Supporting Information

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Currephila A, a New Chromanol Derivative from the Endophytic Fungus *Curreya pityophila*

Fan Xu [1,†], Xiao-Yan Pan [1,†], Bai-Xiang Cai [3], Yin-Zhong Fan [1], Bao-Bao Shi, [1,2,*] and Ji-Kai Liu [1,2,*]

[1]School of Pharmaceutical Sciences, South-Central MinZu University, Wuhan 430074, People's Republic of China

[2]International Cooperation Base for Active Substances in Traditional Chinese Medicine in Hubei Province, School of Pharmaceutical Sciences, South-Central Minzu University

[3] School of Pharmacy, Anhui University of Chinese Medicine, Hefei, 230012, PR China

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[†]These authors contribute equally to this work.
[*]Corresponding author(s): shibb0505@163.com (B. B. Shi); liujikai@mail.scuec.edu.cn (J.K. Liu)

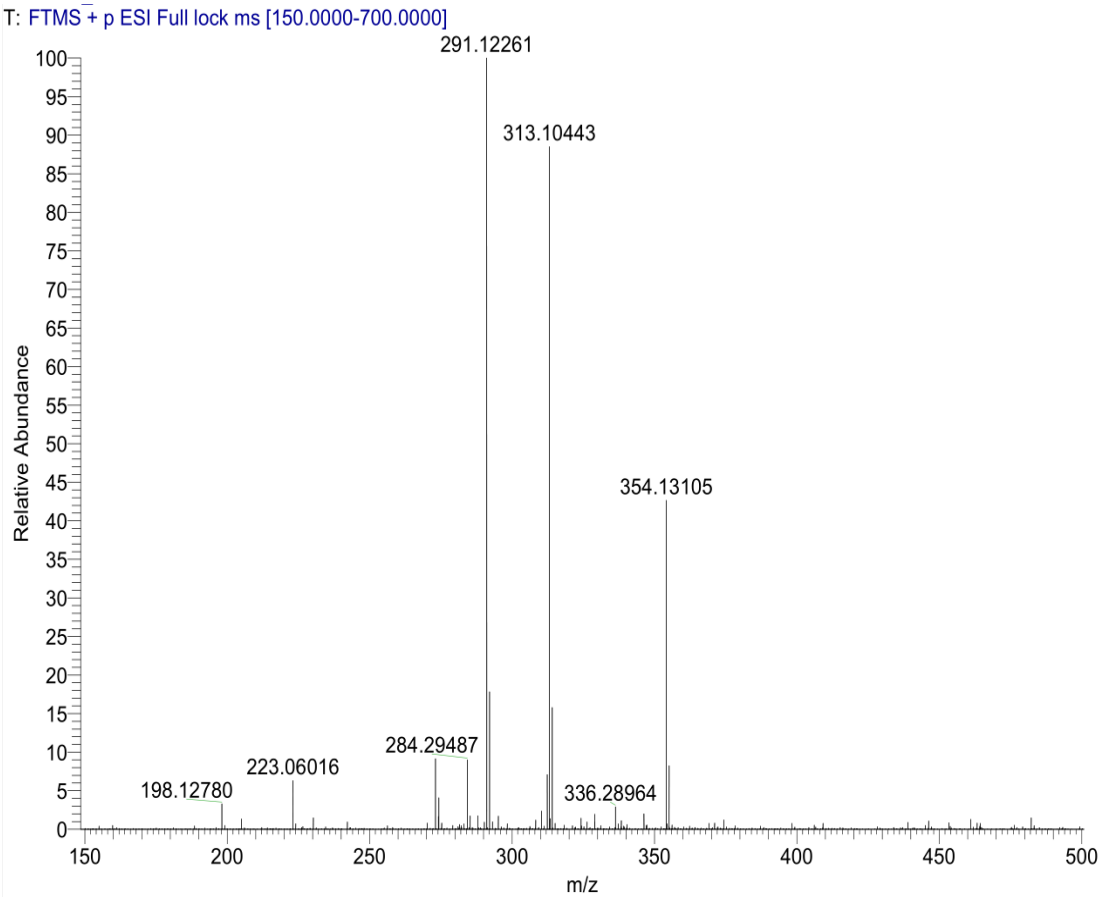


Figure S1: HRESIMS spectrum of **1.**

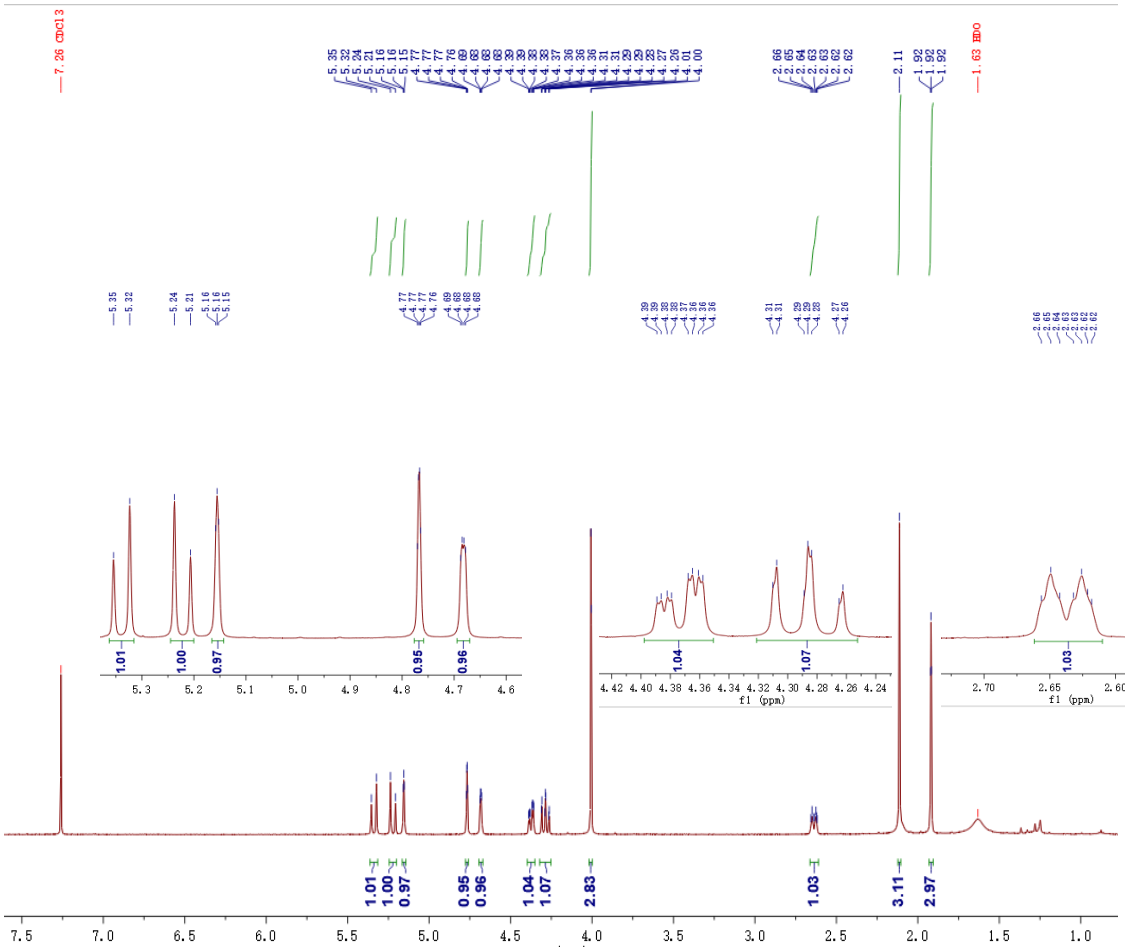


Figure S2: ^{1}H NMR spectrum of **1.**

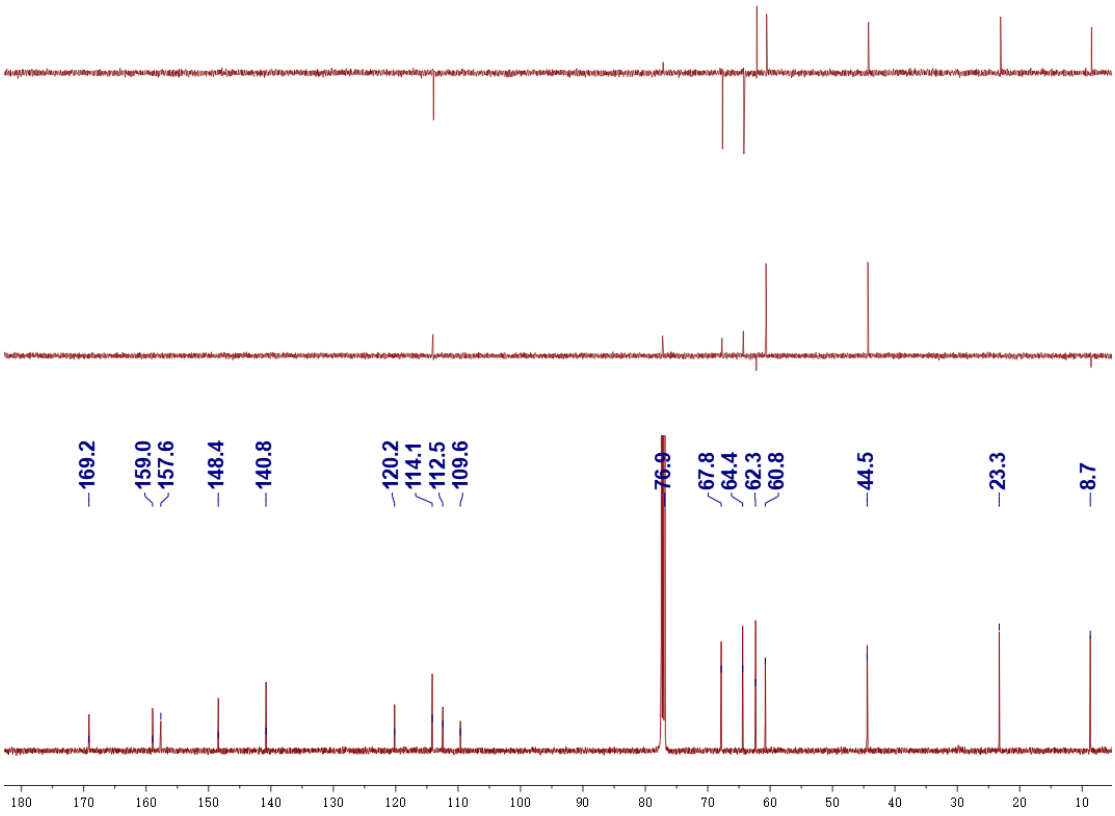


Figure S3: ^{13}C NMR spectrum of **1.**

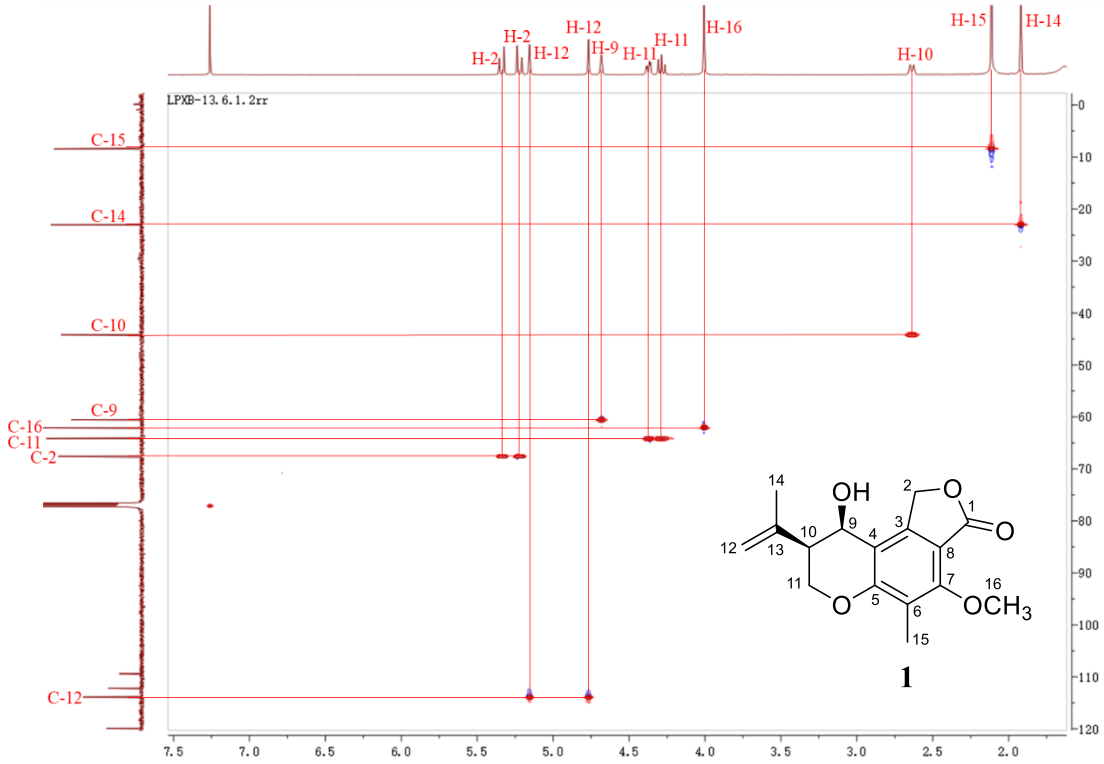


Figure S4: HSQC spectrum of **1.**

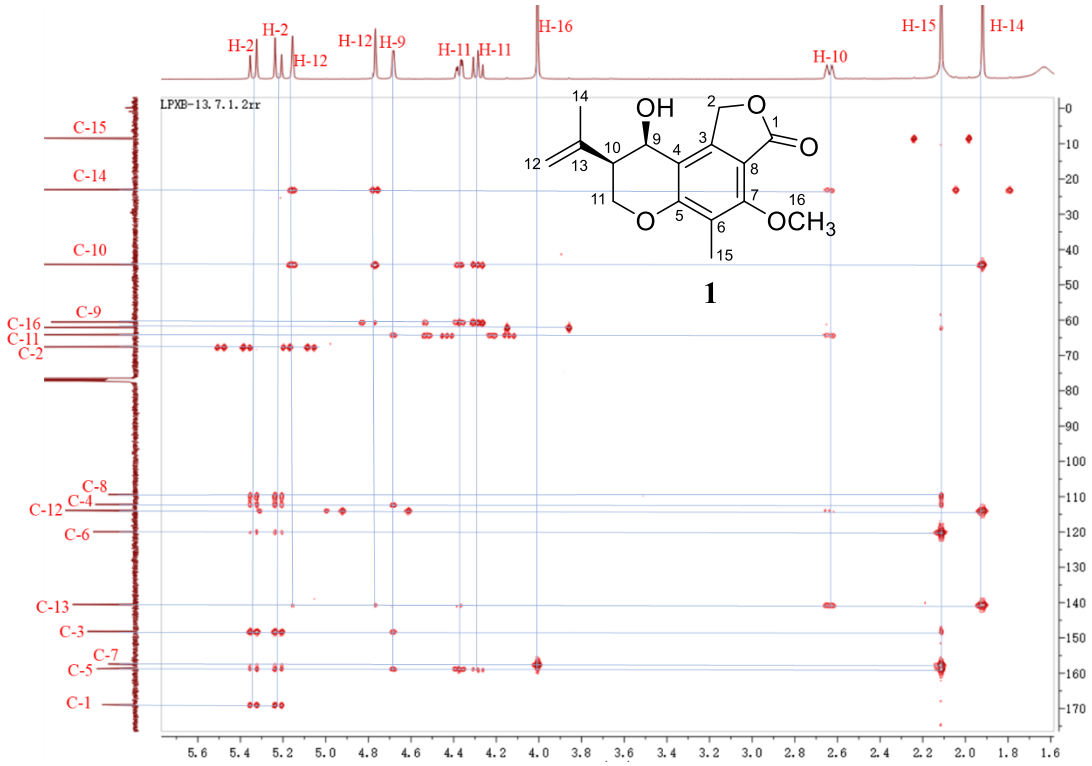
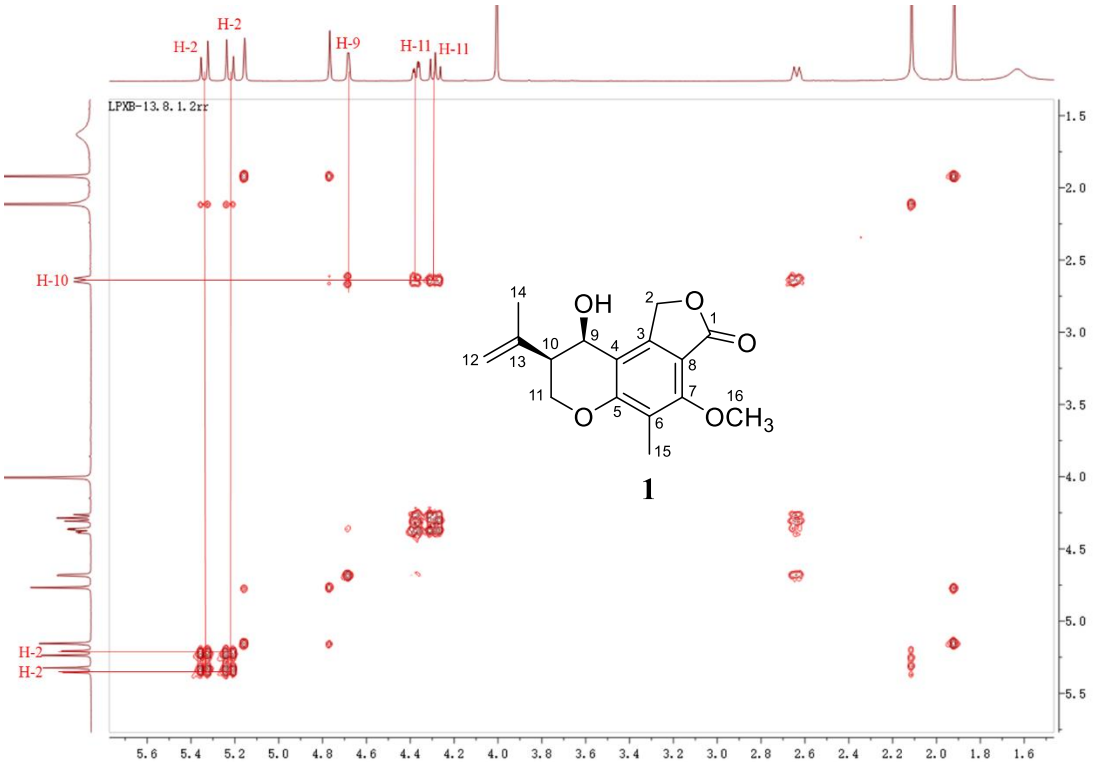


