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Electronic Supplementary Information

(*Organic Chemistry Frontiers*)

Commiphorines A and B, unprecedented sesquiterpenoid dimers from *Resina Commiphora* with striking activities on anti-inflammation and lipogenesis inhibition

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1. Computational data of **1**−**4**

1.1 NMR calculation for compounds **1** and **2**

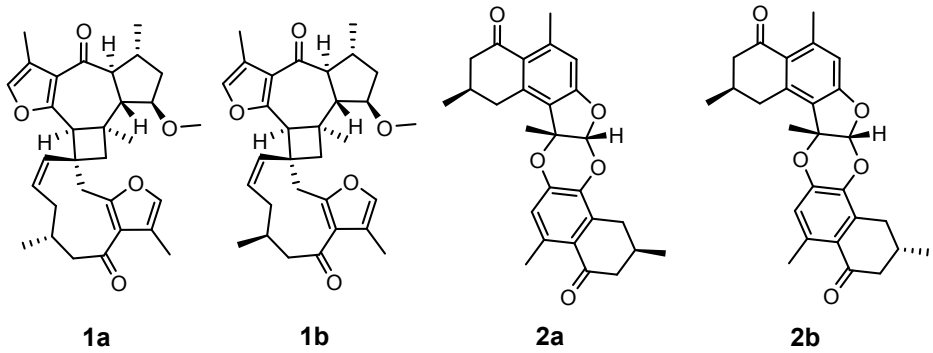


Figure S1. Four model compounds designed for the quantum chemical NMR calculation of compounds **1** and **2**.

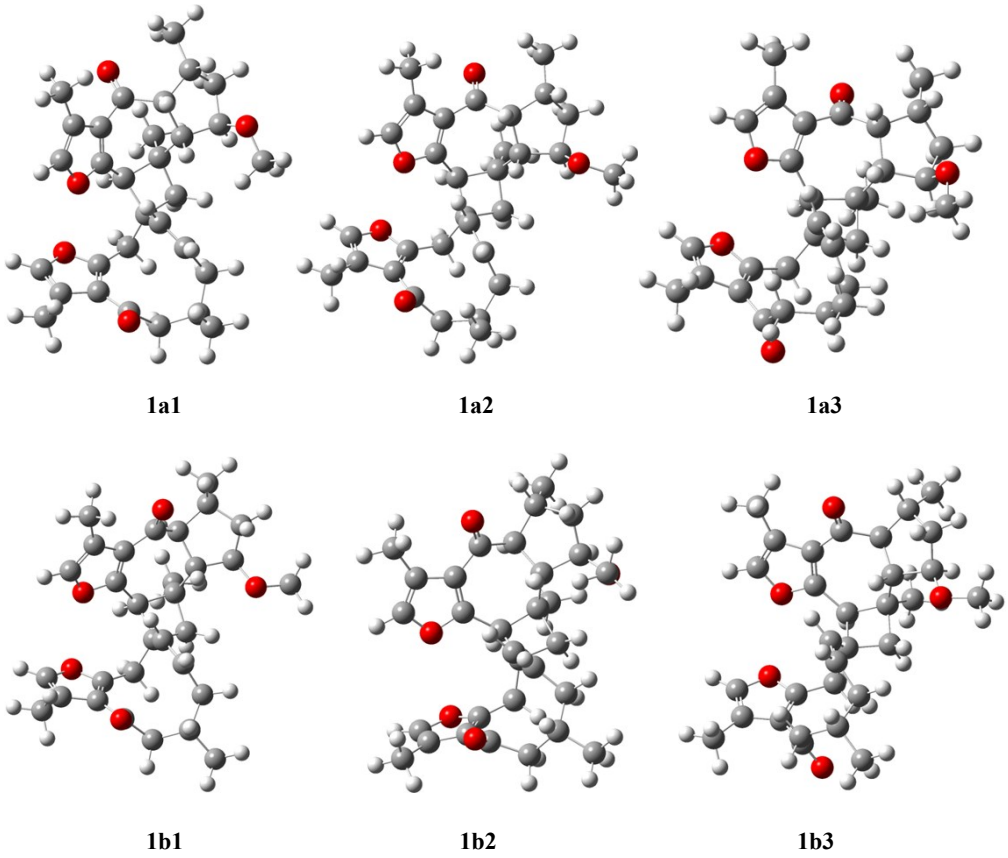
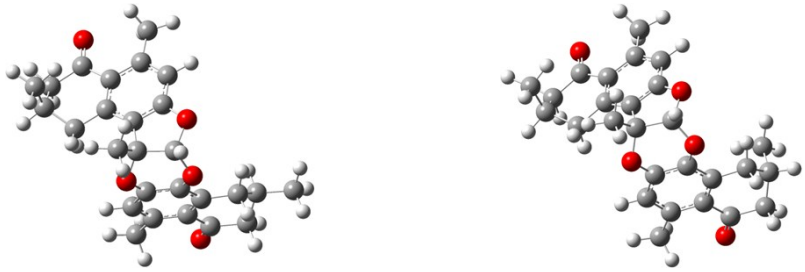


Figure S2. B3LYP/6-31+G(d,p) optimized lowest energy conformers for **1a** and **1b**.



2a **2b**

Figure S3. B3LYP/6-31+G(d,p) optimized lowest energy conformers for **2a** and **2b**.

Table S1. Extracted heats and weighting factors of the optimized conformers of **1a**, **1b**, **2a** and **2b** at B3LYP/6-31+G(d,p) level

		B3LYP/6-31+G(d,p)	
	Conformer	Extracted heats	Boltzmann-calculated contribution (%)
1a	1	-1580.2233480	52.46%
	2	-1580.2231462	42.36%
	3	-1580.2211634	5.18%
1b	1	-1580.2674452	47.66%
	2	-1580.2671938	36.54%
	3	-1580.2664053	15.8%
2a	1	-1421.9029575	100%
2b	1	-1421.9007865	100%

Table S2. The Cartesian coordinates of the lowest energy conformers for **1a, 1b**, **2a**, and **2b**

1a1	X axis(Å)	Y axis(Å)	Z axis(Å)	**1a2**	X axis(Å)	Y axis(Å)	Z axis(Å)
C	1.226308	2.041557	-0.46275	C	1.232369	1.922932	-0.46437
C	0.410056	3.227693	-1.04949	C	0.370462	3.119203	-0.95235
C	-0.56967	2.874926	-2.17199	C	-0.59892	2.813631	-2.09465
C	-1.59549	1.907679	-1.82724	C	-1.64713	1.861419	-1.77933
C	-1.35903	0.597407	-1.46883	C	-1.43674	0.540791	-1.44289
C	0.015617	-0.12543	-1.51281	C	-0.07722	-0.20901	-1.50098
C	1.307983	0.751884	-1.32875	C	1.23623	0.642952	-1.34823
C	2.625058	2.628145	-0.16423	C	2.657973	2.496307	-0.27462
C	2.79016	3.765269	-1.16806	C	2.719614	3.695006	-1.21872
C	1.40436	4.40064	-1.23477	C	1.335775	4.321071	-1.08093
C	-3.0141	2.081771	-1.80728	C	-3.06165	2.063072	-1.76192
C	-3.52629	0.871298	-1.39138	C	-3.59863	0.855634	-1.36878
O	-2.53373	-0.02769	-1.18779	O	-2.62454	-0.06611	-1.17727
C	1.25793	5.318373	-2.43759	C	1.065462	5.376383	-2.14076
O	2.653196	3.208233	1.145711	O	2.767241	2.923424	1.089106
C	2.941798	2.266234	2.170668	C	4.113206	3.079641	1.519543
C	2.061619	0.919173	-2.65699	C	1.945082	0.803445	-2.70296
C	-3.77183	3.307937	-2.15338	C	-3.7936	3.310191	-2.0873
C	0.972706	-3.37601	3.214118	C	0.909989	-3.44283	3.22791

C	0.11118	-4.28051	2.313059	C	0.013507	-4.33732	2.351562
C	-1.30041	-3.80217	1.99491	C	-1.39582	-3.83625	2.059397
C	-0.13811	-0.65552	1.048131	C	-0.18878	-0.71908	1.061418
C	-1.71989	-3.62812	0.601783	C	-1.84114	-3.66223	0.674092
C	-0.98826	-3.11866	-0.46262	C	-1.12241	-3.17548	-0.40962
C	0.367291	-2.5316	-0.63082	C	0.241014	-2.61799	-0.61175
C	0.447649	-1.02447	-0.29397	C	0.36153	-1.11075	-0.2885
C	-3.0266	-3.90809	0.066077	C	-3.16457	-3.91935	0.168368
C	-2.9619	-3.60046	-1.2745	C	-3.12237	-3.62309	-1.17561
O	-1.73499	-3.13852	-1.60191	O	-1.8936	-3.18912	-1.53271
C	-4.20832	-4.42631	0.799546	C	-4.34059	-4.40793	0.930742
O	-0.56939	3.404295	-3.27688	O	-0.56204	3.356494	-3.19242
C	0.365557	-3.17547	4.606908	C	0.333451	-3.21727	4.629816
C	1.890135	-0.45645	-0.51944	C	1.812959	-0.57802	-0.55394
O	-2.11583	-3.66384	2.908936	O	-2.19073	-3.6821	2.988957
H	0.045809	-0.69276	-2.4563	H	-0.07547	-0.78322	-2.44105
H	-0.25929	3.573852	-0.24352	H	-0.29912	3.395235	-0.12074
H	0.744963	1.785955	0.487464	H	0.84544	1.653708	0.526284
C	0.285052	-1.10418	2.240078	C	0.25029	-1.16588	2.248144
C	1.406228	-2.04397	2.566543	C	1.358113	-2.12612	2.559387
H	3.448246	1.912754	-0.26342	H	3.444019	1.764102	-0.48538
H	3.091958	3.391189	-2.15053	H	2.897153	3.375628	-2.25046
H	3.538012	4.496199	-0.84093	H	3.498052	4.414134	-0.94748
H	1.301439	5.043142	-0.34711	H	1.312178	4.847891	-0.11476
H	-4.52771	0.503865	-1.21341	H	-4.60752	0.504788	-1.19988
H	0.25492	5.754312	-2.48074	H	0.039343	5.75079	-2.07085
H	1.971887	6.146965	-2.3692	H	1.738204	6.230128	-2.00118
H	1.463461	4.797084	-3.37769	H	1.240571	4.99868	-3.1526
H	2.96984	2.798613	3.12522	H	4.102076	3.413569	2.56059
H	2.167907	1.497429	2.228611	H	4.642219	2.123126	1.46887
H	3.919484	1.80463	2.002769	H	4.635699	3.830334	0.921007
H	1.623527	1.703099	-3.27955	H	1.486946	1.586073	-3.31223
H	3.116815	1.156595	-2.49178	H	3.005837	1.041094	-2.58066
H	2.046734	-0.00463	-3.24739	H	1.906795	-0.1226	-3.28878
H	-3.66395	3.534931	-3.21874	H	-3.66866	3.560749	-3.14549
H	-4.8386	3.190271	-1.93729	H	-4.86486	3.206355	-1.88691
H	-3.40318	4.163058	-1.57779	H	-3.41707	4.144598	-1.48693
H	1.904999	-3.93576	3.38052	H	1.833725	-4.02002	3.381972
H	-0.01603	-5.2509	2.813878	H	-0.12069	-5.30164	2.862265
H	0.651193	-4.52332	1.394801	H	0.529596	-4.59698	1.424241
H	-1.00225	0.007591	1.049745	H	-1.03508	-0.03366	1.075261
H	1.094927	-3.09344	-0.04391	H	0.969558	-3.19098	-0.03684
H	0.691246	-2.69806	-1.66803	H	0.538261	-2.79885	-1.65455

H	-3.67478	-3.64359	-2.08628	H	-3.85316	-3.65756	-1.97166
H	-4.58846	-3.67042	1.493926	H	-4.68938	-3.64007	1.62842
H	-5.01768	-4.68999	0.110815	H	-5.17029	-4.65833	0.261523
H	-3.94722	-5.32427	1.368493	H	-4.08617	-5.30794	1.499481
H	1.078265	-2.66501	5.263957	H	1.068432	-2.71512	5.26846
H	0.126249	-4.1402	5.066854	H	0.083779	-4.17274	5.103413
H	-0.54845	-2.57611	4.585234	H	-0.56877	-2.6	4.61939
H	2.536019	-1.12047	-1.11071	H	2.427285	-1.25613	-1.16232
H	2.457605	-0.20169	0.381396	H	2.409594	-0.33283	0.331768
H	-0.26347	-0.7366	3.109942	H	-0.26748	-0.77458	3.126292
H	2.020728	-2.25875	1.688409	H	1.949055	-2.3618	1.670487
H	2.078784	-1.52061	3.259269	H	2.056139	-1.61159	3.233213
1a3	X axis(Å)	Y axis(Å)	Z axis(Å)	**1b1**	X axis(Å)	Y axis(Å)	Z axis(Å)
C	1.238101	1.979765	-0.58157	C	1.846065	-1.04219	-1.26581
C	0.493772	3.228282	-1.13398	C	2.743589	-0.11063	-2.09512
C	-0.48941	2.968652	-2.27818	C	2.928941	1.191086	-1.33374
C	-1.5802	2.061103	-1.97273	C	1.775883	2.080598	-1.20203
C	-1.43442	0.729836	-1.64372	C	0.421102	1.777211	-1.28249
C	-0.10856	-0.08018	-1.69043	C	-0.35116	0.418953	-1.45651
C	1.235764	0.709307	-1.47938	C	0.376637	-0.93898	-1.71605
C	2.672875	2.470617	-0.27776	C	2.474118	-2.43681	-1.41251
C	2.898875	3.628055	-1.24617	C	3.965689	-2.1183	-1.44774
C	1.5542	4.348186	-1.27287	C	4.062984	-0.88288	-2.341
C	-2.98484	2.325839	-1.97251	C	1.844831	3.497861	-0.93507
C	-3.58108	1.141192	-1.59661	C	0.545397	3.943546	-0.91614
O	-2.65207	0.175591	-1.39764	O	-0.3072	2.924641	-1.1364
C	1.455024	5.328597	-2.43013	C	4.208442	-1.26841	-3.81555
O	2.745508	3.006043	1.049806	O	2.126084	-3.24321	-0.29444
C	2.996011	2.017075	2.039749	C	2.544523	-4.59519	-0.42258
C	2.004531	0.860005	-2.80164	C	0.100211	-1.45445	-3.14077
C	-3.65578	3.605846	-2.30266	C	3.061137	4.325598	-0.73116
C	0.702912	-3.1608	3.403863	C	-2.5345	-1.2575	3.682933
C	-0.60796	-3.85867	2.989298	C	-3.59653	-0.29444	3.121997
C	-0.51245	-4.43705	1.593112	C	-3.11544	1.140179	2.967595
C	-0.31465	-0.64203	0.857923	C	-0.34001	0.143416	1.154264
C	-1.48373	-3.98492	0.613803	C	-3.24133	1.818106	1.675975
C	-1.16735	-3.1615	-0.44938	C	-3.02052	1.298195	0.407131
C	0.104234	-2.52629	-0.87323	C	-2.55521	-0.00618	-0.13673
C	0.257028	-1.03463	-0.48859	C	-1.01936	-0.1884	-0.15352
C	-2.8897	-4.22053	0.530796	C	-3.57262	3.203016	1.4698
C	-3.30825	-3.54147	-0.59653	C	-3.58671	3.390429	0.105774
O	-2.27126	-2.90606	-1.19734	O	-3.2712	2.245551	-0.53955
C	-3.72512	-5.03271	1.4461	C	-3.85072	4.225523	2.508806

