

Supporting Information

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Two undescribed phenylpropanoid derivatives from *Notopterygium incisum* roots with anti-inflammatory potential

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Abstract: Two previously undescribed phenylpropanoid derivatives, including a terpenylated coumarin (1) and a ferulic acid analogue (2), were isolated from the roots of *Notopterygium incisum* (Umbelliferae). Their structures were successfully established using spectroscopic techniques, including mass spectrometry (MS), nuclear magnetic resonance (NMR), and electronic circular dichroism (ECD) spectroscopy. In vitro anti-inflammatory assay using a lipopolysaccharide-stimulated RAW264.7 macrophages indicated compounds 1–2 owed anti-inflammatory potential by inhibiting the secretion of NO at the concentration of 7.5 μ M.

Keywords: *Notopterygium incisum*, Phenylpropanoid derivatives, Nitric oxide, Anti-inflammatory

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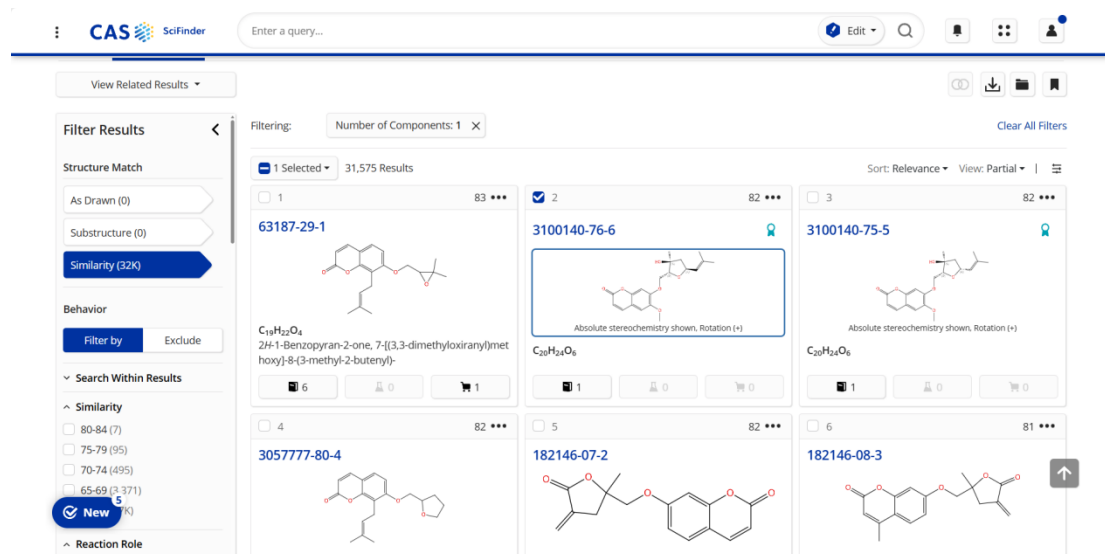


Figure S1: SciFinder search results for compound **1** (similarity >81%).

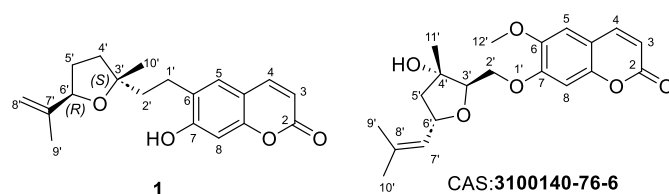


Figure S2: The structures of compound **1** and structurally similar compounds

Table S1: The NMR data of compound **1** and **3100140-76-6** (δ in ppm, J in Hz)

Compound 1			3100140-76-6		
	δ_C	$\delta_H J(\text{Hz})$		δ_C	$\delta_H J(\text{Hz})$
1	-	-	1	-	-
2	161.8	-	2	161.4	-
3	112.7	6.19, d (9.4)	3	114.0	6.30, d (9.5)
4	143.5	7.57, d (9.5)	4	143.3	7.61, d (9.5)
4a	112.0	-	4a	112.1	-
5	128.5	7.12, s	5	108.3	6.85, s
6	126.8	-	6	146.7	-
7	159.1	-	7	151.6	-
8	104.6	6.82, s	8	101.3	6.85, s
8a	154.9	-	8a	149.6	-
1'	24.8	2.76, m; 2.69, m	1'	-	-
2'	41.2	1.83-1.90, m; 1.91-2.00, m	2'	68.9	4.33, dd (9.1, 5.0); 4.00, dd (9.1, 7.8)
3'	84.5	-	3'	81.4	4.19, dd (7.8, 5.0)
4'	37.5	1.82-1.91, m	4'	78.8	-
5'	31.2	1.85-1.95, m; 2.10-2.16, m	5'	47.1	2.24, dd (13.0, 7.0); 1.98, dd (13.0, 8.6)
6'	83.7	4.49, m	6'	74.8	4.86, m,

7'	144.7	-	7'	126.3	4.86, m
8'	111.2	4.87, s; 5.07, s	8'	136.6	-
9'	18.2	1.76, s	9'	18.2	1.70, d (1.3)
10'	26.8	1.30, s	10'	22.1	1.38, s
			11'	26.0	1.75, d (1.3)
			12'	56.4	3.88, s

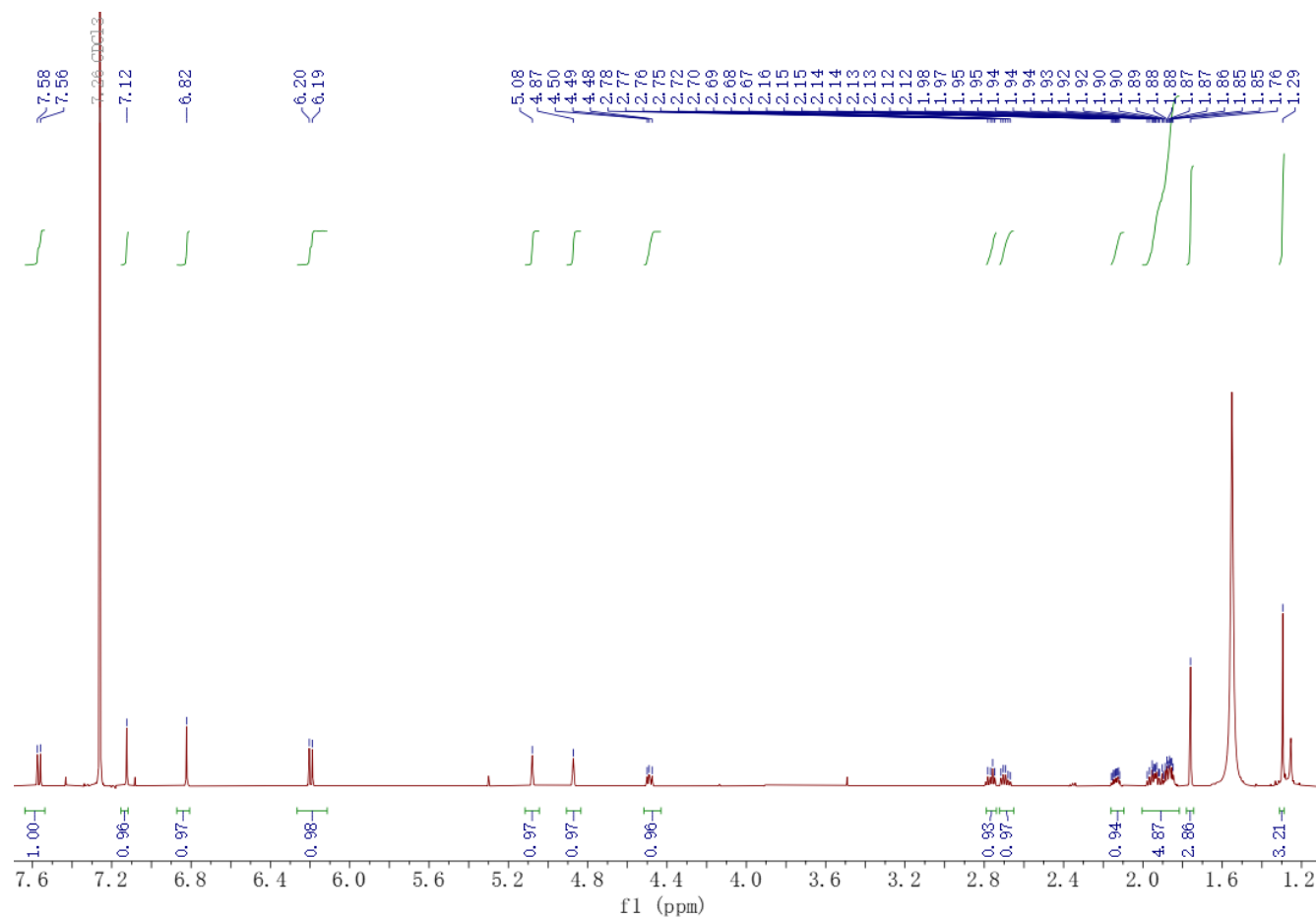


Figure S3: ¹H NMR spectrum of **1** in CDCl₃ (600 MHz)

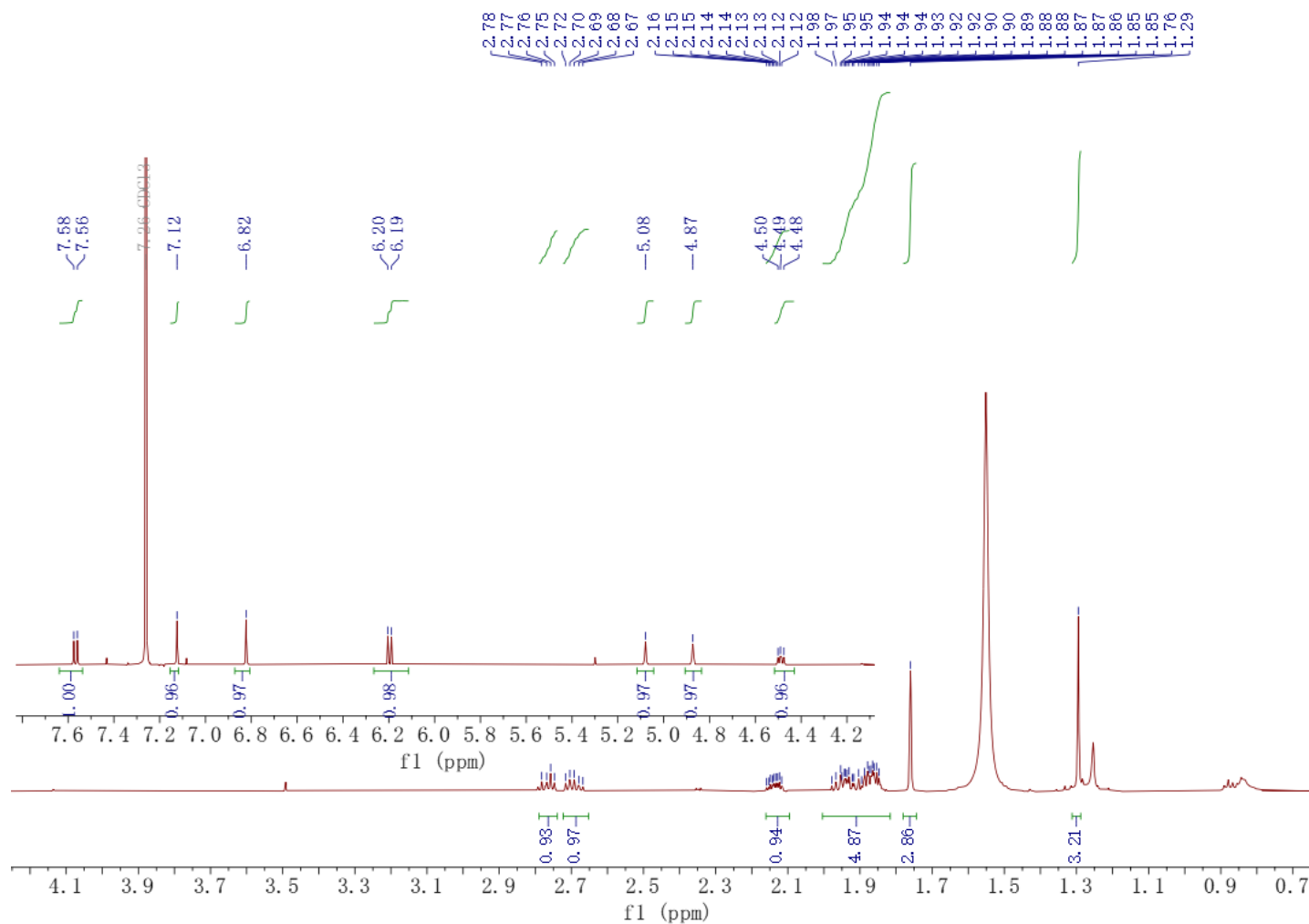


Figure S4: Enlarged ^1H NMR spectrum of **1** in CDCl_3 (600 MHz)

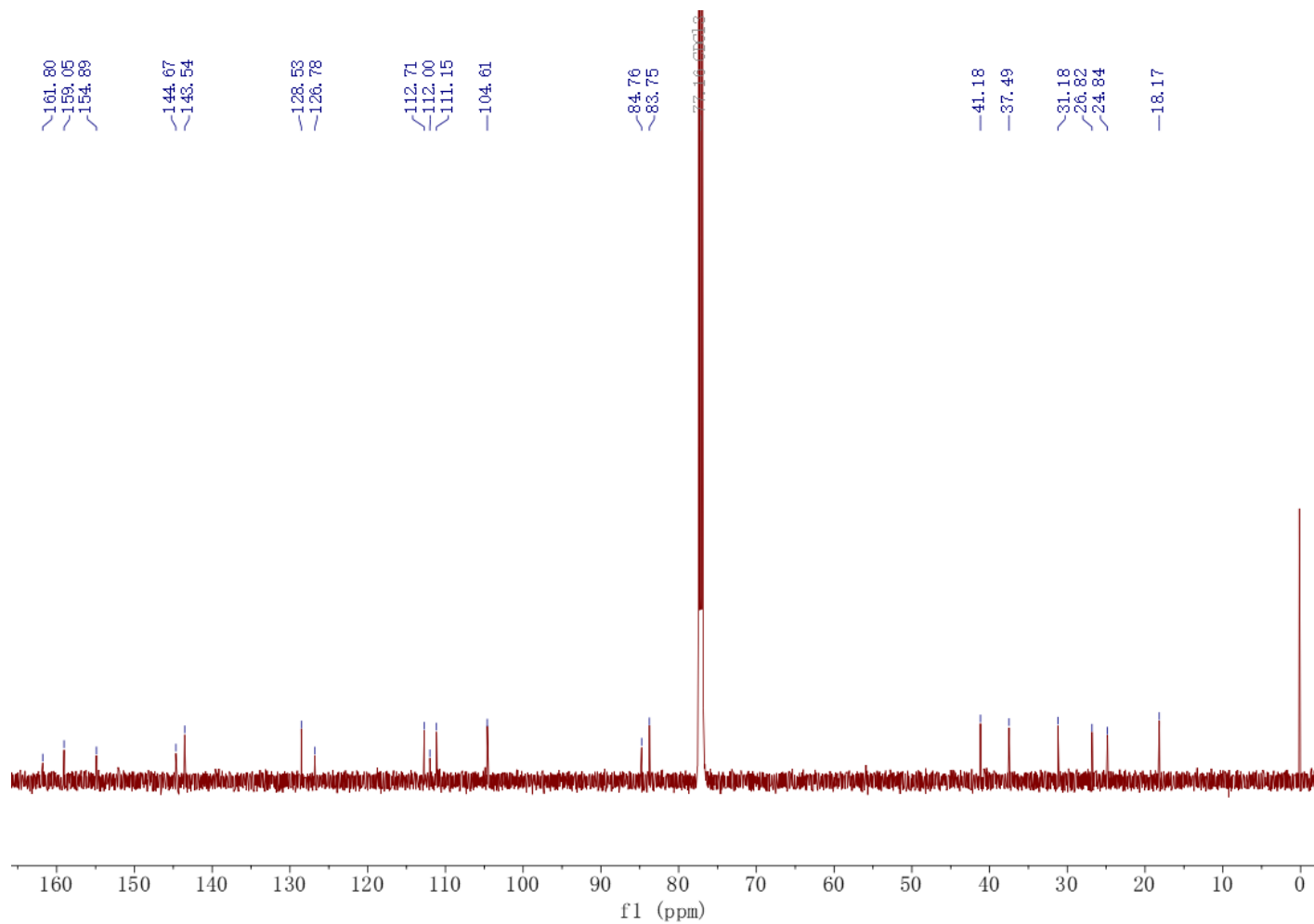


Figure S5: ^{13}C NMR spectrum of **1** in CDCl_3 (150 MHz)