Figure S5: HMBC spectrum of **1.**



1

Figure S6: ^{1}H-^{1}H COSY spectrum of **1.**

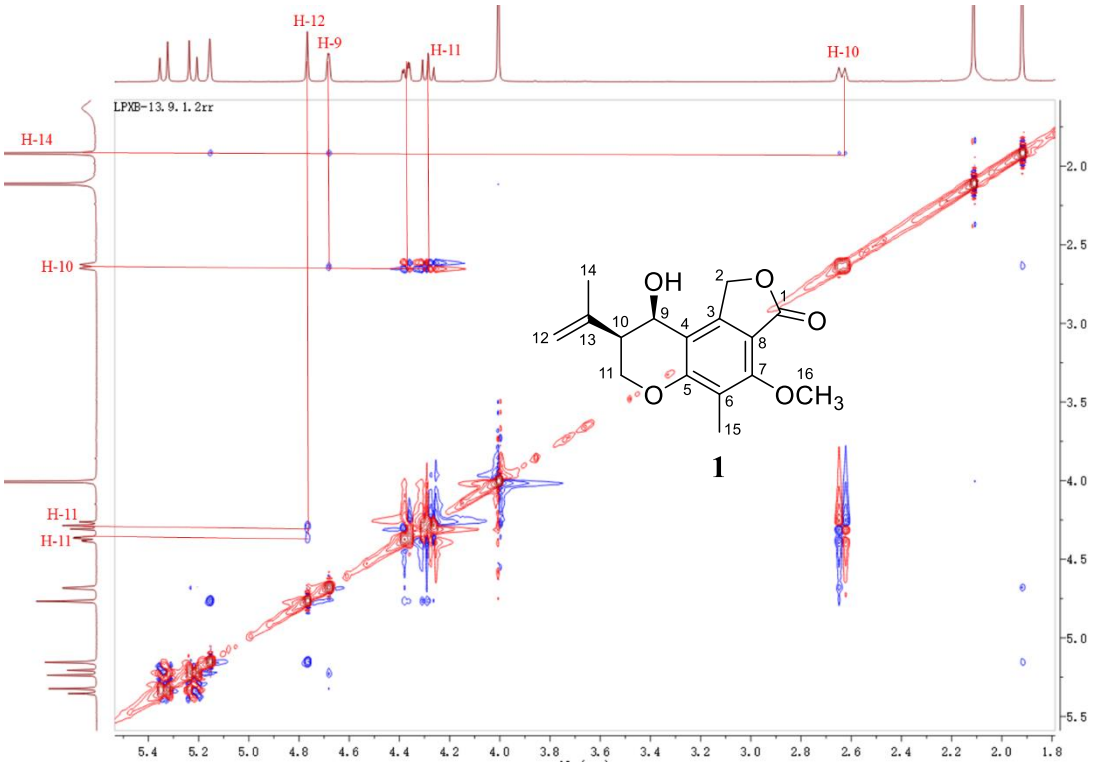


Figure S7: ROESY spectrum of **1.**

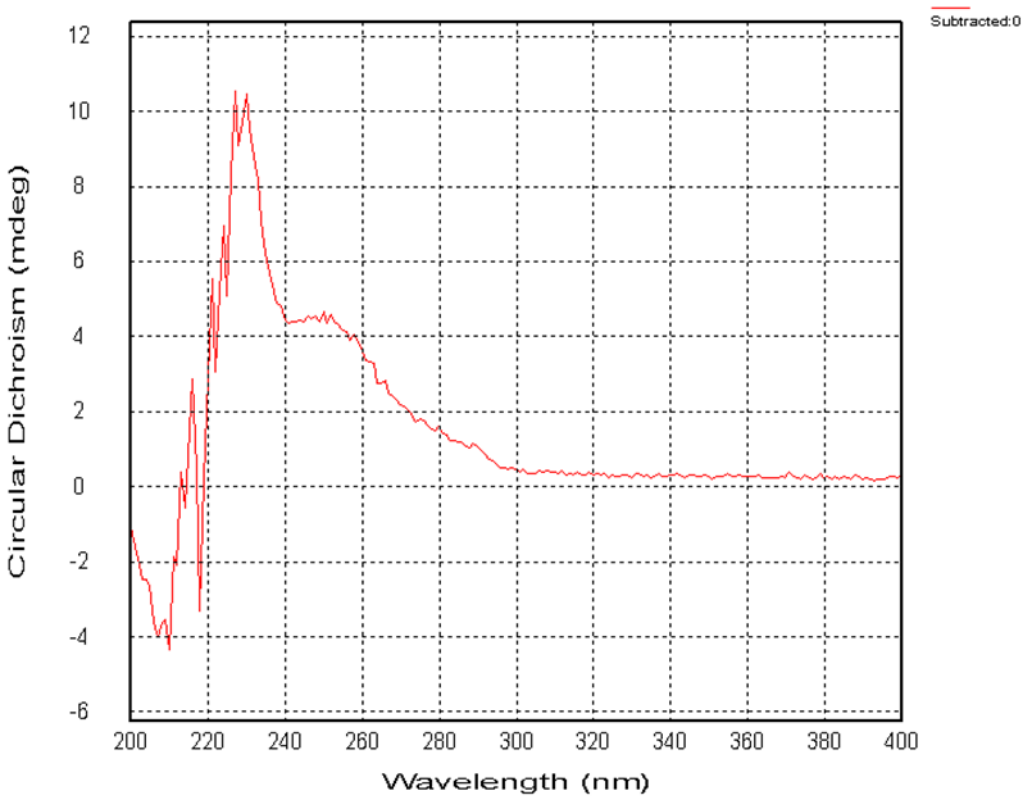


Figure S8: CD spectrum of **1.**

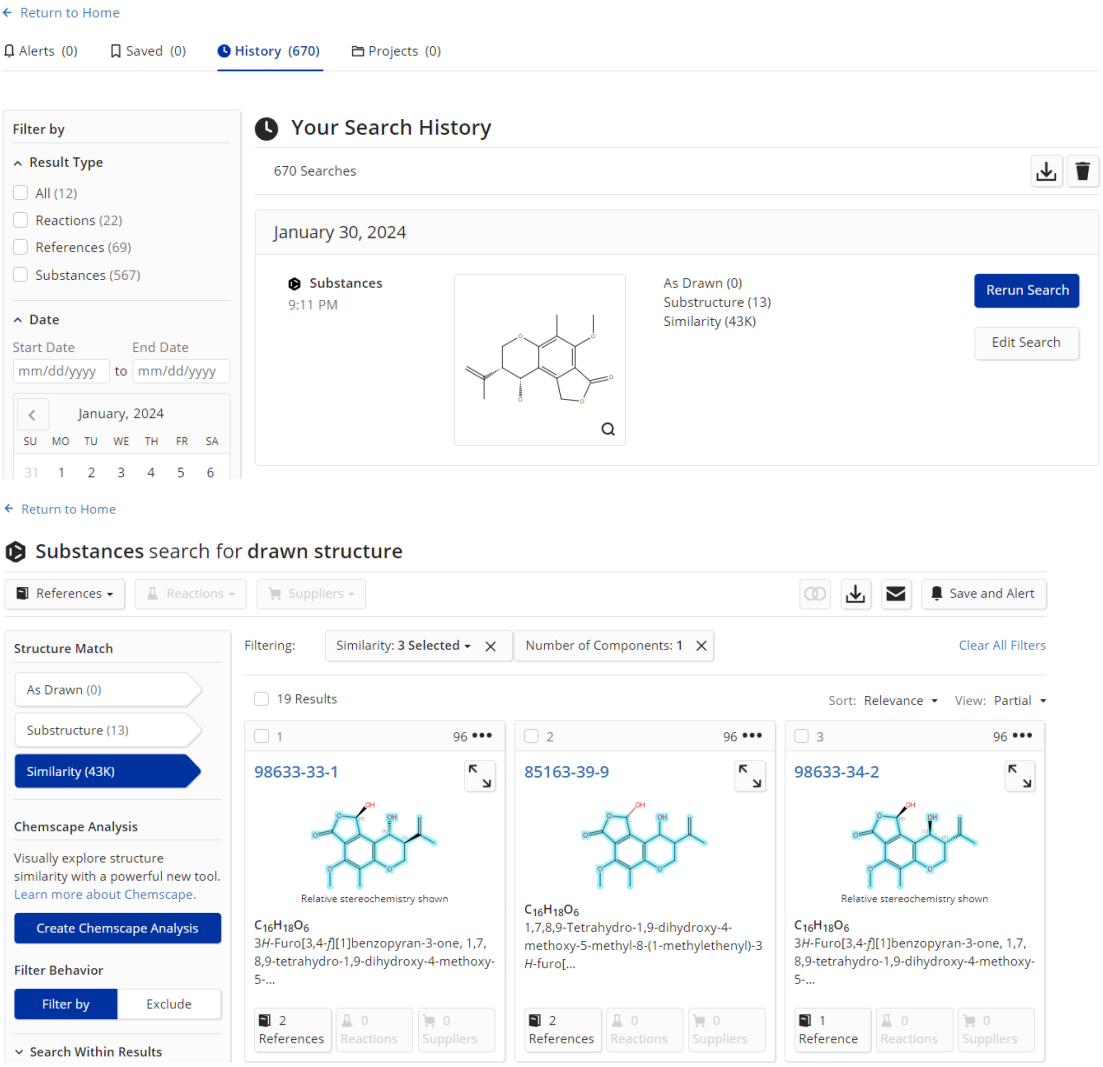


Figure S9: The Scifinder similarity report for **1.**

Table S1: ^{13}C NMR data for compound **1** and chromanol.

Position	**1**	**chromanol**
	δ_C, type	δ_C, type
1	169.2, C	166.8, C
2	67.8, CH_2	96.3, CH
3	148.4, C	148.0, C
4	112.5, C	117.3, C
5	159.0, C	159.4, C
6	120.2, C	121.4, C
7	157.6, C	157.5, C
8	109.6, C	111.0, C
9	60.8, CH	60.3, CH
10	44.5, CH	45.1, CH
11	64.4, CH_2	65.5, CH_2
12	114.1, CH_2	112.8, CH_2
13	140.8, C	142.7, C
14	23.3, CH_3	22.8, CH_3
15	8.7, CH_3	8.8, CH_3
16	62.3, OCH_3	62.4, OCH_3