O	-0.43913	3.525648	-3.36822	O	4.026402	1.517075	-0.88346
C	0.566095	-2.62652	4.834333	C	-3.22501	-2.53751	4.169927
C	1.734853	-0.55291	-0.69917	C	-0.62225	-1.59262	-0.71321
O	0.388904	-5.21606	1.287741	O	-2.70872	1.7508	3.958812
H	-0.107	-0.6232	-2.64836	H	-1.10865	0.605721	-2.23478
H	-0.16423	3.584845	-0.32337	H	2.307722	0.172313	-3.05945
H	0.747389	1.731865	0.365833	H	1.908411	-0.76577	-0.20367
C	0.102555	-1.05941	2.064151	C	-0.54223	-0.48155	2.324304
C	1.171269	-2.04995	2.427123	C	-1.44085	-1.63315	2.660333
H	3.450236	1.710183	-0.40685	H	2.17051	-2.93412	-2.33821
H	3.165356	3.268716	-2.24433	H	4.561771	-2.95926	-1.81665
H	3.69402	4.299991	-0.90456	H	4.327324	-1.89051	-0.43668
H	1.493731	4.953491	-0.35562	H	4.955502	-0.30873	-2.07116
H	-4.60735	0.834625	-1.44784	H	0.087701	4.911037	-0.76267
H	0.474654	5.814765	-2.45167	H	4.277895	-0.37178	-4.44058
H	2.209012	6.116552	-2.32238	H	5.118596	-1.85684	-3.97239
H	1.636642	4.844182	-3.39451	H	3.358619	-1.86103	-4.16959
H	3.065727	2.515758	3.010232	H	3.635473	-4.66657	-0.43485
H	2.181344	1.291042	2.084529	H	2.17431	-5.15022	0.443695
H	3.944433	1.508281	1.842934	H	2.12496	-5.04467	-1.32767
H	1.618408	1.683388	-3.40733	H	0.689867	-0.92469	-3.89317
H	3.07167	1.028347	-2.62855	H	0.306457	-2.52474	-3.23163
H	1.935329	-0.04734	-3.41333	H	-0.95358	-1.32352	-3.41554
H	-3.51746	3.846918	-3.36139	H	3.750728	4.213287	-1.57375
H	-4.73105	3.553856	-2.10356	H	2.807582	5.387563	-0.6467
H	-3.24089	4.423135	-1.70405	H	3.57666	4.029549	0.187836
H	1.501222	-3.91564	3.423029	H	-2.05476	-0.79189	4.554387
H	-1.45469	-3.16565	3.054988	H	-4.43717	-0.2339	3.827741
H	-0.82854	-4.68933	3.670772	H	-4.03696	-0.6766	2.199257
H	-1.14849	0.058474	0.846326	H	0.34806	0.986404	1.165924
H	0.935771	-3.099	-0.4456	H	-3.02569	-0.825	0.409963
H	0.21805	-2.66132	-1.95682	H	-2.95122	-0.11775	-1.15614
H	-4.26669	-3.41781	-1.08186	H	-3.78298	4.242991	-0.52938
H	-3.83444	-4.52706	2.410709	H	-2.93845	4.462166	3.065407
H	-4.72531	-5.19619	1.032054	H	-4.22435	5.15278	2.062149
H	-3.26787	-6.01219	1.618976	H	-4.60665	3.864994	3.21366
H	1.496202	-2.15176	5.16395	H	-3.97259	-2.31001	4.937291
H	0.347047	-3.44364	5.530264	H	-3.72947	-3.05415	3.3462
H	-0.24055	-1.89158	4.91936	H	-2.49905	-3.22886	4.610952
H	2.339246	-1.24047	-1.30758	H	-1.45437	-2.12754	-1.19161
H	2.315783	-0.36059	0.208476	H	-0.18883	-2.29243	0.007482
H	-0.41737	-0.62361	2.918883	H	0.025312	-0.10102	3.177007
H	1.591489	-2.52045	1.535209	H	-1.89538	-2.07884	1.771713

H	2.002627	-1.49953	2.88565	H	-0.80377	-2.41775	3.089509
1b2	X axis(Å)	Y axis(Å)	Z axis(Å)	**1b3**	X axis(Å)	Y axis(Å)	Z axis(Å)
C	1.870208	-1.0644	-1.33183	C	1.793549	-1.08521	-1.29101
C	2.748812	-0.10393	-2.15312	C	2.816221	-0.24781	-2.07339
C	2.867199	1.203839	-1.38946	C	3.038119	1.061486	-1.33466
C	1.682784	2.0559	-1.30294	C	1.957353	2.045481	-1.34709
C	0.341636	1.702076	-1.40437	C	0.592106	1.841837	-1.51283
C	-0.37658	0.312642	-1.56477	C	-0.26879	0.536845	-1.66187
C	0.406247	-1.01821	-1.80902	C	0.369161	-0.8785	-1.84169
C	2.561082	-2.42963	-1.4697	C	2.317967	-2.52701	-1.36765
C	4.043432	-2.0643	-1.48049	C	3.828675	-2.32556	-1.29513
C	4.104782	-0.82402	-2.37461	C	4.090009	-1.11949	-2.19592
C	1.6966	3.478985	-1.06376	C	2.123017	3.467554	-1.16597
C	0.382036	3.878299	-1.08052	C	0.866684	4.012279	-1.27997
O	-0.42966	2.825207	-1.29607	O	-0.04905	3.048902	-1.49969
C	4.297684	-1.19932	-3.84608	C	4.326751	-1.5466	-3.64691
O	2.16951	-3.39699	-0.50696	O	1.829085	-3.278	-0.26386
C	2.626772	-3.21946	0.824524	C	2.1277	-4.66458	-0.35023
C	0.17287	-1.55143	-3.23431	C	0.148473	-1.41224	-3.26948
C	2.879133	4.352489	-0.85272	C	3.386067	4.209887	-0.92241
C	-2.46887	-1.44646	3.584532	C	-2.34916	-1.09711	3.737029
C	-3.56574	-0.51497	3.036715	C	-3.0909	0.256049	3.719552
C	-3.13051	0.934541	2.885647	C	-3.90627	0.488853	2.46133
C	-0.34499	0.04332	1.04768	C	-0.35386	0.326588	0.954102
C	-3.2903	1.615701	1.599609	C	-3.55348	1.630001	1.634627
C	-3.06342	1.110893	0.325683	C	-2.97786	1.519785	0.383208
C	-2.56179	-0.17487	-0.23034	C	-2.54865	0.345484	-0.41711
C	-1.02129	-0.31027	-0.25669	C	-1.03371	0.02794	-0.36696
C	-3.66749	2.990461	1.405122	C	-3.67263	3.029202	1.896729
C	-3.69818	3.185938	0.042492	C	-3.18239	3.655681	0.768157
O	-3.35082	2.055956	-0.61262	O	-2.76839	2.749851	-0.1523
C	-3.97041	3.996899	2.452876	C	-4.2203	3.67767	3.111193
O	3.932742	1.556764	-0.88644	O	4.10866	1.313883	-0.78383
C	-3.11355	-2.75196	4.066472	C	-3.29788	-2.26193	4.0391
C	-0.58489	-1.70243	-0.81876	C	-0.74635	-1.41893	-0.89496
O	-2.72814	1.550688	3.875201	O	-4.80908	-0.27692	2.130139
H	-1.14013	0.460075	-2.34562	H	-0.97602	0.743154	-2.48138
H	2.318938	0.158428	-3.1259	H	2.475358	0.032221	-3.07608
H	1.902405	-0.76818	-0.27754	H	1.810285	-0.78944	-0.23306
C	-0.51434	-0.5937	2.216524	C	-0.56468	-0.30483	2.120131
C	-1.36937	-1.77845	2.552959	C	-1.53126	-1.40195	2.459451
H	2.326274	-2.88009	-2.43825	H	2.045235	-3.01943	-2.30557
H	4.667336	-2.89217	-1.83257	H	4.382223	-3.21786	-1.60499

H	4.39843	-1.79994	-0.47802	H	4.131096	-2.10587	-0.26302
H	4.966341	-0.212	-2.08716	H	4.997313	-0.60565	-1.86141
H	-0.11261	4.831829	-0.95688	H	0.48017	5.020776	-1.229
H	4.347718	-0.29848	-4.46692	H	4.511851	-0.67123	-4.27847
H	5.232635	-1.75269	-3.98338	H	5.201375	-2.20171	-3.71839
H	3.479172	-1.82151	-4.22202	H	3.467512	-2.08501	-4.06006
H	2.106863	-3.94464	1.457236	H	3.206624	-4.83524	-0.3029
H	3.697825	-3.42809	0.893056	H	1.662868	-5.16729	0.502272
H	2.406834	-2.22023	1.206149	H	1.716638	-5.09065	-1.27042
H	0.758192	-1.00729	-3.9798	H	0.830282	-0.95506	-3.99099
H	0.416652	-2.61496	-3.31288	H	0.270761	-2.49805	-3.31908
H	-0.87948	-1.45777	-3.52891	H	-0.86942	-1.20483	-3.62146
H	3.595429	4.237982	-1.67243	H	4.125994	3.977662	-1.69489
H	2.589012	5.407454	-0.80772	H	3.218087	5.291904	-0.93539
H	3.378166	4.100785	0.088334	H	3.802963	3.94634	0.054677
H	-1.99946	-0.97125	4.456427	H	-1.64473	-1.04963	4.579959
H	-4.40217	-0.48441	3.749303	H	-2.36103	1.06708	3.831659
H	-4.00055	-0.9065	2.115254	H	-3.76909	0.338439	4.577296
H	0.303088	0.917628	1.057847	H	0.376923	1.132489	0.962613
H	-3.0034	-1.01116	0.314224	H	-3.11261	-0.52862	-0.06876
H	-2.96031	-0.29189	-1.24809	H	-2.88191	0.485555	-1.45345
H	-3.92698	4.03561	-0.58568	H	-3.0664	4.691116	0.479016
H	-3.06158	4.260801	3.002818	H	-3.52069	3.573058	3.946448
H	-4.37909	4.913645	2.015314	H	-4.39677	4.74549	2.946287
H	-4.70731	3.606922	3.162197	H	-5.17231	3.219706	3.398077
H	-3.86351	-2.55467	4.83984	H	-3.87781	-2.06863	4.947551
H	-3.60569	-3.27935	3.242107	H	-3.99786	-2.44373	3.218332
H	-2.36234	-3.42187	4.498205	H	-2.73058	-3.18539	4.199072
H	-1.39975	-2.25397	-1.308	H	-1.59816	-1.87143	-1.4219
H	-0.14106	-2.39579	-0.09876	H	-0.42997	-2.15311	-0.14853
H	0.03807	-0.19089	3.069004	H	0.050702	0.023297	2.960004
H	-1.81516	-2.23482	1.665374	H	-2.2051	-1.62221	1.627973
H	-0.702	-2.54232	2.973384	H	-0.94871	-2.31682	2.628148
2a	X axis(Å)	Y axis(Å)	Z axis(Å)	**2b**	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-2.92642	3.835293	-0.81698	C	-2.8583	3.72255	-0.72111
C	-3.57289	2.794044	0.08324	C	-3.47446	2.691931	0.212003
C	-2.58516	1.658709	0.34205	C	-2.47363	1.566064	0.461636
C	-1.24382	2.135291	0.835223	C	-1.12237	2.057444	0.911249
C	-0.75784	3.43832	0.551219	C	-0.65165	3.358468	0.594325
C	-1.61709	4.360594	-0.27163	C	-1.53794	4.263287	-0.21916
C	-0.41451	1.272289	1.554342	C	-0.26914	1.210154	1.620929
C	0.835509	1.689824	1.999215	C	0.990006	1.641123	2.025501
C	1.309606	2.961529	1.775574	C	1.450651	2.911697	1.769731

C	0.517039	3.857817	1.037564	C	0.633421	3.792209	1.039665
C	-0.61162	-0.13361	2.048614	C	-0.44455	-0.18915	2.141482
C	0.87025	-0.50422	2.2821	C	1.045196	-0.54819	2.339619
O	1.536741	0.726037	2.687705	O	1.715021	0.691607	2.709238
O	-1.34123	-0.98291	1.175128	O	-1.19238	-1.05627	1.301649
C	-1.37425	-0.10312	3.383087	C	-1.17059	-0.14244	3.495737
O	1.560657	-1.0256	1.141326	O	1.707919	-1.08205	1.188253
C	0.729994	-3.359	-1.5559	C	0.817898	-3.43192	-1.47502
C	1.469334	-2.54005	-0.67004	C	1.57613	-2.60583	-0.61265
C	0.790174	-1.76111	0.289653	C	0.918573	-1.82607	0.361614
C	-0.59653	-1.73955	0.32411	C	-0.46667	-1.81288	0.434402
C	-1.32408	-2.52389	-0.56716	C	-1.21345	-2.60729	-0.4314
C	-0.68296	-3.34369	-1.5109	C	-0.5934	-3.42697	-1.38912
O	-1.26351	5.502854	-0.5521	O	-1.19865	5.402994	-0.52638
C	1.080596	5.233878	0.791481	C	1.182303	5.167241	0.75733
C	-4.10937	3.405663	1.382071	C	-3.97956	3.320727	1.515206
C	-1.55226	-4.16649	-2.4251	C	-1.48295	-4.25865	-2.27547
C	1.473652	-4.24674	-2.51567	C	1.538773	-4.307	-2.46284
C	2.985057	-4.22963	-2.4955	C	3.050783	-4.28704	-2.48559
C	3.529636	-2.87288	-2.07806	C	3.64056	-2.95543	-2.0492
C	2.981951	-2.51767	-0.6978	C	3.087133	-2.57716	-0.67716
C	5.056761	-2.87863	-2.07252	H	4.727142	-3.08001	-1.95166
O	0.888376	-5.02093	-3.26849	O	0.935479	-5.07388	-3.20911
H	0.98257	-1.23497	3.092529	H	1.183801	-1.26658	3.15697
H	-2.724	3.413709	-1.80886	H	-2.67999	3.286721	-1.71147
H	-3.60954	4.682608	-0.94978	H	-3.54962	4.564014	-0.84858
H	-4.43751	2.374124	-0.44757	H	-4.35052	2.2592	-0.28893
H	-3.0388	0.967041	1.059658	H	-2.90385	0.883156	1.20171
H	2.287973	3.245806	2.151839	H	2.437153	3.206933	2.115035
H	-2.39758	0.264775	3.245703	H	-2.19944	0.217679	3.380832
H	-1.46237	-1.11584	3.793516	H	-1.2415	-1.14923	3.923726
H	-0.88919	0.529318	4.134932	H	-0.66896	0.504089	4.22436
H	-2.41167	-2.49352	-0.52121	H	-2.2995	-2.58397	-0.35506
H	2.060057	5.356821	1.267528	H	2.17351	5.302724	1.204803
H	1.225135	5.40405	-0.27984	H	1.296977	5.321524	-0.32
H	0.425479	5.999733	1.218045	H	0.534556	5.936155	1.189608
H	-4.84783	4.184314	1.1629	H	-4.7281	4.091919	1.303984
H	-3.31946	3.856618	1.990546	H	-3.17628	3.785285	2.095289
H	-4.60442	2.641152	1.990491	H	-4.45375	2.563098	2.148345
H	-2.61623	-3.9687	-2.25242	H	-2.5428	-4.07887	-2.06249
H	-1.35307	-3.91854	-3.47232	H	-1.32599	-4.00226	-3.32782
H	-1.39426	-5.23462	-2.24691	H	-1.30247	-5.32513	-2.10905
H	3.337496	-4.46596	-3.50673	H	3.383326	-4.52225	-3.50355

