

SUPPORTING INFORMATION

Bioassay-guided Isolation of Terpenoids from the Soft Coral *Sclerophyllum humesi* and Assessment of their Antidiabetic and Cytotoxic activities

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Figure S1. ^1H NMR spectrum of compound **1**

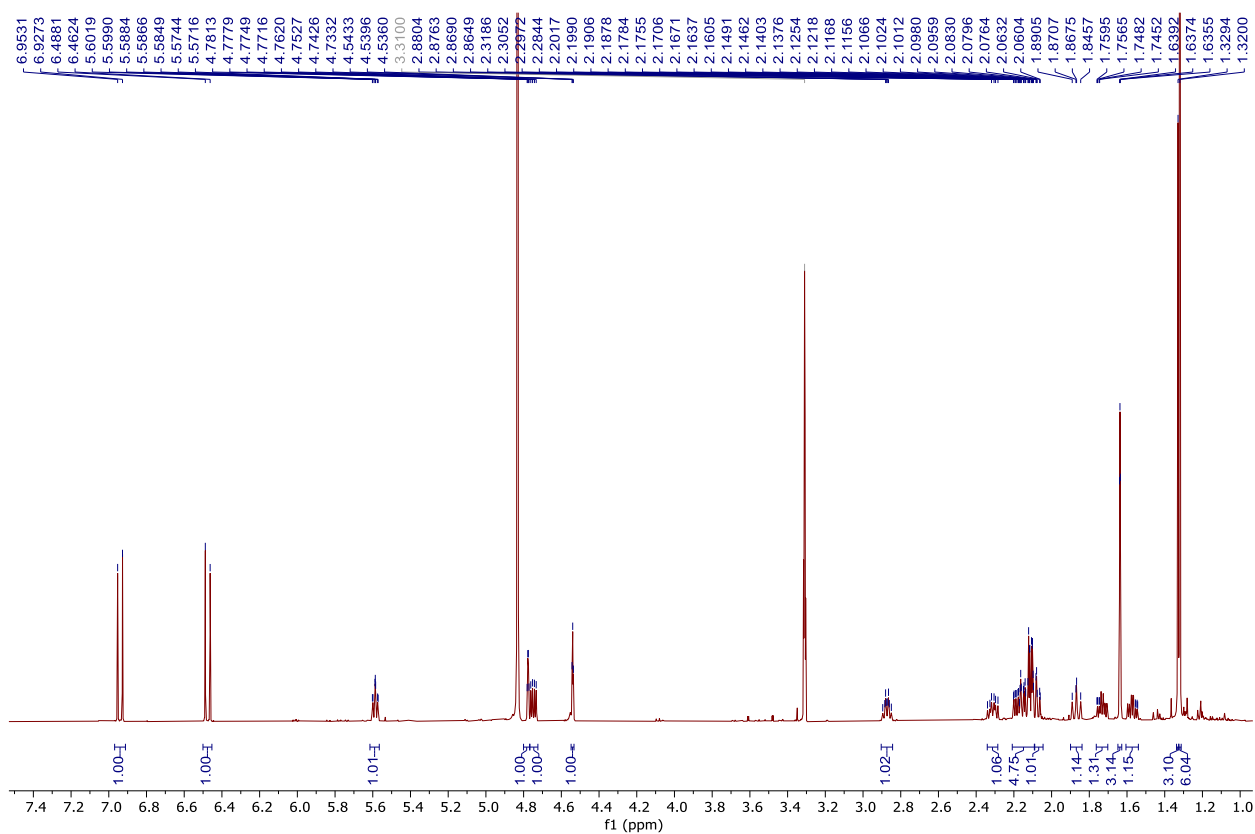


Figure S2. ^{13}C NMR spectrum of compound **1**

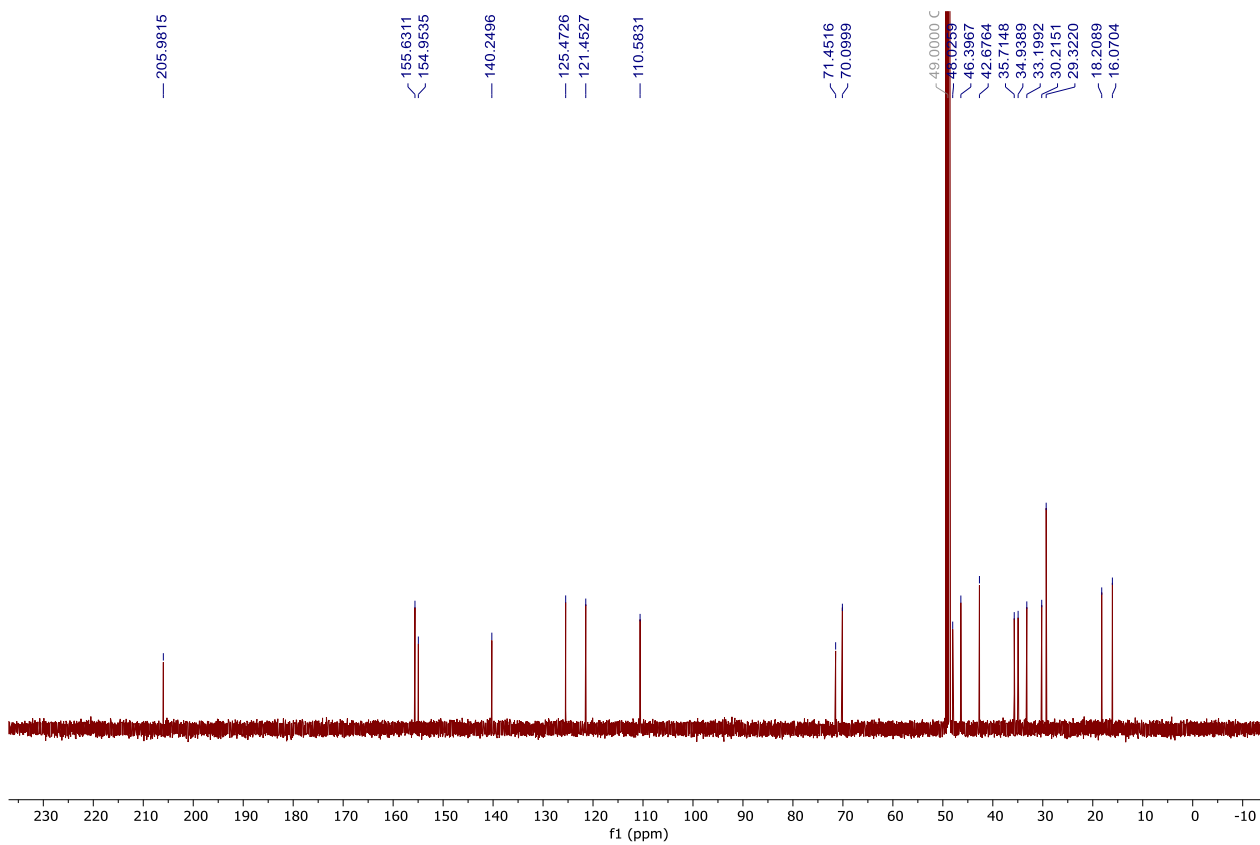


Figure S3. DEPT NMR spectrum of compound **1**

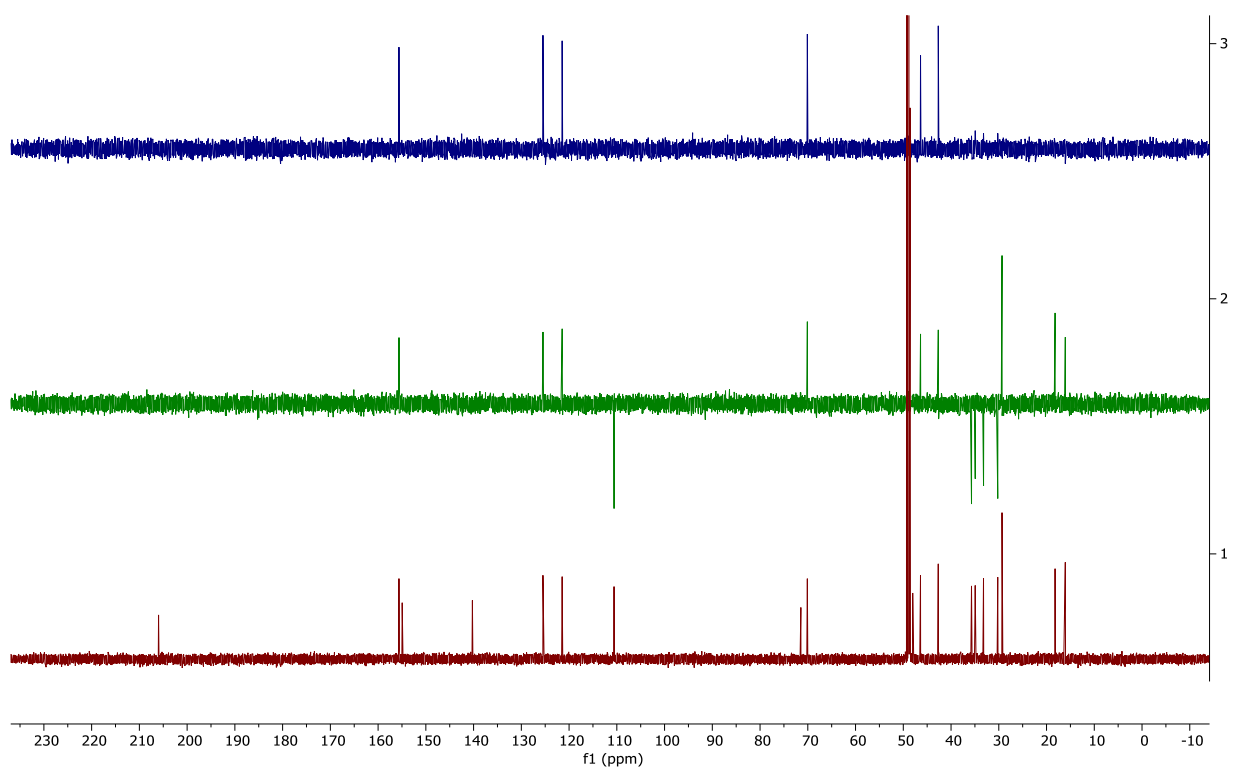


Figure S4. HSQC spectrum of compound **1**

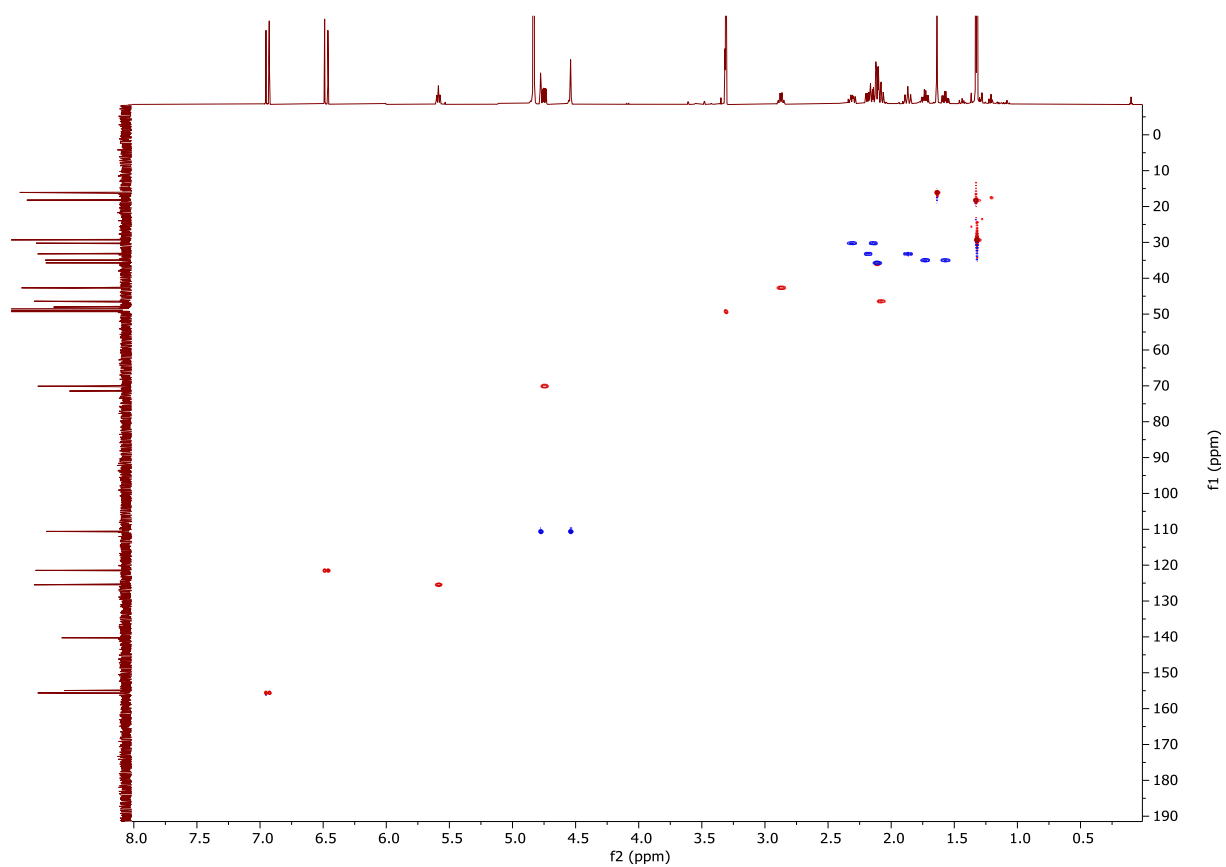


Figure S5. HMBC spectrum of compound **1**

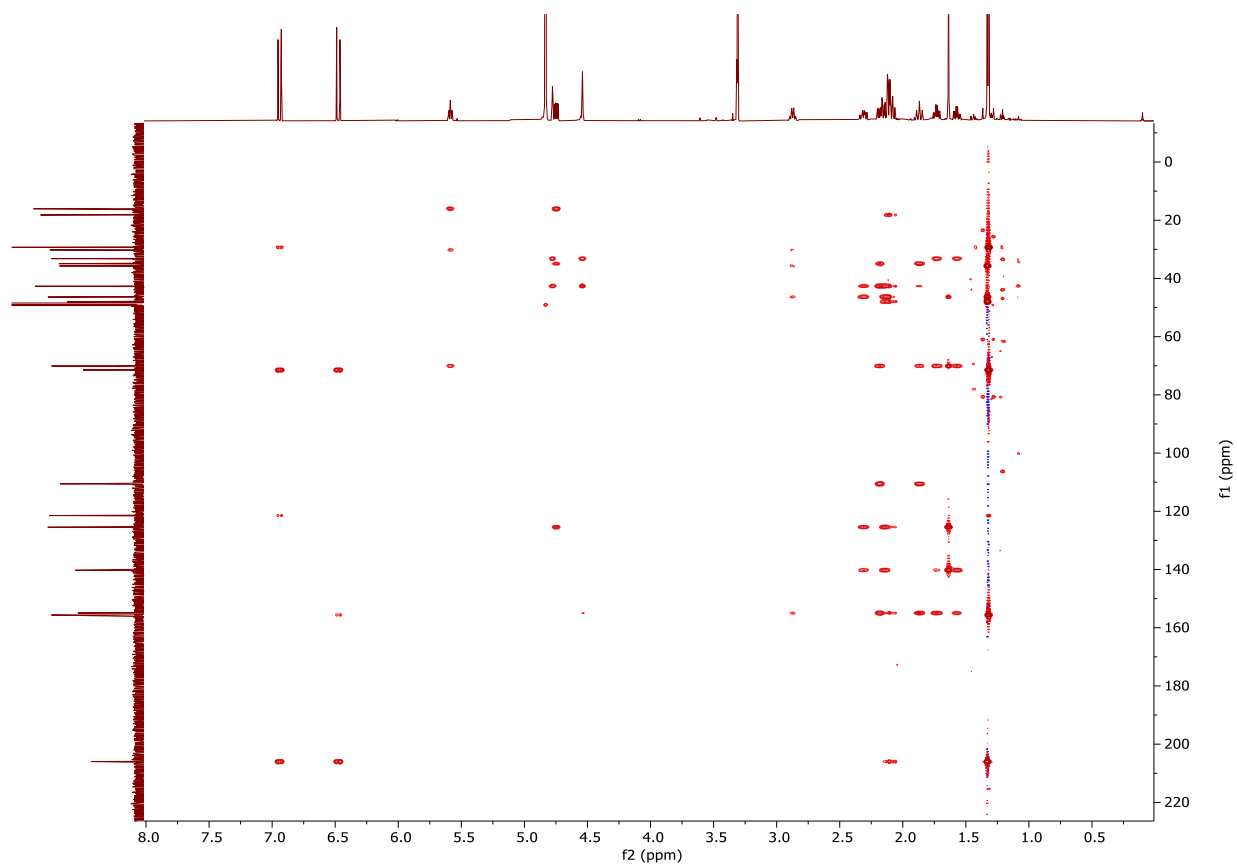


Figure S6. COSY spectrum of compound **1**

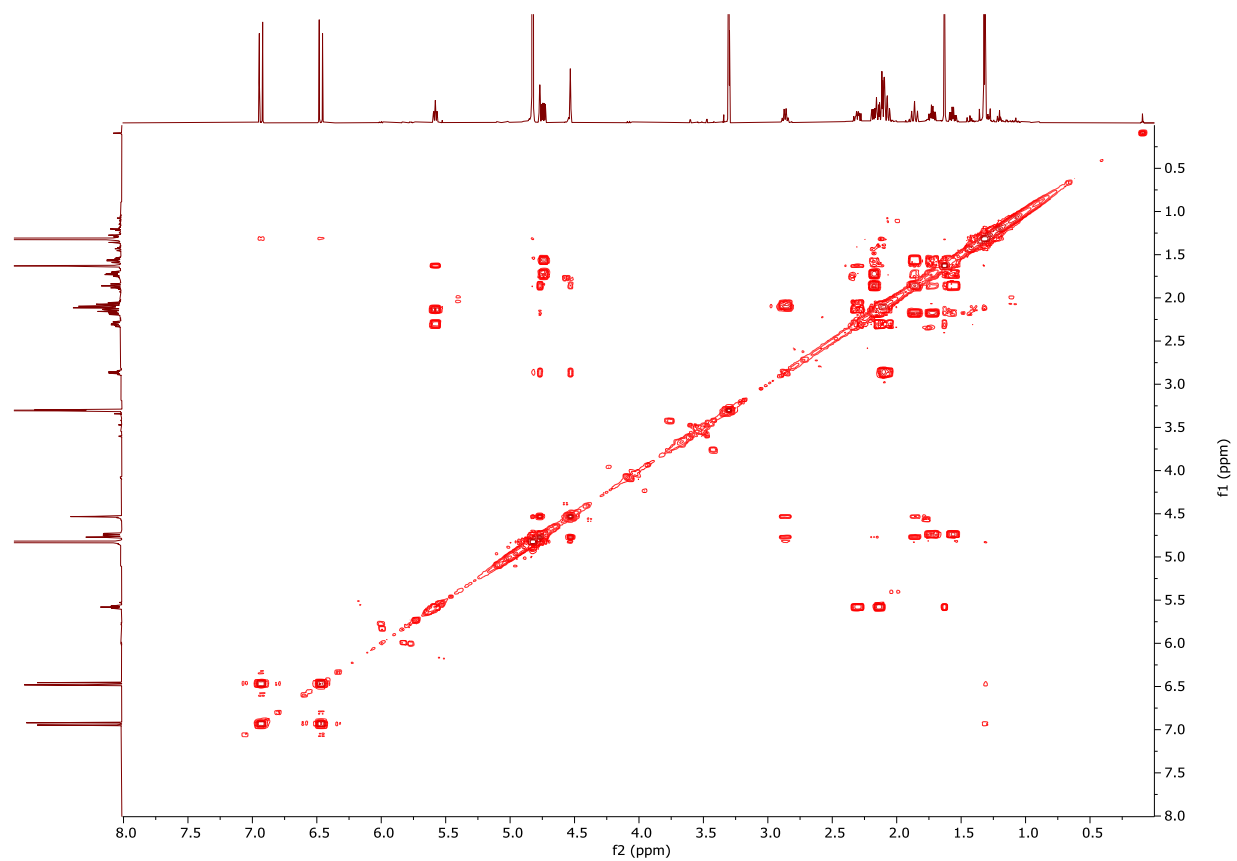


Figure S7. NOESY spectrum of compound 1

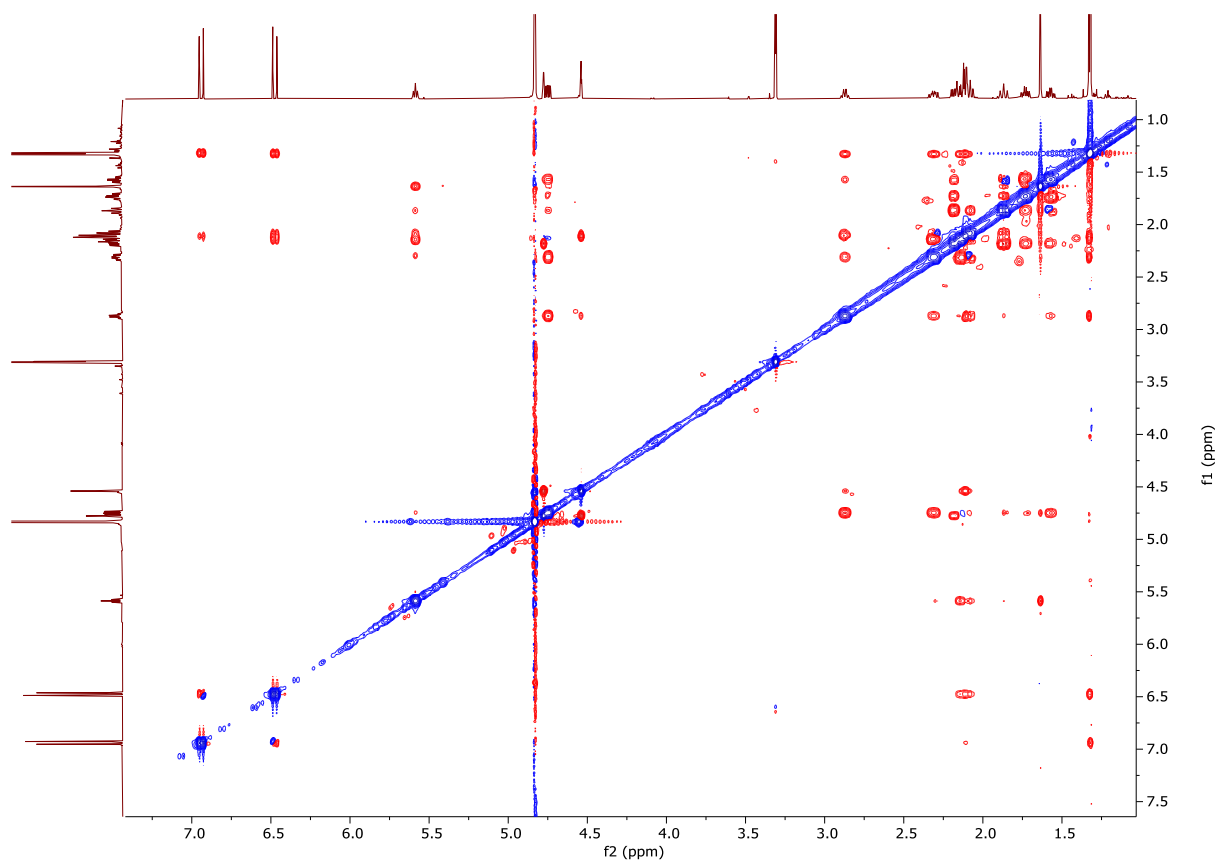


Figure S8. HRESIMS spectra of compound 1

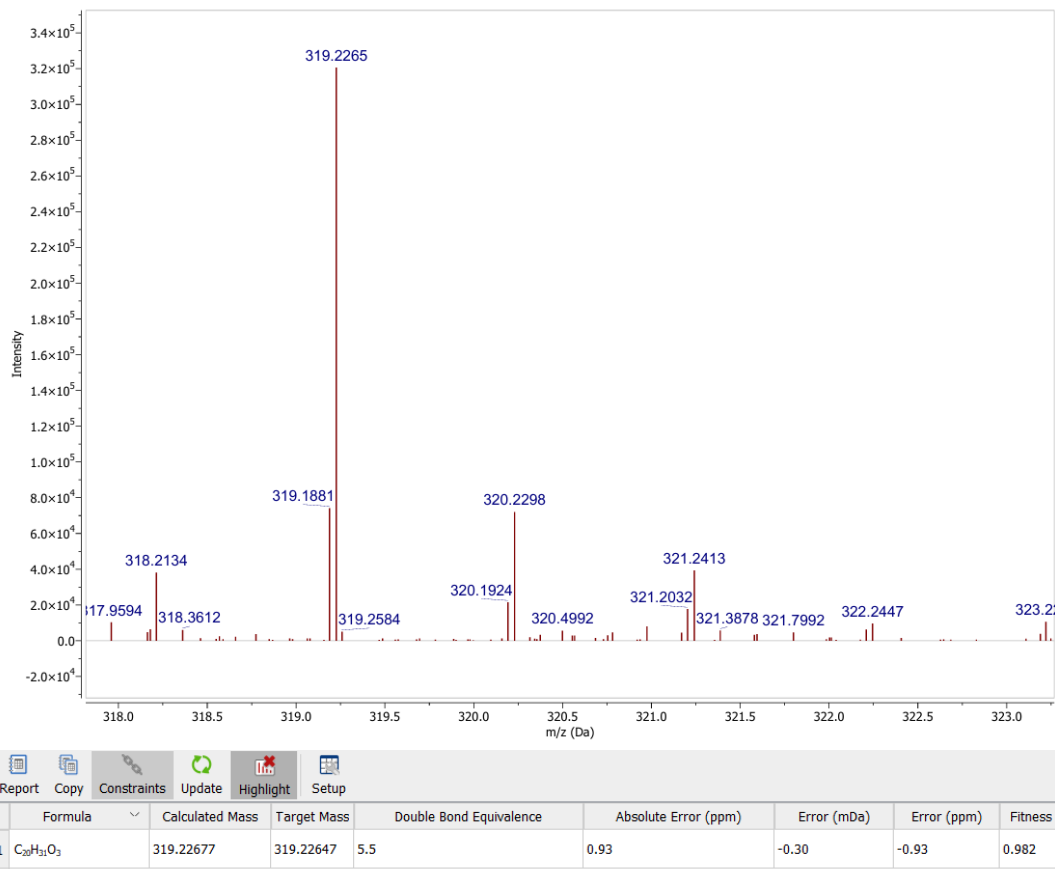


Figure S9. UV spectrum of compound **1**

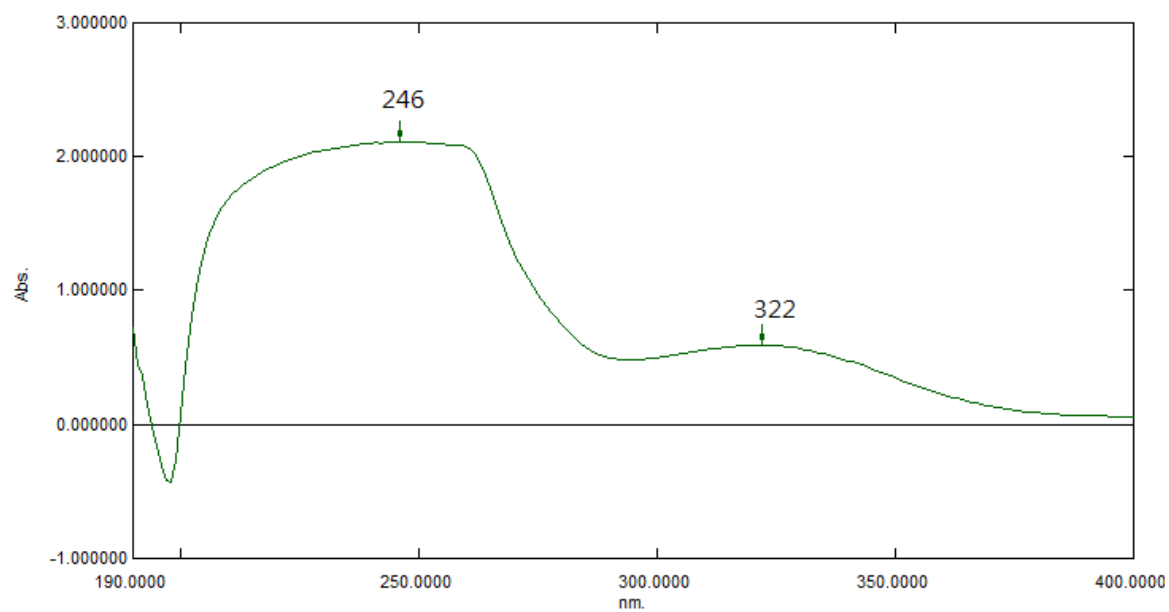


Figure S10. IR spectrum of compound **1**

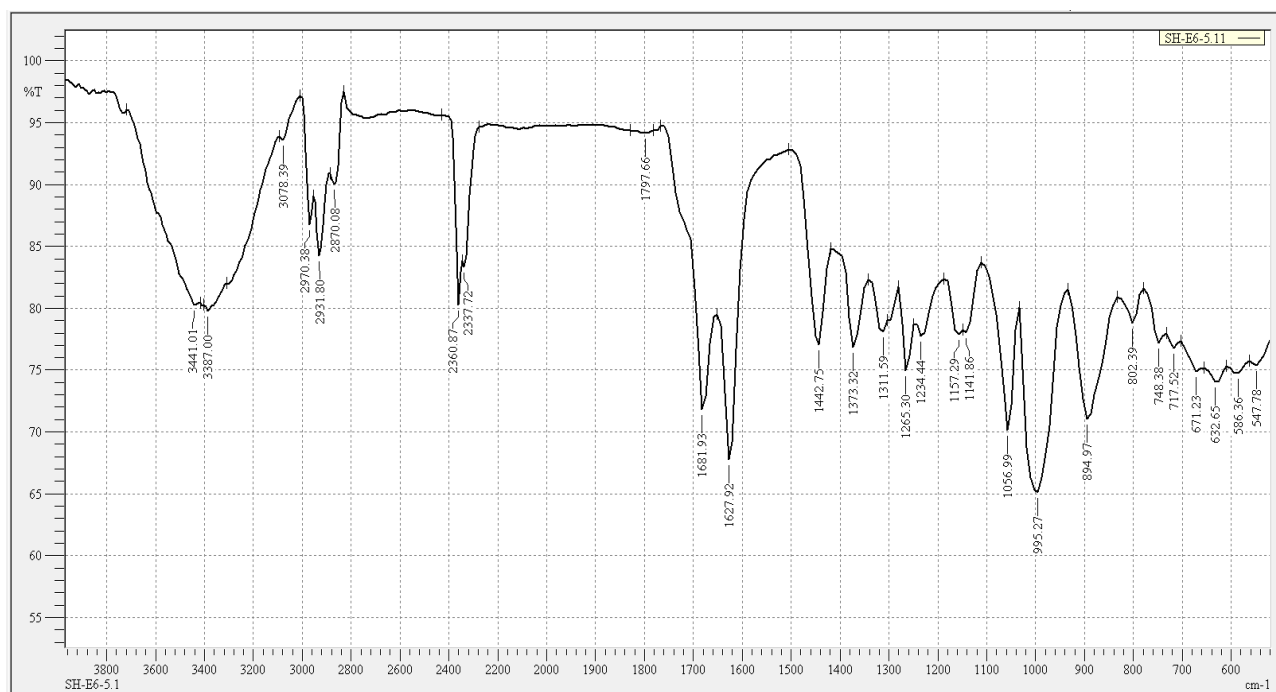


Figure S11. ^1H NMR spectrum of compound **2**

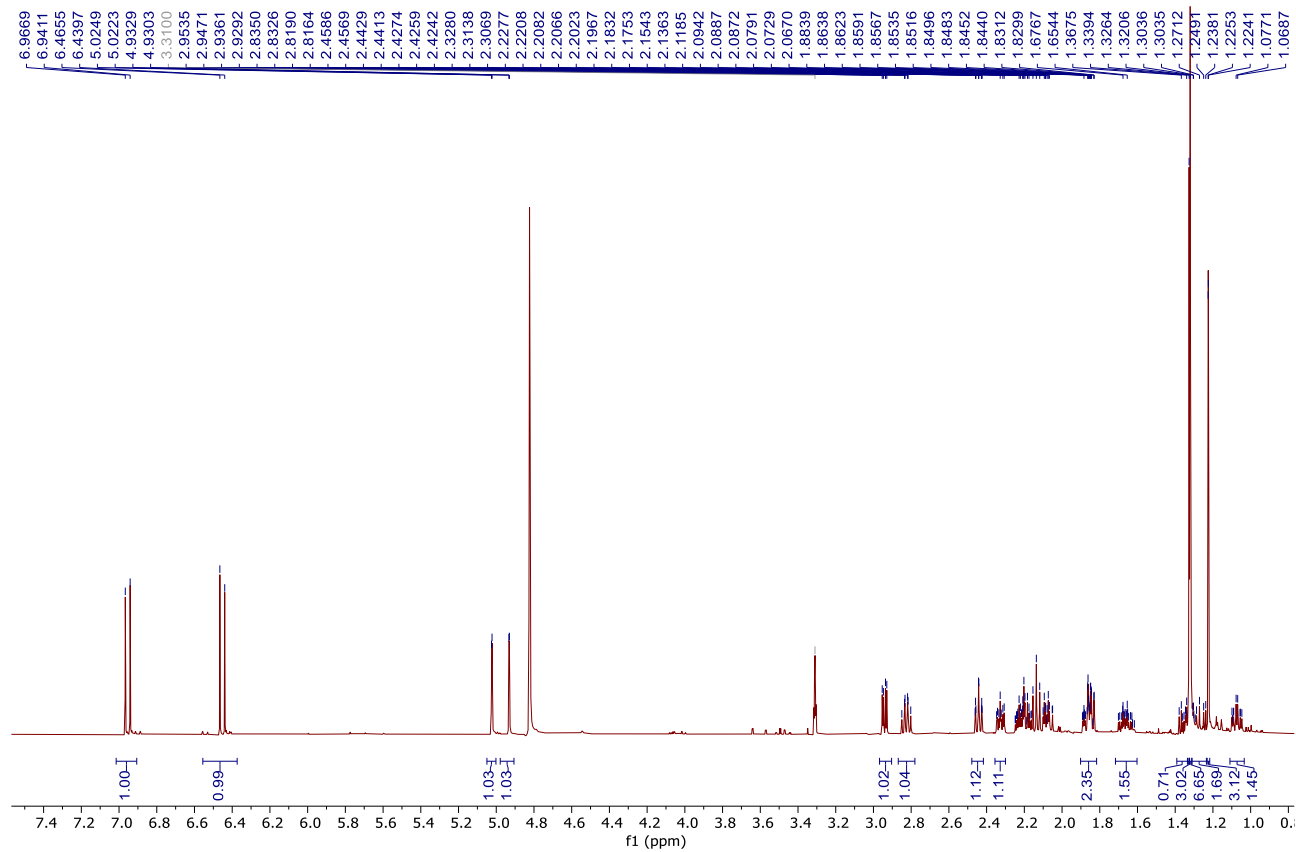


Figure S12. ^{13}C NMR spectrum of compound **2**

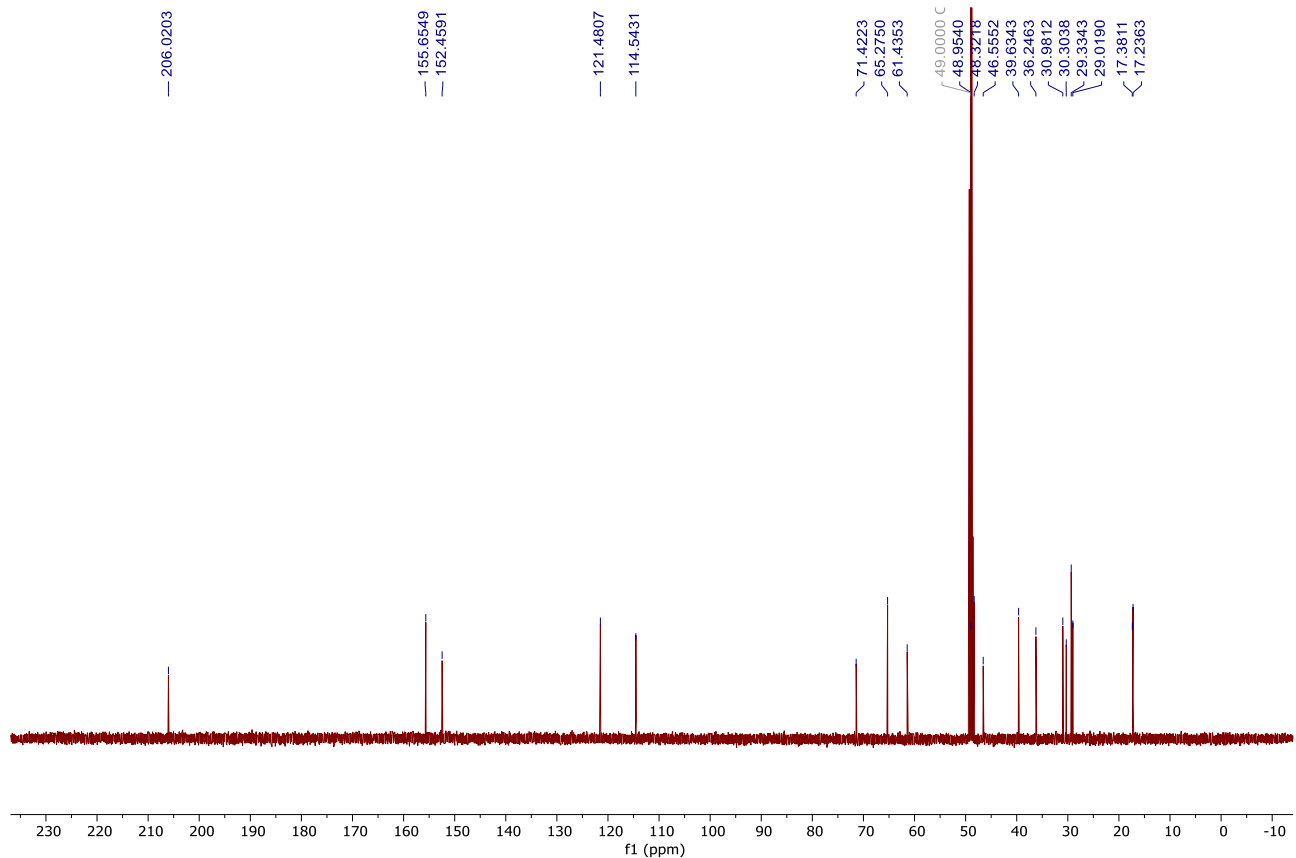


Figure S13. DEPT spectrum of compound **2**

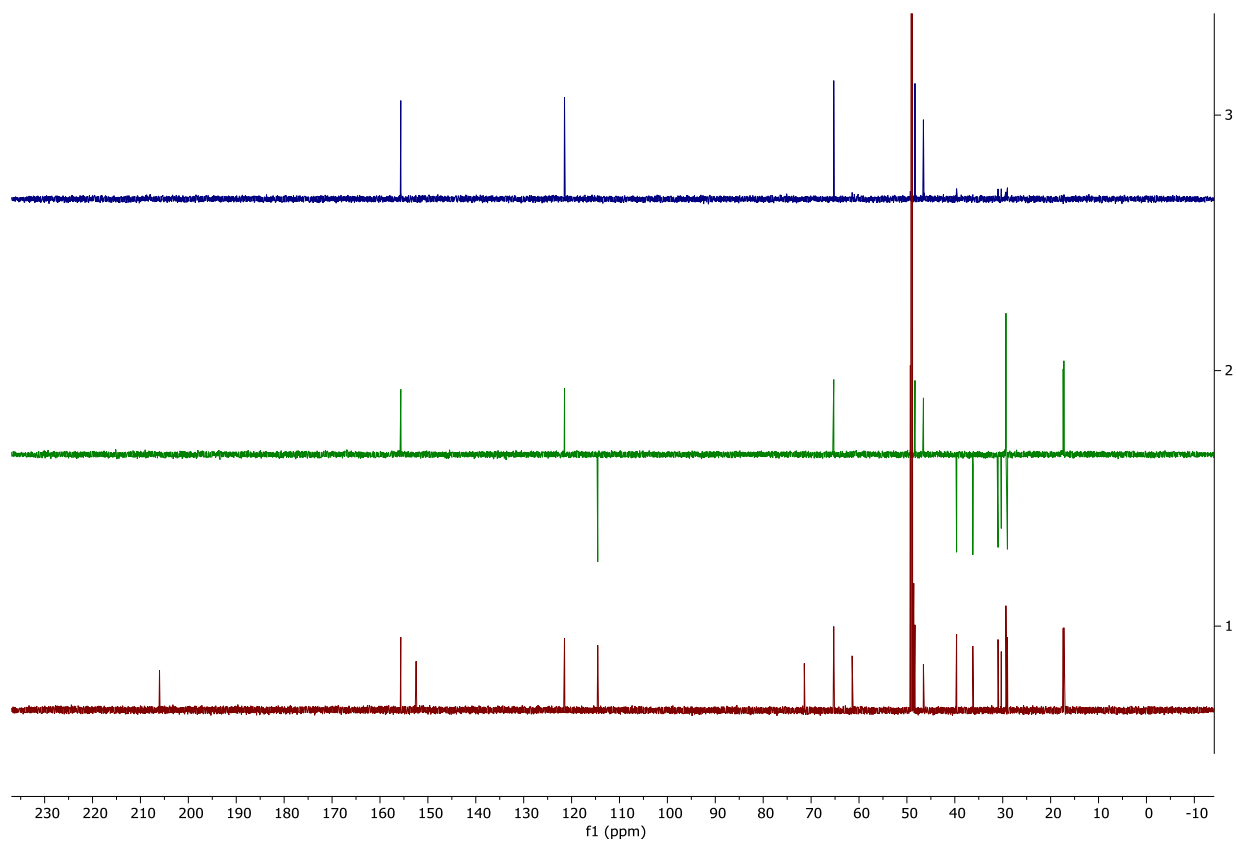


Figure S14. ESI-MS spectrum of compound **2**

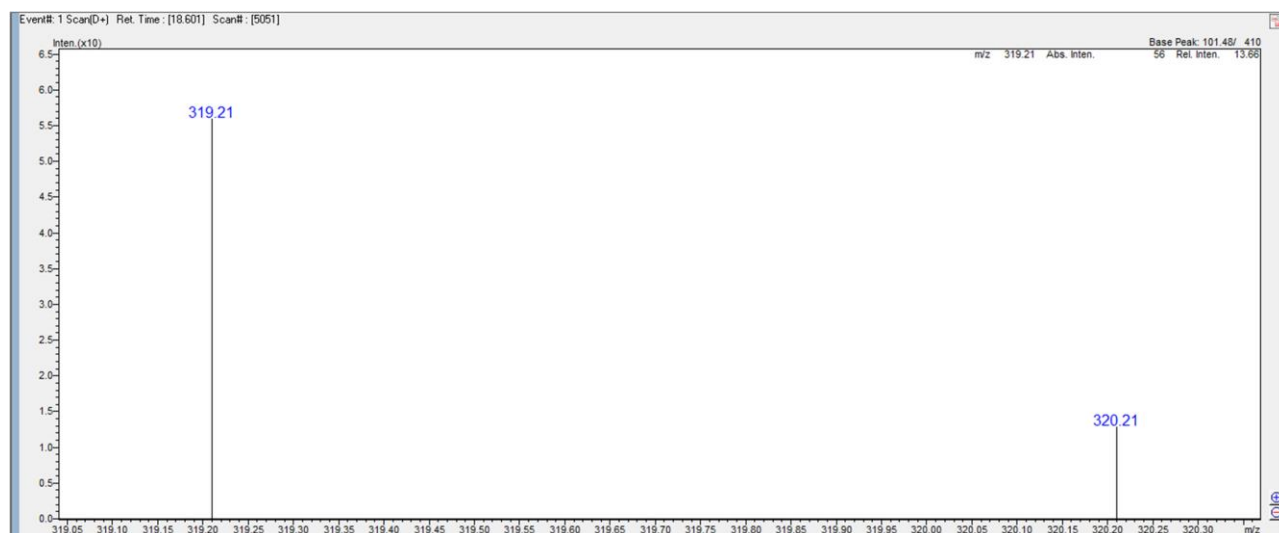


Figure S15. ^1H NMR spectrum of compound **3**

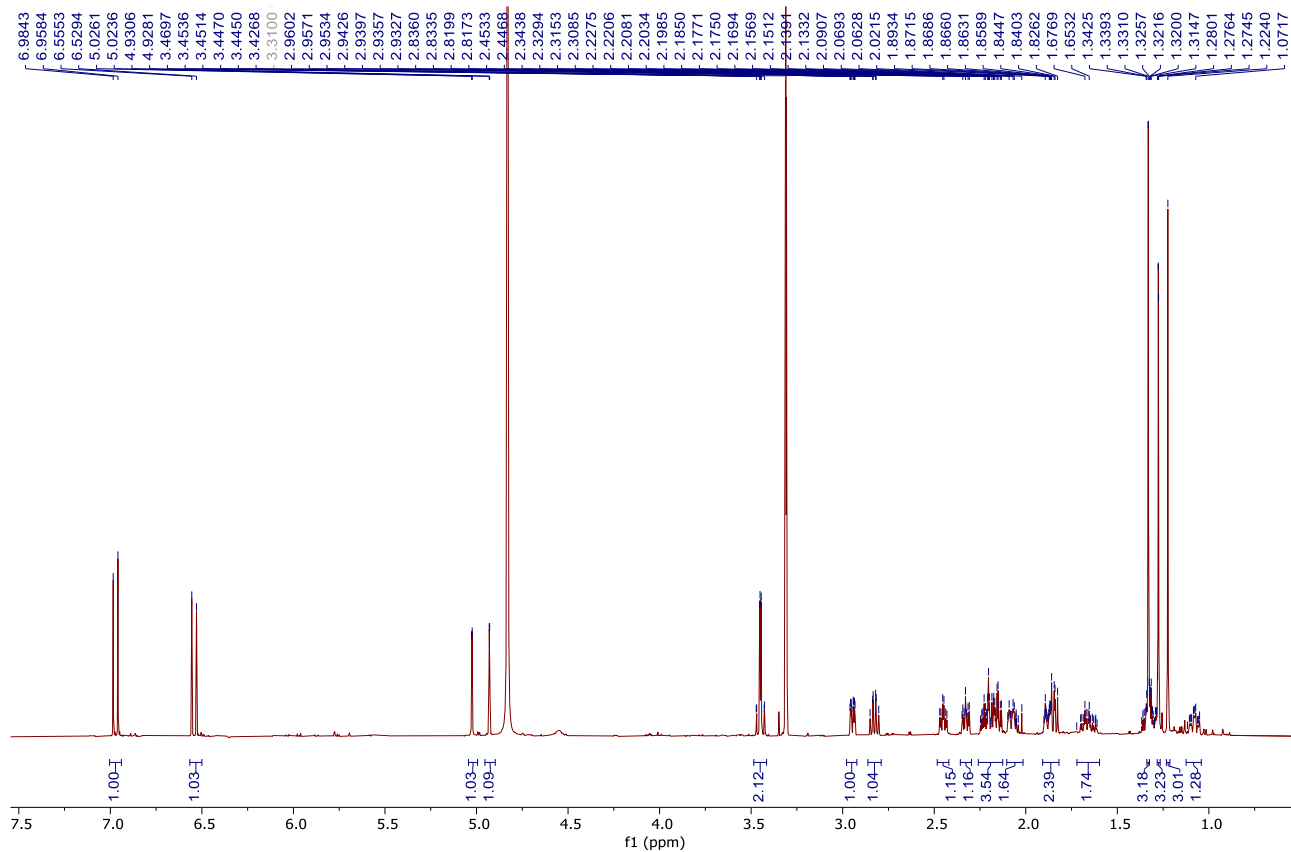


Figure S16. ^{13}C NMR spectrum of compound **3**

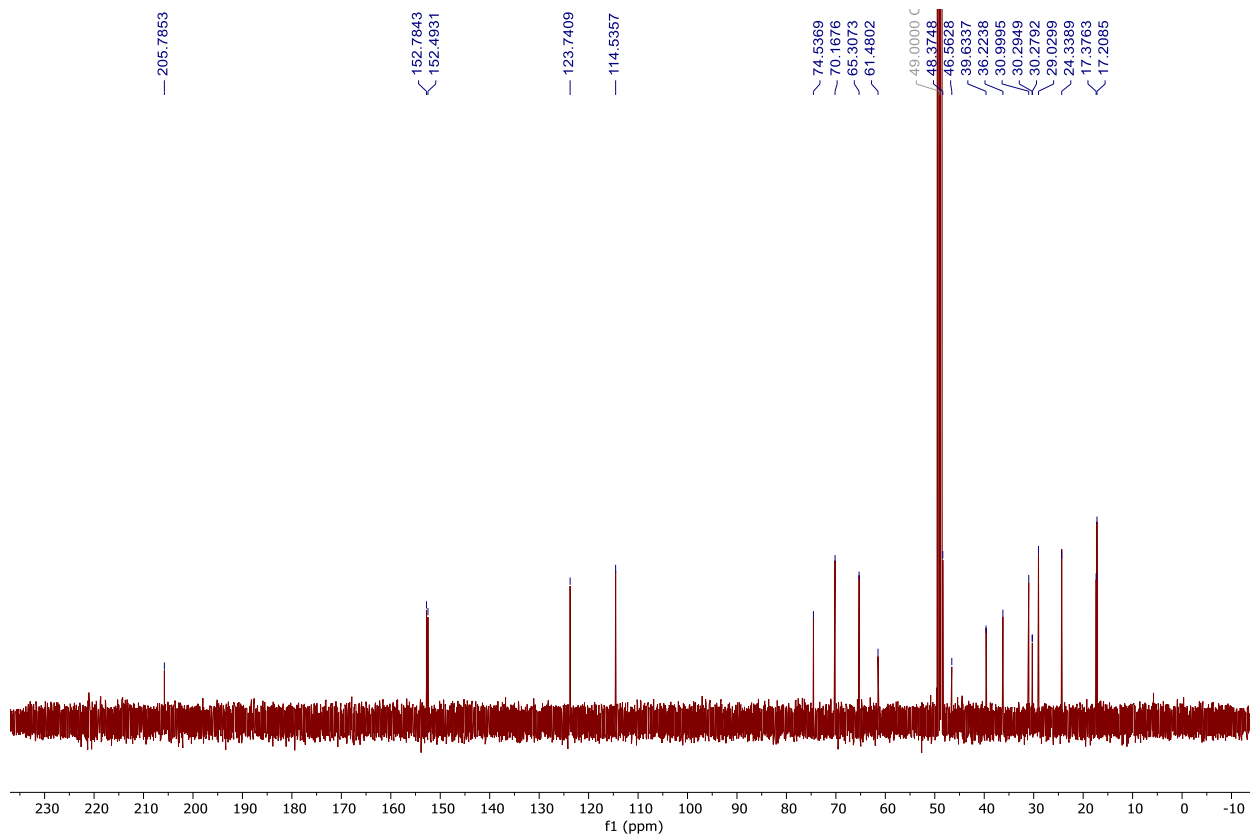


Figure S17. DEPT spectrum of compound **3**

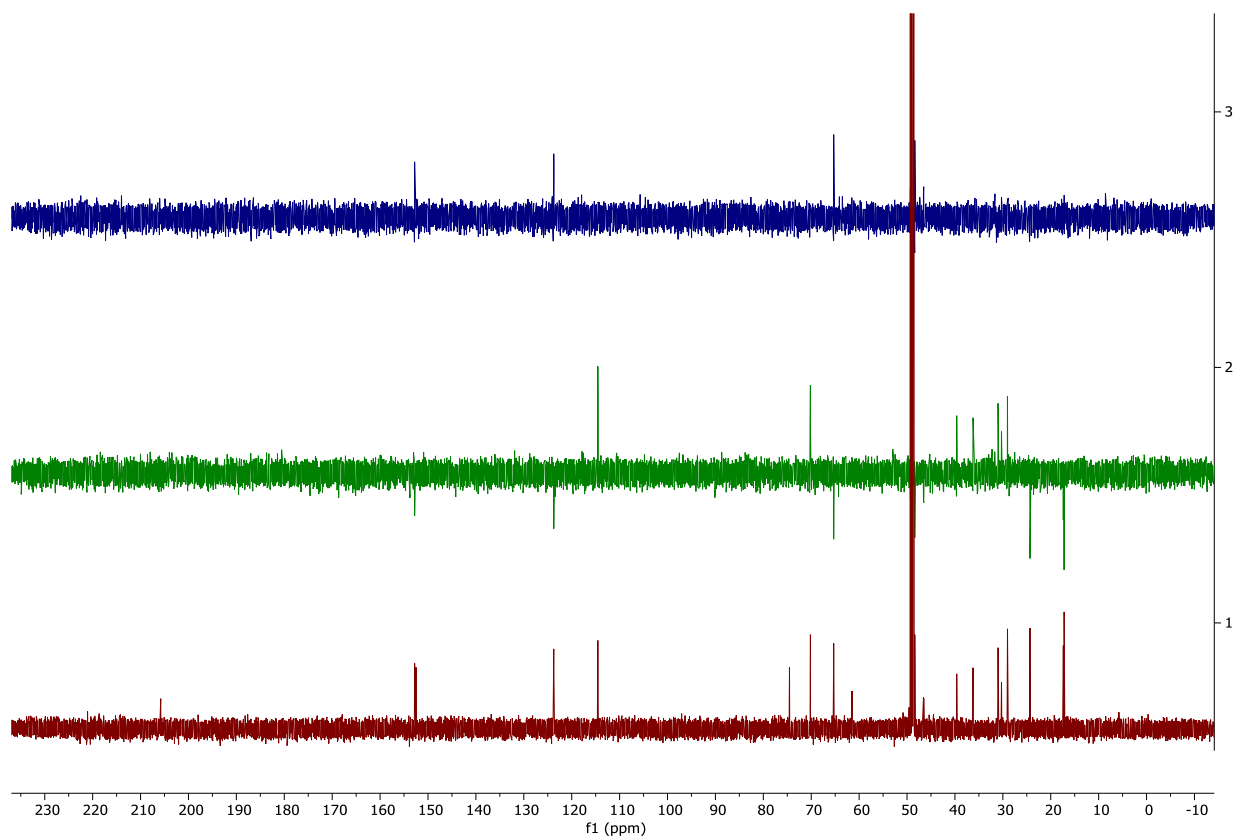


Figure S18. ESI-MS spectrum of compound **3**

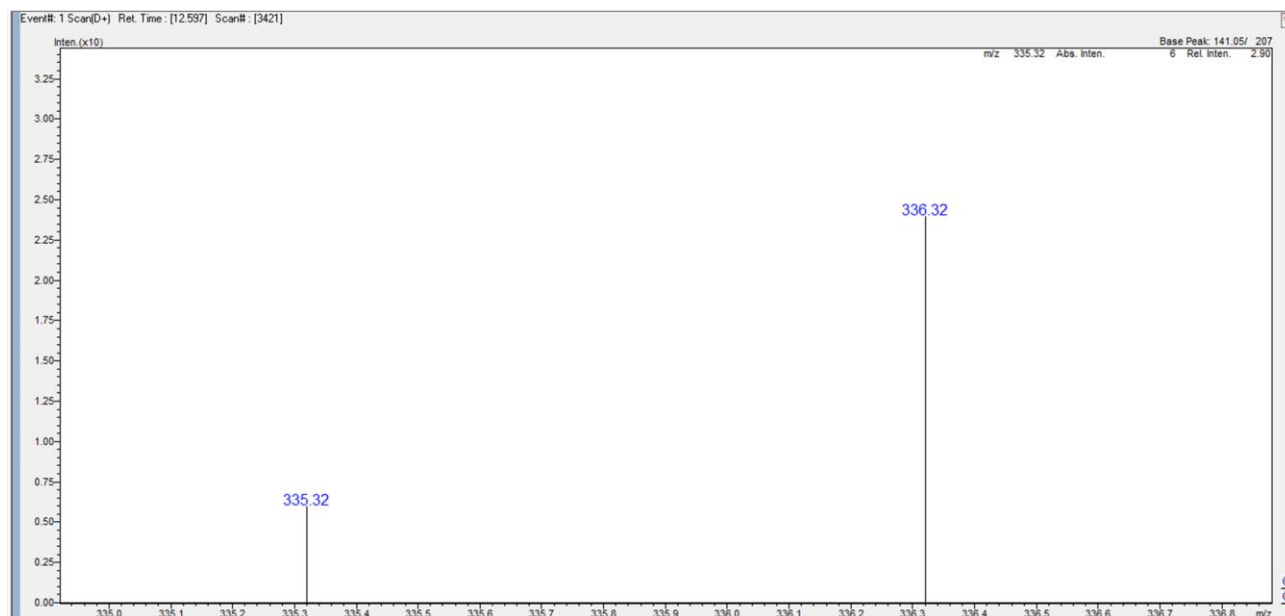


Figure S19. ^1H NMR spectrum of compound **4**

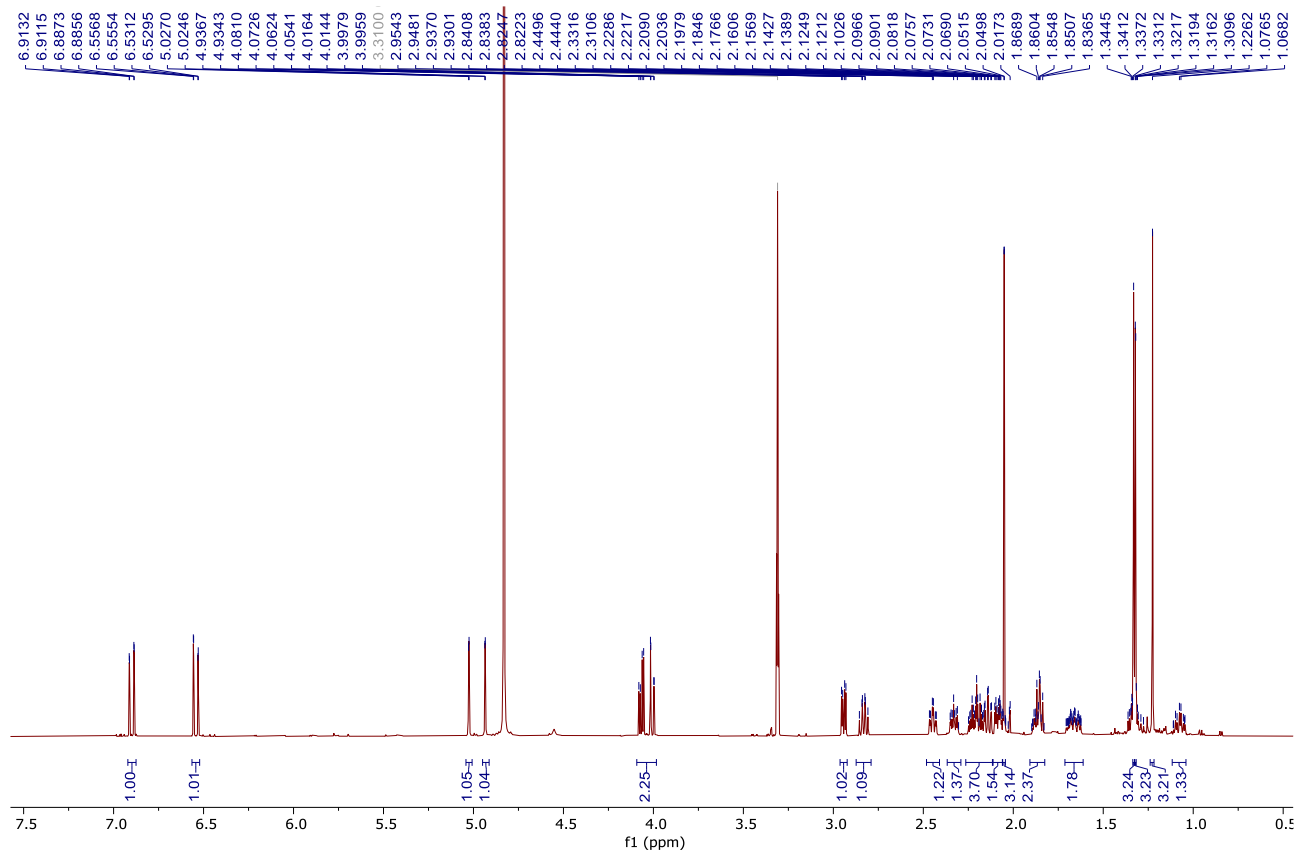


Figure S20. ^{13}C NMR spectrum of compound **4**

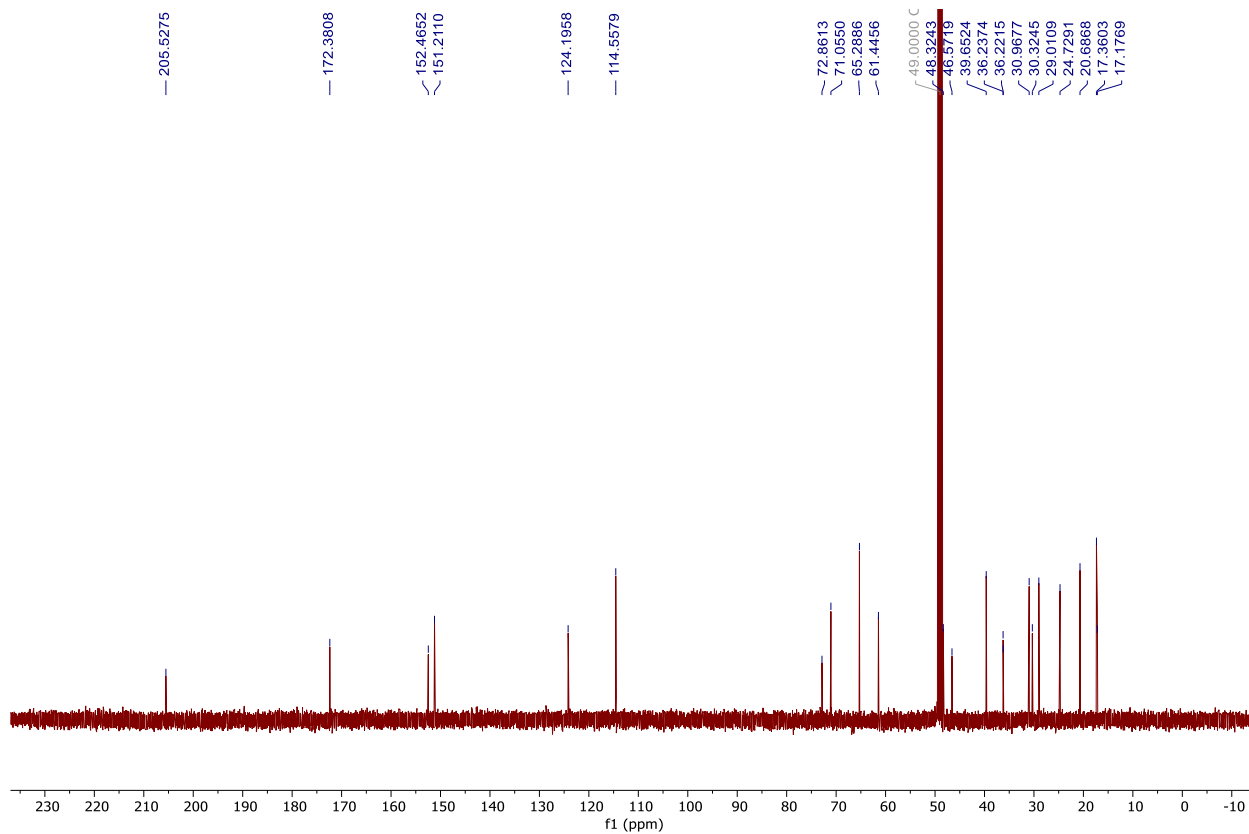


Figure S21. DEPT spectrum of compound **4**

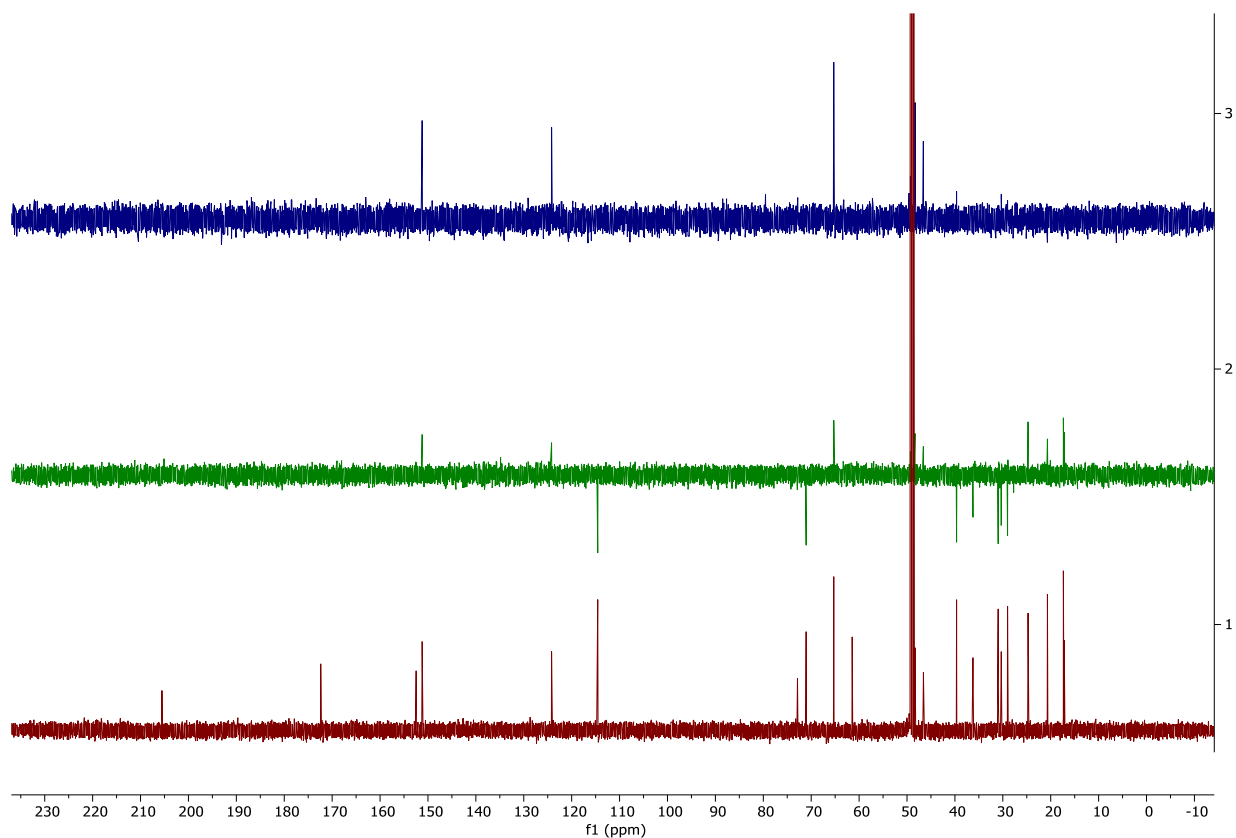


Figure S22. ESI-MS spectrum of compound **4**



Figure S23. ^1H NMR spectrum of compound **5**

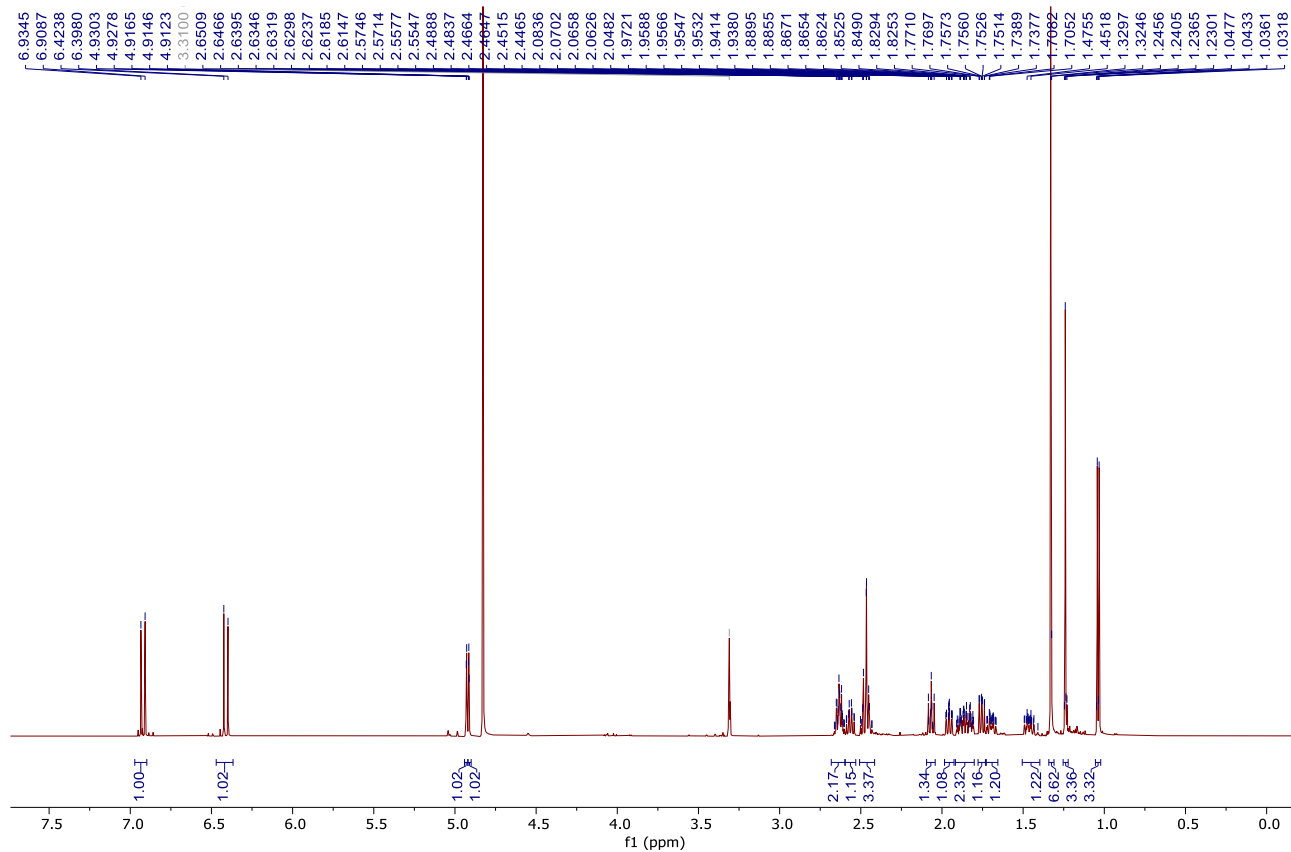


Figure S24. ^{13}C NMR spectrum of compound **5**

