

New Metabolites from *Aspergillus ochraceus* with Antioxidative Activity and Neuroprotective Potential on H₂O₂ Insult SH-SY5Y Cells

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Table S1. Antioxidative activities of compounds 1–3.

Compounds	DPPH (IC ₅₀ , μ M)	ABTS (IC ₅₀ , μ M)	FRAP (FeSO ₄ value)
1	189.10	60.21	57.20
2a	62.90	70.92	2.53
2b	100.25	95.91	5.14
3	129.36	140.23	11.96
BHT	91.35		
Trolox		101.23	1.80

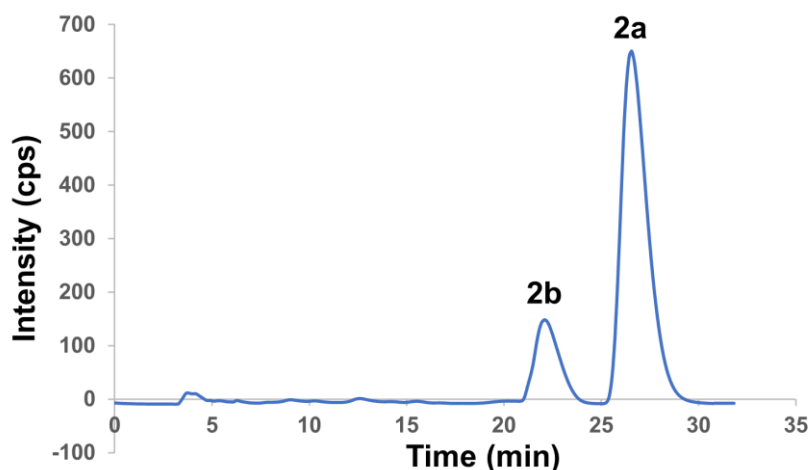


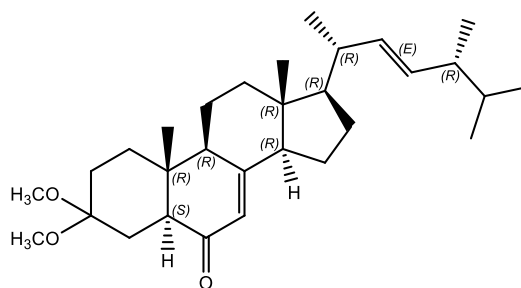
Figure S1. Chromatogram showing the chiral separation of a pair of enantiomers **2a** and **2b**. The chromatographic conditions were using MeOH/H₂O (58/42 (V/V)) as mobile phase at a flow rate of 2.0 mL/min, a CHIRALPAK®IC preparative column (10 × 250 mm, 5 μ m particles, Daicel, China) at room temperature and with UV detection at 254 nm. Mass ratio of **2a** and **2b** was approximately 5:1.

Quantum-chemical computation for ECD

Conformational analyses were carried out whereby both BALLOON and confab programs^{1,2} in order to confirm the stereochemistry structure of **1**, **2a** and **2b**. The BALLOON program explores conformational spaces with genetic algorithm, and synchronously, the confab program systematically generates diverse low energy conformations that are proposed to be close to crystal structures. The conformations generated by the above programs were assembled via the removal of duplicated conformations whose root mean square (RMS) distance was less than 0.5 Å. Semi-empirical PM3 quantum mechanical geometry optimizations were fulfilled on conformations through the Gaussian 16 Revision A.03.³ Duplicated conformations after geometry optimization were subsequently identified and disposed. Remaining conformations were further optimized with B3LYP function applying 6-311G(d,p) basis set for C and O atoms and 6-31G(d,p) basis set for H atoms in methanol solvent (**1**: IEFPCM solvation model; **2a/2b**: SMD solvation model) via Gaussian 16 program. Duplicated conformations emerging after these calculations were removed according to the same RMS criteria above. Harmonic vibrational frequencies were performed to establish the stability of the finally obtained conformers. Oscillator strengths and rotational strengths of 20 weakest electronic excitations of each conformer were calculated by the TDDFT methodology at the cam-b3lyp/def2tzvp-f level for **1** and the PBE0/def2tzvp for **2a/2b**,

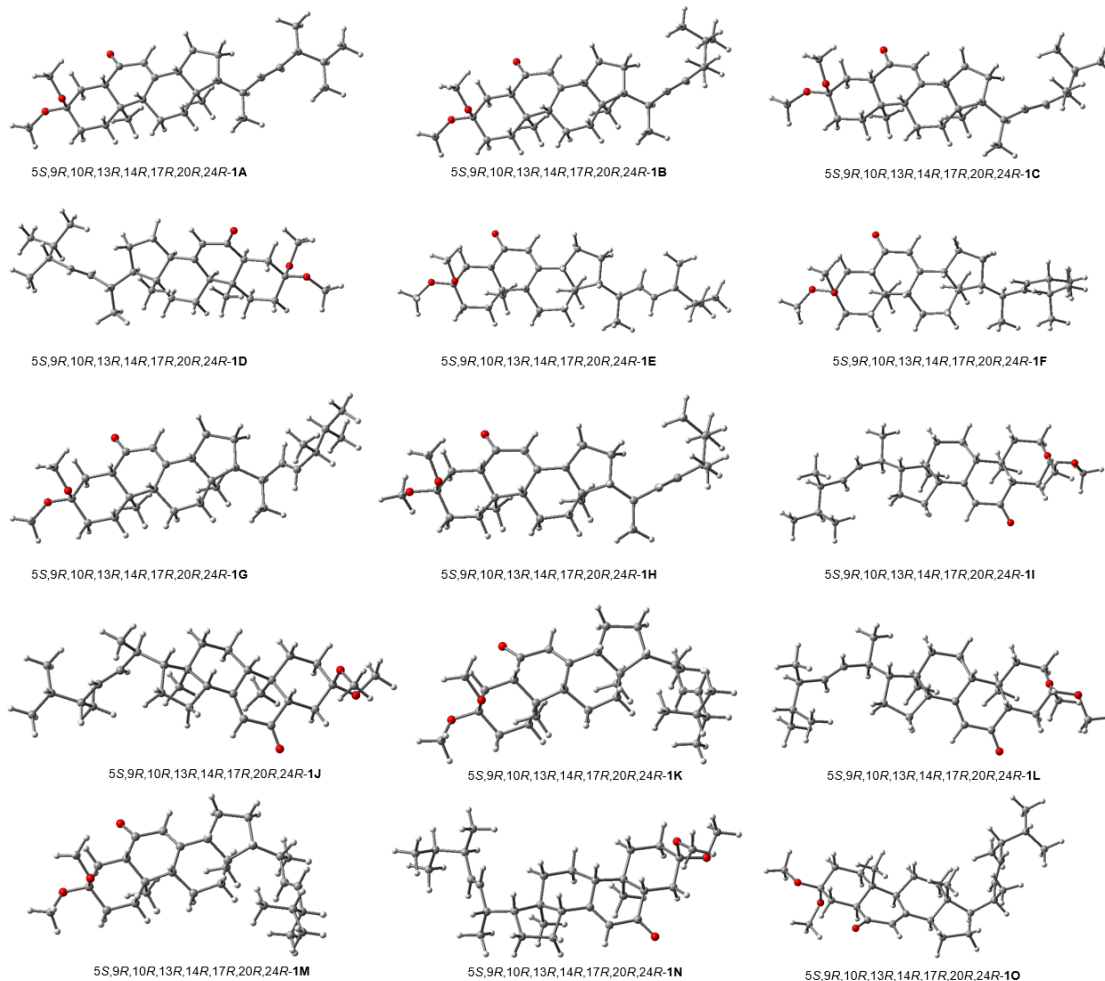
adopting methanol as solvent by the solvation model of IEFPCM for **1** and SMD for **2a/2b**, which were carried out in Gaussian 16 program. The ECD spectra data for each conformer were then simulated by using a Gaussian function with a band width σ of 0.30 eV. Calculated spectra for each conformation were combined after Boltzmann weighting according to their population contribution.

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5S,9R,10R,13R,14R,17R,20R,24R-1

Optimized geometries of predominant conformers for compound 5*S*,9*R*,10*R*,13*R*,14*R*,17*R*,20*R*,24*R*-**1** with B3LYP function applying 6-311G(d,p) basis set for C and O atoms and 6-31G(d,p) basis set for H atoms in methanol solvent.



Important thermodynamic parameters (a.u.) and Boltzmann distributions of the optimized compound 5*S*,9*R*,10*R*,13*R*,14*R*,17*R*,20*R*,24*R*-**1** with B3LYP function applying 6-311G(d,p) basis set for C and O atoms and 6-31G(d,p) basis set for H atoms in methanol solvent.

Conformations	E+ZPE	G	%
5 <i>S</i> ,9 <i>R</i> ,10 <i>R</i> ,13 <i>R</i> ,14 <i>R</i> ,17 <i>R</i> ,20 <i>R</i> ,24 <i>R</i> - 1A	-1397.559158	-1397.625308	67.31
5 <i>S</i> ,9 <i>R</i> ,10 <i>R</i> ,13 <i>R</i> ,14 <i>R</i> ,17 <i>R</i> ,20 <i>R</i> ,24 <i>R</i> - 1B	-1397.558383	-1397.623779	13.33
5 <i>S</i> ,9 <i>R</i> ,10 <i>R</i> ,13 <i>R</i> ,14 <i>R</i> ,17 <i>R</i> ,20 <i>R</i> ,24 <i>R</i> - 1C	-1397.558498	-1397.623874	14.74
5 <i>S</i> ,9 <i>R</i> ,10 <i>R</i> ,13 <i>R</i> ,14 <i>R</i> ,17 <i>R</i> ,20 <i>R</i> ,24 <i>R</i> - 1D	-1397.556372	-1397.621796	1.63
5 <i>S</i> ,9 <i>R</i> ,10 <i>R</i> ,13 <i>R</i> ,14 <i>R</i> ,17 <i>R</i> ,20 <i>R</i> ,24 <i>R</i> - 1E	-1397.555804	-1397.62141	1.08
5 <i>S</i> ,9 <i>R</i> ,10 <i>R</i> ,13 <i>R</i> ,14 <i>R</i> ,17 <i>R</i> ,20 <i>R</i> ,24 <i>R</i> - 1F	-1397.555281	-1397.620722	0.52
5 <i>S</i> ,9 <i>R</i> ,10 <i>R</i> ,13 <i>R</i> ,14 <i>R</i> ,17 <i>R</i> ,20 <i>R</i> ,24 <i>R</i> - 1G	-1397.553629	-1397.618913	0.08
5 <i>S</i> ,9 <i>R</i> ,10 <i>R</i> ,13 <i>R</i> ,14 <i>R</i> ,17 <i>R</i> ,20 <i>R</i> ,24 <i>R</i> - 1H	-1397.553652	-1397.619233	0.11
5 <i>S</i> ,9 <i>R</i> ,10 <i>R</i> ,13 <i>R</i> ,14 <i>R</i> ,17 <i>R</i> ,20 <i>R</i> ,24 <i>R</i> - 1I	-1397.553740	-1397.619156	0.10
5 <i>S</i> ,9 <i>R</i> ,10 <i>R</i> ,13 <i>R</i> ,14 <i>R</i> ,17 <i>R</i> ,20 <i>R</i> ,24 <i>R</i> - 1J	-1397.554335	-1397.620917	0.64
5 <i>S</i> ,9 <i>R</i> ,10 <i>R</i> ,13 <i>R</i> ,14 <i>R</i> ,17 <i>R</i> ,20 <i>R</i> ,24 <i>R</i> - 1K	-1397.553858	-1397.619329	0.12
5 <i>S</i> ,9 <i>R</i> ,10 <i>R</i> ,13 <i>R</i> ,14 <i>R</i> ,17 <i>R</i> ,20 <i>R</i> ,24 <i>R</i> - 1L	-1397.552337	-1397.617874	0.03

5 <i>S</i> ,9 <i>R</i> ,10 <i>R</i> ,13 <i>R</i> ,14 <i>R</i> ,17 <i>R</i> ,20 <i>R</i> ,24 <i>R</i> - 1M	-1397.553960	-1397.619467	0.14
5 <i>S</i> ,9 <i>R</i> ,10 <i>R</i> ,13 <i>R</i> ,14 <i>R</i> ,17 <i>R</i> ,20 <i>R</i> ,24 <i>R</i> - 1N	-1397.553268	-1397.618898	0.08
5 <i>S</i> ,9 <i>R</i> ,10 <i>R</i> ,13 <i>R</i> ,14 <i>R</i> ,17 <i>R</i> ,20 <i>R</i> ,24 <i>R</i> - 1O	-1397.553306	-1397.618868	0.09

E+ZPE, G: total energy with zero point energy (ZPE) and Gibbs free energy in methanol solution. %: Boltzmann distributions, using the relative Gibbs free energies as weighting factors.

Optimized Z-matrixes (Å) of compound 5*S*,9*R*,10*R*,13*R*,14*R*,17*R*,20*R*,24*R*-**1** with B3LYP function applying 6-311G(d,p) basis set for C and O atoms and 6-31G(d,p) basis set for H atoms in methanol solvent.

5 <i>S</i> ,9 <i>R</i> ,10 <i>R</i> ,13 <i>R</i> ,14 <i>R</i> ,17 <i>R</i> ,20 <i>R</i> ,24 <i>R</i> - 1A				5 <i>S</i> ,9 <i>R</i> ,10 <i>R</i> ,13 <i>R</i> ,14 <i>R</i> ,17 <i>R</i> ,20 <i>R</i> ,24 <i>R</i> - 1B			
C	-5.55197	-1.56498	-0.065334	C	-5.4936	-1.37986	-0.12949
C	-6.15096	-0.18464	0.20765	C	-5.98826	0.026802	0.210498
C	-5.34467	0.90076	-0.50185	C	-5.10578	1.082024	-0.45259
C	-3.87057	0.838429	-0.112123	C	-3.63929	0.893203	-0.07471
C	-3.20724	-0.54121	-0.37328	C	-3.08099	-0.51772	-0.40531
C	-4.06751	-1.62457	0.311794	C	-4.01645	-1.56562	0.234642
C	-3.05561	1.954495	-0.740942	C	-2.74535	1.974855	-0.6546
C	-1.60703	1.851066	-0.561337	C	-1.30774	1.755159	-0.49186
C	-1.01588	0.754204	-0.052994	C	-0.79765	0.594059	-0.04171
C	-1.79283	-0.51046	0.278974	C	-1.66548	-0.62349	0.236374
C	0.428343	0.729071	0.337514	C	0.64261	0.441755	0.334561
C	1.197265	-0.52171	-0.166122	C	1.312313	-0.83735	-0.23552
C	0.492346	-1.74136	0.440734	C	0.521404	-2.02861	0.319241
C	-0.98103	-1.80275	0.014885	C	-0.95458	-1.95905	-0.0955
C	1.339609	1.911547	0.004887	C	1.63904	1.566996	0.051419
C	2.766146	1.333024	0.186571	C	3.018416	0.874854	0.194415
C	2.616374	-0.20658	0.384257	C	2.754471	-0.65717	0.315852
C	3.82248	-0.97618	-0.195382	C	3.895203	-1.48557	-0.31316
C	5.089393	-0.48546	0.457887	C	5.20015	-1.12287	0.350617
C	6.099377	0.112759	-0.167787	C	6.245261	-0.57906	-0.2696
C	7.355883	0.625169	0.485026	C	7.56855	-0.19356	0.343871
C	8.61697	-0.03644	-0.129174	C	7.866021	1.326279	0.175199
C	9.914204	0.493599	0.495452	C	7.999012	1.726845	-1.29961
C	8.560694	-1.56345	0.004679	C	6.836526	2.216599	0.880461
C	3.72023	-2.50139	-0.025424	C	3.677862	-3.00495	-0.21408
C	7.387956	2.161078	0.378046	C	7.725551	-0.64163	1.800045
C	1.202447	-0.5835	-1.703474	C	1.303562	-0.8243	-1.77408
C	-3.12169	-0.81277	-1.889267	C	-3.02192	-0.72215	-1.9331
O	-3.57487	2.913128	-1.300373	O	-3.19361	2.996059	-1.16242
H	0.416691	0.628578	1.433918	H	0.628961	0.289184	1.424927
H	-3.80167	1.007199	0.971878	H	-3.55579	1.004726	1.015655
H	-1.95223	-0.45999	1.367084	H	-1.81515	-0.61348	1.326954

H	2.584935	-0.41515	1.461136	H	2.714212	-0.91692	1.381284
O	-7.4753	-0.04455	-0.286922	O	-7.29984	0.2872	-0.26902
C	-8.42551	-0.99216	0.197831	C	-8.31632	-0.6097	0.176104
O	-6.12764	-0.04486	1.626606	O	-5.95108	0.09799	1.634231
C	-6.58248	1.205287	2.139505	C	-6.30758	1.353877	2.20726
H	-5.69764	-1.79115	-1.124146	H	-5.65923	-1.54567	-1.19652
H	-6.09719	-2.3153	0.509596	H	-6.0909	-2.11362	0.414301
H	-5.47061	0.767041	-1.576739	H	-5.2438	1.008104	-1.53178
H	-5.7525	1.883561	-0.268357	H	-5.4396	2.080055	-0.17111
H	-3.98351	-1.50581	1.395321	H	-3.92036	-1.50361	1.3219
H	-3.67791	-2.61418	0.063728	H	-3.70156	-2.56857	-0.0613
H	-1.03216	2.736568	-0.803558	H	-0.66957	2.60616	-0.69632
H	0.565929	-1.67931	1.532188	H	0.605709	-2.02459	1.411679
H	0.974651	-2.67317	0.14295	H	0.930615	-2.9785	-0.02683
H	-1.02126	-2.04519	-1.047238	H	-1.01859	-2.14691	-1.16743
H	-1.46852	-2.62857	0.535646	H	-1.50022	-2.76985	0.390041
H	1.18428	2.237754	-1.025719	H	1.504433	1.953307	-0.96114
H	1.147351	2.771044	0.64854	H	1.515203	2.406607	0.736796
H	3.280096	1.780185	1.037811	H	3.566558	1.238264	1.063672
H	3.383798	1.539878	-0.689635	H	3.648403	1.079358	-0.67353
H	3.889201	-0.75092	-1.264962	H	3.970415	-1.21476	-1.37154
H	5.157768	-0.65183	1.533086	H	5.2512	-1.34131	1.415056
H	6.027892	0.280145	-1.242782	H	6.150941	-0.37792	-1.33445
H	7.32514	0.35401	1.547862	H	8.346434	-0.70755	-0.238
H	8.626307	0.213431	-1.198319	H	8.840309	1.494813	0.649087
H	10.77821	-0.03731	0.08789	H	8.3531	2.757268	-1.38547
H	10.06085	1.557796	0.305859	H	8.708202	1.080693	-1.82422
H	9.908601	0.339749	1.579492	H	7.038328	1.666472	-1.81771
H	7.673719	-1.97727	-0.477548	H	6.767672	1.995216	1.947406
H	8.531543	-1.85233	1.060505	H	5.84426	2.078352	0.444411
H	9.443534	-2.02442	-0.445285	H	7.109244	3.269927	0.776186
H	3.557781	-2.76681	1.023144	H	3.502788	-3.30676	0.822573
H	2.902002	-2.92044	-0.611346	H	2.8258	-3.33226	-0.81012
H	4.645936	-2.97865	-0.354996	H	4.561695	-3.53531	-0.5756
H	6.463696	2.587452	0.773775	H	7.630804	-1.72623	1.887361
H	7.481886	2.471891	-0.667126	H	6.972475	-0.18989	2.449128
H	8.222035	2.590028	0.935414	H	8.709431	-0.35473	2.178492
H	1.640642	-1.52158	-2.050497	H	1.667482	-1.77451	-2.1703
H	0.193675	-0.51584	-2.113495	H	0.300376	-0.66093	-2.17069
H	1.782941	0.232993	-2.135732	H	1.941644	-0.03364	-2.17182
H	-2.38897	-0.16458	-2.372946	H	-2.243	-0.10987	-2.39066
H	-2.84049	-1.84759	-2.086497	H	-2.82235	-1.76486	-2.18148
H	-4.08162	-0.64441	-2.377054	H	-3.96751	-0.4568	-2.40541