H	3.324591	-5.02582	-1.82262	H	3.398301	-5.09277	-1.8278
H	3.19198	-2.11646	-2.80028	C	3.41669	-1.85491	-3.09206
H	3.350877	-1.5183	-0.43645	H	3.46798	-1.58223	-0.41665
H	3.352739	-3.21815	0.061314	H	3.46674	-3.27801	0.077638
H	5.447508	-1.89636	-1.78677	H	3.882971	-0.91827	-2.7681
H	5.447432	-3.11811	-3.06713	H	2.355525	-1.65582	-3.27042
H	5.450854	-3.61807	-1.36702	H	3.868716	-2.13627	-4.04925
H	-2.42057	1.100922	-0.58892	H	-2.33078	0.994826	-0.46475

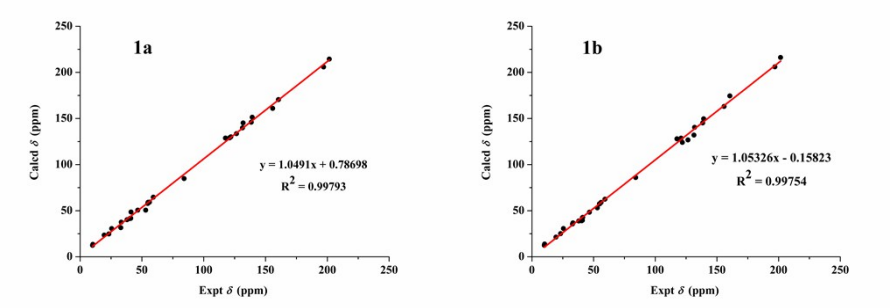


Figure S4. Correlation plots of experimental ^{13}C NMR chemical shifts versus corresponding calculated ^{13}C NMR chemical shifts for **1**.

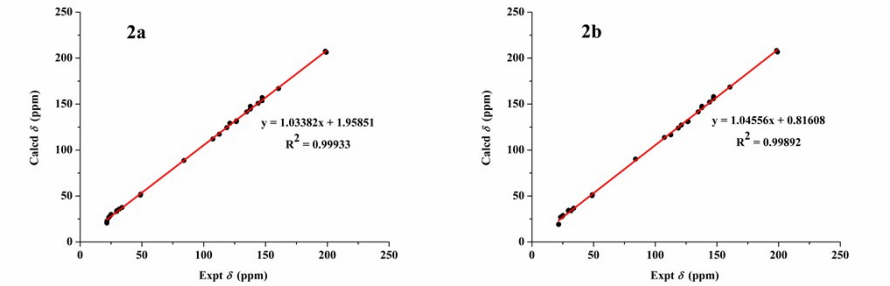


Figure S5. Correlation plots of experimental ^{13}C NMR chemical shifts versus corresponding calculated ^{13}C NMR chemical shifts for **2**.

Table S3. DP4+ analysis results of **1a** (isomer1**)** and **1b** (Isomer 2)

Functional	Solvent?	Basis Set	Type of Data
mPW1PW91	PCM	6-311+G(d,p)	Unscaled Shifts

		DP4+	100.00%	0.00%	-	-	-
Nuclei	sp2?	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5
C	x	201.59	214.4	216.2			
C	x	196.98	205.9	206.0			
C	x	160.47	170.5	174.5			
C	x	155.84	160.9	163.0			
C	x	139.26	151.3	149.6			
C	x	138.49	145.9	145.2			
C	x	131.87	145.2	140.4			
C	x	131.36	139.8	132.0			
C	x	126.53	133.5	126.7			
C	x	121.95	130.1	124.1			
C	x	120.93	129.0	128.6			
C	x	117.56	128.72	127.95			
C		84.1	84.87	85.94			
C		59.25	64.61	62.49			
C		56.08	59.24	59.00			
C		54.99	59.08	57.48			
C		54.74	57.86	57.43			
C		53.06	50.62	53.03			
C		46.63	50.57	48.35			
C		41.21	48.55	42.82			
C		40.93	41.93	42.45			
C		40.93	41.72	39.61			
C		40.3	41.45	39.03			
C		37.95	40.23	38.79			
C		33.3	37.55	36.78			
C		32.91	31.6	35.57			
C		25.54	30.58	30.66			
C		23.26	24.2	25.12			
C		19.51	23.51	21.31			
C		10.28	13.51	13.8			
C		10.02	12.45	12.44			
H	x	7.13	7.03	7.2			
H	x	7.06	6.92	6.42			
H		4.5	5.75	5.34			
H		4.5	4.53	6.33			
H		3.36	3.84	3.91			
H		3.34	3.58	3.89			
H		3.33	3.43	3.45			
H		3.1	3.38	3.41			
H		3.1	3.28	3.33			
H		3.1	3.27	3.08			
H		2.89	3.02	2.84			
H		2.74	2.94	2.84			
H		2.61	2.92	2.78			
H		2.55	2.76	2.54			
H		2.3	2.76	2.4			
H		2.19	2.46	2.39			
H		2.17	2.36	2.32			
H		2.17	2.34	2.39			
H		2.17	2.2	2.12			
H		2.1	2.15	1.97			
H		2.06	2.13	1.9			
H		2.06	2.04	1.88			
H		2.06	2.01	1.84			
H		2.02	1.98	1.82			
H		1.95	1.93	1.79			
H		1.92	1.91	1.7			
H		1.91	1.86	1.64			
H		1.73	1.83	1.62			
H		1.23	1.69	1.47			
H		1.23	1.57	1.41			
H		1.23	1.45	1.34			
H		1.11	1.22	1.19			
H		1.08	1.19	1.18			
H		1.08	1.18	1.09			
H		1.08	1.07	1.07			
H		1.01	1.03	1.06			
H		1.01	1.02	1.04			
H		1.01	1.02	0.86			

Functional	Solvent?	Basis Set	Type of Data
mPW1PW91	PCM	6-311+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)	96.88%	3.12%	-	-	-	-
sDP4+ (all data)	100.00%	0.00%	-	-	-	-
uDP4+ (H data)	99.80%	0.20%	-	-	-	-
uDP4+ (C data)	100.00%	0.00%	-	-	-	-
uDP4+ (all data)	100.00%	0.00%	-	-	-	-
DP4+ (H data)	100.00%	0.00%	-	-	-	-
DP4+ (C data)	100.00%	0.00%	-	-	-	-
DP4+ (all data)	100.00%	0.00%	-	-	-	-

Table S4. DP4+ analysis results of **2a** (Isomer 1) and **2b** (Isomer 2)

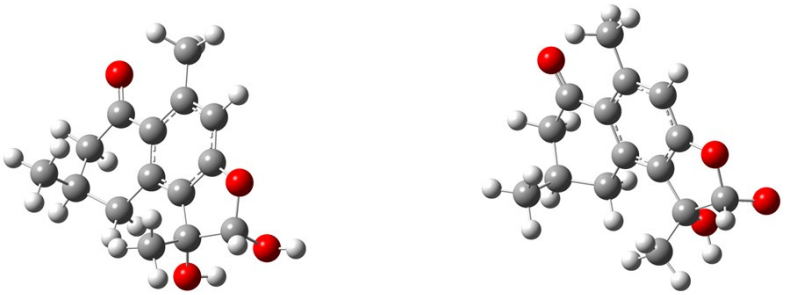
Functional	Solvent?	Basis Set	Type of Data
mPW1PW91	PCM	6-311+G(d,p)	Unscaled Shifts

		DP4+	100.00%	0.00%	-	-	-
Nuclei	sp2?	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5
C	x	198.4	207.5	208.3			
C	x	199.1	206.4	206.6			
C	x	160.5	166.8	168.5			
C	x	147.3	157.1	158.1			
C	x	147.2	153.5	155.7			
C	x	144	150.8	152.1			
C	x	137.8	147.5	147.5			
C	x	137.7	144.5	146.0			
C	x	134.8	141.5	141.5			
C	x	126.6	131.7	131.1			
C	x	126.3	130.9	130.8			
C	x	121.2	129.12	127.26			
C	x	118.7	124.35	123.96			
C	x	112.6	117.27	116.56			
C		107.4	112.00	113.68			
C		84	88.65	90.15			
C		49	51.92	51.43			
C		48.8	50.85	50.34			
C		33.9	37.47	36.74			
C		31.7	35.72	34.00			
C		29.8	34.11	34.44			
C		29.5	33.09	33.88			
C		25.1	29.98	28.83			
C		24.4	28.59	27.58			
C		23.2	26.66	26.91			
C		21.7	22.67	19.24			
C		21.6	20.54	19.01			
H	x	6.53	6.85	6.96			
H	x	6.53	6.66	6.73			
H		5.97	6.01	6.01			
H		3.45	3.43	3.4			
H		3.16	3.3	3.23			
H		2.67	3.21	3.17			
H		2.6	2.92	3.03			
H		2.56	2.77	2.92			
H		2.55	2.75	2.91			
H		2.55	2.75	2.83			
H		2.55	2.73	2.79			
H		2.49	2.55	2.79			
H		2.49	2.5	2.72			
H		2.49	2.45	2.52			
H		2.36	2.44	2.48			
H		2.25	2.42	2.44			
H		2.25	2.25	2.43			
H		2.18	2.18	2.38			
H		1.98	2.14	2.1			
H		1.98	2.08	2.08			
H		1.98	2.06	2.01			
H		1.25	1.49	1.49			
H		1.2	1.26	1.16			
H		1.2	1.23	1.08			
H		1.2	1.08	1.02			
H		1.13	1.03	0.96			
H		1.13	1.02	0.94			
H		1.13	1.02	0.94			

Functional	Solvent?	Basis Set	Type of Data
mPW1PW91	PCM	6-311+G(d,p)	Unscaled Shifts

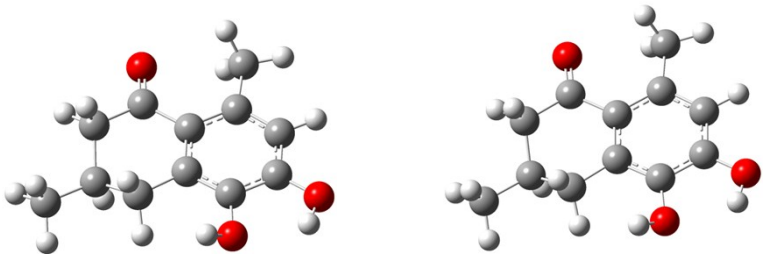
	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6
sDP4+ (H data)	99.99%	0.01%	-	-	-	-
sDP4+ (C data)	99.92%	0.08%	-	-	-	-
sDP4+ (all data)	100.00%	0.00%	-	-	-	-
uDP4+ (H data)	100.00%	0.00%	-	-	-	-
uDP4+ (C data)	99.99%	0.01%	-	-	-	-
uDP4+ (all data)	100.00%	0.00%	-	-	-	-
DP4+ (H data)	100.00%	0.00%	-	-	-	-
DP4+ (C data)	100.00%	0.00%	-	-	-	-
DP4+ (all data)	100.00%	0.00%	-	-	-	-

1.2 ECD calculation for compounds **3** and **4**



3-1 **3-2**

Figure S6. B3LYP/6-31+G(d) optimized lowest energy conformers for **3**.



4-1 **4-2**

Figure S7. B3LYP/6-31+G(d) optimized lowest energy conformers for **4**.

Table S5. Extracted heats and weighting factors of the optimized conformers of **3** and **4** at B3LYP/6-31+G(d) level

		B3LYP/6-31+G(d)	
	Conformer	Extracted heats	Boltzmann-calculated contribution (%)
3	1	-883.3502246	68.47%
	2	-883.3482307	31.53%
4	1	-691.3994484	37.4%
	2	-691.3999324	62.6%

Table S6. The Cartesian coordinates of the lowest energy conformers for **3** and **4**

3-1	X axis(Å)	Y axis(Å)	Z axis(Å)	**3-2**	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-3.11222	0.40646	-0.77058	C	-3.07013	0.40048	-0.82438
C	-2.64506	-0.93697	-0.2325	C	-2.60012	-0.93012	-0.25794
C	-1.19779	-1.17884	-0.65419	C	-1.14669	-1.16899	-0.65943
C	-0.27658	-0.04395	-0.28693	C	-0.23641	-0.02496	-0.29252
C	-0.74754	1.28875	-0.15922	C	-0.71759	1.30727	-0.19701
C	-2.21351	1.55639	-0.37244	C	-2.18047	1.56356	-0.44439
C	1.09256	-0.27611	-0.12515	C	1.13092	-0.24788	-0.09969
C	1.9614	0.77054	0.15371	C	1.98734	0.80959	0.17786
C	1.52341	2.06594	0.31698	C	1.53894	2.10514	0.30843
C	0.15475	2.3456	0.1618	C	0.17231	2.37442	0.12284
C	1.89367	-1.53984	-0.1643	C	1.93682	-1.50916	-0.10525
C	3.31651	-0.92067	-0.29664	C	3.36074	-0.88296	-0.20207

