Supporting Information

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Euphebranone F, a new acetophenone derivative from the *Euphorbia fischeriana*

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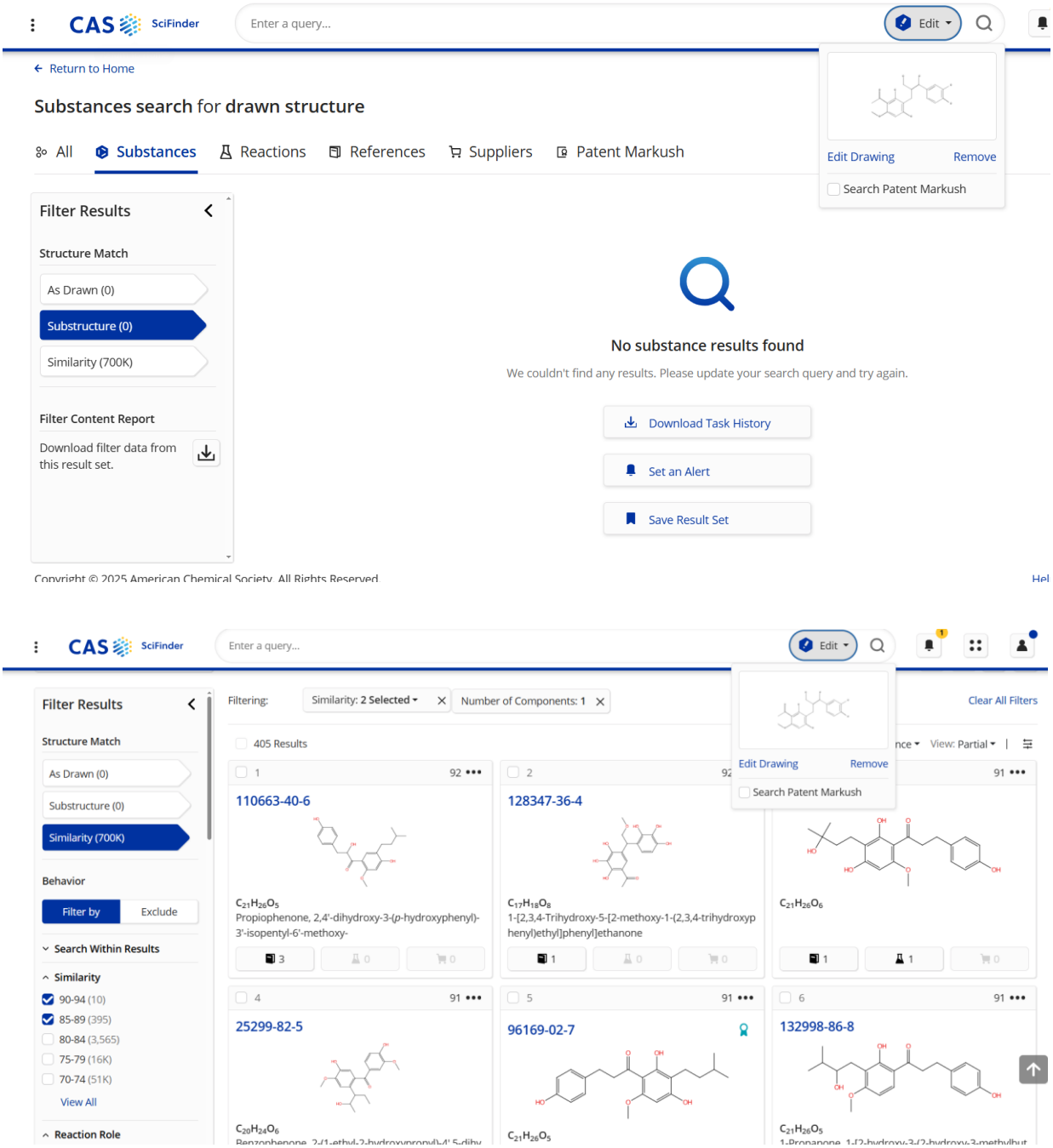


Figure S1: New compound (**1**) search report of SciFinder

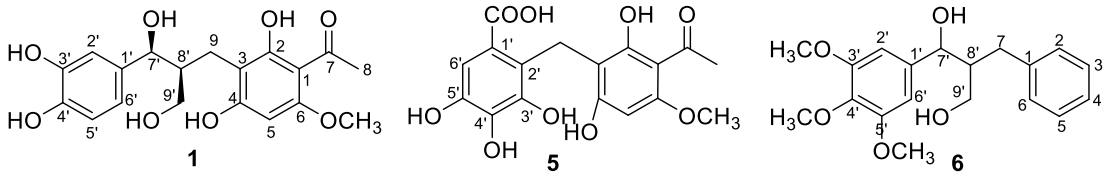
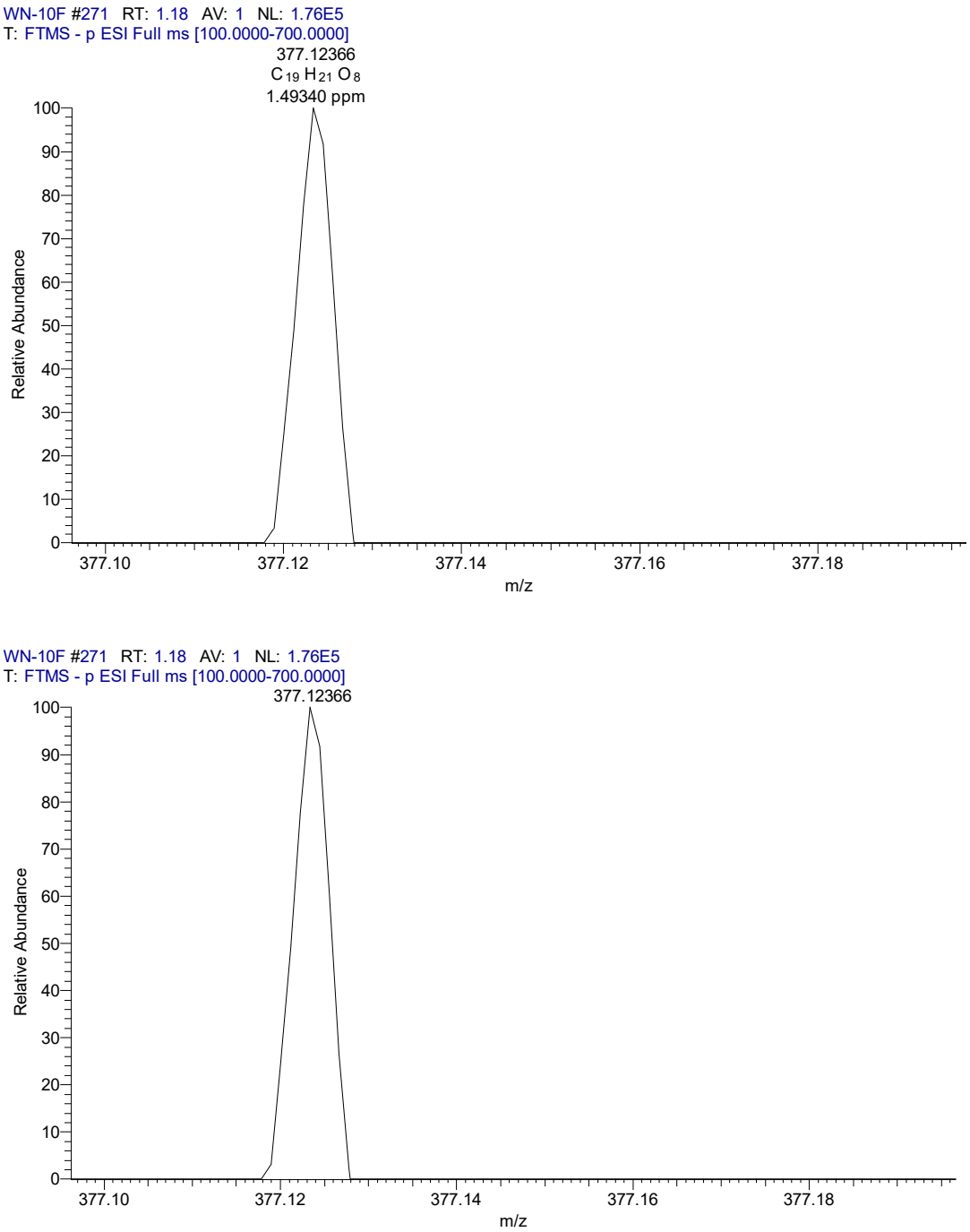