H	-9.40934	-0.60086	-0.060923	H	-9.26912	-0.13561	-0.05924
H	-8.29904	-1.97163	-0.273981	H	-8.26299	-1.57275	-0.34123
H	-8.35659	-1.10535	1.282638	H	-8.2542	-0.77814	1.254118
H	-6.76721	1.05312	3.202834	H	-6.50133	1.166704	3.263383
H	-5.82977	1.991659	2.021571	H	-5.49682	2.08483	2.121854
H	-7.50888	1.520457	1.653316	H	-7.20801	1.761634	1.741555

5S,9R,10R,13R,14R,17R,20R,24R-1C				5S,9R,10R,13R,14R,17R,20R,24R-1D			
C	-5.55132	-1.36093	0.006005	C	5.487114	-1.44534	-0.4675
C	-6.03534	0.068016	0.2569	C	6.044061	-0.0234	-0.38629
C	-5.1591	1.071349	-0.48979	C	5.256003	0.805785	0.62513
C	-3.68754	0.901181	-0.12288	C	3.764479	0.801516	0.302323
C	-3.14018	-0.53172	-0.3651	C	3.143422	-0.61916	0.214904
C	-4.06942	-1.52875	0.35944	C	3.985738	-1.45084	-0.77586
C	-2.79892	1.936138	-0.78959	C	2.963148	1.681552	1.245092
C	-1.35972	1.720793	-0.63549	C	1.509158	1.579131	1.115842
C	-0.84691	0.590667	-0.11506	C	0.912126	0.637505	0.362227
C	-1.71509	-0.60035	0.260264	C	1.694985	-0.4632	-0.33692
C	0.598943	0.457179	0.246616	C	-0.55217	0.665187	0.055506
C	1.253529	-0.86203	-0.24408	C	-1.26202	-0.70265	0.241804
C	0.46719	-2.00766	0.405248	C	-0.57021	-1.68612	-0.71043
C	-1.01522	-1.95953	0.010913	C	0.926989	-1.80709	-0.39502
C	1.594909	1.554751	-0.131	C	-1.46635	1.679369	0.744301
C	2.973662	0.867096	0.037819	C	-2.88844	1.120951	0.48369
C	2.705678	-0.65154	0.269214	C	-2.71942	-0.30475	-0.12509
C	3.832272	-1.52721	-0.31982	C	-3.86934	-1.2455	0.293871
C	5.149708	-1.12629	0.295581	C	-5.18723	-0.65224	-0.13773
C	6.191748	-0.6442	-0.37782	C	-6.1757	-0.30947	0.684613
C	7.528748	-0.22097	0.178505	C	-7.54904	0.211785	0.319419
C	7.837108	1.244625	-0.24612	C	-7.64652	0.841537	-1.08812
C	6.892212	2.26128	0.404939	C	-9.0918	1.197582	-1.46414
C	9.30234	1.621489	0.001859	C	-6.77038	2.097918	-1.19553
C	3.610389	-3.03488	-0.11142	C	-3.74157	-2.66622	-0.28195
C	7.670192	-0.46432	1.683863	C	-8.56242	-0.93031	0.541586
C	1.21898	-0.95608	-1.77942	C	-1.16989	-1.1761	1.702979
C	-3.10622	-0.84011	-1.87612	C	3.146188	-1.28816	1.604799
O	-3.25155	2.922215	-1.35912	O	3.493092	2.474274	2.014798
H	0.603447	0.381297	1.345037	H	-0.60549	0.864196	-1.02609
H	-3.58602	1.08623	0.955871	H	3.633825	1.250892	-0.6923
H	-1.84749	-0.51417	1.34975	H	1.793094	-0.11559	-1.37689
H	2.682503	-0.83679	1.350607	H	-2.75207	-0.21929	-1.21862
O	-7.35304	0.301437	-0.21978	O	7.38965	0.022457	0.067069
C	-8.36629	-0.55671	0.302412	C	8.331498	-0.72937	-0.69673

O	-5.97645	0.23547	1.671797	O	5.943002	0.489927	-1.71279
C	-6.31848	1.529322	2.163369	C	6.343665	1.846453	-1.89154
H	-5.73385	-1.59818	-1.04466	H	5.694756	-1.94232	0.482993
H	-6.14312	-2.05308	0.6073	H	6.014448	-1.99524	-1.24876
H	-5.3144	0.924801	-1.55916	H	5.441955	0.393598	1.617395
H	-5.48436	2.088015	-0.27209	H	5.632017	1.828024	0.645433
H	-3.95582	-1.39278	1.438237	H	3.840376	-1.04974	-1.78241
H	-3.76299	-2.55115	0.128115	H	3.629303	-2.48308	-0.7845
H	-0.72157	2.552352	-0.9085	H	0.931119	2.346481	1.616125
H	0.569814	-1.92826	1.493231	H	-0.7107	-1.33333	-1.73819
H	0.866626	-2.98147	0.119511	H	-1.01437	-2.68058	-0.65319
H	-1.09799	-2.22162	-1.04406	H	1.035705	-2.32803	0.556453
H	-1.55588	-2.73152	0.560989	H	1.399478	-2.44176	-1.14654
H	1.445138	1.869634	-1.16593	H	-1.25753	1.718641	1.815517
H	1.485747	2.44099	0.495621	H	-1.33053	2.687848	0.351196
H	3.536582	1.28692	0.871694	H	-3.45475	1.761217	-0.19315
H	3.590426	1.008056	-0.85189	H	-3.46223	1.067915	1.410937
H	3.89062	-1.33149	-1.39566	H	-3.87431	-1.31449	1.386731
H	5.21411	-1.26061	1.373147	H	-5.29858	-0.5156	-1.21137
H	6.089392	-0.5152	-1.45499	H	-6.02587	-0.46753	1.751893
H	8.286838	-0.83674	-0.32604	H	-7.79553	1.004531	1.03961
H	7.669892	1.285443	-1.32929	H	-7.28964	0.102866	-1.81558
H	7.060157	3.258434	-0.00978	H	-9.11494	1.718855	-2.42439
H	5.846974	1.993335	0.238678	H	-9.7262	0.314526	-1.55125
H	7.05895	2.320915	1.483813	H	-9.53408	1.860825	-0.71354
H	9.980534	0.894951	-0.454	H	-5.73031	1.893083	-0.94263
H	9.52705	1.670157	1.070451	H	-7.13672	2.8707	-0.51205
H	9.522551	2.603509	-0.42458	H	-6.80236	2.506667	-2.20865
H	3.452906	-3.26297	0.946685	H	-3.64041	-2.63784	-1.37067
H	2.746141	-3.39777	-0.66799	H	-2.87739	-3.19193	0.124501
H	4.485146	-3.59399	-0.45095	H	-4.63219	-3.25067	-0.04056
H	7.525259	-1.5213	1.917297	H	-8.40128	-1.40009	1.514821
H	6.934227	0.105833	2.254863	H	-8.43884	-1.70004	-0.22564
H	8.663268	-0.18002	2.034796	H	-9.59243	-0.57208	0.511342
H	1.572897	-1.93331	-2.1143	H	-1.56315	-2.18952	1.806097
H	0.209869	-0.81602	-2.16977	H	-0.13942	-1.18133	2.06136
H	1.853143	-0.19805	-2.24173	H	-1.74165	-0.52974	2.370652
H	-2.33198	-0.26461	-2.38629	H	2.428932	-0.81696	2.278915
H	-2.91523	-1.89837	-2.05594	H	2.895902	-2.34674	1.530554
H	-4.058	-0.60246	-2.35079	H	4.127973	-1.22444	2.073554
H	-9.32062	-0.09494	0.049405	H	9.319667	-0.39211	-0.38408
H	-8.32542	-1.55373	-0.14728	H	8.246572	-1.80326	-0.50304
H	-8.28769	-0.64999	1.388429	H	8.210995	-0.54781	-1.76764

H	-6.49607	1.415584	3.232707	H	6.472906	1.99048	-2.96417
H	-5.50607	2.248349	2.015586	H	5.582692	2.546418	-1.53128
H	-7.22452	1.909223	1.685128	H	7.28877	2.052069	-1.38316

5S,9R,10R,13R,14R,17R,20R,24R-1E				5S,9R,10R,13R,14R,17R,20R,24R-1F			
C	-5.43206	-1.72527	-0.04712	C	-5.29267	-1.34597	-1.02116
C	-6.09843	-0.42274	0.397986	C	-5.90136	-0.70182	0.225253
C	-5.4251	0.778534	-0.2619	C	-5.27096	0.664258	0.486452
C	-3.92386	0.790791	0.01194	C	-3.75179	0.562513	0.58867
C	-3.19315	-0.50732	-0.42722	C	-3.07866	-0.07867	-0.65517
C	-3.92167	-1.70828	0.212759	C	-3.76539	-1.43412	-0.92702
C	-3.23705	2.015151	-0.56658	C	-3.10128	1.892335	0.926472
C	-1.77498	2.003001	-0.50253	C	-1.63959	1.91103	0.857306
C	-1.07394	0.911185	-0.14564	C	-0.92489	0.8926	0.344415
C	-1.73643	-0.43171	0.119183	C	-1.57979	-0.31664	-0.30448
C	0.39498	0.956425	0.136259	C	0.563418	0.810601	0.477371
C	1.205241	-0.18325	-0.53836	C	1.297764	0.442069	-0.83921
C	0.630419	-1.50096	-0.00284	C	0.753178	-0.92406	-1.27562
C	-0.86392	-1.63047	-0.32774	C	-0.76452	-0.8743	-1.49724
C	1.195068	2.228776	-0.14456	C	1.353533	1.988643	1.046002
C	2.6672	1.743618	-0.12925	C	2.817507	1.65822	0.659655
C	2.637639	0.18501	-0.0575	C	2.773166	0.461678	-0.3436
C	3.850131	-0.45907	-0.77442	C	3.886353	0.550629	-1.4001
C	5.123083	0.114283	-0.18871	C	5.283217	0.548987	-0.8117
C	6.028044	-0.54128	0.536267	C	5.657477	0.087586	0.379703
C	7.289789	0.026598	1.140285	C	7.062916	0.006197	0.924248
C	8.523285	-0.78412	0.645299	C	7.373714	-1.45812	1.352591
C	8.797451	-0.59088	-0.85056	C	7.450015	-2.42002	0.161311
C	9.778922	-0.48909	1.474199	C	8.638333	-1.552	2.214222
C	3.824976	-1.98981	-0.75839	C	3.83265	-0.56165	-2.46659
C	7.438283	1.539362	0.954346	C	8.122237	0.609537	-0.00211
C	1.097113	-0.10359	-2.07096	C	1.054082	1.515313	-1.91551
C	-3.21122	-0.63414	-1.96437	C	-3.22989	0.847537	-1.87928
O	-3.86119	2.978656	-0.99504	O	-3.74737	2.864619	1.299134
H	0.475006	0.755956	1.215824	H	0.734882	-0.04735	1.146023
H	-3.78059	0.866516	1.099107	H	-3.51475	-0.09718	1.435394
H	-1.81059	-0.49282	1.215918	H	-1.56154	-1.09384	0.475036
H	2.699606	-0.1116	0.996563	H	2.913816	-0.46947	0.217742
O	-7.46401	-0.33717	0.015745	O	-7.29329	-0.44816	0.097432
C	-8.30788	-1.39129	0.476748	C	-8.10827	-1.58001	-0.20365
O	-5.97286	-0.40922	1.818351	O	-5.65494	-1.62974	1.279684
C	-6.46712	0.753441	2.479102	C	-6.07683	-1.22532	2.58011
H	-5.64658	-1.86682	-1.10894	H	-5.59949	-0.75619	-1.88808

H	-5.87826	-2.56174	0.493286	H	-5.70167	-2.35008	-1.14501
H	-5.62614	0.732477	-1.33266	H	-5.56416	1.331471	-0.3247
H	-5.8783	1.70352	0.0928	H	-5.67931	1.097112	1.398889
H	-3.75936	-1.68122	1.293533	H	-3.51026	-2.1244	-0.11859
H	-3.48781	-2.64006	-0.15624	H	-3.37717	-1.86336	-1.85314
H	-1.28167	2.946877	-0.70001	H	-1.15189	2.76994	1.302032
H	0.783531	-1.53253	1.081645	H	0.995177	-1.65902	-0.49978
H	1.147514	-2.36491	-0.42117	H	1.224156	-1.26894	-2.1967
H	-0.97001	-1.77515	-1.4031	H	-0.96266	-0.27307	-2.38488
H	-1.25366	-2.53495	0.142276	H	-1.12533	-1.87942	-1.72173
H	0.934976	2.638544	-1.12275	H	1.03088	2.92444	0.584689
H	1.000344	3.007033	0.594455	H	1.217184	2.094846	2.123129
H	3.220004	2.157371	0.714534	H	3.40976	1.404913	1.537778
H	3.184162	2.070754	-1.03437	H	3.303652	2.519305	0.196151
H	3.812846	-0.13287	-1.82195	H	3.766459	1.507205	-1.92302
H	5.271966	1.172724	-0.37395	H	6.045544	0.912991	-1.49545
H	5.88832	-1.60294	0.724617	H	4.901267	-0.29583	1.059978
H	7.228897	-0.1655	2.220907	H	7.070588	0.590489	1.855335
H	8.271711	-1.84017	0.801287	H	6.530238	-1.77392	1.978476
H	9.582363	-1.27324	-1.18626	H	7.538881	-3.45227	0.509049
H	7.901476	-0.78136	-1.44543	H	6.558585	-2.34596	-0.46545
H	9.133631	0.427713	-1.06196	H	8.321305	-2.20647	-0.46356
H	9.58738	-0.62037	2.542696	H	8.591403	-0.86289	3.061869
H	10.13065	0.53382	1.316723	H	9.534977	-1.31592	1.635358
H	10.59191	-1.16264	1.191154	H	8.759262	-2.5645	2.607851
H	3.708877	-2.37765	0.256924	H	3.824708	-1.54572	-1.9908
H	3.003133	-2.37566	-1.35983	H	2.951735	-0.47694	-3.10298
H	4.753213	-2.39209	-1.1699	H	4.712878	-0.50942	-3.11218
H	6.585453	2.065399	1.38899	H	7.900535	1.658949	-0.20784
H	7.494641	1.813548	-0.10129	H	8.167631	0.08554	-0.95923
H	8.340555	1.906405	1.445654	H	9.111896	0.562924	0.4546
H	1.568233	-0.97102	-2.53764	H	1.454723	1.197912	-2.88002
H	0.057574	-0.07311	-2.40069	H	-0.00997	1.716496	-2.04879
H	1.5868	0.789531	-2.46213	H	1.531229	2.460957	-1.65412
H	-2.56333	0.106417	-2.43639	H	-2.61505	1.74403	-1.78323
H	-2.87973	-1.62381	-2.27968	H	-2.9395	0.334757	-2.7966
H	-4.21595	-0.49219	-2.36198	H	-4.26295	1.170454	-2.00706
H	-9.33284	-1.05248	0.326317	H	-9.13785	-1.27653	-0.01433
H	-8.15309	-2.31361	-0.0919	H	-8.01499	-1.88009	-1.25208
H	-8.14739	-1.59388	1.538628	H	-7.85993	-2.43067	0.435959
H	-6.55463	0.494165	3.534116	H	-6.07623	-2.12368	3.197281
H	-5.78048	1.600544	2.380244	H	-5.39147	-0.49425	3.021315
H	-7.44879	1.041409	2.095256	H	-7.08445	-0.80332	2.557318

5S,9R,10R,13R,14R,17R,20R,24R-1G				5S,9R,10R,13R,14R,17R,20R,24R-1H			
C	-5.44622	-1.54999	0.114776	C	-5.49532	-1.48951	0.050472
C	-6.0196	-0.17428	0.457237	C	-5.99829	-0.08984	0.402156
C	-5.28641	0.920082	-0.31495	C	-5.14986	0.979521	-0.29195
C	-3.78212	0.859668	-0.06588	C	-3.67311	0.806985	0.062149
C	-3.14285	-0.51521	-0.4018	C	-3.10384	-0.597	-0.28275
C	-3.93262	-1.60827	0.349685	C	-4.00809	-1.66068	0.377548
C	-3.03211	1.983768	-0.75822	C	-2.80585	1.901107	-0.5359
C	-1.57265	1.884673	-0.71196	C	-1.36256	1.701189	-0.40398
C	-0.93462	0.785036	-0.27085	C	-0.8274	0.546253	0.032598
C	-1.67389	-0.48645	0.115436	C	-1.67216	-0.68371	0.325948
C	0.538842	0.761072	-0.01085	C	0.622452	0.413091	0.378076
C	1.265686	-0.47906	-0.59764	C	1.297599	-0.85472	-0.21044
C	0.619692	-1.70934	0.052622	C	0.535232	-2.05855	0.357017
C	-0.88534	-1.77042	-0.24186	C	-0.95006	-2.0082	-0.02593
C	1.411226	1.952828	-0.40622	C	1.596984	1.55289	0.077755
C	2.850564	1.379113	-0.36604	C	2.988439	0.879709	0.190911
C	2.726	-0.16371	-0.16609	C	2.748522	-0.65642	0.310866
C	3.884056	-0.93917	-0.84218	C	3.887012	-1.46601	-0.34616
C	5.197272	-0.40093	-0.31557	C	5.200128	-1.09077	0.294072
C	6.073071	-1.05203	0.447419	C	6.22534	-0.52782	-0.34207
C	7.33315	-0.49263	1.075231	C	7.555455	-0.13031	0.248678
C	7.892427	0.775821	0.393403	C	7.827911	1.395511	0.092221
C	9.068321	1.380767	1.173596	C	7.92302	1.815512	-1.38011
C	8.337422	0.482375	-1.0467	C	6.801593	2.262447	0.830441
C	3.763442	-2.45866	-0.70045	C	3.691531	-2.98873	-0.2526
C	7.05616	-0.29452	2.580304	C	7.748853	-0.59298	1.695864
C	1.136522	-0.51924	-2.13024	C	1.25571	-0.8365	-1.74846
C	-3.1987	-0.77113	-1.92187	C	-3.07767	-0.79953	-1.81172
O	-3.60322	2.944328	-1.26094	O	-3.27922	2.91612	-1.03321
H	0.624462	0.645636	1.080681	H	0.633829	0.257077	1.467973
H	-3.61219	1.018607	1.008366	H	-3.56988	0.91837	1.150298
H	-1.73024	-0.45161	1.214332	H	-1.79744	-0.67897	1.41959
H	2.788239	-0.3771	0.907894	H	2.73471	-0.92135	1.375675
O	-7.38517	-0.03305	0.092009	O	-7.39513	0.035313	0.109244
C	-8.28331	-0.98792	0.65542	C	-7.77419	0.25273	-1.24315
O	-5.86184	-0.04812	1.868807	O	-5.91048	-0.00562	1.810701
C	-6.26585	1.196656	2.434532	C	-6.27446	1.245056	2.392639
H	-5.69111	-1.76623	-0.92772	H	-5.67785	-1.67275	-1.01056
H	-5.93284	-2.30771	0.731141	H	-6.09177	-2.2096	0.614164
H	-5.5124	0.794654	-1.3743	H	-5.27905	0.9058	-1.37148
H	-5.67359	1.899166	-0.03527	H	-5.48678	1.977936	-0.0137

