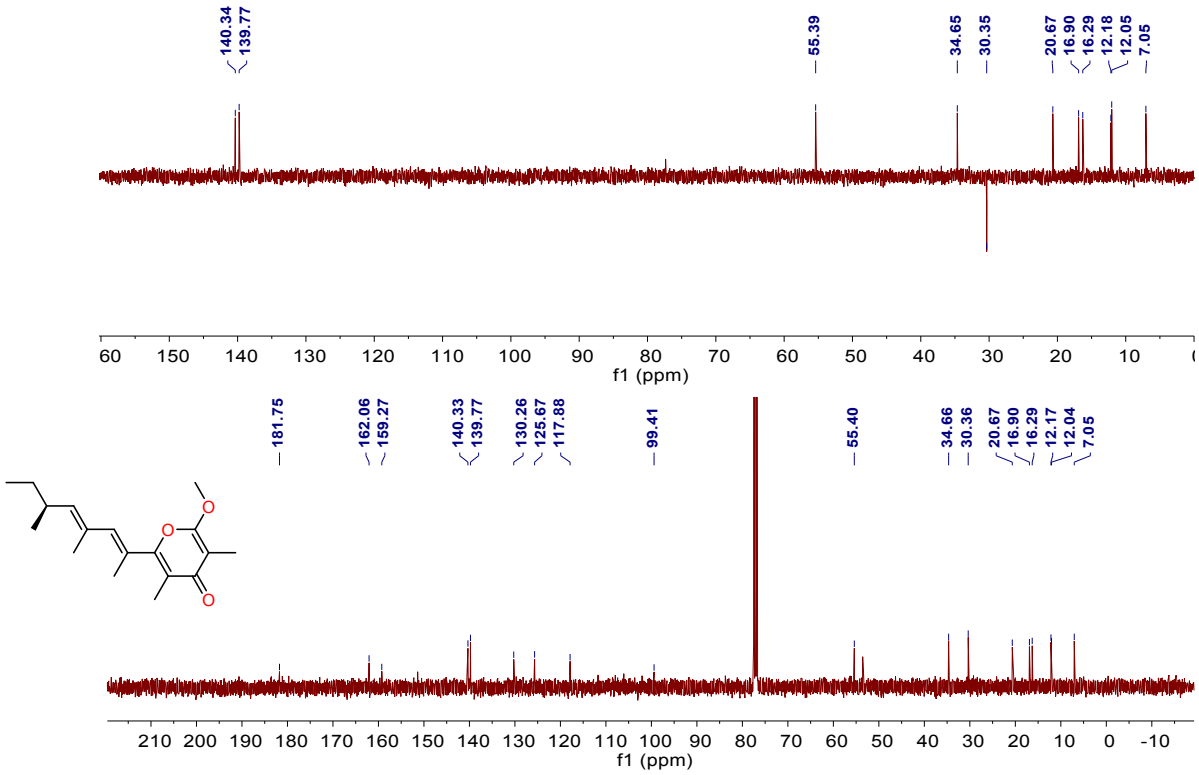


Figure S42. HSQC Spectrum of **5** in $CDCl_3$

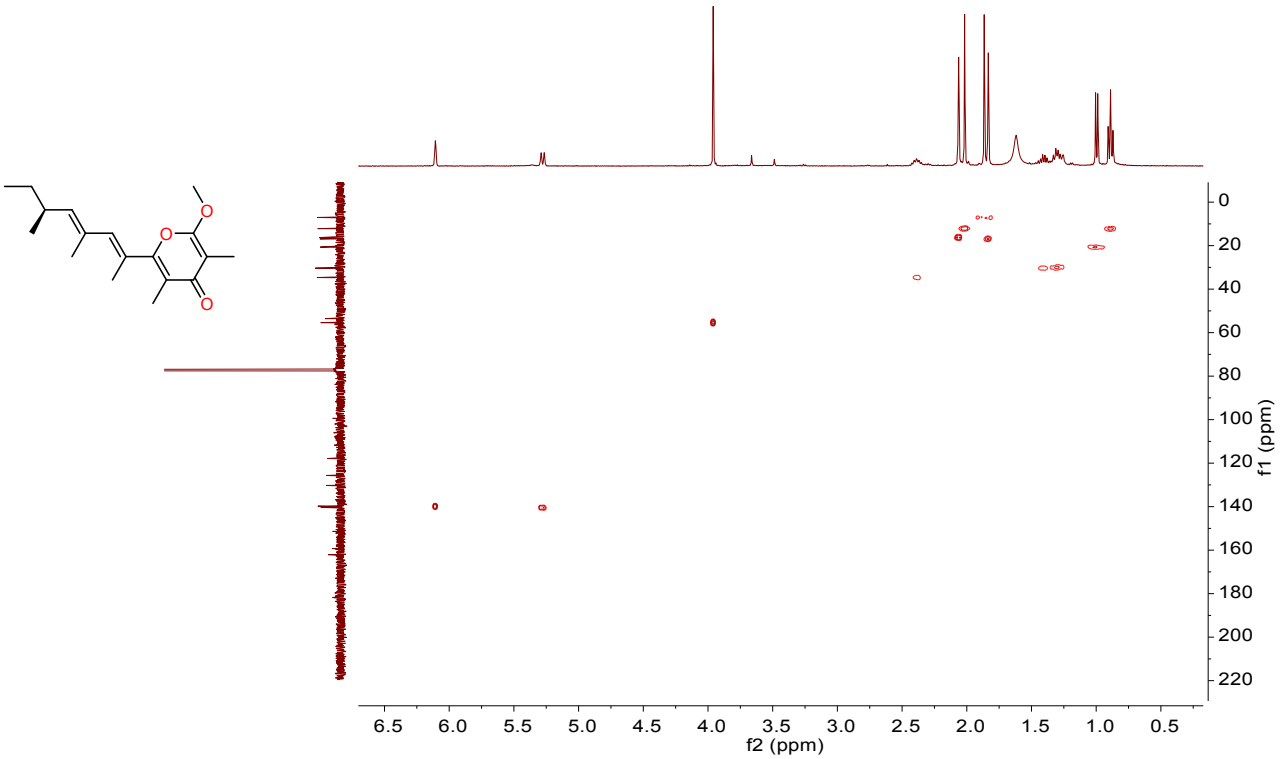


Figure S43. HMBC Spectrum of **5** in $CDCl_3$

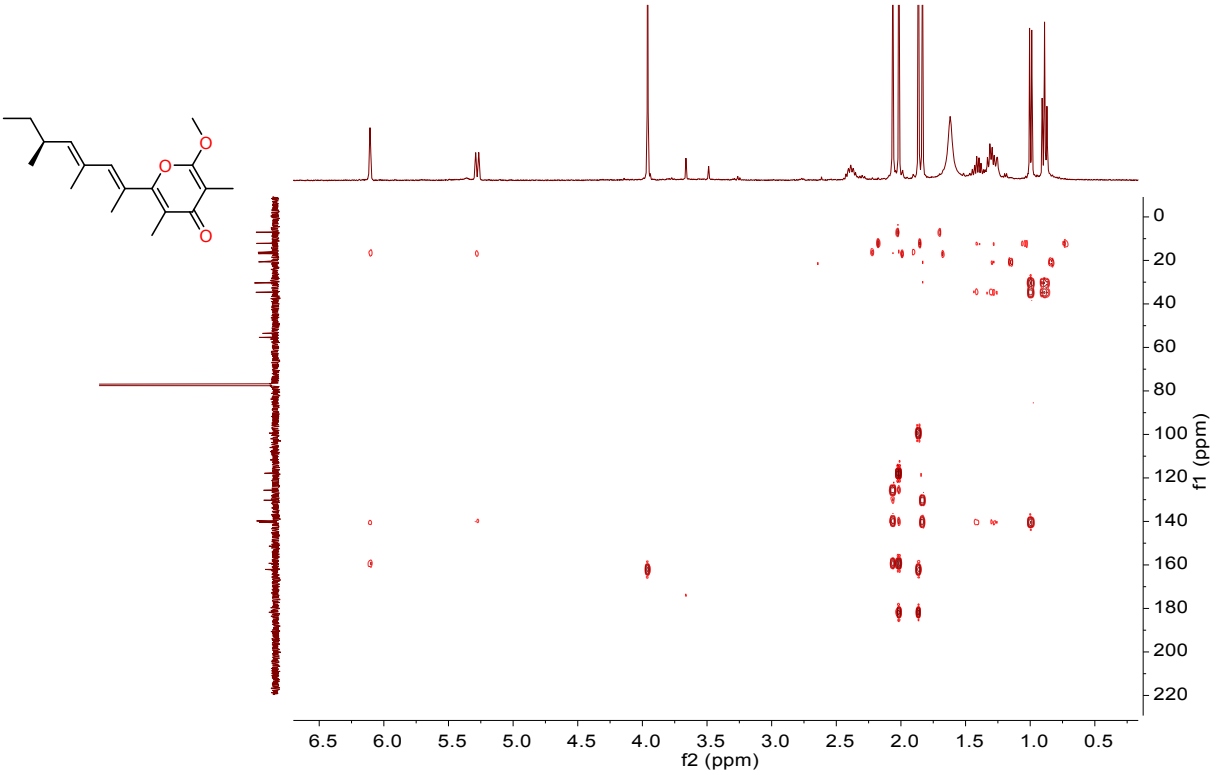