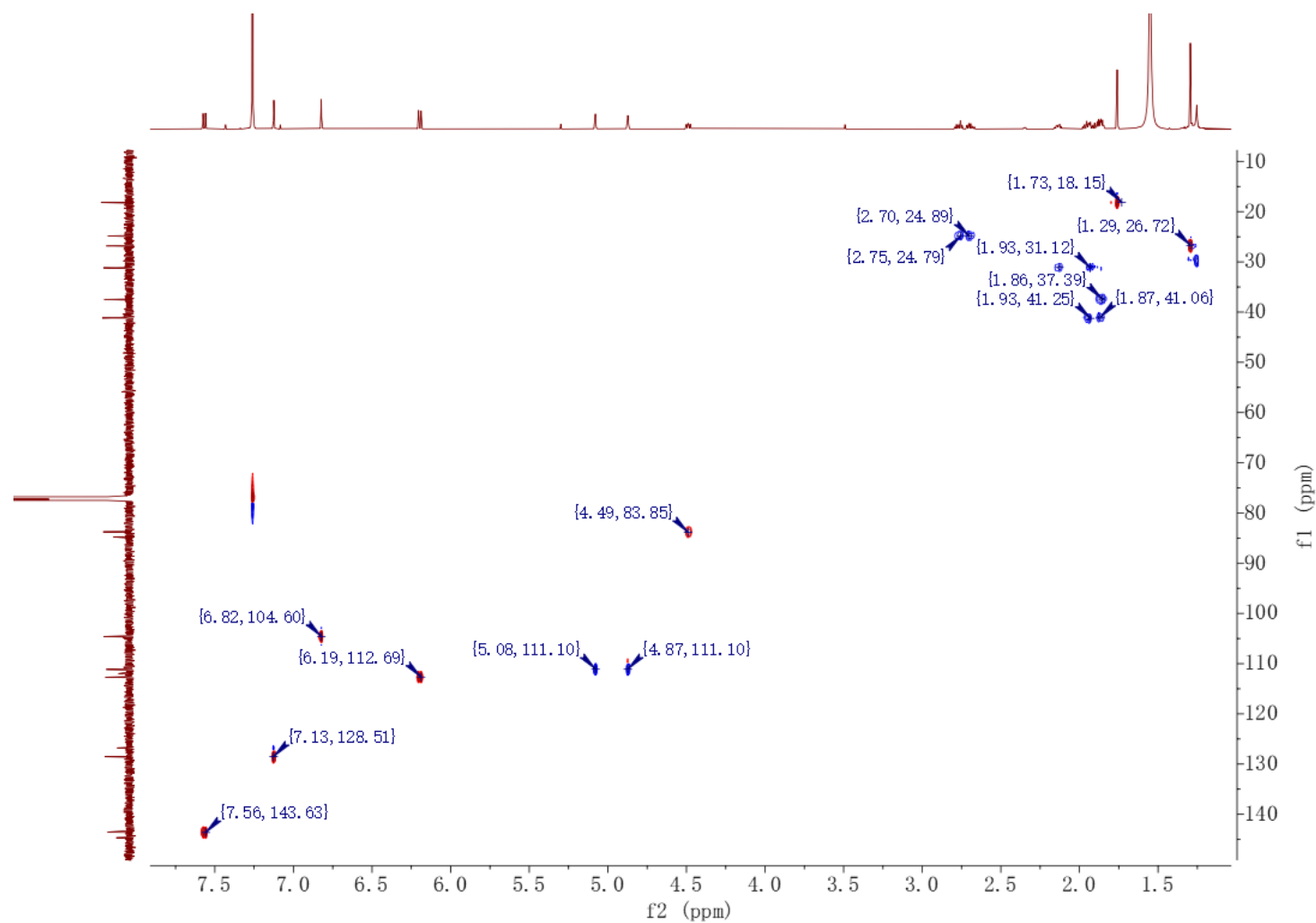


Figure S6: HSQC spectrum of **1** in CDCl₃

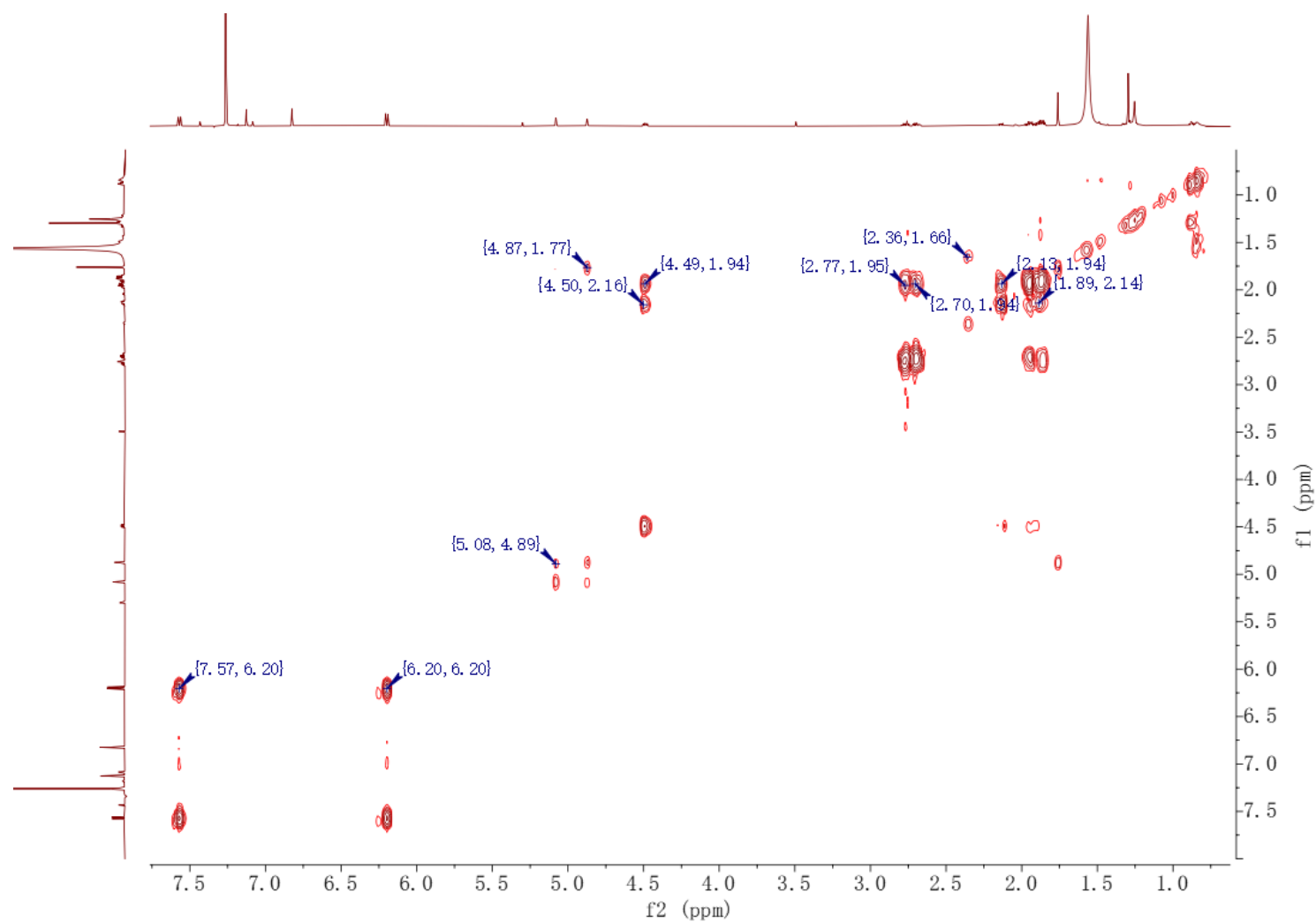


Figure S7: ^1H - ^1H COSY spectrum of **1** in CDCl_3

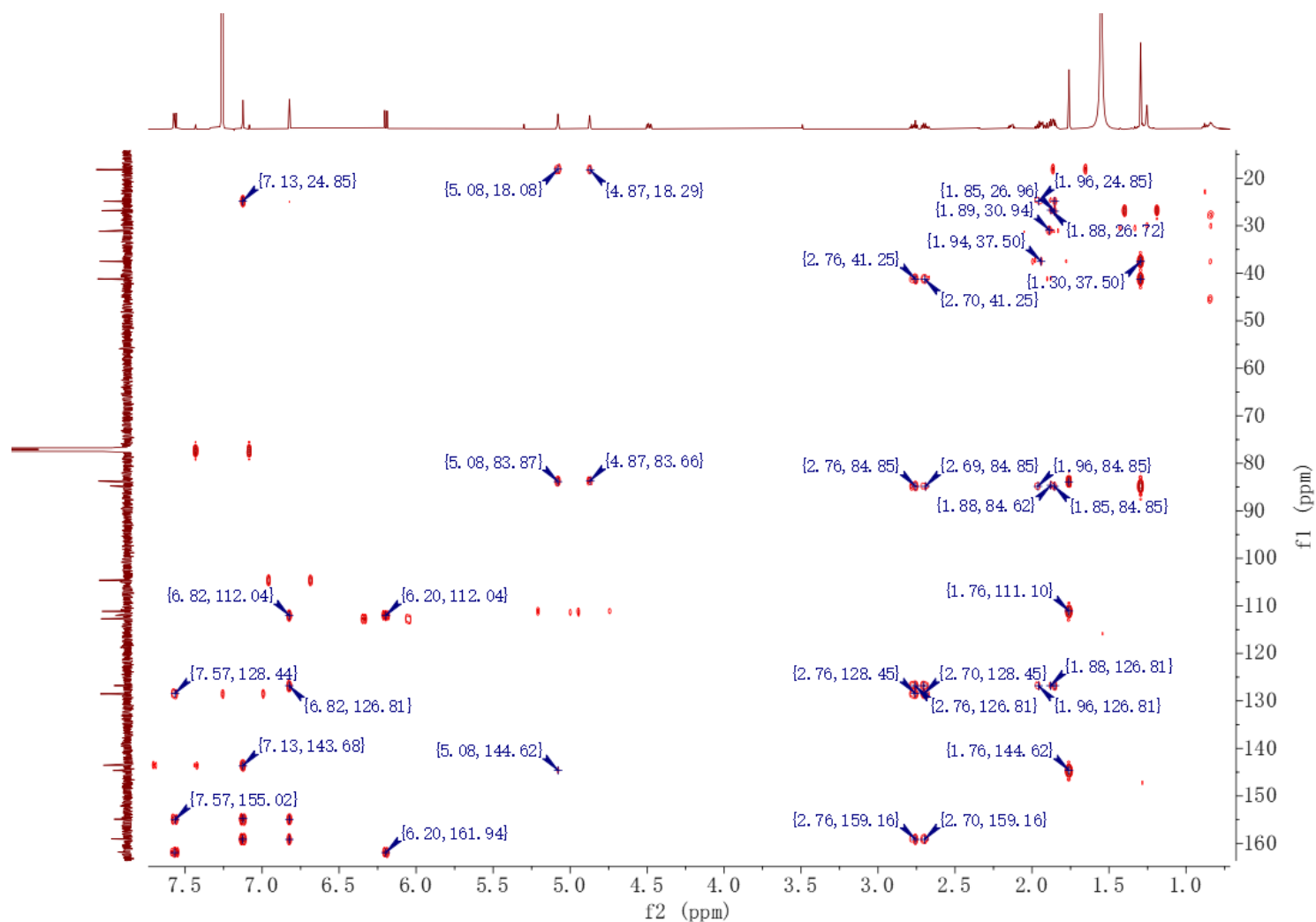


Figure S8: HMBC spectrum of **1** in CDCl_3

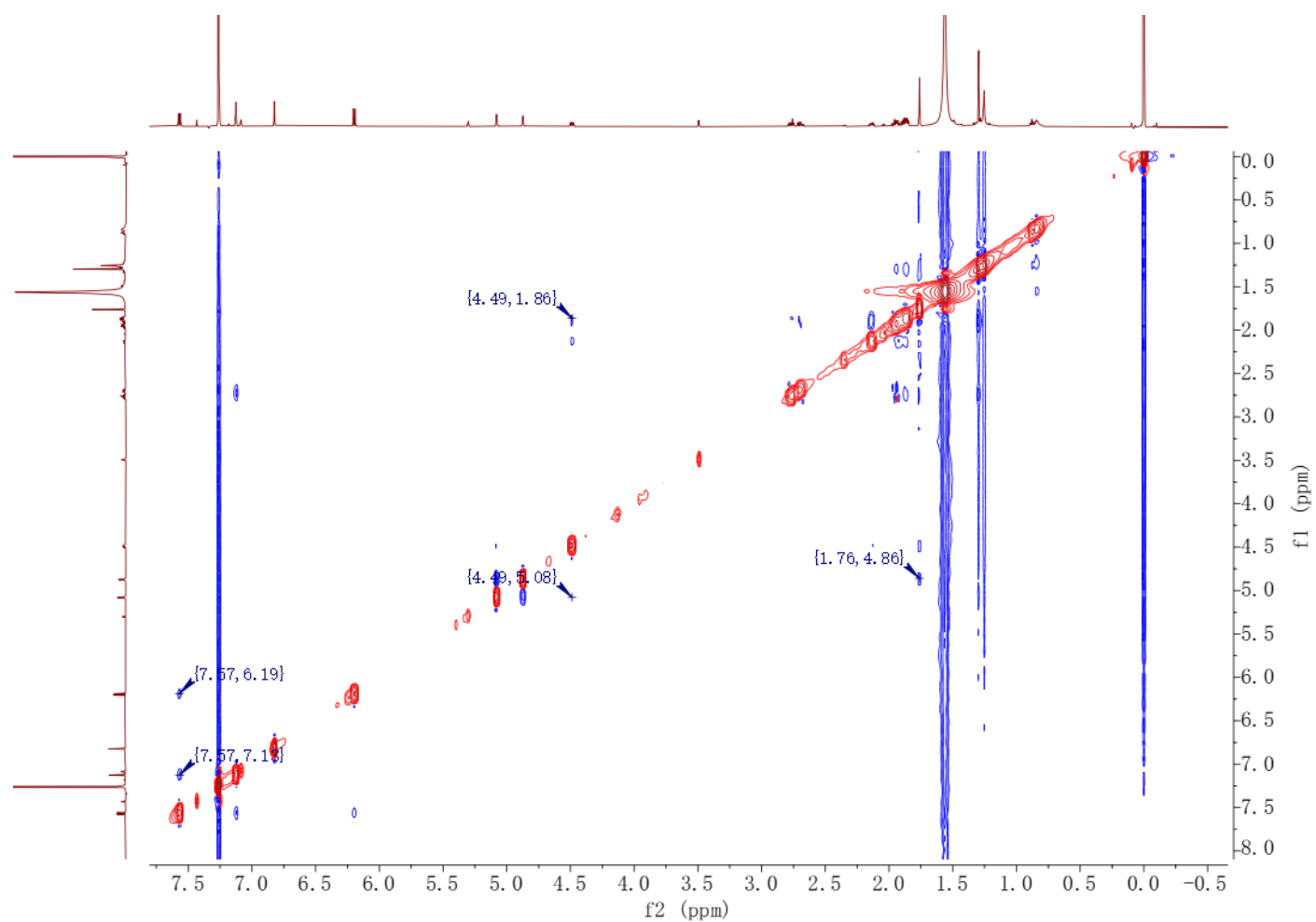


Figure S9: NOESY spectrum of **1** in CDCl₃

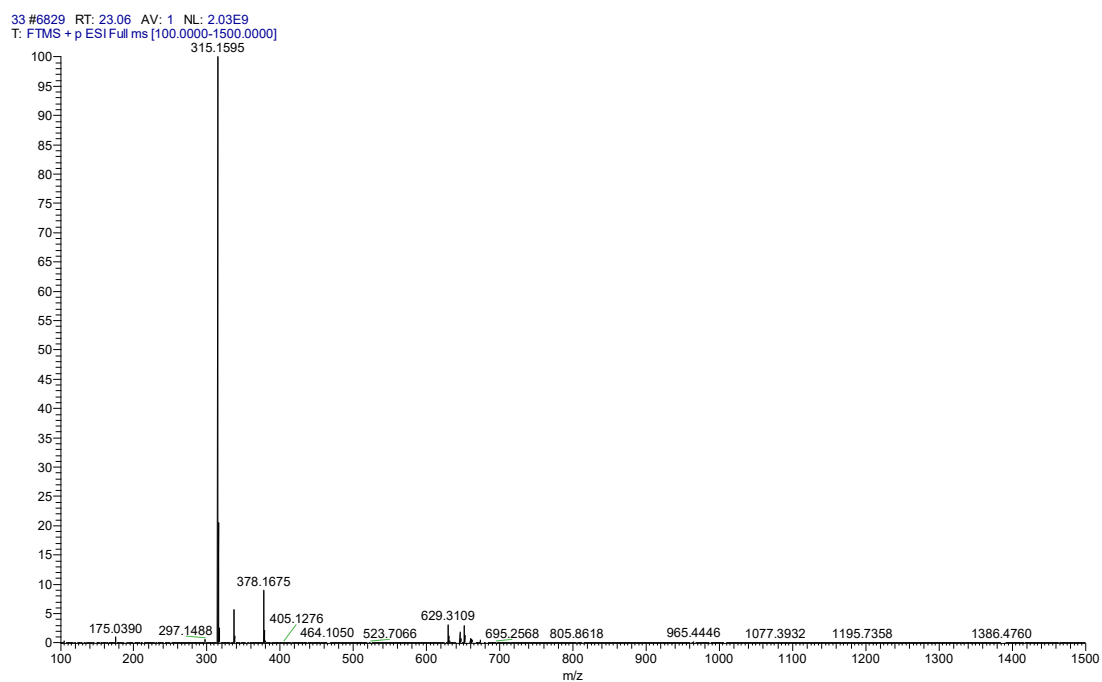


Figure S10: HRESIMS spectrum of 1

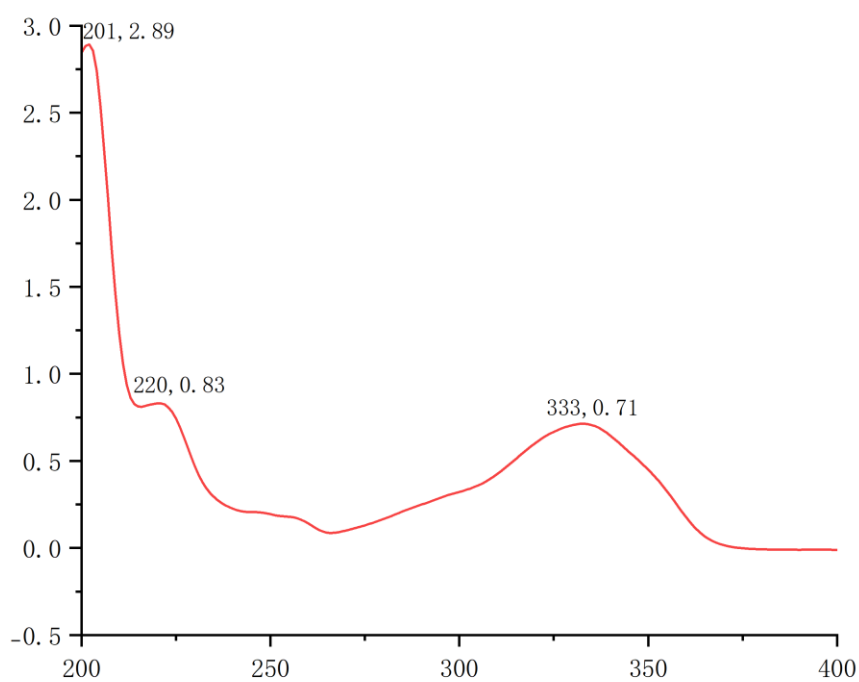


Figure S11: UV spectrum of compound 1

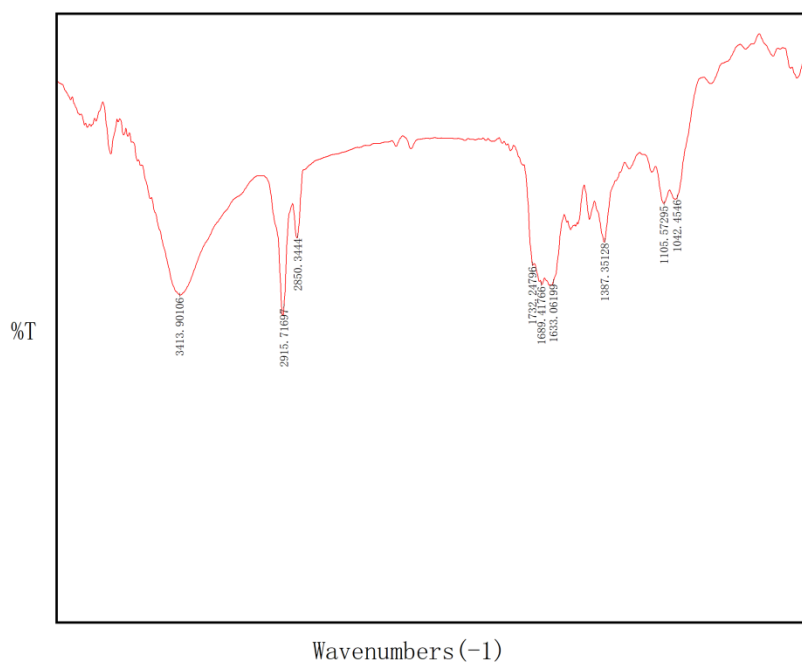


Figure S12: IR spectrum of compound **1**

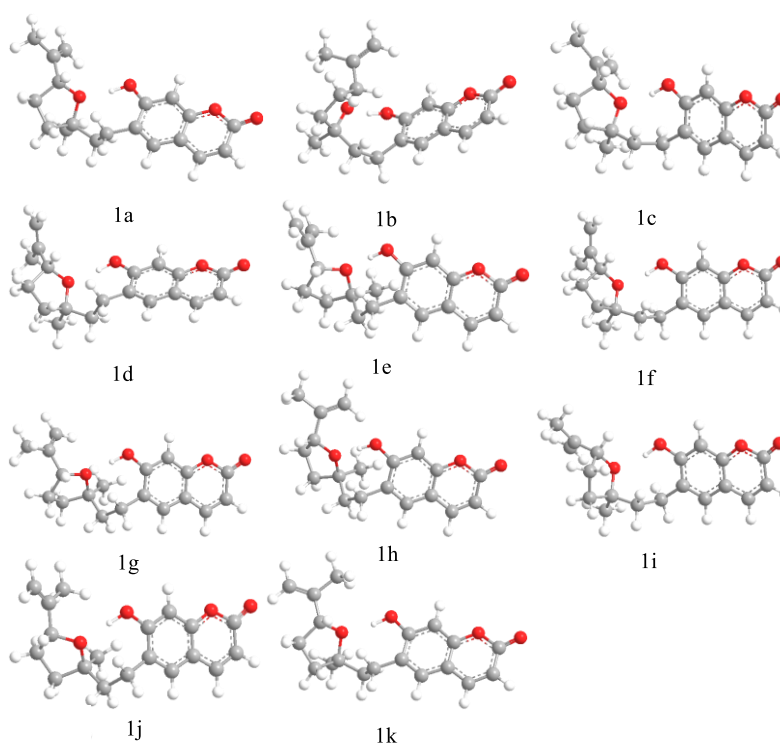


Figure S13: Most stable conformers of 3'S, 6'R-1 calculated at the CAM-B3LYP/DGTZVP level

Table S2: Energies and atomic Cartesian coordinates of geometry-optimized conformers of

3'S, 6'R-1 at wb97xd/dgdzvp in methanol

	1a			1b			1c			1d		
Gibbs free energy (hartrees)	-1037.62544			-1037.625272			-1037.62518			-1037.624962		
ΔG (kcal/mol)				0.105			0.163			0.3		
Population Proportion	21.38%			17.89%			16.23%			12.88%		
Element	X	Y	Z	X	Y	Z	X	Y	Z	X	Y	Z
C	-0.903317	-0.739538	-0.406076	-0.466451	-1.243795	0.794577	0.975951	-0.872120	-0.497121	-0.891282	-0.741806	-0.431011
C	-0.913758	0.611570	0.031474	-0.330934	-0.032569	1.517074	0.916064	0.533358	-0.303395	-0.906826	0.602000	0.028095
C	-2.115816	1.281371	0.256734	-1.281262	0.980678	1.415777	2.074402	1.275264	-0.077785	-2.111019	1.257571	0.281842
C	-3.313726	0.611047	0.056903	-2.364497	0.810545	0.566104	3.298469	0.623399	-0.036192	-3.305962	0.579771	0.089394
C	-3.346832	-0.722215	-0.364623	-2.518944	-0.353453	-0.193956	3.399958	-0.760292	-0.214013	-3.333819	-0.747017	-0.352575
C	-2.120954	-1.371382	-0.588967	-1.556995	-1.365432	-0.053682	2.216506	-1.482632	-0.443664	-2.105910	-1.381636	-0.605681
O	-4.467399	1.308050	0.292112	-3.268491	1.834800	0.487369	4.408040	1.391422	0.189131	-4.461928	1.262680	0.352746
C	-5.710853	0.748165	0.133197	-4.367036	1.783944	-0.332974	5.671549	0.858409	0.255256	-5.702778	0.694347	0.203329
C	-5.765484	-0.635703	-0.304694	-4.548639	0.579784	-1.127297	5.797376	-0.576824	0.070431	-5.751960	-0.682945	-0.255326
C	-4.633793	-1.335169	-0.542326	-3.665686	-0.439554	-1.058419	4.709829	-1.347202	-0.153799	-4.617947	-1.368574	-0.520606
O	-6.672347	1.457605	0.372123	-5.106272	2.752089	-0.331994	6.589034	1.632730	0.463657	-6.666658	1.391507	0.467409
O	0.211610	1.326689	0.237981	0.723823	0.189334	2.343300	-0.239732	1.229704	-0.343595	0.215568	1.323358	0.229031