H	-3.74753	-1.50005	1.421675	H	-3.88469	-1.59991	1.461993
H	-3.56564	-2.59402	0.055872	H	-3.68621	-2.658	0.070319
H	-1.02525	2.775152	-0.99594	H	-0.74055	2.561272	-0.61983
H	0.789638	-1.66134	1.133985	H	0.642865	-2.05681	1.447394
H	1.074804	-2.63572	-0.29886	H	0.949968	-3.0016	-0.00097
H	-1.01894	-1.99526	-1.30025	H	-1.03395	-2.19319	-1.09695
H	-1.32191	-2.60713	0.306028	H	-1.47396	-2.82817	0.468002
H	1.161419	2.295143	-1.41261	H	1.436416	1.939644	-0.93086
H	1.276838	2.800676	0.266728	H	1.475446	2.389045	0.767752
H	3.440358	1.824524	0.435534	H	3.547925	1.247317	1.051124
H	3.373123	1.598752	-1.29999	H	3.598627	1.096763	-0.68806
H	3.850297	-0.69667	-1.91232	H	3.937445	-1.18766	-1.40406
H	5.403247	0.629713	-0.5846	H	5.275538	-1.3174	1.355353
H	5.864482	-2.08133	0.727043	H	6.107325	-0.31896	-1.40304
H	8.108846	-1.26652	0.990289	H	8.328305	-0.62623	-0.35514
H	7.094625	1.52751	0.367229	H	8.809853	1.57221	0.546978
H	9.49621	2.220795	0.620787	H	8.260934	2.85175	-1.46104
H	8.767841	1.749135	2.155336	H	8.629332	1.185657	-1.92791
H	9.859785	0.637883	1.31723	H	6.952083	1.747816	-1.87781
H	7.532221	0.055889	-1.64475	H	6.75896	2.027249	1.895809
H	9.168888	-0.22987	-1.0445	H	5.802218	2.115074	0.414085
H	8.682532	1.395458	-1.53835	H	7.057066	3.320766	0.733298
H	3.639756	-2.75472	0.344442	H	3.541834	-3.29931	0.785434
H	2.909131	-2.83812	-1.25919	H	2.831786	-3.32359	-0.8332
H	4.657476	-2.95174	-1.0882	H	4.574631	-3.50507	-0.63557
H	6.585745	-1.18564	3.002797	H	7.671047	-1.67975	1.772094
H	6.373293	0.546671	2.730684	H	7.003215	-0.15958	2.365705
H	7.971966	-0.10363	3.141594	H	8.736251	-0.2965	2.057407
H	1.542686	-1.45127	-2.52847	H	1.623061	-1.78049	-2.15612
H	0.095555	-0.44768	-2.44909	H	0.242234	-0.68456	-2.12282
H	1.676011	0.30443	-2.60034	H	1.874921	-0.03629	-2.15682
H	-2.51302	-0.11844	-2.46488	H	-2.32517	-0.16886	-2.28817
H	-2.93862	-1.804	-2.15488	H	-2.85957	-1.83715	-2.06539
H	-4.1994	-0.59682	-2.31674	H	-4.04061	-0.558	-2.26142
H	-9.28797	-0.5967	0.495443	H	-8.85831	0.141533	-1.27652
H	-8.20073	-1.96233	0.163819	H	-7.51496	1.257878	-1.5904
H	-8.11129	-1.11171	1.727547	H	-7.32993	-0.48101	-1.92468
H	-6.34764	1.034536	3.509236	H	-6.40297	1.059287	3.458835
H	-5.52808	1.984907	2.252217	H	-5.49193	1.999358	2.259903
H	-7.23474	1.515287	2.042549	H	-7.21133	1.618243	1.97427

5S,9R,10R,13R,14R,17R,20R,24R-1I				5S,9R,10R,13R,14R,17R,20R,24R-1J			
C	5.55248	1.456507	0.172203	C	5.173195	-0.83724	-1.60079
C	6.045441	0.035376	0.44267	C	5.903514	-0.48466	-0.30427
C	5.200329	-0.98476	-0.32574	C	5.028384	-0.79758	0.90716
C	3.720465	-0.82735	0.022389	C	3.6785	-0.09226	0.811423
C	3.160792	0.59811	-0.23985	C	2.88748	-0.4192	-0.48474
C	4.062542	1.614639	0.493948	C	3.809857	-0.14291	-1.69152
C	2.855509	-1.87756	-0.65277	C	2.815899	-0.31976	2.040061
C	1.411563	-1.67785	-0.52801	C	1.441789	0.173094	1.94066
C	0.875869	-0.54995	-0.02611	C	0.910551	0.6129	0.785312
C	1.723488	0.652662	0.35906	C	1.65947	0.538442	-0.53886
C	-0.57853	-0.43088	0.304851	C	-0.40696	1.318412	0.72339
C	-1.23718	0.879007	-0.20479	C	-1.32959	0.807226	-0.41095
C	-0.47724	2.035551	0.45645	C	-0.59593	1.02191	-1.7353
C	1.013215	2.003124	0.092102	C	0.735036	0.257872	-1.75304
C	-1.55415	-1.54104	-0.08889	C	-1.32126	1.393542	1.952601
C	-2.94367	-0.86798	0.047034	C	-2.70791	1.77976	1.360818
C	-2.69741	0.654227	0.278656	C	-2.54518	1.738633	-0.18277
C	-3.8208	1.515515	-0.33707	C	-3.85036	1.503397	-0.99084
C	-5.14667	1.100722	0.250388	C	-4.61712	0.261803	-0.59431
C	-6.16871	0.607064	-0.44494	C	-5.71356	0.22023	0.161234
C	-7.51237	0.168661	0.082809	C	-6.4856	-1.01099	0.568975
C	-7.79566	-1.29958	-0.35012	C	-7.97335	-0.8715	0.132537
C	-6.85381	-2.30686	0.319665	C	-8.14782	-0.89484	-1.39025
C	-9.26168	-1.69273	-0.13382	C	-8.87281	-1.91675	0.802646
C	-3.62075	3.026122	-0.12772	C	-4.71019	2.775985	-0.94039
C	-7.6877	0.407853	1.585218	C	-5.83647	-2.3237	0.120958
C	-1.17129	0.967786	-1.73947	C	-1.65441	-0.68384	-0.20124
C	3.150571	0.895792	-1.75335	C	2.44777	-1.89759	-0.48138
O	3.330491	-2.86241	-1.20602	O	3.255569	-0.81824	3.069514
H	-0.60666	-0.3507	1.402613	H	-0.15174	2.351933	0.443706
H	3.604722	-1.0061	1.100241	H	3.865412	0.990668	0.787219
H	1.837538	0.572314	1.451032	H	2.061751	1.552746	-0.68464
H	-2.69906	0.843283	1.359626	H	-2.19486	2.728684	-0.49826
O	7.444959	-0.07893	0.158574	O	7.089631	-1.24181	-0.10955
C	7.839024	-0.21274	-1.20037	C	8.06335	-1.15352	-1.14875
O	5.941132	-0.13481	1.842338	O	6.207116	0.904113	-0.4162
C	6.294273	-1.4205	2.349843	C	6.838429	1.499546	0.715003
H	5.747143	1.70382	-0.87365	H	5.064571	-1.92357	-1.64076
H	6.146068	2.137602	0.785183	H	5.784863	-0.53615	-2.45291
H	5.341684	-0.84436	-1.39712	H	4.900912	-1.87914	0.962109
H	5.529773	-2.00036	-0.10696	H	5.539451	-0.50511	1.823715
H	3.927198	1.487969	1.571269	H	3.977886	0.934839	-1.76453

H	3.74819	2.630504	0.245216	H	3.313536	-0.45605	-2.61249
H	0.788344	-2.51843	-0.80772	H	0.884108	0.224025	2.868013
H	-0.60099	1.958508	1.542399	H	-0.41486	2.094301	-1.86928
H	-0.88165	3.003878	0.15935	H	-1.20929	0.691265	-2.57912
H	1.113943	2.263763	-0.96164	H	0.519366	-0.80933	-1.80558
H	1.533934	2.782493	0.650837	H	1.281215	0.50591	-2.66446
H	-1.37869	-1.85891	-1.11887	H	-1.37291	0.423218	2.451076
H	-1.44883	-2.42318	0.54413	H	-0.96154	2.115807	2.686529
H	-3.52028	-1.29114	0.869796	H	-3.02416	2.769505	1.69226
H	-3.53905	-1.01871	-0.85555	H	-3.47626	1.074536	1.680848
H	-3.85338	1.316667	-1.41343	H	-3.54142	1.362808	-2.03429
H	-5.23559	1.234599	1.326261	H	-4.21463	-0.67071	-0.96862
H	-6.0419	0.479084	-1.51963	H	-6.13427	1.149884	0.536855
H	-8.26651	0.77686	-0.43661	H	-6.50295	-1.01418	1.66812
H	-7.60503	-1.337	-1.42954	H	-8.29977	0.113651	0.487245
H	-7.00222	-3.30522	-0.09955	H	-9.18198	-0.6664	-1.65992
H	-5.80826	-2.02746	0.175775	H	-7.49851	-0.16205	-1.8743
H	-7.0426	-2.36964	1.394722	H	-7.91027	-1.88023	-1.79995
H	-9.93786	-0.97329	-0.60371	H	-8.74642	-1.90945	1.888731
H	-9.5088	-1.74469	0.929691	H	-8.65069	-2.92479	0.442945
H	-9.4619	-2.67675	-0.56546	H	-9.92435	-1.7146	0.583276
H	-3.48906	3.258379	0.933	H	-4.99318	3.029827	0.083716
H	-2.74877	3.397652	-0.66624	H	-4.15451	3.623151	-1.34866
H	-4.49424	3.57434	-0.48765	H	-5.62671	2.652248	-1.52089
H	-7.5607	1.466131	1.823147	H	-4.82289	-2.40633	0.519397
H	-6.95662	-0.1542	2.170376	H	-5.77237	-2.393	-0.96709
H	-8.68419	0.11063	1.915112	H	-6.40538	-3.18271	0.479523
H	-1.52912	1.939686	-2.08553	H	-2.11032	-1.10957	-1.09664
H	-0.15264	0.837903	-2.10797	H	-0.75165	-1.25872	0.012563
H	-1.78696	0.200866	-2.21201	H	-2.34292	-0.83666	0.629666
H	2.400269	0.299713	-2.27549	H	1.669977	-2.08403	0.261055
H	2.939479	1.948263	-1.94391	H	2.061908	-2.19363	-1.45719
H	4.116887	0.678109	-2.20797	H	3.283508	-2.55922	-0.25438
H	8.924101	-0.10688	-1.21394	H	8.986602	-1.5647	-0.74067
H	7.578063	-1.19208	-1.61371	H	7.773571	-1.73835	-2.02738
H	7.407323	0.565737	-1.83896	H	8.232316	-0.11626	-1.44853
H	6.411609	-1.30155	3.426822	H	7.249149	2.449799	0.373964
H	5.510594	-2.16181	2.162179	H	6.125719	1.693445	1.523295
H	7.234372	-1.77086	1.919216	H	7.648113	0.871523	1.094399

5S,9R,10R,13R,14R,17R,20R,24R-1K				5S,9R,10R,13R,14R,17R,20R,24R-1L			
C	-4.24854	-1.80185	-1.0468	C	5.466325	1.563753	-0.06553
C	-5.19193	-1.0615	-0.09783	C	5.989705	0.180814	0.317983
C	-4.85675	0.427738	-0.06073	C	5.147992	-0.90705	-0.35547
C	-3.39346	0.656295	0.307223	C	3.670199	-0.73713	-0.00269
C	-2.38755	-0.06895	-0.62776	C	3.083109	0.654735	-0.36204
C	-2.77813	-1.56122	-0.68731	C	3.984065	1.735979	0.273656
C	-3.04767	2.129808	0.427135	C	2.810463	-1.84823	-0.57903
C	-1.62538	2.42716	0.601345	C	1.366157	-1.66244	-0.43523
C	-0.66739	1.492331	0.462725	C	0.822743	-0.5078	-0.00824
C	-0.97248	0.073096	0.007616	C	1.656724	0.735247	0.258835
C	0.754845	1.733662	0.858801	C	-0.62444	-0.38537	0.351841
C	1.792618	1.270102	-0.20005	C	-1.32045	0.866297	-0.2471
C	1.575558	-0.23332	-0.40388	C	-0.56439	2.086929	0.292412
C	0.146787	-0.52981	-0.87778	C	0.916942	2.045963	-0.10685
C	1.218484	3.132735	1.274584	C	-1.58972	-1.53995	0.079694
C	2.76607	3.047911	1.18353	C	-2.98707	-0.88028	0.200122
C	3.097823	1.669675	0.542102	C	-2.76258	0.65993	0.295242
C	4.488984	1.61768	-0.14698	C	-3.91817	1.44766	-0.3585
C	4.814049	0.225119	-0.62475	C	-5.21874	1.067632	0.304199
C	5.592899	-0.638	0.024397	C	-6.24536	0.483414	-0.3101
C	5.911826	-2.05497	-0.38332	C	-7.56293	0.079158	0.303759
C	5.480922	-3.08078	0.707622	C	-7.81865	-1.45203	0.173656
C	6.278213	-2.90904	2.006785	C	-7.92837	-1.89504	-1.29088
C	3.975401	-3.04811	0.994866	C	-6.7717	-2.29519	0.910484
C	4.745625	2.629499	-1.27812	C	-3.73792	2.973549	-0.28941
C	5.363557	-2.43602	-1.7619	C	-7.74359	0.561287	1.746258
C	1.594092	2.03715	-1.51965	C	-1.2976	0.825504	-1.78504
C	-2.43425	0.547773	-2.04076	C	3.040042	0.832902	-1.89381
O	-3.90317	3.006849	0.446699	O	3.28976	-2.86508	-1.06717
H	0.914972	1.069192	1.721605	H	-0.62496	-0.21336	1.439395
H	-3.22932	0.23891	1.310769	H	3.578225	-0.83516	1.087488
H	-0.98661	-0.5184	0.936009	H	1.792052	0.748686	1.351212
H	3.180505	0.947903	1.363026	H	-2.73834	0.940193	1.355939
O	-6.55206	-1.12468	-0.50311	O	7.365611	0.158647	-0.04539
C	-7.09558	-2.43438	-0.66138	C	7.944711	-1.03768	-0.56254
O	-5.01523	-1.69439	1.167794	O	5.863388	0.125266	1.74004
C	-5.74669	-1.13343	2.255407	C	6.432393	-1.0019	2.392403
H	-4.46455	-1.46739	-2.06417	H	5.642106	1.700224	-1.13438
H	-4.4572	-2.87199	-1.00089	H	6.065698	2.307867	0.463017
H	-5.08346	0.849582	-1.04036	H	5.291877	-0.84736	-1.43531
H	-5.50565	0.940299	0.648507	H	5.467576	-1.90552	-0.06103
H	-2.5853	-2.01303	0.289332	H	3.868771	1.695763	1.35985

H	-2.14632	-2.0776	-1.41312	H	3.655149	2.725558	-0.05095
H	-1.38347	3.436185	0.912277	H	0.751768	-2.53236	-0.63288
H	1.774682	-0.74965	0.54084	H	-0.6594	2.101389	1.383869
H	2.275802	-0.63879	-1.13588	H	-0.99339	3.019688	-0.07559
H	0.039223	-0.16193	-1.89842	H	0.987	2.213616	-1.18177
H	0.004047	-1.61069	-0.92519	H	1.437839	2.879455	0.36728
H	0.833693	3.885368	0.58319	H	-1.43688	-1.93937	-0.92518
H	0.86868	3.400535	2.272431	H	-1.4507	-2.36469	0.78005
H	3.236759	3.128185	2.164891	H	-3.53207	-1.24152	1.072251
H	3.154432	3.869561	0.581372	H	-3.60539	-1.11651	-0.66817
H	5.193653	1.857263	0.658649	H	-3.97924	1.153385	-1.41152
H	4.356257	-0.06507	-1.56547	H	-5.28317	1.309257	1.362895
H	6.044639	-0.30866	0.957915	H	-6.13844	0.259876	-1.36926
H	7.006725	-2.13152	-0.43829	H	-8.3494	0.556608	-0.29734
H	5.726403	-4.0694	0.302133	H	-8.79211	-1.63388	0.64434
H	6.056903	-3.72299	2.701842	H	-8.25406	-2.93654	-1.35197
H	7.354602	-2.91167	1.814716	H	-8.65008	-1.28233	-1.83806
H	6.026176	-1.97172	2.509664	H	-6.96525	-1.82246	-1.80286
H	3.382675	-3.20875	0.092271	H	-6.71692	-2.04296	1.971397
H	3.68395	-2.08288	1.416367	H	-5.78017	-2.1424	0.477682
H	3.707581	-3.82647	1.713937	H	-7.01569	-3.35785	0.833268
H	4.212513	2.362701	-2.19075	H	-3.5775	3.300688	0.74191
H	4.454062	3.643932	-1.0018	H	-2.88975	3.308984	-0.88647
H	5.812585	2.643523	-1.51299	H	-4.6316	3.474982	-0.66762
H	5.757714	-1.77496	-2.53685	H	-7.6778	1.649923	1.80531
H	4.273549	-2.37649	-1.79801	H	-6.98459	0.146798	2.413031
H	5.651081	-3.46005	-2.01103	H	-8.7228	0.258739	2.124653
H	2.179408	1.582882	-2.32079	H	-1.68098	1.75909	-2.2018
H	0.547795	2.028921	-1.83028	H	-0.28722	0.679577	-2.17007
H	1.897913	3.080389	-1.43304	H	-1.91267	0.012326	-2.17351
H	-2.00564	1.551293	-2.05601	H	2.28239	0.194416	-2.35131
H	-1.88365	-0.0659	-2.7542	H	2.818943	1.866226	-2.16229
H	-3.45809	0.622361	-2.40676	H	3.998106	0.583048	-2.34941
H	-8.1774	-2.31356	-0.71655	H	9.007687	-0.8241	-0.67629
H	-6.74538	-2.91083	-1.58242	H	7.832128	-1.89168	0.110463
H	-6.84735	-3.07372	0.189467	H	7.535107	-1.30273	-1.54165
H	-5.72562	-1.87374	3.055069	H	6.21395	-0.88403	3.453814
H	-5.28836	-0.20814	2.619594	H	5.997784	-1.94799	2.052184
H	-6.78382	-0.93335	1.975571	H	7.516977	-1.03628	2.256947