Figure S44. ^{1}H–^{1}H COSY Spectrum of **5** in $CDCl_3$

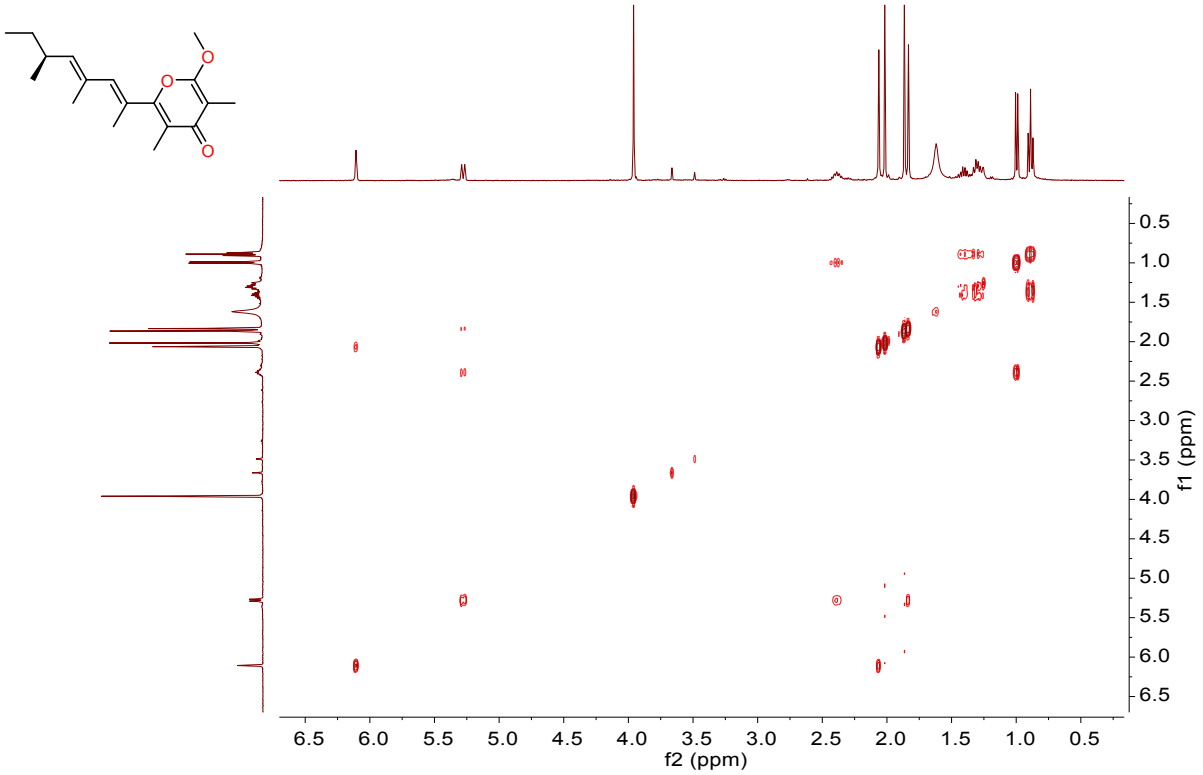


Figure S45. NOESY Spectrum of **5** in $CDCl_3$

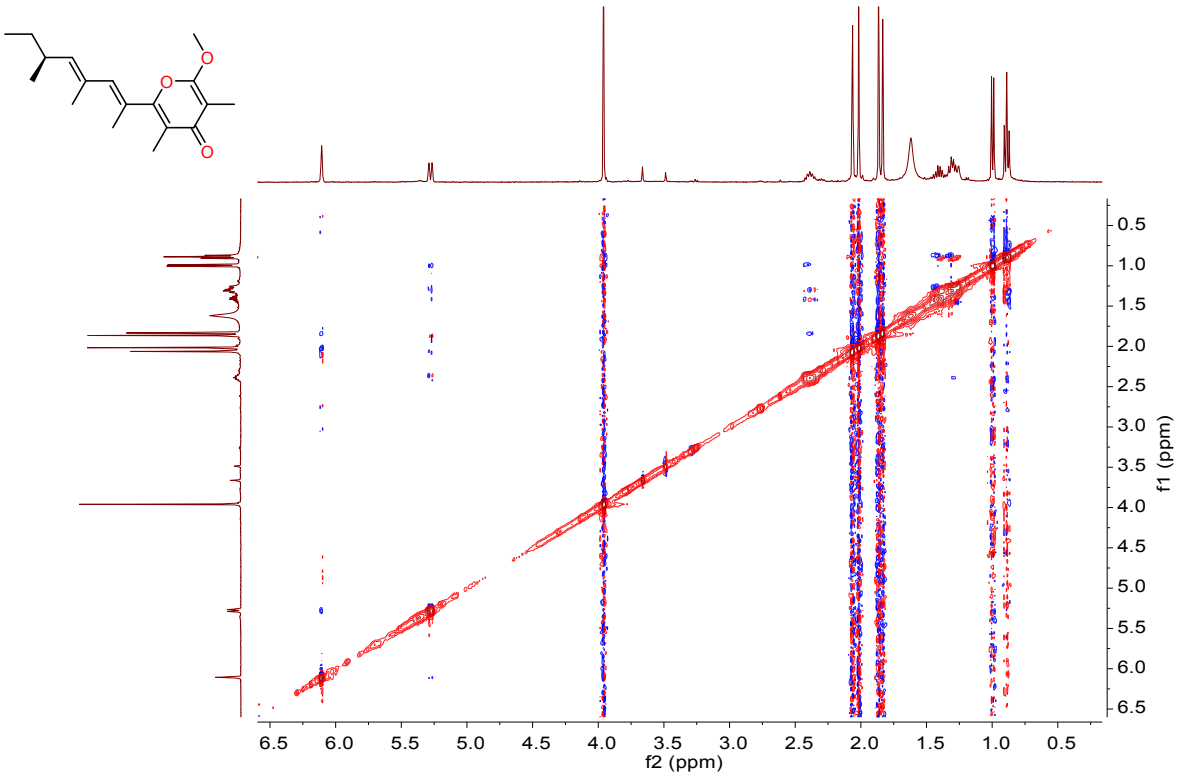
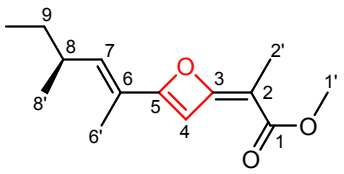


Table S1. ^{1}H (400 MHz) and ^{13}C NMR (100 MHz) data and calculated ^{13}C NMR data of two possible structures 1A and 1B in $CDCl_3$ (δ in ppm, J in Hz).