O	3.28213	0.40878	0.25506	O	3.30868	0.46253	0.30723
C	-2.83743	-1.05179	1.28349	C	-2.80923	-1.02043	1.25747
C	-0.2805	3.7781	0.33326	C	-0.27332	3.80733	0.26212
C	1.7531	-2.34806	1.12332	C	1.76791	-2.31423	1.1809
O	1.56149	-2.35015	-1.28777	O	1.62829	-2.31644	-1.23883
O	3.68557	-0.85364	-1.68137	O	3.83656	-0.8822	-1.55192
O	-2.68836	2.68578	-0.28124	O	-2.6591	2.69396	-0.39665
H	-4.12431	0.61776	-0.40549	H	-4.0857	0.61367	-0.47027
H	-3.15218	0.38687	-1.86634	H	-3.10245	0.35886	-1.91981
H	-3.26464	-1.72021	-0.68895	H	-3.20924	-1.72522	-0.70795
H	-0.86262	-2.11942	-0.2072	H	-0.81288	-2.10307	-0.19841
H	-1.15246	-1.30617	-1.74364	H	-1.08687	-1.30789	-1.74675
H	2.23857	2.85066	0.54589	H	2.2463	2.8976	0.53676
H	4.07399	-1.51673	0.22449	H	4.08975	-1.44744	0.38921
H	-3.89303	-0.92457	1.54657	H	-3.869	-0.89854	1.50592
H	-2.26343	-0.30223	1.83689	H	-2.24892	-0.25591	1.80438
H	-2.52453	-2.04034	1.63644	H	-2.49151	-1.99973	1.63127
H	0.56307	4.42369	0.60287	H	0.56033	4.46069	0.54364
H	-0.69321	4.16902	-0.60186	H	-0.66396	4.18246	-0.6888
H	-1.01226	3.86369	1.1425	H	-1.02564	3.90144	1.05134
H	0.73365	-2.72545	1.25364	H	0.74784	-2.69707	1.28694
H	2.40513	-3.22849	1.09335	H	2.42539	-3.19101	1.17044
H	2.00917	-1.75978	2.01141	H	1.99798	-1.72099	2.07277
H	2.10919	-1.99364	-2.01912	H	2.46215	-2.73895	-1.51917
H	4.58428	-0.48099	-1.67674	H	3.09098	-0.5558	-2.08828
4-1	X axis(Å)	Y axis(Å)	Z axis(Å)	**4-2**	X axis(Å)	Y axis(Å)	Z axis(Å)
C	2.072487	0.526045	-1.06652	C	2.04674	0.470547	-1.09343
C	1.163533	1.742041	-0.96771	C	1.140075	1.687548	-0.98717
C	0.39533	1.687217	0.350828	C	0.38484	1.634573	0.338738
C	-0.36847	0.3948	0.495971	C	-0.38129	0.344096	0.492254
C	0.043135	-0.79725	-0.14285	C	0.027707	-0.85108	-0.14597
C	1.293841	-0.76761	-0.9773	C	1.266704	-0.82176	-0.99818
C	-1.49547	0.355464	1.322028	C	-1.49716	0.306451	1.334649
C	-2.22899	-0.81354	1.494103	C	-2.2394	-0.85727	1.492511
C	-1.85026	-1.98075	0.850306	C	-1.85195	-2.0299	0.868656
C	-0.70942	-1.99122	0.024803	C	-0.71338	-2.04811	0.042845
C	-0.34207	-3.29456	-0.63707	C	-0.34449	-3.35863	-0.60218
C	1.970358	3.034191	-1.07402	C	1.947247	2.978729	-1.10226
O	1.723736	-1.77274	-1.53751	O	1.686021	-1.82447	-1.57022
O	-1.90022	1.482499	1.986829	O	-1.85555	1.421158	2.043692
O	-3.32184	-0.76187	2.314754	O	-3.37704	-0.85459	2.246137
H	2.591707	0.539776	-2.0324	H	2.558157	0.483774	-2.06348
H	2.830188	0.521916	-0.27415	H	2.811004	0.465118	-0.30741

H	0.445112	1.716612	-1.79901	H	0.41364	1.662194	-1.81146
H	1.079071	1.784205	1.203779	H	1.077103	1.730456	1.184927
H	-0.29479	2.539386	0.380502	H	-0.30392	2.487673	0.375232
H	-2.42671	-2.89191	0.985385	H	-2.44444	-2.92948	1.019047
H	-1.07061	-4.08037	-0.40765	H	-1.05607	-4.14946	-0.33911
H	-0.33236	-3.18392	-1.72584	H	-0.36165	-3.26878	-1.69276
H	0.629594	-3.64728	-0.27782	H	0.640165	-3.69169	-0.25989
H	1.312761	3.908018	-1.01763	H	1.291184	3.853322	-1.04015
H	2.70734	3.112408	-0.26746	H	2.692098	3.056731	-0.30293
H	2.506541	3.079407	-2.02779	H	2.474211	3.022656	-2.06121
H	-2.69465	1.204521	2.486356	H	-2.19426	1.099706	2.900562
H	-3.72887	-1.64549	2.337084	H	-3.83631	-0.01953	2.038576

2. Assays for anti-inflammation and lipogenesis inhibition of **1** and **2**

2.1 Assays for anti-inflammation of **1** and **2**

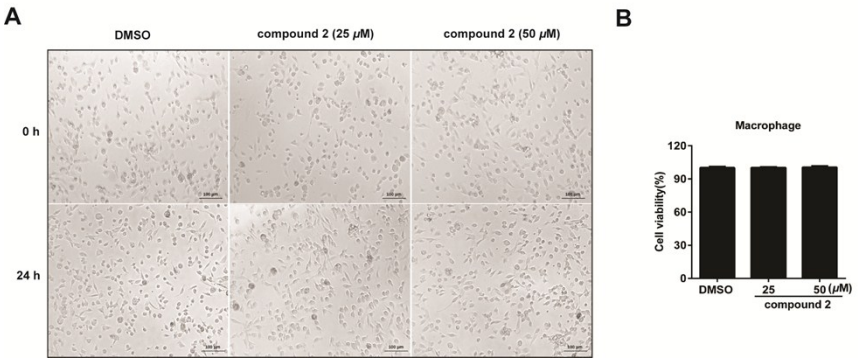


Figure S8. Compound **2** had no obvious impact on cell viability. (A) Macrophages were photographed with microscope at a 200 X enlargement after 24 hours treated with indicated concentration of compound **2**. (B) The cell viability was determined by MTT assay.

2.2 Assays for lipogenesis inhibition of **1** and **2**

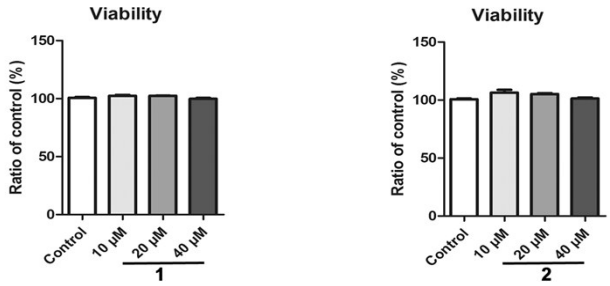
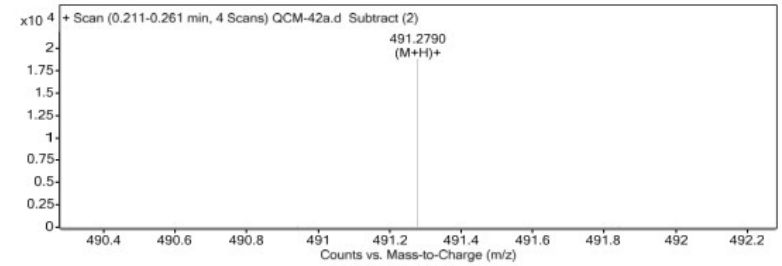


Figure S9. HepG2 cells were treated with the concentration of 10, 20, and 40 μM of **1** and **2** for 24 hours, followed by MTT assay.

3. HRESIMS spectra and NMR spectra of **1**−**4**

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
97.9689		4314.48		
141.9584		5364.05		
193.9299	1	4146.66		
274.2741	1	5282.65		
318.3003	1	4263		
491.279	1	18845.89	C31 H38 O5	(M+H)+
492.2826	1	6389.95	C31 H38 O5	(M+H)+
513.2608	1	4981.58		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C31 H38 O5	490.2719	491.2792	491.2790	0.1	0.2	13.0000