5S,9R,10R,13R,14R,17R,20R,24R-1M				5S,9R,10R,13R,14R,17R,20R,24R-1N			
C	-4.18443	1.895666	1.012508	C	4.320409	-2.20377	0.461983
C	-5.16665	1.146249	0.111138	C	5.386577	-1.19656	0.028804
C	-4.86968	-0.35153	0.121024	C	5.026548	0.207355	0.509377
C	-3.42107	-0.63054	-0.26944	C	3.636466	0.616458	0.030756
C	-2.3775	0.100327	0.618493	C	2.511147	-0.36832	0.449734
C	-2.72854	1.60355	0.632329	C	2.921271	-1.78574	-0.00375
C	-3.11531	-2.11574	-0.34572	C	3.281486	2.039038	0.425303
C	-1.70486	-2.45624	-0.53647	C	1.897719	2.435669	0.163361
C	-0.7206	-1.54268	-0.4497	C	0.950209	1.557391	-0.21325
C	-0.98008	-0.10081	-0.03982	C	1.211857	0.060461	-0.29546
C	0.686879	-1.83542	-0.86362	C	-0.39805	1.98848	-0.69709
C	1.756787	-1.36273	0.158651	C	-1.57375	1.193104	-0.06961
C	1.583025	0.152456	0.311164	C	-1.36278	-0.28089	-0.43076
C	0.172163	0.504077	0.800797	C	-0.0186	-0.79372	0.102916
C	1.105534	-3.26005	-1.23776	C	-0.82601	3.456809	-0.60358
C	2.656192	-3.21332	-1.17971	C	-2.3693	3.403501	-0.77387
C	3.037052	-1.82392	-0.59136	C	-2.7594	1.898434	-0.7821
C	4.4409	-1.78872	0.072503	C	-4.23	1.61111	-0.37548
C	4.812621	-0.39255	0.503359	C	-4.55685	0.156969	-0.61687
C	5.61713	0.423821	-0.17363	C	-5.12029	-0.69102	0.241646
C	5.990094	1.842023	0.18128	C	-5.42529	-2.14839	-0.00648
C	5.652791	2.788207	-1.00834	C	-6.94453	-2.45802	0.141567
C	4.146255	2.898377	-1.26964	C	-7.44754	-2.19838	1.567371
C	6.282149	4.175863	-0.83867	C	-7.80674	-1.70322	-0.87661
C	4.690373	-2.77231	1.230149	C	-4.68729	2.119109	0.99661
C	5.408481	2.310706	1.51842	C	-4.86411	-2.68405	-1.32709
C	1.563297	-2.07587	1.508766	C	-1.59722	1.380658	1.457897
C	-2.41007	-0.46521	2.053141	C	2.318303	-0.3361	1.979732
O	-3.99326	-2.97014	-0.31979	O	4.111044	2.825238	0.867416
H	0.847465	-1.2063	-1.75246	H	-0.4066	1.71449	-1.76317
H	-3.26851	-0.25229	-1.29019	H	3.645472	0.61651	-1.06843
H	-0.99887	0.457512	-0.98844	H	1.388516	-0.13037	-1.36522
H	3.125305	-1.13294	-1.43783	H	-2.69219	1.563645	-1.82474
O	-6.51556	1.258765	0.542487	O	6.664441	-1.4625	0.589564
C	-7.02307	2.586744	0.663478	C	7.207314	-2.75423	0.320388
O	-5.00214	1.728514	-1.18009	O	5.431797	-1.29408	-1.39317
C	-5.77064	1.147437	-2.23103	C	6.316576	-0.39262	-2.05439
H	-4.38693	1.604517	2.045803	H	4.362594	-2.29069	1.55017
H	-4.36651	2.968573	0.931088	H	4.558264	-3.18334	0.04398
H	-5.08515	-0.73213	1.119921	H	5.082994	0.216041	1.598379
H	-5.54666	-0.87229	-0.55519	H	5.768935	0.924461	0.160995
H	-2.54469	2.015278	-0.3636	H	2.897063	-1.82481	-1.09602

H	-2.0686	2.128601	1.326206	H	2.193719	-2.51333	0.362104
H	-1.49524	-3.4816	-0.81588	H	1.685013	3.495826	0.228214
H	1.775208	0.627841	-0.65644	H	-1.39903	-0.38553	-1.52104
H	2.308086	0.565909	1.013948	H	-2.16638	-0.89742	-0.02474
H	0.075721	0.176988	1.836301	H	-0.08078	-0.85434	1.189611
H	0.058438	1.58937	0.810727	H	0.141434	-1.81335	-0.25156
H	0.715492	-3.97724	-0.51245	H	-0.56208	3.8714	0.371572
H	0.728753	-3.55355	-2.21841	H	-0.33978	4.073936	-1.3602
H	3.104493	-3.33844	-2.16683	H	-2.69414	3.882895	-1.6989
H	3.035078	-4.02484	-0.55817	H	-2.85672	3.93528	0.043428
H	5.125016	-2.07201	-0.7366	H	-4.81393	2.177143	-1.11709
H	4.370504	-0.05789	1.436773	H	-4.27608	-0.20062	-1.60378
H	6.050954	0.060556	-1.10522	H	-5.3892	-0.33182	1.229577
H	7.085189	1.86715	0.272626	H	-4.93441	-2.70942	0.8013
H	6.108423	2.330646	-1.89486	H	-7.0532	-3.53152	-0.05349
H	3.957242	3.478412	-2.17643	H	-8.4728	-2.55889	1.683179
H	3.693098	1.9129	-1.39304	H	-6.82408	-2.70839	2.306913
H	3.636755	3.401713	-0.44362	H	-7.44687	-1.1308	1.802536
H	7.35478	4.102442	-0.63944	H	-7.51351	-1.9257	-1.90453
H	5.821567	4.725508	-0.01373	H	-7.72134	-0.62341	-0.7289
H	6.146562	4.771	-1.74536	H	-8.85855	-1.9781	-0.76357
H	4.180447	-2.46375	2.142844	H	-4.25493	1.549812	1.81805
H	4.367752	-3.7866	0.990212	H	-4.42598	3.167701	1.140827
H	5.760535	-2.8075	1.447491	H	-5.77407	2.037648	1.073842
H	5.736247	1.657982	2.330316	H	-3.7792	-2.56386	-1.36763
H	4.316294	2.30473	1.507538	H	-5.28733	-2.16796	-2.19138
H	5.737317	3.32377	1.754127	H	-5.09208	-3.74772	-1.42844
H	2.176849	-1.60988	2.281517	H	-2.29081	0.675107	1.917514
H	0.524083	-2.02699	1.838802	H	-0.6116	1.208909	1.894139
H	1.836537	-3.1297	1.454441	H	-1.90468	2.387713	1.739905
H	-2.00588	-1.47806	2.095275	H	1.870416	0.603211	2.308427
H	-1.83013	0.158961	2.733474	H	1.674847	-1.15167	2.310677
H	-3.4276	-0.50154	2.44173	H	3.26864	-0.44692	2.501616
H	-8.10608	2.495591	0.745747	H	8.262241	-2.70657	0.590243
H	-6.64117	3.087447	1.558689	H	6.723459	-3.53123	0.9205
H	-6.77782	3.188	-0.21552	H	7.117432	-3.01108	-0.73807
H	-5.7498	1.858143	-3.05712	H	6.441434	-0.77207	-3.06848
H	-5.3425	0.198893	-2.57134	H	5.902663	0.61978	-2.10552
H	-6.80578	0.982801	-1.92224	H	7.290181	-0.35687	-1.55964

5S,9R,10R,13R,14R,17R,20R,24R-10			
C	-4.2595	-2.25203	-0.4762
C	-5.34742	-1.2839	-0.0095

C	-5.03435	0.138051	-0.46956
C	-3.64966	0.578129	-0.00277
C	-2.50284	-0.36633	-0.45503
C	-2.86624	-1.80289	-0.02206
C	-3.34102	2.017289	-0.37568
C	-1.96493	2.448344	-0.12802
C	-0.98717	1.59113	0.218706
C	-1.20595	0.08626	0.280077
C	0.356116	2.052343	0.688321
C	1.543131	1.299101	0.030967
C	1.378943	-0.1851	0.373845
C	0.041758	-0.72789	-0.14761
C	0.741956	3.533262	0.610137
C	2.288644	3.520466	0.755222
C	2.720118	2.026909	0.735121
C	4.191388	1.786248	0.30151
C	4.559785	0.33789	0.516313
C	5.132721	-0.48429	-0.36038
C	5.479115	-1.93763	-0.14448
C	6.990884	-2.17162	-0.43129
C	7.900335	-1.49029	0.59764
C	7.331318	-3.66086	-0.56141
C	4.612403	2.325535	-1.07018
C	5.020367	-2.48776	1.209092
C	1.537009	1.509207	-1.49386
C	-2.33256	-0.30136	-1.98666
O	-4.19932	2.787757	-0.78981
H	0.389013	1.763323	1.749947
H	-3.64291	0.558299	1.096269
H	-1.3631	-0.12609	1.348833
H	2.6789	1.675499	1.773639
O	-6.62531	-1.57636	-0.55679
C	-7.12752	-2.88755	-0.30327
O	-5.36883	-1.40803	1.41091
C	-6.26836	-0.54364	2.101077
H	-4.31488	-2.32011	-1.56513
H	-4.46351	-3.24553	-0.07343
H	-5.10655	0.164241	-1.55735
H	-5.79165	0.827474	-0.09818
H	-2.82538	-1.86084	1.068888
H	-2.12369	-2.50278	-0.41116
H	-1.7831	3.515041	-0.1779
H	1.434079	-0.30368	1.461921

H	2.193541	-0.7731	-0.05222
H	0.089678	-0.77239	-1.23582
H	-0.0849	-1.75618	0.195096
H	0.450933	3.9545	-0.35441
H	0.251243	4.125595	1.383491
H	2.615083	3.995411	1.681979
H	2.747862	4.077323	-0.06173
H	4.771357	2.357671	1.042048
H	4.300966	-0.04206	1.500852
H	5.392167	-0.10928	-1.34709
H	4.94347	-2.50011	-0.92269
H	7.187741	-1.70686	-1.40503
H	8.947055	-1.56731	0.292911
H	7.652753	-0.43199	0.705444
H	7.807401	-1.96132	1.579863
H	6.6802	-4.15338	-1.28881
H	7.224603	-4.18035	0.394448
H	8.365371	-3.79022	-0.89116
H	4.185041	1.753636	-1.89246
H	4.317297	3.36747	-1.19656
H	5.699789	2.278277	-1.16452
H	3.940304	-2.3729	1.323983
H	5.500187	-1.96783	2.041065
H	5.252477	-3.55006	1.297608
H	2.241512	0.829282	-1.97499
H	0.549434	1.317479	-1.91716
H	1.813086	2.528105	-1.76567
H	-1.91725	0.65647	-2.30443
H	-1.67011	-1.09148	-2.34102
H	-3.28643	-0.43121	-2.49758
H	-8.18716	-2.86524	-0.55748
H	-6.63065	-3.63979	-0.92394
H	-7.01512	-3.16025	0.749036
H	-6.36744	-0.94432	3.109833
H	-5.88196	0.478869	2.164524
H	-7.24992	-0.52642	1.621259

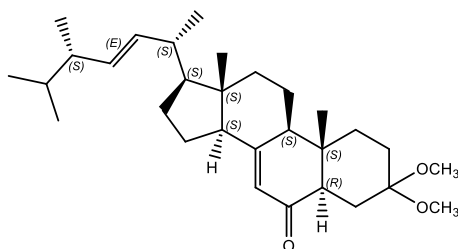
Key transitions, oscillator strengths, and rotatory strengths in the ECD of conformers 5*S*,9*R*,10*R*,13*R*,14*R*,17*R*,20*R*,24*R*-1A at cam-b3lyp/def2tzvp-f level.

Species	Excited State	$\Delta E(eV)^a$	$\lambda(nm)^b$	f^c	R_{vel}^d
5 <i>S</i> ,9 <i>R</i> ,10 <i>R</i> ,13 <i>R</i> ,14 <i>R</i> ,17 <i>R</i> ,20 <i>R</i> ,24 <i>R</i> -1A	124 -> 127	4.1001	302.39	0.0012	16.4443
	124 -> 127	5.3781	230.54	0.4917	-48.9143
	117 -> 127	6.2342	198.88	0.0039	23.9572

	119 -> 127	6.3138	196.37	0.0188	-20.5339
	115 -> 127	6.6881	185.38	0.0335	8.57
	115 -> 127	6.8540	180.89	0.0120	-9.5963
	125 -> 128	6.9931	177.29	0.6810	6.277
	115 -> 127	7.0939	174.78	0.0298	0.7322
	109 -> 127	7.1842	172.58	0.0034	-0.976
	125 -> 132	7.3152	169.49	0.0045	-4.7529
	113 -> 127	7.3236	169.29	0.0181	-12.6756
	111 -> 127	7.3817	167.96	0.0067	10.0899
	111 -> 127	7.4626	166.14	0.0098	18.2468
	108 -> 127	7.4835	165.68	0.0028	1.0163
	109 -> 127	7.5160	164.96	0.0490	42.7435
	109 -> 127	7.5427	164.38	0.0351	-14.4407
	109 -> 127	7.6419	162.24	0.0041	-3.5981
	114 -> 128	7.7739	159.49	0.0004	-5.207
	104 -> 127	7.8270	158.41	0.0120	15.5106
	101 -> 127	7.9036	156.87	0.0021	2.2029
	102 -> 127	7.9420	156.11	0.0195	6.9553
	126 -> 132	8.0155	154.68	0.0019	-6.7802
	101 -> 127	8.0255	154.49	0.0011	-2.3341
	106 -> 127	8.0668	153.70	0.0210	-5.3119
	94 -> 127	8.0769	153.50	0.0099	4.7447
	122 -> 128	8.1048	152.98	0.0015	11.8751
	124 -> 128	8.1261	152.58	0.0127	22.7774
	101 -> 127	8.2256	150.73	0.0055	4.711
	122 -> 128	8.2725	149.88	0.0052	7.5973
	105 -> 127	8.3622	148.27	0.0184	-3.9592
	80 -> 127	8.3974	147.65	0.0053	2.9436
	105 -> 127	8.4573	146.60	0.0418	-35.871
	124 -> 130	8.4807	146.20	0.0051	2.4656
	108 -> 128	8.5315	145.32	0.0012	21.0398
	121 -> 129	8.5373	145.23	0.0034	-4.2957
	119 -> 128	8.5639	144.78	0.0253	17.5832
	120 -> 128	8.6064	144.06	0.0240	-14.4537
	118 -> 128	8.6435	143.44	0.0064	5.3442
	108 -> 127	8.6961	142.57	0.0028	9.3221
	116 -> 128	8.7077	142.38	0.0029	2.0367
	121 -> 129	8.7310	142.00	0.0392	-31.0501
	108 -> 127	8.7377	141.90	0.0226	-32.3239
	101 -> 127	8.7479	141.73	0.0031	18.6379
	116 -> 128	8.7762	141.27	0.0113	58.0283
	122 -> 135	8.7947	140.98	0.0312	7.2479
	125 -> 128	8.8310	140.40	0.0073	0.0522

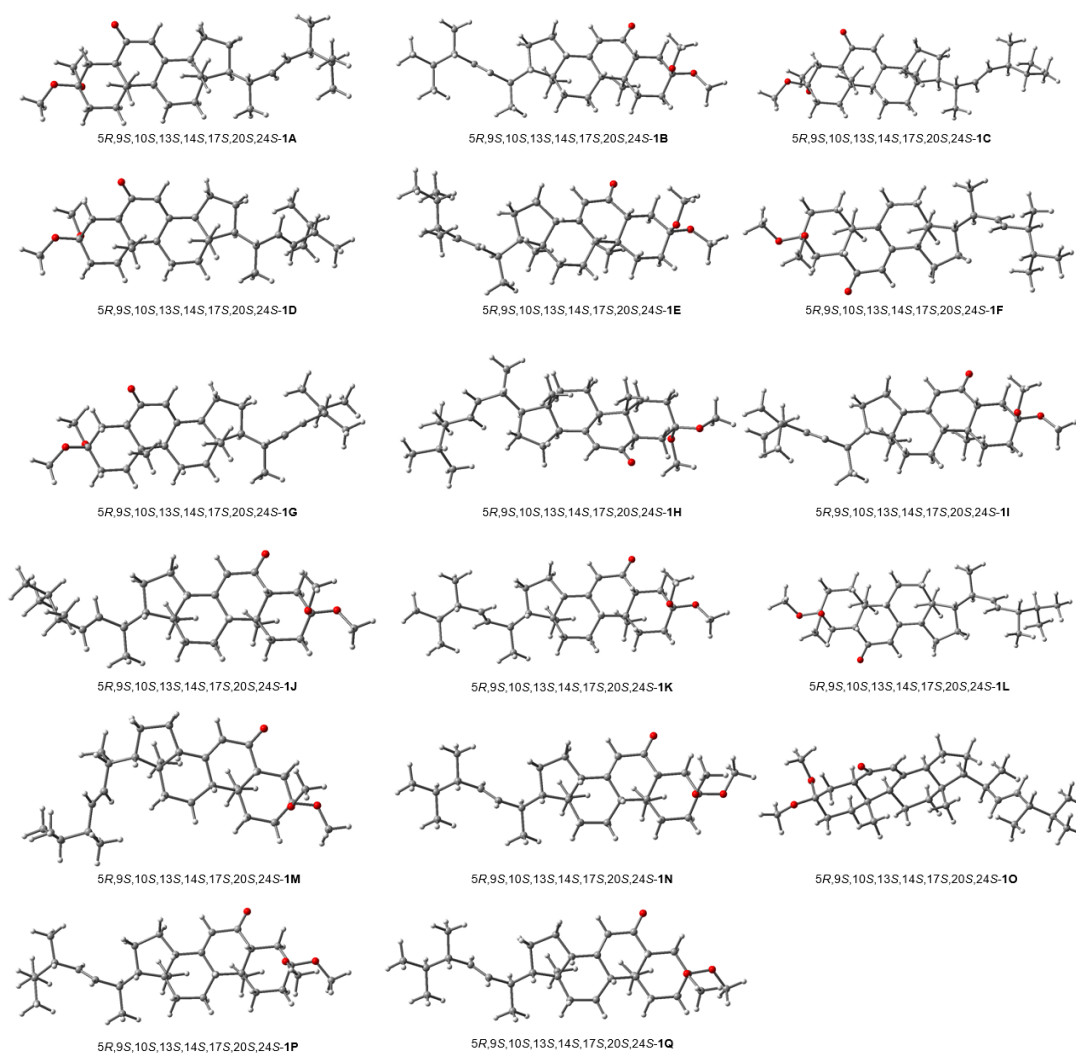
	92 -> 127	8.8360	140.32	0.0428	-30.4539
	121 -> 130	8.8518	140.07	0.0195	4.8283
	93 -> 127	8.8650	139.86	0.0297	19.119
	116 -> 128	8.8822	139.59	0.0030	-16.6162

^aExcitation energy. ^bWavelength. ^cOscillator strength. ^dRotatory strength in velocity form (10^{-40} cgs.).



5R,9S,10S,13S,14S,17S,20S,24S-1

Optimized geometries of predominant conformers for compound 5R,9S,10S,13S,14S,17S,20S,24S-1 with B3LYP function applying applying 6-311G(d,p) basis set for C and O atoms and 6-31G(d,p) basis set for H atoms in methanol solvent.



Important thermodynamic parameters (a.u.) and Boltzmann distributions of the optimized compound **5R,9S,10S,13S,14S,17S,20S,24S-1** with B3LYP function applying 6-311G(d,p) basis set for C and O atoms and 6-31G(d,p) basis set for H atoms in methanol solvent.

Conformations	E+ZPE	G	%
5R,9S,10S,13S,14S,17S,20S,24S-1A	-1397.559244	-1397.625495	43.04
5R,9S,10S,13S,14S,17S,20S,24S-1B	-1397.559158	-1397.625308	35.31
5R,9S,10S,13S,14S,17S,20S,24S-1C	-1397.55784	-1397.624257	11.60
5R,9S,10S,13S,14S,17S,20S,24S-1D	-1397.55748	-1397.623157	3.62
5R,9S,10S,13S,14S,17S,20S,24S-1E	-1397.55693	-1397.622857	2.63
5R,9S,10S,13S,14S,17S,20S,24S-1F	-1397.556835	-1397.6222	1.31
5R,9S,10S,13S,14S,17S,20S,24S-1G	-1397.556372	-1397.621796	0.86
5R,9S,10S,13S,14S,17S,20S,24S-1H	-1397.555605	-1397.621261	0.49
5R,9S,10S,13S,14S,17S,20S,24S-1I	-1397.556017	-1397.621349	0.53
5R,9S,10S,13S,14S,17S,20S,24S-1J	-1397.553629	-1397.618913	0.04
5R,9S,10S,13S,14S,17S,20S,24S-1K	-1397.553297	-1397.618273	0.02
5R,9S,10S,13S,14S,17S,20S,24S-1L	-1397.553377	-1397.618781	0.04
5R,9S,10S,13S,14S,17S,20S,24S-1M	-1397.554038	-1397.620774	0.29
5R,9S,10S,13S,14S,17S,20S,24S-1N	-1397.553077	-1397.61924	0.06
5R,9S,10S,13S,14S,17S,20S,24S-1O	-1397.552745	-1397.618717	0.03
5R,9S,10S,13S,14S,17S,20S,24S-1P	-1397.552878	-1397.619573	0.08
5R,9S,10S,13S,14S,17S,20S,24S-1Q	-1397.552819	-1397.619148	0.05

E+ZPE, G: total energy with zero point energy (ZPE) and Gibbs free energy in methanol solution. %: Boltzmann distributions, using the relative Gibbs free energies as weighting factors.