No.	1A			No.	1B		
	δ_H (exptl)	δ_C (exptl)	δ_C (adj_calcd)		δ_H (exptl)	δ_C (exptl)	δ_C (adj_calcd)
1		162.6	168.1	2		162.6	161.3
2		101.0	103.9	3		101.0	102.6
2'	1.85, s	6.8	10.1	3'	1.85, s	6.8	5.8
3		181.8	166.3	4		181.8	178.3
4	6.22, d (1.3)	109.4	95.1	5	6.22, d (1.3)	109.4	109.1
5		159.2	169.5	6		159.2	158.9
6		125.6	124.6	7		125.6	128.4
6'	1.89, s	13.1	10.7	7'	1.89, s	13.1	11.3
7	6.08, d (9.8)	139.9	147.0	8	6.08, d (9.8)	139.9	142.9
8	2.49, m	34.8	39.1	9	2.49, m	34.8	38.0
8'	1.02, dd (6.6, 1.3)	20.3	21.4	9'	1.02, dd (6.6, 1.3)	20.3	20.2
9	1.34, m; 1.45, m	30.2	33.3	10	1.34, m; 1.45, m	30.2	32.0
10	0.87, dd (8.1, 6.8)	12.0	13.0	11	0.87, dd (8.1, 6.8)	12.0	11.2
$-OCH_3$	4.02, s	55.8	50.5	$-OCH_3$	4.02, s	55.8	52.4

"m" means overlapped or multiplet with other signals

^{13}C NMR Calculation Data



1A

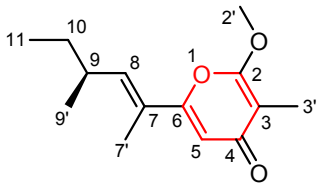
Table S2. Important thermodynamic parameters (a.u.) and boltzmann distribution of the optimized compound **1A** at B3LYP/6-31G(d) level in chloroform.

Conformation	Internal Energy	%
1	-771.031782	58.74%
2	-771.031435	40.67%

Table S3. Optimized coordinates of compound **1A** at B3LYP/6-31G(d) level in chloroform.

Conformation 1							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-0.943	-1.075	-0.082	H	1.441	-2.86	-1.067
C	0.294	-0.514	-0.167	H	3.023	-2.587	-0.324
C	-1.47	0.278	-0.076	H	1.592	-2.824	0.69
C	2.605	0.111	-0.319	H	-3.142	2.894	-0.914
C	1.684	-0.879	-0.245	H	-3.048	2.93	0.843
C	-2.598	1.01	-0.022	H	-1.552	2.888	-0.117
C	-3.923	0.367	0.071	H	5.033	0.719	2.905
C	1.959	-2.366	-0.237	H	3.434	0.191	2.358
C	-2.576	2.515	-0.054	H	4.829	-0.885	2.184
C	4.504	0.161	2.124	H	4.29	1.617	-1.889
C	4.567	0.561	-1.784	H	5.657	0.488	-1.873
C	-5.145	-1.652	0.184	H	4.117	0.011	-2.617
C	4.792	0.75	0.74	H	-5.773	-1.4	-0.675
C	4.1	-0.001	-0.424	H	-4.917	-2.717	0.19
O	-4.971	0.991	0.122	H	-5.665	-1.368	1.102
O	-0.159	0.84	-0.165	H	5.874	0.738	0.554
O	-3.874	-0.987	0.094	H	4.486	1.805	0.714
H	-1.364	-2.065	-0.038	H	4.402	-1.054	-0.37
H	2.227	1.134	-0.316				
Conformation 2							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-0.782	-1.276	-0.036	H	3.282	-2.526	-0.174
C	0.417	-0.64	-0.143	H	1.828	-2.83	0.789
C	-1.392	0.04	-0.083	H	1.754	-2.931	-0.971
C	2.681	0.132	-0.322	H	-1.678	2.627	-0.223
C	1.828	-0.913	-0.206	H	-3.261	2.489	-1.016

C	-2.575	0.682	-0.056	H	-3.17	2.598	0.74
C	-3.786	-0.156	0.065	H	5.051	1.024	2.877
C	2.201	-2.377	-0.137	H	3.497	0.358	2.348
C	-2.672	2.182	-0.144	H	4.969	-0.617	2.218
C	4.568	0.399	2.117	H	5.707	0.652	-1.888
C	4.614	0.655	-1.803	H	4.205	0.044	-2.615
C	-6.145	-0.119	0.197	H	4.267	1.685	-1.949
C	4.817	0.954	0.712	H	-6.272	-0.799	-0.649
C	4.18	0.116	-0.423	H	-6.17	-0.695	1.126
O	-3.814	-1.375	0.139	H	-6.927	0.64	0.198
O	-0.126	0.684	-0.194	H	5.898	1.01	0.526
O	-4.908	0.603	0.084	H	4.44	1.984	0.647
H	-1.142	-2.286	0.047	H	4.551	-0.912	-0.329
H	2.235	1.127	-0.363				



1B

Table S4. Important thermodynamic parameters (a.u.) and boltzmann distribution of the optimized compound **1B** at B3LYP/6-31G(d) level in chloroform.