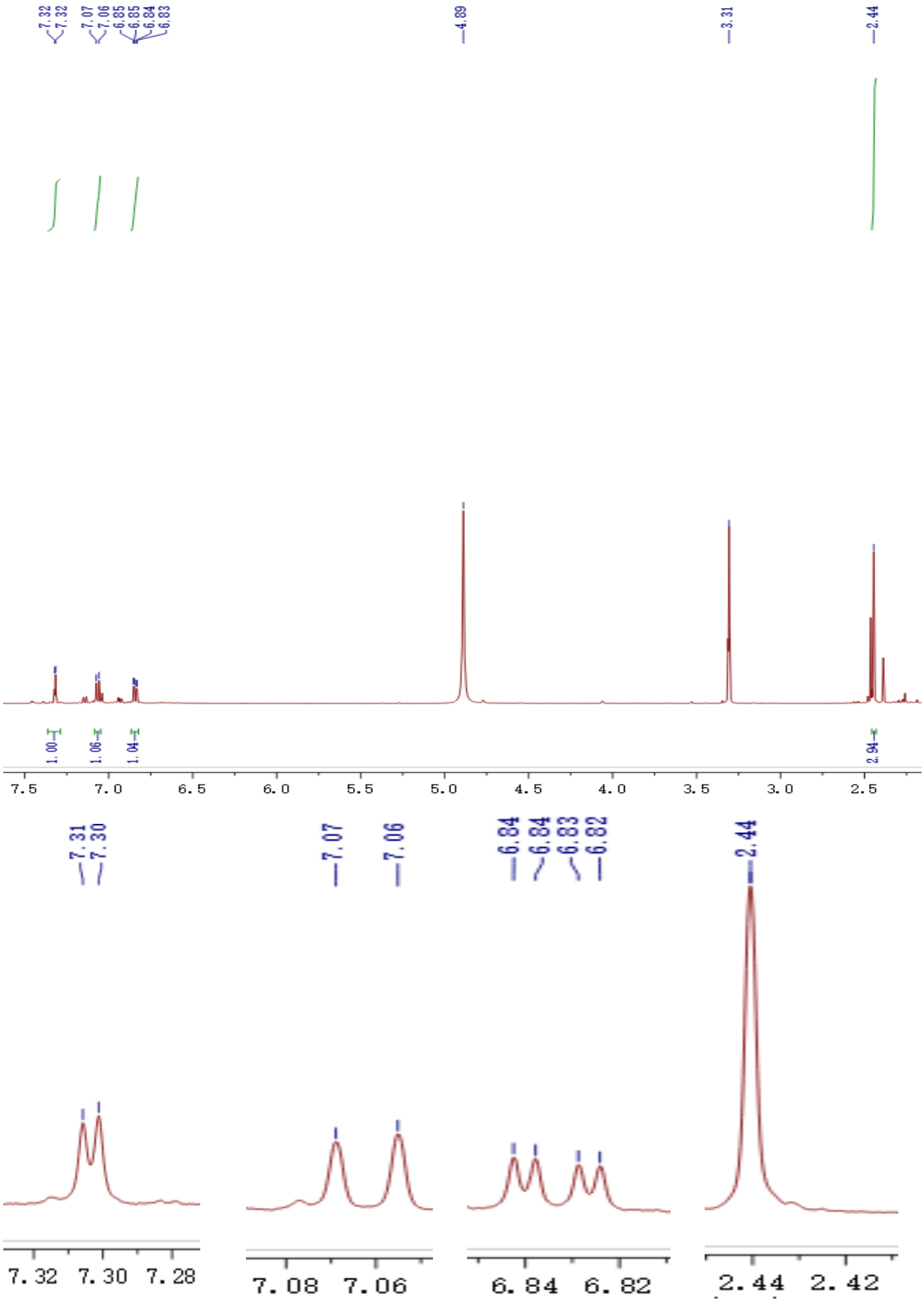


Figure S10: ^{1}H NMR spectrum of **2.**

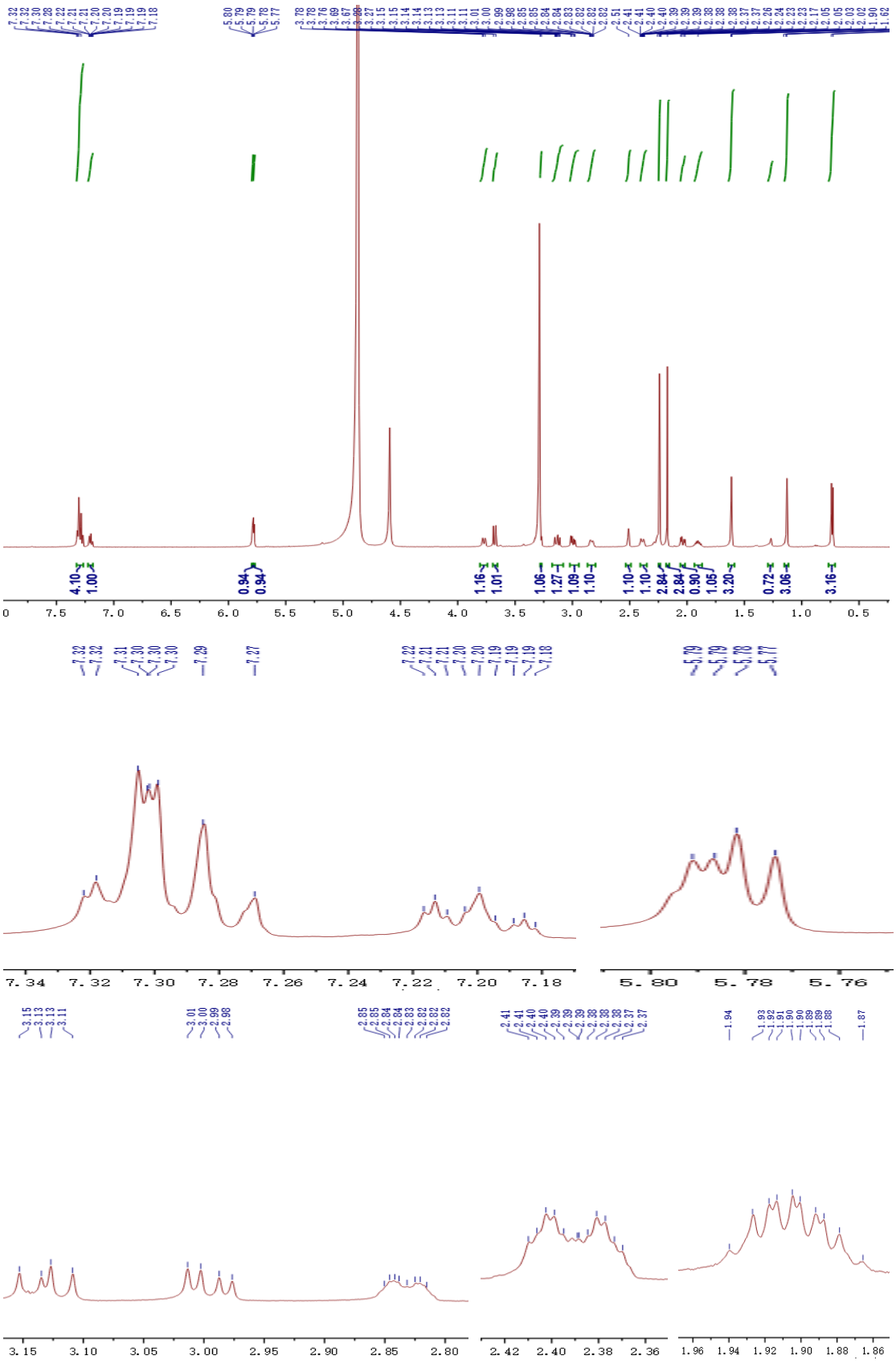


Figure S11: ^{1}H NMR spectrum of **3.**

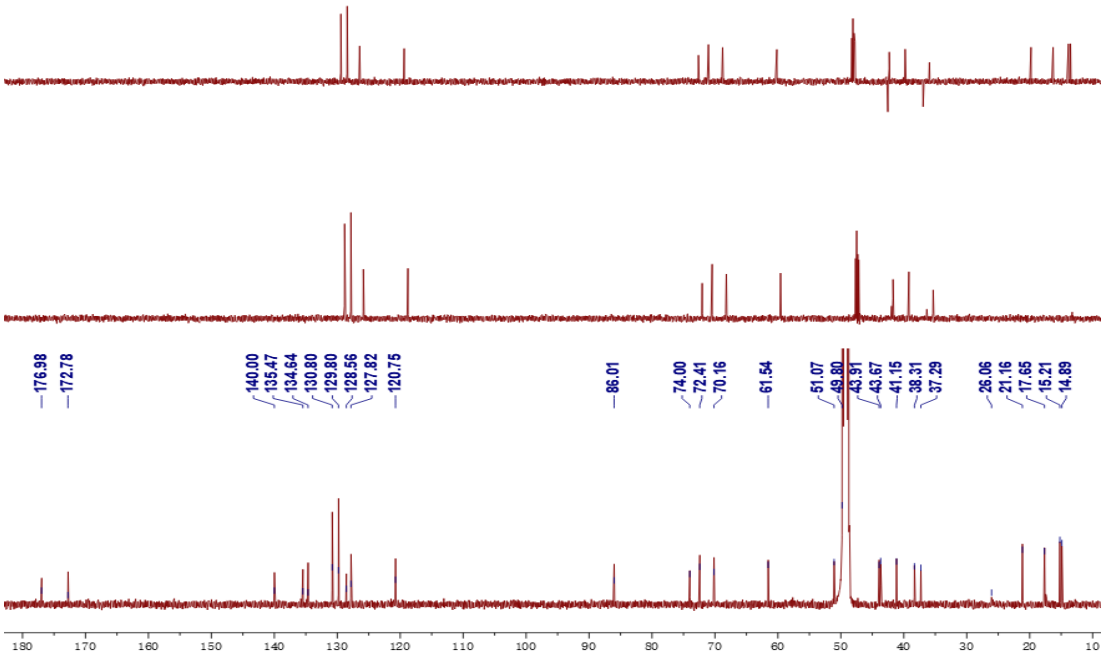


Figure S12: ^{13}C NMR spectrum of **3.**

Quantum chemical calculation

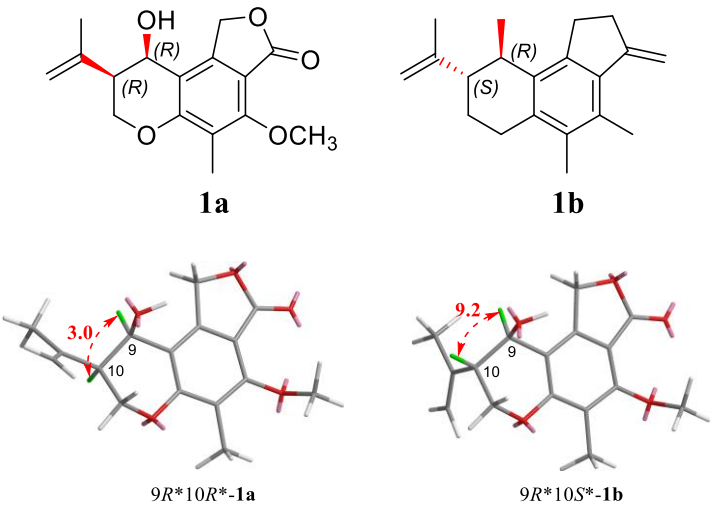


Figure S13: Calculated spin-spin coupling constants of compound **1**.

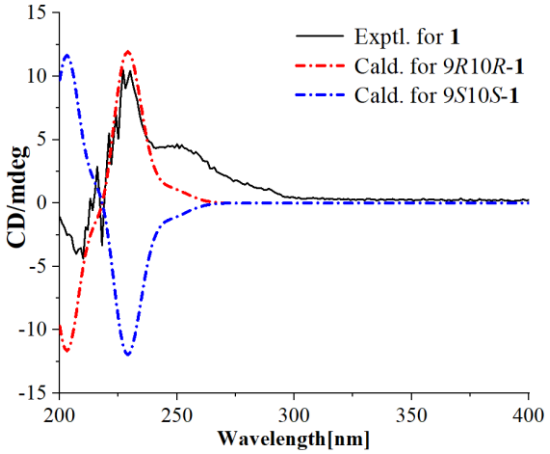


Figure S14: Experimental and calculated ECD spectra of **1** at the M062X/def2svp level in methanol.

Table S2: Important thermodynamic parameters of the wb97xd/Def2SVP optimized conformers of **1a** in the gas phase

Conformers	E[a](Hartree)	C[b](Hartree)	G[c](kcal/mol)
1a_1	-995.6179639	0.270943	-995.347021
1a_2	-995.6190602	0.27258	-995.346481
1a _3	-995.618917	0.272627	-995.34629
1a_4	-995.6182202	0.271988	-995.346232
1a_5	-995.6183233	0.272353	-995.34597
1a_6	-995.6180694	0.272614	-995.345456
1a_7	-995.6176966	0.272619	-995.345077
1a_8	-995.6179095	0.272996	-995.344913
1a_9	-995.6164512	0.271853	-995.344598
1a_10	-995.6162761	0.272153	-995.344123

[a]Electronic energy; [b]Thermal correction to Gibbs free energy ; [c]Gibbs free energy (E + C).

Table S3: Conformational analysis of the wb97xd/Def2SVP optimized conformers of **1a** in the gas phase (T=298.15 K)

Conformers	ΔG (kcal/mol)[a]	Population[b]
1a_1	0.000000	29.99%
1a_2	0.338850	16.92%
1a _3	0.458703	13.82%
1a_4	0.495098	13.00%
1a_5	0.659503	9.84%
1a_6	0.982038	5.71%