C	0.398004	-1.463070	-0.651657	0.500370	-2.401634	0.939927	-0.283676	-1.665092	-0.741339	0.412760	-1.448819	-0.707842
C	1.166271	-1.802344	0.648935	1.550600	-2.525455	-0.182298	-1.165869	-1.805376	0.525793	1.205225	-1.799300	0.575098
C	2.623802	-1.337412	0.656243	2.851172	-1.729932	0.034067	-2.629732	-1.427375	0.305020	2.659013	-1.322177	0.565648
C	3.491570	-1.953475	-0.448683	3.578981	-1.482304	-1.290272	-3.428820	-1.345848	1.611970	3.513941	-1.918656	-0.560923
C	4.470463	-0.833160	-0.790765	2.856725	-0.264420	-1.876747	-4.411544	-0.207395	1.350830	4.467711	-0.780684	-0.917940
C	3.606952	0.425212	-0.625418	2.250706	0.453182	-0.647374	-3.575048	0.759686	0.503086	3.581293	0.456835	-0.749461
O	2.616549	0.083543	0.352279	2.555738	-0.390898	0.481242	-2.634596	-0.062659	-0.199650	2.638967	0.104575	0.283589
C	4.382871	1.656086	-0.227726	2.795062	1.832278	-0.368764	-4.385675	1.610365	-0.442523	4.300163	1.729657	-0.370985
C	4.241000	2.232066	0.968360	1.980426	2.890798	-0.401092	-4.314235	1.468338	-1.768224	4.377973	2.735983	-1.246781
C	5.328784	2.163452	-1.283762	4.265396	1.929265	-0.062583	-5.280406	2.614366	0.234852	4.913543	1.790577	1.002518
C	3.239788	-1.523198	2.041030	3.737577	-2.365101	1.095167	-3.315017	-2.324668	-0.724681	3.297684	-1.524366	1.937571
H	-2.108438	2.314247	0.586357	-1.154604	1.900185	1.975898	2.014251	2.348485	0.063968	-2.107589	2.285185	0.627580
H	-2.135814	-2.405751	-0.921970	-1.685219	-2.283173	-0.622278	2.284439	-2.557526	-0.588498	-2.116756	-2.410636	-0.955029
H	-6.752802	-1.062442	-0.426541	-5.422161	0.553665	-1.766112	6.799793	-0.981967	0.122966	-6.737252	-1.116527	-0.369172
H	-4.686903	-2.369153	-0.869784	-3.811967	-1.333948	-1.656540	4.816125	-2.419183	-0.290585	-4.667050	-2.397837	-0.863259
H	1.039555	0.789296	0.205485	1.531111	-0.119972	1.870130	-1.045754	0.659818	-0.356879	1.047396	0.793474	0.176077
H	0.190898	-2.375818	-1.212200	0.985237	-2.362622	1.919240	-0.851305	-1.182074	-1.543278	0.205538	-2.355381	-1.278296
H	1.023490	-0.848183	-1.307542	-0.093366	-3.318956	0.941059	-0.014388	-2.651230	-1.122394	1.020907	-0.818479	-1.365289
H	0.663216	-1.346225	1.508215	1.831218	-3.577062	-0.295075	-1.117710	-2.829367	0.905847	0.712549	-1.359512	1.448816
H	1.147495	-2.880624	0.826455	1.085864	-2.232840	-1.129950	-0.773693	-1.163430	1.321187	1.197767	-2.880138	0.737645
H	3.986724	-2.864653	-0.108996	4.627182	-1.247031	-1.086242	-3.921543	-2.290165	1.848695	4.029177	-2.823688	-0.234867