Figure S2: Most similar compounds **5** and **6** for the new compound **1**

Table S1. ^{1}H and ^{13}C NMR spectroscopic data for **1**, **5** and **6** (δ in ppm and J in Hz)

No.	**1**[a]		**5**[b]		**6**[c]	
	δ_H	δ_C, type	δ_H	δ_C, type	δ_H	δ_C, type
1		106.4, C		105.3, C		139.8, C
2		165.6, C		166.5, C		128.5, CH
3		103.4, C		107.1, C		127.8, CH
4		162.9, C		164.3, C		125.4, CH
5	6.03 (s)	91.9, CH	5.97 (s)	93.4, CH		127.8, CH
6		162.8, C		163.6, C		128.5, CH
6-OCH_3	3.88 (s)	56.1, CH_3	3.83 (s)	55.9, CH_3		
7		204.6, C		204.4, C		30.5, CH_2
8	2.60 (s)	33.1, CH_3	2.58 (s)	32.8, CH_3		
9	2.52 (dd, J = 16.7, 9.5 Hz) 2.79 (dd, J = 16.7, 5.4 Hz)	22.0, CH_2	4.16 (s)	20.3, CH_2		
1′		132.3, C		118.5, C		138.0, C
2′	6.81 (d, J = 2.1 Hz)	114.8, CH		125.6, C	6.63 (s)	102.6, CH
3′		146.5, C		145.4, C		152.5, C
4′		146.5, C		144.4, C		136.8, C
5′	6.78 (d, J = 8.0 Hz)	116.2, CH		137.1, C		152.5, C
6′	6.70 (dd, J = 8.0, 2.1 Hz)	119.6, CH	6.87 (s)	110.2, CH	6.63 (s)	102.6, CH
7′	4.85 (d, J = 8.4 Hz)	81.4, CH				75.8, CH
8′	2.15 (m)	41.0, CH				47.9, CH
9′	3.35 (dd, J = 10.9, 6.8 Hz) 3.48 (dd, J = 10.9, 4.5 Hz)	63.6, CH_2				62.8, CH_2
-OCH_3					3.85 (s, 3H), 3.87 (s, 6H)	55.6/60.4, CH_3

a): the ^{1}H and ^{13}C NMR data of compound **1** were recorded at 600 MHz and 150 MHz, with CD_3OD as solvent, respectively. b): the ^{1}H and ^{13}C NMR data of the compound **5** reported in the literature [1] were recorded with a Bruker DRX-600, with CD_3OD as solvent . c): the ^{1}H and ^{13}C NMR data of the compound **6** reported in the literature [2] were recorded with a Bruker DRX-300, with $CDCl_3$ as solvent .



m/z	Calc Mass	Formula	RDB	Delta ppm	Ion
377.12366	377.12419	$C_{19}H_{22}O_8$	9.5	0.566	$[M-H]^-$

Figure S3: HR-ESI-MS spectrum of **1** (Euphebranone F)

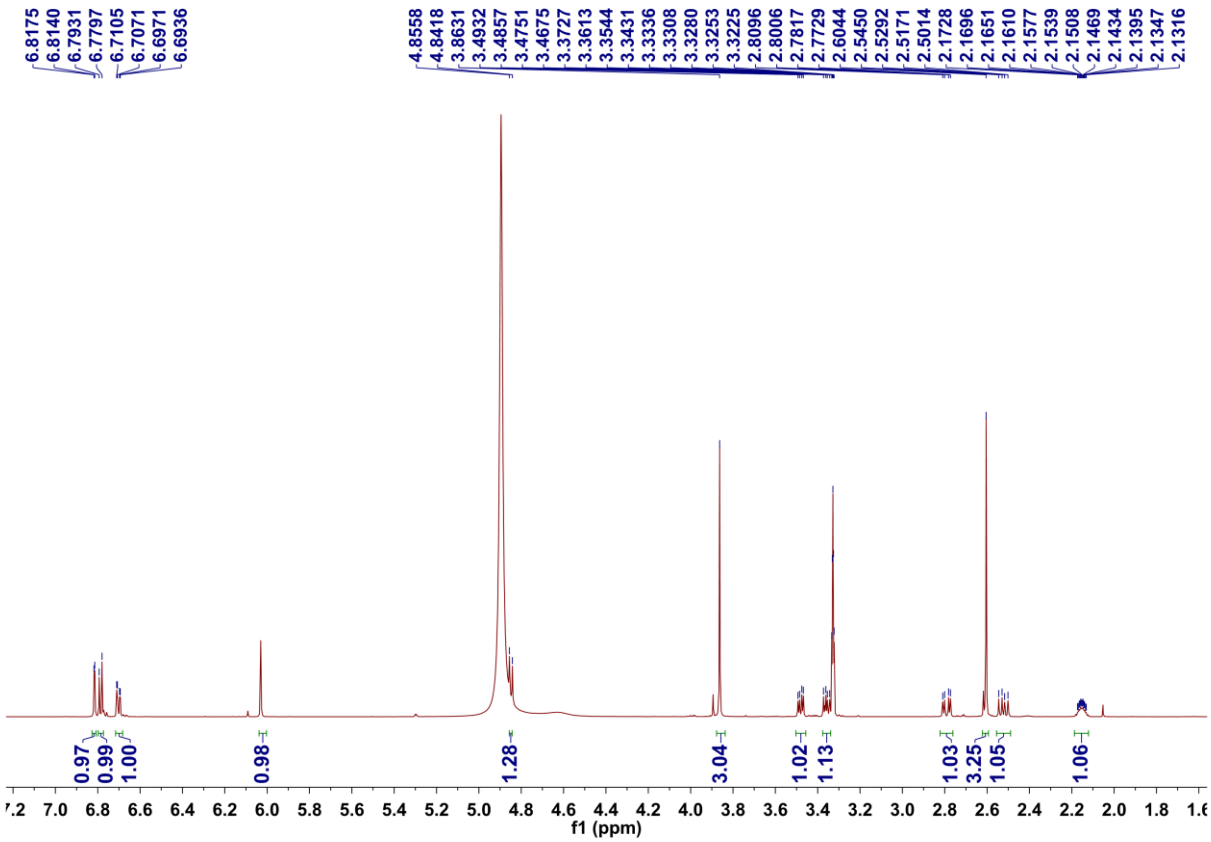


Figure S4: ^{1}H-NMR (600 MHz, CD_3OD) spectrum of **1** (Euphebranone F)