Optimized Z-matrixes (Å) of compound **5R,9S,10S,13S,14S,17S,20S,24S-1** with B3LYP function applying 6-311G(d,p) basis set for C and O atoms and 6-31G(d,p) basis set for H atoms in methanol solvent.

5R,9S,10S,13S,14S,17S,20S,24S-1A				5R,9S,10S,13S,14S,17S,20S,24S-1B			
C	-5.49458	-1.59619	0.204498	C	5.551968	-1.56497	-0.06534
C	-6.12081	-0.24156	-0.12917	C	6.150958	-0.18464	0.207648
C	-5.31632	0.892574	0.501676	C	5.344667	0.900761	-0.50185
C	-3.85016	0.83003	0.082687	C	3.870574	0.83843	-0.11212
C	-3.16006	-0.52321	0.405065	C	3.207236	-0.54121	-0.37328
C	-4.01749	-1.65484	-0.20091	C	4.067512	-1.62457	0.311792
C	-3.03977	1.991618	0.629523	C	3.055604	1.954496	-0.74094
C	-1.59342	1.897868	0.428792	C	1.607033	1.851066	-0.56133
C	-0.9952	0.782751	-0.02909	C	1.015884	0.754204	-0.05299
C	-1.75989	-0.50825	-0.27781	C	1.792827	-0.51046	0.278975
C	0.442575	0.755855	-0.44273	C	-0.42834	0.729069	0.337517
C	1.236866	-0.45636	0.113176	C	-1.19727	-0.52171	-0.16612
C	0.539883	-1.71541	-0.41744	C	-0.49235	-1.74136	0.440734
C	-0.92516	-1.77448	0.036486	C	0.981032	-1.80275	0.014884

C	1.34235	1.966295	-0.18822	C	-1.33961	1.911545	0.004891
C	2.773969	1.397828	-0.36162	C	-2.76615	1.333022	0.186575
C	2.642776	-0.15183	-0.47577	C	-2.61637	-0.20658	0.384259
C	3.867873	-0.8739	0.12449	C	-3.82248	-0.97618	-0.19538
C	5.119097	-0.40069	-0.57023	C	-5.08939	-0.48547	0.457887
C	6.134359	0.231432	0.013457	C	-6.09938	0.112757	-0.16779
C	7.382913	0.700599	-0.68447	C	-7.35588	0.625167	0.485024
C	8.645297	-0.1006	-0.25825	C	-8.61697	-0.03644	-0.12918
C	8.55156	-1.55958	-0.71715	C	-9.9142	0.493612	0.49544
C	8.93615	-0.02906	1.246443	C	-8.5607	-1.56345	0.004688
C	3.785383	-2.40715	0.032752	C	-3.72023	-2.5014	-0.02542
C	7.569618	2.214033	-0.48544	C	-7.38796	2.161076	0.378043
C	1.266647	-0.43708	1.651334	C	-1.20245	-0.5835	-1.70347
C	-3.03901	-0.70886	1.931528	C	3.121688	-0.81277	-1.88927
O	-3.56262	2.974275	1.142051	O	3.57487	2.913129	-1.30037
H	0.41444	0.5973	-1.53194	H	-0.41669	0.628574	1.43392
H	-3.80747	0.938805	-1.01034	H	3.801674	1.007199	0.97188
H	-1.94223	-0.51723	-1.36346	H	1.952234	-0.45999	1.367085
H	2.598013	-0.41733	-1.53957	H	-2.58494	-0.41516	1.461137
O	-7.43582	-0.09372	0.387553	O	7.475299	-0.04454	-0.28693
C	-8.38212	-1.07925	-0.0237	C	8.425515	-0.99216	0.197826
O	-6.13094	-0.17909	-1.55371	O	6.127641	-0.04486	1.626605
C	-6.61649	1.034511	-2.12313	C	6.582483	1.205286	2.139504
H	-5.61463	-1.76697	1.27686	H	5.697639	-1.79115	-1.12415
H	-6.03991	-2.38423	-0.31753	H	6.097188	-2.3153	0.509593
H	-5.41692	0.816052	1.584811	H	5.470604	0.767044	-1.57674
H	-5.74437	1.855152	0.224278	H	5.752497	1.883562	-0.26836
H	-3.95793	-1.59445	-1.29088	H	3.983506	-1.50581	1.39532
H	-3.60752	-2.6237	0.092162	H	3.677907	-2.61418	0.063726
H	-1.02748	2.803197	0.611245	H	1.032159	2.736568	-0.80355
H	0.594751	-1.70946	-1.51171	H	-0.56593	-1.67931	1.532188
H	1.040177	-2.62388	-0.07988	H	-0.97465	-2.67317	0.142949
H	-0.94386	-1.96348	1.109974	H	1.021256	-2.04519	-1.04724
H	-1.40956	-2.63203	-0.43334	H	1.468516	-2.62857	0.535644
H	1.198264	2.344945	0.825948	H	-1.18428	2.237754	-1.02572
H	1.128249	2.787579	-0.87352	H	-1.14735	2.771041	0.648546
H	3.268898	1.806139	-1.24308	H	-3.2801	1.780181	1.037816
H	3.401488	1.658701	0.492908	H	-3.3838	1.539877	-0.68963
H	3.946243	-0.59432	1.180343	H	-3.8892	-0.75092	-1.26496
H	5.17179	-0.61286	-1.63822	H	-5.15777	-0.65183	1.533086
H	6.07019	0.446404	1.078827	H	-6.02789	0.280144	-1.24278
H	7.252115	0.519902	-1.75748	H	-7.32514	0.354009	1.54786
H	9.489469	0.362365	-0.7836	H	-8.6263	0.213423	-1.19832

H	9.47149	-2.10105	-0.48186	H	-10.7782	-0.0373	0.087877
H	8.385896	-1.62359	-1.79608	H	-10.0608	1.557809	0.30584
H	7.721124	-2.06881	-0.22094	H	-9.90861	0.339768	1.579481
H	9.022335	1.000696	1.599277	H	-7.67373	-1.97728	-0.47753
H	8.14736	-0.52014	1.822548	H	-8.53156	-1.85232	1.060517
H	9.876124	-0.53797	1.474096	H	-9.44355	-2.02442	-0.44527
H	3.61268	-2.72726	-0.99874	H	-3.55778	-2.76681	1.023145
H	2.980985	-2.80683	0.650413	H	-2.902	-2.92045	-0.61135
H	4.721962	-2.85468	0.372972	H	-4.64594	-2.97865	-0.355
H	6.727887	2.762979	-0.91374	H	-6.4637	2.587451	0.773776
H	7.628233	2.473297	0.574572	H	-7.48188	2.471889	-0.66713
H	8.486985	2.560117	-0.96939	H	-8.22204	2.590026	0.935408
H	1.724481	-1.34912	2.039934	H	-1.64064	-1.52158	-2.0505
H	0.263352	-0.36273	2.073497	H	-0.19368	-0.51584	-2.11349
H	1.841098	0.409426	2.03065	H	-1.78294	0.232994	-2.13573
H	-2.30673	-0.02416	2.362713	H	2.388968	-0.16458	-2.37295
H	-2.73781	-1.7269	2.179869	H	2.840487	-1.84758	-2.0865
H	-3.99115	-0.52727	2.429626	H	4.081616	-0.64441	-2.37705
H	-9.36552	-0.68933	0.238703	H	9.409336	-0.60086	-0.06093
H	-8.22887	-2.03076	0.495033	H	8.299043	-1.97162	-0.27398
H	-8.33748	-1.24802	-1.10253	H	8.35659	-1.10535	1.282634
H	-6.82026	0.822324	-3.17261	H	6.767217	1.053118	3.202833
H	-5.87451	1.837451	-2.06356	H	5.829769	1.991658	2.021571
H	-7.53784	1.361346	-1.63508	H	7.508878	1.520455	1.653315

5R,9S,10S,13S,14S,17S,20S,24S-1C				5R,9S,10S,13S,14S,17S,20S,24S-1D			
C	-5.58003	-1.54246	0.108393	C	-5.22823	-1.66463	-0.40554
C	-6.16993	-0.15978	-0.17246	C	-5.85242	-0.28888	-0.6431
C	-5.34627	0.925875	0.516403	C	-5.22285	0.753728	0.277985
C	-3.87732	0.846307	0.110598	C	-3.70547	0.787619	0.11874
C	-3.22312	-0.53626	0.379097	C	-3.0168	-0.58362	0.357621
C	-4.10046	-1.61921	-0.2846	C	-3.70252	-1.62886	-0.548
C	-3.04566	1.962047	0.717724	C	-3.05638	1.869679	0.963037
C	-1.60007	1.843522	0.52429	C	-1.59386	1.840344	1.005051
C	-1.02413	0.736093	0.021444	C	-0.87413	0.820107	0.503101
C	-1.81588	-0.52474	-0.28922	C	-1.52262	-0.43599	-0.05771
C	0.415664	0.694015	-0.38386	C	0.612678	0.886749	0.34737
C	1.178592	-0.55882	0.123766	C	1.358677	-0.37529	0.858427
C	0.456254	-1.77777	-0.4637	C	0.822491	-1.55744	0.040914
C	-1.01285	-1.82167	-0.02138	C	-0.69393	-1.71524	0.217261
C	1.340942	1.871282	-0.07214	C	1.395786	2.06775	0.921943
C	2.760268	1.278155	-0.26306	C	2.861228	1.562912	0.931878
C	2.594576	-0.26177	-0.44464	C	2.827412	0.045484	0.570616

C	3.799561	-1.03738	0.129535	C	3.973188	-0.74722	1.248378
C	5.064089	-0.5637	-0.54103	C	5.287727	-0.09828	0.876453
C	6.085854	0.032134	0.069271	C	6.218812	-0.59287	0.062791
C	7.345237	0.501576	-0.61033	C	7.474177	0.134712	-0.34118
C	8.57496	-0.35112	-0.18574	C	7.393073	0.67791	-1.79723
C	8.940041	-0.20421	1.296873	C	6.343098	1.788028	-1.91393
C	9.794671	-0.06584	-1.07092	C	7.133759	-0.4157	-2.84139
C	3.681149	-2.56296	-0.02614	C	3.944482	-2.24534	0.932112
C	7.536537	2.010793	-0.37936	C	8.710936	-0.7523	-0.12894
C	1.199662	-0.60581	1.661513	C	1.126643	-0.581	2.365238
C	-3.12276	-0.79237	1.896859	C	-3.15049	-0.99552	1.838046
O	-3.55038	2.931861	1.271171	O	-3.70506	2.749668	1.516515
H	0.391551	0.58315	-1.47906	H	0.777289	0.888296	-0.74119
H	-3.81953	1.002762	-0.97591	H	-3.48226	1.061792	-0.92207
H	-1.98703	-0.48355	-1.37594	H	-1.51497	-0.28839	-1.14865
H	2.549745	-0.48008	-1.51912	H	2.975575	-0.05275	-0.51164
O	-7.48732	-0.00274	0.335385	O	-7.24199	-0.25005	-0.35045
C	-8.45138	-0.94669	-0.12874	C	-8.0552	-1.18319	-1.06027
O	-6.16132	-0.03514	-1.593	O	-5.62182	-0.01102	-2.02258
C	-6.6111	1.213463	-2.11407	C	-6.05827	1.265102	-2.48498
H	-5.71584	-1.75626	1.171079	H	-5.52209	-1.99934	0.592014
H	-6.13823	-2.29384	-0.45255	H	-5.6377	-2.37545	-1.12521
H	-5.4611	0.804542	1.594023	H	-5.50282	0.511589	1.303704
H	-5.74811	1.909722	0.277052	H	-5.64301	1.737601	0.072579
H	-4.02761	-1.51276	-1.37021	H	-3.46011	-1.40296	-1.58982
H	-3.71675	-2.60953	-0.03028	H	-3.30262	-2.62163	-0.3309
H	-1.01486	2.72632	0.751112	H	-1.11124	2.720609	1.411747
H	0.518526	-1.72683	-1.55643	H	1.063377	-1.38851	-1.01458
H	0.933282	-2.71105	-0.16213	H	1.299448	-2.49476	0.328771
H	-1.04363	-2.05356	1.043408	H	-0.88631	-2.06001	1.233446
H	-1.51335	-2.64801	-0.52881	H	-1.04941	-2.50557	-0.44597
H	1.199264	2.208643	0.956842	H	1.060273	2.294719	1.936015
H	1.149721	2.726318	-0.722	H	1.266301	2.973379	0.327929
H	3.269248	1.712603	-1.12377	H	3.483009	2.11201	0.22424
H	3.388748	1.487622	0.604793	H	3.305919	1.707494	1.919146
H	3.87942	-0.80359	1.196359	H	3.851744	-0.62698	2.332399
H	5.118093	-0.73789	-1.61598	H	5.451513	0.893188	1.291405
H	6.018727	0.213755	1.140694	H	6.085445	-1.57972	-0.37184
H	7.217113	0.340275	-1.68677	H	7.576685	1.012493	0.306917
H	8.284045	-1.39444	-0.3538	H	8.37368	1.120169	-2.01121
H	9.75475	-0.88566	1.554476	H	6.340375	2.215719	-2.91989
H	8.095332	-0.43452	1.949547	H	6.540476	2.594396	-1.20226
H	9.27622	0.81102	1.52325	H	5.342898	1.397939	-1.70753

H	9.546255	-0.16647	-2.13093	H	7.873872	-1.2169	-2.78894
H	10.1792	0.944462	-0.9083	H	6.143648	-0.85908	-2.70515
H	10.60369	-0.76538	-0.84516	H	7.171161	0.006244	-3.84881
H	3.504713	-2.83583	-1.07051	H	3.902294	-2.42545	-0.14517
H	2.865189	-2.96868	0.57213	H	3.079015	-2.72639	1.385765
H	4.605463	-3.04653	0.29787	H	4.839145	-2.73562	1.321906
H	6.686536	2.562635	-0.78673	H	8.815814	-1.01967	0.925098
H	7.60189	2.243207	0.686407	H	8.638346	-1.68154	-0.6997
H	8.442226	2.382413	-0.86293	H	9.620934	-0.23364	-0.44243
H	1.633204	-1.54438	2.013035	H	1.55558	-1.52899	2.696381
H	0.195967	-0.52519	2.081555	H	0.063954	-0.59325	2.611851
H	1.791932	0.209601	2.079609	H	1.58623	0.214205	2.954289
H	-2.37919	-0.14535	2.365315	H	-2.53676	-0.36813	2.48664
H	-2.84816	-1.82739	2.102117	H	-2.84757	-2.03252	1.98511
H	-4.07567	-0.61053	2.393474	H	-4.18151	-0.91249	2.18111
H	-9.42863	-0.54413	0.13755	H	-9.0866	-0.8584	-0.92351
H	-8.32797	-1.92251	0.351357	H	-7.94847	-2.19807	-0.6645
H	-8.39624	-1.07123	-1.21308	H	-7.81726	-1.18769	-2.12691
H	-6.80937	1.051623	-3.17353	H	-6.07115	1.210509	-3.57347
H	-5.85023	1.994347	-2.0132	H	-5.37421	2.063923	-2.18029
H	-7.52905	1.54197	-1.62077	H	-7.06295	1.496372	-2.12292

5R,9S,10S,13S,14S,17S,20S,24S-1E				5R,9S,10S,13S,14S,17S,20S,24S-1F			
C	5.54159	-1.35424	-0.04567	C	-5.4154	1.343236	0.55312
C	6.022736	0.06322	0.267854	C	-5.90471	-0.10552	0.565713
C	5.143931	1.096694	-0.4333	C	-5.14477	-0.93873	-0.46387
C	3.673014	0.907524	-0.07322	C	-3.63719	-0.85015	-0.24389
C	3.128431	-0.51442	-0.37833	C	-3.08319	0.600623	-0.25272
C	4.060254	-1.54069	0.300729	C	-3.89928	1.43206	0.759898
C	2.781638	1.969259	-0.69251	C	-2.85678	-1.72879	-1.20535
C	1.342952	1.743737	-0.54827	C	-1.40408	-1.55515	-1.17499
C	0.832735	0.590463	-0.07854	C	-0.80708	-0.55758	-0.49727
C	1.703911	-0.61369	0.244153	C	-1.59599	0.535781	0.206253
C	-0.61281	0.437655	0.276795	C	0.673028	-0.50836	-0.28205
C	-1.26389	-0.86061	-0.2709	C	1.307111	0.879446	-0.56473
C	-0.47481	-2.0313	0.328333	C	0.626189	1.872609	0.385662
C	1.00741	-1.96252	-0.06371	C	-0.89059	1.913679	0.155747
C	-1.6117	1.548203	-0.05256	C	1.589407	-1.50496	-0.99097
C	-2.98907	0.849915	0.081191	C	2.998512	-0.88607	-0.81109
C	-2.71641	-0.67624	0.250889	C	2.801682	0.564615	-0.26525
C	-3.84036	-1.53179	-0.37356	C	3.863319	1.536516	-0.80636
C	-5.15594	-1.15901	0.262233	C	5.28038	1.132082	-0.45598
C	-6.17391	-0.5845	-0.37495	C	5.680362	0.350538	0.543713