H	2.884923	-2.205035	-1.322713	3.546280	-2.353521	-1.947604	-2.765636	-1.088145	2.442846	2.894001	-2.176399	-1.423792
H	4.877928	-0.916734	-1.798773	2.057258	-0.563607	-2.556673	-4.772413	0.261071	2.267044	4.857904	-0.848902	-1.933889
H	5.306229	-0.810250	-0.086119	3.532287	0.383810	-2.436820	-5.277912	-0.554577	0.781146	5.316977	-0.753412	-0.231359
H	3.084471	0.633089	-1.570475	1.161663	0.513988	-0.750678	-3.005486	1.423794	1.168656	3.017130	0.625685	-1.674718
H	4.818117	3.112812	1.236267	2.349789	3.898584	-0.230872	-4.914829	2.086694	-2.429651	4.920341	3.648972	-1.016627
H	3.546542	1.836828	1.702378	0.917685	2.780687	-0.603162	-3.655066	0.733464	-2.218561	3.907016	2.675064	-2.224669
H	4.794208	2.374445	-2.215551	4.867832	1.515422	-0.877813	-4.700241	3.272747	0.889435	5.664514	1.006576	1.140772
H	5.831967	3.076114	-0.960456	4.571077	2.964811	0.096345	-5.808746	3.230883	-0.494181	5.395321	2.754508	1.175358
H	6.093419	1.415288	-1.516608	4.504176	1.351612	0.834385	-6.024482	2.114215	0.863223	4.148383	1.638069	1.767982
H	2.696045	-0.925796	2.777118	3.206486	-2.495710	2.041602	-2.827426	-2.249286	-1.699186	2.770256	-0.931806	2.689287
H	3.193865	-2.573248	2.341919	4.078475	-3.346728	0.758020	-3.279351	-3.367940	-0.399630	3.251682	-2.577239	2.228430
H	4.285743	-1.206220	2.049221	4.611413	-1.734911	1.276630	-4.361599	-2.036732	-0.851787	4.345666	-1.213917	1.931524
	1e			1f			1g			1h		
Gibbs free energy (hartrees)	-1037.624738			-1037.624465			-1037.624209			-1037.623222		
ΔG (kcal/mol)	0.441			0.612			0.772			1.392		
Population Proportion	10.16%			7.61%			5.8%			2.04%		
Element	X	Y	Z	X	Y	Z	X	Y	Z	X	Y	Z
C	0.715581	0.596545	-0.911660	0.940542	-0.873607	-0.503609	0.737808	0.702366	-0.866438	-0.725870	-0.889418	-1.072114
C	0.749523	-0.795356	-0.642767	0.903774	0.528061	-0.279237	0.769463	-0.712228	-0.770596	-0.636586	0.524260	-1.090093
C	1.933929	-1.423949	-0.259227	2.074985	1.247221	-0.046788	1.950948	-1.384599	-0.459084	-1.711792	1.319326	-0.697846
C	3.086948	-0.667926	-0.112646	3.289114	0.575938	-0.029106	3.103508	-0.654041	-0.213257	-2.878076	0.709932	-0.258823
C	3.089851	0.713146	-0.337511	3.368019	-0.804896	-0.237874	3.108570	0.744185	-0.267011	-2.998486	-0.682878	-0.198808
C	1.888486	1.315184	-0.741619	2.171842	-1.504050	-0.473598	1.910161	1.392884	-0.601572	-1.905660	-1.457011	-0.618362
O	4.223637	-1.325378	0.272098	4.411996	1.321959	0.204162	4.237238	-1.355255	0.095183	-3.905805	1.527316	0.125631
C	5.419611	-0.678563	0.459424	5.667534	0.768496	0.248984	5.432384	-0.737971	0.367872	-5.101063	1.037566	0.589404
C	5.443579	0.755851	0.227112	5.770047	-0.664047	0.031587	5.458771	0.714077	0.313098	-5.247167	-0.407064	0.655156
C	4.329537	1.417698	-0.154442	4.669182	-1.412755	-0.200846	4.347534	1.419239	0.008713	-4.242004	-1.226104	0.277029
O	6.369473	-1.358455	0.805365	6.598369	1.523918	0.467444	6.379525	-1.456483	0.634039	-5.947847	1.852690	0.909400
O	-0.342626	-1.584572	-0.757549	-0.241758	1.241998	-0.294917	-0.321868	-1.480552	-0.989784	0.479872	1.170073	-1.504167
C	-0.531167	1.298171	-1.404225	-0.333656	-1.641065	-0.753380	-0.505178	1.462260	-1.275691	0.405222	-1.765583	-1.558916
C	-1.394750	2.003233	-0.345746	-1.208428	-1.790276	0.517622	-1.366947	2.040843	-0.141789	1.334923	-2.365157	-0.490203
C	-2.084505	1.093876	0.694560	-2.668490	-1.386486	0.315812	-2.060962	1.015995	0.781588	2.139121	-1.383003	0.376790
C	-3.435003	1.673925	1.123516	-3.456159	-1.329904	1.632316	-3.415239	1.534250	1.270058	3.468443	-1.983885	0.857101
C	-4.382648	1.241417	0.002366	-4.404619	-0.151484	1.424109	-4.352534	1.218785	0.105614	4.391888	-0.773336	0.954212
C	-3.760108	-0.065719	-0.538345	-3.536757	0.825053	0.627203	-3.776865	-0.098613	-0.455519	3.910198	0.118395	-0.203430
O	-2.462577	-0.161281	0.083305	-2.662019	-0.009585	-0.159136	-2.426302	-0.160351	0.019051	2.554496	-0.272812	-0.459946
C	-4.538930	-1.318007	-0.211115	-4.281982	1.773116	-0.281456	-4.556582	-1.322301	-0.024989	4.052481	1.591616	0.097633
C	-5.043743	-2.071413	-1.192161	-4.305921	3.080375	-0.005008	-4.114353	-2.150718	0.924258	3.018467	2.371742	0.421120
C	-4.714948	-1.641031	1.248489	-4.982183	1.175424	-1.472680	-5.858462	-1.525777	-0.754090	5.472156	2.092288	0.044991

C	-1.186324	0.770916	1.881734	-3.374126	-2.249148	-0.728968	-1.163022	0.563184	1.926817	1.325926	-0.838525	1.555644
H	1.941831	-2.489789	-0.061036	2.032524	2.317888	0.118701	1.956858	-2.466720	-0.393093	-1.625061	2.399772	-0.718990
H	1.886135	2.383690	-0.942000	2.221918	-2.576492	-0.642066	1.909694	2.477973	-0.668726	-1.997566	-2.540060	-0.596395
H	6.394909	1.250289	0.376356	6.766527	-1.085323	0.067397	6.409467	1.185233	0.527492	-6.196851	-0.777140	1.019768
H	4.359727	2.489551	-0.325835	4.758032	-2.482957	-0.361866	4.379632	2.503958	-0.029996	-4.362848	-2.303903	0.330075
H	-1.166721	-1.067619	-0.584357	-1.056003	0.684187	-0.318420	-1.145877	-0.990136	-0.752684	1.282182	0.646635	-1.275215
H	-0.218149	2.064061	-2.118580	-0.899032	-1.133691	-1.541773	-0.187508	2.305805	-1.894158	-0.034171	-2.608101	-2.099657
H	-1.153799	0.601797	-1.972823	-0.083725	-2.624202	-1.154864	-1.131483	0.840557	-1.921244	1.008642	-1.224773	-2.292083
H	-0.793165	2.745222	0.189137	-1.172405	-2.821361	0.879708	-0.762047	2.710715	0.477901	0.757478	-3.015179	0.174686
H	-2.158749	2.565616	-0.892267	-0.800755	-1.168443	1.321216	-2.127709	2.667272	-0.618242	2.037175	-3.010564	-1.026075
H	-3.734118	1.227830	2.076099	-3.975589	-2.267835	1.834980	-3.717388	0.980830	2.163685	3.360051	-2.514090	1.804815
H	-3.393232	2.757365	1.252606	-2.780404	-1.126392	2.468097	-3.384507	2.596851	1.518149	3.851589	-2.687946	0.113782
H	-4.421913	1.987254	-0.793542	-4.746396	0.295545	2.358189	-4.316939	2.001953	-0.654443	5.444761	-1.037505	0.850114
H	-5.403655	1.090897	0.356194	-5.284579	-0.454415	0.851873	-5.389913	1.114184	0.424909	4.266709	-0.253540	1.907399
H	-3.618796	-0.001785	-1.622039	-2.915532	1.404249	1.320699	-3.749958	-0.069663	-1.551283	4.484879	-0.110392	-1.109721
H	-5.632477	-2.959987	-0.980480	-4.864111	3.781204	-0.619847	-4.695663	-3.017529	1.226156	3.165680	3.422128	0.657192
H	-4.888699	-1.819428	-2.238169	-3.772978	3.489372	0.849649	-3.158724	-1.987789	1.411822	2.003576	1.989899	0.458286
H	-5.245108	-0.837002	1.769632	-5.738991	0.446086	-1.167750	-5.678637	-1.670801	-1.824379	5.901371	1.937965	-0.950192
H	-5.279721	-2.564768	1.385463	-5.475448	1.946691	-2.066826	-6.395327	-2.396453	-0.374214	5.528577	3.155268	0.284766
H	-3.741457	-1.749551	1.734050	-4.267205	0.646103	-2.107688	-6.511911	-0.652863	-0.658034	6.105309	1.547904	0.753392
H	-0.230115	0.344940	1.571032	-2.903007	-2.146642	-1.709096	-0.209093	0.169626	1.569364	0.448637	-0.285580	1.214783
H	-0.978835	1.685492	2.442579	-3.338601	-3.301846	-0.435890	-0.950613	1.411493	2.582393	0.983361	-1.661007	2.189180
H	-1.686273	0.060756	2.544946	-4.421567	-1.953363	-0.829217	-1.663185	-0.211864	2.512519	1.933097	-0.163979	2.164963
	1i			1j			1k					
Gibbs free energy (hartrees)	-1037.62309			-1037.622926			-1037.622753					
ΔG (kcal/mol)	1.475			1.578			1.686					
Population Proportion	1.77%			1.49%			1.24%					
Element	X	Y	Z	X	Y	Z	X	Y	Z			
C	-0.981967	-0.964395	0.474921	-0.672124	-0.875050	-1.039072	-0.848499	-0.759362	-0.380449			
C	-0.953430	0.449648	0.585050	-0.596450	0.540345	-0.998568	-0.868647	0.578506	0.094114			
C	-2.114389	1.205981	0.439787	-1.695695	1.308803	-0.618608	-2.074742	1.235207	0.334096			
C	-3.312440	0.557354	0.175457	-2.871265	0.673150	-0.247728	-3.267942	0.563308	0.111504			
C	-3.383014	-0.834237	0.051003	-2.978732	-0.721870	-0.243380	-3.291579	-0.757859	-0.347116			
C	-2.196365	-1.570835	0.207413	-1.862605	-1.468732	-0.650817	-2.061216	-1.393551	-0.585284			
O	-4.427696	1.337700	0.038881	-3.921399	1.465931	0.127513	-4.426466	1.246481	0.362167			
C	-5.667579	0.810748	-0.225716	-5.127161	0.947910	0.529288	-5.666137	0.683824	0.183997			
C	-5.761268	-0.632900	-0.356753	-5.259584	-0.499428	0.537410	-5.710944	-0.687699	-0.292270			
C	-4.667907	-1.415821	-0.223756	-4.232336	-1.294266	0.166556	-4.574305	-1.373435	-0.545665			
O	-6.592766	1.596753	-0.329637	-5.993881	1.742689	0.847335	-6.632509	1.380612	0.439554			

O	0.180897	1.132081	0.853705	0.526836	1.216337	-1.336988	0.252803	1.292819	0.325467
C	0.286906	-1.763634	0.631499	0.480297	-1.729598	-1.518130	0.460047	-1.464002	-0.639055
C	1.225064	-1.667059	-0.598594	1.394996	-2.343211	-0.442675	1.233243	-1.811901	0.655970
C	2.674950	-1.305029	-0.252441	2.174500	-1.359306	0.444075	2.691555	-1.348964	0.661095
C	3.498106	-1.014909	-1.514513	3.504168	-1.934435	0.956276	3.552052	-1.963464	-0.451699
C	3.305494	0.482160	-1.733254	4.407585	-0.705541	1.043799	4.518016	-0.835839	-0.807384
C	3.264237	1.016700	-0.296560	3.966401	0.116987	-0.171461	3.631592	0.397839	-0.680102
O	2.640587	-0.030750	0.462506	2.588896	-0.246683	-0.390505	2.695467	0.078359	0.375658
C	4.613905	1.412686	0.270162	4.089983	1.616027	-0.026624	4.289732	1.724414	-0.381611
C	5.149817	0.805123	1.331325	4.973734	2.284315	-0.774090	5.600601	1.920559	-0.548759
C	5.276697	2.579212	-0.417188	3.199680	2.294299	0.981200	3.353210	2.826239	0.039163
C	3.323456	-2.358083	0.637998	1.332421	-0.828164	1.608906	3.311119	-1.550795	2.041939
H	-2.077810	2.285649	0.531578	-1.619486	2.389994	-0.594998	-2.074640	2.258573	0.692198
H	-2.240766	-2.653078	0.119380	-1.944288	-2.552635	-0.673172	-2.068619	-2.418512	-0.946321
H	-6.745296	-1.033584	-0.563859	-6.217535	-0.891960	0.853696	-6.695234	-1.116966	-0.428839
H	-4.750194	-2.493933	-0.323754	-4.342916	-2.374404	0.176392	-4.620061	-2.398309	-0.901680
H	0.988558	0.570737	0.793367	1.328771	0.682790	-1.123524	1.084945	0.765153	0.266123
H	0.808356	-1.424348	1.532742	0.061076	-2.564061	-2.086546	0.263767	-2.370663	-1.213217
H	0.028093	-2.806743	0.819051	1.094214	-1.166536	-2.225375	1.076130	-0.831523	-1.287101
H	1.222200	-2.617221	-1.139168	0.810979	-3.006870	0.202628	0.733840	-1.361673	1.520521
H	0.842986	-0.916104	-1.297884	2.112578	-2.974179	-0.975698	1.213413	-2.891464	0.826129
H	4.552795	-1.238977	-1.333096	3.386134	-2.447837	1.911986	4.058003	-2.868750	-0.112310
H	3.164779	-1.615804	-2.362350	3.911340	-2.646661	0.233450	2.939243	-2.225417	-1.318403
H	2.352095	0.686112	-2.226598	5.468349	-0.951698	0.986178	4.940420	-0.933634	-1.808038
H	4.094992	0.928628	-2.337209	4.240536	-0.160347	1.975306	5.340423	-0.793597	-0.088963
H	2.609400	1.893198	-0.231402	4.531284	-0.204130	-1.052929	3.047203	0.519858	-1.604867
H	6.105754	1.125558	1.736468	5.110761	3.357106	-0.668926	6.044167	2.898749	-0.383514
H	4.639939	-0.012682	1.828542	5.593621	1.777636	-1.509424	6.272531	1.128197	-0.863923
H	4.580468	3.418227	-0.517382	3.392043	1.929956	1.995060	2.882925	2.588705	0.997106
H	6.148606	2.921710	0.142477	3.355296	3.374562	0.976173	3.877954	3.778404	0.135985
H	5.606758	2.316623	-1.426630	2.146804	2.094804	0.763487	2.545774	2.946658	-0.690618
H	2.782537	-2.482853	1.578870	0.467307	-0.262984	1.258520	2.774608	-0.956248	2.785584
H	3.332685	-3.320600	0.119058	0.969022	-1.660950	2.216731	3.258579	-2.602802	2.334289
H	4.354952	-2.083649	0.868160	1.925548	-0.171147	2.249751	4.359484	-1.241916	2.047945

CAS SciFinder

Enter a query...