--- End Of Report ---

Figure S10. HRESIMS of **1**

The 1D and 2D NMR spectra of **1**

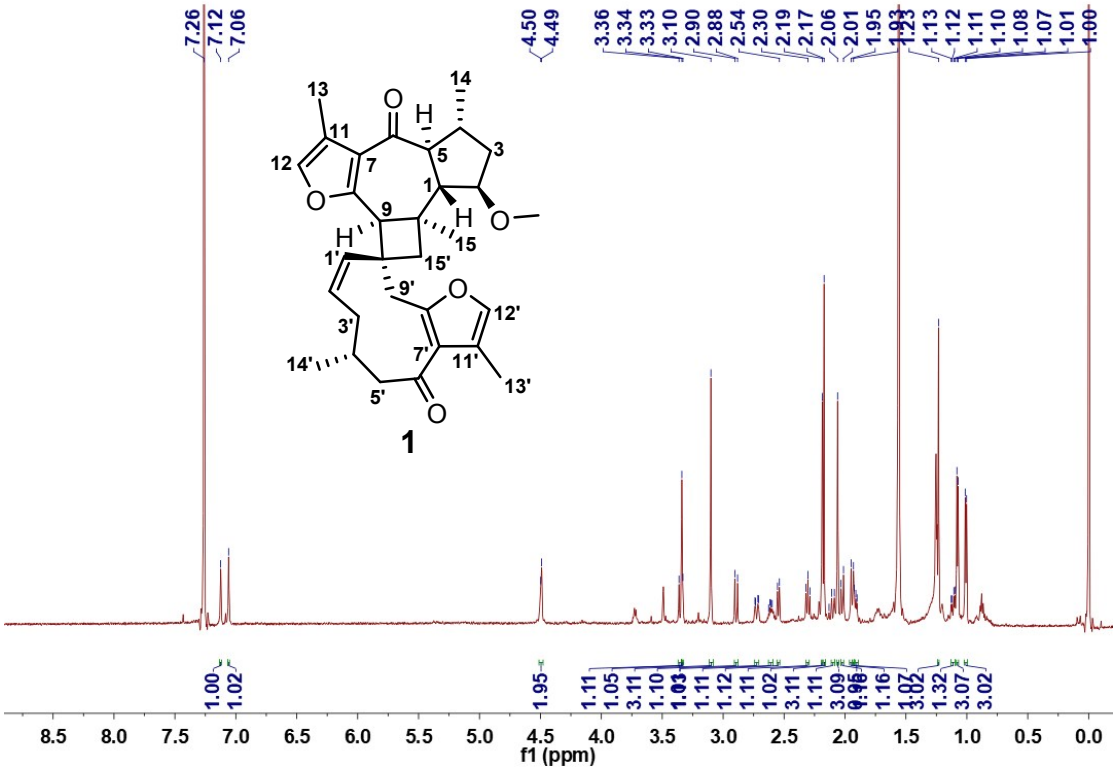


Figure S11. ^{1}H NMR spectrum (AV-600, 600 MHz) of **1** in $CDCl_3$

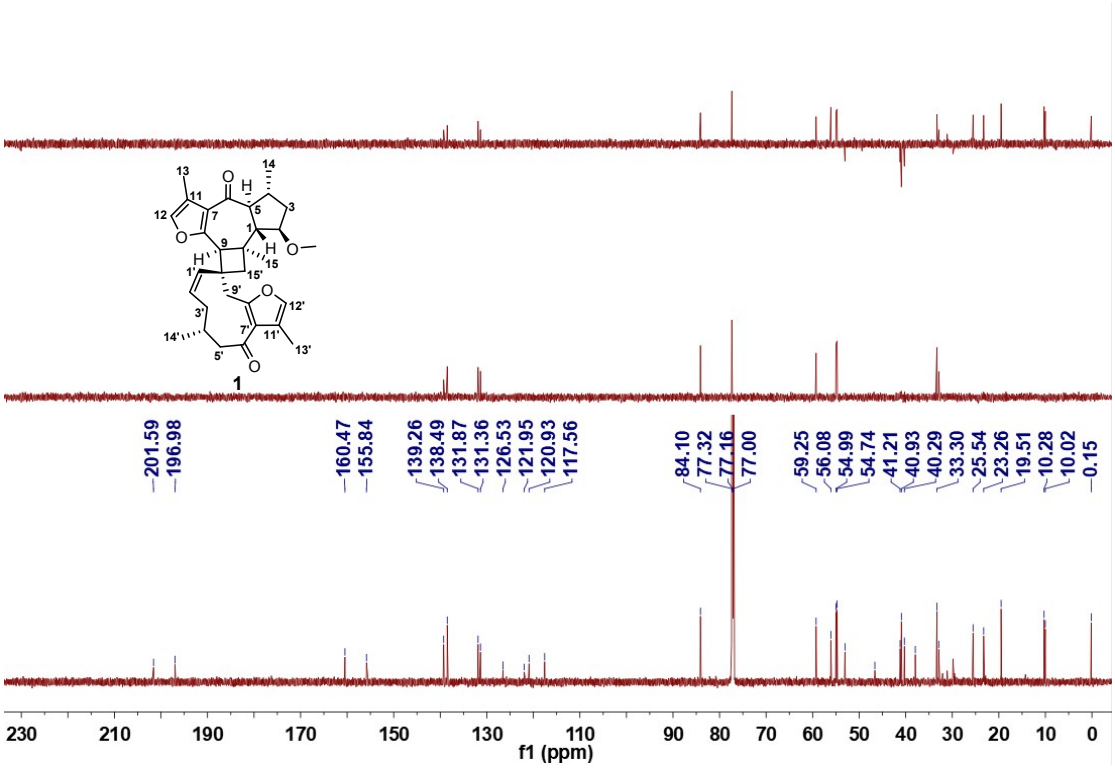


Figure S12. ^{13}C NMR and DEPT spectra (AV-600, 150 MHz) of **1** in $CDCl_3$

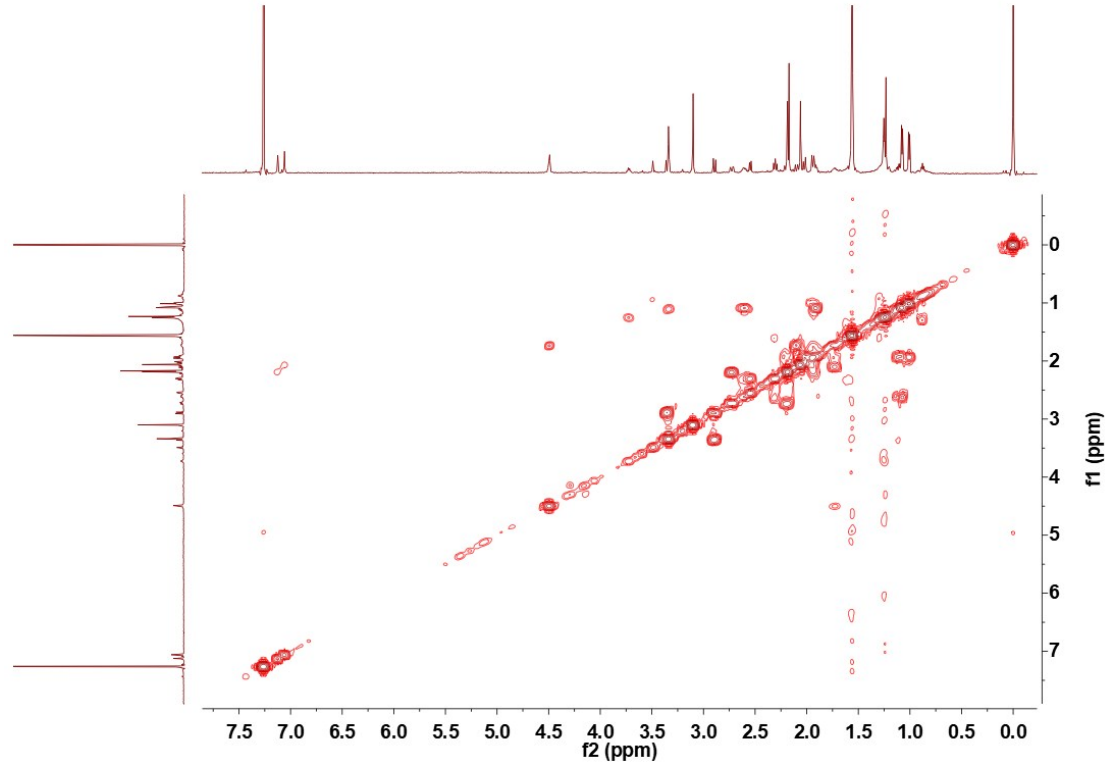


Figure S13. ^{1}H-^{1}H COSY spectrum (AV-600) of **1** in $CDCl_3$

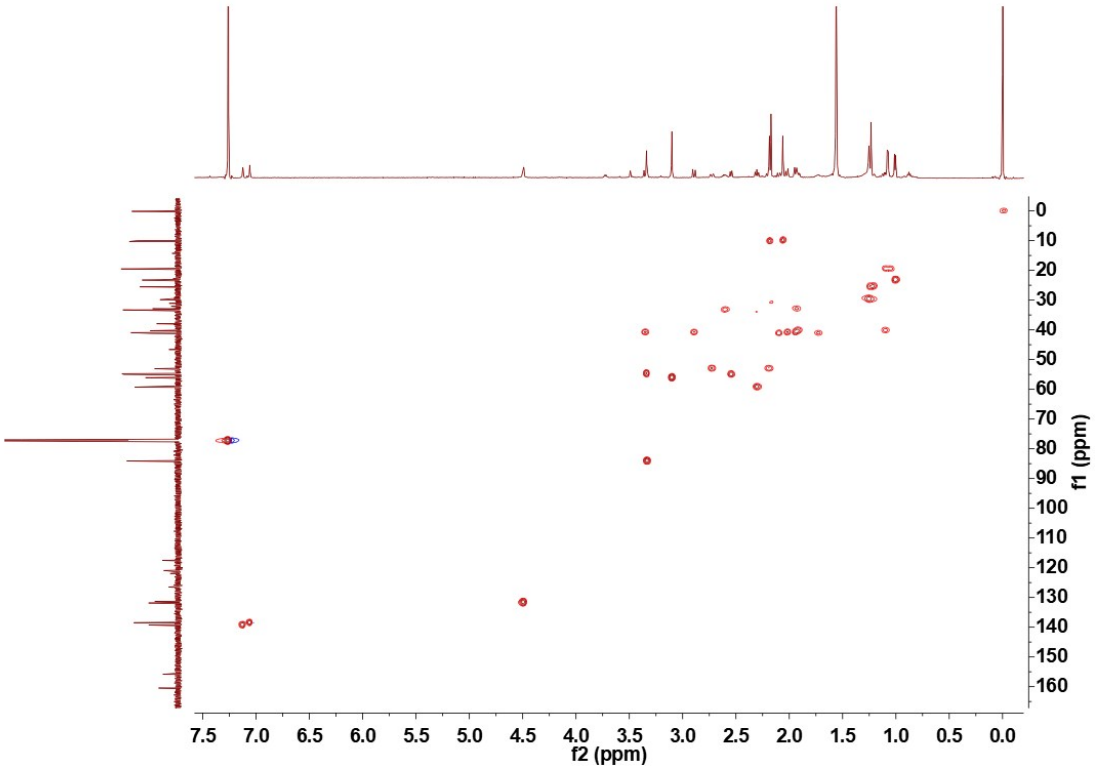


Figure S14. HSQC spectrum (AV-600) of **1** in $CDCl_3$

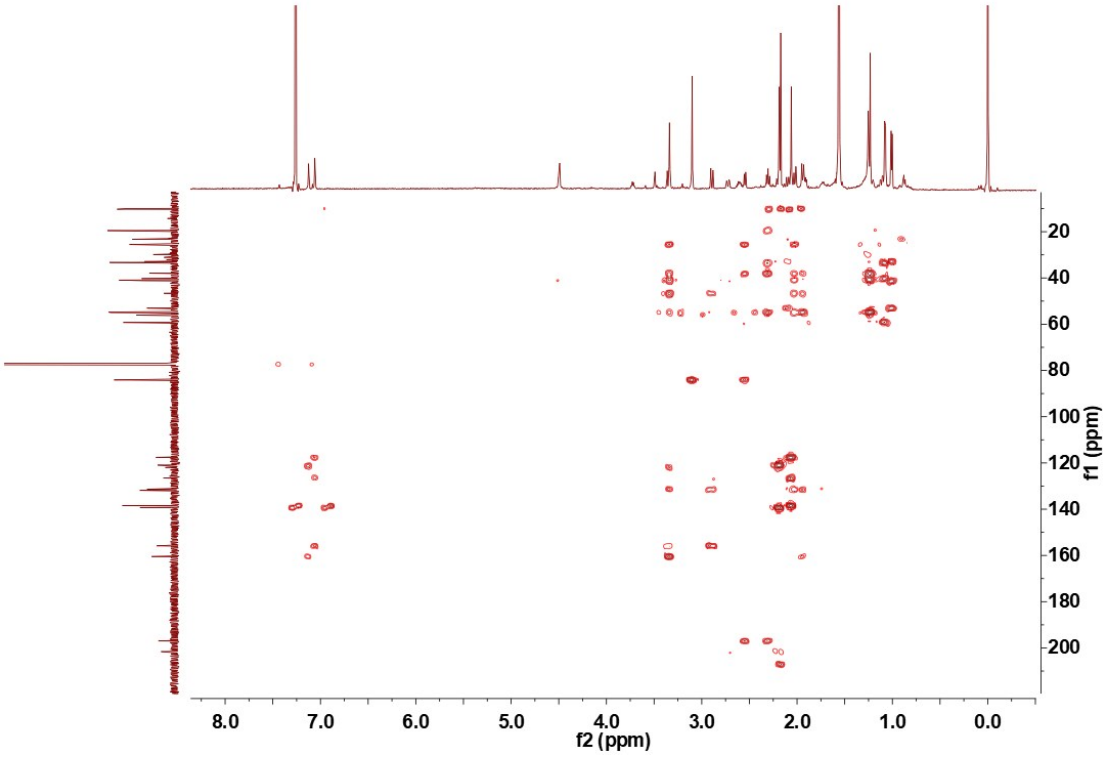


Figure S15. HMBC spectrum (AV-600) of **1** in $CDCl_3$

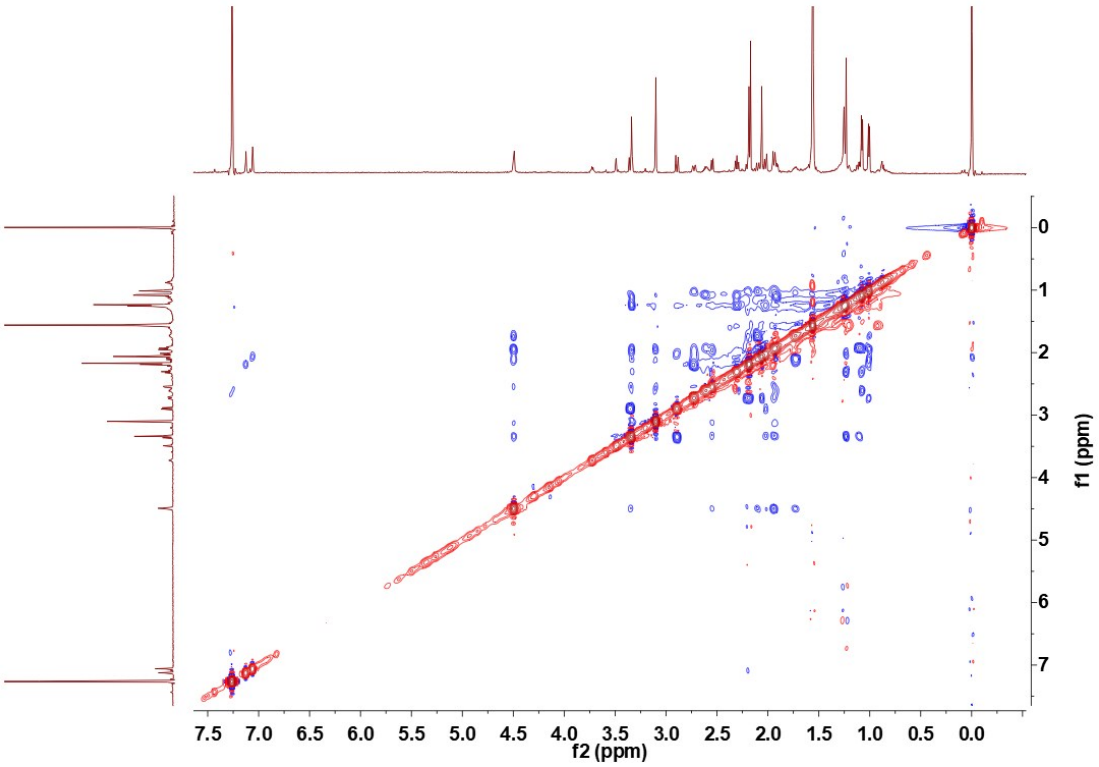
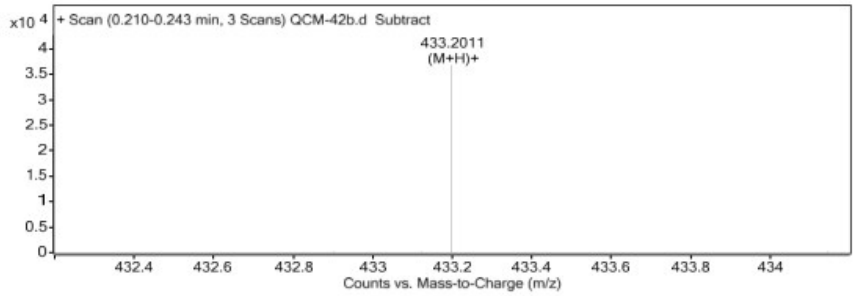


Figure S16. NOESY spectrum (AV-600) of **1** in $CDCl_3$

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
113.964		4164.03		
141.9584		6876.82		
193.9301		4187.9		
212.1184	1	4675.28		
274.2741	1	4529.78		
433.2011	1	36831.23	C27 H28 O5	(M+H)+
434.2047	1	9782.65	C27 H28 O5	(M+H)+
455.1829	1	4168.02		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C27 H28 O5	432.1937	433.2010	433.2011	-0.2	-0.5	14.0000