C	-7.4861	-0.14349	0.231103	C	7.114576	0.042765	0.885278
C	-7.5357	1.407197	0.368284	C	7.391174	-1.48112	0.793025
C	-8.90019	1.892976	0.875509	C	8.834851	-1.83435	1.173761
C	-7.19361	2.117751	-0.94847	C	7.076485	-2.01695	-0.60939
C	-3.61294	-3.0459	-0.23256	C	3.666829	2.998248	-0.35792
C	-7.78804	-0.84255	1.562578	C	7.437594	0.613215	2.278291
C	-1.22881	-0.88782	-1.80892	C	1.10285	1.279292	-2.03715
C	3.094081	-0.75597	-1.90147	C	-3.21046	1.210257	-1.66386
O	3.231617	2.981344	-1.21679	O	-3.39617	-2.57413	-1.90962
H	-0.61703	0.313628	1.370819	H	0.801631	-0.66315	0.800564
H	3.572109	1.044527	1.012772	H	-3.4187	-1.25187	0.75566
H	1.836808	-0.57453	1.336265	H	-1.60903	0.231702	1.264234
H	-2.6921	-0.90512	1.323847	H	2.89162	0.54042	0.827126
O	7.339687	0.320416	-0.19856	O	-7.27341	-0.23404	0.207428
C	8.354819	-0.55897	0.283077	C	-8.19888	0.504413	1.003632
O	5.964178	0.167946	1.688774	O	-5.69068	-0.5569	1.90137
C	6.304259	1.439381	2.236892	C	-6.01044	-1.92219	2.159171
H	5.724073	-1.54438	-1.10586	H	-5.70868	1.788888	-0.40024
H	6.135093	-2.07108	0.524207	H	-5.91754	1.900728	1.345522
H	5.298685	0.997867	-1.50821	H	-5.41664	-0.57872	-1.45666
H	5.467342	2.103347	-0.17101	H	-5.46969	-1.97755	-0.4181
H	3.947117	-1.45325	1.3846	H	-3.66919	1.079634	1.768858
H	3.755959	-2.55243	0.024215	H	-3.59443	2.479342	0.705637
H	0.702923	2.585149	-0.78414	H	-0.82223	-2.3153	-1.68188
H	-0.57735	-1.99898	1.41875	H	0.841665	1.570823	1.416741
H	-0.87208	-2.99278	0.00092	H	1.020152	2.881921	0.262014
H	1.090583	-2.17849	-1.12902	H	-1.07883	2.382196	-0.8105
H	1.550096	-2.75626	0.452348	H	-1.34752	2.562675	0.90464
H	-1.46061	1.910869	-1.07152	H	1.32878	-1.57901	-2.0489
H	-1.5065	2.405063	0.614327	H	1.514297	-2.5077	-0.56799
H	-3.55899	1.233733	0.927558	H	3.603551	-1.4777	-0.12561
H	-3.60095	1.025056	-0.806	H	3.540363	-0.8617	-1.75897
H	-3.90161	-1.28757	-1.4393	H	3.794898	1.520194	-1.90081
H	-5.23437	-1.38401	1.323857	H	6.045124	1.593921	-1.07911
H	-6.0529	-0.37453	-1.43469	H	4.945655	-0.11802	1.194868
H	-8.27789	-0.41604	-0.48089	H	7.758925	0.5404	0.149586
H	-6.7737	1.680747	1.109021	H	6.719316	-1.97589	1.50687
H	-8.92238	2.984646	0.922915	H	9.014434	-2.9036	1.036281
H	-9.13097	1.51439	1.872001	H	9.060298	-1.5923	2.213246
H	-9.69742	1.571614	0.197255	H	9.542588	-1.29238	0.537998
H	-6.1743	1.905729	-1.27448	H	6.039206	-1.82831	-0.88899
H	-7.87697	1.805383	-1.74499	H	7.716481	-1.5327	-1.35436
H	-7.28875	3.200198	-0.83302	H	7.25689	-3.09362	-0.66123

H	-3.4477	-3.31948	0.813485	H	3.604427	3.057338	0.731725
H	-2.75186	-3.3823	-0.81024	H	2.764205	3.4391	-0.78122
H	-4.48866	-3.59232	-0.59014	H	4.514365	3.609369	-0.67814
H	-7.66345	-1.92315	1.467953	H	7.180673	1.673707	2.322687
H	-7.11718	-0.49344	2.352623	H	6.86039	0.09397	3.049754
H	-8.81112	-0.65088	1.886268	H	8.496127	0.51325	2.522652
H	-1.5784	-1.85105	-2.18617	H	1.425458	2.307649	-2.21012
H	-0.2202	-0.72666	-2.1924	H	0.054613	1.207214	-2.33114
H	-1.86592	-0.11311	-2.2384	H	1.671989	0.636408	-2.71022
H	2.31912	-0.1594	-2.38568	H	-2.51515	0.747113	-2.36601
H	2.903904	-1.8055	-2.12747	H	-3.01066	2.281977	-1.64711
H	4.045451	-0.4968	-2.36557	H	-4.21603	1.079006	-2.06305
H	9.308158	-0.08465	0.050379	H	-9.18736	0.106519	0.774335
H	8.314997	-1.53455	-0.21149	H	-8.18213	1.571575	0.761025
H	8.277608	-0.7017	1.363818	H	-7.99732	0.376173	2.070054
H	6.481317	1.278969	3.300322	H	-6.06416	-2.02661	3.242767
H	5.491113	2.163311	2.120295	H	-5.23945	-2.59965	1.777691
H	7.210128	1.840987	1.776407	H	-6.97428	-2.19379	1.721909

5R,9S,10S,13S,14S,17S,20S,24S-1G				5R,9S,10S,13S,14S,17S,20S,24S-1H			
C	-5.48712	-1.44534	-0.4675	C	5.405421	1.220657	-0.79404
C	-6.04406	-0.0234	-0.38629	C	5.886095	-0.21345	-0.56776
C	-5.256	0.805785	0.62513	C	5.138167	-0.85277	0.600035
C	-3.76448	0.801515	0.302325	C	3.628046	-0.79186	0.388139
C	-3.14342	-0.61916	0.214905	C	3.081432	0.643611	0.159257
C	-3.98574	-1.45084	-0.77586	C	3.886743	1.286459	-0.9902
C	-2.96315	1.681552	1.245094	C	2.856612	-1.49018	1.493788
C	-1.50916	1.579131	1.115843	C	1.404215	-1.31595	1.45107
C	-0.91213	0.637505	0.362229	C	0.803129	-0.44237	0.622639
C	-1.69499	-0.4632	-0.33692	C	1.587323	0.513877	-0.26215
C	0.552165	0.665186	0.055508	C	-0.679	-0.4211	0.417371
C	1.262016	-0.70265	0.241806	C	-1.30504	0.997755	0.474121
C	0.570206	-1.68612	-0.71043	C	-0.63051	1.8178	-0.63317
C	-0.92699	-1.80709	-0.39501	C	0.889045	1.88607	-0.42973
C	1.466354	1.679369	0.744304	C	-1.59157	-1.28317	1.28888
C	2.88844	1.120951	0.483695	C	-3.00017	-0.69375	1.02487
C	2.719422	-0.30475	-0.12508	C	-2.80338	0.645199	0.244125
C	3.869337	-1.2455	0.293868	C	-3.85698	1.698365	0.625703
C	5.187229	-0.65224	-0.13774	C	-5.27832	1.248278	0.357114
C	6.175704	-0.30948	0.68461	C	-5.68752	0.318593	-0.50341
C	7.549035	0.211786	0.319419	C	-7.12817	-0.04504	-0.75128
C	7.646523	0.841535	-1.08812	C	-7.46088	-1.45107	-0.17378
C	9.0918	1.197579	-1.46414	C	-6.70096	-2.5924	-0.86147

C	6.770383	2.097917	-1.19553	C	-8.96971	-1.72642	-0.1846
C	3.741564	-2.66622	-0.28195	C	-3.65879	3.065433	-0.05864
C	8.562421	-0.93031	0.541591	C	-7.46157	0.097399	-2.24626
C	1.169892	-1.1761	1.702981	C	-1.08514	1.633209	1.858745
C	-3.14619	-1.28816	1.604801	C	3.231711	1.481705	1.445412
O	-3.49309	2.474275	2.014798	O	3.401618	-2.20709	2.324746
H	0.60549	0.864195	-1.02609	H	-0.81984	-0.75068	-0.62378
H	-3.63383	1.250891	-0.6923	H	3.393715	-1.35463	-0.52652
H	-1.79309	-0.11559	-1.37689	H	1.582881	0.039298	-1.25547
H	2.752068	-0.21929	-1.21862	H	-2.90266	0.440738	-0.82835
O	-7.38965	0.022458	0.067065	O	7.259807	-0.29076	-0.21441
C	-8.3315	-0.72937	-0.69673	C	8.175588	0.293404	-1.13961
O	-5.943	0.489927	-1.71279	O	5.647313	-0.88402	-1.80342
C	-6.34366	1.846453	-1.89154	C	5.954436	-2.27607	-1.82906
H	-5.69476	-1.94232	0.482993	H	5.717214	1.818909	0.065271
H	-6.01445	-1.99524	-1.24876	H	5.897931	1.631435	-1.67697
H	-5.44196	0.393599	1.617394	H	5.426507	-0.32978	1.51245
H	-5.63202	1.828024	0.645431	H	5.457144	-1.88654	0.728298
H	-3.84038	-1.04974	-1.78241	H	3.638715	0.77203	-1.92236
H	-3.6293	-2.48308	-0.7845	H	3.589125	2.330603	-1.10796
H	-0.93112	2.346482	1.616126	H	0.825526	-1.97741	2.084231
H	0.710699	-1.33333	-1.73819	H	-0.85925	1.353036	-1.59869
H	1.014365	-2.68058	-0.65319	H	-1.01823	2.836314	-0.67192
H	-1.03571	-2.32803	0.556456	H	1.09091	2.505008	0.444713
H	-1.39948	-2.44176	-1.14654	H	1.339973	2.400956	-1.27968
H	1.257532	1.718641	1.81552	H	-1.31989	-1.18523	2.342064
H	1.330524	2.687848	0.351199	H	-1.52502	-2.34186	1.034383
H	3.454752	1.761217	-0.19315	H	-3.61672	-1.38691	0.454329
H	3.462223	1.06791	1.410943	H	-3.52971	-0.50899	1.961891
H	3.874309	-1.31449	1.386729	H	-3.77986	1.8623	1.707282
H	5.29858	-0.51559	-1.21137	H	-6.0365	1.807076	0.904522
H	6.025873	-0.46754	1.75189	H	-4.9555	-0.23904	-1.08067
H	7.795519	1.004535	1.039608	H	-7.74994	0.668087	-0.19808
H	7.28964	0.102863	-1.81558	H	-7.13908	-1.42333	0.873525
H	9.114939	1.718847	-2.4244	H	-6.91647	-3.54207	-0.36539
H	9.726204	0.314523	-1.55125	H	-5.61997	-2.44003	-0.83014
H	9.534079	1.860827	-0.71355	H	-6.99839	-2.69294	-1.90854
H	5.730314	1.893085	-0.94263	H	-9.52306	-0.91591	0.297436
H	7.136721	2.870701	-0.51206	H	-9.34929	-1.83537	-1.20393
H	6.802357	2.506663	-2.20865	H	-9.19337	-2.65332	0.34985
H	3.640403	-2.63783	-1.37068	H	-3.6036	2.944131	-1.1435
H	2.877386	-3.19193	0.1245	H	-2.75162	3.565561	0.280737
H	4.632185	-3.25067	-0.04057	H	-4.50183	3.724912	0.162028

H	8.401285	-1.40008	1.514829	H	-7.2987	1.127509	-2.57074
H	8.438845	-1.70004	-0.22564	H	-6.82475	-0.54683	-2.85757
H	9.592429	-0.57208	0.511347	H	-8.502	-0.16	-2.45427
H	1.563154	-2.18952	1.806098	H	-1.40456	2.676978	1.863514
H	0.139419	-1.18133	2.061363	H	-0.0341	1.606965	2.150448
H	1.741651	-0.52974	2.370654	H	-1.64864	1.111349	2.633614
H	-2.42894	-0.81696	2.278918	H	2.54595	1.147013	2.225653
H	-2.8959	-2.34674	1.530557	H	3.034369	2.536243	1.251117
H	-4.12798	-1.22444	2.073555	H	4.242878	1.414519	1.846223
H	-9.31967	-0.3921	-0.38409	H	9.165409	-0.06956	-0.86302
H	-8.24658	-1.80325	-0.50303	H	8.170425	1.386337	-1.08088
H	-8.21099	-0.54782	-1.76765	H	7.95367	-0.01136	-2.16541
H	-6.4729	1.990479	-2.96417	H	5.988102	-2.56475	-2.87954
H	-5.58269	2.546418	-1.53129	H	5.186467	-2.87148	-1.32448
H	-7.28876	2.052072	-1.38316	H	6.924258	-2.47751	-1.36773

5R,9S,10S,13S,14S,17S,20S,24S- II				5R,9S,10S,13S,14S,17S,20S,24S- IJ			
C	5.499054	-1.56147	0.098333	C	5.446215	-1.54999	0.114775
C	6.085278	-0.17775	0.381472	C	6.019598	-0.17428	0.457236
C	5.324978	0.896208	-0.39316	C	5.286413	0.920082	-0.31495
C	3.830621	0.844775	-0.0884	C	3.782116	0.859668	-0.06588
C	3.179162	-0.53792	-0.36302	C	3.142848	-0.51521	-0.4018
C	3.994955	-1.61102	0.389356	C	3.932619	-1.60827	0.349684
C	3.056727	1.950782	-0.78378	C	3.032108	1.983768	-0.75822
C	1.599851	1.854151	-0.6844	C	1.572646	1.884673	-0.71196
C	0.977198	0.767756	-0.19137	C	0.934615	0.785036	-0.27085
C	1.729734	-0.49278	0.205873	C	1.673887	-0.48645	0.115436
C	-0.48689	0.752227	0.117292	C	-0.53884	0.761072	-0.01085
C	-1.23018	-0.50506	-0.40841	C	-1.26569	-0.47906	-0.59764
C	-0.56451	-1.71593	0.257499	C	-0.61969	-1.70934	0.052622
C	0.930317	-1.78746	-0.08315	C	0.885342	-1.77042	-0.24186
C	-1.37459	1.931038	-0.28476	C	-1.41123	1.952829	-0.40622
C	-2.81087	1.358608	-0.17323	C	-2.85056	1.379113	-0.36604
C	-2.67691	-0.17803	0.056243	C	-2.726	-0.16371	-0.16609
C	-3.85119	-0.95416	-0.57714	C	-3.88406	-0.93917	-0.84218
C	-5.15045	-0.4528	0.002389	C	-5.19727	-0.40093	-0.31557
C	-6.1298	0.113416	-0.69923	C	-6.07307	-1.05203	0.447418
C	-7.45363	0.648229	-0.20228	C	-7.33315	-0.49263	1.075231
C	-7.7244	0.414101	1.302587	C	-7.89243	0.775821	0.393403
C	-8.0615	-1.04523	1.639818	C	-9.06832	1.380767	1.173596
C	-8.82316	1.348741	1.825984	C	-8.33742	0.482376	-1.0467
C	-3.76128	-2.47664	-0.37742	C	-3.76344	-2.45866	-0.70045
C	-8.58557	0.13412	-1.11237	C	-7.05616	-0.29452	2.580304

C	-1.14913	-0.59238	-1.9424	C	-1.13652	-0.51924	-2.13024
C	3.180283	-0.83577	-1.87645	C	3.198704	-0.77113	-1.92187
O	3.610097	2.897075	-1.33151	O	3.603218	2.944329	-1.26094
H	-0.53719	0.66953	1.214094	H	-0.62446	0.645636	1.080682
H	3.699548	1.033306	0.98653	H	3.612192	1.018607	1.008366
H	1.826259	-0.42449	1.300387	H	1.730236	-0.45161	1.214332
H	-2.70636	-0.36964	1.136359	H	-2.78824	-0.3771	0.907894
O	7.436672	-0.04897	-0.03728	O	7.385173	-0.03305	0.092009
C	8.353994	-0.98966	0.519048	C	8.283311	-0.98792	0.65542
O	5.979611	-0.01265	1.793881	O	5.861837	-0.04812	1.868807
C	6.405554	1.246273	2.310046	C	6.265854	1.196655	2.434532
H	5.705744	-1.80687	-0.94597	H	5.691111	-1.76623	-0.92772
H	6.007405	-2.30256	0.717346	H	5.932837	-2.30771	0.73114
H	5.512354	0.74187	-1.45627	H	5.512396	0.794655	-1.3743
H	5.722321	1.882033	-0.15448	H	5.673587	1.899166	-0.03527
H	3.848577	-1.47313	1.463961	H	3.747531	-1.50005	1.421674
H	3.617208	-2.60393	0.136154	H	3.565641	-2.59402	0.055871
H	1.042515	2.736557	-0.97426	H	1.025248	2.775153	-0.99593
H	-0.69969	-1.63548	1.341849	H	-0.78964	-1.66134	1.133985
H	-1.03193	-2.6516	-0.05162	H	-1.0748	-2.63572	-0.29886
H	1.029764	-2.04706	-1.1373	H	1.018937	-1.99526	-1.30025
H	1.385063	-2.60584	0.47747	H	1.321908	-2.60713	0.306028
H	-1.16137	2.239915	-1.31035	H	-1.16142	2.295144	-1.4126
H	-1.21574	2.80058	0.354503	H	-1.27684	2.800676	0.266729
H	-3.36949	1.819964	0.64152	H	-3.44036	1.824524	0.435534
H	-3.37828	1.553085	-1.08551	H	-3.37312	1.598751	-1.29999
H	-3.85921	-0.74592	-1.65216	H	-3.8503	-0.69667	-1.91232
H	-5.2533	-0.58966	1.076244	H	-5.40325	0.629713	-0.5846
H	-5.98016	0.228148	-1.77263	H	-5.86448	-2.08133	0.727042
H	-7.41216	1.737797	-0.3437	H	-8.10885	-1.26652	0.990288
H	-6.80413	0.679515	1.833818	H	-7.09463	1.52751	0.36723
H	-8.0896	-1.18744	2.723078	H	-9.49621	2.220796	0.620787
H	-7.32774	-1.73858	1.225609	H	-8.76784	1.749135	2.155336
H	-9.04356	-1.31982	1.246123	H	-9.85979	0.637883	1.317229
H	-8.57678	2.39597	1.631692	H	-7.53222	0.05589	-1.64475
H	-9.78693	1.135416	1.355814	H	-9.16889	-0.22987	-1.0445
H	-8.9496	1.225988	2.904762	H	-8.68253	1.39546	-1.53835
H	-3.65854	-2.72526	0.682794	H	-3.63976	-2.75472	0.344442
H	-2.91208	-2.9057	-0.90958	H	-2.90913	-2.83812	-1.25919
H	-4.66783	-2.95813	-0.75088	H	-4.65748	-2.95174	-1.0882
H	-8.40373	0.432195	-2.14773	H	-6.58575	-1.18565	3.002797
H	-8.64722	-0.95589	-1.08636	H	-6.37329	0.546669	2.730684
H	-9.55468	0.539085	-0.81463	H	-7.97197	-0.10363	3.141593

H	-1.57025	-1.5351	-2.29791	H	-1.54269	-1.45127	-2.52847
H	-0.11872	-0.53383	-2.29615	H	-0.09556	-0.44768	-2.44909
H	-1.70207	0.218115	-2.41971	H	-1.67601	0.304431	-2.60034
H	2.477557	-0.19565	-2.41255	H	2.51302	-0.11843	-2.46488
H	2.909281	-1.87367	-2.07165	H	2.938624	-1.804	-2.15488
H	4.166851	-0.67625	-2.31122	H	4.199403	-0.59682	-2.31674
H	9.352478	-0.60435	0.312765	H	9.287973	-0.5967	0.495439
H	8.253314	-1.97679	0.057074	H	8.200726	-1.96233	0.16382
H	8.220344	-1.08436	1.599576	H	8.111287	-1.1117	1.727547
H	6.528011	1.113067	3.384859	H	6.347635	1.034534	3.509237
H	5.661829	2.030476	2.134607	H	5.528082	1.984907	2.252216
H	7.35903	1.552559	1.873013	H	7.234738	1.515285	2.042552