Substances search for drawn structure

All Substances Reactions References Suppliers Patent Markush

View Related Results

Filter Results

Structure Match

As Drawn (0)

Substructure (0)

Similarity (331K)

Behavior

5 Exclude

Search Within Results

Filtering: Similarity: 85-89 Number of Components: 1

1 Selected 21 Results

Sort: Relevance View: Partial

1 89

2 88

3 88

2131055-67-7

C₁₈H₂₄O₄
2-Cyclohexylethyl 3-(4-hydroxy-3-methoxyphenyl)-2-propenoate

2795766-78-6

C₁₇H₂₂O₄
2-Cyclopentylethyl 3-(4-hydroxy-3-methoxyphenyl)-2-propenoate

1428244-58-9

C₁₉H₂₆O₄
(trans-4-Ethylcyclohexyl)methyl (2E)-3-(4-hydroxy-3-methoxyphenyl)-2-propenoate

Figure S14: SciFinder search results for compound 2 (similarity >87%).

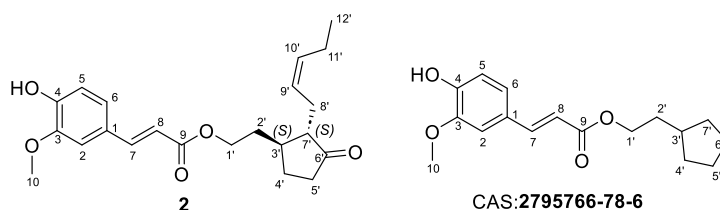


Figure S15: The structures of compound 2 and structurally similar compounds

Table S3: The NMR data of compound 2 and 2795766-78-6 (δ in ppm, J in Hz)

Compound 1			2795766-78-6		
	δ_C	δ_H J(Hz)		δ_C	δ_H J(Hz)
1	127.1	-	1	127.6	-
2	109.5	7.03, d (1.9)	2	109.9	7.04, d (1.9)
3	148.2	-	3	148.1	-
4	146.9	-	4	146.9	-
5	114.9	6.92, d (8.2)	5	114.8	6.89, d (8.2)
6	123.2	7.08, dd (8.2, 1.9)	6	123.1	7.09, dd (8.2, 1.9)
7	145.2	7.61, d (15.9)	7	145.1	7.61, d (15.9)
8	115.4	6.28, d (16.0)	8	115.2	6.28, d (16.0)
9	167.4	-	9	167.5	-
10	56.1	3.93, s	10	56.1	3.93, s
1'	62.6	4.25-4.33, m	1'	68.1	4.26, m
2'	33.8	1.61-1.68, m; 2.13-2.18, m	2'	32.3	1.55, m
3'	38.5	2.00-2.06	3'	34.4	1.41, m
4'	27.3	1.46-1.52, m; 2.22-2.27, m	4'	32.5	1.65, m; 1.90, m
5'	38.1	2.08-2.13, m; 2.34-2.41, m	5'	25.1	1.63, m; 1.73, m
6'	219.9	-	6'	25.1	1.63, m; 1.73, m
7'	55.0	1.84-1.90, m	7'	32.5	1.65, m; 1.90, m

8'	25.6	2.34-2.40, m	8'
9'	125.3	5.26, dtt (10.5, 8.0, 1.8)	9'
10'	134.0	5.44, dtt (10.5, 7.2, 1.6)	10'
11'	20.8	2.01-2.12, m	11'
12'	14.3	0.96, t (7.6)	12'

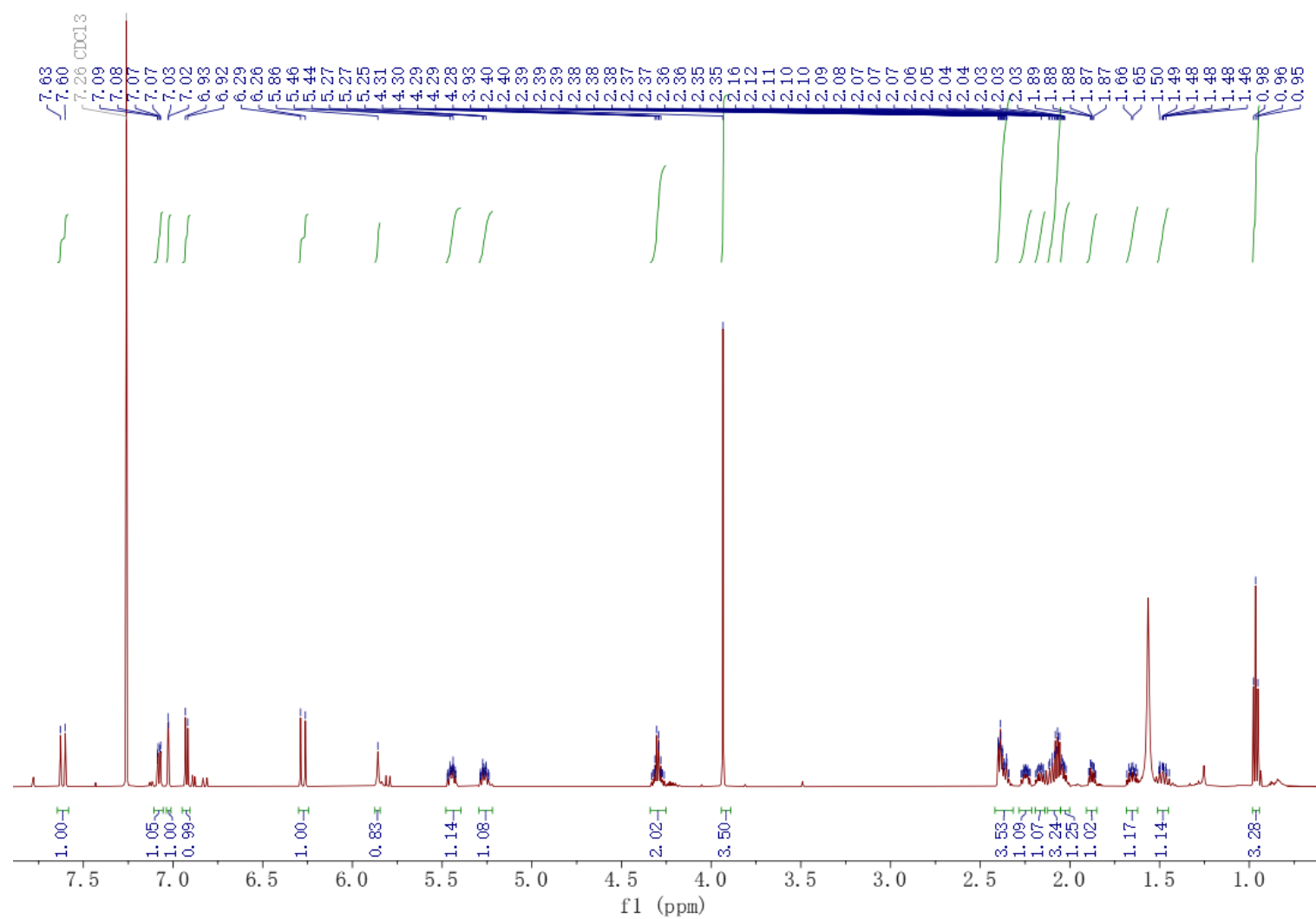


Figure S16: ¹H NMR spectrum of **2** in CDCl₃ (600 MHz)

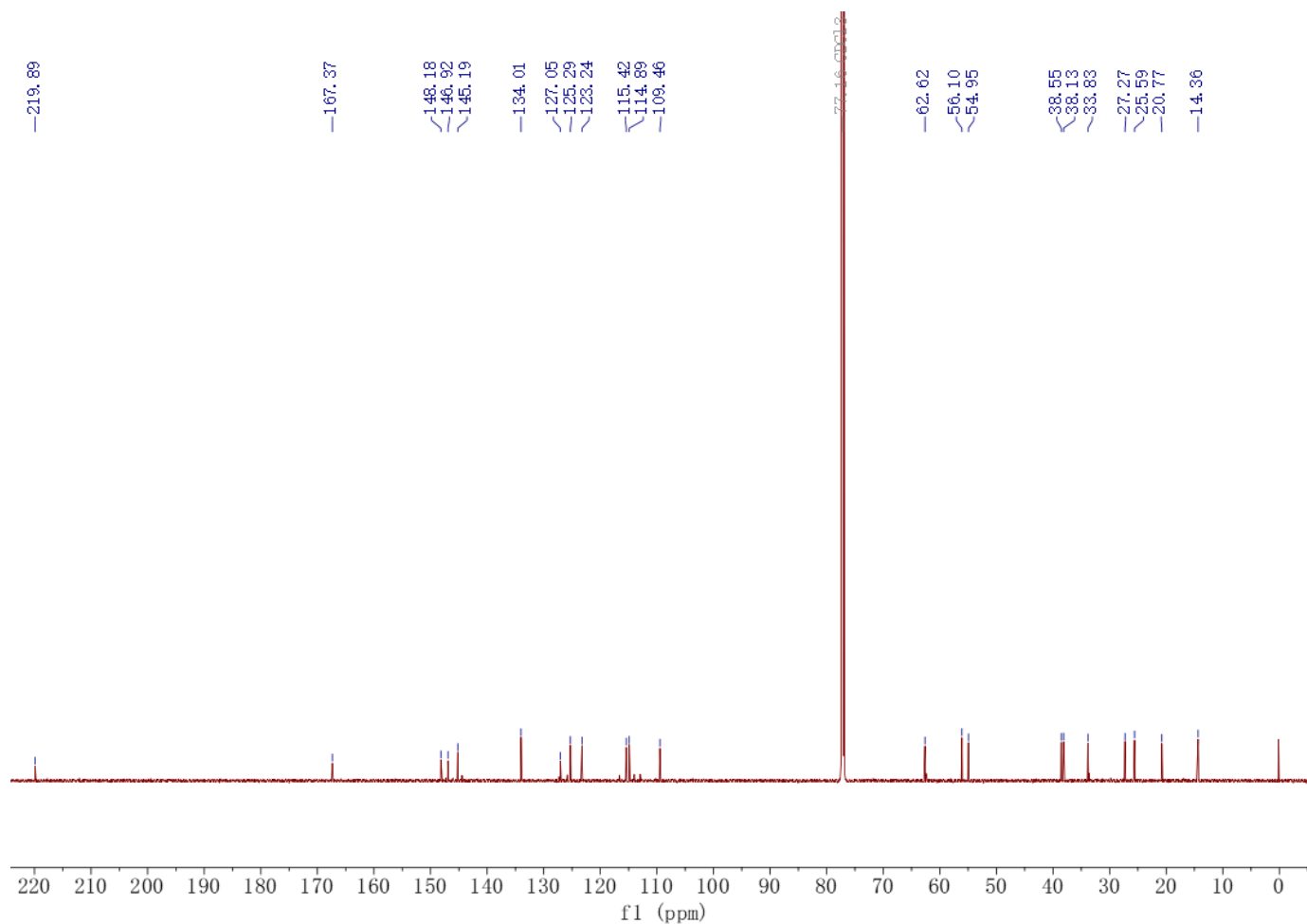


Figure S18: ¹³C NMR spectrum of **2** in CDCl₃ (150 MHz)