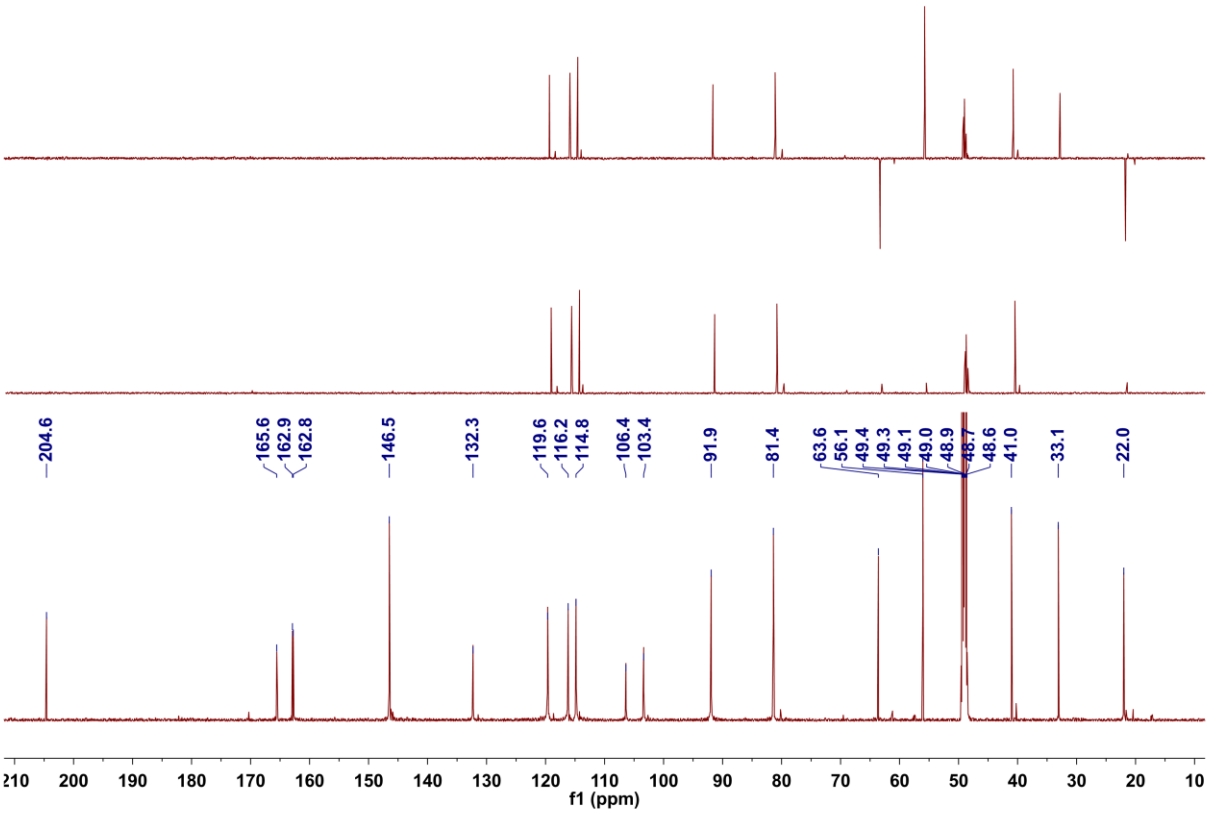


Figure S5: ^{13}C-NMR and DEPT (150 MHz, CD_3OD) spectrum of **1** (Euphebranone F)

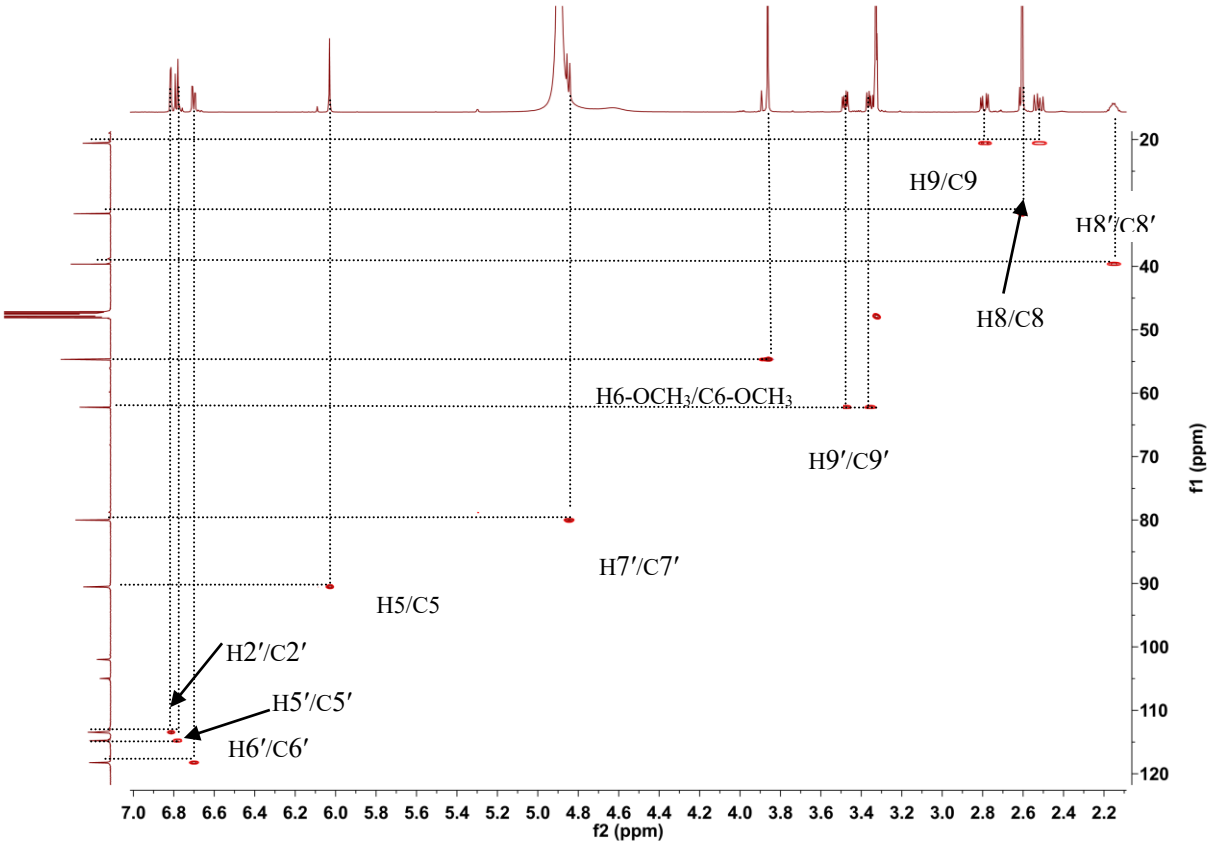


Figure S6: HSQC spectrum of **1** (Euphebranone F)