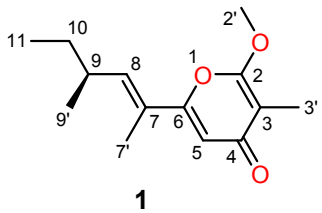
Conformation	Internal Energy	%
1	-771.069838	86.32%
2	-771.067475	7.07%
3	-771.067412	6.61%

Table S5. Optimized coordinates of compound **1B** at B3LYP/6-31G(d) level in chloroform.

Conformation 1							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-1.382	-1.716	-0.038	H	-5.104	0.04	-0.527
C	-3.053	0.097	0.078	H	-4.551	1.652	-0.009
C	-0.388	-0.799	-0.119	H	-4.88	0.379	1.183
C	-1.99	0.944	-0.002	H	0.973	-3.055	-1.091
C	-2.791	-1.336	0.07	H	2.516	-2.668	-0.324
C	1.934	-0.049	-0.312	H	1.103	-3.04	0.669
C	1.055	-1.071	-0.229	H	4.257	-0.931	2.153
C	-4.472	0.58	0.185	H	2.812	0.072	2.345
C	1.437	-2.534	-0.245	H	4.392	0.686	2.862
C	3.878	0.097	2.094	H	3.522	1.516	-1.925
C	3.851	0.475	-1.816	H	3.413	-0.103	-2.637
C	-0.976	3.115	-0.127	H	4.941	0.453	-1.926
C	4.112	0.691	0.701	H	-1.364	4.133	-0.098
C	3.433	-0.097	-0.445	H	-0.474	2.932	-1.08
O	-3.697	-2.182	0.146	H	-0.276	2.959	0.698
O	-0.703	0.543	-0.1	H	3.757	1.731	0.676
O	-2.134	2.275	0.015	H	5.19	0.73	0.495
H	-1.153	-2.773	-0.05	H	3.787	-1.133	-0.39
H	1.53	0.962	-0.297				
Conformation 2							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	0.668	1.49	0.173	H	4.522	1.702	-1.255
C	2.963	0.672	-0.225	H	4.909	0.001	-0.882
C	0.24	0.215	0.314	H	4.955	1.238	0.387
C	2.447	-0.573	-0.029	H	-0.675	-1.423	2.361
C	2.063	1.816	-0.124	H	-2.275	-1.749	1.678
C	-2.171	0.442	0.104	H	-0.824	-2.382	0.891
C	-1.13	-0.261	0.594	H	-4.134	-2.111	-1.258

C	4.419	0.905	-0.512	H	-2.879	-1.17	-2.08
C	-1.239	-1.52	1.426	H	-4.505	-1.276	-2.775
C	-3.947	-1.196	-1.835	H	-4.107	2.346	0.55
C	-4.244	1.404	1.095	H	-3.768	1.51	2.075
C	2.584	-2.967	0.038	H	-5.32	1.259	1.25
C	-4.372	0.048	-1.049	H	3.403	-3.68	-0.055
C	-3.647	0.219	0.307	H	1.859	-3.121	-0.766
O	2.45	2.987	-0.271	H	2.093	-3.085	1.008
O	1.142	-0.824	0.223	H	-4.203	0.947	-1.658
O	3.206	-1.675	-0.07	H	-5.452	0.007	-0.855
H	-0.028	2.311	0.297	H	-3.814	-0.694	0.892
H	-1.941	1.306	-0.521				
Conformation 3							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	0.525	1.374	-0.026	H	4.617	1.944	-0.582
C	2.926	0.816	0.101	H	5.04	0.365	0.121
C	0.225	0.057	-0.088	H	4.561	1.725	1.16
C	2.53	-0.483	0.005	H	-0.608	-2.659	-0.456
C	1.901	1.854	0.099	H	-2.203	-2.218	-1.078
C	-2.155	0.033	0.41	H	-0.741	-1.755	-1.963
C	-1.109	-0.571	-0.189	H	-4.473	0.238	-2.214
C	4.369	1.222	0.204	H	-3.257	1.439	-1.757
C	-1.176	-1.87	-0.962	H	-4.959	1.909	-1.892
C	-4.285	1.107	-1.572	H	-3.876	0.069	2.558
C	-4.011	-0.773	1.867	H	-3.408	-1.61	2.235
C	2.914	-2.848	-0.119	H	-5.066	-1.069	1.9
C	-4.506	0.761	-0.096	H	3.808	-3.471	-0.105
C	-3.603	-0.379	0.431	H	2.373	-2.99	-1.059
O	2.176	3.062	0.182	H	2.266	-3.104	0.723
O	1.239	-0.877	-0.084	H	-4.348	1.656	0.523
O	3.401	-1.5	-0.004	H	-5.553	0.465	0.057
H	-0.266	2.112	-0.08	H	-3.758	-1.252	-0.215
H	-1.949	0.937	0.985				

ECD Calculation Data



1

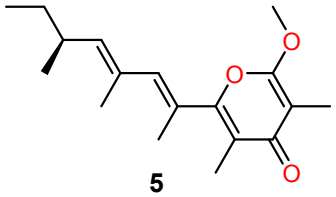
Table S6. Important thermodynamic parameters (a.u.) and Boltzmann distributions of the optimized **1** at B3LYP/6-31G(d) level in methanol.