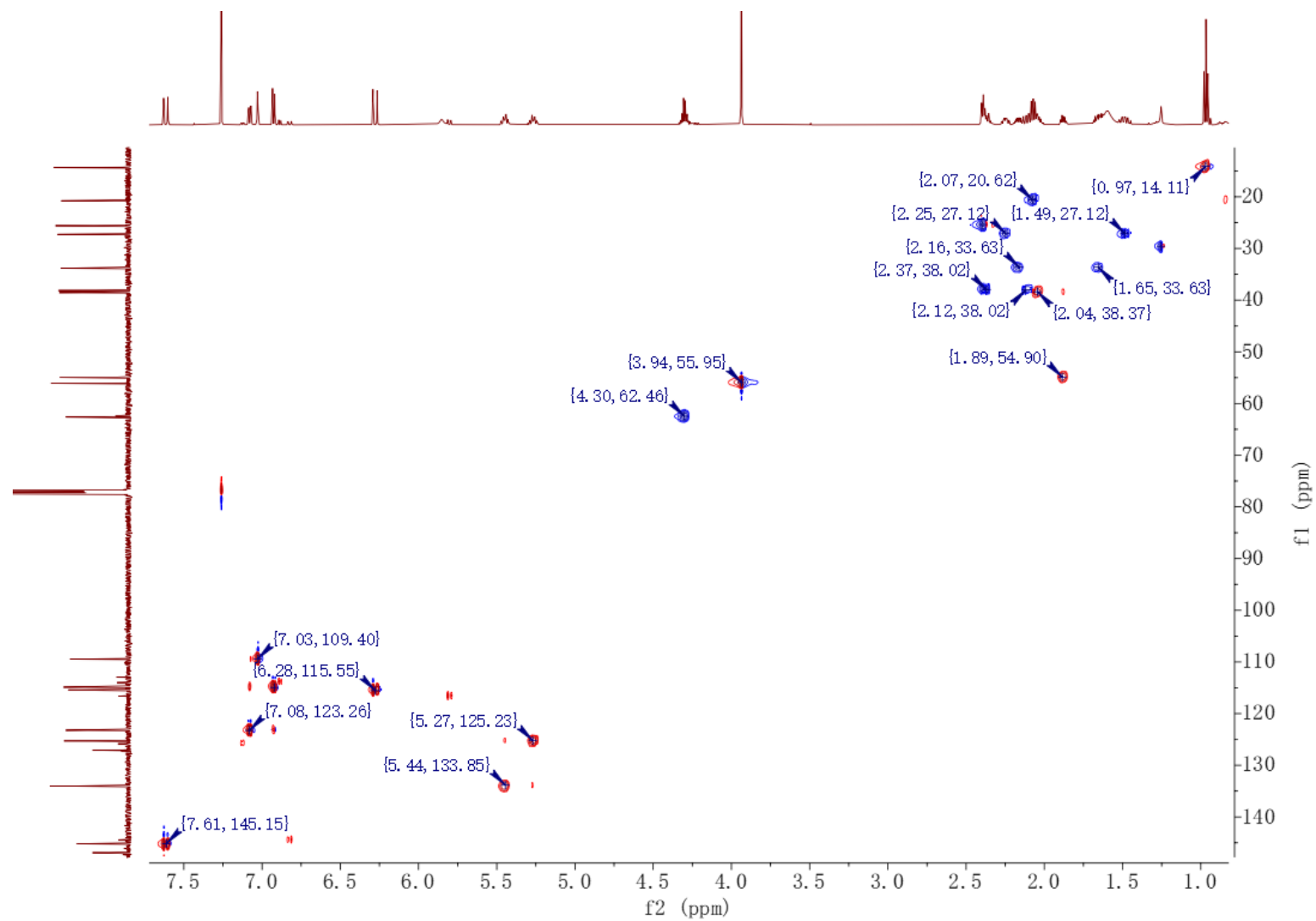


Figure S19: HSQC spectrum of **2** in CDCl_3

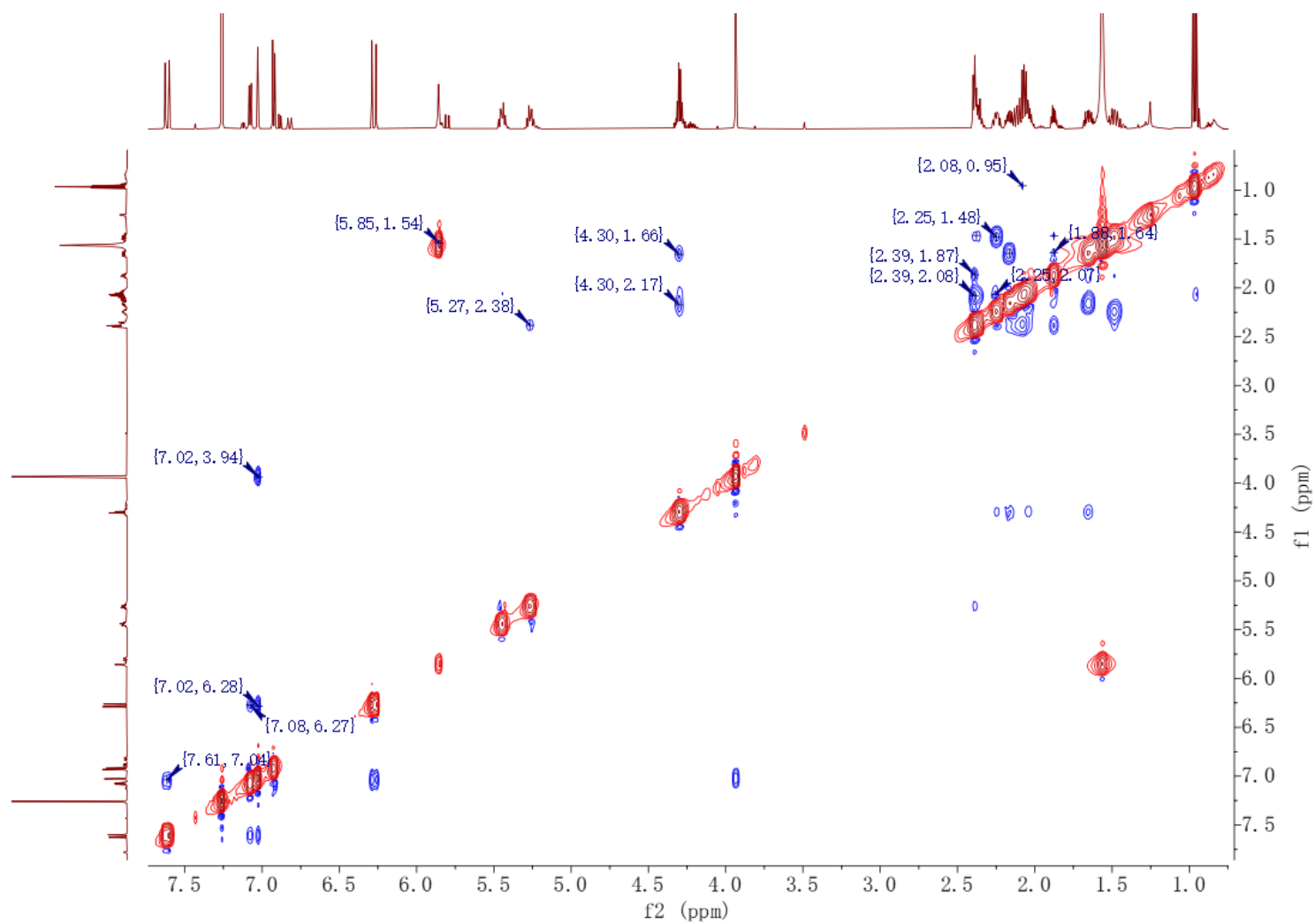


Figure S20: ^1H - ^1H COSY spectrum of **2** in CDCl_3

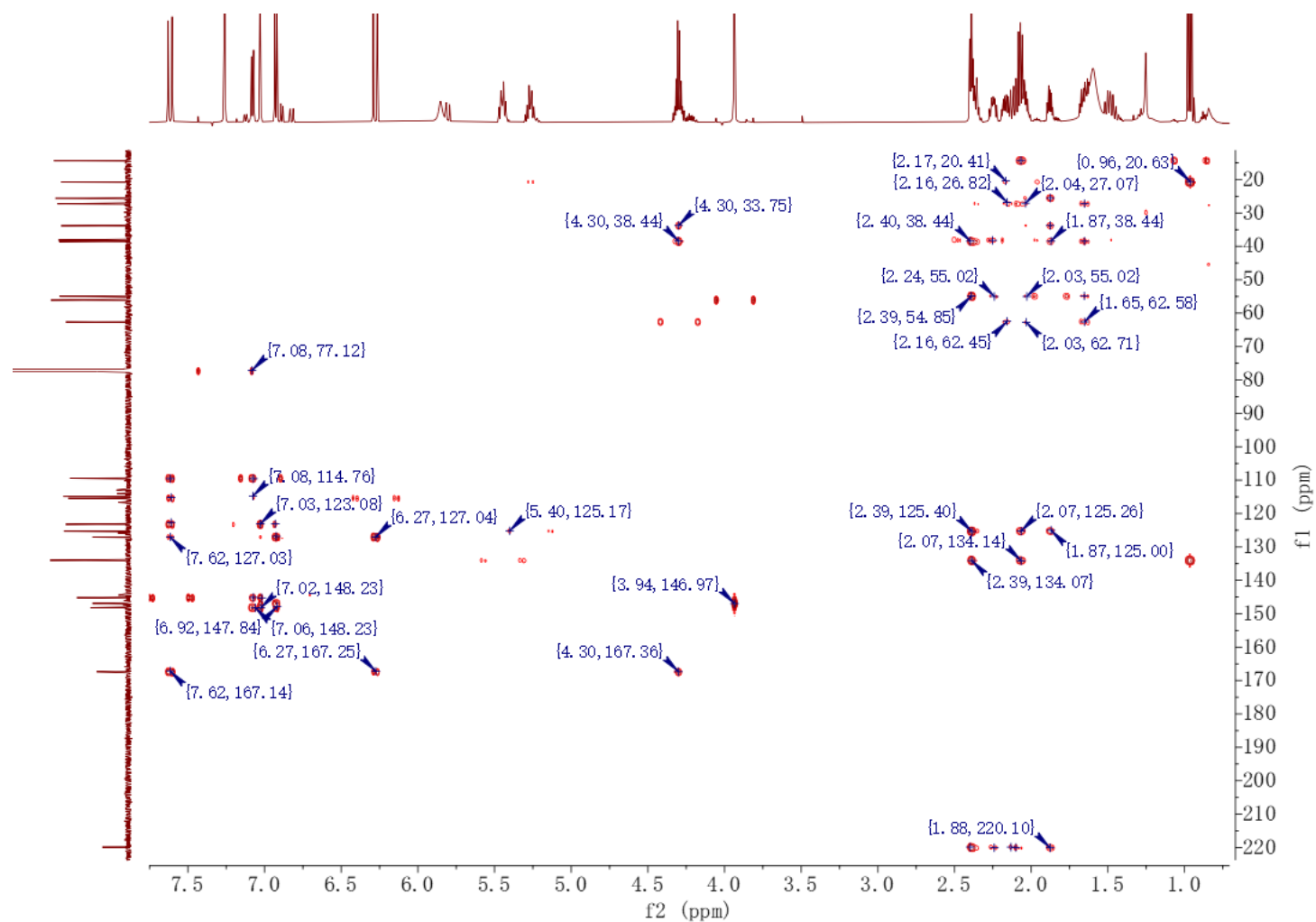


Figure S21: HMBC spectrum of **2** in CDCl_3

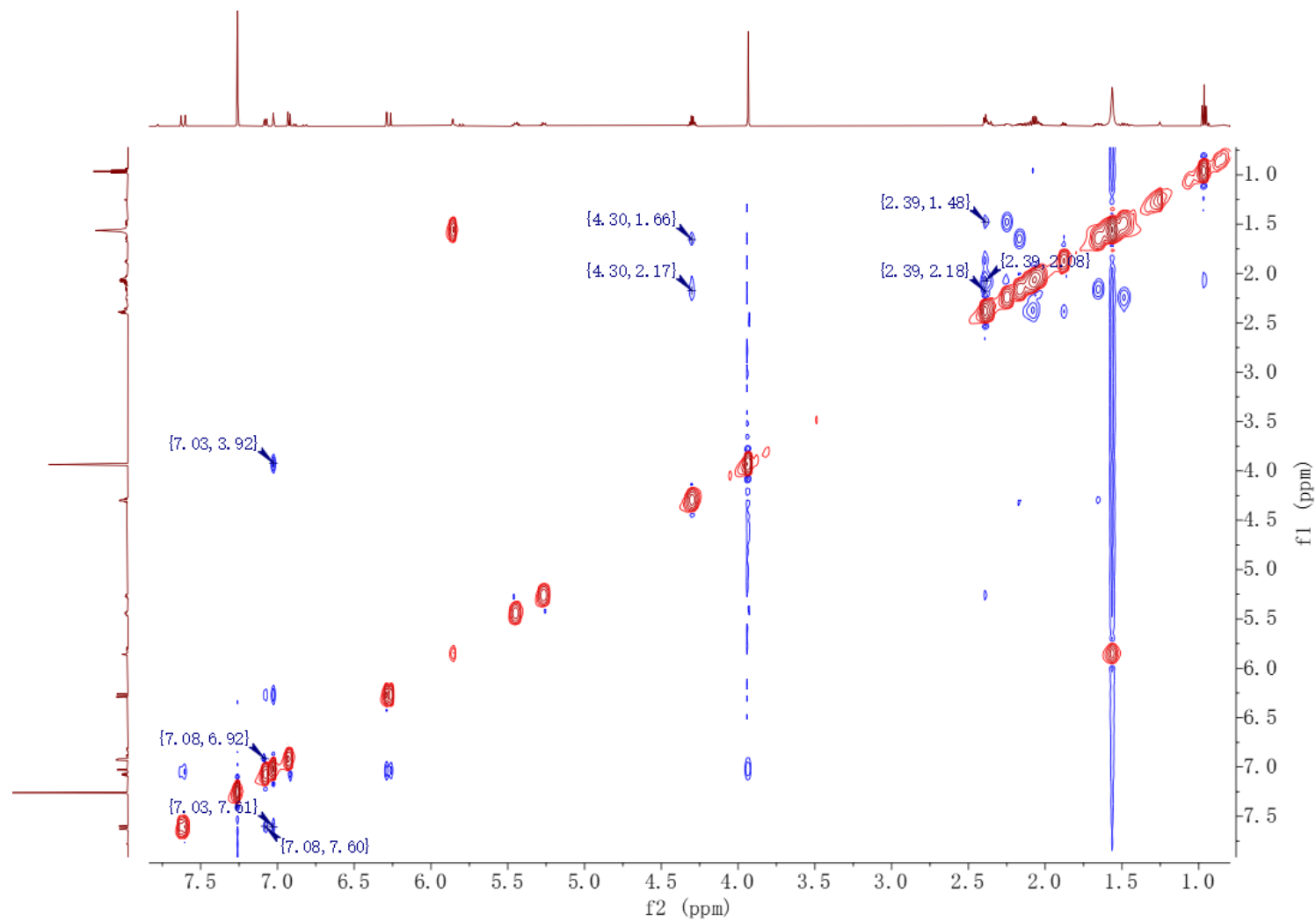


Figure S22: NOESY spectrum of **2** in CDCl_3

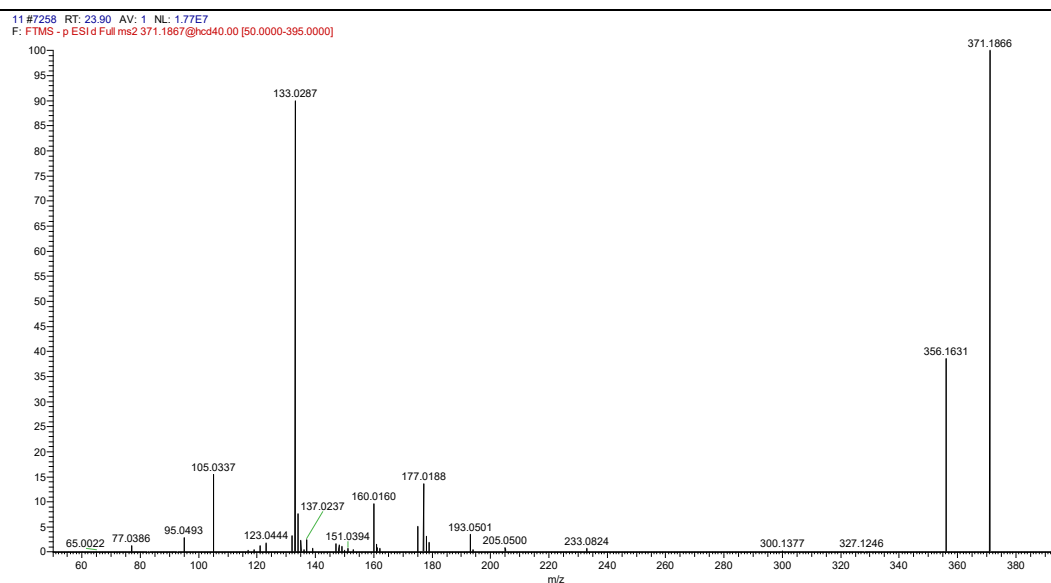


Figure S23: HRESIMS spectrum of **2**

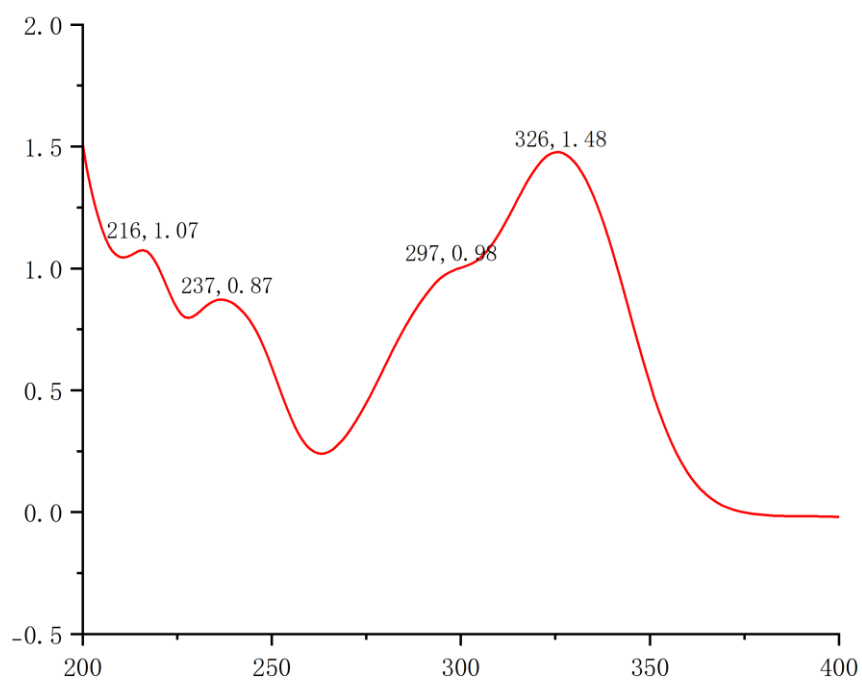


Figure S24: UV spectrum of compound **2**

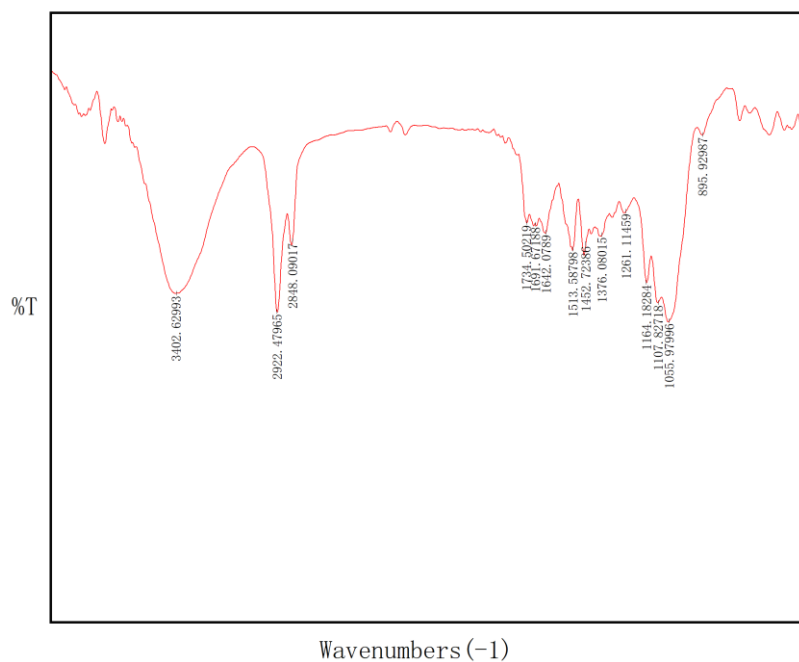


Figure S25: IR spectrum of compound **2**

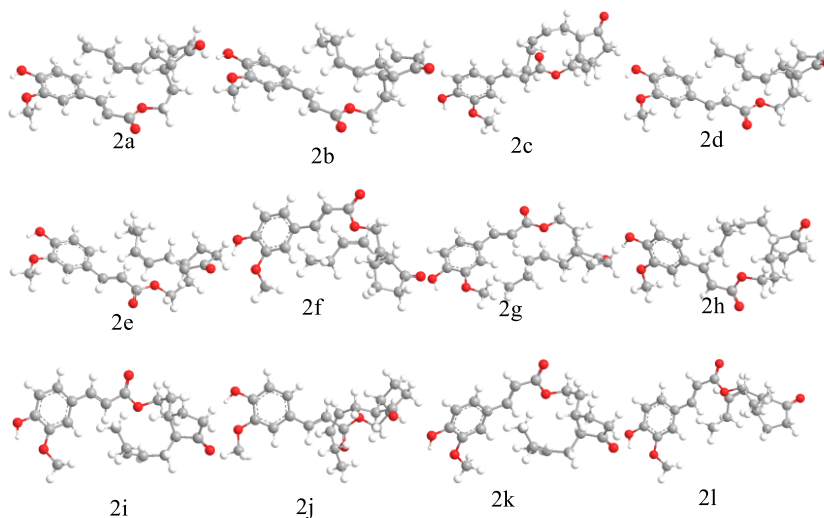


Figure S26: Most stable conformers of 3'S, 7'S-**2** calculated at the CAM-B3LYP/DGTZVP level

Table S4: Energies and atomic Cartesian coordinates of geometry-optimized conformers of 3'S, 7'S-**2** at wb97xd/dgdzvp in methanol

	2a	2b	2c	2d
Gibbs free energy	-1230.648202	-1230.647924	-1230.647272	-1230.6472

(hartrees)												
ΔG (kcal/mol)				0.174			0.584			0.629		
Population Proportion	25.68%			19.13%			9.59%			8.89%		
Element	X	Y	Z	X	Y	Z	X	Y	Z	X	Y	Z
C	4.539048	-0.923505	-0.051929	4.866176	-0.526678	0.036907	-4.784637	-0.357193	0.584566	-5.238318	0.644847	0.114706
C	4.737587	-0.722080	-1.436108	5.213029	-0.069107	-1.253791	-5.659911	-0.747423	-0.453167	-5.300288	0.840179	-1.278096
C	3.830120	0.034838	-2.160205	4.333353	0.736670	-1.959367	-5.284098	-0.569687	-1.775448	-4.236792	0.444111	-2.080148
C	2.724027	0.590493	-1.517818	3.110376	1.090964	-1.390069	-4.042025	-0.009314	-2.074133	-3.113342	-0.146467	-1.510325
C	2.513155	0.399111	-0.150599	2.753786	0.647884	-0.114579	-3.166761	0.384651	-1.059166	-3.037438	-0.350144	-0.128113
C	3.441228	-0.369142	0.581563	3.652211	-0.172162	0.598201	-3.557333	0.205416	0.284197	-4.116176	0.057408	0.679728
C	1.299188	0.949659	0.451831	1.442233	1.023816	0.414344	-1.866228	0.945046	-1.426664	-1.869053	-0.939286	0.529299
O	5.502401	-1.688320	0.532325	5.819087	-1.310892	0.612987	-5.273526	-0.594236	1.833339	-6.342653	1.079370	0.784283
C	5.380117	-1.978481	1.920939	5.563981	-1.833796	1.912503	-4.443355	-0.284000	2.947964	-6.370038	0.931952	2.200191
O	5.813150	-1.272211	-2.053051	6.403931	-0.421131	-1.800278	-6.863274	-1.297862	-0.154143	-6.393567	1.417750	-1.837920
C	0.897166	0.834006	1.728587	0.920577	0.693585	1.607457	-0.902209	1.367485	-0.593354	-0.762137	-1.414795	-0.062386
C	-0.420429	1.293240	2.200338	-0.435469	1.080300	2.033089	0.396135	1.827881	-1.116802	0.384613	-1.865055	0.748291
O	-1.153200	1.884961	1.248250	-1.116300	1.757069	1.097594	1.249261	2.066852	-0.108073	1.459871	-2.060820	-0.029257
O	-0.815744	1.121387	3.344444	-0.890710	0.800589	3.132596	0.683356	1.967777	-2.295221	0.388633	-2.021739	1.959121
C	-2.527522	2.187679	1.551815	-2.480177	2.123544	1.379381	2.602895	2.429789	-0.441217	2.709928	-2.354721	0.624113
C	-3.275765	2.266464	0.233149	-3.250600	2.097575	0.071295	3.499514	1.951848	0.686897	3.819273	-2.016073	-0.355331
C	-3.251997	0.951283	-0.558410	-3.295385	0.711260	-0.585570	3.503645	0.426029	0.851249	3.876408	-0.520258	-0.693310
C	-3.871553	1.107178	-1.965481	-3.984863	0.746331	-1.967928	4.287556	-0.025654	2.103879	4.829531	-0.213030	-1.870712
C	-5.370717	0.874796	-1.766959	-5.476979	0.580761	-1.670930	5.740291	-0.148901	1.640002	6.201649	-0.003521	-1.229316
C	-5.443314	-0.103782	-0.612524	-5.515988	-0.260499	-0.410766	5.629937	-0.550498	0.183317	5.879870	0.614017	0.114722
C	-4.093929	-0.161600	0.097669	-4.127847	-0.305538	0.219257	4.209611	-0.297221	-0.312941	4.421287	0.335262	0.471013
C	-3.481276	-1.572467	-0.053442	-3.576352	-1.747384	0.153372	3.542469	-1.632777	-0.706652	3.644375	1.649317	0.695659
O	-6.419793	-0.760906	-0.297397	-6.497411	-0.829898	0.033493	6.526978	-1.017800	-0.496041	6.652042	1.247830	0.812071
C	-2.243056	-1.722291	0.786818	-2.241684	-1.852929	0.837461	2.199553	-1.404696	-1.343660	2.310608	1.378690	1.336536
C	-0.973938	-1.759075	0.364517	-1.059835	-2.133107	0.275536	0.997664	-1.733567	-0.855756	1.103317	1.399674	0.760457
C	-0.466720	-1.672285	-1.050354	-0.768386	-2.419463	-1.172440	0.680652	-2.411879	0.449101	0.759258	1.718479	-0.669098
C	0.727250	-2.596152	-1.301709	0.277605	-1.461461	-1.751652	-0.296726	-1.593886	1.299952	-0.482298	2.607538	-0.780081
H	3.992213	0.179402	-3.222948	4.610366	1.079148	-2.950632	-5.964364	-0.875928	-2.562895	-4.298630	0.608532	-3.150691
H	2.012609	1.171875	-2.096033	2.424259	1.715189	-1.953862	-3.754621	0.118959	-3.112969	-2.292102	-0.433492	-2.157657
H	3.288750	-0.538783	1.640521	3.390858	-0.533163	1.585646	-2.893606	0.504553	1.086266	-4.058243	-0.092467	1.752316
H	0.638872	1.474903	-0.234061	0.828332	1.622638	-0.253804	-1.656839	0.996413	-2.493537	-1.894730	-0.964950	1.617314
H	6.235993	-2.600284	2.172466	6.439514	-2.423156	2.174284	-5.007237	-0.575799	3.830768	-7.325561	1.337521	2.524267