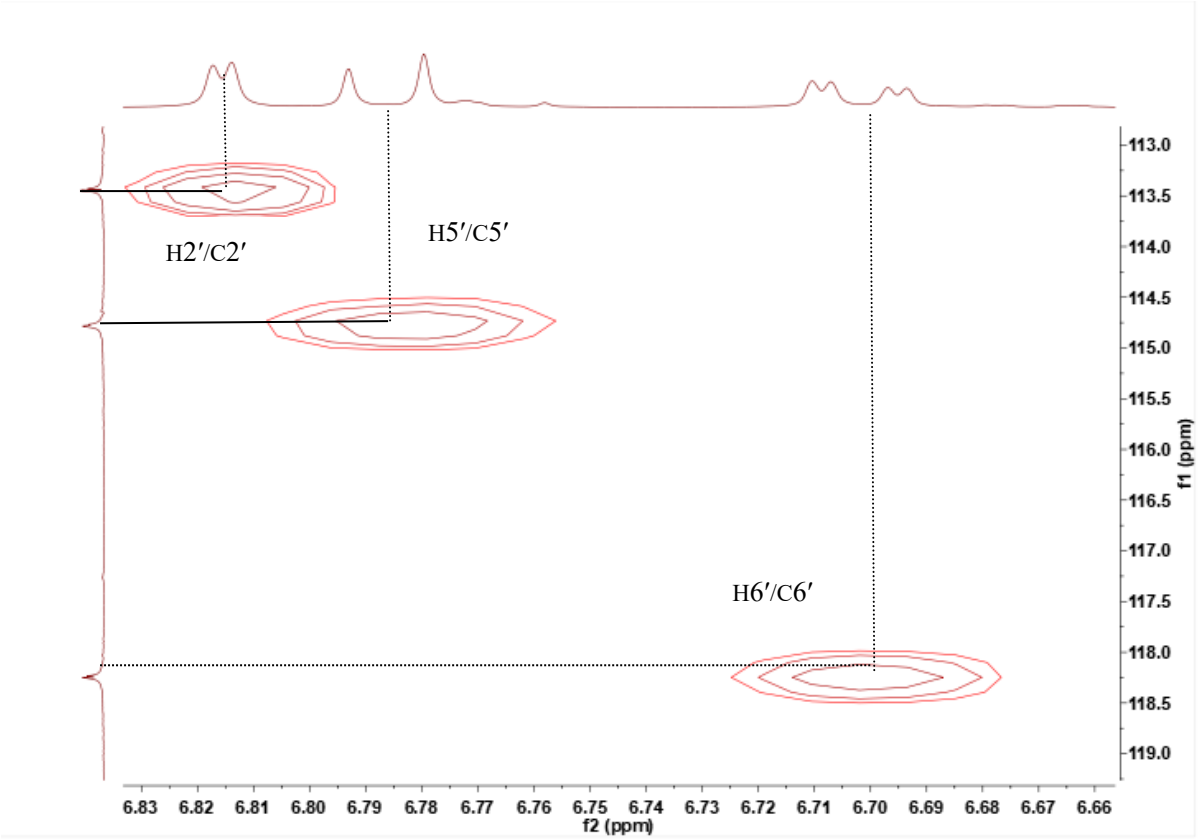


Figure S7: HSQC spectrum of **1** (Euphebranone F) (From δ_C110 ppm to δ_C 120 ppm)

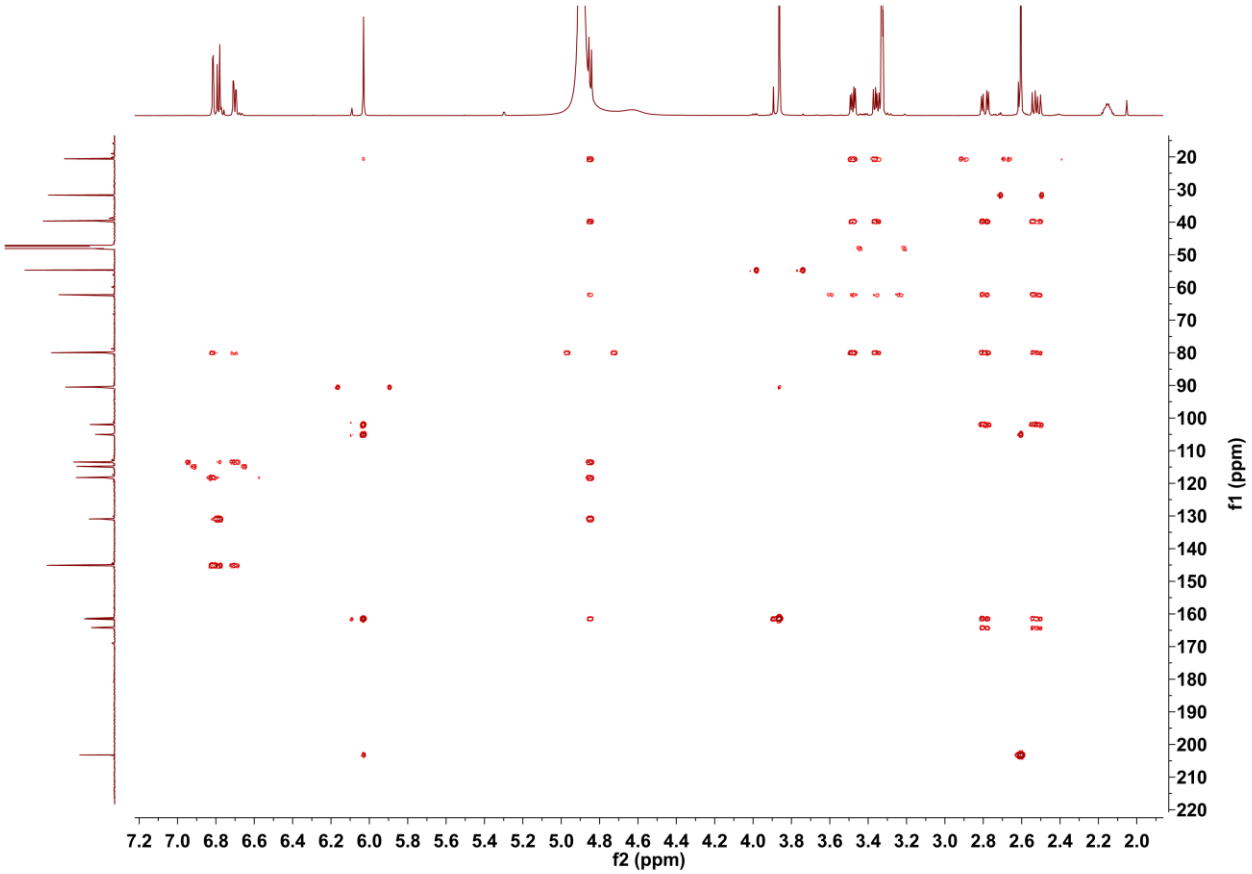


Figure S8: HMBC spectrum of **1** (Euphebranone F)