1a_7	1.219860	3.82%
1a_8	1.322770	3.21%
1a_9	1.520433	2.30%
1a_10	1.818495	1.39%

[a]The relative Gibbs free energy; [b]The Boltzmann distribution of each conformer.

Table S4: Cartesian coordinates for the low-energy optimized conformers of **1a** at wb97xd/Def2SVP level.

Conformer **1a_1**							
C	-0.050553	1.58905	1.272994	C	3.054392	3.218446	1.466749
C	-0.675818	0.438136	0.755247	H	2.11487	-2.738015	1.055677
C	0.026047	-0.730191	0.41735	H	2.581115	-2.08169	-0.526412
C	1.390497	-0.718288	0.686134	H	-2.899395	-1.168312	1.226483
C	2.044515	0.383289	1.228219	H	-3.713412	-0.290452	-0.096286
C	1.331076	1.566641	1.514983	H	-2.668471	-2.478717	-0.737516
C	2.402896	-1.817143	0.525157	H	-0.81391	-2.690488	0.622189
O	3.593894	-1.301425	1.0901	H	-0.252528	3.632898	1.900582
C	3.441657	-0.026925	1.52601	H	-1.437781	3.12056	0.660616
O	-2.004374	0.550961	0.550344	H	-1.635258	2.591972	2.333016
C	-2.737233	-0.62597	0.276675	H	0.289569	-1.953152	-1.844273
C	-2.064004	-1.558382	-0.724036	H	-2.190716	-1.694186	-4.221168
C	-0.668237	-1.94137	-0.174708	H	-1.693603	-2.971982	-3.069707
O	4.33978	0.560944	2.060012	H	-3.373169	-2.412904	-3.094907
C	-0.883733	2.806405	1.557926	H	-1.385226	0.952583	-1.736092
C	-1.991112	-1.049648	-2.156267	H	-1.571321	0.499249	-3.533146
O	0.12948	-2.587843	-1.133908	H	3.137046	4.243196	1.849812
C	-2.327213	-2.080298	-3.201609	H	3.940226	2.636687	1.750859
C	-1.62261	0.194856	-2.483922	H	2.967386	3.254187	0.367637
O	1.875231	2.67732	2.039186				