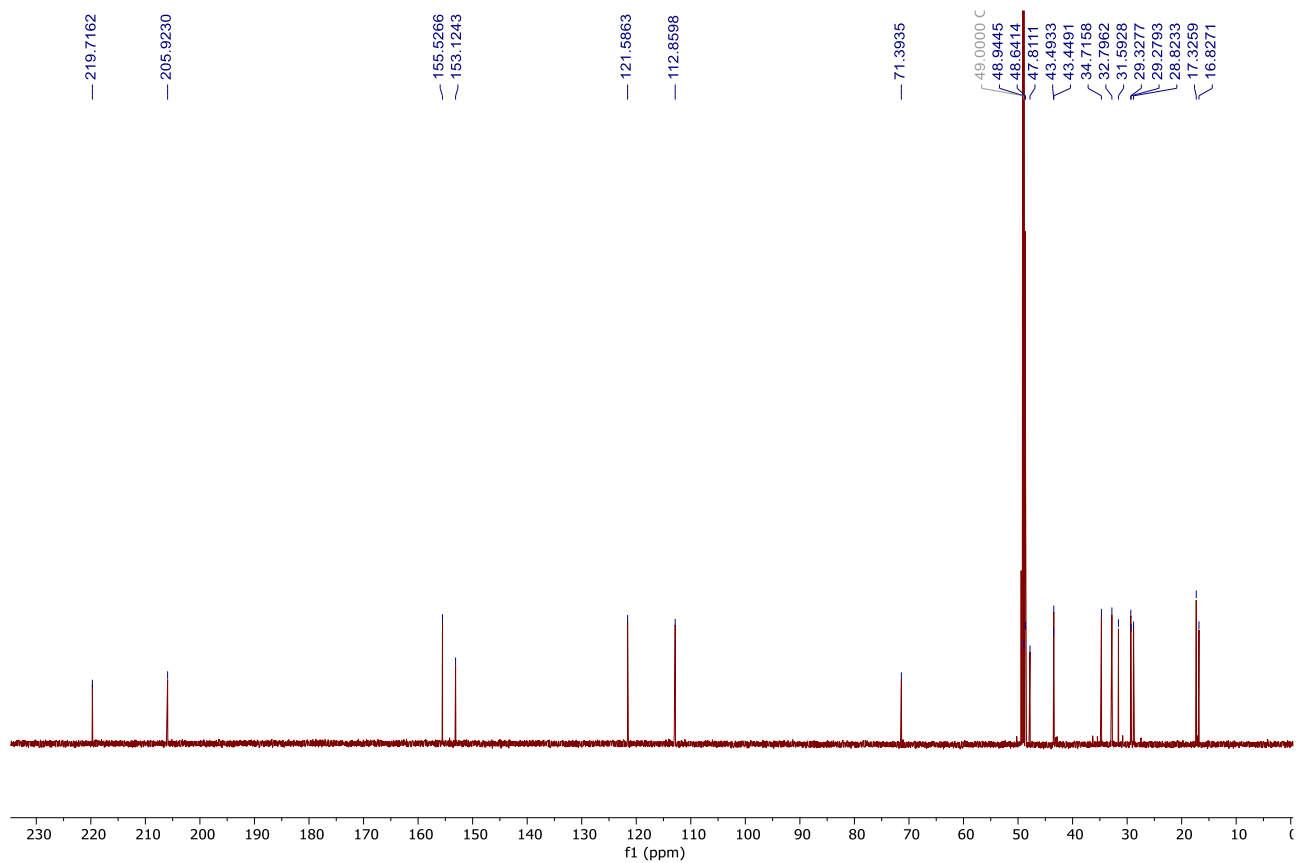


Figure S25. DEPT spectrum of compound **5**

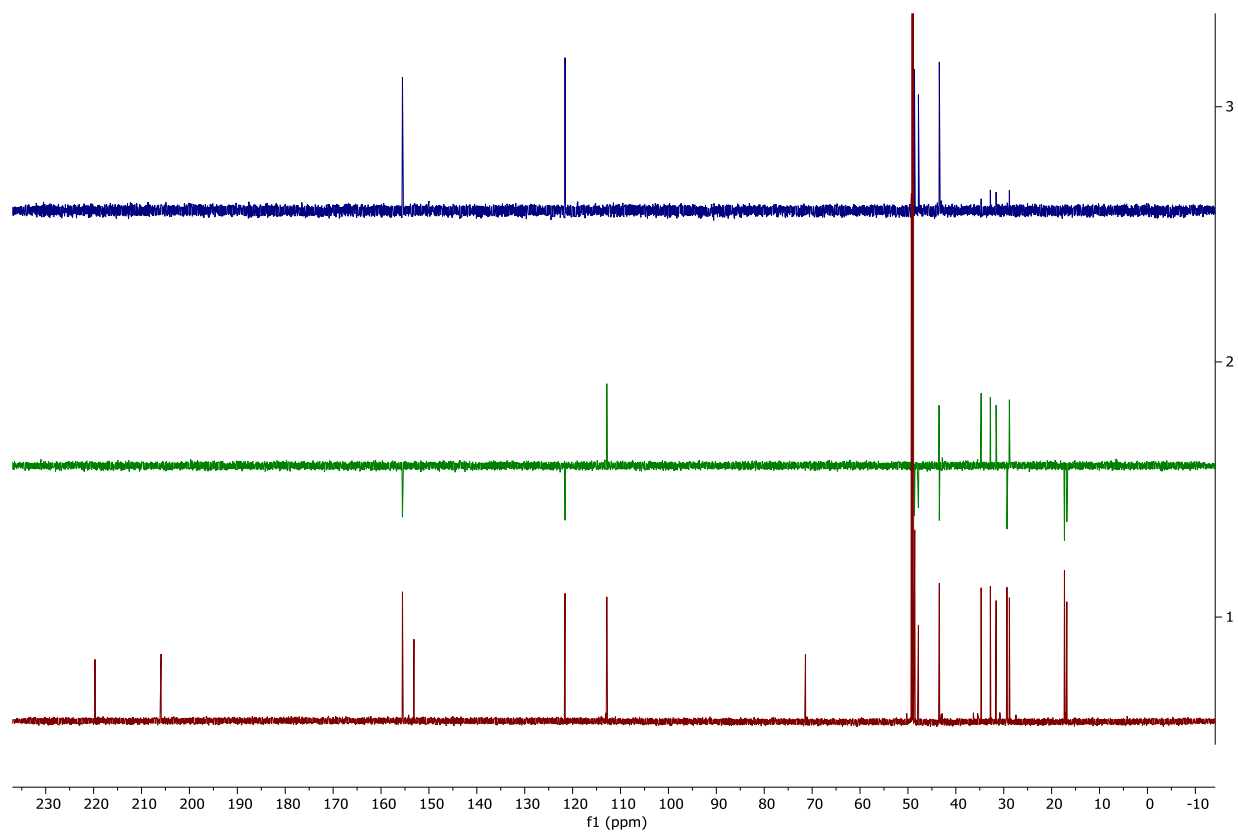


Figure S26. ESI-MS spectrum of compound **5**

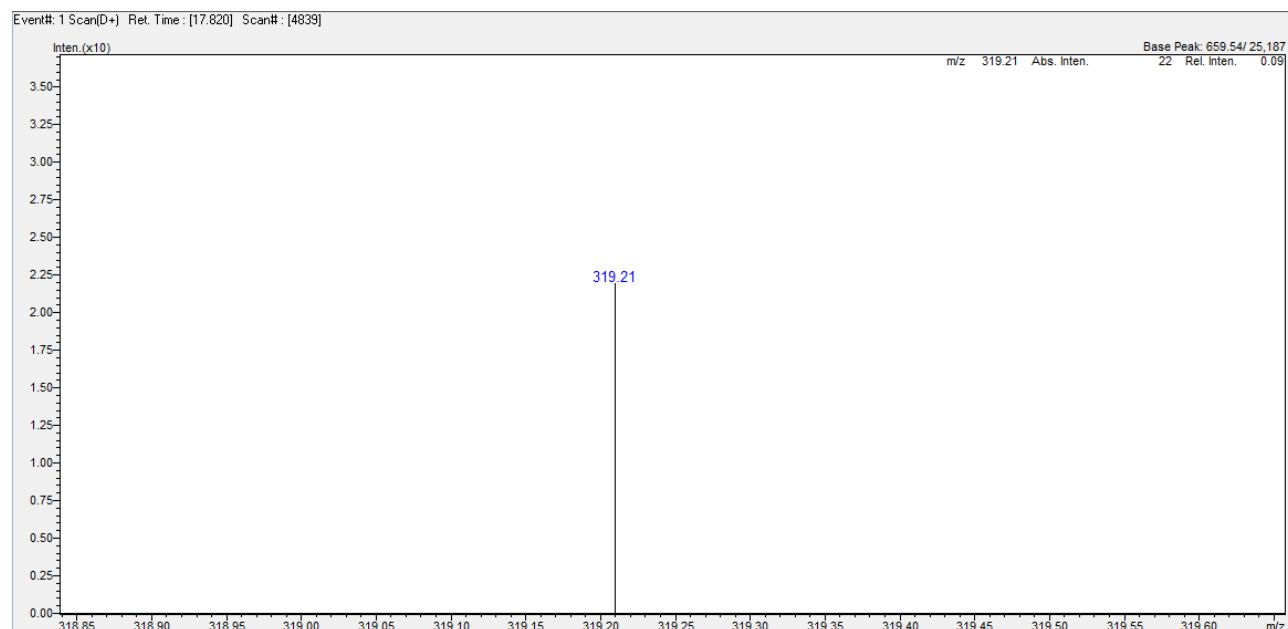


Figure S27. ^1H NMR spectrum of compound **6**

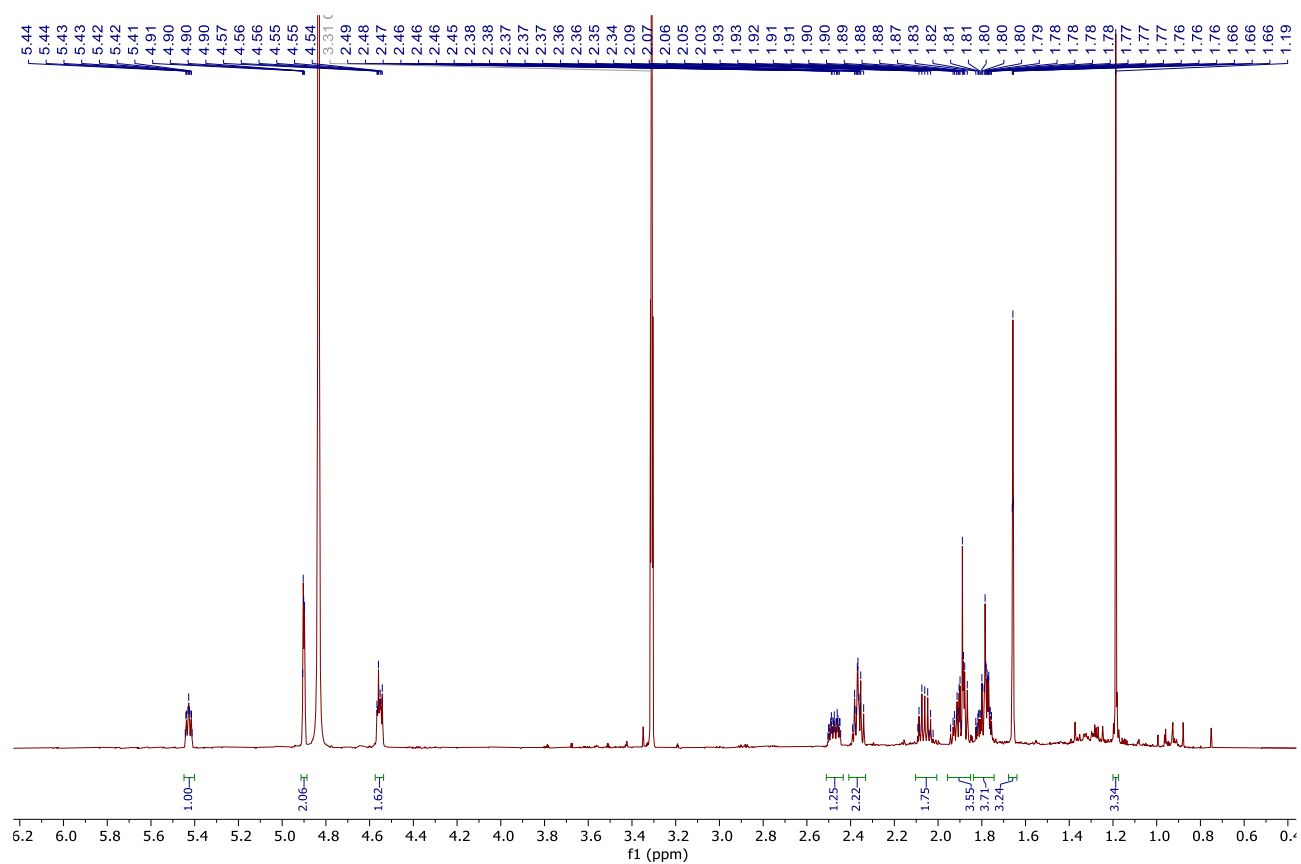


Figure S28. ^{13}C NMR spectrum of compound **6**

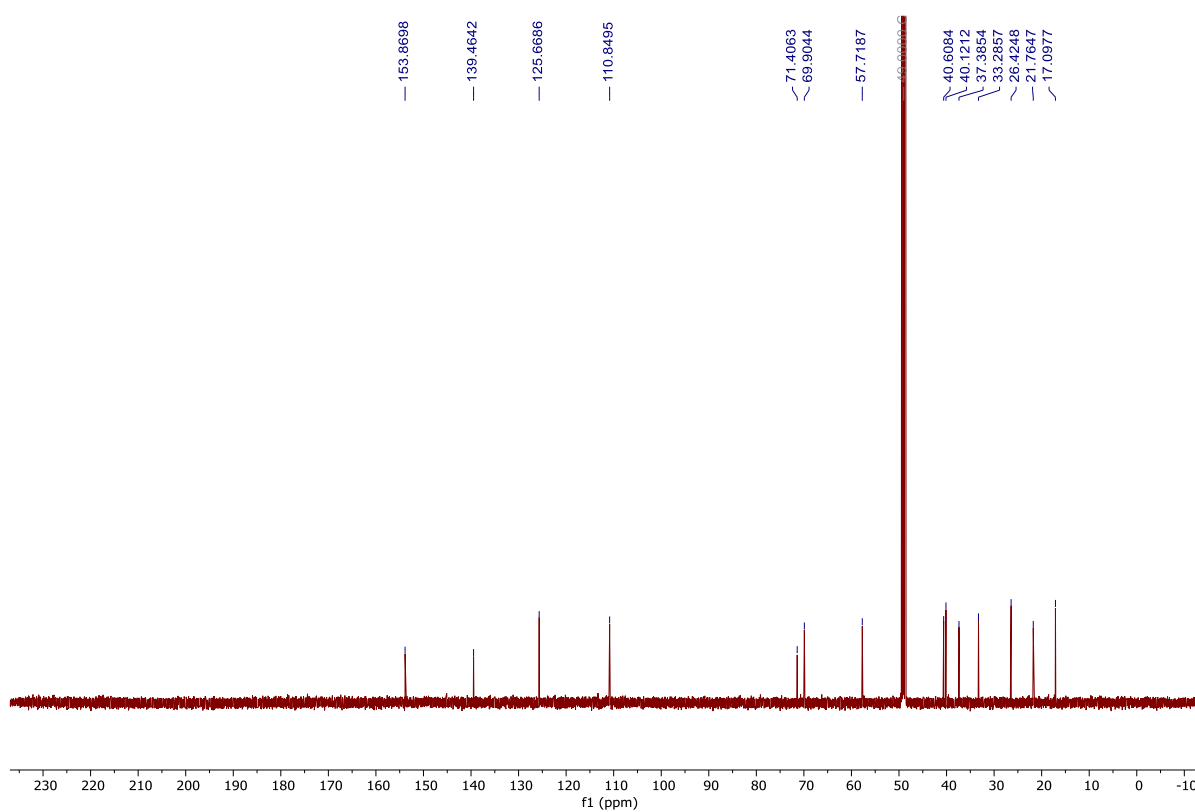


Figure S29. DEPT spectrum of compound **6**

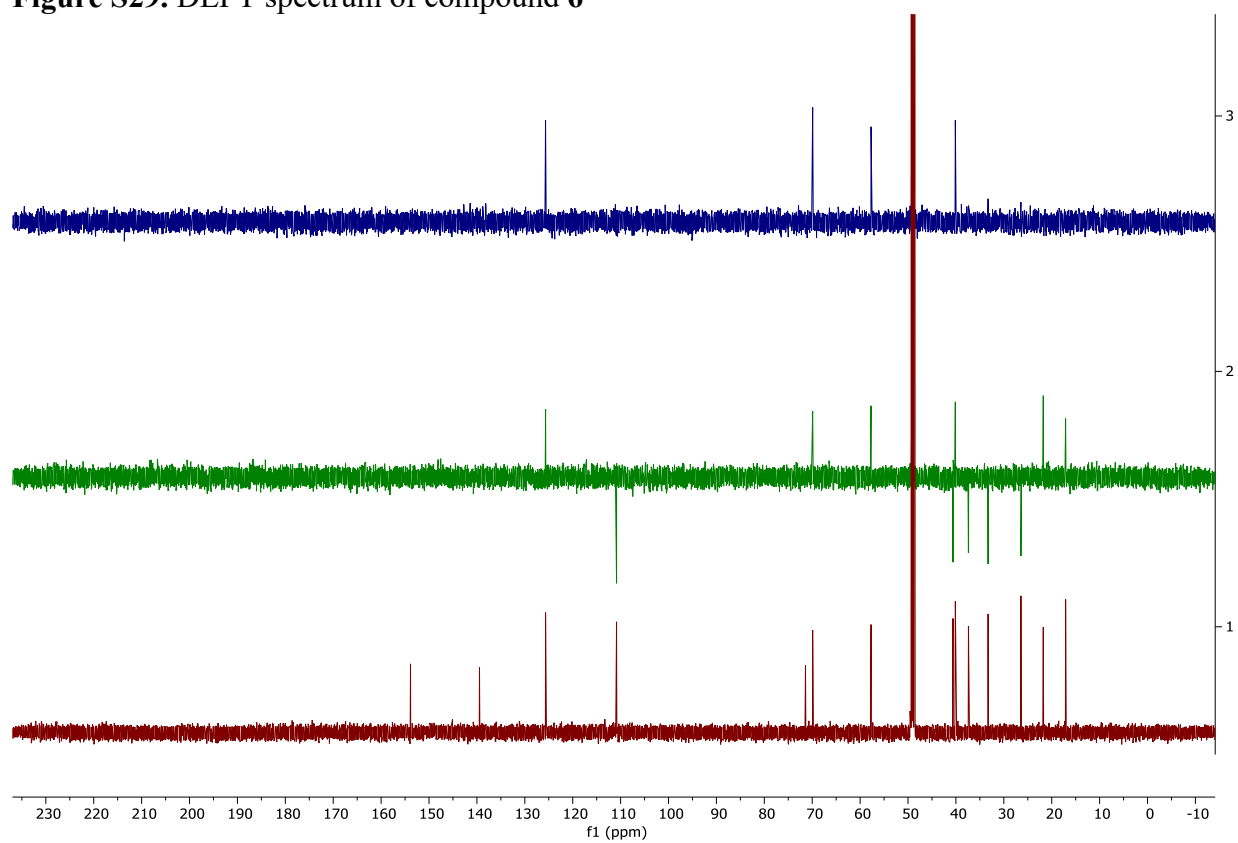


Figure S30. HSQC spectrum of compound **6**

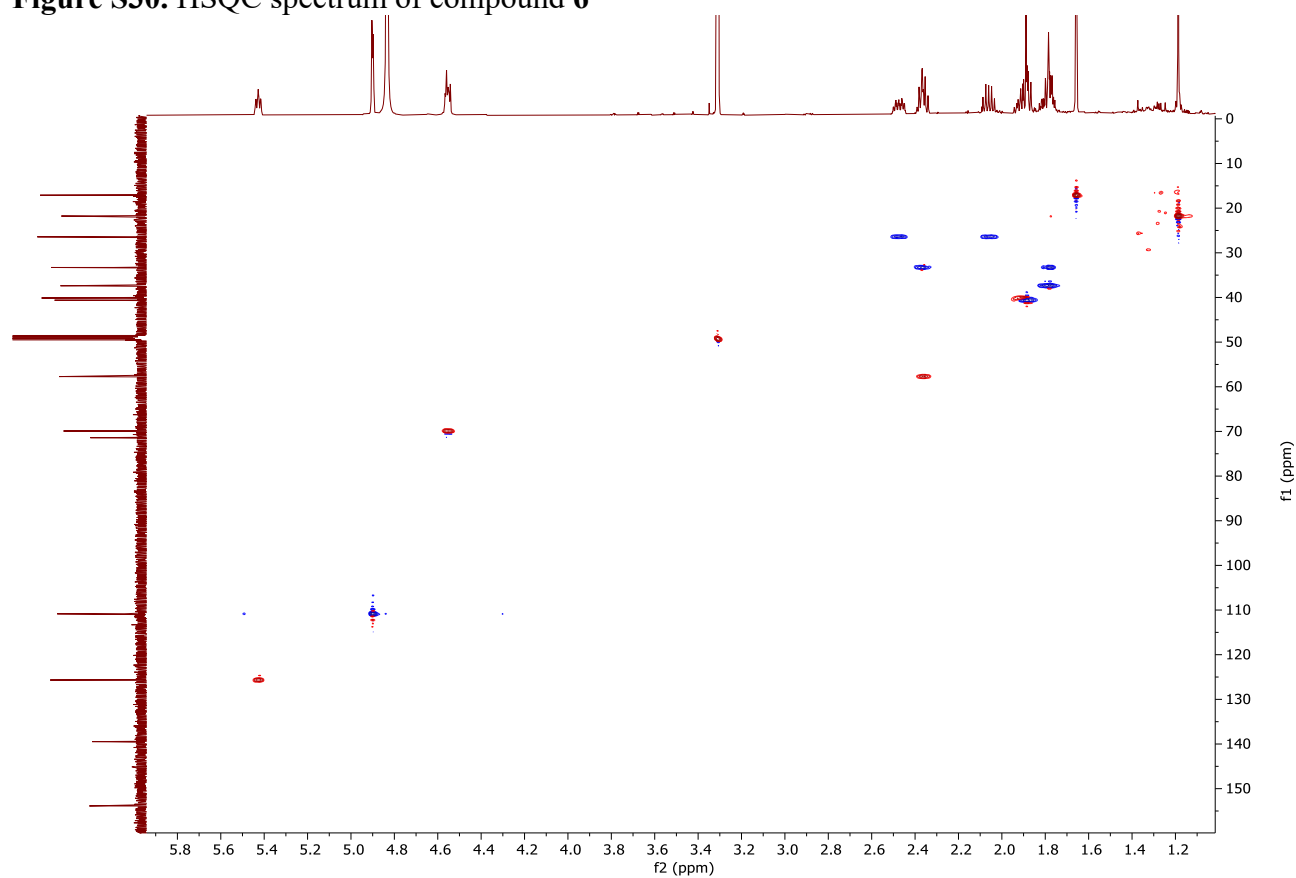


Figure S31. HMBC spectrum of compound **6**

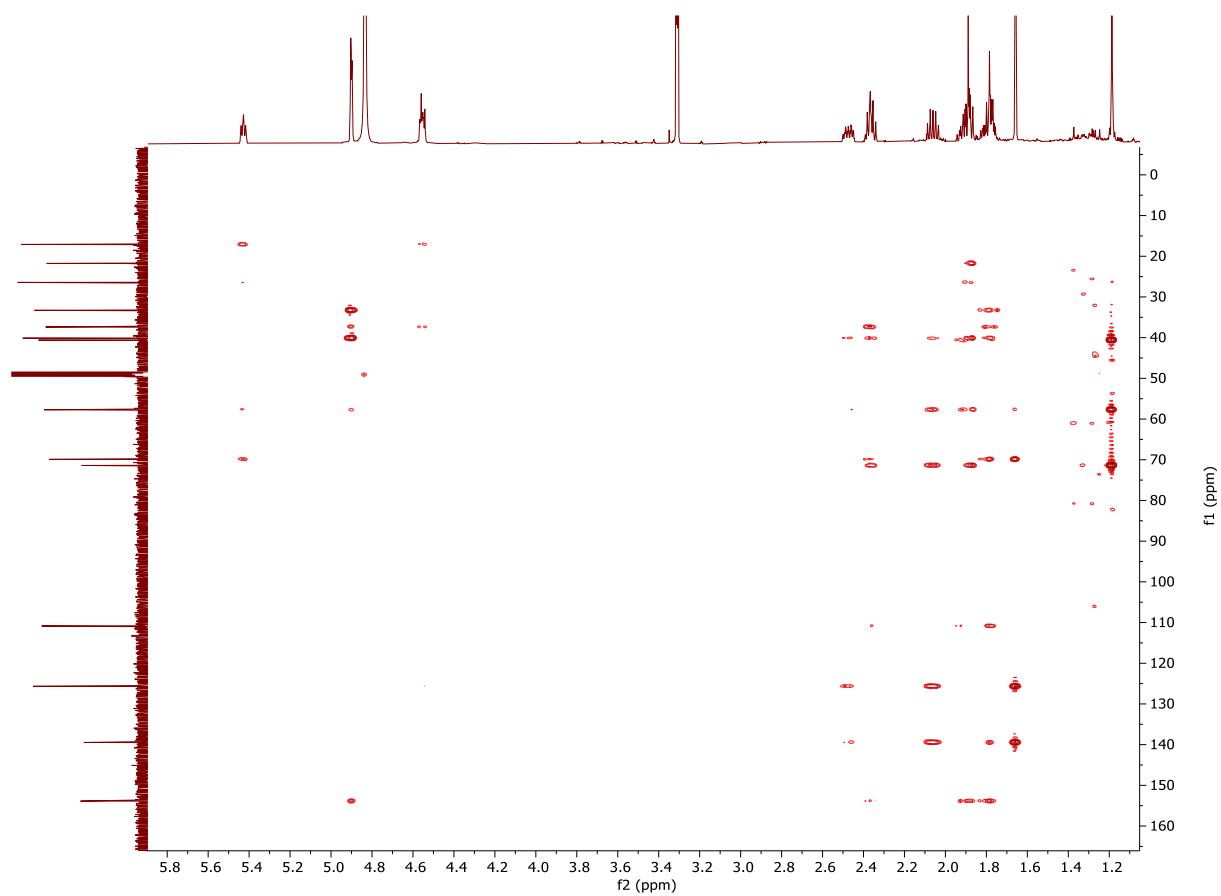


Figure S32. COSY spectrum of compound **6**

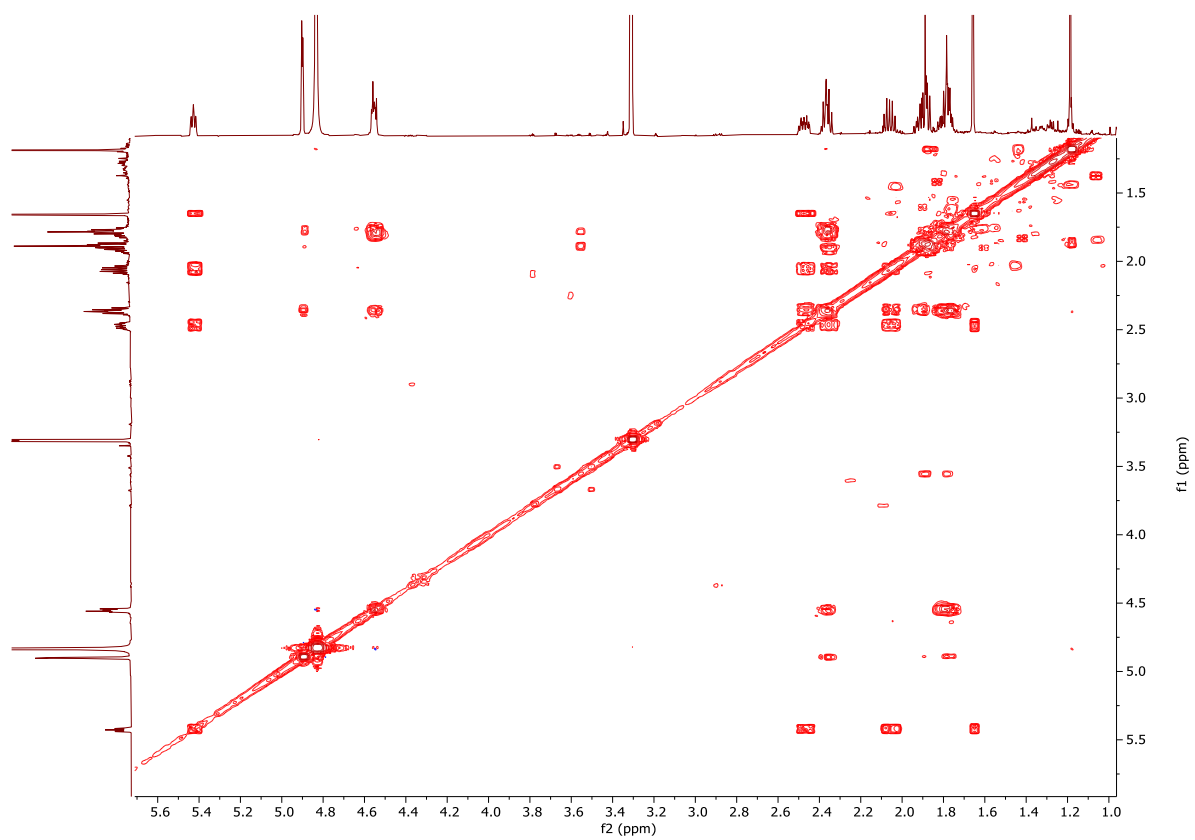


Figure S33. NOESY spectrum of compound **6**

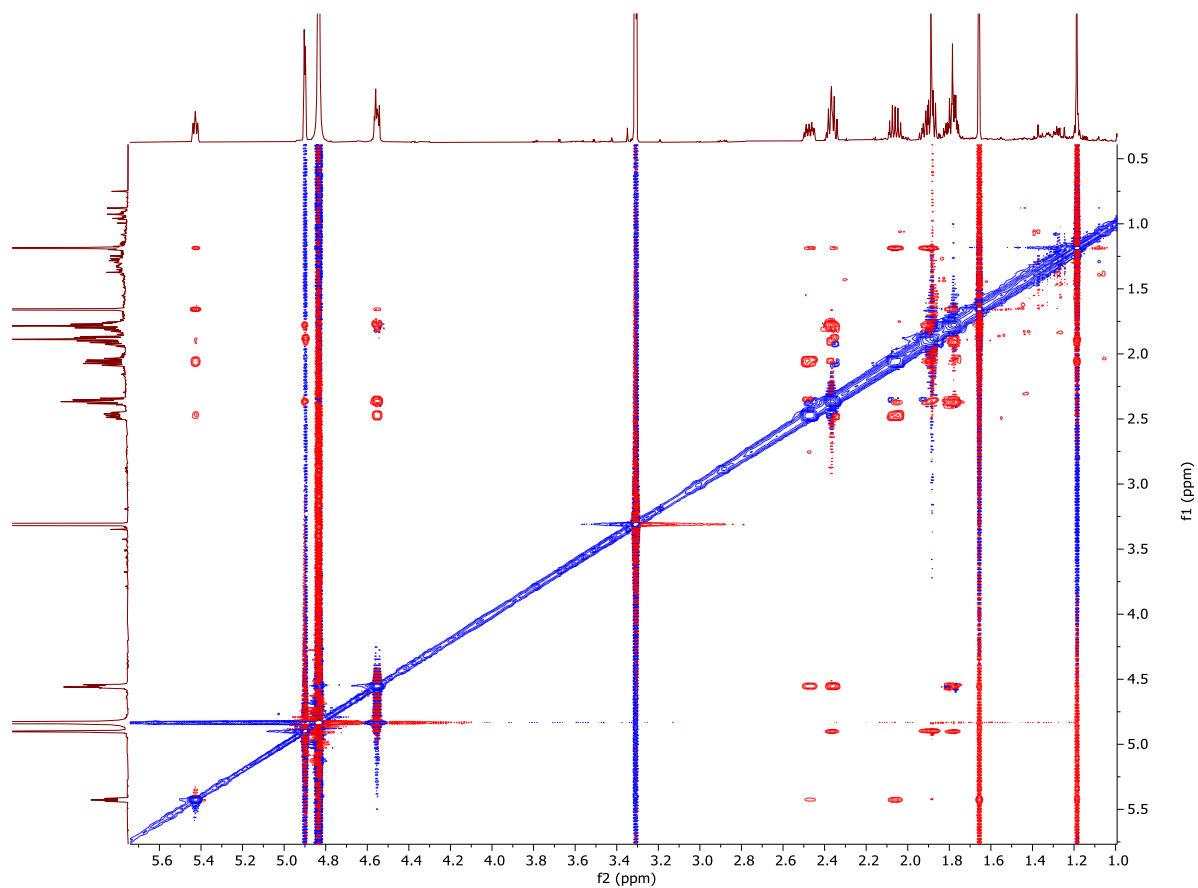


Figure S34. HR-ESI-MS spectra of compound **6**

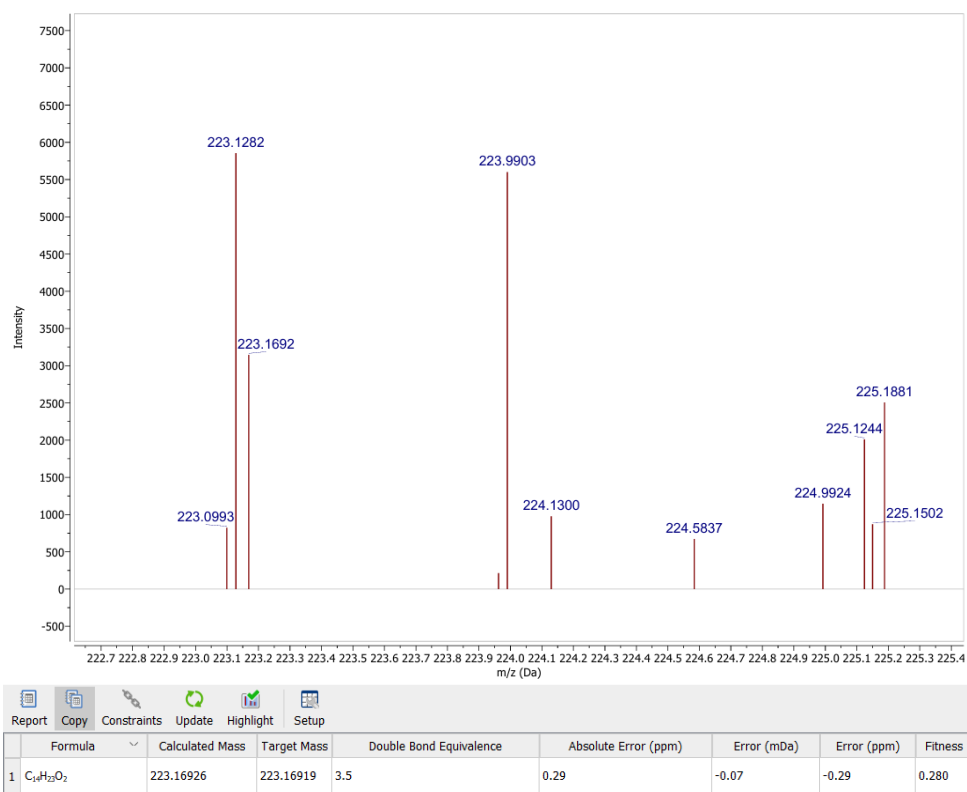


Figure S35. UV spectrum of compound **6**

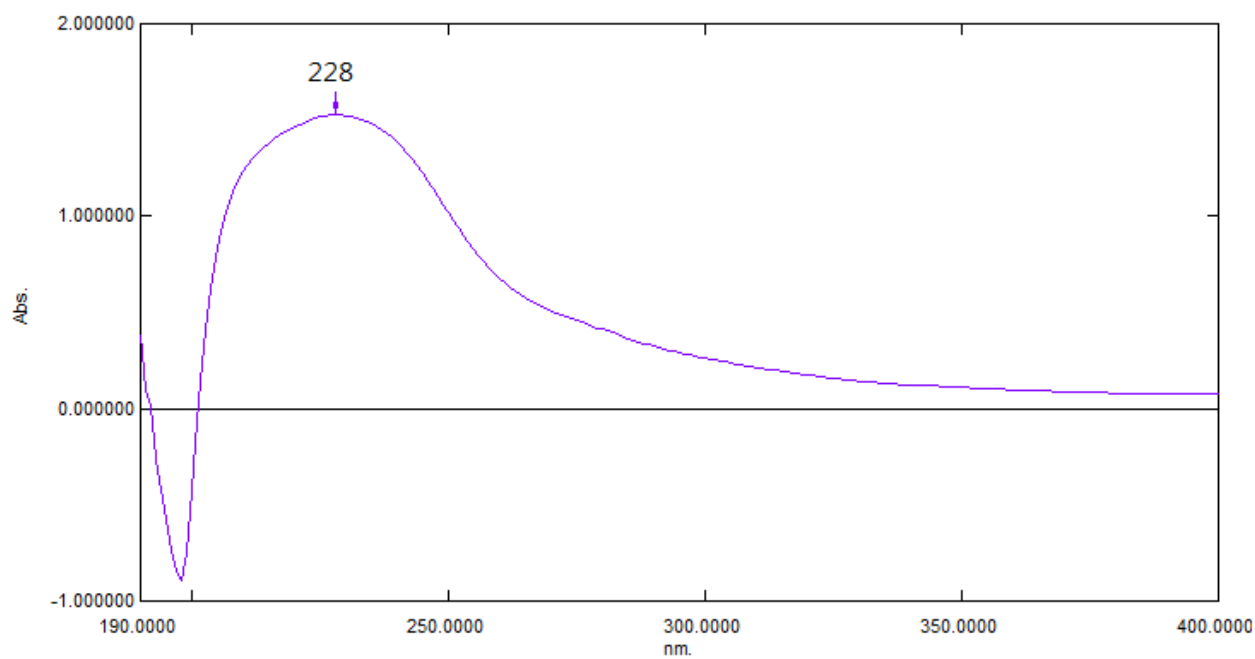


Figure S36. IR spectrum of compound **6**

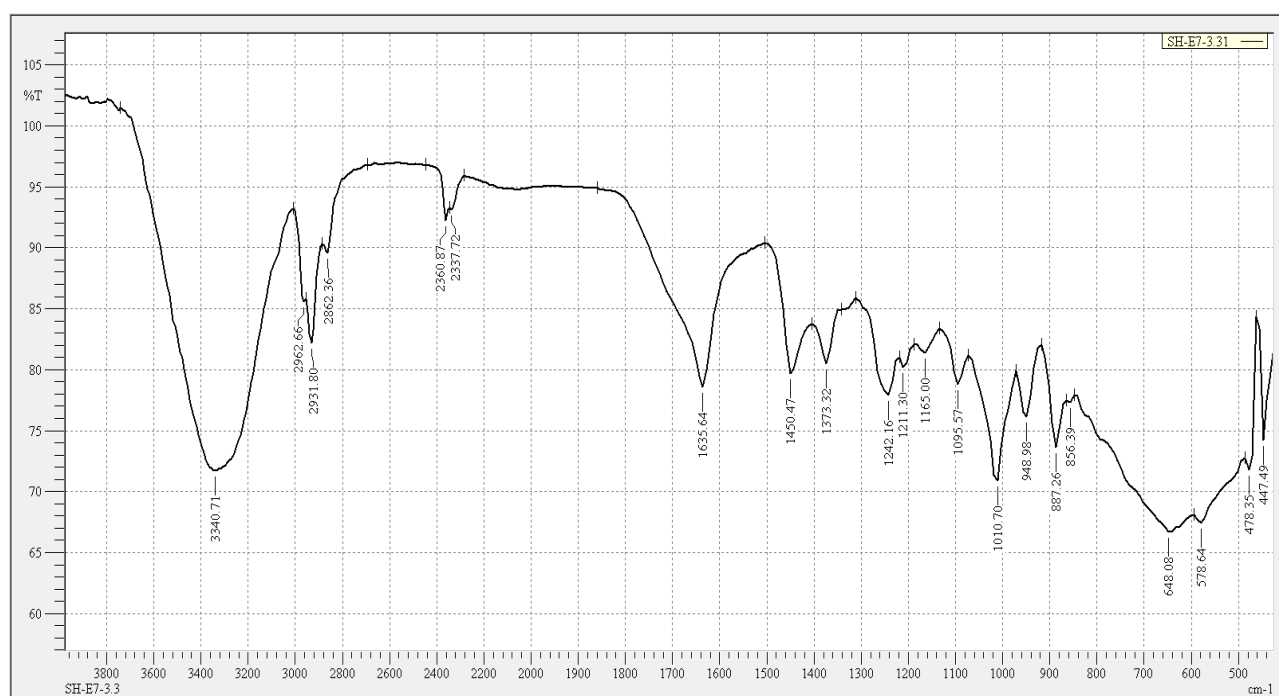


Figure S37. ^1H NMR spectrum of compound 7

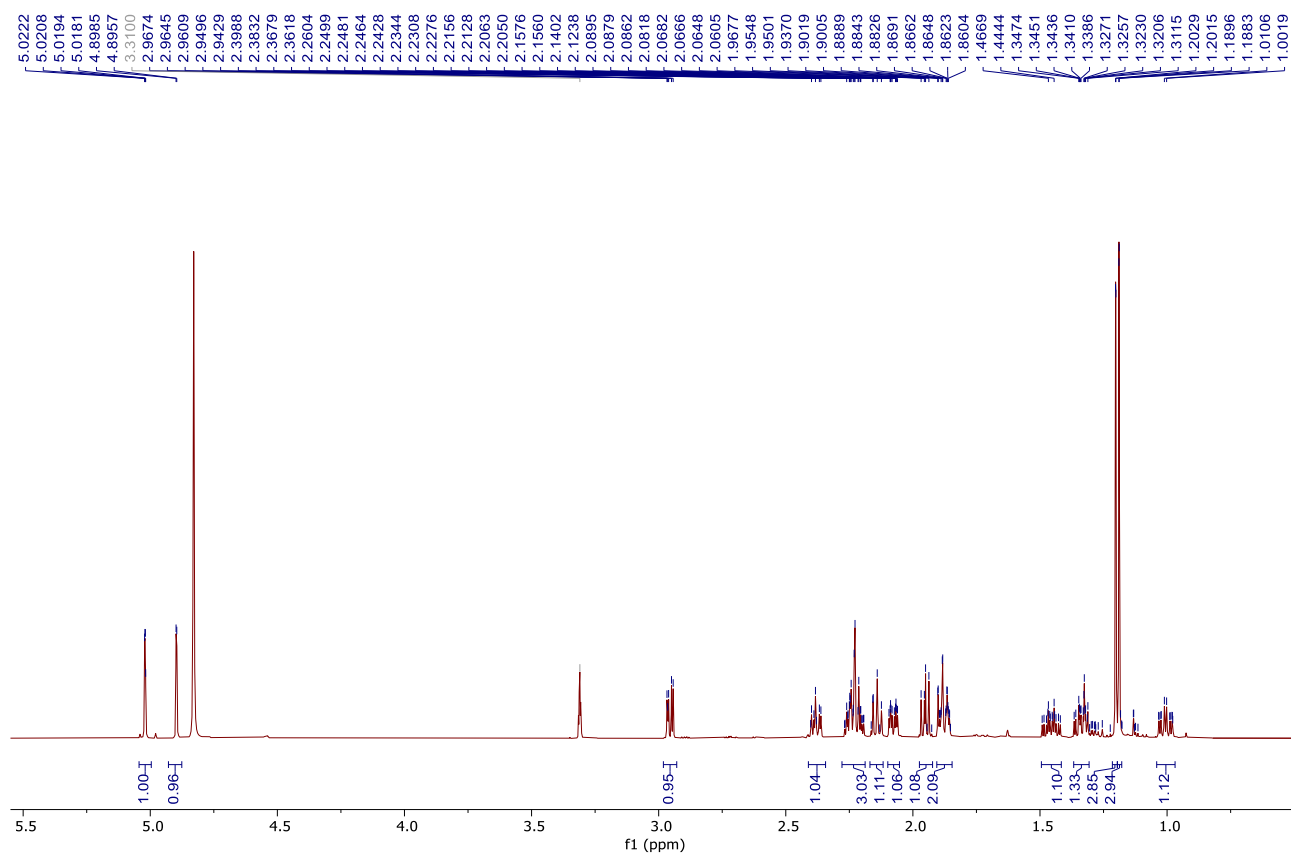


Figure S38. ^{13}C NMR spectrum of compound 7

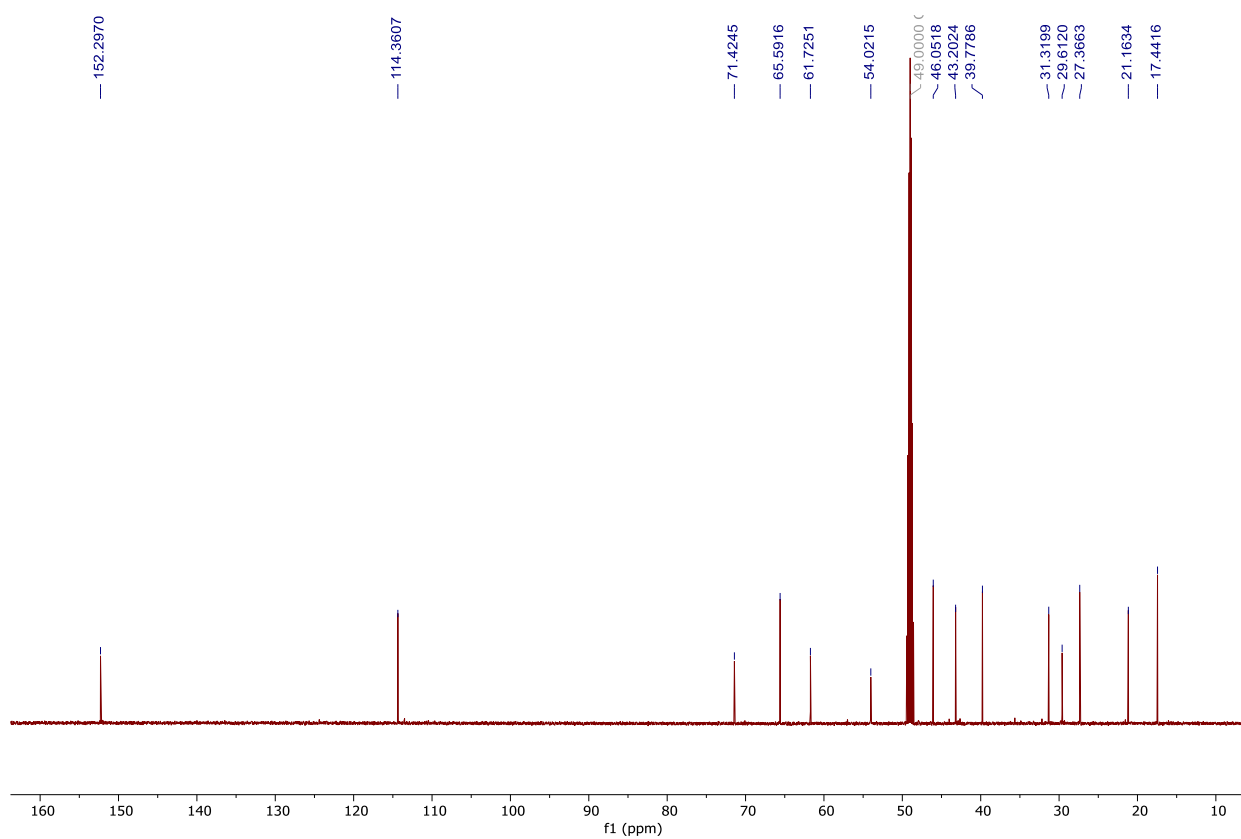


Figure S39. DEPT spectrum of compound **7**

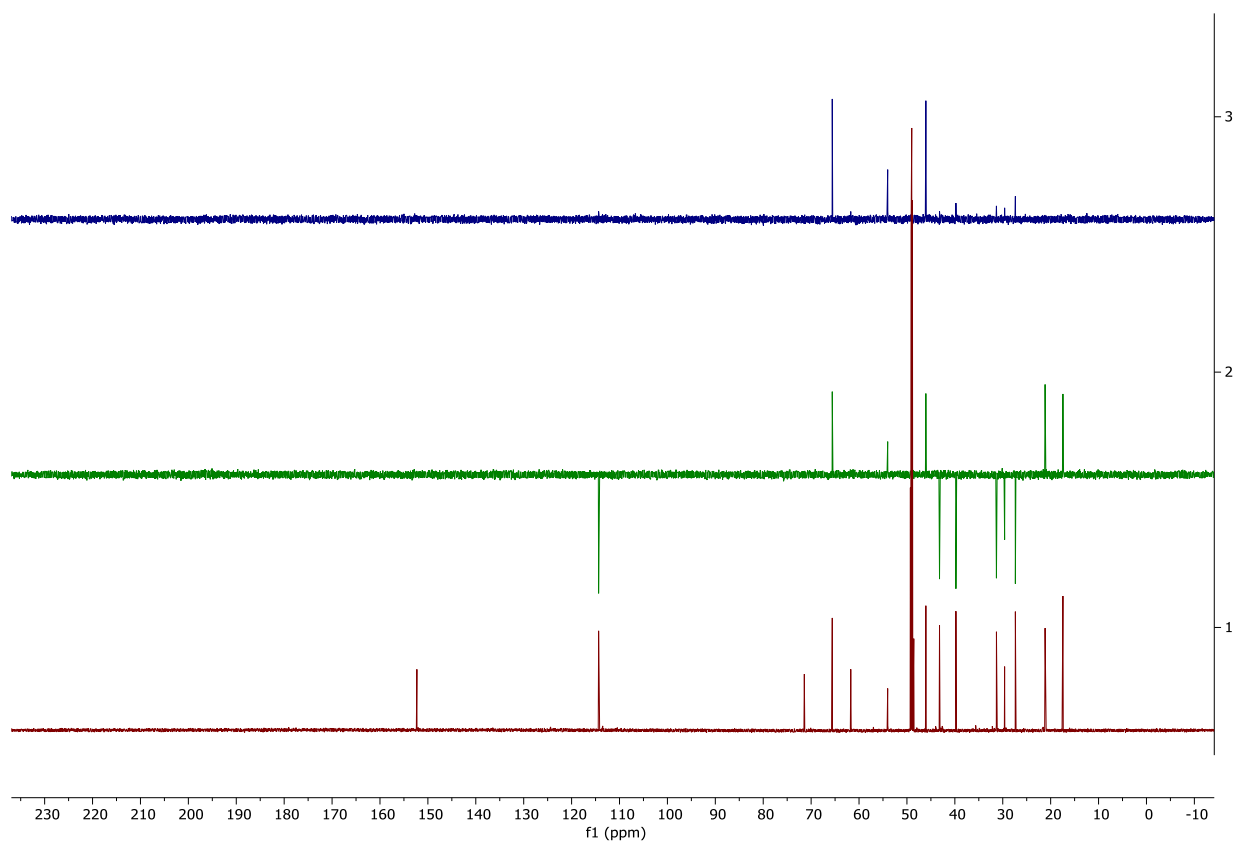


Figure S40. ESI-MS spectrum of compound **7**

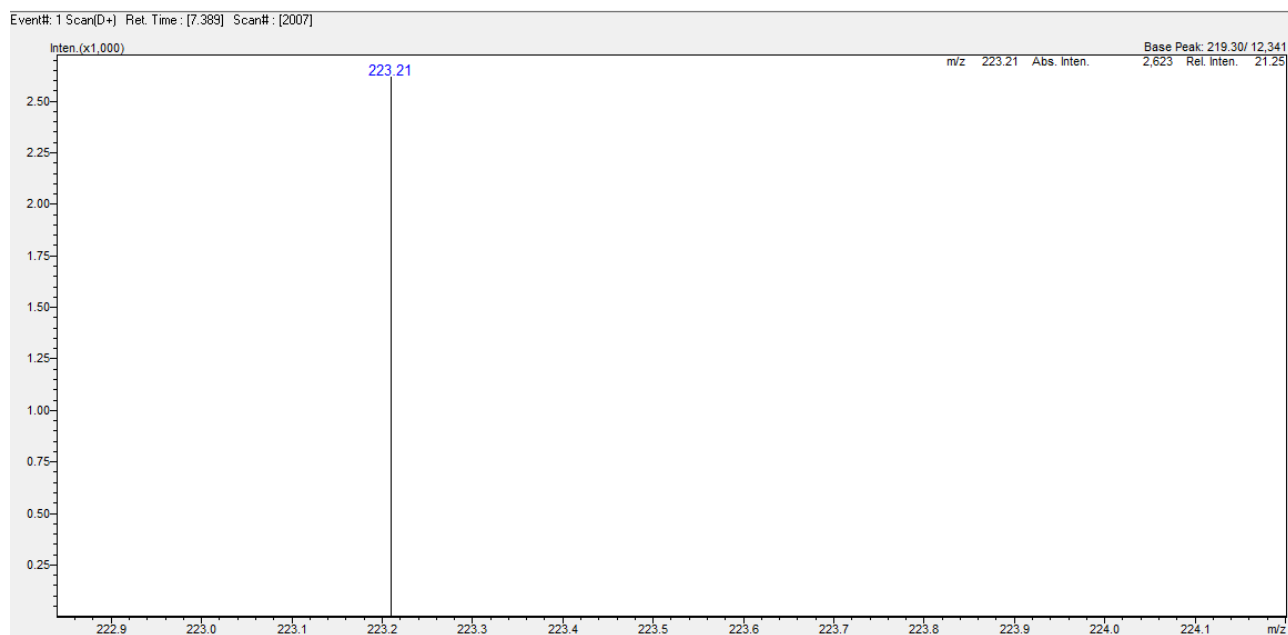


Figure S41. ^1H NMR spectrum of compound **8**

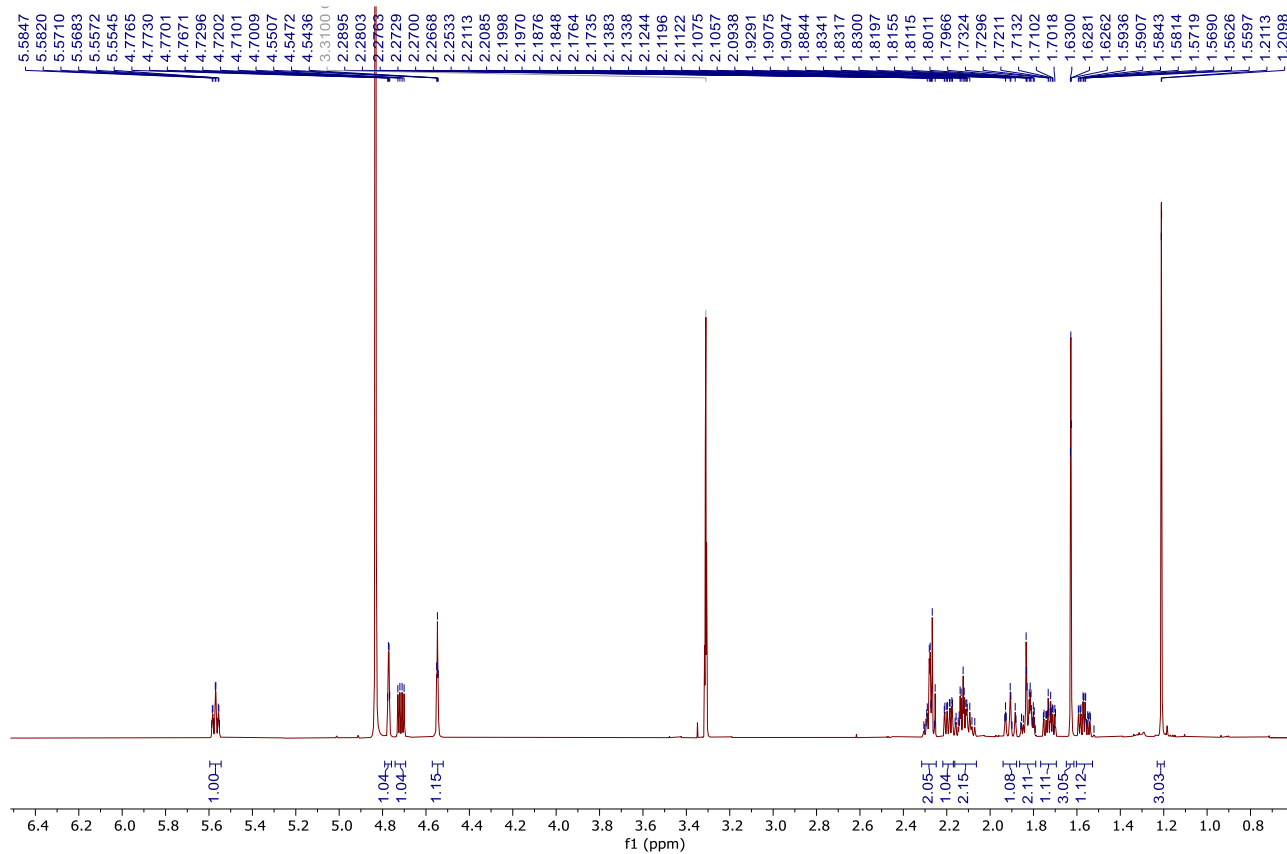


Figure S42. ^{13}C NMR spectrum of compound **8**

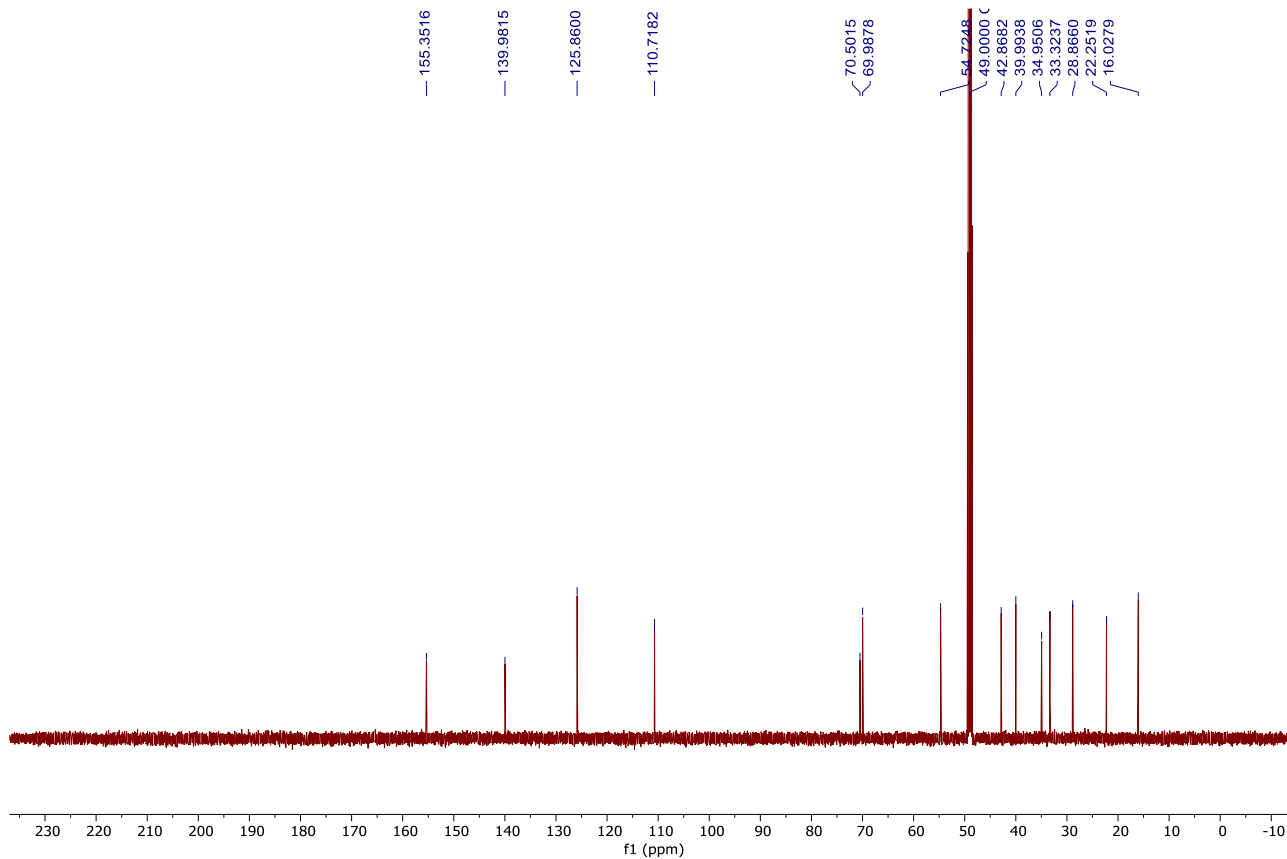


Figure S43. DEPT spectrum of compound **8**

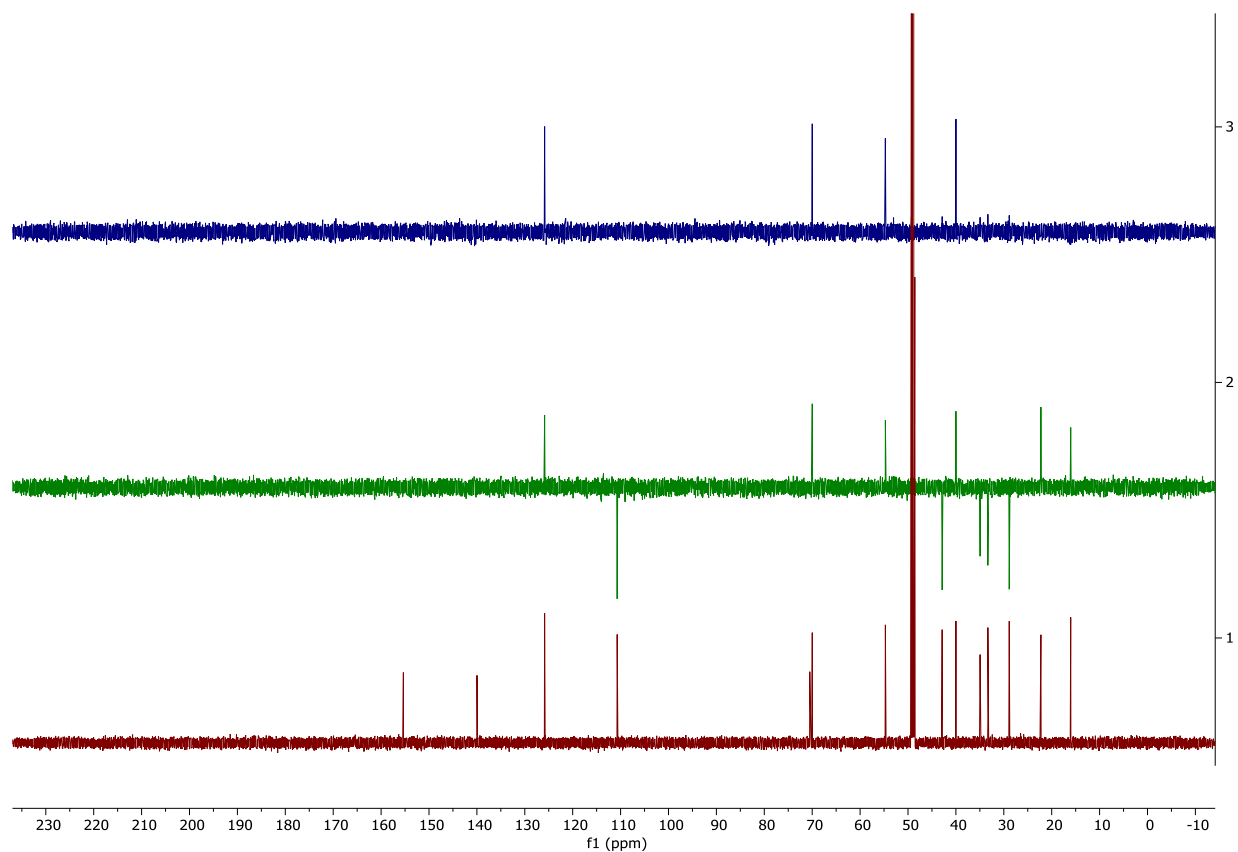


Figure S44. ESI-MS spectra of compound **8**

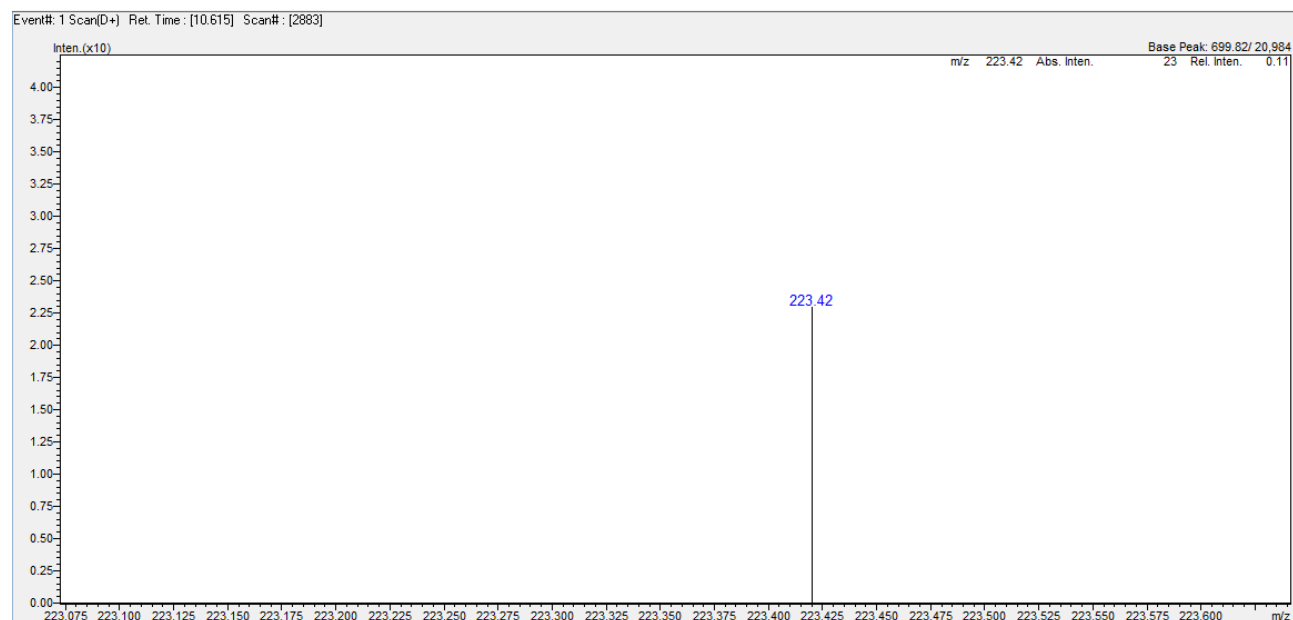


Figure S45. ^1H NMR spectrum of compound **9**

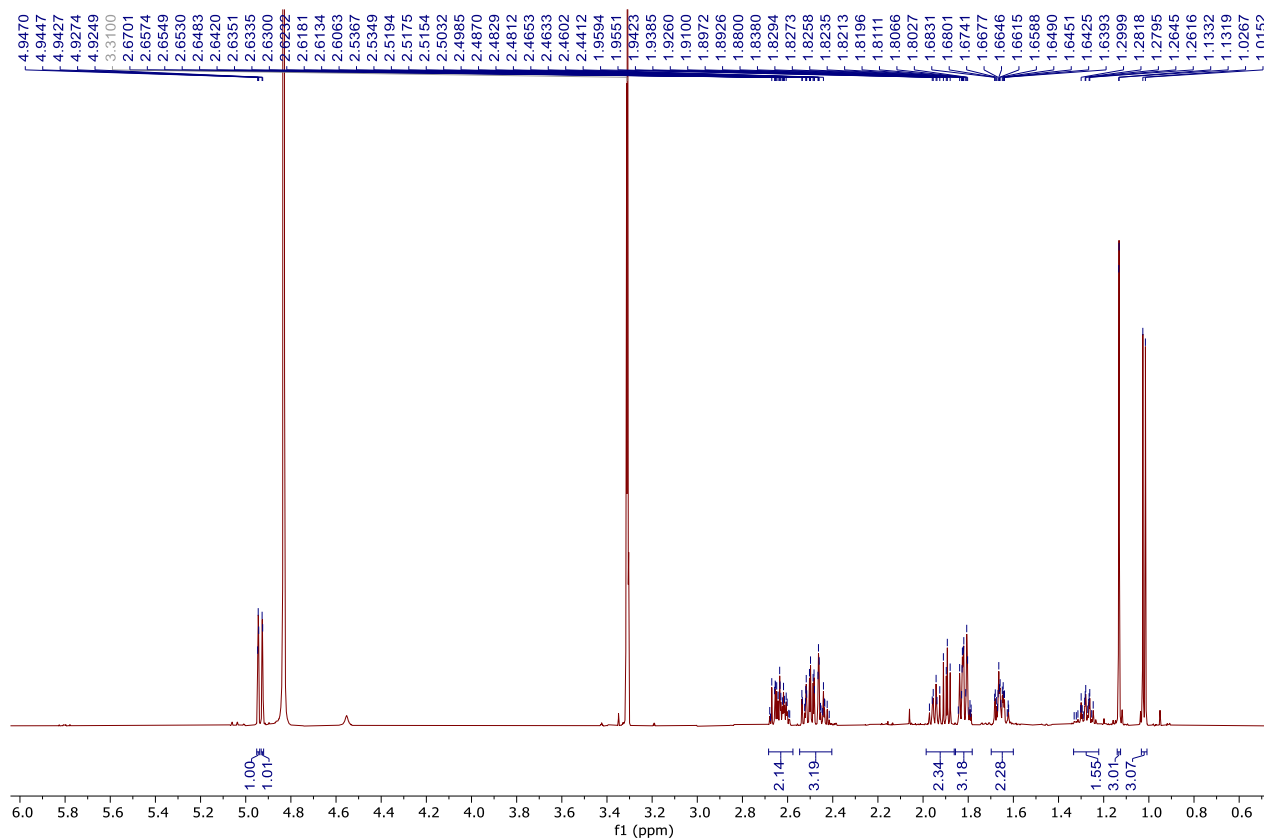


Figure S46. ^{13}C NMR spectrum of compound **9**

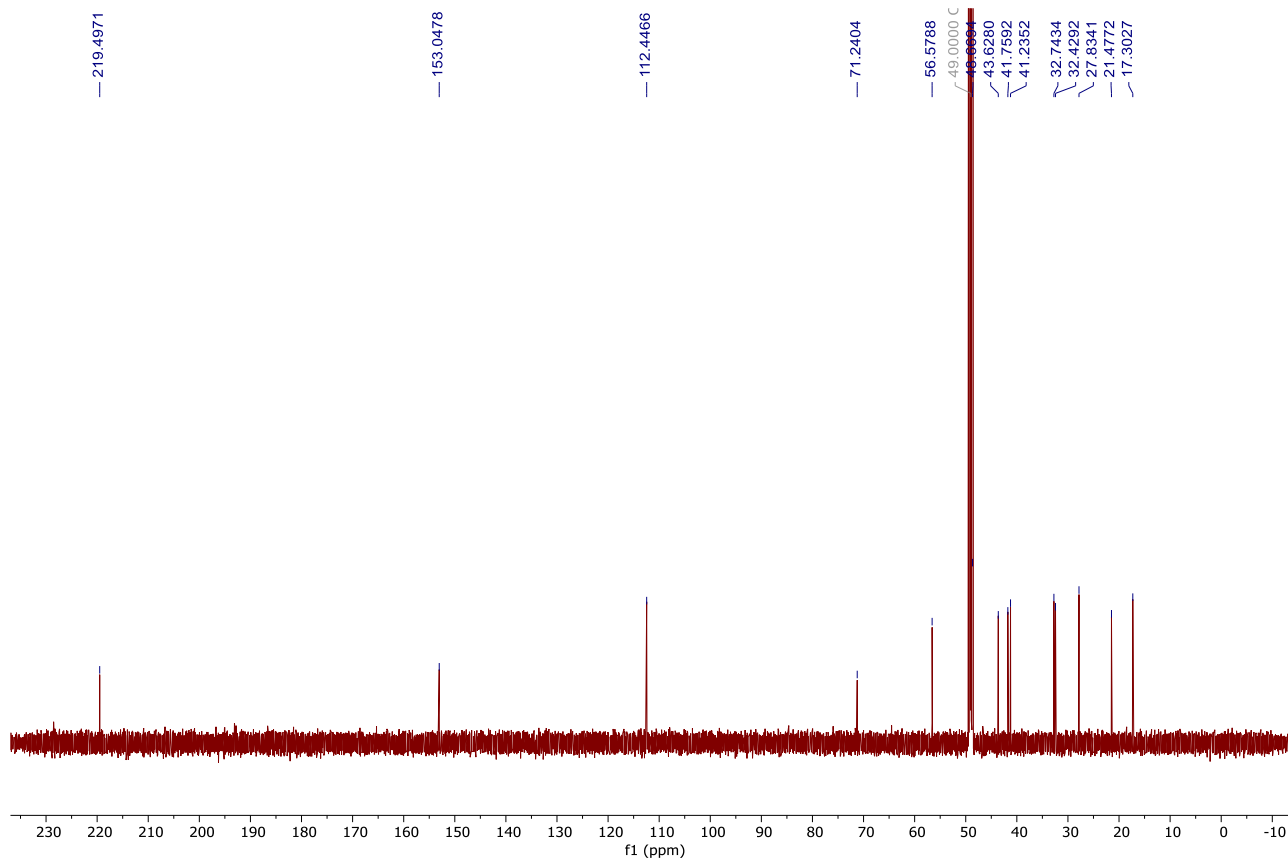


Figure S47. DEPT spectrum of compound **9**

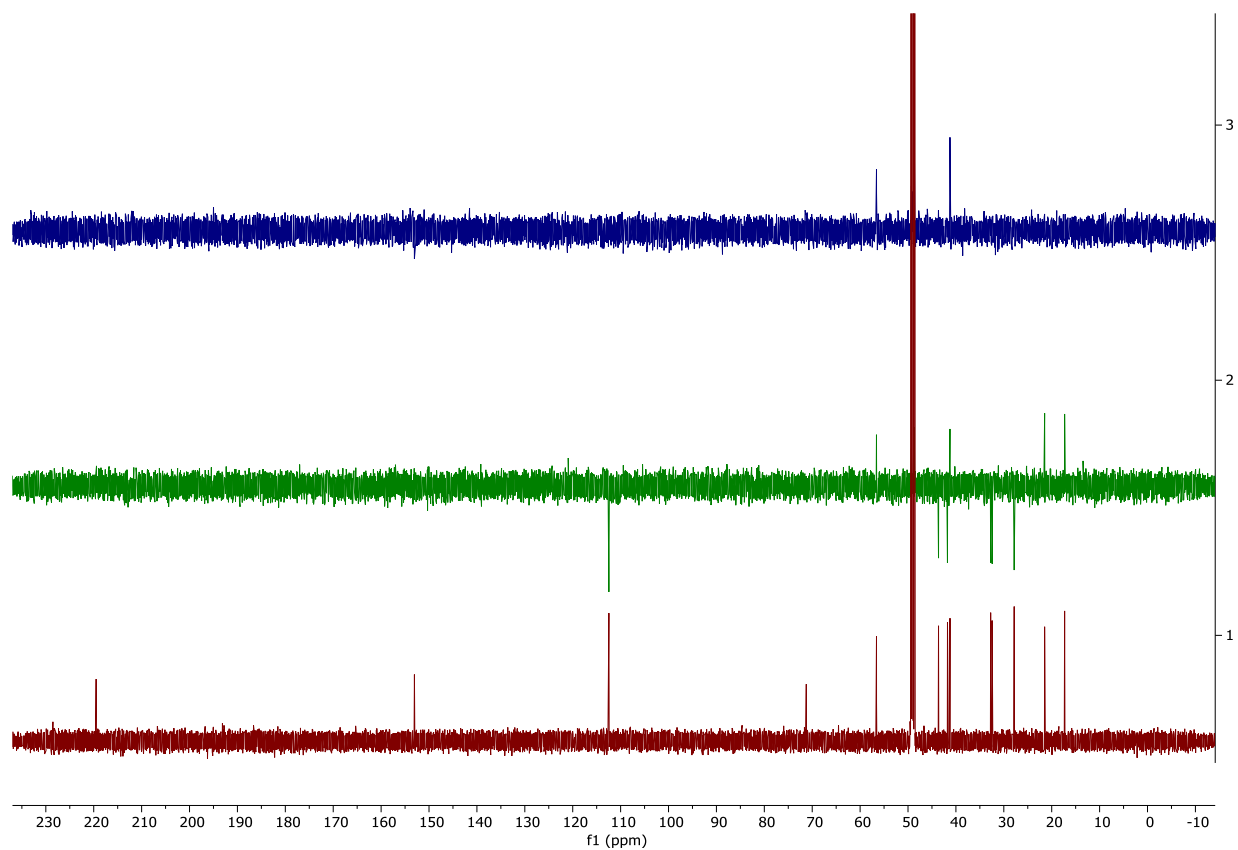
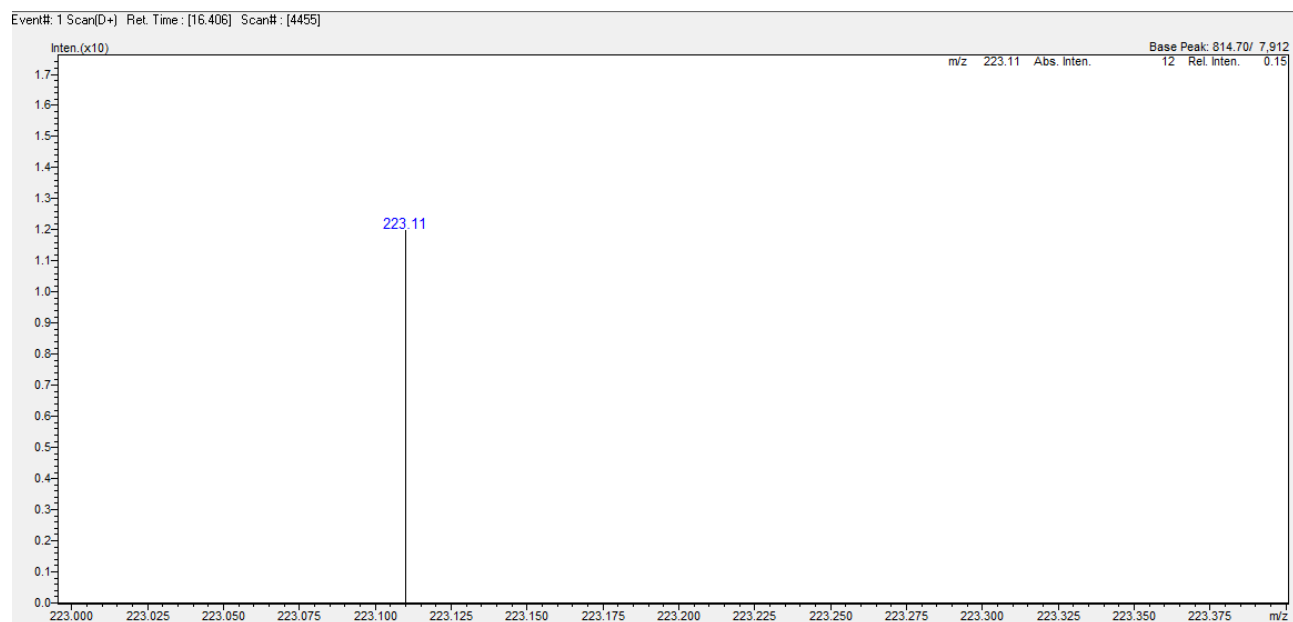


Figure S48. ESI-MS spectrum of compound **9**



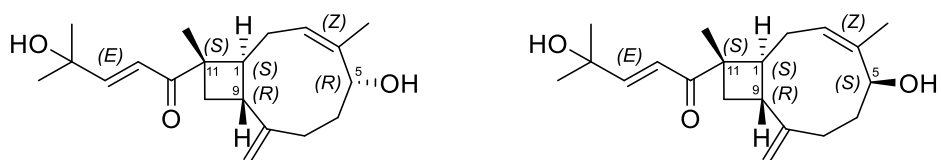


Figure S49. Structures of isomers 1 and 2 of compound **1**