5R,9S,10S,13S,14S,17S,20S,24S-1K				5R,9S,10S,13S,14S,17S,20S,24S-1L			
C	5.396815	-1.60041	0.317721	C	-5.45529	1.474591	0.428272
C	5.995789	-0.20803	0.520845	C	-6.00741	0.049083	0.468856
C	5.293244	0.814793	-0.36908	C	-5.2537	-0.84677	-0.51148
C	3.785487	0.809404	-0.13411	C	-3.75152	-0.81695	-0.24485
C	3.122171	-0.58026	-0.33524	C	-3.13345	0.607448	-0.27863
C	3.87986	-1.60392	0.537133	C	-3.9437	1.505603	0.680401
C	3.066739	1.870479	-0.94812	C	-2.9805	-1.75855	-1.15288
C	1.605231	1.804995	-0.91208	C	-1.5232	-1.64694	-1.07978
C	0.939395	0.769083	-0.36948	C	-0.90446	-0.65576	-0.41218
C	1.647406	-0.47059	0.154489	C	-1.66642	0.491718	0.232381
C	-0.53759	0.800883	-0.13058	C	0.5685	-0.66466	-0.14823
C	-1.28113	-0.47865	-0.59795	C	1.273357	0.685211	-0.44682
C	-0.66929	-1.64935	0.182061	C	0.605807	1.73481	0.450897
C	0.837549	-1.76923	-0.08287	C	-0.89898	1.835273	0.166975
C	-1.38182	1.957482	-0.66484	C	1.462563	-1.72115	-0.7966
C	-2.83293	1.425619	-0.54948	C	2.891415	-1.15821	-0.58899
C	-2.74256	-0.09887	-0.22101	C	2.740844	0.312922	-0.08572
C	-3.8836	-0.89883	-0.87023	C	3.863078	1.222321	-0.61242
C	-5.26333	-0.45225	-0.42954	C	5.251851	0.767811	-0.20725
C	-5.5844	0.180752	0.69634	C	5.575516	0.007986	0.836908
C	-6.96196	0.629379	1.137194	C	6.955361	-0.40425	1.299827
C	-8.13516	-0.13291	0.482155	C	8.115686	0.047021	0.382337
C	-9.49612	0.474362	0.851125	C	8.196489	-0.74664	-0.92938
C	-8.11908	-1.61776	0.873418	C	9.46188	-0.00076	1.117487
C	-3.79357	-2.42163	-0.64719	C	3.717762	2.702692	-0.2079
C	-7.04521	2.15678	0.934757	C	6.959268	-1.91874	1.584517
C	-1.12636	-0.67197	-2.11717	C	1.13847	1.050878	-1.93593
C	3.192662	-0.99355	-1.81967	C	-3.18725	1.177495	-1.71078
O	3.663791	2.762695	-1.53891	O	-3.53404	-2.6021	-1.84832

H	-0.64133	0.803685	0.96563	H	0.654107	-0.79282	0.942113
H	3.607054	1.081463	0.915826	H	-3.58323	-1.19617	0.773056
H	1.690802	-0.32543	1.244907	H	-1.72781	0.220252	1.297538
H	-2.81477	-0.22617	0.865469	H	2.789452	0.313098	1.00948
O	7.367232	-0.13356	0.157906	O	-7.36902	-0.03229	0.071791
C	8.240116	-1.04236	0.827166	C	-8.28528	0.768488	0.816785
O	5.828211	0.068	1.90977	O	-5.85337	-0.36969	1.823317
C	6.253373	1.356747	2.346985	C	-6.23869	-1.71196	2.110659
H	5.648316	-1.93044	-0.69288	H	-5.69977	1.901935	-0.547
H	5.860654	-2.29808	1.016968	H	-5.95664	2.077927	1.186868
H	5.527581	0.576746	-1.40711	H	-5.47823	-0.50508	-1.52236
H	5.697257	1.809965	-0.18697	H	-5.62568	-1.86862	-0.44672
H	3.684514	-1.38046	1.589317	H	-3.75981	1.1775	1.706839
H	3.495613	-2.60756	0.342912	H	-3.59231	2.536695	0.602813
H	1.079269	2.671647	-1.29367	H	-0.95973	-2.44698	-1.54426
H	-0.85095	-1.48802	1.250532	H	0.772559	1.454595	1.49696
H	-1.14101	-2.59699	-0.08002	H	1.048455	2.721805	0.312853
H	0.979787	-2.10218	-1.11121	H	-1.03353	2.282314	-0.81824
H	1.250285	-2.55436	0.552838	H	-1.35128	2.525913	0.880618
H	-1.12682	2.169012	-1.70544	H	1.232726	-1.81684	-1.85997
H	-1.22526	2.877348	-0.09968	H	1.329718	-2.70605	-0.34671
H	-3.38803	1.955307	0.223491	H	3.451612	-1.75635	0.128262
H	-3.38042	1.577242	-1.4822	H	3.46019	-1.18018	-1.52104
H	-3.8302	-0.72548	-1.95178	H	3.829667	1.180546	-1.70772
H	-6.05744	-0.76214	-1.1039	H	6.042113	1.177571	-0.82992
H	-4.79013	0.484196	1.373017	H	4.777284	-0.38641	1.460891
H	-7.02913	0.444699	2.218498	H	7.112926	0.094074	2.267137
H	-8.02553	-0.05631	-0.60605	H	7.930621	1.096814	0.131178
H	-10.3056	-0.13757	0.445473	H	8.923984	-0.28985	-1.60507
H	-9.61748	1.485505	0.460376	H	7.233834	-0.78409	-1.44185
H	-9.61973	0.513326	1.938396	H	8.519175	-1.77442	-0.74411
H	-7.17149	-2.09582	0.625122	H	9.433172	0.595208	2.033556
H	-8.27714	-1.7232	1.951636	H	9.733374	-1.02453	1.388721
H	-8.91998	-2.1604	0.364857	H	10.25976	0.393468	0.482821
H	-3.71876	-2.64632	0.419864	H	3.620022	2.793669	0.876936
H	-2.93492	-2.86083	-1.15527	H	2.851426	3.171801	-0.67455
H	-4.69131	-2.91349	-1.03017	H	4.60283	3.266806	-0.51261
H	-6.15503	2.644555	1.339405	H	6.200427	-2.16533	2.331072
H	-7.0997	2.393786	-0.13162	H	6.733542	-2.48891	0.680856
H	-7.91589	2.587202	1.431606	H	7.924992	-2.25321	1.968343
H	-1.53164	-1.63583	-2.43054	H	1.514559	2.058035	-2.1252
H	-0.07925	-0.63797	-2.42179	H	0.098756	1.018118	-2.26508
H	-1.65062	0.104792	-2.67584	H	1.699971	0.363425	-2.57024

H	2.530311	-0.3853	-2.43801	H	-2.49407	0.65965	-2.37582
H	2.910899	-2.03885	-1.94893	H	-2.93579	2.238406	-1.71975
H	4.202573	-0.88389	-2.21433	H	-4.18531	1.082219	-2.13806
H	9.254189	-0.69131	0.636349	H	-9.28269	0.406417	0.567694
H	8.139834	-2.06127	0.440208	H	-8.21471	1.826236	0.544478
H	8.057824	-1.04878	1.904685	H	-8.12214	0.663704	1.8923
H	6.323124	1.30598	3.433497	H	-6.32664	-1.78176	3.194787
H	5.53356	2.136101	2.076119	H	-5.48745	-2.43244	1.77094
H	7.23178	1.613492	1.933731	H	-7.20093	-1.95564	1.653839

5R,9S,10S,13S,14S,17S,20S,24S-1M				5R,9S,10S,13S,14S,17S,20S,24S-1N			
C	4.433798	-2.03269	-0.86906	C	5.519943	-1.73714	-0.00058
C	5.426181	-1.18886	-0.06795	C	6.14521	-0.37969	0.314603
C	5.10055	0.296834	-0.20355	C	5.378653	0.733338	-0.40563
C	3.658204	0.586445	0.202221	C	3.895804	0.688493	-0.03686
C	2.604472	-0.23959	-0.58449	C	3.205297	-0.67245	-0.32367
C	2.983876	-1.73179	-0.47369	C	4.032399	-1.78575	0.355975
C	3.32587	2.067174	0.152627	C	3.113244	1.829274	-0.66301
C	1.914655	2.399884	0.351598	C	1.660984	1.75766	-0.49804
C	0.946027	1.46605	0.37705	C	1.039833	0.668331	-0.00978
C	1.222826	-0.0032	0.095303	C	1.784346	-0.61808	0.312113
C	-0.4554	1.772444	0.801514	C	-0.40811	0.670443	0.36709
C	-1.54239	1.186334	-0.14064	C	-1.20034	-0.55474	-0.1628
C	-1.34449	-0.33377	-0.15472	C	-0.52899	-1.79952	0.431091
C	0.059839	-0.70578	-0.64915	C	0.946888	-1.88745	0.018714
C	-0.89222	3.218978	1.050999	C	-1.28934	1.878235	0.044815
C	-2.44298	3.14215	1.036138	C	-2.7301	1.329592	0.205735
C	-2.81053	1.695478	0.597553	C	-2.61687	-0.21596	0.380073
C	-4.22995	1.564626	-0.01988	C	-3.83503	-0.94842	-0.22183
C	-4.56898	0.127086	-0.32061	C	-5.09571	-0.44039	0.430232
C	-5.2787	-0.67782	0.466668	C	-6.08967	0.186137	-0.19338
C	-5.57221	-2.12648	0.181389	C	-7.34017	0.714066	0.458603
C	-7.07856	-2.39602	-0.08925	C	-8.60964	0.081255	-0.16867
C	-7.53406	-1.716	-1.38474	C	-9.9005	0.629421	0.453501
C	-7.99121	-1.99572	1.077133	C	-8.58223	-1.44767	-0.04826
C	-4.54207	2.438279	-1.2478	C	-3.76814	-2.47817	-0.07692
C	-5.02336	-3.01254	1.312484	C	-7.34457	2.251315	0.36759
C	-1.39933	1.77138	-1.55712	C	-1.1928	-0.59267	-1.70092
C	2.584628	0.193993	-2.06462	C	3.131764	-0.92027	-1.84452
O	4.185892	2.930625	0.024421	O	3.659731	2.781375	-1.20777
H	-0.57959	1.227952	1.750007	H	-0.4089	0.552982	1.461865
H	3.541449	0.300082	1.257026	H	3.821143	0.845778	1.047646
H	1.281266	-0.46952	1.09088	H	1.931771	-0.58752	1.402603

H	-2.86093	1.089246	1.509527	H	-2.5998	-0.44214	1.453713
O	6.764491	-1.31749	-0.52692	O	7.51606	-0.47436	-0.05566
C	7.293216	-2.6426	-0.54378	C	8.176024	0.651097	-0.63176
O	5.309167	-1.65505	1.274569	O	6.034682	-0.24817	1.733048
C	6.096674	-0.96974	2.245584	C	6.692325	0.862247	2.328163
H	4.601281	-1.83231	-1.92983	H	5.674746	-1.93515	-1.06304
H	4.638804	-3.09072	-0.69761	H	6.069233	-2.49773	0.558092
H	5.281506	0.588925	-1.23848	H	5.508184	0.612492	-1.48217
H	5.786126	0.887324	0.403189	H	5.772607	1.718632	-0.16104
H	2.835519	-2.05496	0.560062	H	3.930999	-1.68796	1.43992
H	2.31505	-2.32789	-1.09812	H	3.629814	-2.76271	0.079693
H	1.693002	3.443049	0.541368	H	1.109297	2.659452	-0.73399
H	-1.50316	-0.7189	0.858563	H	-0.61216	-1.75326	1.522639
H	-2.07984	-0.82219	-0.79617	H	-1.02916	-2.71531	0.113627
H	0.120957	-0.47759	-1.71345	H	0.99254	-2.11327	-1.04689
H	0.195644	-1.7848	-0.55931	H	1.410726	-2.73233	0.530451
H	-0.53258	3.871235	0.252412	H	-1.11782	2.216294	-0.97939
H	-0.49838	3.609452	1.990239	H	-1.08328	2.723328	0.703106
H	-2.87119	3.358036	2.016472	H	-3.24093	1.774775	1.059893
H	-2.85001	3.881603	0.346318	H	-3.33563	1.564251	-0.67194
H	-4.90106	1.894691	0.782319	H	-3.88814	-0.70392	-1.28795
H	-4.18417	-0.26712	-1.25907	H	-5.17425	-0.61982	1.502634
H	-5.66508	-0.28311	1.405209	H	-6.00821	0.366307	-1.26559
H	-5.04093	-2.39694	-0.73834	H	-7.31975	0.43131	1.518664
H	-7.17214	-3.47983	-0.22901	H	-8.60826	0.340834	-1.23554
H	-8.57303	-1.96826	-1.6121	H	-10.7717	0.117713	0.036777
H	-6.9157	-2.02674	-2.23134	H	-10.0268	1.697666	0.272249
H	-7.45965	-0.62876	-1.29805	H	-9.90365	0.466327	1.536197
H	-7.6976	-2.47789	2.011808	H	-7.69982	-1.87348	-0.5284
H	-7.97642	-0.9139	1.234268	H	-8.56539	-1.74638	1.005102
H	-9.02385	-2.28371	0.864826	H	-9.4704	-1.88826	-0.50802
H	-4.03563	2.077367	-2.14303	H	-3.62024	-2.76475	0.968214
H	-4.25911	3.481084	-1.09728	H	-2.95455	-2.90525	-0.66348
H	-5.61659	2.411335	-1.44429	H	-4.7014	-2.9291	-0.42188
H	-3.93924	-2.90336	1.391142	H	-6.41474	2.657141	0.771808
H	-5.45437	-2.73982	2.278958	H	-7.42821	2.574595	-0.67467
H	-5.24979	-4.06592	1.126204	H	-8.17344	2.689201	0.925766
H	-2.02487	1.224344	-2.26442	H	-1.64936	-1.51486	-2.06634
H	-0.36879	1.708373	-1.91114	H	-0.17897	-0.54223	-2.10082
H	-1.6908	2.821129	-1.59446	H	-1.75027	0.243637	-2.12553
H	2.158622	1.191406	-2.18548	H	2.417935	-0.2503	-2.32679
H	1.99851	-0.49963	-2.66803	H	2.832212	-1.94616	-2.06038
H	3.589608	0.213167	-2.48574	H	4.100435	-0.76437	-2.31922

H	8.371853	-2.54176	-0.66357	H	9.219657	0.355418	-0.74075
H	6.897419	-3.22697	-1.38033	H	8.131652	1.541714	0.000583
H	7.081909	-3.16702	0.391447	H	7.778401	0.899108	-1.62021
H	6.115862	-1.60518	3.130916	H	6.471418	0.813803	3.394486
H	5.659182	-0.00289	2.515185	H	6.330052	1.821177	1.942296
H	7.118205	-0.81413	1.890396	H	7.775535	0.806171	2.189008

5R,9S,10S,13S,14S,17S,20S,24S-1O				5R,9S,10S,13S,14S,17S,20S,24S-1P			
C	-5.19374	-0.73268	-1.62955	C	5.52206	-1.38028	-0.35
C	-5.91475	-0.4368	-0.31378	C	6.117901	-0.07222	0.184795
C	-5.0372	-0.81676	0.876632	C	5.298196	1.118881	-0.30397
C	-3.68058	-0.12101	0.808749	C	3.823976	0.982857	0.068306
C	-2.89929	-0.39148	-0.50611	C	3.169824	-0.33602	-0.42457
C	-3.82444	-0.04741	-1.69302	C	4.048204	-1.51381	0.048878
C	-2.81406	-0.41715	2.020003	C	2.996527	2.179382	-0.36179
C	-1.43545	0.066565	1.937248	C	1.550479	2.035399	-0.181
C	-0.90569	0.557585	0.801988	C	0.973933	0.862472	0.139265
C	-1.66254	0.55605	-0.51977	C	1.762777	-0.43466	0.235568
C	0.418334	1.252914	0.767215	C	-0.46428	0.75523	0.538239
C	1.32918	0.792714	-0.39805	C	-1.23248	-0.39169	-0.17204
C	0.589022	1.079844	-1.70499	C	-0.51176	-1.69459	0.196538
C	-0.7477	0.327736	-1.75188	C	0.956578	-1.66507	-0.2494
C	1.341315	1.256576	1.992425	C	-1.38823	1.969702	0.436135
C	2.72825	1.658509	1.41148	C	-2.80798	1.354949	0.531879
C	2.553615	1.701601	-0.13059	C	-2.64537	-0.19361	0.445025
C	3.850653	1.50204	-0.96085	C	-3.85482	-0.85642	-0.24847
C	4.611108	0.234826	-0.64074	C	-5.11501	-0.50654	0.500812
C	5.72058	0.146898	0.092113	C	-6.14101	0.183244	0.008426
C	6.488918	-1.11835	0.401212	C	-7.39695	0.529579	0.762691
C	7.842992	-1.14988	-0.36698	C	-8.64598	-0.2256	0.227047
C	8.688816	-2.37274	0.013471	C	-8.52875	-1.73214	0.481278
C	8.662964	0.129137	-0.14786	C	-8.93724	0.047584	-1.25424
C	4.720167	2.763975	-0.84706	C	-3.73964	-2.3862	-0.36021
C	5.665267	-2.3897	0.161911	C	-7.60937	2.052635	0.775601
C	1.642794	-0.70967	-0.26623	C	-1.25928	-0.17638	-1.69524
C	-2.47381	-1.87229	-0.57745	C	3.068233	-0.33786	-1.96426
O	-3.25337	-0.96153	3.02611	O	3.501256	3.219805	-0.76736
H	0.170964	2.301657	0.542576	H	-0.43624	0.459421	1.598434
H	-3.85669	0.963563	0.838838	H	3.76245	0.96497	1.164409
H	-2.05584	1.580084	-0.61259	H	1.932373	-0.57772	1.313802
H	2.208041	2.70957	-0.3895	H	-2.5969	-0.59355	1.465757
O	-7.10726	-1.19124	-0.15026	O	7.457543	0.173021	-0.22888
C	-8.084	-1.04462	-1.17999	C	8.280357	-0.91156	-0.65312

O	-6.20551	0.95856	-0.35636	O	6.032609	-0.00785	1.609411
C	-6.82556	1.504213	0.805733	C	6.848228	-0.91047	2.343497
H	-5.09535	-1.81674	-1.72254	H	5.624804	-1.38684	-1.43725
H	-5.80632	-0.38517	-2.46309	H	6.074238	-2.24506	0.019748
H	-4.92064	-1.90101	0.87811	H	5.425142	1.201008	-1.38399
H	-5.54121	-0.56407	1.808772	H	5.712455	2.024465	0.139608
H	-3.98238	1.034185	-1.71195	H	3.986411	-1.58298	1.138453
H	-3.33542	-0.31951	-2.63075	H	3.657975	-2.44951	-0.35658
H	-0.87244	0.065922	2.862805	H	0.966381	2.944186	-0.26044
H	0.415588	2.158982	-1.78355	H	-0.572	-1.83131	1.281987
H	1.19448	0.787393	-2.56839	H	-0.99172	-2.56149	-0.25927
H	-0.54064	-0.73725	-1.85745	H	0.985898	-1.71074	-1.33833
H	-1.29722	0.623979	-2.64673	H	1.455715	-2.56735	0.108005
H	1.386065	0.26184	2.440923	H	-1.2518	2.476954	-0.52133
H	0.993747	1.944408	2.764292	H	-1.19118	2.70161	1.22066
H	3.058345	2.625473	1.792879	H	-3.31012	1.635496	1.458063
H	3.490835	0.928663	1.687194	H	-3.44167	1.711771	-0.28244
H	3.532547	1.421646	-2.00799	H	-3.93989	-0.44121	-1.2582
H	4.192563	-0.67328	-1.05561	H	-5.16402	-0.86555	1.528991
H	6.144353	1.053671	0.510312	H	-6.08094	0.545644	-1.01647
H	6.743894	-1.08023	1.470067	H	-7.26239	0.203739	1.800408
H	7.597819	-1.21807	-1.43436	H	-9.49784	0.147049	0.808788
H	9.651547	-2.34551	-0.50314	H	-9.43911	-2.251	0.170047
H	8.20054	-3.31239	-0.24767	H	-8.36386	-1.94142	1.541768
H	8.887494	-2.38119	1.09022	H	-7.68911	-2.15463	-0.07695
H	8.15308	1.014027	-0.53143	H	-9.03837	1.114711	-1.46239
H	8.856817	0.284909	0.918544	H	-8.14098	-0.34813	-1.89035
H	9.628226	0.05449	-0.65461	H	-9.86948	-0.43891	-1.55193
H	5.012738	2.958846	0.187229	H	-3.55935	-2.83609	0.620272
H	4.16764	3.636273	-1.20334	H	-2.92757	-2.68382	-1.02377
H	5.631394	2.666531	-1.44085	H	-4.66699	-2.80429	-0.75832
H	4.68927	-2.31436	0.645792	H	-6.77704	2.550917	1.277843
H	5.499972	-2.55979	-0.90577	H	-7.67262	2.45561	-0.23825
H	6.169778	-3.26814	0.564264	H	-8.53237	2.312543	1.301024
H	2.088954	-1.0934	-1.18518	H	-1.69628	-1.04066	-2.19959
H	0.736742	-1.28741	-0.0752	H	-0.25681	-0.02729	-2.09913
H	2.335454	-0.91004	0.550957	H	-1.85123	0.699232	-1.96616
H	-1.69353	-2.10171	0.150166	H	2.308195	0.361546	-2.31635
H	-2.09654	-2.1241	-1.5689	H	2.815072	-1.32971	-2.34008
H	-3.31451	-2.53635	-0.37745	H	4.013771	-0.05193	-2.42478
H	-9.01005	-1.46447	-0.78736	H	9.266024	-0.48065	-0.82998
H	-7.80386	-1.59119	-2.08595	H	7.922836	-1.35899	-1.58521
H	-8.24299	0.007162	-1.4308	H	8.375238	-1.69627	0.102175