--- End Of Report ---

Figure S17. HRESIMS spectrum of **2**

The 1D and 2D NMR spectra of **2**

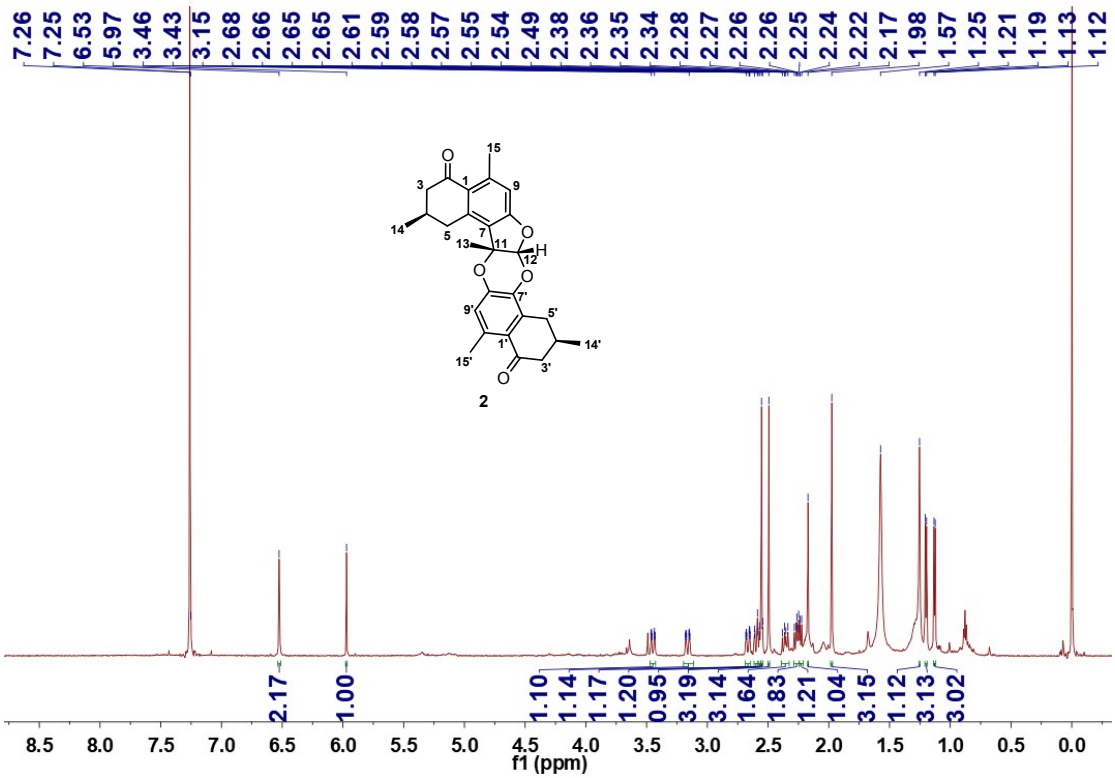


Figure S18. ^{1}H NMR spectrum (AV-600, 600 MHz) of **2** in $CDCl_3$

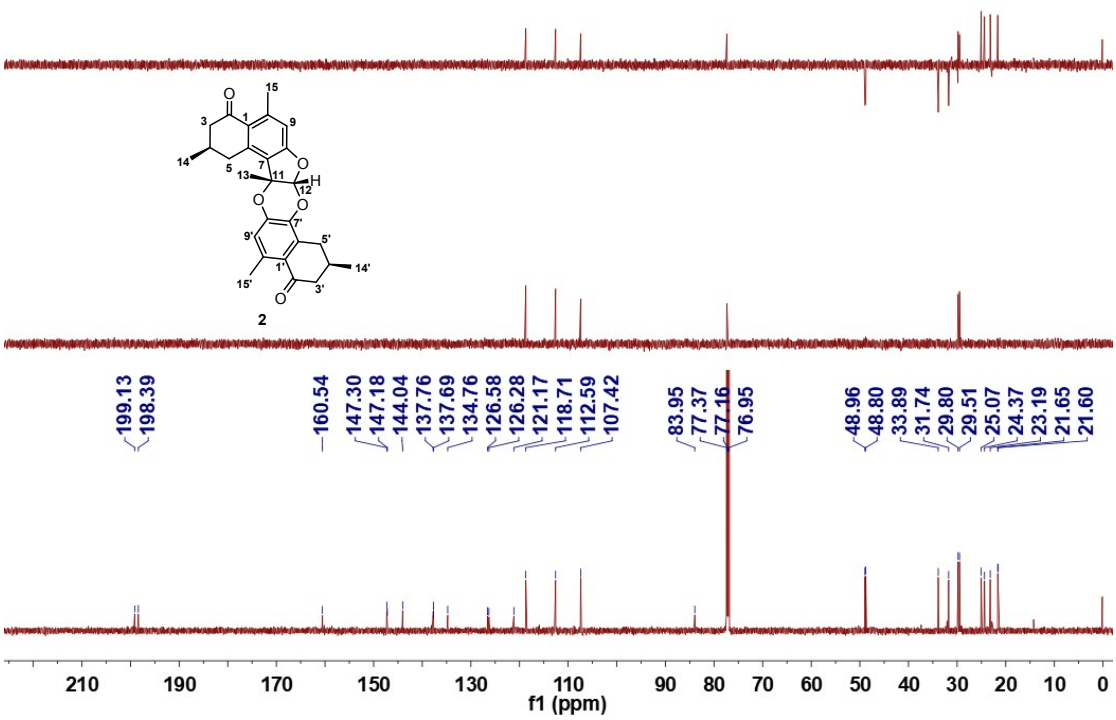


Figure S19. ^{13}C NMR and DEPT spectra (AV-600, 150 MHz) of **2** in $CDCl_3$

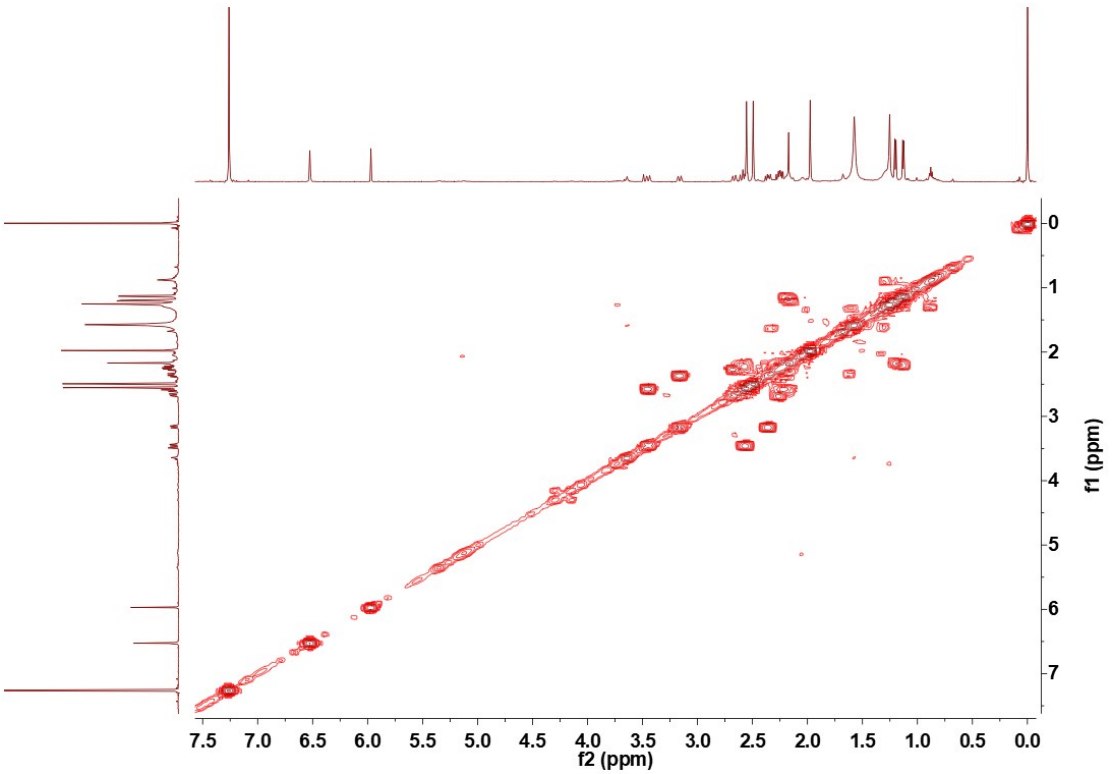


Figure S20. ^{1}H-^{1}H COSY spectrum (AV-600) of **2** in $CDCl_3$

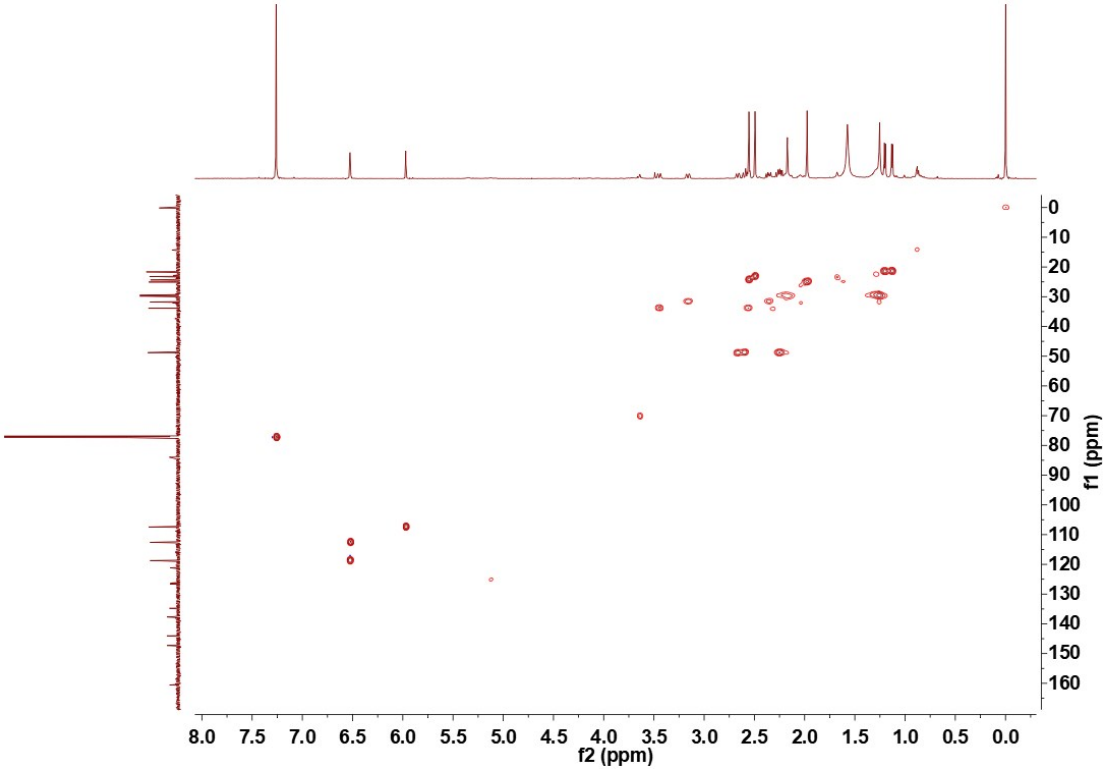


Figure S21. HSQC spectrum (AV-600) of **2** in $CDCl_3$

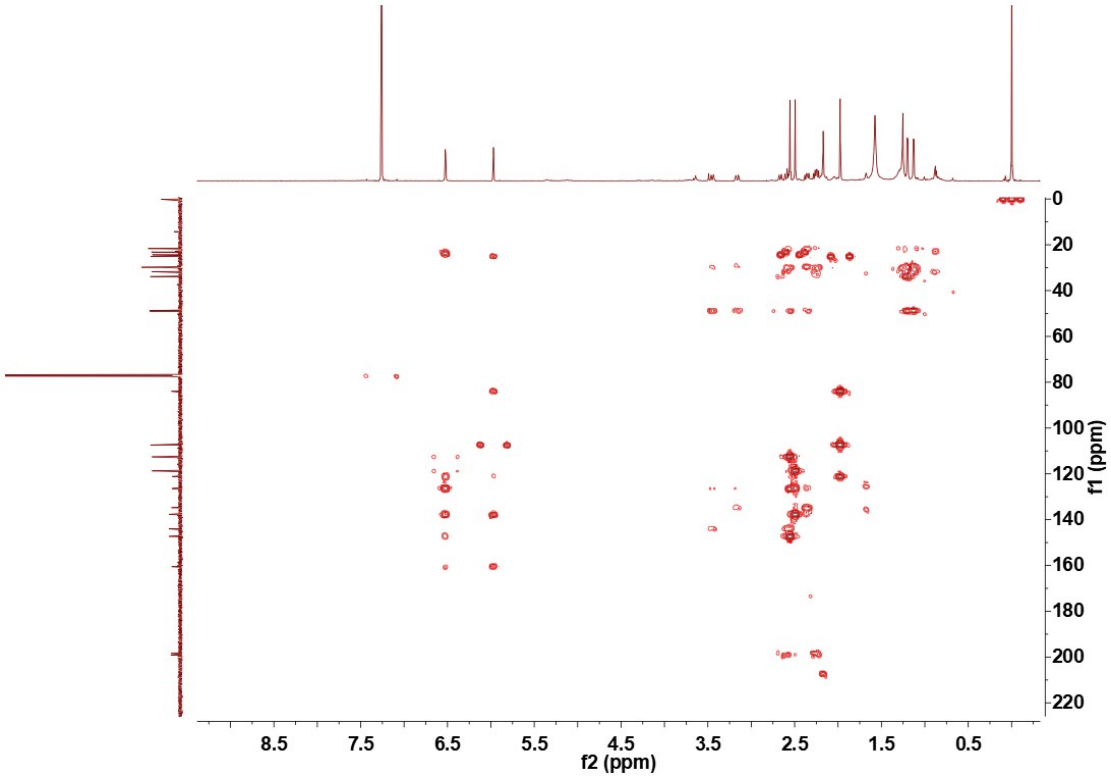


Figure S22. HMBC spectrum (AV-600) of **2** in $CDCl_3$

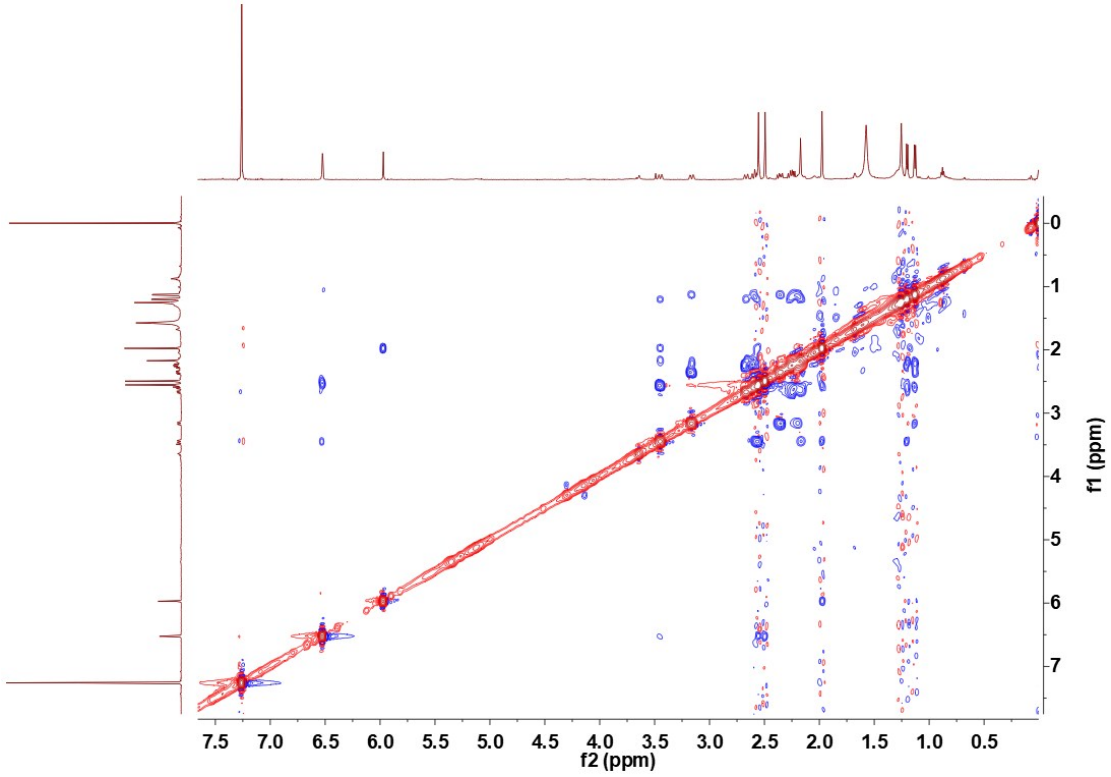
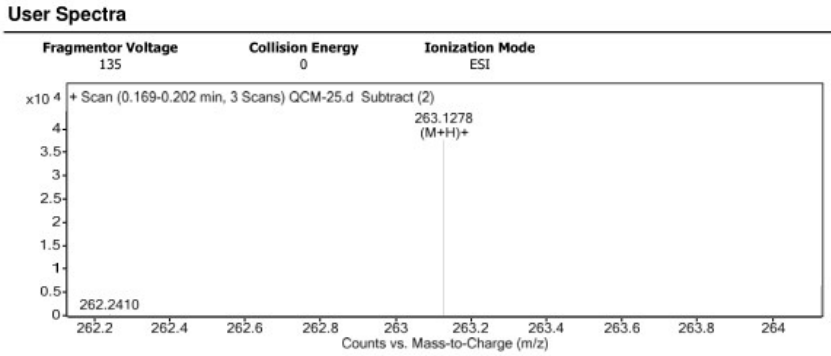


Figure S23. ROESY spectrum (AV-600) of **2** in $CDCl_3$



Peak List

m/z	z	Abund	Formula	Ion
245.1172		2692.4		
246.2425		1165.46		
263.1278	1	37825	C15 H18 O4	(M+H)+
264.1311	1	6289.12	C15 H18 O4	(M+H)+
274.2739	1	5830.16		
285.1103		1848.82		
302.3052	1	1930.42		
318.2997	1	2403.08		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C15 H18 O4	262.1205	263.1278	263.1278	-0.1	-0.3	7.0000