Figure S50. Structures of isomers 1 and 2 of compound **6**

Table S1. Gibbs free energy of the conformers of compound **1** and the Boltzmann distribution of each conformer.

Conformer	Gibbs free energy (Hartree)	Boltzmann population (%)
1-5R-conf. 1	-1005.428633	6.76
1-5R-conf. 2	-1005.428735	7.53
1-5R-conf. 3	-1005.429558	18.00
1-5R-conf. 4	-1005.429125	11.38
1-5R-conf. 5	-1005.425789	0.33
1-5R-conf. 6	-1005.425934	0.39
1-5R-conf. 7	-1005.427765	2.70
1-5R-conf. 8	-1005.428942	9.38
1-5R-conf. 9	-1005.428813	8.18
1-5R-conf. 10	-1005.42827	4.60
1-5R-conf. 11	-1005.426089	0.46
1-5R-conf. 12	-1005.426391	0.63
1-5R-conf. 13	-1005.427298	1.64
1-5R-conf. 14	-1005.427071	1.29
1-5R-conf. 15	-1005.426279	0.56
1-5R-conf. 16	-1005.425557	0.26
1-5R-conf. 17	-1005.428745	7.61
1-5R-conf. 18	-1005.42829	4.70
1-5R-conf. 19	-1005.425648	0.29
1-5R-conf. 20	-1005.425038	0.15
1-5R-conf. 21	-1005.425232	0.18
1-5R-conf. 22	-1005.426556	0.75
1-5R-conf. 23	-1005.426749	0.92

1-5R-conf. 24	-1005.428178	4.17
1-5R-conf. 25	-1005.426087	0.46
1-5R-conf. 26	-1005.427981	3.39
1-5R-conf. 27	-1005.425292	0.20
1-5R-conf. 28	-1005.425468	0.24
1-5R-conf. 29	-1005.426765	0.93
1-5R-conf. 30	-1005.426702	0.87
1-5R-conf. 31	-1005.426773	0.94
1-5R-conf. 32	-1005.424721	0.11
1-5S-conf. 1	-1005.424522	7.92
1-5S-conf. 2	-1005.42404	4.75
1-5S-conf. 3	-1005.424029	4.70
1-5S-conf. 4	-1005.42474	9.97
1-5S-conf. 5	-1005.424876	11.52
1-5S-conf. 6	-1005.424587	8.48
1-5S-conf. 7	-1005.424311	6.33
1-5S-conf. 8	-1005.423726	3.41
1-5S-conf. 9	-1005.42169	0.39
1-5S-conf. 10	-1005.421274	0.25
1-5S-conf. 11	-1005.421464	0.31
1-5S-conf. 12	-1005.421241	0.25
1-5S-conf. 13	-1005.424119	5.17
1-5S-conf. 14	-1005.422816	1.30
1-5S-conf. 15	-1005.42285	1.35
1-5S-conf. 16	-1005.424571	8.34

1-5S-conf. 17	-1005.421925	0.51
1-5S-conf. 18	-1005.421559	0.34
1-5S-conf. 19	-1005.421127	0.22
1-5S-conf. 20	-1005.421506	0.32
1-5S-conf. 21	-1005.420454	0.11
1-5S-conf. 22	-1005.42257	1.00
1-5S-conf. 23	-1005.42252	0.95
1-5S-conf. 24	-1005.422275	0.73
1-5S-conf. 25	-1005.422588	1.02
1-5S-conf. 26	-1005.423148	1.85
1-5S-conf. 27	-1005.42376	3.53
1-5S-conf. 28	-1005.422956	1.51
1-5S-conf. 29	-1005.4207	0.14
1-5S-conf. 30	-1005.420904	0.17
1-5S-conf. 31	-1005.42141	0.29
1-5S-conf. 32	-1005.422588	1.02
1-5S-conf. 33	-1005.421473	0.31
1-5S-conf. 34	-1005.423426	2.48