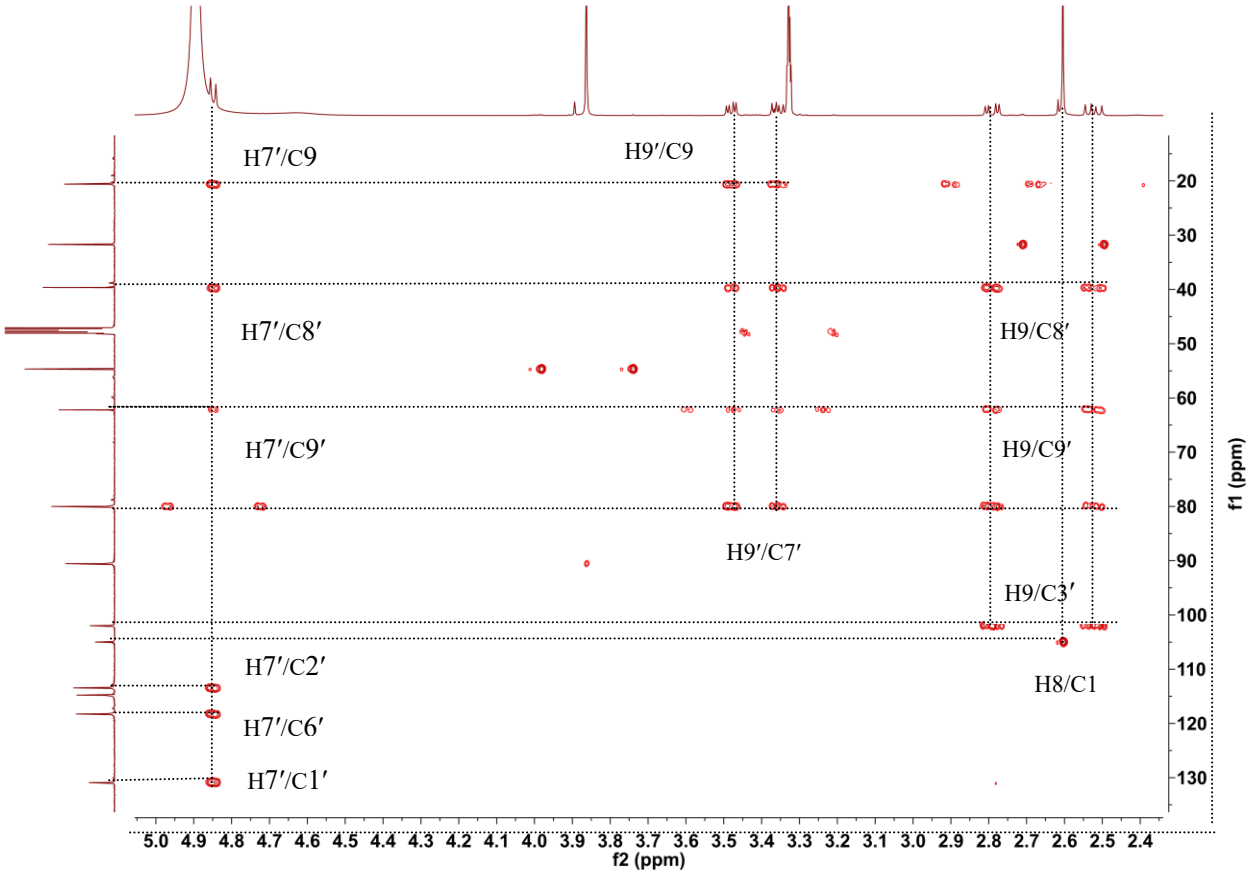


Figure S9: HMBC spectrum of **1** (Euphebranone F) (From δ_C 20 pm to δ_C 140 ppm)

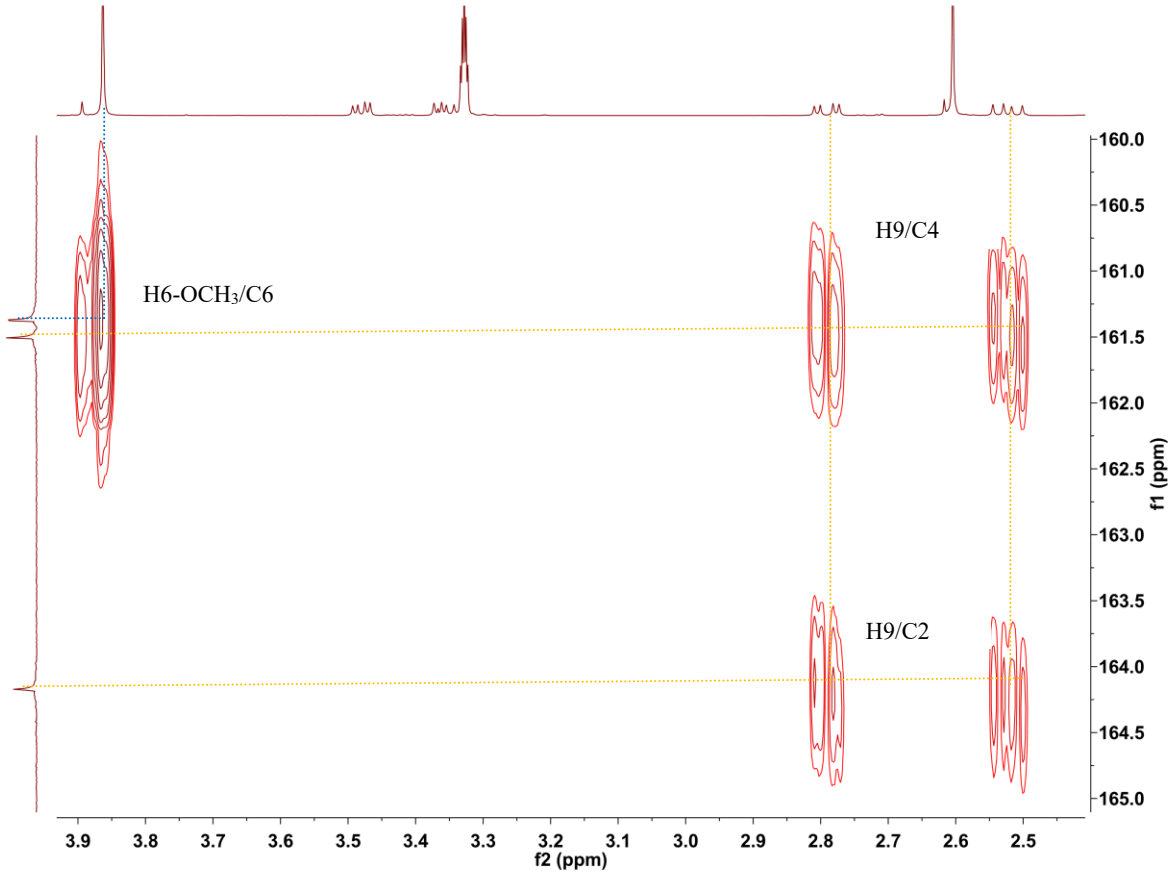


Figure S10: HMBC spectrum of **1** (Euphebranone F) (From δ_C 160 pm to δ_C 165 ppm)

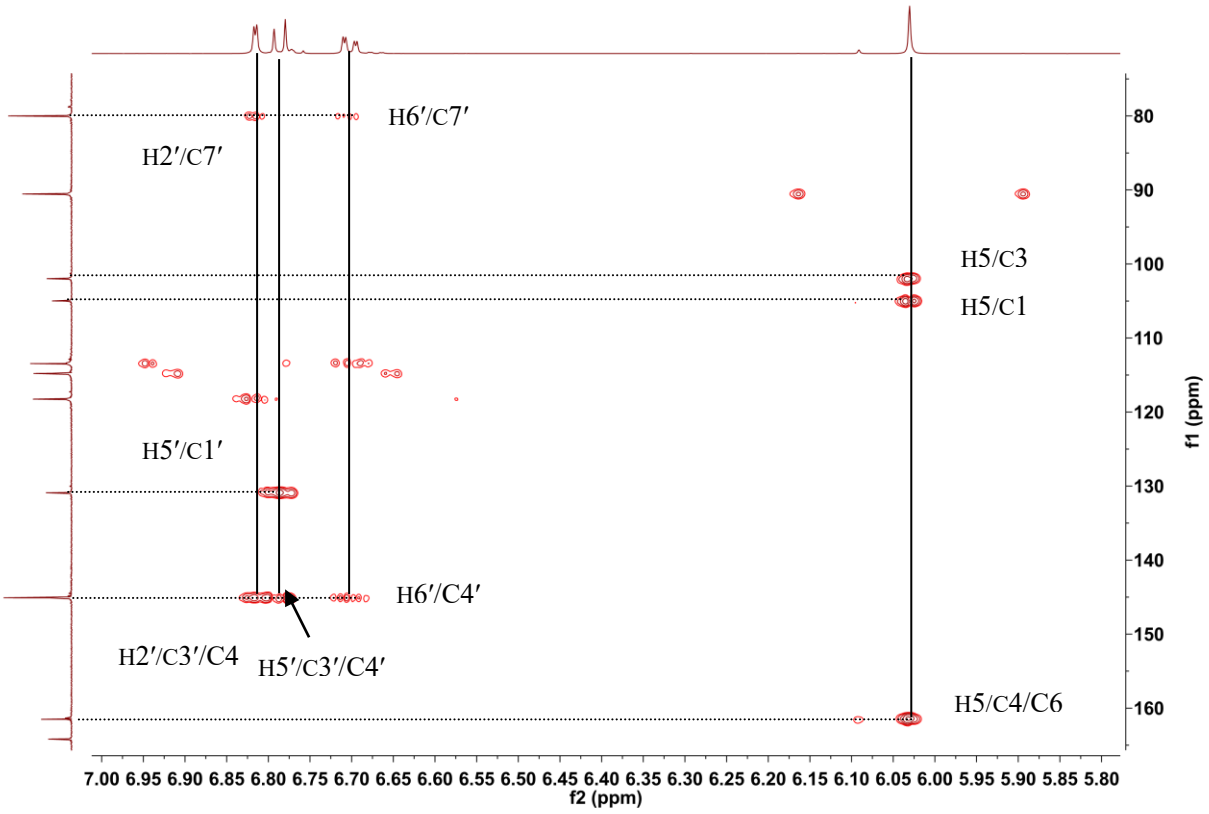


Figure S11: HMBC spectrum of **1** (Euphebranone F) (From δ_C 80 ppm to δ_C 160 ppm)