--- End Of Report ---

Figure S24. HRESIMS of **3**

The 1D and 2D NMR spectra of **3**

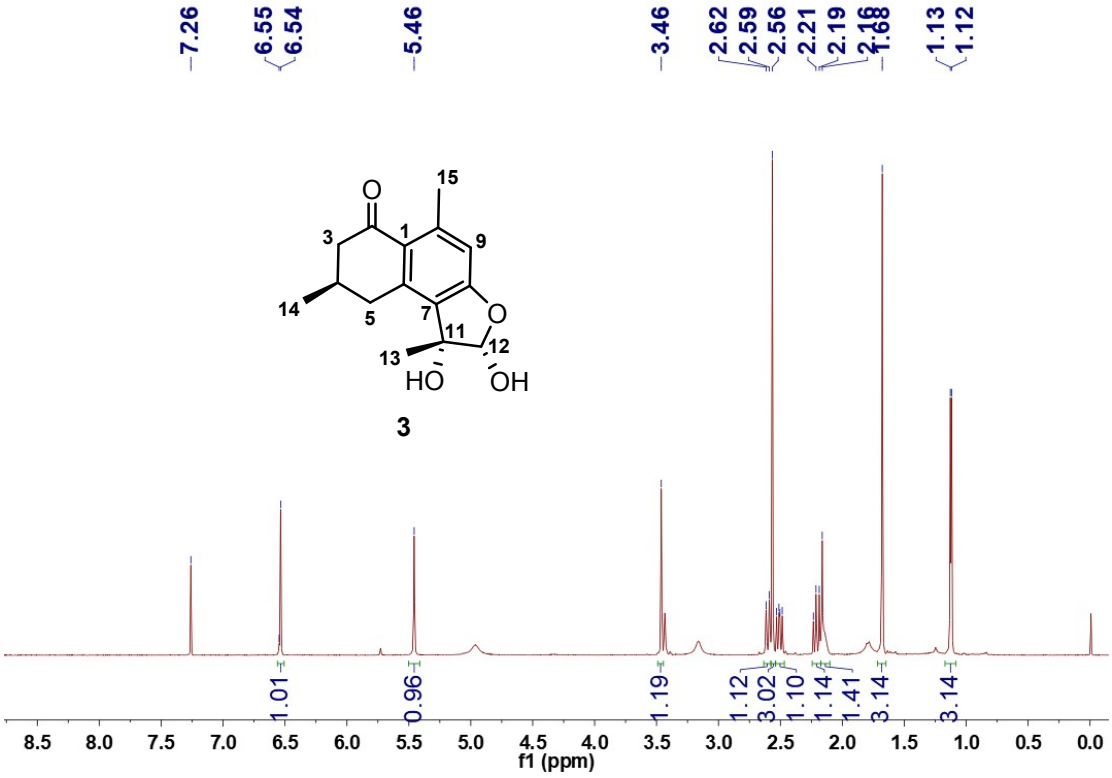


Figure S25. ^{1}H NMR spectrum (AV-600, 600 MHz) of **3** in $CDCl_3$

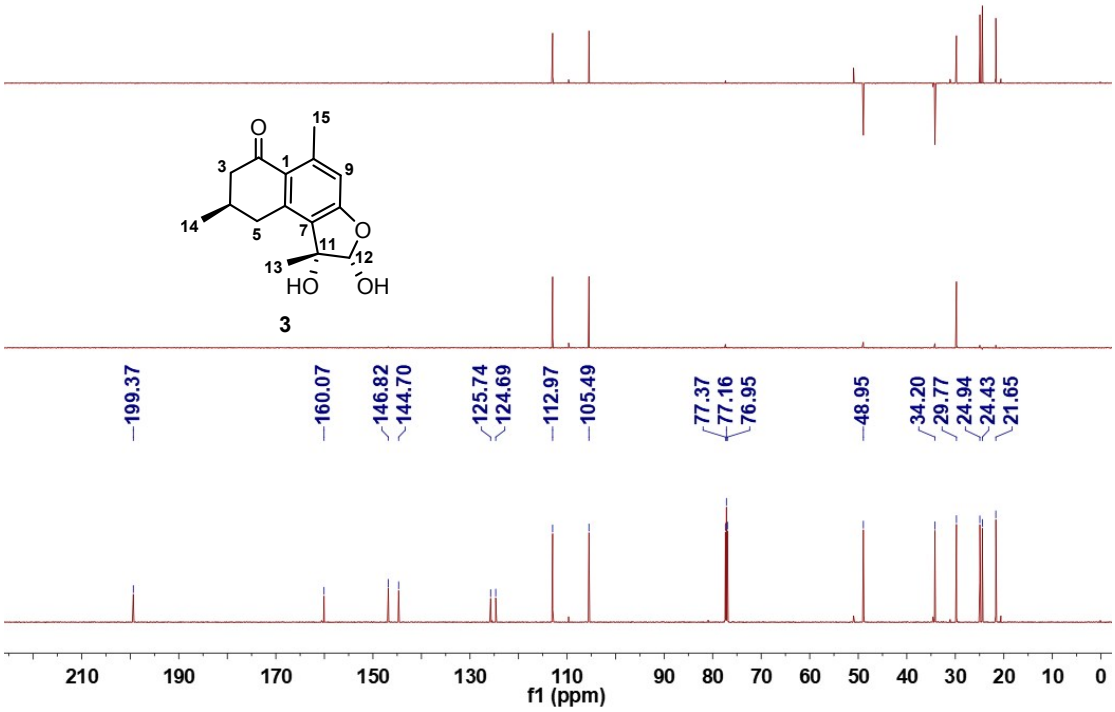


Figure S26. ^{13}C NMR and DEPT spectra (AV-600, 150 MHz) of **3** in $CDCl_3$

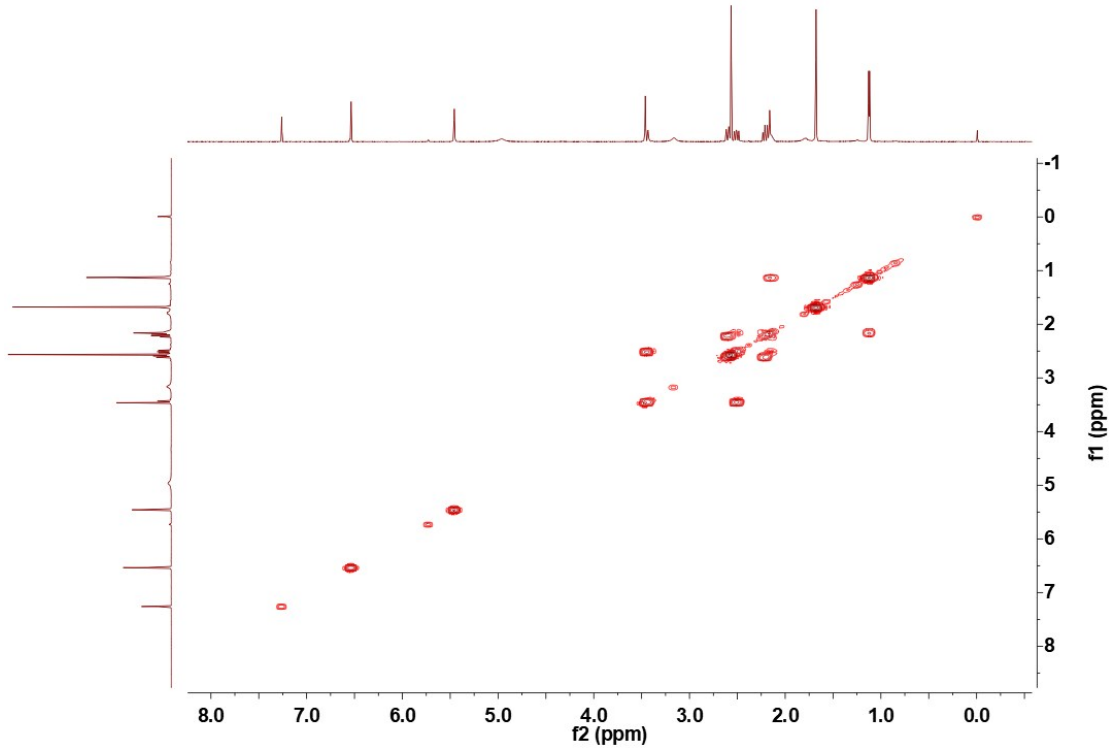


Figure S27. ^{1}H-^{1}H COSY spectrum (AV-600) of **3** in $CDCl_3$

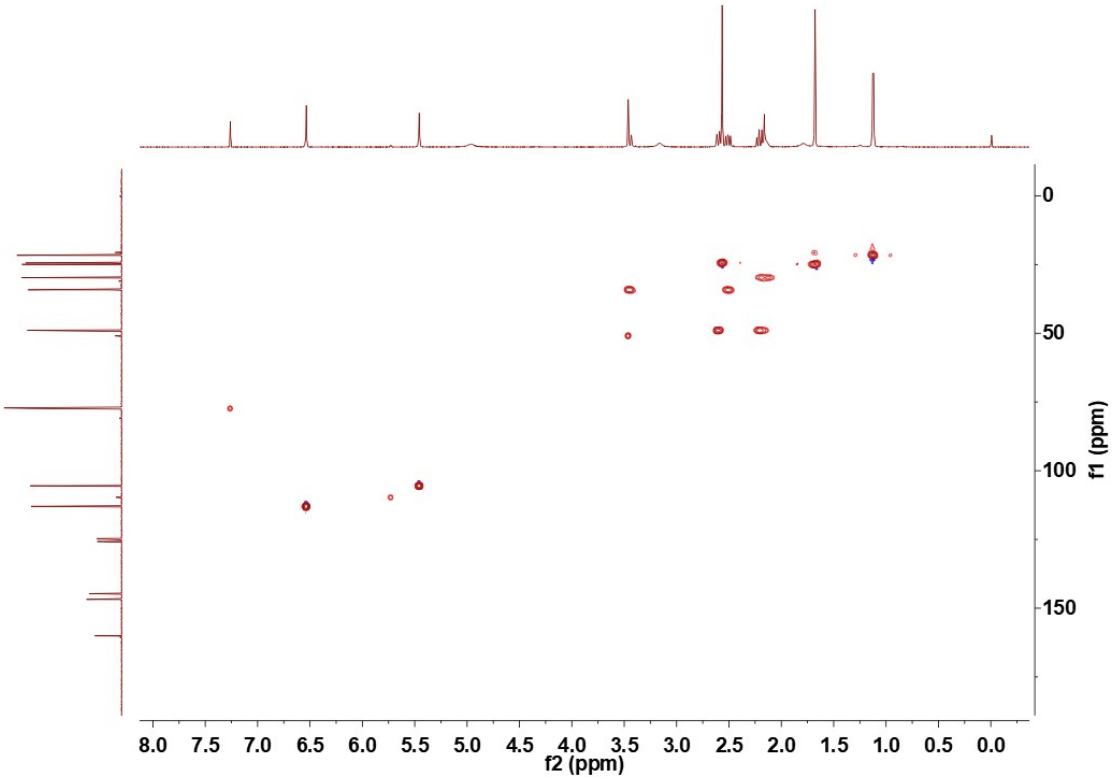


Figure S28. HSQC spectrum (AV-600) of **3** in $CDCl_3$

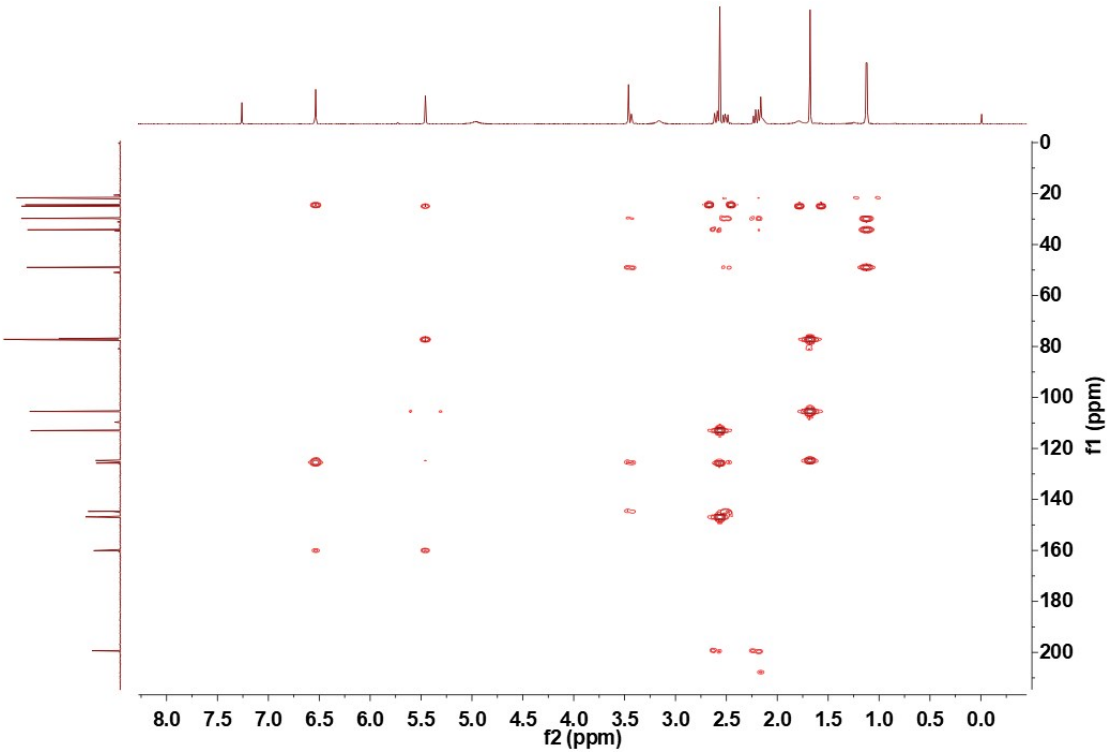


Figure S29. HMBC spectrum (AV-600) of **3** in $CDCl_3$

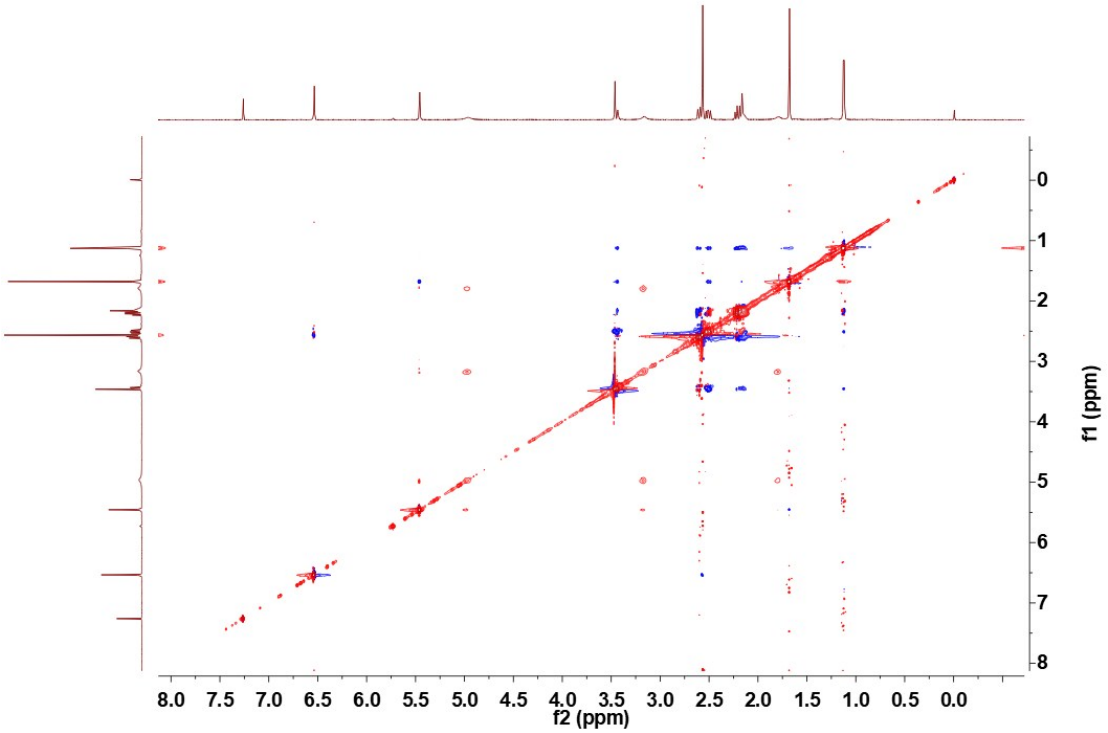
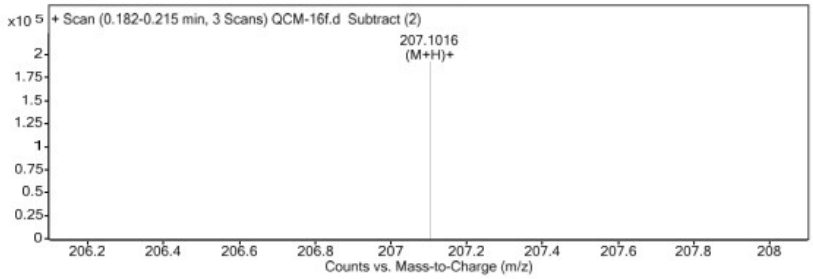