Conformation	Internal Energy	%
1	-771.074	86.09%
2	-771.072	7.40%
3	-771.071	6.52%

Table S7. Optimized coordinates of compound **1** at B3LYP/6-31G(d) level in methanol.

Conformation 1							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-1.383	-1.715	-0.037	H	-5.08	0.166	-0.623
C	-3.052	0.097	0.081	H	-4.533	1.669	0.153
C	-0.388	-0.798	-0.122	H	-4.925	0.236	1.128
C	-1.989	0.946	-0.008	H	2.515	-2.667	-0.337
C	-2.789	-1.334	0.071	H	1.104	-3.044	0.656
C	1.932	-0.047	-0.311	H	0.971	-3.051	-1.103
C	1.054	-1.071	-0.233	H	4.254	-0.949	2.143
C	-4.471	0.58	0.19	H	2.814	0.058	2.348
C	1.436	-2.534	-0.256	H	4.397	0.662	2.865
C	3.879	0.081	2.093	H	3.516	1.53	-1.914
C	3.846	0.488	-1.813	H	3.408	-0.084	-2.638
C	-0.969	3.116	-0.105	H	4.937	0.469	-1.923
C	4.111	0.685	0.705	H	-1.358	4.133	-0.083
C	3.431	-0.095	-0.446	H	-0.44	2.937	-1.045
O	-3.698	-2.181	0.15	H	-0.295	2.953	0.739
O	-0.704	0.542	-0.106	H	3.755	1.726	0.689
O	-2.133	2.274	-0.003	H	5.188	0.725	0.498
H	-1.152	-2.773	-0.048	H	3.785	-1.131	-0.4
H	1.529	0.964	-0.29				
Conformation 2							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	0.666	1.487	0.175	H	4.533	1.541	-1.395
C	2.962	0.676	-0.218	H	4.966	-0.011	-0.643

C	0.239	0.209	0.307	H	4.886	1.473	0.326
C	2.449	-0.574	-0.038	H	-0.662	-1.476	2.32
C	2.059	1.814	-0.118	H	-2.268	-1.783	1.642
C	-2.172	0.44	0.113	H	-0.824	-2.401	0.83
C	-1.129	-0.272	0.584	H	-4.131	-2.082	-1.305
C	4.419	0.921	-0.498	H	-2.883	-1.117	-2.107
C	-1.234	-1.55	1.387	H	-4.511	-1.211	-2.799
C	-3.95	-1.153	-1.86	H	-4.109	2.33	0.612
C	-4.243	1.374	1.133	H	-3.765	1.456	2.115
C	2.589	-2.968	0.056	H	-5.318	1.224	1.287
C	-4.376	0.07	-1.042	H	3.408	-3.679	-0.044
C	-3.647	0.209	0.316	H	1.845	-3.137	-0.727
O	2.448	2.989	-0.26	H	2.123	-3.066	1.039
O	1.144	-0.825	0.21	H	-4.212	0.985	-1.629
O	3.205	-1.674	-0.093	H	-5.455	0.02	-0.844
H	-0.032	2.306	0.302	H	-3.81	-0.717	0.879
H	-1.947	1.318	-0.494				
Conformation 3							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	0.525	1.374	-0.019	H	4.623	1.925	-0.608
C	2.925	0.818	0.1	H	5.037	0.362	0.131
C	0.224	0.056	-0.079	H	4.563	1.745	1.14
C	2.53	-0.483	0.005	H	-0.61	-2.668	-0.399
C	1.9	1.852	0.101	H	-2.198	-2.234	-1.044
C	-2.157	0.039	0.407	H	-0.725	-1.793	-1.924
C	-1.108	-0.575	-0.177	H	-4.461	0.218	-2.225
C	4.369	1.223	0.195	H	-3.253	1.43	-1.772
C	-1.171	-1.887	-0.926	H	-4.956	1.891	-1.92
C	-4.28	1.094	-1.589	H	-3.884	0.092	2.55
C	-4.016	-0.755	1.866	H	-3.414	-1.589	2.243
C	2.915	-2.848	-0.129	H	-5.071	-1.052	1.898
C	-4.508	0.76	-0.112	H	3.811	-3.468	-0.12
C	-3.605	-0.375	0.428	H	2.372	-2.984	-1.067
O	2.175	3.064	0.182	H	2.27	-3.106	0.715
O	1.24	-0.876	-0.078	H	-4.354	1.66	0.501
O	3.401	-1.497	-0.009	H	-5.554	0.462	0.038
H	-0.267	2.111	-0.07	H	-3.757	-1.253	-0.21
H	-1.956	0.954	0.967				



5

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

Conformation	Internal Energy	%
1	-927.046	26.24%
2	-927.046	25.80%
3	-927.046	17.27%
4	-927.046	15.29%
5	-927.046	14.11%
6	-927.043	1.25%

Table S9. Optimized coordinates of compound **5** at B3LYP/6-31G(d) level in methanol.