Conformer **1a_2**							
C	0.019911	1.633719	1.050826	C	3.13106	3.206025	0.666516
C	-0.666661	0.436214	0.774504	H	2.129168	-2.732136	1.230095
C	-0.013666	-0.787289	0.550521	H	2.397645	-2.313827	-0.473913
C	1.370468	-0.770048	0.661884	H	-2.982864	-1.039321	1.534643
C	2.088798	0.38492	0.958956	H	-3.762483	-0.267301	0.133755
C	1.420003	1.612286	1.147666	H	-2.812754	-2.567707	-0.277729
C	2.352108	-1.901397	0.54361	H	-0.998233	-2.571942	1.193236
O	3.604595	-1.333248	0.882189	H	-0.09401	3.75222	1.383951
C	3.509853	-0.007778	1.146161	H	-1.400389	3.094106	0.351581
O	-2.008303	0.556322	0.680607	H	-1.441	2.824232	2.095826
C	-2.798135	-0.607995	0.534596	H	-0.200584	-2.700113	-1.470415
C	-2.175993	-1.674169	-0.360453	H	-1.73185	0.177503	-3.348854
C	-0.801083	-2.046358	0.242097	H	-2.402383	0.82429	-1.827291
O	4.467476	0.632267	1.480021	H	-0.706465	0.348927	-1.90121
C	-0.76594	2.901506	1.229884	H	-2.569829	-3.29697	-2.45511
C	-2.085705	-1.318672	-1.837291	H	-2.214542	-2.075989	-3.819751
O	-0.095381	-2.9614	-0.545629	H	3.266636	4.270816	0.893666
C	-1.714206	0.080509	-2.25503	H	4.041081	2.647585	0.91951
C	-2.294471	-2.279874	-2.748418	H	2.911521	3.095767	-0.409024
O	2.026607	2.774319	1.443813				

Conformer **1a_3**							
C	0.015912	1.535297	1.085383	C	2.688844	2.287641	3.161753
C	-0.69072	0.456708	0.518205	H	1.88536	-2.961762	0.916677
C	-0.100543	-0.787816	0.241281	H	2.272175	-2.351139	-0.704509
C	1.248017	-0.907598	0.557967	H	-3.201242	-0.872436	0.697395
C	1.978321	0.126783	1.13471	H	-3.678399	0.133634	-0.691056
C	1.371132	1.369716	1.404481	H	-2.843713	-2.178464	-1.256717
C	2.184746	-2.065418	0.351797	H	-1.306465	-2.535907	0.461773
O	3.440705	-1.608506	0.821845	H	-0.044854	3.539896	1.849296
C	3.386736	-0.327842	1.259796	H	-1.017708	3.28782	0.376977
O	-1.983488	0.715758	0.226064	H	-1.61161	2.672057	1.921647
C	-2.821888	-0.342314	-0.194565	H	-0.109763	-2.415593	-2.044941
C	-2.138767	-1.345203	-1.117244	H	-1.042529	0.796682	-3.718683
C	-0.914651	-1.916638	-0.364527	H	-1.899291	1.324855	-2.24564
O	4.365275	0.241975	1.654493	H	-0.264323	0.678086	-2.119915
C	-0.699685	2.833356	1.32825	H	-2.331269	-2.64463	-3.451663
C	-1.77782	-0.822883	-2.500086	H	-1.649591	-1.312385	-4.565039
O	-0.158636	-2.788596	-1.154253	H	2.958158	3.301601	3.482418
C	-1.218066	0.566899	-2.659239	H	2.015181	1.842394	3.91353

C	-1.921153	-1.63606	-3.556498	H	3.59672	1.679091	3.058757
O	2.018893	2.430942	1.920084				

Conformer **1a_4**							
C	0.306398	2.198579	0.467894	C	3.344516	3.338505	1.835898
C	-0.373848	1.025904	0.081639	H	2.596165	-2.078685	0.181617
C	0.29013	-0.179202	-0.194409	H	2.506941	-1.581949	-1.531702
C	1.675494	-0.135492	-0.155971	H	-3.479142	0.234896	-0.400646
C	2.393569	1.002601	0.187598	H	-2.256563	0.159546	-1.708381
C	1.708502	2.191781	0.525848	H	-1.954116	-1.255428	0.976027
C	2.653407	-1.216805	-0.503913	H	-0.017123	-2.280847	0.01457
O	3.924657	-0.609823	-0.385414	H	0.163728	4.228485	1.155093
C	3.833686	0.694002	-0.012118	H	-1.02565	3.79312	-0.100308
O	-1.717716	1.120977	0.030256	H	-1.256194	3.211191	1.550941
C	-2.415921	0.075405	-0.619301	H	-0.885038	-2.406127	-2.170907
C	-1.937732	-1.283603	-0.127209	H	-3.323996	-4.49441	-0.065439
C	-0.459537	-1.436236	-0.55173	H	-1.771629	-3.949601	0.623906
O	4.812635	1.37771	0.090307	H	-3.289406	-3.353226	1.305821
C	-0.491327	3.430015	0.791186	H	-3.395284	-1.635045	-2.449183
C	-2.769569	-2.461409	-0.583121	H	-3.980023	-3.360518	-2.073999
O	-0.324043	-1.656872	-1.93441	H	3.452947	4.37666	2.173944
C	-2.794323	-3.632116	0.361514	H	3.066765	2.709439	2.698454
C	-3.404278	-2.484776	-1.762426	H	4.287828	2.979118	1.40619
O	2.305087	3.344238	0.871886				

Conformer **1a_5**							
C	0.336798	2.148637	0.619458	C	3.34672	3.834614	0.000212
C	-0.362955	0.964519	0.309887	H	2.531021	-2.149269	0.186498
C	0.284817	-0.228133	-0.047549	H	2.509163	-1.601389	-1.511946
C	1.668505	-0.174422	-0.119214	H	-3.490314	0.144526	0.092988
C	2.402624	0.970276	0.163358	H	-2.380691	0.093087	-1.313452
C	1.738104	2.157071	0.545815	H	-1.835213	-1.336541	1.32338
C	2.630607	-1.268954	-0.469362	H	0.021738	-2.331952	0.19705
O	3.911958	-0.699167	-0.290595	H	0.225154	4.241054	1.090642
C	3.840426	0.600299	0.102304	H	-1.222033	3.588094	0.258589
O	-1.706812	1.043168	0.384915	H	-0.951894	3.23031	1.966697
C	-2.447805	-0.002318	-0.215617	H	-1.040489	-2.47282	-1.902746
C	-1.915699	-1.359446	0.222857	H	-3.256816	-4.585721	0.387422
C	-0.479216	-1.495177	-0.331147	H	-1.653114	-4.028939	0.935176
O	4.8315	1.229546	0.343248	H	-3.107416	-3.45282	1.757942

C	-0.440335	3.375864	1.002482	H	-3.573329	-1.71312	-1.960142
C	-2.772522	-2.543805	-0.164317	H	-4.103449	-3.44731	-1.545841
O	-0.463188	-1.721006	-1.719312	H	3.490097	4.879537	0.30237
C	-2.698691	-3.720611	0.770139	H	4.291476	3.283415	0.087547
C	-3.511181	-2.567081	-1.281442	H	2.995986	3.810087	-1.045315
O	2.356469	3.305899	0.86702				

Conformer **1a_6**							
C	0.153094	1.548363	1.223625	C	3.401411	2.88003	1.368049
C	-0.580886	0.449883	0.73799	H	1.911284	-2.971271	1.090774
C	0.006806	-0.789583	0.433614	H	2.404241	-2.383462	-0.510244
C	1.366532	-0.900081	0.694296	H	-2.910708	-0.948531	1.262219
C	2.126315	0.149486	1.202474	H	-3.686943	-0.024194	-0.049732
C	1.528484	1.400947	1.462219	H	-2.834072	-2.279676	-0.745447
C	2.271688	-2.088689	0.540082	H	-1.054017	-2.627738	0.687829
O	3.513406	-1.672406	1.07874	H	0.153198	3.622488	1.779092
C	3.483627	-0.382056	1.492582	H	-1.090182	3.179106	0.567974
O	-1.893978	0.681085	0.525749	H	-1.316192	2.73387	2.261728
C	-2.729915	-0.431968	0.301467	H	-0.015739	-2.207753	-1.872391
C	-2.14404	-1.422059	-0.705351	H	-3.195627	-0.653644	-3.95334
C	-0.808415	-1.937082	-0.137598	H	-3.305946	-2.250843	-3.16236
O	4.438821	0.130235	2.005421	H	-4.191926	-0.873311	-2.492004
C	-0.557747	2.84827	1.472122	H	-0.204278	0.189382	-1.919693
C	-2.069297	-0.836915	-2.107354	H	-1.071885	0.333411	-3.560338
O	-0.09199	-2.717223	-1.055488	H	3.574831	3.907817	1.710701
C	-3.248323	-1.164703	-2.982627	H	4.230279	2.232252	1.679707
C	-1.06037	-0.073147	-2.545532	H	3.32176	2.879397	0.267742
O	2.176702	2.470315	1.953301				