H	5.407524	-1.060312	2.514153	5.435562	-1.026166	2.638502	-3.508562	-0.850369	2.905330	-6.304912	-0.122320	2.483268
H	4.456059	-2.527251	2.123188	4.678634	-2.475676	1.906460	-4.229706	0.787691	2.987907	-5.556335	1.494869	2.665885
H	6.322203	-1.763822	-1.388325	6.873588	-0.982461	-1.162351	-6.940801	-1.346108	0.812423	-7.021012	1.625310	-1.126737
H	1.482499	0.327359	2.488386	1.456427	0.102299	2.342176	-1.003077	1.348210	0.485915	-0.625516	-1.424456	-1.138267
H	-2.924407	1.409622	2.206315	-2.889649	1.432306	2.116353	2.865700	1.978800	-1.399111	2.775338	-1.764038	1.540368

H	-2.566005	3.137938	2.089466	-2.476648	3.125054	1.815857	2.646969	3.515866	-0.551480	2.721236	-3.413038	0.895016
H	-4.304463	2.573174	0.454532	-4.262287	2.464559	0.279662	4.510192	2.326166	0.487426	4.766407	-2.354888	0.079411
H	-2.833579	3.062246	-0.374594	-2.793937	2.810847	-0.622128	3.169586	2.418257	1.620549	3.666026	-2.595918	-1.270916
H	-2.209201	0.637023	-0.643330	-2.265737	0.359697	-0.690016	2.463572	0.097848	0.924826	2.863037	-0.203717	-0.950730
H	-3.464901	0.340719	-2.632285	-3.633386	-0.093295	-2.575201	3.921680	-1.003112	2.432699	4.512929	0.710344	-2.365443
H	-3.646715	2.078513	-2.410560	-3.760152	1.662355	-2.518084	4.164986	0.666014	2.939738	4.826615	-1.004083	-2.623116
H	-5.879625	1.791410	-1.447578	-5.948349	1.541199	-1.433876	6.253714	0.818916	1.671147	6.699678	-0.960766	-1.035456
H	-5.903614	0.494453	-2.639751	-6.062387	0.120732	-2.468578	6.350653	-0.859127	2.199810	6.894688	0.618419	-1.797471
H	-4.272341	0.011688	1.164090	-4.228608	-0.036376	1.275412	4.280324	0.318428	-1.215843	4.428307	-0.212548	1.420514
H	-4.230501	-2.303102	0.267818	-4.295632	-2.406400	0.650754	4.199450	-2.142815	-1.418842	4.238415	2.291300	1.353786
H	-3.273390	-1.767925	-1.109088	-3.517854	-2.071725	-0.888795	3.465617	-2.277819	0.172606	3.535592	2.174375	-0.257495
H	-2.419527	-1.764861	1.861270	-2.256825	-1.646297	1.907442	2.230327	-0.888601	-2.303014	2.360502	1.089876	2.386139
H	-0.197437	-1.837798	1.125554	-0.187137	-2.145725	0.929196	0.127025	-1.473218	-1.457965	0.250401	1.138100	1.387361
H	-1.263674	-1.888216	-1.767044	-0.390727	-3.445056	-1.257822	0.228548	-3.387708	0.236807	1.603250	2.186834	-1.182768
H	-0.153937	-0.639511	-1.247628	-1.678336	-2.372784	-1.775076	1.588881	-2.607998	1.024010	0.562755	0.777050	-1.196795
H	1.094029	-2.488947	-2.325904	0.497281	-1.708906	-2.793798	-0.550789	-2.125232	2.221184	-0.737762	2.793649	-1.826555
H	1.553526	-2.354412	-0.625289	-0.075920	-0.426653	-1.714357	0.136670	-0.626919	1.572325	-1.345059	2.128578	-0.305948
H	0.455087	-3.644035	-1.144310	1.213864	-1.510869	-1.188023	-1.225409	-1.402711	0.753141	-0.320231	3.572733	-0.291473
	2e			2f			2g			2h		
Gibbs free energy (hartrees)	-1230.647147			-1230.646861			-1230.646712			-1230.646676		
ΔG (kcal/mol)	0.662			0.841			0.935			0.958		
Population Proportion	8.4%			6.21%			5.3%			5.1%		
Element	X	Y	Z	X	Y	Z	X	Y	Z	X	Y	Z
C	5.325130	-0.434454	0.308292	-4.038125	0.507375	-0.933083	4.583301	0.528147	0.796575	-4.643118	-0.498510	0.007263
C	5.501734	-0.608223	-1.077689	-4.734409	1.513206	-0.236580	5.555522	0.982784	-0.121811	-4.834635	-1.573785	-0.888602
C	4.492004	-0.234096	-1.955804	-4.304273	1.904914	1.025295	5.316805	0.885236	-1.483726	-3.860595	-1.870117	-1.829226
C	3.307589	0.310107	-1.468734	-3.183171	1.311217	1.597990	4.117047	0.338775	-1.940093	-2.696376	-1.104165	-1.885115
C	3.115477	0.488067	-0.093913	-2.480808	0.310708	0.918187	3.151662	-0.125935	-1.044251	-2.497354	-0.031532	-1.012898
C	4.143306	0.107886	0.790664	-2.928803	-0.088916	-0.355223	3.399471	-0.021955	0.339979	-3.489963	0.263352	-0.056528
C	1.884186	1.037932	0.476920	-1.250723	-0.296763	1.428367	1.900441	-0.671954	-1.570953	-1.245455	0.720738	-1.099754
O	6.388964	-0.839791	1.057058	-4.551949	0.226100	-2.163063	4.937559	0.700363	2.100263	-5.669409	-0.329334	0.886120
C	6.305527	-0.701022	2.471620	-3.856970	-0.712003	-2.977910	4.009833	0.304405	3.105066	-5.560970	0.710660	1.852605
O	6.654884	-1.139343	-1.557746	-5.818324	2.105993	-0.798149	6.714942	1.522909	0.330527	-5.966084	-2.319148	-0.820337
C	0.781447	1.412407	-0.190215	-0.634872	-0.039191	2.594126	0.919636	-1.263754	-0.870960	-0.934491	1.856180	-0.451936
C	-0.412623	1.878327	0.537711	0.693430	-0.582033	2.926875	-0.345569	-1.645190	-1.524731	0.386658	2.499624	-0.546017
O	-1.439545	2.053044	-0.309230	1.167926	-1.432356	2.007453	-1.251162	-2.021891	-0.609667	1.257211	1.822110	-1.308793
O	-0.483909	2.074977	1.740578	1.315829	-0.260053	3.928668	-0.572649	-1.608124	-2.723803	0.664676	3.542211	0.028593
C	-2.715530	2.428827	0.244325	2.543079	-1.840957	2.120689	-2.594004	-2.271420	-1.067798	2.618417	2.289904	-1.348532
C	-3.797322	1.857845	-0.654953	2.977747	-2.342878	0.755285	-3.506391	-2.178380	0.141860	3.380697	1.973043	-0.067682