1-5S-conf. 35	-1005.422863	1.37
1-5S-conf. 36	-1005.423099	1.75
1-5S-conf. 37	-1005.421348	0.27
1-5S-conf. 38	-1005.423424	2.47
1-5S-conf. 39	-1005.423296	2.16
1-5S-conf. 40	-1005.420497	0.11
1-5S-conf. 41	-1005.42006	0.07
1-5S-conf. 42	-1005.421156	0.22

1-5S-conf. 43	-1005.421147	0.22
1-5S-conf. 44	-1005.421013	0.19
1-5S-conf. 45	-1005.421106	0.21

Table S2. Gibbs free energy of the conformers of compound **6** and the Boltzmann distribution of each conformer.

Conformer	Gibbs free energy (Hartree)	Boltzmann population (%)
6-6 <i>R</i> -conf. 1	-696.863317	32.89
6-6 <i>R</i> -conf. 2	-696.862955	22.42
6-6 <i>R</i> -conf. 3	-696.862241	10.52
6-6 <i>R</i> -conf. 4	-696.862515	14.07
6-6 <i>R</i> -conf. 5	-696.86218	9.87
6-6 <i>R</i> -conf. 6	-696.861032	2.92
6-6 <i>R</i> -conf. 7	-696.859935	0.92
6-6 <i>R</i> -conf. 8	-696.860402	1.50
6-6 <i>R</i> -conf. 9	-696.85977	0.77
6-6 <i>R</i> -conf. 10	-696.860977	2.76
6-6 <i>R</i> -conf. 11	-696.860314	1.37
6-6 <i>S</i> -conf. 1	-696.862117	41.31
6-6 <i>S</i> -conf. 2	-696.861164	15.06
6-6 <i>S</i> -conf. 3	-696.861683	26.09
6-6 <i>S</i> -conf. 4	-696.860625	8.51
6-6 <i>S</i> -conf. 5	-696.860204	5.45
6-6 <i>S</i> -conf. 6	-696.85914	1.77
6-6 <i>S</i> -conf. 7	-696.859171	1.82

Table S3. The cartesian coordinates of the dominant conformers for **1-5R** and **1-5S**

Conformer 1-5R-conf. 1	Coordinates (Å)			Coordinates (Å)			
	X	Y	Z		X	Y	Z
C	0.572997	-0.28802	0.67108	H	5.506521	1.645542	-1.64243
C	1.757412	-0.69142	-0.19913	H	7.153666	1.117389	-1.23151
C	3.084501	-0.14195	0.183853	H	6.154903	0.132281	-2.31222
C	4.194835	-0.47078	-0.49004	H	6.402596	1.222153	1.106798
C	5.587267	0.019717	-0.19751	H	0.613753	1.687744	1.79083
C	6.488711	-1.18338	0.146338	H	0.815052	1.81907	0.028021
C	6.131375	0.774723	-1.42696	H	1.624963	-0.73488	2.528776
O	1.613074	-1.44127	-1.16236	H	-0.13116	-0.70272	2.696245
O	5.506946	0.906091	0.924299	H	0.658231	-2.08807	1.923276
C	0.338766	1.246023	0.828682	H	-3.5141	2.503369	-1.59992
H	-1.6965	0.886332	1.504952	H	-3.00519	0.824735	-1.65751
C	0.686127	-0.99956	2.032065	H	-4.52685	2.016609	0.723933
H	-0.67039	-0.33769	-1.1103	H	-5.31572	1.335013	-0.68932
C	-3.20565	1.659623	-0.97417	H	-3.58438	-0.15066	1.31536
C	-1.91903	2.052818	-0.2715	H	-2.79747	-2.54493	-1.3806