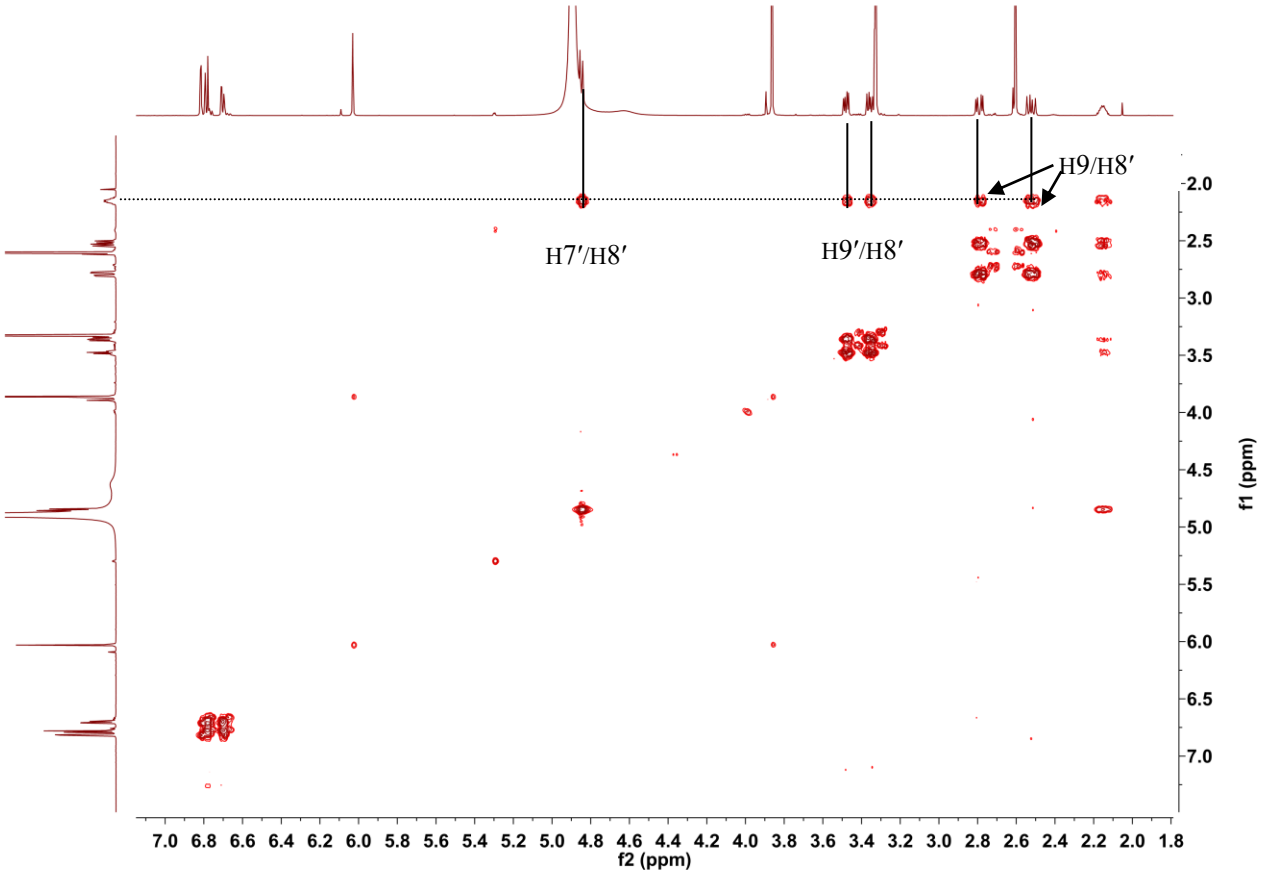


Figure S12: ^{1}H-^{1}H COSY spectrum of **1** (Euphebranone F)

S13: ECD Computational details of compound 1.

The initial conformational analysis of compound **1** was performed using Monte Carlo searching algorithm via the MMFF94 molecular mechanics force field[3], with the aid of the SPARTAN'16 program package, leading to afford a panel of relatively favored conformations in an energy range of 3 kcal/mol above the global minimum. The force field minimum energy conformers thus obtained were subsequently optimized by applying the density functional theory (DFT) with the M06-2X/def2-SVP level in vacuum, implemented in the Gaussian 09 software package. Harmonic vibrational frequencies were also performed to confirm no imaginary frequencies of the finally optimized conformers. These predominant conformers were subjected to theoretical calculation of ECD by utilizing Time-dependent density functional theory (TDDFT) calculations at the CAM-B3LYP/def2-TZVP level in MeOH using the Polarizable Continuum Model (PCM) solvent model. The energies, oscillator strengths, and rotational strengths of each conformer were carried out with Gaussian 09 software package. The theoretical calculations of ECD spectra for each conformer were then approximated by the Gaussian distribution. The final ECD spectrum of the individual conformers was summed up on the basis of Boltzmann-weighed population contribution by the SpecDisv 1.64[4], as well as its enantiomer.

S13-Table S2. Conformational analysis of the optimized conformers of 1 in the gas phase (T=298.15 K)

Conformers	ΔG (kcal/mol)	Population
1-1	0.0000	26.84%
1-2	0.2102	18.82%
1-3	0.4179	13.25%
1-4	0.6288	9.28%
1-5	0.6388	9.12%
1-6	0.6689	8.67%
1-7	0.6721	8.63%
1-8	0.9507	5.39%

S13-Table S3. Cartesian coordinates of low-energy conformers of 1 optimized at B3LYP/def2-SVP level in gas phase