Conformation 1							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	1.694	-1.371	-0.17	H	-0.198	-2.301	-0.673
C	4.031	-0.491	-0.071	H	0.699	-3.124	0.612
C	1.243	-0.092	-0.071	H	5.823	-1.292	0.81
C	3.467	0.749	-0.01	H	6.065	0.236	-0.061
C	3.148	-1.638	-0.152	H	5.823	-1.285	-0.948
C	-1.036	-0.209	0.779	H	-0.535	1.329	-1.963
C	-3.293	0.273	-0.089	H	0.343	2.353	-0.83
C	-0.149	0.407	-0.039	H	-1.398	2.074	-0.608
C	-2.475	0.062	0.964	H	-2.473	0.827	2.989
C	0.803	-2.573	-0.331	H	-4.01	0.083	2.52
C	5.518	-0.709	-0.067	H	-2.6	-0.924	2.88
C	-0.456	1.609	-0.904	H	-5.91	-1.939	0.687
C	-2.926	0.012	2.409	H	-4.445	-2.281	-0.246
C	-5.478	-1.922	-0.321	H	-6.038	-2.636	-0.936
C	-5.033	1.961	-0.683	H	-4.653	2.039	-1.71
C	3.535	3.144	0.104	H	-6.107	2.179	-0.706
C	-5.537	-0.514	-0.922	H	-4.54	2.734	-0.083
C	-4.775	0.555	-0.103	H	4.34	3.874	0.176
O	3.588	-2.802	-0.216	H	2.881	3.217	0.976
O	2.141	0.962	-0.009	H	2.958	3.311	-0.809
O	4.198	1.866	0.064	H	-5.135	-0.531	-1.945
H	-0.64	-0.983	1.436	H	-6.585	-0.198	-1.009
H	-2.847	0.229	-1.084	H	-5.17	0.538	0.919

H	1.261	-3.264	-1.045				
Conformation 2							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-1.852	1.397	0.199	H	-1.664	3.318	1.102
C	-4.056	0.229	0.051	H	-0.095	2.552	0.723
C	-1.24	0.187	0.098	H	-5.952	0.771	0.903
C	-3.338	-0.929	-0.008	H	-5.916	0.817	-0.855
C	-3.327	1.478	0.159	H	-5.98	-0.749	-0.02
C	1.01	0.585	-0.739	H	-0.058	-2.097	0.927
C	3.311	0.393	0.135	H	0.721	-0.955	2.019
C	0.205	-0.13	0.082	H	1.638	-1.636	0.667
C	2.473	0.507	-0.917	H	2.496	1.559	-2.803
C	-1.121	2.7	0.381	H	4.002	0.691	-2.47
C	-5.558	0.257	0.018	H	2.55	-0.192	-2.964
C	0.655	-1.269	0.968	H	5.465	-3.092	0.468
C	2.917	0.647	-2.359	H	3.979	-2.357	-0.152
C	5.056	-2.203	-0.024	H	5.503	-2.14	-1.024
C	5.35	1.594	0.925	H	6.447	1.594	0.945
C	-3.098	-3.31	-0.164	H	5.017	2.528	0.461
C	5.351	-0.94	0.791	H	4.995	1.589	1.963
C	4.819	0.367	0.154	H	-2.504	-3.419	0.747
O	-3.912	2.576	0.228	H	-3.803	-4.136	-0.251
O	-1.995	-0.972	0.014	H	-2.441	-3.282	-1.036
O	-3.92	-2.129	-0.101	H	6.437	-0.839	0.92
H	0.52	1.296	-1.405	H	4.93	-1.042	1.801
H	2.862	0.358	1.129	H	5.208	0.417	-0.869
H	-1.085	3.273	-0.555				
Conformation 3							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	2.048	-1.418	0.165	H	0.628	-2.825	0.999
C	4.016	0.044	-0.32	H	2.313	-3.404	0.881
C	1.286	-0.298	0.278	H	6.094	-0.319	0.078
C	3.167	1.096	-0.146	H	5.763	1.272	-0.643
C	3.482	-1.296	-0.174	H	5.705	-0.201	-1.633
C	-1.043	-0.956	-0.042	H	-0.52	1.914	1.15
C	-3.26	0.12	0.12	H	0.235	0.938	2.407
C	-0.153	-0.154	0.585	H	-1.491	0.728	2.029
C	-2.513	-1.004	0.092	H	-2.731	-2.95	1.014
C	1.534	-2.814	0.391	H	-4.165	-2.437	0.11
C	5.473	0.22	-0.646	H	-2.715	-2.984	-0.746
C	-0.504	0.914	1.599	H	-5.673	-0.654	-2.304
C	-3.074	-2.412	0.12	H	-4.113	0.146	-2.547
C	-5.17	0.321	-2.315	H	-5.601	0.909	-3.133