C	-4.40611	1.280882	-0.07975	H	-1.99038	-1.57872	1.355658
C	-4.37162	-0.12245	0.552868	H	-1.06705	-2.50829	0.192906
C	-4.11128	-1.21036	-0.47268	H	-5.53498	-0.6602	-2.01275
C	-2.91914	-1.82032	-0.57515	H	-6.14134	-1.83645	-0.86058
C	-1.70026	-1.61983	0.298657	H	-4.97333	-2.33818	-2.10191
C	-0.82396	-0.3961	-0.02769	H	-0.54279	3.63374	0.100958
C	-1.17274	1.021346	0.548595	H	-2.00358	4.060709	-0.94296
C	-5.24661	-1.53364	-1.41428	H	-5.62885	-1.12904	1.662905
C	-1.46221	3.307978	-0.37598				
O	-5.64749	-0.2817	1.196621				
H	3.138279	0.539154	1.02638				
H	4.103322	-1.15641	-1.33081				
H	7.510693	-0.8398	0.341387				
H	6.115135	-1.69187	1.039113				
H	6.526551	-1.90275	-0.67707				

Conformer 1-5R-conf. 2	Coordinates (Å)			Coordinates (Å)			
	X	Y	Z		X	Y	Z
C	0.505679	1.447034	0.867679	H	5.950337	-0.35433	1.391557
C	1.864298	1.489714	0.17315	H	6.827183	-1.47593	0.326688
C	2.688558	0.253043	0.228683	H	6.633928	0.21966	-0.14531
C	3.899287	0.198137	-0.34268	H	4.762734	-2.81366	0.34852
C	4.819566	-0.99267	-0.35547	H	-0.64491	3.351324	1.246545
C	5.080293	-1.41838	-1.81453	H	-0.12956	3.089204	-0.43393
C	6.14044	-0.62245	0.348888	H	1.273081	2.177179	2.761103
O	2.252549	2.499477	-0.40973	H	-0.25975	1.312817	2.907169
O	4.167002	-2.05172	0.354027	H	1.242708	0.410243	2.66865
C	-0.45936	2.592853	0.480559	H	-3.79066	0.917998	-2.42649
H	-2.19717	1.455092	1.133225	H	-2.58086	-0.19879	-1.82057
C	0.703211	1.319423	2.388048	H	-4.97741	0.727702	-0.14481
H	-0.20075	0.188124	-0.79948	H	-5.02214	-0.6565	-1.22452
C	-3.28596	0.584352	-1.51406	H	-3.32752	-0.35903	1.277741
C	-2.51339	1.765929	-0.95589	H	-0.93736	-2.72148	-0.25402
C	-4.35493	-0.05197	-0.59898	H	-1.31859	-0.65961	1.917768
C	-3.83892	-0.96981	0.524622	H	0.160957	-1.33853	1.280371
C	-2.88324	-2.03059	0.009876	H	-4.25611	-3.68402	-0.19906
C	-1.55674	-1.95019	0.204133	H	-2.7361	-3.88002	-1.09827
C	-0.79762	-0.89811	0.982912	H	-4.00136	-2.7877	-1.68584
C	-0.51317	0.414854	0.22713	H	-2.12693	3.850088	-1.14651
C	-1.58795	1.559914	0.225027	H	-3.34691	3.140316	-2.33615
C	-3.49541	-3.15866	-0.78555	H	-4.72713	-2.0704	1.875821
C	-2.66556	2.97837	-1.50504				
O	-5.01582	-1.54596	1.115978				
H	2.292051	-0.61579	0.741922				
H	4.271268	1.086675	-0.84989				
H	5.767758	-2.27123	-1.83776				
H	4.143361	-1.71202	-2.29527				
H	5.531562	-0.60647	-2.39249				