Atom	Conformer **1-1**			Conformer **1-2**			Conformer **1-3**			Conformer **1-4**		
	X	Y	Z	X	Y	Z	X	Y	Z	X	Y	Z
O	6.28003	1.720856	-1.6935	-6.66598	1.276379	-1.56328	-6.56389	1.759004	-1.46956	6.401936	1.72722	-1.08603
O	6.251483	-0.83063	-0.93649	-5.02616	2.938704	-0.30255	-6.28789	-0.87245	-1.24026	4.243965	3.145547	-0.46254
C	3.871615	-0.72496	-0.43174	-3.64252	1.093196	0.475739	-4.29731	-0.62513	0.037974	2.902278	1.185527	-0.34488
C	5.065086	-0.16075	-0.86502	-4.7235	1.614023	-0.2178	-5.36737	-0.07628	-0.66143	4.124734	1.806143	-0.56275
C	5.115984	1.181397	-1.27387	-5.61555	0.75967	-0.8955	-5.48299	1.320639	-0.76412	5.248292	1.024354	-0.89382
C	3.948459	1.937834	-1.24682	-5.39593	-0.61067	-0.8597	-4.5384	2.143538	-0.16478	5.12641	-0.35118	-1.00707
C	2.750713	1.369595	-0.81344	-4.30156	-1.13315	-0.16388	-3.47158	1.585063	0.541156	3.890019	-0.96952	-0.78776
O	1.519196	-1.94878	0.381573	-2.34824	-2.19663	1.571926	-2.39042	-1.73549	1.771097	1.442051	-2.24643	-0.44733
C	2.700433	0.037722	-0.39644	-3.41766	-0.29088	0.507486	-3.34232	0.199681	0.643278	2.775616	-0.20711	-0.45093
C	1.401074	-0.55898	0.111937	-2.20313	-0.82336	1.240387	-2.15458	-0.39153	1.377125	1.432211	-0.85432	-0.17176
C	0.85997	0.173991	1.359234	-0.90225	-0.68921	0.432001	-0.8669	-0.38758	0.537375	0.940994	-0.60576	1.271583
O	-1.04365	-2.71108	0.013833	1.969543	-2.94382	-0.09895	1.793806	-2.90891	0.039464	-1.16002	-2.61323	-1.02074
O	-4.11913	2.746794	0.76432	3.171575	3.191831	0.748184	3.513817	3.138293	0.57832	-3.83145	2.351544	1.811234
O	-2.10251	1.610672	1.604201	1.394221	1.556536	1.22392	1.627052	1.673647	1.180984	-1.91769	0.833784	2.121045
C	-5.69081	1.907104	-0.76213	5.24221	2.783233	-0.27655	5.494217	2.522797	-0.51954	-5.42901	2.294099	0.094505
C	-4.4298	1.784729	0.054188	3.896871	2.333482	0.233259	4.146872	2.20338	0.075796	-4.19992	1.764957	0.787923
C	-3.58531	0.584091	0.028575	3.440291	0.941845	0.140066	3.582946	0.848492	0.071569	-3.44851	0.604781	0.292962
C	-2.41668	0.56723	0.847711	2.155353	0.619473	0.671543	2.29253	0.65523	0.650689	-2.29691	0.18851	1.026179
C	-1.55432	-0.54231	0.908462	1.638658	-0.6879	0.654285	1.669657	-0.60411	0.70109	-1.51784	-0.9183	0.64206
C	-1.83092	-1.63506	0.080046	2.393465	-1.68625	0.028079	2.324377	-1.6872	0.103581	-1.86397	-1.58839	-0.53603
C	-2.98271	-1.66086	-0.73165	3.672105	-1.40847	-0.49622	3.610005	-1.53928	-0.45657	-3.0031	-1.21617	-1.27811
C	-3.8459	-0.57909	-0.75335	4.188169	-0.1255	-0.43837	4.228129	-0.30136	-0.47058	-3.78195	-0.14656	-0.87167
C	-0.41023	-0.51398	1.885981	0.31927	-0.95321	1.327137	0.350002	-0.72794	1.413172	-0.38099	-1.34697	1.530736
C	1.923103	0.283524	2.443353	-0.8956	-1.60989	-0.78938	-0.96436	-1.34019	-0.65516	2.003475	-0.98914	2.291966
O	2.387159	-1.02731	2.746319	-0.68204	-2.96471	-0.42349	-0.85556	-2.69774	-0.25345	2.362149	-2.34852	2.074163
O	-4.95463	-0.56687	-1.52127	5.404325	0.178086	-0.93615	5.453145	-0.12114	-1.00619	-4.8743	0.244336	-1.5595

C	-5.23858	-1.68499	-2.3246	6.184866	-0.84634	-1.49964	6.134831	-1.23172	-1.53314	-5.23133	-0.45351	-2.72609
H	6.955308	1.029366	-1.66548	-6.63677	2.238618	-1.47032	-6.57447	2.72107	-1.50844	7.11509	1.134041	-1.34407
H	6.123898	-1.75888	-0.71437	-4.36658	3.468349	0.158128	-6.94045	-0.30763	-1.67703	5.161389	3.379856	-0.65937
H	3.841873	-1.77557	-0.13558	-2.96388	1.771178	1.003224	-4.22162	-1.71196	0.093288	2.048105	1.818916	-0.09649
H	3.999694	2.97504	-1.57919	-6.09464	-1.25785	-1.39034	-4.6417	3.228466	-0.24475	6.001855	-0.94766	-1.27682
H	1.843245	1.977316	-0.80846	-4.1334	-2.21102	-0.15171	-2.7364	2.239055	1.015023	3.791735	-2.04837	-0.89972
H	1.961621	-2.0174	1.247117	-3.16626	-2.31501	2.069027	-3.20536	-1.77663	2.285391	1.884558	-2.66866	0.311123
H	0.645526	-0.47263	-0.68677	-2.07367	-0.23116	2.16568	-1.96201	0.229537	2.271425	0.690775	-0.4185	-0.86241
H	0.586724	1.200541	1.066612	-0.84767	0.353533	0.079625	-0.73748	0.63691	0.152887	0.747892	0.472433	1.39168
H	-0.12268	-2.52095	0.301586	0.986809	-3.02347	-0.05999	0.808211	-2.89892	0.087154	-0.22946	-2.61728	-0.70079
H	-2.82523	2.293448	1.448524	1.921738	2.411085	1.163341	2.219646	2.478802	1.070208	-2.58451	1.575821	2.250067
H	-6.12334	2.892095	-0.55588	5.32855	3.856267	-0.07467	5.525841	2.240714	-1.57935	-6.20077	1.517247	0.028177
H	-5.47198	1.794351	-1.83124	6.048506	2.22727	0.218032	5.66276	3.597953	-0.39562	-5.787	3.153871	0.67102
H	-6.3973	1.108794	-0.50325	5.33664	2.579939	-1.35047	6.282131	1.944655	-0.02066	-5.19319	2.585875	-0.93665
H	-3.13562	-2.54742	-1.34014	4.201624	-2.23493	-0.96177	4.061983	-2.4264	-0.89095	-3.21308	-1.78792	-2.17753
H	-0.16577	-1.53686	2.208504	0.248469	-0.29941	2.207745	0.358891	-0.04057	2.270896	-0.2177	-2.43062	1.436284
H	-0.74204	0.033593	2.779417	0.284458	-1.99074	1.69094	0.232812	-1.74488	1.815266	-0.67447	-1.15579	2.57253
H	2.756636	0.912334	2.08826	-1.83417	-1.50556	-1.35936	-1.90364	-1.17472	-1.20943	2.885017	-0.33645	2.176632
H	1.485971	0.756189	3.339855	-0.0683	-1.33256	-1.45918	-0.13328	-1.15253	-1.35095	1.600067	-0.85368	3.310545
H	3.11657	-0.97719	3.371988	-1.32028	-3.16412	0.280488	-1.48533	-2.82191	0.475083	3.115552	-2.57776	2.627097
H	-6.17111	-1.45853	-2.85318	5.690524	-1.2895	-2.37858	6.300389	-2.00058	-0.76209	-4.43866	-0.38899	-3.48808
H	-4.43697	-1.86301	-3.05871	7.127714	-0.38225	-1.80955	7.10122	-0.86112	-1.89256	-5.43888	-1.51347	-2.51088
H	-5.37572	-2.59142	-1.71413	6.391269	-1.64032	-0.76487	5.580835	-1.68012	-2.37303	-6.14059	0.024449	-3.10708
	Conformer **1-5**			Conformer **1-6**			Conformer **1-7**			Conformer **1-8**		
	X	Y	Z	X	Y	Z	X	Y	Z	X	Y	Z
O	-6.65051	1.338133	-1.5364	6.304198	1.833385	-1.45073	6.3042	1.833591	-1.45046	-6.55731	1.803627	-1.4937
O	-4.96872	2.954064	-0.27249	6.238421	-0.74191	-0.80165	6.238541	-0.74169	-0.80138	-6.2804	-0.83367	-1.32111
C	-3.65345	1.119673	0.473683	3.886268	-0.66983	-0.44797	3.886341	-0.66978	-0.44791	-4.26791	-0.60119	0.030545
C	-4.73981	1.627934	-0.22495	5.082218	-0.0466	-0.79038	5.082276	-0.04647	-0.79023	-5.33776	-0.08159	-0.68606
C	-5.61449	0.740934	-0.8831	5.082074	1.316626	-1.1303	5.082064	1.316748	-1.13018	-5.51422	1.30857	-0.79807