Conformer **1a_7**							
C	-0.013167	1.634225	1.117778	C	2.533017	2.496411	3.304148
C	-0.639983	0.527762	0.509824	H	2.0859	-2.747924	0.97112
C	0.028447	-0.673521	0.223167	H	2.521612	-2.113136	-0.627764
C	1.369113	-0.726404	0.595597	H	-2.961147	-0.968599	0.786607
C	2.019098	0.332575	1.2193	H	-3.633985	-0.044328	-0.583494
C	1.336569	1.538159	1.482133	H	-2.645663	-2.273481	-1.171975
C	2.370135	-1.835282	0.423383	H	-0.910851	-2.595534	0.310588
O	3.579112	-1.32449	0.954041	H	-0.216153	3.612087	1.925386
C	3.441849	-0.052911	1.402471	H	-1.121702	3.343726	0.414134
O	-1.938687	0.710362	0.192923	H	-1.731708	2.654012	1.920309
C	-2.7047	-0.428181	-0.143493	H	0.395363	-1.865132	-2.056685

C	-2.002216	-1.382739	-1.101347	H	-1.889886	-1.474799	-4.600673
C	-0.670961	-1.837798	-0.454455	H	-1.543674	-2.790535	-3.43712
O	4.372388	0.558854	1.846326	H	-3.184836	-2.139514	-3.569006
C	-0.810642	2.882948	1.36464	H	-1.115012	1.097626	-2.030508
C	-1.799539	-0.864463	-2.517929	H	-1.19764	0.670839	-3.841063
O	0.166447	-2.501434	-1.366703	H	2.730709	3.518302	3.65066
C	-2.117482	-1.863906	-3.598702	H	1.856064	2.00099	4.020735
C	-1.340154	0.360386	-2.802102	H	3.477462	1.941803	3.229692
O	1.906501	2.623042	2.038058				

Conformer **1a_8**							
C	0.19921	1.586699	1.066203	C	2.850122	2.239212	3.210165
C	-0.542248	0.53512	0.492724	H	1.842524	-2.996679	1.026768
C	-0.004381	-0.739823	0.247918	H	2.307659	-2.438227	-0.592594
C	1.324588	-0.921187	0.615146	H	-2.981582	-0.722217	0.816778
C	2.087177	0.084062	1.200702	H	-3.592827	0.237816	-0.555738
C	1.53433	1.360744	1.43036	H	-2.814378	-2.065106	-1.180295
C	2.206118	-2.127856	0.455576	H	-1.185942	-2.51351	0.394974
O	3.468475	-1.728226	0.957513	H	0.206174	3.602126	1.807021
C	3.466387	-0.439234	1.375657	H	-0.725799	3.375983	0.303934
O	-1.81515	0.842017	0.16355	H	-1.400134	2.807432	1.83325
C	-2.693052	-0.222039	-0.126289	H	0.070419	-2.157327	-2.073999
C	-2.082486	-1.248035	-1.080243	H	-2.809449	-0.42605	-4.40317
C	-0.831516	-1.83755	-0.402408	H	-3.084107	-2.011069	-3.627979
O	4.461072	0.086033	1.790992	H	-3.93648	-0.579489	-3.031191
C	-0.461764	2.919882	1.270634	H	0.047691	0.237147	-2.124536
C	-1.855167	-0.67287	-2.469921	H	-0.668757	0.429685	-3.831219
O	-0.088007	-2.656939	-1.262603	H	3.149711	3.245028	3.529659
C	-2.974825	-0.930047	-3.441483	H	2.141921	1.826275	3.94852
C	-0.767751	0.025817	-2.820156	H	3.735937	1.595185	3.134379
O	2.216286	2.397219	1.9514				

Conformer **1a_9**							
C	0.327769	2.14628	0.615892	C	3.362745	3.787087	-0.012142
C	-0.359095	0.938721	0.373977	H	2.531565	-2.166767	0.596774
C	0.300692	-0.275693	0.133591	H	2.581672	-1.746336	-1.136583
C	1.687092	-0.221872	0.108403	H	-3.464869	0.12566	-0.014789
C	2.409433	0.943174	0.328574	H	-2.247299	-0.001997	-1.320639
C	1.730594	2.153742	0.595624	H	-1.993577	-1.33714	1.413761
C	2.66121	-1.337341	-0.11782	H	-0.021046	-2.311627	0.674414
O	3.934808	-0.753544	0.071353	H	0.196815	4.270974	0.898921

C	3.848538	0.572427	0.356833	H	-1.22784	3.538767	0.09367
O	-1.704837	1.015984	0.385315	H	-0.996506	3.334995	1.832753
C	-2.402356	-0.050014	-0.227892	H	-0.509335	-2.959653	-1.391693
C	-1.932733	-1.394217	0.314454	H	-3.868379	-3.451651	-1.796409
C	-0.440665	-1.575321	-0.039316	H	-4.150002	-1.711605	-1.574159
O	4.829093	1.221051	0.589237	H	-2.625843	-2.2599	-2.285167
C	-0.463274	3.397571	0.871282	H	-2.451647	-3.692806	1.625004
C	-2.763968	-2.575773	-0.154885	H	-3.455915	-4.532863	0.296169
O	-0.232697	-2.037319	-1.358606	H	3.492034	4.853536	0.210696
C	-3.38482	-2.503145	-1.525882	H	4.302863	3.248325	0.160599
C	-2.894105	-3.654475	0.625128	H	3.058424	3.676818	-1.066649
O	2.335462	3.325946	0.850207				

Conformer **1a_10**							
C	0.320475	2.182317	0.448346	C	3.288938	3.396848	1.890147
C	-0.357505	0.988754	0.125318	H	2.547315	-2.132977	0.635551
C	0.298387	-0.243053	-0.015801	H	2.565164	-1.772545	-1.11321
C	1.682067	-0.211734	0.091473	H	-3.424783	0.227898	-0.562513
C	2.398404	0.94229	0.377855	H	-2.090249	0.053739	-1.742211
C	1.716558	2.163835	0.581973	H	-2.128815	-1.239669	1.02426
C	2.659982	-1.32899	-0.110928	H	-0.115496	-2.274039	0.479839
O	3.93265	-0.730666	0.033905	H	0.175238	4.265144	0.95098
C	3.84249	0.600774	0.290369	H	-0.956067	3.736755	-0.322274
O	-1.694382	1.094184	-0.010649	H	-1.27884	3.302436	1.358747
C	-2.350404	0.028916	-0.668975	H	-0.408724	-2.908277	-1.625997
C	-1.962763	-1.314404	-0.063129	H	-3.729222	-3.366698	-2.322844
C	-0.447677	-1.527293	-0.26787	H	-4.00037	-1.619675	-2.14756
O	4.824718	1.279481	0.3944	H	-2.426929	-2.20121	-2.707823
C	-0.473319	3.445863	0.623452	H	-2.642478	-3.587413	1.217924
C	-2.767522	-2.487752	-0.595536	H	-3.532965	-4.427298	-0.189758
O	-0.123523	-1.990131	-1.563608	H	3.40643	4.460112	2.133854
C	-3.256698	-2.422668	-2.019236	H	2.936483	2.861784	2.788115
C	-2.989008	-3.554214	0.180689	H	4.247357	2.976128	1.561093
O	2.315084	3.333447	0.861631				