Conformer 1-5R-conf. 3	Coordinates (Å)			Coordinates (Å)			
	X	Y	Z		X	Y	Z
C	0.575466	-0.29437	0.664157	H	7.226971	0.990905	-1.23387
C	1.756005	-0.69187	-0.21389	H	5.620473	1.492581	-1.80606
C	3.087328	-0.15408	0.17303	H	6.26941	-0.08722	-2.27238
C	4.198303	-0.47496	-0.50382	H	5.137831	1.774312	0.548991
C	5.592384	0.021099	-0.19258	H	0.62029	1.676353	1.792562
C	6.447268	-1.15092	0.315751	H	0.818168	1.81588	0.029913
C	6.215185	0.641071	-1.45783	H	1.633331	-0.74949	2.517051
O	1.607096	-1.42545	-1.18841	H	-0.12211	-0.71802	2.689276
O	5.587415	0.979852	0.87186	H	0.665063	-2.09992	1.908101
C	0.342953	1.239537	0.828858	H	-3.50939	2.506343	-1.59424
H	-1.69172	0.881021	1.507723	H	-3.00238	0.827232	-1.65418
C	0.693274	-1.01191	2.021505	H	-4.52351	2.017658	0.728328
H	-0.67381	-0.33781	-1.11312	H	-5.31259	1.338456	-0.68597
C	-3.2021	1.661317	-0.96965	H	-3.5825	-0.15142	1.316876
C	-1.91535	2.052045	-0.26585	H	-2.80154	-2.54414	-1.38244
C	-4.40326	1.282712	-0.07613	H	-1.98941	-1.5818	1.353554
C	-4.37033	-0.1213	0.55504	H	-1.06901	-2.51108	0.188354
C	-4.11247	-1.20861	-0.4718	H	-6.14355	-1.83266	-0.85762
C	-2.92124	-1.82001	-0.57628	H	-4.97764	-2.33393	-2.10108
C	-1.7009	-1.6219	0.296068	H	-5.53784	-0.65559	-2.0093
C	-0.82392	-0.39861	-0.03022	H	-0.53857	3.63137	0.11147
C	-1.16937	1.017595	0.550851	H	-1.99905	4.061915	-0.9314
C	-5.24935	-1.52992	-1.4122	H	-5.62824	-1.12704	1.665095
C	-1.45802	3.307312	-0.3666				
O	-5.6459	-0.27924	1.199625				
H	3.144019	0.509544	1.030599				
H	4.105764	-1.15163	-1.35251				
H	7.466324	-0.80404	0.510883				
H	6.027673	-1.54902	1.243486				
H	6.487446	-1.9555	-0.42317				

Conformer 1-5R-conf. 4	Coordinates (Å)			Coordinates (Å)			
	X	Y	Z		X	Y	Z
C	0.573527	-0.31227	0.677152	H	5.363614	1.85825	-1.36392
C	1.755617	-0.71948	-0.19405	H	7.047045	1.337471	-1.12658
C	3.085488	-0.17351	0.186054	H	6.010216	0.49115	-2.29526
C	4.192443	-0.47426	-0.5064	H	5.435301	0.216011	1.738423
C	5.583963	0.034812	-0.2048	H	0.831491	1.796794	0.046598
C	6.555774	-1.15451	-0.08685	H	0.625423	1.656741	1.808176
C	6.028139	0.991064	-1.32332	H	1.619905	-0.77651	2.534065
O	1.608668	-1.46834	-1.15722	H	0.645752	-2.12015	1.918961
O	5.613554	0.813332	0.997461	H	-0.13611	-0.73431	2.698713
C	0.349582	1.222423	0.842911	H	-3.48598	2.518921	-1.59106
H	-1.68985	0.873986	1.512752	H	-2.9887	0.837051	-1.65474
C	0.680318	-1.03251	2.034129	H	-4.51152	2.028652	0.726137
H	-0.66748	-0.34458	-1.10644	H	-5.29939	1.35877	-0.69325
C	-3.186	1.67003	-0.96817	H	-3.58594	-0.14772	1.311347
C	-1.89947	2.050837	-0.25859	H	-2.80707	-2.53629	-1.39212
C	-4.39265	1.295642	-0.08029	H	-2.00179	-1.58734	1.350814
C	-4.37033	-0.11062	0.546296	H	-1.08155	-2.51858	0.186925
C	-4.11424	-1.19597	-0.48305	H	-5.52856	-0.62894	-2.02563
C	-2.92625	-1.81423	-0.58402	H	-6.14737	-1.80583	-0.88076
C	-1.70876	-1.6261	0.294521	H	-4.97863	-2.31048	-2.1202
C	-0.82312	-0.40714	-0.02435	H	-0.51421	3.620554	0.127828
C	-1.16286	1.009883	0.558304	H	-1.9683	4.062999	-0.91894
C	-5.24856	-1.50702	-1.42999	H	-5.63866	-1.1132	1.64732
C	-1.43399	3.303515	-0.35427				
O	-5.6495	-0.26356	1.184997				
H	3.141598	0.496182	1.038953				
H	4.097304	-1.1377	-1.36516				
H	7.563655	-0.78434	0.121499				
H	6.254117	-1.82284	0.727013				
H	6.582236	-1.73969	-1.01081				

Conformer	Coordinates (Å)			Coordinates (Å)			
1-5R-conf. 7	X	Y	Z		X	Y	Z
C	0.575091	-0.28477	0.671557	H	7.156738	1.112588	-1.23252
C	1.760149	-0.69217	-0.19595	H	5.50969	1.63904	-1.64599
C	3.087051	-0.14134	0.185781	H	6.158434	0.123331	-2.30986
C	4.197749	-0.47293	-0.48614	H	6.405012	1.225502	1.105559
C	5.590054	0.018695	-0.19492	H	0.614517	1.695951	1.782632
C	6.491425	-1.18304	0.153819	H	0.818984	1.819947	0.019669
C	6.134551	0.769098	-1.42703	H	1.625807	-0.72385	2.531846
O	1.616479	-1.44589	-1.15624	H	-0.13041	-0.68978	2.698199
O	5.509306	0.909351	0.923479	H	0.658398	-2.07908	1.931909
C	0.341157	1.250287	0.821843	H	-3.50303	2.478947	-1.63309
H	-1.69618	0.894999	1.495754	H	-2.98872	0.800943	-1.66728
C	0.687054	-0.99011	2.035819	H	-4.52271	2.025113	0.684035
H	-0.66659	-0.3437	-1.11076	H	-5.30621	1.315543	-0.72086
C	-3.19485	1.643817	-0.99569	H	-3.59162	-0.14912	1.320418
C	-1.91453	2.048828	-0.28946	H	-2.79909	-2.54335	-1.37109
C	-4.40082	1.270342	-0.10474	H	-1.98994	-1.56776	1.361888
C	-4.37771	-0.12745	0.555975	H	-1.06938	-2.50598	0.203415
C	-4.11992	-1.22559	-0.45352	H	-6.12513	-1.93531	-0.81388
C	-2.92122	-1.82015	-0.56462	H	-4.96469	-2.34583	-2.09431
C	-1.70038	-1.61532	0.305062	H	-5.60384	-0.69959	-1.94712
C	-0.82133	-0.39579	-0.02798	H	-0.54655	3.637233	0.080002
C	-1.16977	1.024488	0.540026	H	-2.00285	4.051691	-0.97549
C	-5.26043	-1.57335	-1.37951	H	-5.82366	0.350751	1.781383
C	-1.4621	3.304999	-0.39998				
O	-5.64476	-0.38702	1.18184				
H	3.140356	0.543137	1.025609				
H	4.106624	-1.16191	-1.32422				
H	7.513331	-0.83867	0.347902				
H	6.117545	-1.68814	1.048385				
H	6.529579	-1.90552	-0.66683				

Conformer	Coordinates (Å)			Coordinates (Å)			
1-5R-conf. 8	X	Y	Z		X	Y	Z
C	0.508736	1.448685	0.863227	H	5.729043	-0.55068	1.567808
C	1.864151	1.495685	0.16323	H	6.72166	-1.57544	0.50664
C	2.690332	0.259359	0.209479	H	6.584411	0.166693	0.186513
C	3.909068	0.208182	-0.34518	H	3.470652	-2.41523	-0.3732
C	4.820776	-0.9982	-0.35398	H	-0.13343	3.09457	-0.43045
C	5.256723	-1.30651	-1.79887	H	-0.64359	3.349577	1.252647
C	6.043557	-0.71738	0.534118	H	1.283043	2.174245	2.755566
O	2.249964	2.507603	-0.4168	H	1.255425	0.407566	2.657876
O	4.185544	-2.14608	0.221827	H	-0.24763	1.30666	2.905447
C	-0.45938	2.594289	0.483251	H	-3.79604	0.922368	-2.4194
H	-2.19371	1.452211	1.137494	H	-2.58308	-0.19433	-1.81976
C	0.713106	1.316653	2.382335	H	-4.97666	0.724333	-0.13547
H	-0.20197	0.192915	-0.80475	H	-5.0218	-0.65746	-1.21824
C	-3.28844	0.586998	-1.50923	H	-3.32096	-0.36281	1.280215
C	-2.51613	1.768258	-0.94995	H	-0.93237	-2.71977	-0.26258
C	-4.35404	-0.05326	-0.59299	H	-1.30936	-0.66269	1.914375
C	-3.8337	-0.9727	0.527294	H	0.168998	-1.33793	1.27105
C	-2.87812	-2.03128	0.007726	H	-3.99992	-2.78648	-1.68634
C	-1.55119	-1.94981	0.198592	H	-4.24965	-3.68579	-0.20051
C	-0.79116	-0.89831	0.97727	H	-2.73191	-3.87854	-1.10421
C	-0.51099	0.416759	0.22355	H	-2.13361	3.853603	-1.13576
C	-1.58721	1.560446	0.227919	H	-3.35565	3.145149	-2.32403
C	-3.49114	-3.15856	-0.78812	H	-4.71666	-2.07674	1.879131
C	-2.67173	2.981981	-1.49528				
O	-5.00807	-1.55166	1.120759				
H	2.289397	-0.61397	0.714044				
H	4.291135	1.104484	-0.83215				
H	5.924054	-2.17307	-1.80252				
H	4.387931	-1.53218	-2.42684				
H	5.783353	-0.45782	-2.24517				

Conformer 1-5R-conf. 9	Coordinates (Å)		
	X	Y	Z
C	0.507865	1.456578	0.864334
C	1.869161	1.502531	0.176003
C	2.688897	0.261787	0.218015
C	3.902592	0.203036	-0.34689
C	4.808471	-1.00763	-0.36029
C	4.922556	-1.54114	-1.79738
C	6.195235	-0.62224	0.188815
O	2.265933	2.519065	-0.3883
O	4.260321	-2.08717	0.40564
C	-0.45847	2.599288	0.470982
H	-2.19552	1.461126	1.124496
C	0.703994	1.335534	2.385666
H	-0.19302	0.188217	-0.79799
C	-3.27744	0.575652	-1.51958
C	-2.50745	1.761432	-0.96676
C	-4.34729	-0.05677	-0.60281
C	-3.83238	-0.96769	0.526969
C	-2.87465	-2.03034	0.019885
C	-1.54849	-1.94702	0.215198
C	-0.79195	-0.88956	0.989147
C	-0.5076	0.419742	0.226893
C	-1.58439	1.562966	0.217268
C	-3.48435	-3.16401	-0.76942
C	-2.65987	2.970504	-1.52319
O	-5.00976	-1.54164	1.119399
H	2.279233	-0.61374	0.711631
H	4.282232	1.094635	-0.84417
H	5.601762	-2.39855	-1.81712
H	3.942001	-1.86085	-2.16007
H	5.310666	-0.77215	-2.47047

Coordinates (Å)			
	X	Y	Z
H	6.851774	-1.49681	0.17067
H	6.118722	-0.26448	1.221399
H	6.65321	0.171122	-0.40924
H	4.266002	-1.81925	1.336124
H	-0.6471	3.360214	1.233732
H	-0.12806	3.093224	-0.44463
H	1.271065	2.196348	2.755832
H	-0.2595	1.328055	2.903694
H	1.245798	0.428798	2.670109
H	-3.78086	0.90337	-2.43485
H	-2.57075	-0.20831	-1.82027
H	-4.97153	0.724711	-0.15419
H	-5.01263	-0.66566	-1.22609
H	-3.32302	-0.35214	1.277599
H	-0.92747	-2.72015	-0.23755
H	-1.31482	-0.6465	1.921751
H	0.166492	-1.32735	1.291039
H	-4.24542	-3.68641	-0.18079
H	-2.7238	-3.88651	-1.07639
H	-3.9893	-2.79924	-1.6728
H	-2.12316	3.844986	-1.16854
H	-3.33961	3.126781	-2.35668
H	-4.72203	-2.06155	1.882711

Conformer 1-5R-conf. 10	Coordinates (Å)			Coordinates (Å)			
	X	Y	Z		X	Y	Z
C	0.508358	1.445805	0.866784	H	5.942978	-0.3706	1.405927
C	1.868366	1.489088	0.175128	H	6.825312	-1.4854	0.338411
C	2.69044	0.250857	0.227357	H	6.637122	0.213857	-0.12224
C	3.904059	0.197537	-0.33799	H	4.758071	-2.82045	0.337673
C	4.822632	-0.99457	-0.35293	H	-0.6414	3.350341	1.247627
C	5.092255	-1.41071	-1.81313	H	-0.12379	3.091471	-0.43267
C	6.139458	-0.63126	0.36255	H	1.273917	2.171306	2.762757
O	2.259629	2.500841	-0.40228	H	-0.26023	1.308538	2.904963
O	4.163803	-2.05739	0.344989	H	1.241379	0.404549	2.666651
C	-0.45517	2.593376	0.480324	H	-3.77219	0.910315	-2.43774
H	-2.19508	1.45521	1.127659	H	-2.56213	-0.20088	-1.82129
C	0.703458	1.315027	2.38721	H	-4.96877	0.731402	-0.17155
H	-0.19648	0.190508	-0.80381	H	-5.00439	-0.66507	-1.23873
C	-3.27071	0.581668	-1.52167	H	-3.33055	-0.36238	1.282784
C	-2.50571	1.766767	-0.96209	H	-0.94719	-2.71656	-0.26629
C	-4.34299	-0.05734	-0.61056	H	-1.31786	-0.65907	1.911649
C	-3.84199	-0.974	0.529859	H	0.158513	-1.34223	1.270618
C	-2.89153	-2.03821	0.024209	H	-4.21482	-3.73456	-0.12643
C	-1.56345	-1.9476	0.199598	H	-2.73886	-3.87197	-1.10521
C	-0.79903	-0.89756	0.975669	H	-4.07071	-2.8222	-1.61977
C	-0.51042	0.415675	0.222706	H	-2.12589	3.852064	-1.15041
C	-1.5837	1.561486	0.221021	H	-3.33883	3.138521	-2.34526
C	-3.50631	-3.17944	-0.74958	H	-5.58069	-0.94556	1.422714
C	-2.6603	2.978743	-1.51143				
O	-4.95957	-1.63367	1.146072				
H	2.290059	-0.62028	0.73366				
H	4.280048	1.088507	-0.83793				
H	5.778247	-2.2647	-1.83759				
H	4.158025	-1.69927	-2.30213				
H	5.548909	-0.59573	-2.38249				

Conformer 1-5R-conf. 17	Coordinates (Å)		
	X	Y	Z
C	0.577583	-0.29164	0.665139
C	1.75886	-0.69454	-0.20941
C	3.089467	-0.15239	0.173875
C	4.201414	-0.47937	-0.49847
C	5.594751	0.020923	-0.19067
C	6.448715	-1.14421	0.334797
C	6.220246	0.624606	-1.46242
O	1.611104	-1.43577	-1.17831
O	5.587189	0.993466	0.861239
C	0.345756	1.243356	0.821805
H	-1.69098	0.889644	1.498605
C	0.693686	-1.00251	2.026063
H	-0.66958	-0.34411	-1.11343
C	-3.19114	1.646064	-0.99106
C	-1.91044	2.04804	-0.28372
C	-4.39772	1.272682	-0.10096
C	-4.37628	-0.126	0.557889
C	-4.12099	-1.22322	-0.45326
C	-2.92334	-1.81951	-0.56629
C	-1.70122	-1.6176	0.302272
C	-0.82114	-0.39868	-0.03036
C	-1.16604	1.020549	0.542272
C	-5.26296	-1.56834	-1.37847
C	-1.45723	3.304267	-0.39034
O	-5.64334	-0.38438	1.18422
H	3.144803	0.519628	1.024987
H	4.110267	-1.1646	-1.34038
H	7.46717	-0.79448	0.527978
H	6.026873	-1.53059	1.266448
H	6.490981	-1.95812	-0.39373

Coordinates (Å)			
	X	Y	Z
H	5.626256	1.471558	-1.82281
H	7.231557	0.977285	-1.24085
H	6.276152	-0.11413	-2.2674
H	5.136013	1.782601	0.527651
H	0.822502	1.815741	0.020906
H	0.621701	1.684634	1.783866
H	1.633774	-0.73882	2.52093
H	0.664207	-2.09103	1.91794
H	-0.12179	-0.70449	2.691905
H	-3.49798	2.48288	-1.62685
H	-2.98605	0.804168	-1.66419
H	-4.51891	2.026521	0.688796
H	-5.30291	1.319708	-0.71723
H	-3.5897	-0.14997	1.321775
H	-2.80316	-2.54197	-1.37371
H	-1.98938	-1.57106	1.359538
H	-1.07169	-2.50906	0.19868
H	-5.60593	-0.69341	-1.94454
H	-6.12746	-1.92996	-0.81233
H	-4.96894	-2.34025	-2.09459
H	-0.54154	3.634518	0.090761
H	-1.9975	4.053116	-0.96348
H	-5.82034	0.352552	1.785362

Conformer 1-5R-conf. 18	Coordinates (Å)		
	X	Y	Z
C	0.575657	-0.30941	0.677783
C	1.758352	-0.72057	-0.19076
C	3.088018	-0.17329	0.188193
C	4.195326	-0.47647	-0.50264
C	5.586652	0.033931	-0.20231
C	6.558948	-1.15459	-0.08071
C	6.030616	0.987097	-1.32357
O	1.612101	-1.47317	-1.15112
O	5.615811	0.816072	0.997666
C	0.352167	1.226345	0.836313
H	-1.68941	0.882599	1.5037
C	0.681256	-1.02365	2.037923
H	-0.66371	-0.35074	-1.10681
C	-3.17489	1.654301	-0.98995
C	-1.89468	2.046799	-0.27648
C	-4.38715	1.285302	-0.10578
C	-4.37642	-0.1153	0.549203
C	-4.12315	-1.21113	-0.46394
C	-2.92853	-1.8141	-0.57344
C	-1.70904	-1.6217	0.301009
C	-0.8205	-0.40705	-0.02452
C	-1.15969	1.01289	0.549908
C	-5.26305	-1.54689	-1.39513
C	-1.43359	3.300572	-0.37799
O	-5.64756	-0.36813	1.169555
H	3.143647	0.499494	1.038683
H	4.10059	-1.143	-1.35905
H	7.566649	-0.78339	0.126639
H	6.257472	-1.82067	0.735054
H	6.585729	-1.74245	-1.00296

Coordinates (Å)			
	X	Y	Z
H	5.365607	1.853764	-1.36694
H	7.049295	1.334591	-1.12757
H	6.013254	0.484251	-2.29401
H	5.436691	0.221038	1.740263
H	0.835699	1.797285	0.038503
H	0.626442	1.66454	1.800262
H	1.620788	-0.76631	2.537294
H	0.645798	-2.11176	1.927503
H	-0.13528	-0.72199	2.700818
H	-3.4744	2.494714	-1.6245
H	-2.97196	0.813236	-1.66477
H	-4.50724	2.037549	0.685646
H	-5.28956	1.339302	-0.72555
H	-3.59319	-0.14589	1.316296
H	-2.80896	-2.53488	-1.38244
H	-2.00155	-1.57633	1.357134
H	-1.08418	-2.51644	0.197622
H	-5.59866	-0.66824	-1.95983
H	-6.13199	-1.90547	-0.83386
H	-4.97031	-2.31814	-2.11248
H	-0.51778	3.624086	0.107433
H	-1.96713	4.054107	-0.95129
H	-5.82298	0.368377	1.771689

Conformer 1-5R-conf. 24	Coordinates (Å)		
	X	Y	Z
C	0.51144	1.446663	0.862209
C	1.867636	1.494062	0.16384
C	2.693788	0.257731	0.210389
C	3.913332	0.207124	-0.34255
C	4.825407	-0.99899	-0.35066
C	5.262836	-1.30689	-1.7952
C	6.047251	-0.71788	0.538641
O	2.254068	2.506263	-0.41532
O	4.190036	-2.14712	0.224388
C	-0.45527	2.594244	0.48396
H	-2.19129	1.451377	1.133383
C	0.713579	1.310486	2.381231
H	-0.19858	0.196209	-0.81011
C	-3.27495	0.5857	-1.51541
C	-2.50969	1.769892	-0.95421
C	-4.34309	-0.05805	-0.6028
C	-3.83668	-0.97765	0.532844
C	-2.88667	-2.03904	0.020376
C	-1.55811	-1.94747	0.191515
C	-0.79223	-0.89888	0.968122
C	-0.50861	0.417321	0.218505
C	-1.58332	1.561739	0.22498
C	-3.50274	-3.17861	-0.7548
C	-2.66805	2.983656	-1.49849
O	-4.95094	-1.64095	1.151076
H	2.292248	-0.61592	0.713908
H	4.295882	1.103797	-0.82845
H	5.930536	-2.17317	-1.79837
H	4.394722	-1.53282	-2.42401
H	5.789532	-0.4579	-2.24086

Coordinates (Å)			
	X	Y	Z
H	5.731682	-0.55148	1.572055
H	6.72565	-1.57573	0.511677
H	6.588158	0.166425	0.191711
H	3.47595	-2.41667	-0.37142
H	-0.6396	3.347692	1.255125
H	-0.12816	3.09655	-0.42824
H	1.284504	2.166132	2.757426
H	-0.24784	1.300776	2.903074
H	1.253877	0.399734	2.655188
H	-3.78013	0.917009	-2.42847
H	-2.56639	-0.19477	-1.82047
H	-4.96847	0.728311	-0.159
H	-5.00574	-0.66466	-1.23071
H	-3.32328	-0.36775	1.285823
H	-0.94274	-2.71449	-0.27877
H	-1.30752	-0.66443	1.907062
H	0.167214	-1.34296	1.25799
H	-4.20804	-3.73677	-0.13073
H	-2.73572	-3.86889	-1.11565
H	-4.07103	-2.81929	-1.62158
H	-2.13379	3.856493	-1.13609
H	-3.34979	3.145493	-2.3293
H	-5.57244	-0.95479	1.43167

Conformer 1-5R-conf. 26	Coordinates (Å)		
	X	Y	Z
C	0.510489	1.456026	0.863621
C	1.873079	1.50212	0.17793
C	2.691179	0.260273	0.218223
C	3.906484	0.201981	-0.34326
C	4.811065	-1.00962	-0.35785
C	4.929082	-1.53842	-1.79638
C	6.196492	-0.62761	0.196926
O	2.272223	2.519814	-0.38263
O	4.259294	-2.09108	0.402708
C	-0.45437	2.60025	0.470369
H	-2.19343	1.461891	1.119162
C	0.70408	1.332547	2.385095
H	-0.1887	0.190655	-0.80164
C	-3.26146	0.57243	-1.52756
C	-2.49987	1.762058	-0.97286
C	-4.33489	-0.06324	-0.61548
C	-3.83518	-0.97202	0.531761
C	-2.88217	-2.03805	0.03476
C	-1.55452	-1.94433	0.21178
C	-0.79323	-0.88846	0.982919
C	-0.50484	0.420894	0.223074
C	-1.58022	1.564794	0.213388
C	-3.49386	-3.18531	-0.73249
C	-2.6554	2.970695	-1.52923
O	-4.95318	-1.62939	1.149644
H	2.279052	-0.61633	0.707872
H	4.288596	1.094758	-0.83653
H	5.607403	-2.39651	-1.81686
H	3.949318	-1.85584	-2.16319
H	5.320154	-0.7676	-2.46565

Coordinates (Å)			
	X	Y	Z
H	6.117094	-0.27349	1.230542
H	6.852214	-1.50276	0.177715
H	6.657134	0.167427	-0.39685
H	4.262325	-1.82631	1.334109
H	-0.64372	3.360005	1.234109
H	-0.12244	3.095543	-0.44398
H	1.271762	2.192025	2.757426
H	-0.26019	1.325501	2.901671
H	1.244182	0.4246	2.6689
H	-3.76122	0.895037	-2.4467
H	-2.5508	-0.21056	-1.82098
H	-4.9634	0.726867	-0.18287
H	-4.99341	-0.67603	-1.24174
H	-3.32631	-0.35503	1.282054
H	-0.93628	-2.71529	-0.24809
H	-1.31435	-0.64517	1.916392
H	0.164189	-1.33013	1.282866
H	-4.05709	-2.83483	-1.60617
H	-4.20283	-3.73703	-0.10684
H	-2.72479	-3.87921	-1.08186
H	-2.1235	3.847046	-1.17187
H	-3.3323	3.124611	-2.36548
H	-5.57702	-0.94058	1.418327

Conformer 1-5S-conf. 1	Coordinates (Å)				Coordinates (Å)		
	X	Y	Z		X	Y	Z
C	0.554758	0.576248	0.918363	H	6.749575	-0.47212	-2.11854
C	1.629829	-0.44112	0.559191	H	5.040624	-0.29192	-2.57385
C	2.978057	0.095831	0.238555	H	5.643507	-1.84519	-1.95514
C	3.995134	-0.71794	-0.07545	H	6.34689	1.405389	-0.57711
C	5.395442	-0.29266	-0.42641	H	0.662843	2.668344	0.004471
C	6.383863	-0.90506	0.586317	H	0.546456	1.334134	-1.16906
C	5.724168	-0.75832	-1.85943	H	1.838594	1.68926	2.288743
O	1.382147	-1.64522	0.536363	H	0.112962	1.930107	2.573152
O	5.444988	1.136704	-0.35387	H	0.888892	0.419824	3.07576
C	0.259051	1.66616	-0.16604	H	-1.38924	-0.12274	-2.08133
H	-1.57717	2.155555	0.889934	H	-2.43522	0.875744	-3.06512
C	0.866257	1.186812	2.294815	H	-4.4503	0.014982	-1.98918
H	-0.87081	-0.66105	-0.07891	H	-3.47037	-1.26291	-2.69027
C	-2.3257	0.446866	-2.06305	H	-2.55583	-1.75919	-0.3731
C	-2.23529	1.582983	-1.05554	H	-3.74252	0.271612	2.513637
C	-3.5082	-0.53228	-1.87378	H	-1.53526	-1.54038	1.999416
C	-3.55491	-1.35145	-0.57035	H	-1.47695	0.008521	2.808429
C	-4.04383	-0.58428	0.651908	H	-5.72665	0.531327	-0.13379
C	-3.26012	-0.25998	1.693542	H	-6.14197	-1.07492	0.444134
C	-1.76729	-0.47406	1.869842	H	-5.80584	0.227517	1.606496
C	-0.91531	0.082314	0.719965	H	-2.94287	3.502207	-0.48788
C	-1.26736	1.463074	0.099828	H	-3.63822	2.820628	-2.06062
C	-5.50842	-0.20666	0.648552	H	-4.50547	-2.98256	-0.04839
C	-2.97453	2.689578	-1.2093				
O	-4.44694	-2.44893	-0.8536				
H	3.123322	1.170648	0.25587				
H	3.812093	-1.79116	-0.08583				
H	7.408674	-0.61595	0.327899				
H	6.163471	-0.54463	1.594634				
H	6.331586	-1.99788	0.585177				

Conformer 1-5S-conf. 2	Coordinates (Å)				Coordinates (Å)		
	X	Y	Z		X	Y	Z
C	0.581619	-0.45847	0.398363	H	7.20173	1.54661	-0.53641
C	1.812329	-0.53831	-0.49503	H	5.558088	2.179095	-0.77978
C	3.11309	-0.1724	0.124472	H	6.261589	1.040224	-1.94889
C	4.255487	-0.22554	-0.57353	H	6.369058	0.745917	1.635717
C	5.625804	0.125998	-0.06019	H	0.555127	1.062542	2.100782
C	6.541658	-1.11025	-0.16431	H	0.746185	1.749686	0.470492
C	6.19436	1.296638	-0.88745	H	1.523365	-1.50692	2.067959
O	1.722929	-0.89031	-1.66954	H	-0.24208	-1.55606	2.096228
O	5.48725	0.517978	1.310161	H	0.653351	-2.57441	0.958012
C	0.295165	0.93595	1.045506	H	-3.84647	2.886302	1.110899
H	-1.67757	0.210199	1.54769	H	-3.5931	1.266572	1.736736
C	0.631798	-1.59102	1.438586	H	-5.55922	1.309668	0.307918
H	-0.56342	0.215303	-1.28836	H	-4.68116	2.073357	-1.00907
C	-3.539	1.873893	0.826017	H	-3.41718	0.098325	-1.47018
C	-2.09586	1.910687	0.336326	H	-2.7377	-2.56711	0.96803
C	-4.58181	1.354986	-0.18709	H	-1.03072	-2.44633	-0.67777
C	-4.29061	-0.0141	-0.81678	H	-2.00583	-1.45381	-1.72341
C	-4.02388	-1.1271	0.182591	H	-6.07067	-1.68407	0.557881
C	-2.85339	-1.78762	0.214637	H	-5.38943	-0.64117	1.797233
C	-1.66129	-1.55108	-0.68839	H	-4.91286	-2.34561	1.732607
C	-0.77783	-0.31763	-0.35681	H	-2.2958	3.780478	-0.64121
C	-1.21044	0.739308	0.712825	H	-0.62771	2.999442	-0.75523
C	-5.15517	-1.47279	1.120583	H	-5.26267	-1.14616	-2.08297
C	-1.6483	2.945114	-0.38671				
O	-5.44627	-0.31451	-1.62399				
H	3.119936	0.148229	1.160744				
H	4.209868	-0.54945	-1.61204				
H	6.623988	-1.46044	-1.19757				
H	6.149281	-1.92406	0.451276				
H	7.548344	-0.85929	0.187928				

Conformer 1-5S-conf. 3	Coordinates (Å)				Coordinates (Å)		
	X	Y	Z		X	Y	Z
C	-0.42757	-1.80868	0.415965	H	-6.72789	1.171733	0.505075
C	-1.69429	-1.52324	-0.38123	H	-5.9164	-0.29934	1.08631
C	-2.55676	-0.41372	0.105032	H	-6.44052	-0.17551	-0.6074
C	-3.70154	-0.0997	-0.51635	H	-4.71606	2.360291	1.275681
C	-4.65262	0.997543	-0.12098	H	0.737971	-3.71087	-0.01676
C	-4.79284	1.996899	-1.28674	H	0.51489	-2.60928	-1.396
C	-6.01994	0.379988	0.236066	H	-1.35037	-3.30408	1.690658
O	-1.97932	-2.17773	-1.3818	H	0.10095	-2.5773	2.389936
O	-4.10096	1.657514	1.024049	H	-1.41859	-1.67355	2.375272
C	0.644433	-2.66177	-0.31188	H	1.742248	-0.42937	-2.18577
H	2.101826	-2.04374	1.179539	H	3.365153	-0.83986	-2.69057
C	-0.79618	-2.36586	1.800171	H	4.346007	0.997083	-1.4206
H	0.484531	-0.0801	-0.50911	H	3.131073	1.553809	-2.56029
C	2.78514	-0.44724	-1.8483	H	1.474358	1.703015	-0.64417
C	2.944094	-1.39164	-0.66645	H	2.568716	0.740565	2.781254
C	3.269071	1.004476	-1.62164	H	0.042217	1.199993	1.428481
C	2.558473	1.831534	-0.53422	H	0.445053	-0.10757	2.51892
C	2.969927	1.498216	0.894318	H	5.120733	1.299678	0.735438
C	2.157892	0.906801	1.785788	H	4.575596	2.941426	1.043464
C	0.750053	0.373703	1.584508	H	4.54959	1.736996	2.351003
C	0.626366	-0.62885	0.426541	H	4.261855	-2.64577	0.427787
C	1.745465	-1.68607	0.207511	H	4.980323	-1.83729	-1.07275
C	4.377154	1.892503	1.282994	H	2.459895	3.752028	-0.16329
C	4.119526	-1.98746	-0.42558				
O	2.887067	3.202577	-0.83572				
H	-2.24069	0.14556	0.978789				
H	-3.99016	-0.68222	-1.3897				
H	-5.49812	2.790021	-1.01461				
H	-3.82509	2.452835	-1.51208				
H	-5.16856	1.507168	-2.19002				