C	-3.804076	0.323862	-0.691593	2.870018	-1.283858	-0.351549	-3.528626	-0.776137	0.765038	3.221451	0.536781	0.451919
C	-4.795603	-0.234411	-1.736993	3.170393	-1.874621	-1.747286	-4.261914	-0.744263	2.125338	4.044386	0.332395	1.744359
C	-6.135928	-0.325948	-1.004791	4.691577	-1.791958	-1.892902	-5.730293	-0.491745	1.781162	5.455700	-0.016817	1.259141
C	-5.752126	-0.602632	0.434541	5.079183	-0.577233	-1.073222	-5.665918	0.379183	0.544726	5.249670	-0.645621	-0.107352
C	-4.270275	-0.301622	0.638106	3.902522	-0.149471	-0.201582	-4.288052	0.252156	-0.101005	3.783306	-0.529828	-0.503518
C	-3.514207	-1.595192	1.010848	3.382217	1.226737	-0.677806	-3.592417	1.626765	-0.190824	3.131981	-1.923879	-0.319672
O	-6.499763	-1.015134	1.303710	6.157952	-0.011749	-1.107905	-6.563863	1.086336	0.122852	6.115211	-1.179663	-0.778400
C	-2.083354	-1.304841	1.371030	2.314610	1.755626	0.239441	-2.381746	1.559126	-1.081147	1.692812	-1.952525	-0.755031
C	-0.983728	-1.657351	0.694712	1.003902	1.852518	-0.010894	-1.094587	1.539264	-0.716776	0.610642	-2.026323	0.028571
C	-0.896130	-2.429542	-0.593313	0.270467	1.471906	-1.269520	-0.519627	1.596934	0.672400	0.550391	-2.060154	1.531012
C	-0.133476	-1.658771	-1.676337	-0.835457	2.469012	-1.623512	0.690787	2.530510	0.759160	-0.319548	-0.928849	2.091450
H	4.645235	-0.374438	-3.020562	-4.849401	2.685603	1.545182	6.068847	1.244031	-2.178220	-4.017134	-2.702114	-2.507343
H	2.536889	0.594333	-2.176729	-2.857122	1.649470	2.575245	3.935925	0.274172	-3.008399	-1.935941	-1.347958	-2.620755
H	3.998226	0.242459	1.857086	-2.382648	-0.858779	-0.889312	2.650570	-0.351626	1.049943	-3.341337	1.075504	0.644938
H	1.857327	1.126456	1.561515	-0.764897	-1.001559	0.757677	1.745813	-0.557900	-2.642396	-0.489855	0.291891	-1.752966
H	7.247686	-1.075877	2.864521	-4.404081	-0.756040	-3.916697	4.481661	0.538535	4.056403	-6.469361	0.660654	2.448199
H	6.183012	0.348545	2.753148	-2.832163	-0.378528	-3.165187	3.074395	0.863491	3.012317	-4.691089	0.553338	2.496534
H	5.479386	-1.294525	2.872955	-3.848778	-1.701713	-2.512989	3.810369	-0.769383	3.049396	-5.494761	1.688007	1.366662
H	7.232637	-1.336483	-0.802968	-5.954265	1.713375	-1.675584	6.694033	1.511358	1.301131	-6.516987	-1.965035	-0.103572
H	0.693217	1.347594	-1.268768	-1.029859	0.651009	3.331703	0.975305	-1.428496	0.199626	-1.627367	2.368252	0.207223
H	-2.784801	2.051970	1.265560	3.137526	-0.989472	2.457536	-2.846883	-1.533776	-1.832539	3.043873	1.777548	-2.210850
H	-2.761504	3.519860	0.278318	2.617381	-2.627257	2.875495	-2.629645	-3.264052	-1.522752	2.628676	3.363909	-1.543005
H	-4.759755	2.244452	-0.300539	4.006969	-2.707593	0.850913	-4.511376	-2.482729	-0.171569	4.435226	2.199225	-0.267129
H	-3.655317	2.246844	-1.668136	2.361500	-3.206855	0.487065	-3.173456	-2.907203	0.887531	3.057641	2.661706	0.717197
H	-2.789320	-0.005670	-0.929031	1.855507	-0.879103	-0.326419	-2.491282	-0.461551	0.899975	2.160437	0.355566	0.642121
H	-4.476486	-1.234248	-2.046752	2.691488	-1.261218	-2.516488	-3.879862	0.085856	2.727488	3.630956	-0.497715	2.324262
H	-4.842251	0.385464	-2.634569	2.787397	-2.891227	-1.856850	-4.109856	-1.660636	2.699000	4.024750	1.215321	2.386359
H	-6.667446	0.632400	-1.020725	5.186239	-2.659501	-1.441825	-6.237509	-1.421106	1.496587	6.074006	0.876217	1.121105
H	-6.822885	-1.084845	-1.382336	5.057509	-1.706963	-2.917340	-6.322118	-0.022295	2.568105	6.011673	-0.692270	1.911955
H	-4.187354	0.388054	1.484743	4.266128	-0.032417	0.824320	-4.450545	-0.105421	-1.124315	3.712225	-0.257879	-1.560016
H	-4.019824	-2.048391	1.869830	4.228665	1.920911	-0.691645	-4.306042	2.345574	-0.605749	3.700089	-2.638125	-0.924407
H	-3.583706	-2.310651	0.187170	3.018391	1.144001	-1.705670	-3.335567	1.970052	0.815250	3.234497	-2.245297	0.720225
H	-1.950155	-0.715156	2.277753	2.663810	2.052968	1.227931	-2.603226	1.474823	-2.144794	1.535294	-1.896948	-1.831705
H	-0.023953	-1.341603	1.104011	0.369715	2.231043	0.790863	-0.354708	1.453325	-1.512962	-0.362396	-2.049023	-0.462623
H	-0.374357	-3.374384	-0.401731	0.960084	1.365486	-2.111057	-1.277311	1.897196	1.401179	0.124255	-3.019855	1.845728
H	-1.889601	-2.692276	-0.964687	-0.183996	0.483869	-1.125132	-0.203724	0.586173	0.958690	1.549901	-2.003365	1.969380
H	-0.045109	-2.255170	-2.588432	-1.385399	2.143823	-2.510809	1.118052	2.524601	1.765553	-0.394359	-0.999400	3.179903
H	-0.647199	-0.725848	-1.926923	-1.553293	2.560374	-0.801804	1.473888	2.216385	0.061753	0.098653	0.050136	1.839994
H	0.876078	-1.403485	-1.339302	-0.420576	3.461385	-1.823286	0.412381	3.559434	0.513565	-1.331983	-0.970216	1.677299
	2i			2j			2k			2l		
Gibbs free energy (hartrees)	-1230.646525			-1230.64638			-1230.646042			-1230.645163		

ΔG (kcal/mol)	1.052			1.143			1.355			1.907		
Population Proportion	4.35%			3.73%			2.61%			1.03%		
Element	X	Y	Z	X	Y	Z	X	Y	Z	X	Y	Z
C	5.526587	-0.119172	-0.366181	-4.408880	-1.187520	-0.288468	-4.590629	-0.175470	-0.698983	-4.349665	-1.002242	-0.651002
C	5.609991	0.953184	-1.274529	-5.511410	-0.571416	0.344397	-5.342595	0.890996	-0.170309	-5.186517	-0.458157	0.342092
C	4.516917	1.791614	-1.457150	-5.423605	0.751538	0.748492	-4.823279	1.655829	0.866949	-4.770951	0.654459	1.063297
C	3.341484	1.573930	-0.744849	-4.245717	1.466671	0.530866	-3.560710	1.373523	1.380573	-3.530689	1.231587	0.806812
C	3.242488	0.512953	0.162148	-3.149535	0.873907	-0.100006	-2.801408	0.317901	0.865624	-2.689062	0.704439	-0.177887
C	4.353844	-0.333200	0.342509	-3.247189	-0.471435	-0.511966	-3.336949	-0.458693	-0.179611	-3.115685	-0.423514	-0.904564
C	2.032681	0.232011	0.938489	-1.930682	1.660928	-0.287320	-1.453044	-0.008463	1.335600	-1.357494	1.240329	-0.466570
O	6.665119	-0.863018	-0.281896	-4.624833	-2.489948	-0.622245	-5.210263	-0.842561	-1.712970	-4.870843	-2.091960	-1.280804
C	6.675577	-1.976178	0.605820	-3.539802	-3.229570	-1.172890	-4.507720	-1.911271	-2.338489	-4.070853	-2.743784	-2.262005
O	6.754160	1.169257	-1.971818	-6.649413	-1.277040	0.560796	-6.572317	1.173535	-0.671048	-6.394269	-1.020988	0.600066
C	0.870062	0.903180	0.907830	-0.806215	1.274681	-0.911511	-0.718458	0.674647	2.228820	-0.809625	2.362671	0.028698
C	-0.268278	0.455511	1.731695	0.374555	2.155319	-0.951638	0.650027	0.287836	2.613694	0.573110	2.776281	-0.265020
O	-1.357629	1.198050	1.484351	1.387950	1.550208	-1.592244	1.097627	-0.803070	1.976867	1.222831	1.927430	-1.075612
O	-0.253011	-0.468456	2.529502	0.453341	3.273597	-0.467163	1.310627	0.910342	3.432535	1.079842	3.788846	0.195343
C	-2.589296	0.761126	2.087273	2.675975	2.193314	-1.566642	2.448106	-1.229874	2.237508	2.622786	2.166101	-1.313113
C	-3.725682	1.513168	1.418342	3.368881	2.036181	-0.217129	2.950430	-1.958885	1.004339	3.486698	1.745847	-0.131354
C	-3.767763	1.346263	-0.106249	3.301052	0.624683	0.383037	3.010417	-1.072731	-0.247230	3.206536	0.337306	0.412468
C	-4.909100	2.170972	-0.746756	4.058487	0.557601	1.728756	3.406790	-1.872327	-1.508541	4.120469	0.025366	1.619437
C	-6.121922	1.239631	-0.756581	5.514904	0.275312	1.346915	4.937184	-1.867246	-1.517737	5.426095	-0.485489	1.000504
C	-5.520048	-0.137529	-0.936578	5.426504	-0.478905	0.033407	5.310468	-0.561613	-0.844532	5.013209	-1.079202	-0.334226
C	-4.041796	-0.105260	-0.558089	3.990966	-0.448465	-0.477093	4.086831	0.025485	-0.148644	3.540696	-0.781840	-0.588793
C	-3.158975	-0.574177	-1.733297	3.377708	-1.859150	-0.301838	3.685747	1.349964	-0.835166	2.744362	-2.087677	-0.342596
O	-6.110218	-1.128574	-1.329214	6.352470	-1.040430	-0.525173	6.413145	-0.043432	-0.861095	5.737152	-1.713570	-1.081256
C	-1.712872	-0.712694	-1.324426	1.987577	-1.941783	-0.868194	2.526111	2.000013	-0.132921	1.276799	-1.935309	-0.633526
C	-1.140110	-1.809111	-0.814450	0.842071	-2.103678	-0.195910	1.297053	2.211179	-0.618551	0.276708	-1.894148	0.254665
C	-1.795637	-3.134375	-0.539215	0.643459	-2.224668	1.290113	0.768552	1.859698	-1.982771	0.363432	-1.946608	1.755280
C	-1.738132	-3.504050	0.947605	-0.247210	-1.107687	1.846165	-0.460880	0.948763	-1.906688	-0.320168	-0.739443	2.407541
H	4.598798	2.612589	-2.161566	-6.275702	1.211379	1.237445	-5.417486	2.472190	1.263700	-5.425185	1.055392	1.830214
H	2.503720	2.243090	-0.907119	-4.184653	2.499618	0.858679	-3.179020	1.987002	2.189160	-3.222236	2.086968	1.397525
H	4.281346	-1.156940	1.044270	-2.406837	-0.951067	-0.998968	-2.748338	-1.274615	-0.584621	-2.467174	-0.832611	-1.671713
H	2.084999	-0.624290	1.608731	-1.940386	2.660046	0.144607	-1.002450	-0.891716	0.889684	-0.749640	0.645093	-1.143426
H	7.663333	-2.421716	0.514375	-3.913672	-4.238998	-1.326834	-5.165824	-2.285081	-3.119351	-4.657646	-3.589649	-2.612292
H	6.513971	-1.652955	1.637921	-3.224789	-2.806660	-2.130790	-3.574834	-1.554763	-2.784597	-3.858844	-2.073754	-3.099796
H	5.915562	-2.708801	0.320348	-2.695477	-3.253306	-0.477491	-4.297740	-2.711354	-1.623142	-3.134880	-3.102644	-1.824292
H	7.396774	0.489172	-1.712899	-6.514692	-2.176928	0.222068	-6.760022	0.540735	-1.382847	-6.503548	-1.783220	0.008945
H	0.697801	1.763165	0.269527	-0.687672	0.300611	-1.373143	-1.075235	1.574043	2.719068	-1.337191	3.029247	0.702496
H	-2.673990	-0.319582	1.953648	3.229460	1.701248	-2.365687	3.056032	-0.357633	2.480588	2.840679	1.578625	-2.204579
H	-2.555454	0.967326	3.159680	2.563726	3.248648	-1.821097	2.434628	-1.888641	3.109042	2.778245	3.221098	-1.545046

H	-4.659589	1.164993	1.874477	4.409941	2.350786	-0.357983	3.940297	-2.364215	1.244022	4.530187	1.836687	-0.456883
H	-3.635763	2.577739	1.656460	2.924824	2.735465	0.496313	2.298082	-2.816145	0.810208	3.350594	2.466039	0.679890
H	-2.807915	1.688250	-0.498504	2.249010	0.367889	0.529654	2.023181	-0.624314	-0.384582	2.155023	0.285560	0.706300
H	-4.640636	2.432261	-1.774613	3.665762	-0.263348	2.335855	3.030270	-1.361304	-2.399817	3.668725	-0.755152	2.238493
H	-5.093983	3.104063	-0.210620	3.943389	1.474279	2.310689	2.985057	-2.879491	-1.508244	4.268448	0.898352	2.258212
H	-6.636074	1.244018	0.211663	6.071903	1.198979	1.156648	5.345582	-2.677278	-0.902996	6.127845	0.329607	0.795337
H	-6.867282	1.451564	-1.524302	6.082971	-0.295554	2.083485	5.397136	-1.946020	-2.504030	5.960960	-1.224216	1.600187
H	-3.909967	-0.827870	0.254341	3.999199	-0.215606	-1.545400	4.367317	0.257922	0.883536	3.405138	-0.492773	-1.634496
H	-3.555181	-1.521006	-2.107874	4.022000	-2.571522	-0.827587	4.551857	2.019419	-0.808670	3.158328	-2.858232	-1.000991
H	-3.238916	0.148789	-2.552165	3.394163	-2.140137	0.754387	3.460871	1.164783	-1.888603	2.908290	-2.432615	0.681716
H	-1.095922	0.178853	-1.422166	1.927772	-1.838339	-1.950968	2.723007	2.302916	0.895403	1.021813	-1.844253	-1.688877
H	-0.087616	-1.744075	-0.536304	-0.075609	-2.139513	-0.784338	0.571716	2.681186	0.046158	-0.736551	-1.795538	-0.135509
H	-2.835921	-3.133476	-0.873867	0.171213	-3.190378	1.504084	0.488655	2.785205	-2.499173	-0.128189	-2.861414	2.106149
H	-1.280066	-3.911355	-1.115369	1.600530	-2.222671	1.817096	1.538022	1.383260	-2.594504	1.402376	-2.002203	2.089519
H	-2.187429	-4.485509	1.121068	-0.407573	-1.238291	2.919787	-0.852090	0.735820	-2.905368	-0.283167	-0.814623	3.497580
H	-0.704934	-3.535579	1.304803	0.206660	-0.125548	1.685521	-0.212333	-0.003694	-1.428717	0.166116	0.194851	2.112025
H	-2.275535	-2.769846	1.554246	-1.226904	-1.102481	1.358208	-1.260566	1.414142	-1.323369	-1.370442	-0.672738	2.106741