Figure S30. ROESY spectrum (AV-600) of **3** in $CDCl_3$

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
123.0284	2	4471.34		
143.5415	2	9729.2		
207.1016	1	192594.69	C12 H14 O3	(M+H)+
208.1048	1	27186.25	C12 H14 O3	(M+H)+
229.0837	1	8268.66		
274.2742	1	10604		
302.3051	1	3905.54		
318.2996	1	5292.57		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C12 H14 O3	206.0943	207.1016	207.1016	0.0	0.1	6.0000

--- End Of Report ---

Figure S31. HRESIMS of **4**

The 1D and 2D NMR spectra of **4**

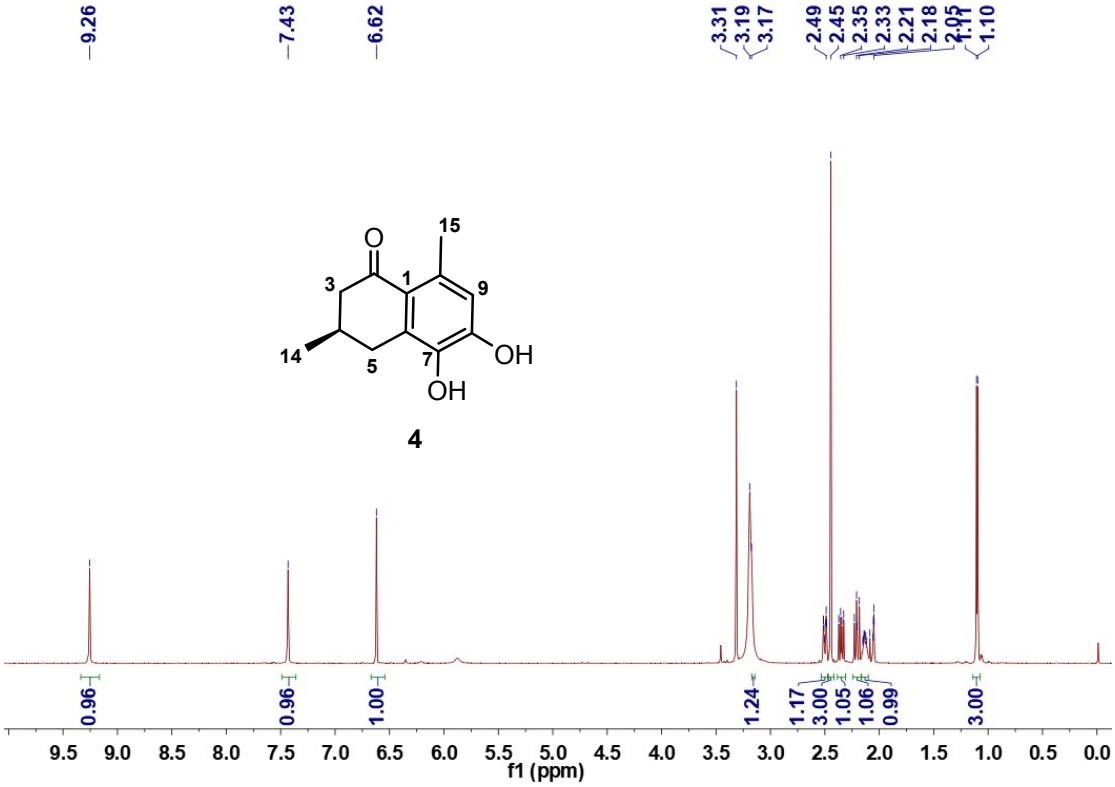


Figure S32. [1]H NMR spectrum (AV-600, 600 MHz) of **4** in acetone-d_6

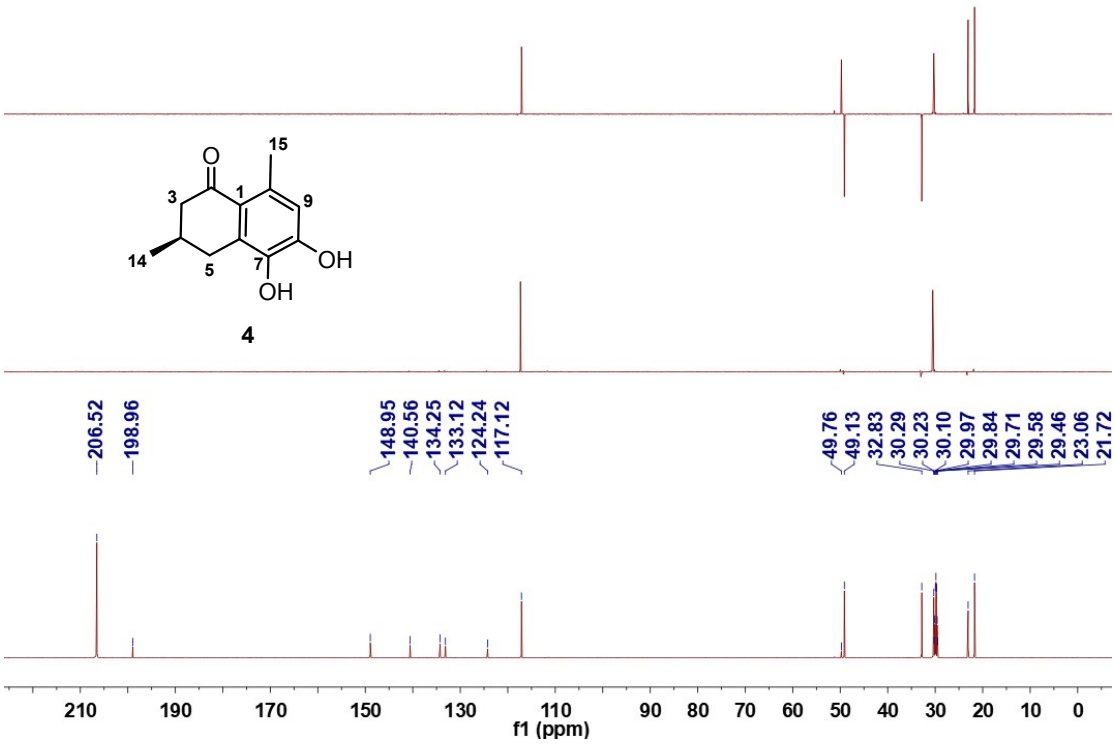


Figure S33. [13]C NMR and DEPT spectra (AV-600, 150 MHz) of **4** in acetone-d_6

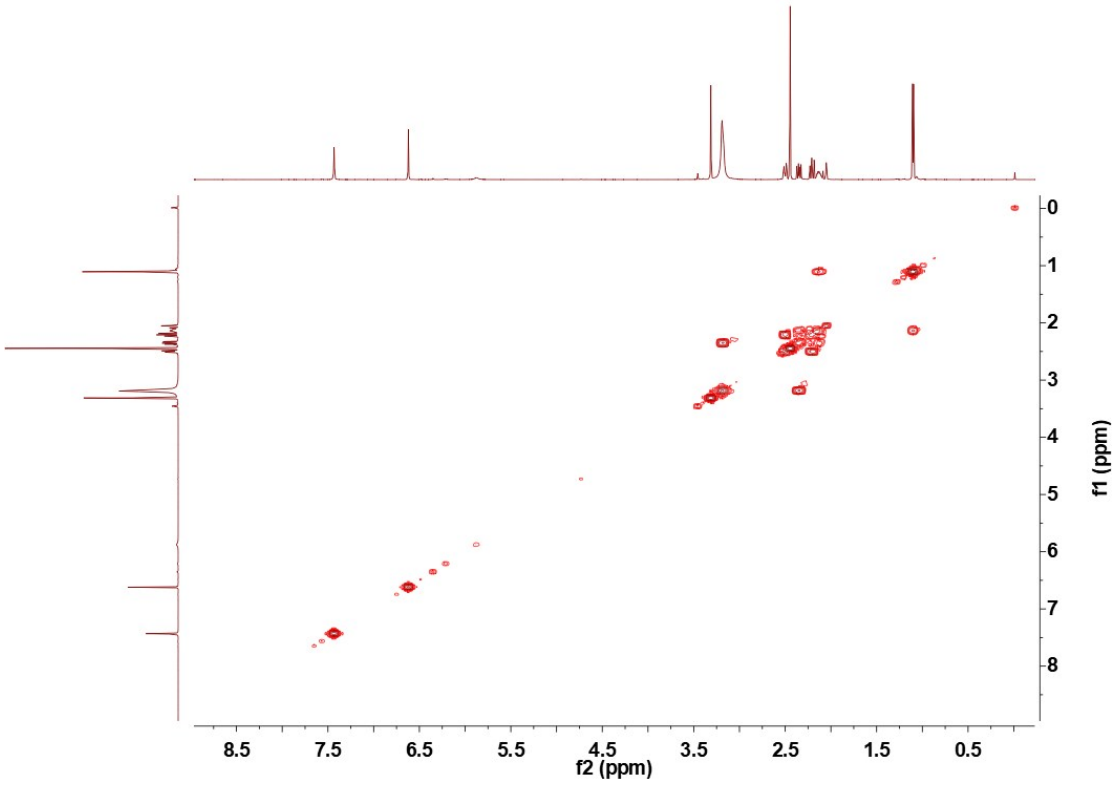


Figure S34. ^{1}H-^{1}H COSY spectrum (AV-600) of **4** in acetone-d_6

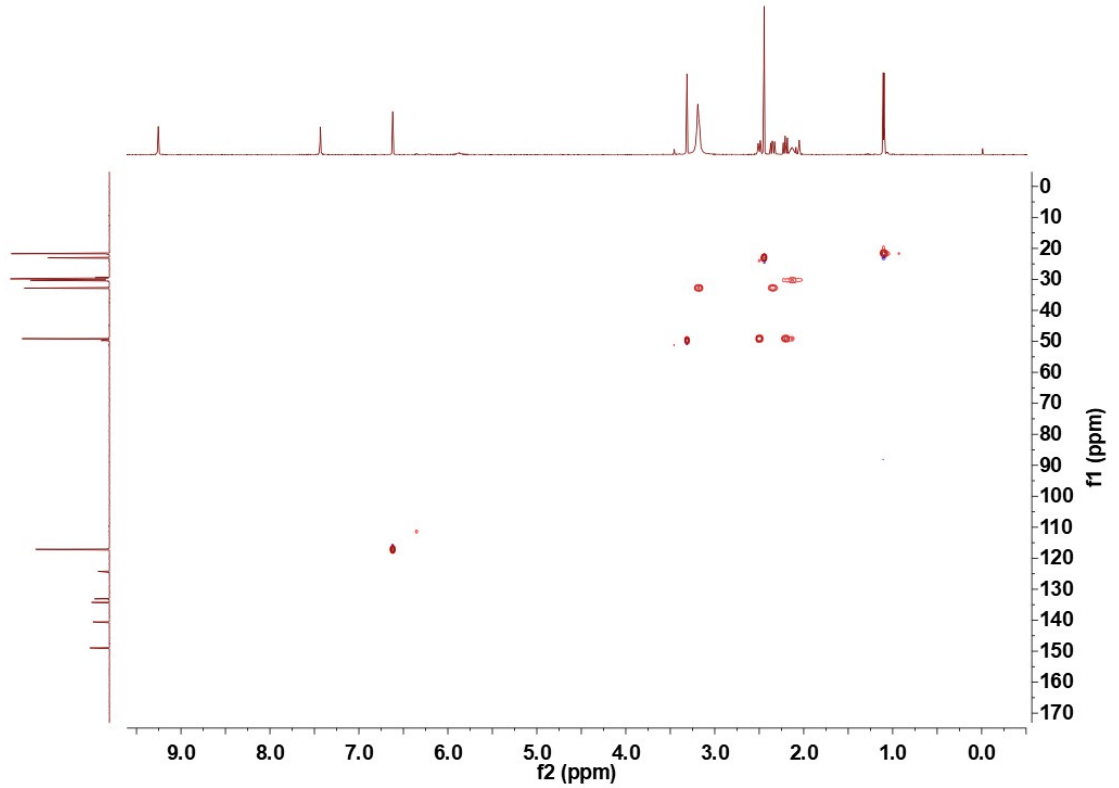


Figure S35. HSQC spectrum (AV-600) of **4** in acetone-d_6

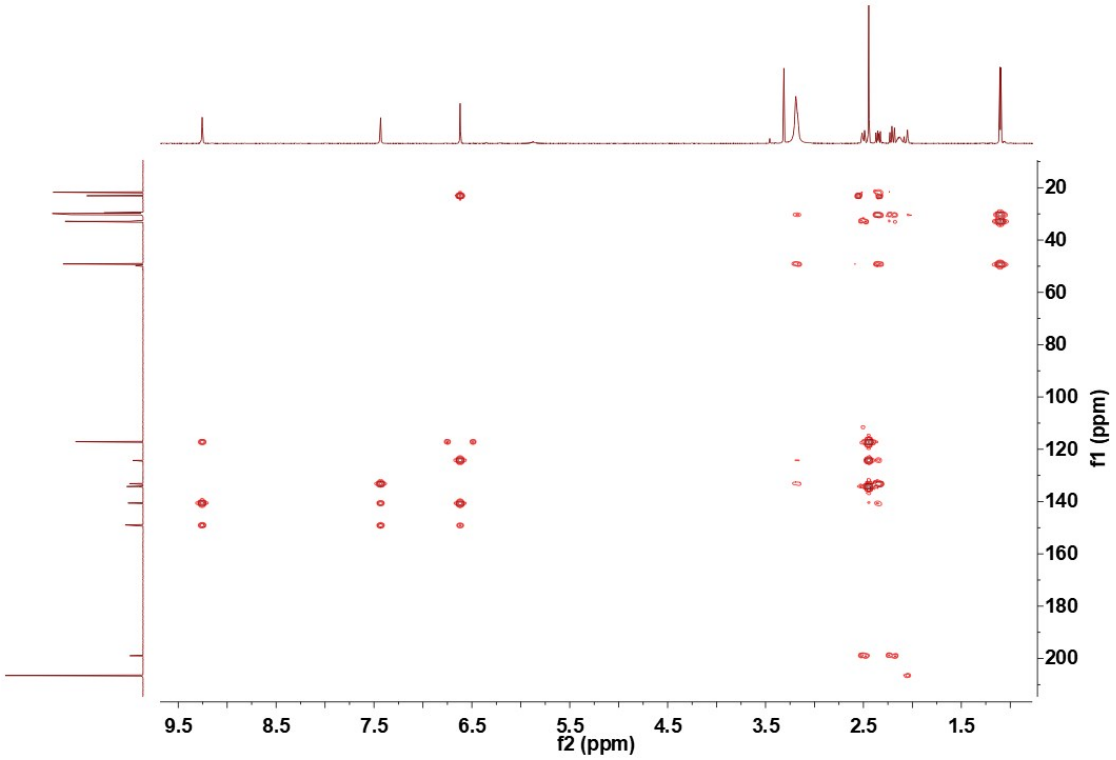


Figure S36. HMBC spectrum (AV-600) of **4** in acetone-d_6