Conformer 1-5S-conf. 4	Coordinates (Å)				Coordinates (Å)		
	X	Y	Z		X	Y	Z
C	0.559828	0.489641	0.938485	H	6.882689	-0.45255	-2.01727
C	1.62816	-0.4936	0.47874	H	5.20573	-0.41742	-2.60552
C	2.980418	0.063367	0.211428	H	5.840448	-1.88044	-1.83725
C	4.006549	-0.72207	-0.14319	H	4.996114	1.520492	-1.15461
C	5.413499	-0.2524	-0.43685	H	0.663622	2.654131	0.212208
C	6.355495	-0.74739	0.672583	H	0.533926	1.429325	-1.07407
C	5.862138	-0.78697	-1.81023	H	1.860724	1.474841	2.388375
O	1.374396	-1.68788	0.33695	H	0.138951	1.693409	2.710411
O	5.510721	1.176621	-0.40994	H	0.91509	0.143104	3.070181
C	0.256368	1.671508	-0.04299	H	-1.41493	0.056851	-2.09204
H	-1.56973	2.068716	1.068108	H	-2.46808	1.138867	-2.97486
C	0.887032	0.975866	2.36003	H	-4.47464	0.191057	-1.95654
H	-0.87757	-0.65347	-0.14918	H	-3.50524	-1.022	-2.77717
C	-2.34968	0.62437	-2.01498	H	-2.56636	-1.71822	-0.52126
C	-2.24604	1.668853	-0.91378	H	-3.72261	0.051903	2.543287
C	-3.53273	-0.36562	-1.89949	H	-1.52335	-1.70977	1.851507
C	-3.56716	-1.29543	-0.6723	H	-1.45475	-0.23711	2.791407
C	-4.04343	-0.63766	0.616827	H	-5.73229	0.541997	-0.05354
C	-3.24915	-0.40623	1.675076	H	-6.14424	-1.1075	0.388798
C	-1.75496	-0.63603	1.8173	H	-5.79467	0.090348	1.65513
C	-0.91306	0.017375	0.71185	H	-2.942	3.533522	-0.17545
C	-1.268	1.447457	0.217961	H	-3.65418	2.99233	-1.79448
C	-5.50738	-0.26034	0.660592	H	-4.51045	-2.96773	-0.28573
C	-2.98299	2.786431	-0.96411				
O	-4.46208	-2.36465	-1.04107				
H	3.124511	1.134446	0.317315				
H	3.82868	-1.7935	-0.22771				
H	7.380681	-0.43827	0.448296				
H	6.061664	-0.31958	1.634807				
H	6.328439	-1.83733	0.751532				

Conformer 1-5S-conf. 5	Coordinates (Å)				Coordinates (Å)		
	X	Y	Z		X	Y	Z
C	-0.5566	-0.52917	0.949255	H	-6.67526	0.187184	-2.19147
C	-1.62869	0.476823	0.552192	H	-4.95807	-0.11526	-2.53991
C	-2.97801	-0.06798	0.24791	H	-5.52168	1.538236	-2.21874
C	-3.99401	0.729026	-0.10997	H	-5.49568	-1.29604	0.721322
C	-5.39473	0.270312	-0.4476	H	-0.67291	-2.65709	0.123753
C	-6.41502	1.054746	0.398779	H	-0.55719	-1.37343	-1.10487
C	-5.65185	0.487273	-1.94758	H	-1.84124	-1.57998	2.367289
O	-1.3795	1.678725	0.487818	H	-0.11599	-1.81472	2.657963
O	-5.5568	-1.13662	-0.23181	H	-0.88553	-0.28209	3.099026
C	-0.26731	-1.66392	-0.08982	H	1.379772	0.041057	-2.08188
H	1.571265	-2.11459	0.979337	H	2.420043	-0.99967	-3.02717
C	-0.86723	-1.0809	2.350589	H	4.440741	-0.10104	-1.99408
H	0.870086	0.662195	-0.10127	H	3.461601	1.150252	-2.74277
C	2.314813	-0.52986	-2.04316	H	2.556167	1.741223	-0.44421
C	2.224477	-1.6236	-0.98978	H	3.746809	-0.17527	2.517633
C	3.500484	0.452997	-1.89764	H	1.543787	1.622776	1.937751
C	3.55362	1.323506	-0.62823	H	1.483086	0.108122	2.809134
C	4.044627	0.604231	0.621964	H	5.720348	-0.54692	-0.12625
C	3.263554	0.324824	1.678463	H	6.143661	1.078735	0.388098
C	1.771952	0.551302	1.85085	H	5.80719	-0.17684	1.600912
C	0.914473	-0.04826	0.727048	H	2.929018	-3.5196	-0.34552
C	1.260446	-1.45419	0.16262	H	3.621725	-2.90501	-1.94675
C	5.507799	0.221311	0.628045	H	4.50844	2.972241	-0.17446
C	2.960635	-2.7374	-1.09983				
O	4.447137	2.406761	-0.95744				
H	-3.12229	-1.14268	0.305446				
H	-3.80986	1.800896	-0.17209				
H	-7.42795	0.72907	0.145503				
H	-6.24925	0.880036	1.467386				
H	-6.33817	2.130905	0.217625				

Conformer 1-5S-conf. 6	Coordinates (Å)		
	X	Y	Z
C	-0.58551	-0.44009	-0.37497
C	-1.81342	-0.50888	0.52296
C	-3.11661	-0.15315	-0.09859
C	-4.26597	-0.22648	0.586208
C	-5.63578	0.114825	0.044213
C	-6.47155	-1.17019	-0.06989
C	-6.32319	1.130728	0.975985
O	-1.7223	-0.84393	1.701881
O	-5.56219	0.641539	-1.286
C	-0.29386	0.951589	-1.02653
H	1.670893	0.210986	-1.53632
C	-0.64568	-1.57487	-1.41231
H	0.570502	0.231643	1.305114
C	3.54626	1.865335	-0.83538
C	2.107851	1.912062	-0.33283
C	4.59481	1.33879	0.167911
C	4.299055	-0.02695	0.802816
C	4.012968	-1.14008	-0.1911
C	2.837143	-1.79169	-0.20907
C	1.655975	-1.54229	0.704712
C	0.777756	-0.30493	0.374057
C	1.212008	0.745912	-0.70068
C	5.13162	-1.4973	-1.13989
C	1.672915	2.949797	0.393139
O	5.460668	-0.33518	1.598464
H	-3.11977	0.166329	-1.13639
H	-4.22716	-0.56191	1.621937
H	-6.56195	-1.66552	0.900353
H	-6.00318	-1.86313	-0.77396
H	-7.47418	-0.92457	-0.43219

Coordinates (Å)			
	X	Y	Z
H	-7.31776	1.368372	0.587924
H	-5.7417	2.057107	1.036553
H	-6.42932	0.732684	1.989504
H	-5.12279	1.502951	-1.23645
H	-0.55839	1.077549	-2.08075
H	-0.73655	1.769344	-0.45068
H	-1.53859	-1.4878	-2.0393
H	0.226279	-1.5463	-2.07272
H	-0.67093	-2.5569	-0.92918
H	3.858306	2.875612	-1.12283
H	3.587749	1.257918	-1.74671
H	5.566728	1.284848	-0.33692
H	4.708436	2.057341	0.987876
H	3.433499	0.093801	1.46515
H	2.707575	-2.57236	-0.95895
H	1.01921	-2.43327	0.706031
H	2.01149	-1.44079	1.735579
H	6.050864	-1.71605	-0.58623
H	5.366449	-0.66877	-1.82013
H	4.875281	-2.36876	-1.7481
H	2.327581	3.781448	0.641327
H	0.655883	3.010486	0.770479
H	5.275369	-1.16465	2.060695

Conformer 1-5S-conf. 7	Coordinates (Å)		
	X	Y	Z
C	0.583683	-0.46644	0.387286
C	1.812361	-0.5509	-0.5081
C	3.114993	-0.18466	0.108288
C	4.25897	-0.22521	-0.5882
C	5.626968	0.134039	-0.05331
C	6.608675	-1.02163	-0.32418
C	6.112292	1.428051	-0.72622
O	1.721836	-0.9068	-1.68096
O	5.586684	0.424628	1.348961
C	0.303021	0.928889	1.035083
H	-1.67004	0.207836	1.541806
C	0.632212	-1.59948	1.427247
H	-0.56285	0.21151	-1.29694
C	-3.52858	1.877335	0.828945
C	-2.08752	1.910125	0.33293
C	-4.57725	1.360417	-0.17914
C	-4.29183	-0.00909	-0.81058
C	-4.02271	-1.12326	0.186897
C	-2.85358	-1.78649	0.212947
C	-1.66507	-1.55161	-0.6952
C	-0.77684	-0.32123	-0.36516
C	-1.2039	0.736333	0.706033
C	-5.15033	-1.46719	1.129936
C	-1.63994	2.943088	-0.39215
O	-5.45193	-0.30679	-1.61238
H	3.119459	0.136777	1.145494
H	4.215492	-0.538	-1.63083
H	6.689215	-1.23235	-1.39466
H	6.276908	-1.93799	0.175915
H	7.599536	-0.75659	0.055527

Coordinates (Å)			
	X	Y	Z
H	7.1155	1.674724	-0.36617
H	5.43875	2.25446	-0.48413
H	6.149111	1.313768	-1.81274
H	5.374164	-0.39836	1.812828
H	0.565932	1.054872	2.089694
H	0.754787	1.741286	0.458768
H	1.525046	-1.51848	2.05529
H	-0.24032	-1.5617	2.086445
H	0.649612	-2.58278	0.946373
H	-3.83223	2.890691	1.114546
H	-3.58016	1.270753	1.740308
H	-5.55233	1.316976	0.320593
H	-4.67919	2.079046	-1.00057
H	-3.4213	0.101835	-1.4681
H	-2.73614	-2.56686	0.965146
H	-1.03685	-2.44856	-0.68941
H	-2.01406	-1.45117	-1.72841
H	-6.06887	-1.67625	0.571379
H	-5.37971	-0.63549	1.808145
H	-4.90698	-2.34088	1.740315
H	-2.28598	3.780354	-0.64405
H	-0.62073	2.994308	-0.76493
H	-5.27219	-1.13855	-2.0727

Conformer 1-5S-conf. 8	Coordinates (Å)		
	X	Y	Z
C	0.529925	1.320591	0.891021
C	1.916061	1.445445	0.268804
C	2.736183	0.207291	0.193615
C	3.98282	0.226816	-0.29709
C	4.903764	-0.95681	-0.42386
C	5.27916	-1.15402	-1.90649
C	6.164595	-0.71393	0.430045
O	2.32881	2.523431	-0.15373
O	4.200346	-2.10671	0.059833
C	-0.44073	2.488784	0.58491
H	-2.09007	1.253956	1.254148
C	0.657614	1.023515	2.393984
H	-0.17732	0.385527	-0.94242
C	-4.02391	1.194144	-0.50089
C	-2.61158	1.703781	-0.76349
C	-4.37414	-0.1714	-1.12891
C	-3.43254	-1.33225	-0.78084
C	-3.21035	-1.52836	0.708834
C	-1.99322	-1.41234	1.266472
C	-0.69459	-1.10633	0.54795
C	-0.46602	0.369504	0.114789
C	-1.57214	1.461741	0.313805
C	-4.42738	-1.88111	1.529282
C	-2.32408	2.345128	-1.90343
O	-4.03161	-2.50112	-1.37266
H	2.306523	-0.7241	0.545365
H	4.387746	1.177542	-0.63968
H	5.969029	-1.99922	-2.00776
H	4.383751	-1.36131	-2.4985
H	5.771835	-0.2667	-2.31506

Coordinates (Å)			
	X	Y	Z
H	6.852259	-1.56086	0.328638
H	5.892579	-0.60922	1.483714
H	6.693746	0.189613	0.113073
H	4.797645	-2.86365	-0.01606
H	-0.62013	3.211597	1.386548
H	-0.12595	3.028764	-0.31011
H	1.17566	1.846612	2.897552
H	-0.32878	0.917779	2.856095
H	1.219622	0.105607	2.591269
H	-4.74415	1.920807	-0.89311
H	-4.19299	1.14388	0.580751
H	-5.39093	-0.44711	-0.82484
H	-4.3885	-0.07964	-2.22106
H	-2.46772	-1.1396	-1.26588
H	-1.91963	-1.55223	2.344984
H	-0.61745	-1.73852	-0.34312
H	0.129976	-1.4202	1.196347
H	-5.16334	-1.06718	1.533846
H	-4.93342	-2.75651	1.108577
H	-4.15963	-2.09798	2.566699
H	-1.32904	2.719373	-2.12634
H	-3.08292	2.516372	-2.66289
H	-3.4254	-3.23941	-1.2195

Conformer	Coordinates (Å)			Coordinates (Å)			
1-5S-conf. 13	X	Y	Z		X	Y	Z
C	-0.42693	-1.82566	0.411132	H	-6.74839	1.260911	0.275906
C	-1.69431	-1.54191	-0.38535	H	-6.11988	-0.33656	0.737831
C	-2.56317	-0.43907	0.106231	H	-6.40013	0.041234	-0.96894
C	-3.68895	-0.09419	-0.53346	H	-4.36738	0.935588	1.818488
C	-4.63189	1.012763	-0.11911	H	0.748635	-3.71931	-0.03091
C	-4.56386	2.15131	-1.1496	H	0.518705	-2.61288	-1.40513
C	-6.06504	0.457841	-0.01447	H	-1.34227	-3.33191	1.678684
O	-1.97501	-2.18947	-1.39122	H	0.106459	-2.60232	2.380275
O	-4.24128	1.601668	1.127102	H	-1.41678	-1.70536	2.372371
C	0.649315	-2.66945	-0.32137	H	1.730747	-0.42479	-2.18668
H	2.10503	-2.05059	1.171533	H	3.355828	-0.82208	-2.69484
C	-0.79221	-2.39181	1.792586	H	4.325459	1.017243	-1.42003
H	0.47533	-0.08772	-0.5058	H	3.104877	1.569382	-2.55587
C	2.774136	-0.43652	-1.85047	H	1.450209	1.700546	-0.63651
C	2.941125	-1.38408	-0.67224	H	2.558275	0.733544	2.783773
C	3.248181	1.017778	-1.61935	H	0.025457	1.178996	1.439763
C	2.533586	1.836192	-0.52795	H	0.441311	-0.13111	2.522477
C	2.949993	1.500792	0.898735	H	5.101958	1.31936	0.734962
C	2.144214	0.900146	1.789724	H	4.544817	2.955641	1.050366
C	0.739916	0.35726	1.589652	H	4.530643	1.746059	2.353312
C	0.620815	-0.64021	0.427014	H	4.268851	-2.63277	0.416163
C	1.745453	-1.69015	0.201725	H	4.980111	-1.81354	-1.08197
C	4.35492	1.904316	1.286247	H	2.421332	3.754766	-0.15096
C	4.121015	-1.97232	-0.43461				
O	2.852029	3.210448	-0.82532				
H	-2.25781	0.101344	0.996887				
H	-3.96029	-0.6477	-1.43155				
H	-5.26877	2.940309	-0.87131				
H	-3.55609	2.574184	-1.17831				
H	-4.82007	1.790178	-2.14901				

Conformer 1-5S-conf. 16	Coordinates (Å)		
	X	Y	Z
C	-0.43185	-1.80834	0.410952
C	-1.69371	-1.52421	-0.39405
C	-2.56049	-0.41497	0.086491
C	-3.71044	-0.10526	-0.5277
C	-4.65417	1.002829	-0.11793
C	-4.95013	1.906308	-1.3298
C	-5.95146	0.387533	0.431116
O	-1.97256	-2.17743	-1.39674
O	-4.11721	1.78412	0.956226
C	0.643451	-2.66403	-0.30887
H	2.093794	-2.04158	1.187615
C	-0.80778	-2.36087	1.795096
H	0.485589	-0.08289	-0.51519
C	2.791409	-0.45519	-1.84246
C	2.945007	-1.39518	-0.65637
C	3.274047	0.997431	-1.61894
C	2.558367	1.828526	-0.53793
C	2.963288	1.500591	0.89372
C	2.147479	0.912116	1.783701
C	0.74084	0.377366	1.578309
C	0.622467	-0.62867	0.422948
C	1.742265	-1.68695	0.212739
C	4.36861	1.89672	1.287329
C	4.119509	-1.98947	-0.40744
O	2.888125	3.198359	-0.84317
H	-2.24535	0.145251	0.961373
H	-4.00616	-0.69506	-1.39442
H	-5.64241	2.699795	-1.03426
H	-4.02976	2.367788	-1.70381
H	-5.3991	1.337852	-2.14963

Coordinates (Å)			
	X	Y	Z
H	-6.65109	1.184895	0.698743
H	-5.7383	-0.20746	1.323182
H	-6.42452	-0.25708	-0.31431
H	-3.34753	2.262081	0.614475
H	0.7351	-3.71211	-0.00969
H	0.519282	-2.61515	-1.39377
H	-1.36203	-3.29904	1.68583
H	0.086415	-2.57097	2.389724
H	-1.43238	-1.66642	2.365221
H	1.750134	-0.43888	-2.18498
H	3.375449	-0.85081	-2.68052
H	4.350013	0.990948	-1.41282
H	3.140433	1.54325	-2.56028
H	1.47474	1.699396	-0.65236
H	2.553832	0.749792	2.781619
H	0.03308	1.202844	1.417084
H	0.432345	-0.10118	2.512955
H	5.114715	1.301072	0.746331
H	4.568391	2.944404	1.043554
H	4.535843	1.746504	2.35691
H	4.257917	-2.64454	0.449045
H	4.983433	-1.84119	-1.05086
H	2.460886	3.750302	-0.17282

Conformer	Coordinates (Å)			Coordinates (Å)			
1-5S-conf. 27	X	Y	Z		X	Y	Z
C	0.533167	1.326312	0.889301	H	6.750068	-1.66258	0.460792
C	1.915329	1.454205	0.2593	H	5.693249	-0.78725	1.591535
C	2.741457	0.219225	0.18711	H	6.626341	0.107768	0.373712
C	3.987735	0.235228	-0.3049	H	3.55161	-2.35164	-0.70842
C	4.901278	-0.96391	-0.42306	H	-0.61987	3.212841	1.393257
C	5.422139	-1.07737	-1.86823	H	-0.13069	3.03579	-0.30547
C	6.0689	-0.81289	0.565163	H	1.185235	1.849904	2.89433
O	2.320982	2.529926	-0.17471	H	-0.31733	0.917996	2.856457
O	4.235305	-2.17505	-0.04585	H	1.231682	0.10956	2.585194
C	-0.4414	2.492711	0.589049	H	-4.74712	1.916126	-0.88031
H	-2.08648	1.252761	1.260031	H	-4.19063	1.135563	0.589606
C	0.667203	1.026621	2.391107	H	-5.38613	-0.45374	-0.82052
H	-0.1784	0.393293	-0.94384	H	-4.38626	-0.07832	-2.21645
C	-4.02374	1.190427	-0.49214	H	-2.46137	-1.13622	-1.26691
C	-2.61366	1.705803	-0.75558	H	-1.90839	-1.55745	2.342313
C	-4.3705	-0.17389	-1.12465	H	0.139504	-1.41495	1.192847
C	-3.42512	-1.33314	-0.7814	H	-0.60791	-1.73352	-0.34681
C	-3.20081	-1.53307	0.707436	H	-4.91945	-2.76788	1.105434
C	-1.98355	-1.41482	1.2643	H	-5.15457	-1.08043	1.535235
C	-0.68652	-1.10297	0.54534	H	-4.14662	-2.11058	2.564628
C	-0.46342	0.3743	0.114324	H	-3.09145	2.523124	-2.65128
C	-1.57128	1.46374	0.318897	H	-1.33728	2.730522	-2.11747
C	-4.41596	-1.89192	1.528009	H	-3.41401	-3.23936	-1.22428
C	-2.33053	2.351939	-1.89391				
O	-4.02146	-2.50184	-1.37619				
H	2.315831	-0.71022	0.552142				
H	4.39277	1.185586	-0.65004				
H	5.972952	-0.17968	-2.16423				
H	4.592045	-1.21074	-2.57044				
H	6.089721	-1.93986	-1.94993				

Conformer 1-5S-conf. 34	Coordinates (Å)		
	X	Y	Z
C	-0.59045	-0.44711	-0.38331
C	-1.81435	-0.50951	0.520605
C	-3.11977	-0.15443	-0.09669
C	-4.26634	-0.22357	0.593217
C	-5.63792	0.117643	0.055607
C	-6.47549	-1.16676	-0.05172
C	-6.32071	1.136794	0.987226
O	-1.71844	-0.83912	1.700667
O	-5.56889	0.640605	-1.27634
C	-0.30096	0.940439	-1.04453
H	1.662436	0.197771	-1.5582
C	-0.65644	-1.5876	-1.41392
H	0.574125	0.23337	1.287508
C	3.54433	1.846883	-0.8546
C	2.102616	1.904118	-0.36337
C	4.585693	1.332545	0.163788
C	4.297498	-0.03163	0.819876
C	4.027637	-1.14986	-0.16847
C	2.845835	-1.78741	-0.21244
C	1.656002	-1.54462	0.691208
C	0.776569	-0.30877	0.358653
C	1.205986	0.736519	-0.72349
C	5.159459	-1.5156	-1.09779
C	1.666425	2.95228	0.346792
O	5.428369	-0.43422	1.61553
H	-3.12699	0.160975	-1.13572
H	-4.22361	-0.55514	1.630045
H	-6.56274	-1.65925	0.920257
H	-6.01057	-1.8622	-0.75558
H	-7.47924	-0.92106	-0.4109

Coordinates (Å)			
	X	Y	Z
H	-7.31645	1.374554	0.602232
H	-5.73797	2.062672	1.043239
H	-6.42353	0.74151	2.00216
H	-5.12834	1.501655	-1.23081
H	-0.56956	1.059834	-2.09848
H	-0.74165	1.76175	-0.47227
H	-1.55149	-1.50227	-2.03812
H	0.213143	-1.56424	-2.0777
H	-0.68175	-2.56693	-0.9254
H	3.860498	2.852141	-1.15496
H	3.592689	1.224945	-1.75558
H	5.562653	1.279115	-0.33083
H	4.683886	2.070135	0.971824
H	3.423748	0.088166	1.471789
H	2.72143	-2.55773	-0.97368
H	1.022536	-2.43799	0.682135
H	2.003763	-1.44763	1.725012
H	6.054207	-1.78792	-0.52796
H	5.443909	-0.67573	-1.74402
H	4.88785	-2.35723	-1.74056
H	2.322547	3.784441	0.589482
H	0.647044	3.021641	0.715987
H	5.635303	0.300459	2.210314

Conformer 1-5S-conf. 38	Coordinates (Å)		
	X	Y	Z
C	-0.5641	-0.63276	0.846178
C	-1.63179	0.412914	0.553223
C	-2.98504	-0.09352	0.202693
C	-4.01087	0.738526	-0.02278
C	-5.41774	0.32145	-0.38781
C	-6.36395	0.649607	0.778246
C	-5.85807	1.053969	-1.66938
O	-1.37741	1.614369	0.603661
O	-5.51775	-1.09547	-0.57428
C	-0.26422	-1.63872	-0.31616
H	1.5597	-2.21842	0.715329
C	-0.88974	-1.34422	2.16975
H	0.878065	0.668365	-0.04156
C	2.346018	-0.28235	-2.08063
C	2.239856	-1.49767	-1.17266
C	3.530911	0.674332	-1.80156
C	3.587405	1.396543	-0.43432
C	4.052347	0.523767	0.721193
C	3.248448	0.103441	1.710524
C	1.757976	0.32601	1.892926
C	0.910217	-0.13416	0.698562
C	1.260505	-1.46536	-0.02159
C	5.516408	0.14721	0.712244
C	2.974539	-2.5924	-1.4097
O	4.531241	2.482075	-0.51238
H	-3.1302	-1.16768	0.137857
H	-3.83262	1.809788	0.062528
H	-7.38861	0.379425	0.506351
H	-6.07567	0.084337	1.668528
H	-6.33524	1.716018	1.016822

Coordinates (Å)			
	X	Y	Z
H	-6.87918	0.758708	-1.92708
H	-5.19933	0.800416	-2.50713
H	-5.83093	2.139476	-1.53627
H	-5.01044	-1.3233	-1.36693
H	-0.6752	-2.64844	-0.22619
H	-0.54021	-1.229	-1.29338
H	-1.86365	-1.84085	2.118661
H	-0.14134	-2.10941	2.397042
H	-0.91568	-0.63819	3.006084
H	1.41205	0.291221	-2.06099
H	2.463952	-0.62677	-3.11389
H	4.473112	0.137722	-1.95817
H	3.493189	1.457643	-2.57099
H	2.595306	1.807494	-0.2081
H	3.712753	-0.51667	2.476965
H	1.541268	1.383878	2.096346
H	1.452991	-0.21854	2.792102
H	6.151678	1.037703	0.689856
H	5.774029	-0.44576	-0.1742
H	5.773693	-0.44444	1.594675
H	2.930238	-3.46166	-0.75838
H	3.647404	-2.65676	-2.26147
H	4.235527	3.066278	-1.2242

Conformer 1-5S-conf. 39	Coordinates (Å)		
	X	Y	Z
C	0.428943	1.825446	0.410357
C	1.69394	1.529367	-0.38578
C	2.551582	0.419326	0.107524
C	3.689896	0.089371	-0.51751
C	4.633588	-1.01219	-0.11642
C	4.747858	-2.03133	-1.26782
C	6.01226	-0.40516	0.21394
O	1.980753	2.175559	-1.39122
O	4.088769	-1.64768	1.045472
C	-0.64154	2.675497	-0.32356
H	-2.10363	2.072229	1.170811
C	0.800906	2.393687	1.789188
H	-0.48712	0.089602	-0.49698
C	-2.76329	0.451747	-1.84743
C	-2.93858	1.399918	-0.67207
C	-3.22684	-1.00786	-1.61943
C	-2.53467	-1.8457	-0.52076
C	-2.95325	-1.50456	0.905935
C	-2.16073	-0.8836	1.793825
C	-0.75621	-0.3394	1.600898
C	-0.62813	0.648672	0.432706
C	-1.74466	1.705828	0.203029
C	-4.34306	-1.94638	1.305681
C	-4.12023	1.98612	-0.43911
O	-2.76632	-3.24501	-0.78086
H	2.236339	-0.12862	0.988712
H	3.977777	0.659781	-1.39906
H	5.44733	-2.82817	-0.99144
H	3.772211	-2.47945	-1.4739
H	5.118054	-1.5605	-2.18332

	Coordinates (Å)		
	X	Y	Z
H	6.714438	-1.20076	0.486658
H	5.927239	0.288501	1.054626
H	6.428463	0.132184	-0.64336
H	4.69382	-2.3599	1.294808
H	-0.73283	3.726803	-0.03569
H	-0.51222	2.615458	-1.40732
H	1.35808	3.329026	1.670615
H	-0.09496	2.61344	2.377831
H	1.421488	1.704363	2.369791
H	-3.34603	0.83073	-2.69406
H	-1.71942	0.446198	-2.18172
H	-4.30916	-1.00667	-1.43693
H	-3.06893	-1.55355	-2.55729
H	-1.45104	-1.74045	-0.6198
H	-2.58123	-0.71345	2.784551
H	-0.04046	-1.16227	1.463216
H	-0.46542	0.15642	2.532247
H	-4.4528	-3.03393	1.2232
H	-5.11405	-1.49771	0.666626
H	-4.56395	-1.66486	2.33809
H	-4.27177	2.64751	0.410236
H	-4.97725	1.82438	-1.08851
H	-3.7153	-3.36218	-0.92889

Table S4. The cartesian coordinates of the dominant conformers for **6-6R** and **6-6S**

Conformer 6-6R-conf. 1	Coordinates (Å)			Coordinates (Å)			
	X	Y	Z		X	Y	Z
C	2.736942	-0.28785	-0.02118	H	-3.01831	-3.14968	-1.19099
C	2.411468	1.227629	0.03737	H	-3.94169	-2.56188	0.205726
O	3.656355	-0.72363	-1.0157	H	0.949586	3.563069	0.007118
H	0.701875	0.78718	1.311555	H	-0.6787	3.776048	-0.84133
H	1.085578	-0.58418	-1.39749	H	2.636584	-0.53981	2.14054
C	-1.40298	1.192299	-0.97934	H	3.325709	-1.92783	1.275826
C	-0.12979	1.774654	-0.39609	H	4.274849	-0.44361	1.472778
C	-2.4796	0.814858	0.06627	H	-1.91984	2.333638	1.1444
C	-2.15977	-0.45982	0.885657				
C	-1.97443	-1.68842	0.022587				
C	-0.77365	-2.23318	-0.23306				
C	0.568185	-1.80847	0.323575				
C	1.21927	-0.56467	-0.3076				
C	0.910983	0.869444	0.236405				
C	-3.23298	-2.26873	-0.57987				
C	0.054978	3.104039	-0.40445				
C	3.267912	-0.83562	1.298464				
O	-2.76801	1.912647	0.931622				
H	2.909131	1.821137	0.810071				
H	2.571894	1.704286	-0.93547				
H	3.359693	-0.36954	-1.86573				
H	-1.84722	1.936096	-1.64831				
H	-1.18118	0.304668	-1.58035				
H	-3.40965	0.634276	-0.48505				
H	-1.27564	-0.27437	1.503076				
H	-3.0012	-0.60819	1.574741				
H	-0.74826	-3.09154	-0.90456				
H	1.262945	-2.64619	0.188345				
H	0.49621	-1.6508	1.407448				
H	-3.75838	-1.54195	-1.21222				

Conformer 6-6R-conf. 2	Coordinates (Å)		
	X	Y	Z
C	2.736944	-0.27352	-0.02511
C	2.4023	1.229795	0.058843
O	3.622336	-0.5515	-1.1082
H	0.682329	0.779316	1.316123
H	1.096177	-0.58372	-1.3948
C	-1.4072	1.189663	-0.98057
C	-0.13606	1.773167	-0.39403
C	-2.48631	0.8107	0.06171
C	-2.1671	-0.46256	0.883606
C	-1.97368	-1.69142	0.022696
C	-0.7702	-2.233	-0.22691
C	0.568495	-1.8035	0.333927
C	1.218081	-0.56244	-0.30565
C	0.901039	0.867597	0.243117
C	-3.22762	-2.27601	-0.58529
C	0.049783	3.102358	-0.40462
C	3.292393	-0.84997	1.275393
O	-2.77974	1.908741	0.92535
H	2.89293	1.80924	0.846183
H	2.575033	1.711673	-0.90723
H	3.782642	-1.5064	-1.12037
H	-1.85055	1.932933	-1.65075
H	-1.18193	0.302438	-1.58093
H	-3.4143	0.627865	-0.49238
H	-1.28672	-0.27402	1.505366
H	-3.01162	-0.61277	1.56851
H	-0.73944	-3.0915	-0.89802
H	1.261553	-2.64491	0.211505
H	0.490147	-1.63772	1.416278
H	-3.7518	-1.55141	-1.22115

	Coordinates (Å)		
	X	Y	Z
H	-3.0075	-3.15706	-1.19434
H	-3.93951	-2.57019	0.197052
H	0.943655	3.56151	0.008438
H	-0.68175	3.774175	-0.84539
H	2.661996	-0.60196	2.134729
H	3.374261	-1.94192	1.226345
H	4.291444	-0.44078	1.455522
H	-1.93309	2.332117	1.139417

Conformer 6-6R-conf. 3	Coordinates (Å)		
	X	Y	Z
C	2.698445	-0.32684	0.03011
C	2.39553	1.192056	0.125
O	3.554924	-0.73885	-1.03373
H	0.582342	0.769671	1.261647
H	1.145235	-0.56323	-1.44055
C	-1.46575	1.257605	-0.89418
C	-0.10112	1.779543	-0.48894
C	-2.43861	0.863273	0.241887
C	-2.15499	-0.49203	0.920821
C	-2.01978	-1.63706	-0.05661
C	-0.8328	-2.18088	-0.3705
C	0.515929	-1.82687	0.215999
C	1.205088	-0.57089	-0.34586
C	0.879471	0.86185	0.208166
C	-3.29814	-2.12577	-0.6952
C	0.221289	3.053619	-0.75113
C	3.16554	-0.93108	1.3527
O	-2.46206	1.830303	1.294638
H	2.844725	1.747037	0.954267
H	2.645048	1.683077	-0.8192
H	4.467581	-0.55739	-0.76569
H	-1.95768	2.034338	-1.49145
H	-1.35514	0.386612	-1.55157
H	-3.43658	0.800895	-0.2204
H	-1.25521	-0.38934	1.53206
H	-2.98624	-0.68143	1.612766
H	-0.82591	-2.97513	-1.11713
H	1.18931	-2.67448	0.03945
H	0.439591	-1.72668	1.306038
H	-3.80586	-1.32884	-1.25331