C	-5.38971	-0.62573	-0.83038	3.892216	2.032731	-1.12919	3.892165	2.032777	-1.1292	-4.60409	2.157612	-0.17709
C	-4.29002	-1.12954	-0.12691	2.696539	1.40095	-0.78221	2.696495	1.400912	-0.78234	-3.53159	1.633178	0.544406
O	-2.33249	-2.14019	1.621736	1.497477	-2.016	0.087006	1.497522	-2.01607	0.086734	-2.38568	-1.63257	1.842831
C	-3.41795	-0.26068	0.526222	2.688223	0.049118	-0.43418	2.688246	0.049097	-0.43427	-3.34925	0.254614	0.652566
C	-2.19667	-0.77134	1.264496	1.39126	-0.60445	0.003704	1.391293	-0.60451	0.003561	-2.15262	-0.30184	1.396901
C	-0.90065	-0.64544	0.44676	0.876904	-0.03198	1.343264	0.876973	-0.03214	1.343179	-0.86864	-0.32978	0.551209
O	1.939291	-2.93362	-0.10253	-1.06166	-2.69754	-0.33947	-1.06163	-2.69743	-0.33982	1.75295	-2.89456	0.094058
O	3.237149	3.182592	0.752112	-4.09439	2.631236	1.145628	-4.09439	2.63115	1.145919	3.57012	3.133495	0.51949
O	1.436707	1.571595	1.232991	-2.0823	1.38195	1.815437	-2.08228	1.381789	1.81557	1.662354	1.709853	1.154043
C	5.292717	2.746819	-0.29106	-5.67983	2.016036	-0.46958	-5.67985	2.016091	-0.46934	5.534674	2.46897	-0.57832
C	3.944688	2.315677	0.228291	-4.41436	1.775622	0.313101	-4.41438	1.775618	0.313329	4.186368	2.180931	0.030415
C	3.466193	0.930954	0.133614	-3.57711	0.585093	0.12155	-3.57713	0.585112	0.12162	3.601455	0.834457	0.053241
C	2.180144	0.626481	0.672617	-2.40599	0.451741	0.926736	-2.40597	0.451686	0.926743	2.310169	0.672632	0.639564
C	1.643461	-0.6734	0.654671	-1.54982	-0.66052	0.835177	-1.54979	-0.66055	0.835053	1.667041	-0.57575	0.713483
C	2.380705	-1.68138	0.023563	-1.83821	-1.63362	-0.12816	-1.8382	-1.63356	-0.12837	2.303072	-1.67931	0.1343
C	3.660079	-1.42113	-0.50814	-2.99315	-1.54373	-0.9312	-2.99317	-1.5436	-0.93135	3.588605	-1.56263	-0.43216
C	4.194533	-0.14569	-0.45169	-3.84685	-0.46136	-0.80828	-3.84689	-0.46126	-0.80829	4.226485	-0.33493	-0.4701
C	0.324117	-0.92028	1.335025	-0.39563	-0.76678	1.796196	-0.39559	-0.76692	1.796043	0.347333	-0.66656	1.430554
C	-0.90768	-1.5658	-0.77443	1.957023	-0.07797	2.415643	1.957093	-0.07825	2.415545	-0.97765	-1.30341	-0.62199
O	-0.71632	-2.92457	-0.40865	2.400448	-1.42383	2.54471	2.400399	-1.42416	2.544544	-0.90556	-2.65545	-0.19156
O	5.412026	0.141251	-0.95685	-4.95539	-0.33562	-1.56602	-4.95547	-0.33546	-1.56596	5.452475	-0.18424	-1.012
C	6.176203	-0.89469	-1.52092	-5.26114	-1.34206	-2.49832	-5.26138	-1.34192	-2.49819	6.113635	-1.3131	-1.52607
H	-7.2025	0.678636	-1.9695	6.219254	2.754118	-1.71902	6.219122	2.754093	-1.71948	-7.06108	1.058644	-1.84937
H	-5.76518	3.102364	-0.80077	6.943468	-0.14213	-1.08175	6.94354	-0.14189	-1.08155	-6.0753	-1.77101	-1.23955
H	-2.99246	1.826255	0.980596	3.905308	-1.73298	-0.21008	3.905406	-1.73293	-0.21001	-4.14002	-1.68452	0.105474
H	-6.07496	-1.30411	-1.34459	3.900254	3.090382	-1.40476	3.900159	3.090427	-1.40478	-4.75869	3.232989	-0.26808
H	-4.11089	-2.20488	-0.09719	1.765674	1.971813	-0.78874	1.765578	1.971689	-0.78898	-2.82651	2.311762	1.030016
H	-3.14	-2.25145	2.137138	1.954986	-2.20465	0.92617	1.955033	-2.20481	0.925874	-3.16086	-1.64105	2.416434
H	-2.06747	-0.16092	2.177165	0.628094	-0.40573	-0.76679	0.628102	-0.40572	-0.76688	-1.95367	0.351699	2.265731
H	-0.84243	0.397211	0.094817	0.616249	1.027357	1.1869	0.61637	1.027223	1.186883	-0.7312	0.685564	0.145695

H	0.95628	-3.00085	-0.05625	-0.1325	-2.55386	-0.04612	-0.13249	-2.55378	-0.04635	0.769347	-2.86913	0.148185
H	1.972897	2.419862	1.171277	-2.80282	2.081465	1.759509	-2.80279	2.081281	1.75977	2.266251	2.504385	1.028866
H	5.397216	3.817484	-0.08517	-6.3925	1.196702	-0.31247	-5.47073	2.045032	-1.54585	5.719063	3.543811	-0.47678
H	6.09449	2.175878	0.193633	-6.10043	2.967962	-0.1278	-6.39245	1.196659	-0.31248	6.317077	1.889777	-0.07207
H	5.374385	2.547319	-1.36677	-5.47081	2.044712	-1.54611	-6.10053	2.967924	-0.1274	5.556127	2.165934	-1.63257
H	4.175455	-2.25428	-0.97764	-3.15416	-2.33988	-1.65254	-3.15419	-2.33967	-1.65279	4.025079	-2.46482	-0.85114
H	0.265799	-0.26307	2.213961	-0.15941	-1.82475	1.984033	-0.1594	-1.82492	1.983764	0.367105	0.038083	2.273896
H	0.279107	-1.95624	1.702216	-0.71189	-0.33356	2.755557	-0.71183	-0.33381	2.755455	0.218382	-1.67318	1.854756
H	-1.84407	-1.44678	-1.34503	2.796386	0.577232	2.128363	2.796506	0.576896	2.128288	-1.90665	-1.12532	-1.18943
H	-0.07585	-1.30114	-1.44382	1.543045	0.285994	3.372059	1.543151	0.285713	3.371977	-0.13631	-1.14913	-1.31368
H	-1.34275	-3.108	0.310248	3.202133	-1.45342	3.076568	3.202076	-1.45387	3.076408	-1.51401	-2.74091	0.56022
H	6.37525	-1.68955	-0.78498	-4.46788	-1.44009	-3.25614	-5.40682	-2.31488	-2.00301	7.084358	-0.96306	-1.89428
H	5.672221	-1.33386	-2.39645	-5.40673	-2.31502	-2.00316	-6.19438	-1.03909	-2.98627	6.270246	-2.07392	-0.74524
H	7.123827	-0.44428	-1.83655	-6.19402	-1.0392	-2.98659	-4.46828	-1.4399	-3.25619	5.548978	-1.76378	-2.3576

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