C	-5.109	0.99	1.553	H	-4.655	1.988	1.587
C	2.614	3.427	-0.045	H	-6.195	1.112	1.649
C	-5.334	1.041	-0.973	H	-4.75	0.428	2.422
C	-4.756	0.268	0.236	H	3.182	4.345	-0.191
O	4.199	-2.307	-0.311	H	2.208	3.393	0.969
O	1.861	0.956	0.139	H	1.8	3.368	-0.772
O	3.567	2.367	-0.253	H	-4.857	2.03	-1.023
H	-0.637	-1.7	-0.727	H	-6.401	1.224	-0.786
H	-2.734	1.071	0.036	H	-5.232	-0.72	0.258
H	1.309	-3.32	-0.557				
Conformation 4							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-2.034	-1.411	0.186	H	-1.397	-3.346	-0.543
C	-4.046	0.038	-0.127	H	-0.516	-2.787	0.888
C	-1.266	-0.289	0.172	H	-5.885	-0.336	-1.175
C	-3.185	1.093	-0.086	H	-6.064	-0.22	0.57
C	-3.497	-1.298	0.008	H	-5.812	1.255	-0.388
C	1.014	-0.954	-0.393	H	1.674	0.762	1.603
C	3.241	0.112	-0.488	H	-0.006	1.013	2.128
C	0.198	-0.138	0.313	H	0.646	1.94	0.779
C	2.489	-1.007	-0.432	H	2.802	-2.965	0.436
C	-1.494	-2.798	0.404	H	2.582	-2.977	-1.31
C	-5.531	0.205	-0.29	H	4.124	-2.447	-0.622
C	0.656	0.952	1.257	H	5.716	-0.614	1.939
C	3.041	-2.417	-0.485	H	5.634	0.962	2.743
C	5.196	0.352	1.945	H	4.148	0.163	2.204
C	5.101	0.929	-1.936	H	6.188	1.033	-2.037
C	-2.625	3.424	-0.158	H	4.732	0.351	-2.79
C	5.322	1.052	0.588	H	4.661	1.933	-1.996
C	4.74	0.248	-0.6	H	-1.915	3.327	-0.983
O	-4.222	-2.311	-0.01	H	-3.207	4.338	-0.269
O	-1.855	0.961	0.053	H	-2.088	3.433	0.794
O	-3.597	2.361	-0.189	H	6.382	1.249	0.38
H	0.531	-1.711	-1.011	H	4.83	2.034	0.629
H	2.717	1.068	-0.504	H	5.21	-0.743	-0.589
H	-2.202	-3.363	1.018				
Conformation 5							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	1.553	-1.307	0.373	H	-0.254	-1.932	1.391
C	3.896	-0.808	-0.339	H	0.095	-2.84	-0.088
C	1.299	0.029	0.36	H	5.798	-1.712	0.128
C	3.544	0.506	-0.268	H	5.219	-2.029	-1.502
C	2.894	-1.802	-0.003	H	5.884	-0.43	-1.095

C	-1.097	0.299	0.112	H	0.615	2.835	0.958
C	-3.377	0.015	-0.562	H	0.99	1.785	2.32
C	0.051	0.76	0.671	H	-0.675	2.294	2.037
C	-2.495	0.748	0.163	H	-2.747	1.806	2.039
C	0.55	-2.352	0.784	H	-2.338	2.848	0.673
C	5.277	-1.259	-0.725	H	-3.967	2.193	0.828
C	0.244	1.984	1.544	H	-4.493	-1.545	1.489
C	-2.91	1.961	0.965	H	-5.927	-0.548	1.78
C	-5.532	-1.379	1.182	H	-6.106	-2.277	1.439
C	-5.155	0.518	-2.236	H	-6.233	0.643	-2.396
C	3.945	2.859	-0.494	H	-4.653	1.44	-2.548
C	-5.631	-1.074	-0.316	H	-4.81	-0.292	-2.892
C	-4.86	0.194	-0.756	H	4.819	3.456	-0.751
O	3.148	-3.022	-0.019	H	3.151	3.019	-1.229
O	2.311	0.928	0.061	H	3.586	3.126	0.503
O	4.406	1.495	-0.525	H	-6.686	-0.945	-0.594
H	-0.974	-0.572	-0.529	H	-5.263	-1.933	-0.895
H	-2.975	-0.839	-1.113	H	-5.227	1.03	-0.15
H	1.065	-3.137	1.346				
Conformation 6							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	2.315	-1.514	0.004	H	0.946	-3.103	0.553
C	4.092	0.23	-0.116	H	2.666	-3.428	0.87
C	1.386	-0.529	-0.072	H	6.065	0.246	0.736
C	3.076	1.138	-0.156	H	5.658	1.717	-0.175
C	3.751	-1.178	-0.035	H	6.044	0.205	-1.022
C	-0.789	0.016	0.862	H	-1.713	-1.808	-0.935
C	-3.095	0.298	0.032	H	-0.093	-2.371	-1.406
C	-0.095	-0.651	-0.088	H	-0.761	-0.914	-2.127
C	-2.248	0.104	1.065	H	-2.112	0.758	3.117
C	1.961	-2.967	0.172	H	-3.732	0.205	2.668
C	5.541	0.632	-0.146	H	-2.43	-0.963	2.939
C	-0.701	-1.487	-1.192	H	-7.222	0.127	-1.178
C	-2.666	0.023	2.519	H	-7.125	-0.831	0.309
C	-6.766	-0.761	-0.726	H	-7.142	-1.635	-1.269
C	-5.003	1.826	-0.474	H	-4.674	1.962	-1.513
C	2.165	3.351	-0.301	H	-6.088	1.967	-0.444
C	-5.234	-0.712	-0.776	H	-4.545	2.618	0.129
C	-4.598	0.433	0.051	H	2.604	4.347	-0.359
O	4.624	-2.066	0.015	H	1.535	3.269	0.588
O	1.773	0.798	-0.143	H	1.571	3.148	-1.196
O	3.291	2.456	-0.217	H	-4.835	-1.666	-0.406
H	-0.201	0.531	1.624	H	-4.901	-0.625	-1.821

H	-2.658	0.398	-0.962	H	-4.967	0.338	1.08
H	2.052	-3.517	-0.774				