	Coordinates (Å)		
	X	Y	Z
H	-3.11374	-2.95361	-1.38546
H	-4.00931	-2.46819	0.067921
H	1.191118	3.469573	-0.4957
H	-0.4811	3.727851	-1.23415
H	2.510425	-0.65152	2.183415
H	3.20712	-2.02281	1.296137
H	4.170622	-0.56264	1.592153
H	-2.52996	2.70534	0.887825

Conformer 6-6R-conf. 4	Coordinates (Å)		
	X	Y	Z
C	2.703836	-0.33885	0.037831
C	2.405043	1.180747	0.109729
O	3.677512	-0.77229	-0.90581
H	0.597146	0.766842	1.257492
H	1.134641	-0.56803	-1.44661
C	-1.4604	1.26375	-0.89034
C	-0.09156	1.778596	-0.49015
C	-2.43041	0.87108	0.248769
C	-2.15168	-0.48835	0.921297
C	-2.02713	-1.63042	-0.06114
C	-0.84432	-2.17979	-0.38113
C	0.507381	-1.83448	0.203571
C	1.203967	-0.57939	-0.3503
C	0.888193	0.856086	0.20231
C	-3.31056	-2.1092	-0.69693
C	0.23575	3.051268	-0.75327
C	3.139571	-0.92512	1.37579
O	-2.44332	1.834232	1.305228
H	2.864132	1.747318	0.925536
H	2.645596	1.668772	-0.84049
H	3.438533	-0.39947	-1.7659
H	-1.95112	2.044287	-1.48358
H	-1.35697	0.393831	-1.55034
H	-3.43076	0.816295	-0.20926
H	-1.24875	-0.39312	1.529074
H	-2.98105	-0.67571	1.615996
H	-0.84389	-2.97149	-1.1305
H	1.177944	-2.68336	0.021021
H	0.434051	-1.73986	1.294081
H	-3.81587	-1.30715	-1.24989

Coordinates (Å)			
	X	Y	Z
H	-3.1334	-2.93528	-1.39118
H	-4.02081	-2.45069	0.067455
H	1.208026	3.463392	-0.50088
H	-0.46545	3.728784	-1.23337
H	2.464947	-0.62949	2.183669
H	3.174016	-2.0178	1.334878
H	4.142438	-0.56013	1.61896
H	-2.51304	2.710942	0.902331

Conformer 6-6R-conf. 5	Coordinates (Å)		
	X	Y	Z
C	2.705822	-0.32284	0.032385
C	2.393917	1.183637	0.132355
O	3.653142	-0.59126	-1.00046
H	0.576778	0.757733	1.26173
H	1.143931	-0.56894	-1.4427
C	-1.46473	1.259733	-0.89335
C	-0.0986	1.776535	-0.48658
C	-2.43981	0.866291	0.241037
C	-2.16058	-0.49055	0.9188
C	-2.0257	-1.63485	-0.05956
C	-0.8393	-2.18101	-0.37169
C	0.509312	-1.82938	0.216902
C	1.203565	-0.57714	-0.34804
C	0.877626	0.85372	0.20968
C	-3.30383	-2.12022	-0.70116
C	0.228808	3.049524	-0.74801
C	3.170384	-0.94062	1.349593
O	-2.46214	1.832034	1.295047
H	2.844208	1.73474	0.963156
H	2.645564	1.678838	-0.80908
H	3.800016	-1.548	-1.02464
H	-1.95383	2.039106	-1.4895
H	-1.35637	0.389582	-1.55224
H	-3.43735	0.807009	-0.22258
H	-1.26197	-0.39045	1.532145
H	-2.99375	-0.67899	1.608683
H	-0.83262	-2.97442	-1.11925
H	1.177787	-2.68312	0.048137
H	0.430078	-1.72437	1.306207
H	-3.80874	-1.32165	-1.25951

	Coordinates (Å)		
	X	Y	Z
H	-3.11989	-2.9478	-1.39185
H	-4.01727	-2.46181	0.060206
H	1.199792	3.46219	-0.49166
H	-0.47058	3.726508	-1.23153
H	2.496861	-0.69537	2.17633
H	3.230535	-2.03302	1.281223
H	4.165961	-0.55861	1.596446
H	-2.52844	2.707688	0.889296

Conformer 6-6R-conf. 6	Coordinates (Å)		
	X	Y	Z
C	2.703618	-0.32156	0.038857
C	2.398232	1.196183	0.137654
O	3.564151	-0.72855	-1.02393
H	0.58319	0.76803	1.267089
H	1.155358	-0.55555	-1.43771
C	-1.46725	1.276944	-0.88942
C	-0.0958	1.785978	-0.48375
C	-2.44687	0.865103	0.225265
C	-2.14962	-0.49262	0.908071
C	-2.00975	-1.64064	-0.06565
C	-0.82097	-2.18137	-0.37802
C	0.524667	-1.82552	0.213255
C	1.212044	-0.56634	-0.34288
C	0.881794	0.864706	0.214263
C	-3.28571	-2.13283	-0.70675
C	0.242315	3.051536	-0.76434
C	3.168049	-0.92981	1.360512
O	-2.47646	1.917709	1.192154
H	2.843816	1.749482	0.970033
H	2.65133	1.689533	-0.80426
H	4.475675	-0.54653	-0.75242
H	-1.95533	2.064629	-1.47228
H	-1.35724	0.413394	-1.55656
H	-3.43417	0.782993	-0.25511
H	-1.25162	-0.38297	1.520476
H	-2.98128	-0.69446	1.599223
H	-0.8107	-2.97456	-1.12572
H	1.200884	-2.67085	0.036554
H	0.44462	-1.72853	1.303388
H	-3.79468	-1.33818	-1.26691

	Coordinates (Å)		
	X	Y	Z
H	-3.09729	-2.96065	-1.39591
H	-3.99769	-2.47706	0.054877
H	1.21963	3.457665	-0.52238
H	-0.45724	3.730553	-1.24436
H	2.510061	-0.65459	2.190407
H	3.212121	-2.02125	1.300181
H	4.171689	-0.56014	1.604171
H	-3.16116	1.697126	1.83896

Conformer 6-6R-conf. 10	Coordinates (Å)		
	X	Y	Z
C	2.710933	-0.31759	0.041127
C	2.39653	1.187737	0.145099
O	3.662209	-0.58082	-0.98969
H	0.577499	0.755851	1.266938
H	1.154189	-0.56115	-1.44019
C	-1.46607	1.278921	-0.88882
C	-0.0933	1.78298	-0.48144
C	-2.44785	0.868236	0.22437
C	-2.15511	-0.49107	0.90608
C	-2.01579	-1.63846	-0.06847
C	-0.82765	-2.18151	-0.37936
C	0.518025	-1.82808	0.213711
C	1.210526	-0.57254	-0.34539
C	0.879922	0.856549	0.21562
C	-3.29172	-2.12744	-0.71211
C	0.249499	3.04758	-0.76084
C	3.172627	-0.93968	1.357249
O	-2.47562	1.919758	1.192479
H	2.843125	1.73705	0.97913
H	2.651873	1.685423	-0.79391
H	3.812252	-1.53701	-1.01539
H	-1.95136	2.069084	-1.47065
H	-1.35818	0.416129	-1.55728
H	-3.43486	0.789322	-0.25716
H	-1.25823	-0.38406	1.52054
H	-2.98868	-0.69176	1.59526
H	-0.81778	-2.97395	-1.1279
H	1.189257	-2.67957	0.044474
H	0.43528	-1.72641	1.303142
H	-3.7982	-1.33117	-1.27223

Coordinates (Å)			
	X	Y	Z
H	-3.10395	-2.95496	-1.40182
H	-4.0056	-2.47098	0.048045
H	1.227786	3.450609	-0.51766
H	-0.44715	3.729248	-1.24132
H	2.496265	-0.69893	2.182989
H	3.235173	-2.0317	1.284874
H	4.166741	-0.55669	1.608517
H	-3.16152	1.700253	1.83838

Conformer 6-6S-conf. 1	Coordinates (Å)		
	X	Y	Z
C	2.793418	-0.32963	-0.0316
C	2.531932	1.179457	0.211528
O	3.710364	-0.67906	-1.06275
H	0.775243	0.675771	1.39824
H	1.149004	-0.37825	-1.45099
C	-1.37797	1.422937	-0.57357
C	0.021558	1.874777	-0.20488
C	-2.28515	0.956936	0.581067
C	-2.03676	-0.49353	1.070343
C	-1.97275	-1.53251	-0.02801
C	-0.81216	-2.05585	-0.45729
C	0.571635	-1.79274	0.09401
C	1.271661	-0.50304	-0.36658
C	1.014505	0.872685	0.343946
C	-3.28803	-1.94159	-0.6468
C	0.364843	3.15945	-0.36899
C	3.28097	-1.05912	1.214906
O	-3.62402	1.118744	0.088654
H	3.04112	1.650001	1.058074
H	2.738544	1.759559	-0.69366
H	3.436505	-0.21828	-1.8681
H	-1.89588	2.263342	-1.04479
H	-1.32805	0.618237	-1.31734
H	-2.13393	1.627252	1.441894
H	-1.11389	-0.49866	1.657123
H	-2.84431	-0.74072	1.775137
H	-0.85906	-2.76778	-1.2816
H	1.213462	-2.63235	-0.20071
H	0.550333	-1.80387	1.191085
H	-3.9521	-2.38045	0.110428

	Coordinates (Å)		
	X	Y	Z
H	-3.81534	-1.07247	-1.05285
H	-3.14866	-2.67845	-1.44312
H	1.35892	3.527596	-0.13425
H	-0.34554	3.89168	-0.74323
H	2.653173	-0.83841	2.082264
H	3.289641	-2.14197	1.059536
H	4.302258	-0.73822	1.443281
H	-4.22845	0.809586	0.777895

Conformer 6-6S-conf. 2	Coordinates (Å)		
	X	Y	Z
C	2.79605	-0.3048	-0.03418
C	2.514228	1.189218	0.222768
O	3.691247	-0.48517	-1.13051
H	0.750539	0.67122	1.392806
H	1.164489	-0.38746	-1.45147
C	-1.39821	1.410548	-0.57185
C	0.003316	1.866971	-0.21399
C	-2.29809	0.938269	0.594581
C	-2.04422	-0.50867	1.074288
C	-1.96484	-1.54257	-0.02963
C	-0.79856	-2.0619	-0.4482
C	0.581153	-1.79053	0.109199
C	1.274283	-0.50233	-0.36679
C	0.998294	0.870872	0.3408
C	-3.27078	-1.95963	-0.66304
C	0.34287	3.152277	-0.38243
C	3.308686	-1.0515	1.195448
O	-3.67661	0.996074	0.201576
H	3.011729	1.653885	1.079108
H	2.729739	1.76814	-0.67905
H	3.822663	-1.43695	-1.25028
H	-1.90876	2.255643	-1.04779
H	-1.35475	0.606968	-1.31701
H	-2.1387	1.607863	1.454435
H	-1.12525	-0.51227	1.665673
H	-2.86356	-0.75414	1.761959
H	-0.83587	-2.77385	-1.27311
H	1.223468	-2.63561	-0.16954
H	0.553593	-1.78798	1.206259
H	-3.94689	-2.38752	0.089379

	Coordinates (Å)		
	X	Y	Z
H	-3.79291	-1.09687	-1.08833
H	-3.11748	-2.70699	-1.44707
H	1.336487	3.523561	-0.15108
H	-0.36925	3.881922	-0.75864
H	2.677225	-0.87809	2.072121
H	3.346667	-2.13294	1.020727
H	4.320813	-0.70778	1.431194
H	-3.86623	1.904646	-0.07062

Conformer 6-6S-conf. 3	Coordinates (Å)		
	X	Y	Z
C	2.786893	-0.31975	-0.03772
C	2.524334	1.1879	0.220893
O	3.582363	-0.64012	-1.17752
H	0.763729	0.680924	1.400401
H	1.160289	-0.37823	-1.4463
C	-1.3845	1.419668	-0.57751
C	0.012869	1.876239	-0.20648
C	-2.29294	0.953997	0.576251
C	-2.03997	-0.49363	1.071614
C	-1.96753	-1.53613	-0.02278
C	-0.80344	-2.05636	-0.44624
C	0.578101	-1.78671	0.107496
C	1.272275	-0.49684	-0.3622
C	1.007025	0.878206	0.346832
C	-3.27887	-1.95214	-0.64541
C	0.352978	3.161603	-0.37147
C	3.301326	-1.06094	1.194496
O	-3.63121	1.108466	0.079695
H	3.025746	1.650237	1.076649
H	2.739031	1.764752	-0.68243
H	4.511215	-0.51246	-0.9356
H	-1.90376	2.257312	-1.05219
H	-1.33021	0.613198	-1.31903
H	-2.14687	1.628057	1.435068
H	-1.11912	-0.49269	1.661578
H	-2.84895	-0.7418	1.774467
H	-0.84511	-2.77066	-1.26878
H	1.221674	-2.62704	-0.18047
H	0.554045	-1.79102	1.204774
H	-3.94476	-2.39006	0.110765

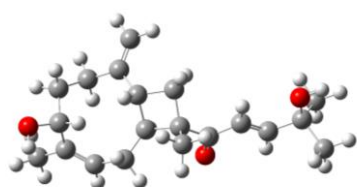
	Coordinates (Å)		
	X	Y	Z
H	-3.80732	-1.08643	-1.05725
H	-3.1337	-2.69172	-1.43816
H	1.346009	3.531983	-0.13587
H	-0.35852	3.891632	-0.74792
H	2.692034	-0.85421	2.079645
H	3.315498	-2.14211	1.028208
H	4.324559	-0.73605	1.420086
H	-4.2361	0.798829	0.768319

Conformer 6-6S-conf. 4	Coordinates (Å)		
	X	Y	Z
C	2.791089	-0.34268	-0.04615
C	2.54425	1.166949	0.208891
O	3.693733	-0.69317	-1.08923
H	0.792063	0.672421	1.407238
H	1.131195	-0.37499	-1.44893
C	-1.36089	1.446553	-0.57011
C	0.038927	1.88536	-0.1857
C	-2.29452	0.976599	0.568173
C	-2.05006	-0.47092	1.071407
C	-1.98652	-1.53122	-0.00708
C	-0.82684	-2.05734	-0.43683
C	0.560634	-1.78725	0.101898
C	1.264072	-0.50242	-0.36609
C	1.025403	0.871584	0.352086
C	-3.30165	-1.99998	-0.58634
C	0.386166	3.172156	-0.32302
C	3.286629	-1.08279	1.190912
O	-3.6636	1.157115	0.173007
H	3.064228	1.627032	1.054575
H	2.747846	1.752232	-0.69361
H	3.415697	-0.22463	-1.88866
H	-1.86209	2.298318	-1.0405
H	-1.30559	0.646243	-1.32088
H	-2.16754	1.645682	1.42768
H	-1.12523	-0.47266	1.656105
H	-2.86552	-0.69473	1.770635
H	-0.87933	-2.79278	-1.2398
H	1.198696	-2.63005	-0.19138
H	0.544053	-1.7927	1.199228
H	-3.95016	-2.39936	0.204279

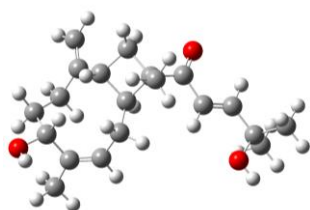
	Coordinates (Å)		
	X	Y	Z
H	-3.86844	-1.18885	-1.05671
H	-3.15424	-2.78369	-1.33456
H	1.379394	3.532544	-0.07321
H	-0.31906	3.91346	-0.68893
H	2.669286	-0.86309	2.065983
H	3.286978	-2.16474	1.02933
H	4.312218	-0.76957	1.410436
H	-3.74577	0.884733	-0.75077

Conformer 6-6S-conf. 5	Coordinates (Å)		
	X	Y	Z
C	2.792278	-0.32837	-0.04888
C	2.534407	1.166538	0.227547
O	3.670695	-0.50874	-1.15853
H	0.772457	0.664643	1.408483
H	1.142392	-0.37981	-1.44744
C	-1.367	1.444656	-0.57273
C	0.03212	1.883094	-0.18553
C	-2.30329	0.975188	0.56349
C	-2.05823	-0.47083	1.070959
C	-1.98675	-1.53325	-0.00486
C	-0.82414	-2.05803	-0.42826
C	0.561237	-1.7842	0.114467
C	1.263378	-0.50209	-0.36483
C	1.015069	0.868557	0.356116
C	-3.29826	-2.00583	-0.58932
C	0.381068	3.169292	-0.32406
C	3.310918	-1.09449	1.166173
O	-3.67152	1.152247	0.163298
H	3.046269	1.61324	1.084916
H	2.74967	1.753729	-0.66893
H	3.786259	-1.46086	-1.29146
H	-1.8671	2.296228	-1.04468
H	-1.30973	0.643958	-1.32293
H	-2.18053	1.646284	1.422071
H	-1.13652	-0.46931	1.660507
H	-2.8769	-0.69489	1.766383
H	-0.87193	-2.79442	-1.23069
H	1.196468	-2.63385	-0.16594
H	0.539456	-1.7794	1.211847
H	-3.94818	-2.4082	0.198672

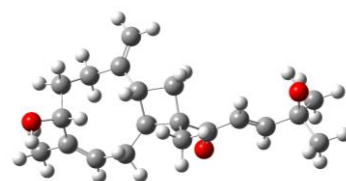
	Coordinates (Å)		
	X	Y	Z
H	-3.86607	-1.19593	-1.0605
H	-3.14577	-2.78827	-1.33785
H	1.374321	3.528789	-0.07318
H	-0.32232	3.910866	-0.69298
H	2.691852	-0.92399	2.052188
H	3.335555	-2.17424	0.979224
H	4.329376	-0.76409	1.393409
H	-3.74933	0.880025	-0.76091



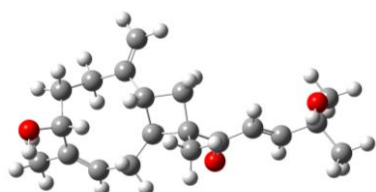
1-5R-conf. 1 (6.76%)



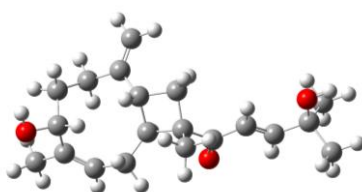
1-5R-conf. 2 (7.53%)



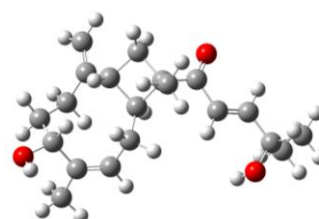
1-5R-conf. 3 (18.00%)



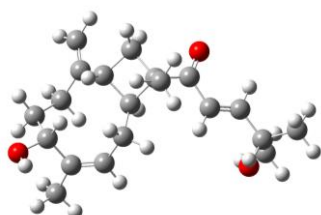
1-5R-conf. 4 (11.38%)



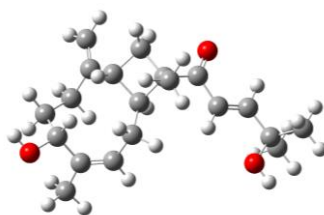
1-5R-conf. 7 (2.70%)



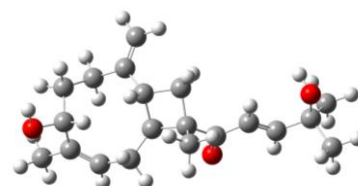
1-5R-conf. 8 (9.38%)



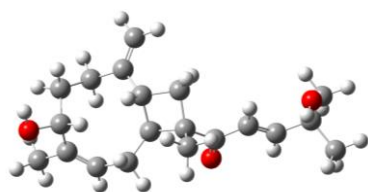
1-5R-conf. 9 (8.18%)



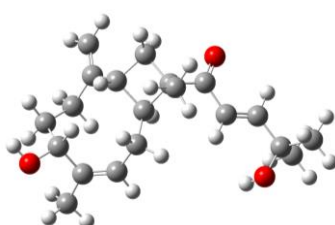
1-5R-conf. 10 (4.60%)



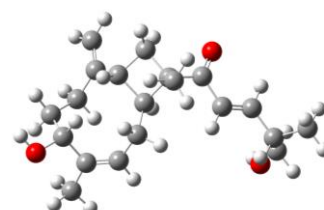
1-5R-conf. 17 (7.61%)



1-5R-conf. 18 (4.70%)

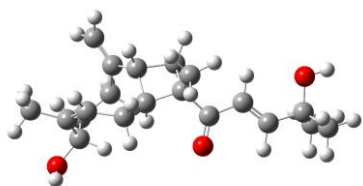


1-5R-conf. 24 (4.17%)

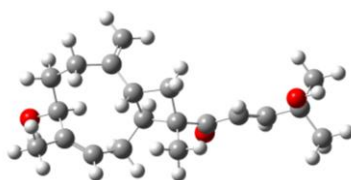


1-5R-conf. 26 (3.39%)

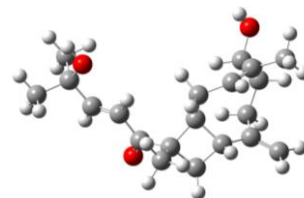
Figure S51. The cartesian coordinates of the dominant conformers for 1-5R



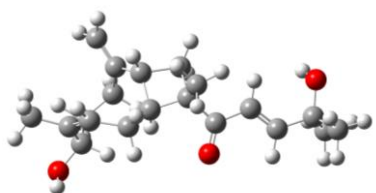
1-5*S*-conf. 1 (7.92%)



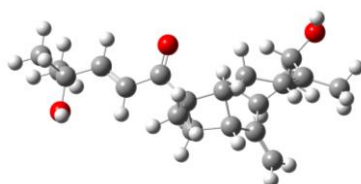
1-5*S*-conf. 2 (4.75%)



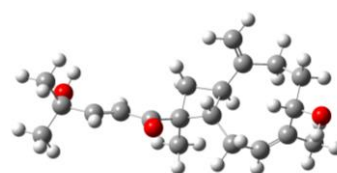
1-5*S*-conf. 3 (4.70%)



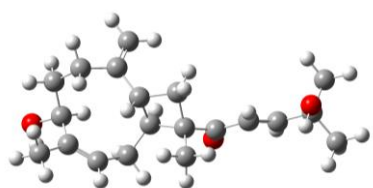
1-5*S*-conf. 4 (9.97%)



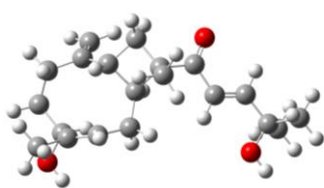
1-5*S*-conf. 5 (11.52%)



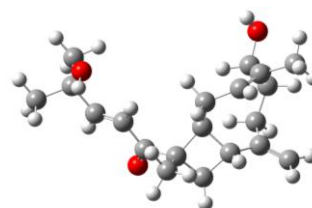
1-5*S*-conf. 6 (8.48%)



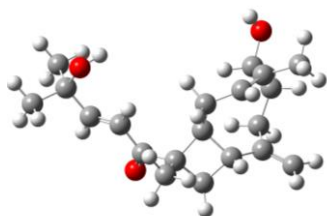
1-5*S*-conf. 7 (6.33%)



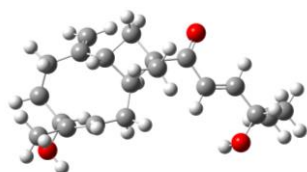
1-5*S*-conf. 8 (3.41%)



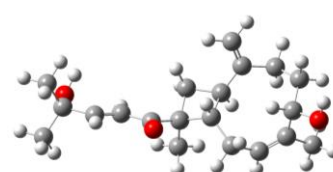
1-5*S*-conf. 13 (5.17%)



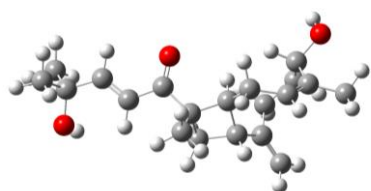
1-5*S*-conf. 16 (8.34%)



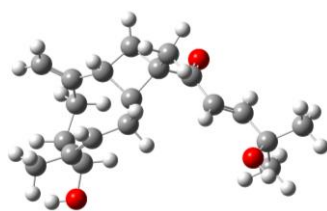
1-5*S*-conf. 27 (3.53%)



1-5*S*-conf. 34 (2.48%)

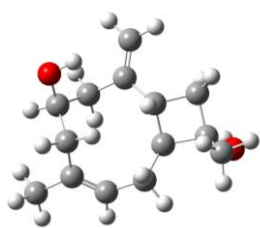


1-5S-conf. 38 (2.47%)

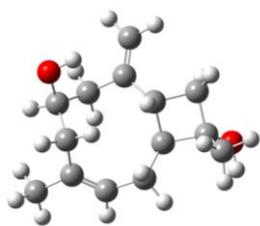


1-5S-conf. 39 (2.16%)

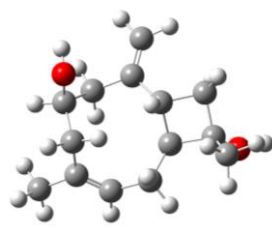
Figure S52. The cartesian coordinates of the dominant conformers for **1-5S**



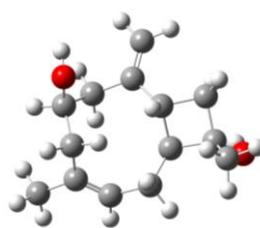
6-6R-conf. 1 (32.89%)



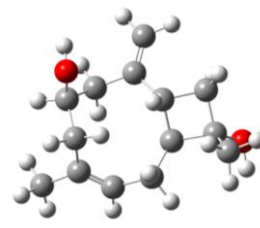
6-6R-conf. 2 (22.42%)



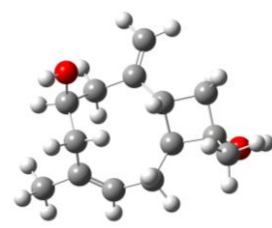
6-6R-conf. 3 (10.52%)



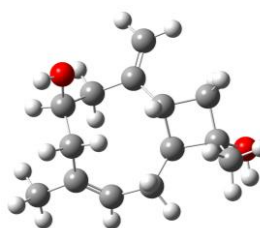
6-6R-conf. 4 (14.07%)



6-6R-conf. 5 (9.87%)

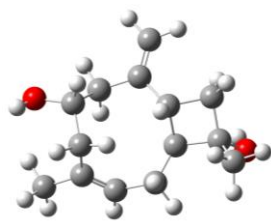


6-6R-conf. 6 (2.92%)

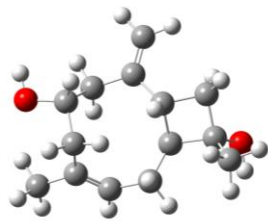


6-6R-conf. 10 (2.76%)

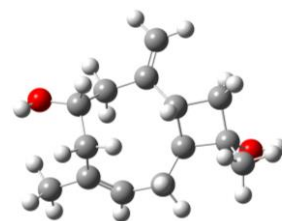
Figure S53. The cartesian coordinates of the dominant conformers for **6-6R**



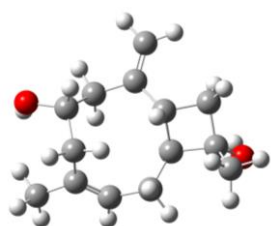
6-6*S*-conf. 1 (41.31%)



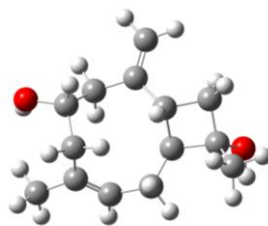
6-6*S*-conf. 2 (15.06%)



6-6*S*-conf. 3 (26.09%)



6-6*S*-conf. 4 (8.51%)



6-6*S*-conf. 5 (5.45%)

Figure S54. The cartesian coordinates of the dominant conformers for **6-6*S***

Functional		Solvent?		Basis Set		Type of Data	
mPW1PW91		PCM		6-31+G(d,p)		Unscaled Shifts	
		DP4+	100.00%	0.00%	-	-	-
Nuclei	sp2?	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5
C		46.4	43.4	44.5			
C		30.2	27.4	22.5			
C	x	125.5	128.6	128.5			
C	x	140.3	145.3	146.9			
C		70.1	68.8	68.7			
C		34.9	32.0	33.8			
C		33.2	31.3	28.5			
C		155	162.2	159.8			
C		42.7	39.6	38.2			
C		35.7	31.1	31.6			
C		48	46.9	49.6			
C	x	206	208.49	209.21			
C	x	121.5	119.82	119.94			
C	x	155.6	161.90	161.48			
C		71.5	71.97	71.96			
C		29.3	24.24	24.40			
C		29.3	24.44	24.36			
C		18.2	13.71	12.69			
C	x	110.6	109.78	111.32			
C		16.1	13.59	13.43			
H		2.07	2.17	2.82			
H		2.31	2.42	2.46			
H		2.14	2.35	2.40			
H		5.59	6.20	5.98			
H		4.75	4.98	4.78			
H		1.73	1.87	1.94			
H		1.57	1.65	1.97			
H		2.19	2.02	2.17			
H		1.87	2.29	2.41			
H		2.87	2.89	2.59			
H		2.11	2.25	1.95			
H		2.11	2.14	1.84			
H		6.48	6.83	6.81			
H		6.94	7.85	7.85			
H		1.32	1.39	1.27			
H		1.32	1.24	1.29			
H		1.33	1.41	1.42			
H		4.78	5.21	5.286			
H		4.54	4.87	5.28			
H		1.64	1.59	1.78			
Functional		Solvent?		Basis Set		Type of Data	
mPW1PW91		PCM		6-31+G(d,p)		Unscaled Shifts	
		Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6
sDP4+ (H data)		100.00%	0.00%	-	-	-	-
sDP4+ (C data)		97.89%	2.11%	-	-	-	-
sDP4+ (all data)		100.00%	0.00%	-	-	-	-
uDP4+ (H data)		100.00%	0.00%	-	-	-	-
uDP4+ (C data)		88.17%	11.83%	-	-	-	-
uDP4+ (all data)		100.00%	0.00%	-	-	-	-
DP4+ (H data)		100.00%	0.00%	-	-	-	-
DP4+ (C data)		99.71%	0.29%	-	-	-	-
DP4+ (all data)		100.00%	0.00%	-	-	-	-

Figure S55. DP4+ results obtained using experimental data of compound **1** *versus* isomers 1 and 2

Functional		Solvent?	Basis Set		Type of Data		
mPW1PW91		PCM	6-31+G(d,p)		Unscaled Shifts		
		DP4+	99.07%	0.93%	-	-	-
Nuclei	sp2?	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5
C		57.7	51.7	52.1			
C		26.4	26.4	26.4			
C	x	125.7	128.5	128.6			
C	x	139.5	143.0	142.4			
C		37.4	37.4	36.5			
C		69.9	65.4	72.8			
C		33.4	36.7	39.6			
C	x	153.9	156.5	158.9			
C		40.1	37.9	36.6			
C		40.7	40.3	39.1			
C		71.4	69.1	69.2			
C		21.8	16.90	17.01			
C	x	110.9	115.60	111.93			
C		17.1	20.22	23.29			
H		2.36	1.95	1.84			
H		2.07	2.17	2.11			
H		2.48	2.27	2.27			
H		5.43	6.07	6.20			
H		1.78	2.38	2.76			
H		4.55	4.11	4.01			
H		2.37	2.36	2.31			
H		1.79	2.71	2.66			
H		1.91	2.47	2.33			
H		1.88	1.77	1.80			
H		1.19	1.17	1.21			
H		4.9	5.26	4.99			
H		1.66	1.81	1.83			

Functional		Solvent?	Basis Set		Type of Data		
mPW1PW91		PCM	6-31+G(d,p)		Unscaled Shifts		
		Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6
sDP4+ (H data)		86.17%	13.83%	-	-	-	-
sDP4+ (C data)		94.08%	5.92%	-	-	-	-
sDP4+ (all data)		99.00%	1.00%	-	-	-	-
uDP4+ (H data)		49.61%	50.39%	-	-	-	-
uDP4+ (C data)		52.20%	47.80%	-	-	-	-
uDP4+ (all data)		51.81%	48.19%	-	-	-	-
DP4+ (H data)		85.99%	14.01%	-	-	-	-
DP4+ (C data)		94.55%	5.45%	-	-	-	-
DP4+ (all data)		99.07%	0.93%	-	-	-	-

Figure S56. DP4+ results obtained using experimental data of compound **6** *versus* isomers 1 and 2