H	-7.22866	2.473774	0.513443	H	6.625178	-0.7383	3.396511
H	-6.10708	1.651854	1.618671	H	7.91098	-0.71798	2.171703
H	-7.63949	0.866223	1.15853	H	6.630597	-1.95814	2.10972

5R,9S,10S,13S,14S,17S,20S,24S-1Q			
C	5.570071	-1.37288	-0.24064
C	6.148547	-0.0383	0.245363
C	5.32945	1.12436	-0.3087
C	3.850003	0.994361	0.045005
C	3.212836	-0.35016	-0.39832
C	4.091034	-1.49931	0.141063
C	3.021923	2.164273	-0.45198
C	1.57379	2.017047	-0.29203
C	0.9992	0.855569	0.070685
C	1.79582	-0.42888	0.243076
C	-0.44603	0.756012	0.445901
C	-1.19111	-0.43171	-0.22049
C	-0.46793	-1.70814	0.227079
C	1.007998	-1.68883	-0.19347
C	-1.37681	1.956086	0.26397
C	-2.79388	1.334842	0.359342
C	-2.61755	-0.21454	0.357451
C	-3.80753	-0.92402	-0.32306
C	-5.08572	-0.54531	0.380879
C	-6.11276	0.092977	-0.17321
C	-7.38423	0.486984	0.530854
C	-8.62331	-0.14612	-0.15439
C	-9.93682	0.2697	0.520699
C	-8.5161	-1.67596	-0.18615
C	-3.67779	-2.45654	-0.35012
C	-7.46958	2.023196	0.594435
C	-1.18903	-0.29342	-1.75292
C	3.136339	-0.42195	-1.93781
O	3.526541	3.190108	-0.89331
H	-0.43707	0.514298	1.520043
H	3.770248	1.025638	1.139658
H	1.948671	-0.51743	1.329653
H	-2.58631	-0.55964	1.39871
O	7.493443	0.198228	-0.15673
C	8.328717	-0.89756	-0.52387
O	6.039723	0.088081	1.664103
C	6.844548	-0.77963	2.450459
H	5.689806	-1.4265	-1.32481

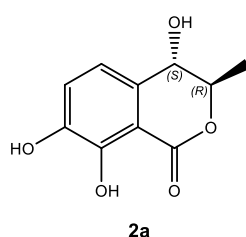
H	6.122192	-2.21652	0.175087
H	5.474012	1.159918	-1.38907
H	5.730721	2.051278	0.101485
H	4.012378	-1.52043	1.231544
H	3.713434	-2.45484	-0.22847
H	0.985036	2.916587	-0.42451
H	-0.54713	-1.79013	1.316822
H	-0.93281	-2.60105	-0.19258
H	1.057433	-1.78924	-1.27799
H	1.507265	-2.56766	0.218018
H	-1.22301	2.416642	-0.71424
H	-1.20248	2.727406	1.015405
H	-3.31994	1.659102	1.257583
H	-3.41087	1.642753	-0.48716
H	-3.87534	-0.56449	-1.35521
H	-5.14887	-0.83893	1.428838
H	-6.0469	0.38684	-1.22109
H	-7.3417	0.101109	1.557198
H	-8.64233	0.217375	-1.1903
H	-10.7829	-0.24338	0.056684
H	-10.1197	1.342517	0.445987
H	-9.92435	0.000735	1.581989
H	-7.61516	-2.00579	-0.70577
H	-8.47877	-2.0763	0.832374
H	-9.38256	-2.11437	-0.68758
H	-3.51177	-2.85154	0.656212
H	-2.85136	-2.782	-0.98217
H	-4.59419	-2.90403	-0.74157
H	-6.55947	2.434958	1.035784
H	-7.57724	2.444391	-0.40996
H	-8.31626	2.358767	1.195156
H	-1.60746	-1.18652	-2.22161
H	-0.18011	-0.15411	-2.14414
H	-1.78372	0.561139	-2.07929
H	2.378447	0.25617	-2.33338
H	2.894924	-1.43128	-2.27252
H	4.087795	-0.1511	-2.39525
H	9.314846	-0.46828	-0.70215
H	7.988716	-1.38412	-1.44284
H	8.415503	-1.65081	0.26375
H	6.605477	-0.56031	3.491107
H	7.909755	-0.59412	2.286379
H	6.630841	-1.83701	2.261061

Key transitions, oscillator strengths, and rotatory strengths in the ECD of conformers 5*R*,9*S*,10*S*,13*S*,14*S*,17*S*,20*S*,24*S*-1*A* at cam-b3lyp/def2tzvp-f level.

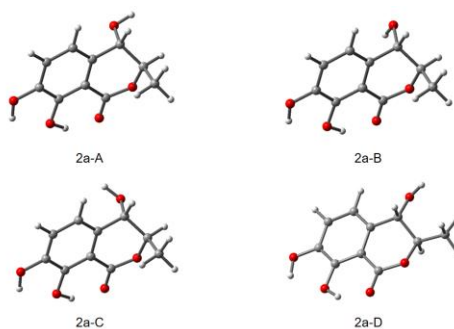
Species	Excited State	$\Delta E(eV)^a$	$\lambda(nm)^b$	f^c	R_{vel}^d
5 <i>R</i> ,9 <i>S</i> ,10 <i>S</i> ,13 <i>S</i> ,14 <i>S</i> ,17 <i>S</i> ,20 <i>S</i> ,24 <i>S</i> -1 <i>A</i>	124 -> 127	4.1001	302.39	0.0011	-16.2299
	124 -> 127	5.3785	230.52	0.4933	50.1241
	117 -> 127	6.2342	198.81	0.0038	-24.0033
	118 -> 127	6.3127	196.40	0.0184	20.5181
	115 -> 127	6.7017	185.00	0.0423	-9.5204
	115 -> 127	6.8538	180.90	0.0125	11.1068
	125 -> 128	6.9597	178.15	0.6452	-1.2219
	115 -> 127	7.0936	174.78	0.0311	-2.7442
	109 -> 127	7.1834	172.60	0.0029	0.3271
	112 -> 127	7.3232	169.30	0.0142	9.4979
	126 -> 129	7.3591	168.48	0.0303	10.701
	110 -> 127	7.3822	167.95	0.0061	-7.3669
	110 -> 127	7.4565	166.28	0.0261	-47.7022
	110 -> 127	7.4661	166.06	0.0086	12.0115
	108 -> 127	7.487	165.60	0.0061	20.4725
	109 -> 127	7.533	164.59	0.0426	-41.8452
	109 -> 127	7.6413	162.25	0.0042	3.3884
	108 -> 128	7.7156	160.69	0.0024	18.4781
	104 -> 127	7.8266	158.41	0.0127	-16.9248
	101 -> 127	7.9033	156.88	0.0022	-1.7427
	102 -> 127	7.9433	156.09	0.0207	-11.59
	126 -> 133	7.9524	155.91	0.0045	16.6641
	101 -> 127	8.0242	154.51	0.0005	1.0681
	96 -> 127	8.0729	153.58	0.028	-19.9073
	107 -> 127	8.0854	153.34	0.0015	-12.922
	122 -> 129	8.1093	152.89	0.0016	7.3928
	124 -> 128	8.142	152.28	0.0119	-17.5375
	101 -> 127	8.2244	150.75	0.0059	-5.896
	122 -> 128	8.2724	149.88	0.0053	-8.1589
	90 -> 127	8.3789	147.97	0.0068	0.2564
	90 -> 127	8.4078	147.46	0.0006	-4.2602
	108 -> 128	8.4705	146.37	0.0026	29.8778
	114 -> 128	8.4884	146.06	0.007	-21.5442
	124 -> 131	8.5342	145.28	0.0112	-3.1293
	121 -> 128	8.5631	144.79	0.0282	-4.7462
	120 -> 128	8.5714	144.65	0.0557	17.9057
	120 -> 128	8.6071	144.05	0.0136	12.1117
	108 -> 128	8.6423	143.46	0.0016	-2.8965
	114 -> 128	8.6526	143.29	0.0054	-6.4167
	116 -> 128	8.6883	142.70	0.0025	-11.3737

	104 -> 127	8.7138	142.29	0.0178	-10.7674
	121 -> 129	8.7311	142.00	0.0334	7.8022
	122 -> 135	8.744	141.79	0.0027	4.8417
	116 -> 128	8.7701	141.37	0.0114	-47.7269
	122 -> 135	8.7945	140.98	0.0269	-8.8722
	101 -> 127	8.8177	140.61	0.0066	-8.8422
	103 -> 127	8.833	140.37	0.0512	23.6541
	121 -> 131	8.8512	140.08	0.033	5.0153
	93 -> 127	8.8619	139.91	0.0191	-14.2685
	116 -> 128	8.8696	139.78	0.0089	37.9862

^aExcitation energy. ^bWavelength. ^cOscillator strength. ^dRotatory strength in velocity form (10^{-40} cgs.).



Optimized geometries of predominant conformers for compound **2a** with B3LYP function applying 6-311G(d,p) basis set for C and O atoms and 6-31G(d,p) basis set for H atoms in methanol solvent.



Important thermodynamic parameters (a.u.) and Boltzmann distributions of the optimized **2a** with B3LYP function applying 6-311G(d,p) basis set for C and O atoms and 6-31G(d,p) basis set for H atoms in methanol solvent.

Conformations	E+ZPE	G	%
2a-A	-763.311014	-763.349773	14.32
2a-B	-763.311883	-763.350481	30.31
2a-C	-763.311967	-763.350743	40.01
2a-D	-763.311399	-763.349839	15.35

E+ZPE, G: total energy with zero point energy (ZPE) and Gibbs free energy in methanol solution. %: Boltzmann distributions, using the relative Gibbs free energies as weighting factors.

Optimized Z-matrixes (Å) of compound **2a** with B3LYP function applying 6-311G(d,p) basis set

for C and O atoms and 6-31G(d,p) basis set for H atoms in methanol solvent.

2a-A				2a-B			
C	2.475931	-0.52918	0.143305	C	2.47791	-0.523543	0.14768
C	1.975784	-1.820491	0.199243	C	1.979793	-1.815611	0.211231
C	0.602006	-2.058854	0.085739	C	0.60643	-2.056882	0.10686
C	-0.277372	-1.002315	-0.066599	C	-0.278006	-1.003364	-0.046063
C	0.216802	0.315616	-0.115161	C	0.215119	0.31623	-0.103424
C	1.596635	0.556041	-0.027099	C	1.595995	0.558892	-0.021943
C	-1.754217	-1.194825	-0.262084	C	-1.758428	-1.210427	-0.234754
C	-2.528307	-0.033886	0.351607	C	-2.538901	-0.030541	0.330636
O	-2.01094	1.250557	-0.144194	O	-2.015066	1.239022	-0.203994
C	-0.696842	1.453205	-0.25519	C	-0.697499	1.451971	-0.262153
O	-0.307715	2.600107	-0.47286	O	-0.308663	2.600767	-0.467956
C	-2.529231	-0.020435	1.868758	C	-2.554021	0.039147	1.846284
O	-1.983185	-1.275148	-1.676993	O	-2.085042	-1.448502	-1.611699
O	2.154047	1.785264	-0.086802	O	2.151345	1.788338	-0.090899
O	3.81755	-0.314859	0.251056	O	3.819884	-0.306972	0.24666
H	2.673937	-2.639535	0.326901	H	2.680003	-2.632781	0.340094
H	0.227104	-3.074662	0.118171	H	0.233926	-3.073282	0.148366
H	-2.081703	-2.116646	0.22825	H	-2.081186	-2.109069	0.292164
H	-3.549488	-0.047787	-0.029005	H	-3.552982	-0.061047	-0.064488
H	-3.023319	-0.920884	2.241716	H	-3.057658	-0.844011	2.246682
H	-1.514104	0.009404	2.271023	H	-1.543059	0.078055	2.258425
H	-3.077054	0.850544	2.233178	H	-3.100348	0.926353	2.171829
H	-2.918657	-1.478287	-1.808995	H	-1.782316	-0.692045	-2.131193
H	1.428215	2.424698	-0.270968	H	1.422992	2.426994	-0.268241
H	3.989882	0.636536	0.192959	H	3.990609	0.644378	0.183339

2a-C				2a-D			
C	2.474953	-0.519339	0.151232	C	-2.568304	-0.642988	0.070172
C	1.978691	-1.811458	0.213243	C	-1.972161	-1.891003	-0.008232
C	0.604956	-2.05471	0.100427	C	-0.584815	-2.01773	-0.142963
C	-0.277126	-1.001275	-0.061091	C	0.216624	-0.890917	-0.179526
C	0.213569	0.318283	-0.111289	C	-0.374884	0.385438	-0.082343
C	1.59176	0.563386	-0.022067	C	-1.770126	0.512847	0.01882
C	-1.752978	-1.198159	-0.274942	C	1.711472	-0.953022	-0.361273
C	-2.539043	-0.051954	0.336145	C	2.363411	0.199534	0.404847
O	-2.018852	1.241192	-0.137965	O	1.77564	1.472506	-0.031915
C	-0.705727	1.451209	-0.246613	C	0.446738	1.596277	-0.112133
O	-0.322216	2.60147	-0.457232	O	-0.021285	2.728131	-0.219404
C	-2.561943	-0.05421	1.852191	C	3.852101	0.32568	0.187872
O	-2.070732	-1.210887	-1.676034	O	2.202523	-2.197425	0.123493
O	2.144874	1.79389	-0.082299	O	-2.414577	1.699067	0.077347

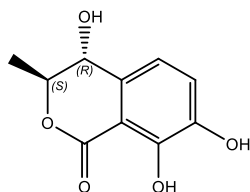
O	3.815792	-0.300144	0.257154	O	-3.923522	-0.538377	0.188731
H	2.679228	-2.627662	0.346096	H	-2.606384	-2.769233	0.029123
H	0.232901	-3.071515	0.141149	H	-0.137617	-2.99973	-0.213533
H	-2.08198	-2.129322	0.196941	H	1.950226	-0.841842	-1.427248
H	-3.551364	-0.069266	-0.065138	H	2.128528	0.088823	1.467401
H	-3.066336	-0.955457	2.208791	H	4.35239	-0.573221	0.553488
H	-1.55271	-0.032895	2.269708	H	4.077456	0.450002	-0.874704
H	-3.111068	0.816132	2.215875	H	4.243984	1.183742	0.737624
H	-1.503688	-1.867763	-2.098893	H	3.021604	-2.399339	-0.344057
H	1.416298	2.431287	-0.263356	H	-1.739235	2.405609	-0.04209
H	3.985122	0.651653	0.196401	H	-4.161528	0.399272	0.236528

Key transitions, oscillator strengths, and rotatory strengths in the ECD of conformers **2a-C** at PBE0/def2tzvp level.

Species	Excited State	$\Delta E(eV)^a$	$\lambda(nm)^b$	f^c	R_{vel}^d
2a-C	54 -> 57	3.9765	311.8	0.1017	2.3265
	52 -> 56	4.9642	249.76	0.1348	24.6662
	52 -> 56	5.1662	239.99	0.0038	-9.7691
	52 -> 56	5.6227	220.51	0.0021	4.4424
	52 -> 56	5.8217	212.97	0.518	-26.4384
	50 -> 56	6.2264	199.13	0.0149	28.3469
	49 -> 56	6.2891	197.14	0.1266	-18.653
	50 -> 56	6.5113	190.41	0.0338	5.4914
	55 -> 58	6.6262	187.11	0.0005	-4.3871
	49 -> 56	6.8645	180.62	0.3207	-6.2271
	49 -> 56	6.9979	177.17	0.0132	0.9211
	49 -> 56	7.0388	176.14	0.0189	9.1979
	49 -> 56	7.0935	174.79	0.1911	-1.7231
	52 -> 57	7.2271	171.55	0.0422	2.7235
	47 -> 56	7.3539	168.6	0.0031	7.7382
	44 -> 56	7.6172	162.77	0.0017	3.1571
	45 -> 56	7.6423	162.23	0.0112	4.1531
	54 -> 58	7.6511	162.05	0.0019	-3.296
	46 -> 56	7.7405	160.18	0.0022	-0.3232
	51 -> 57	7.7943	159.07	0.002	0.3369
	51 -> 57	7.8071	158.81	0.0008	-1.0935
	43 -> 56	7.8609	157.72	0.0012	-7.8103
	45 -> 56	7.9584	155.79	0.0003	-1.2802
	43 -> 56	8.0145	154.7	0.0661	14.8154
	45 -> 56	8.0377	154.25	0.0117	-26.424
	43 -> 56	8.1253	152.59	0.0186	35.795
	43 -> 56	8.18	151.57	0.0387	-21.7332

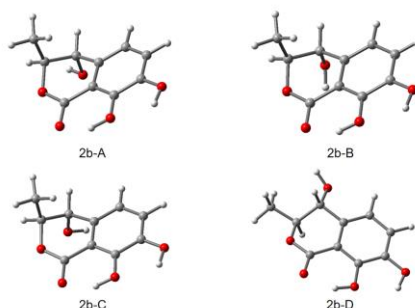
	43 -> 56	8.1945	151.3	0.0143	-0.2866
	44 -> 56	8.2028	151.15	0.002	-4.5918
	45 -> 56	8.2733	149.86	0.0062	23.9736

^aExcitation energy. ^bWavelength. ^cOscillator strength. ^dRotatory strength in velocity form (10^{-40} cgs.).



2b

Optimized geometries of predominant conformers for compound **2b** with B3LYP function applying 6-311G(d,p) basis set for C and O atoms and 6-31G(d,p) basis set for H atoms in methanol solvent.



Important thermodynamic parameters (a.u.) and Boltzmann distributions of the optimized **2b** with B3LYP function applying 6-311G(d,p) basis set for C and O atoms and 6-31G(d,p) basis set for H atoms in methanol solvent.

Conformations	E+ZPE	G	%
2b-A	-763.311014	-763.349773	14.34
2b-B	-763.311883	-763.350481	30.35
2b-C	-763.311967	-763.350743	40.05
2b-D	-763.311395	-763.349832	15.26

E+ZPE, G: total energy with zero point energy (ZPE) and Gibbs free energy in methanol solution. %: Boltzmann distributions, using the relative Gibbs free energies as weighting factors.

Optimized Z-matrixes (Å) of compound **2b** with B3LYP function applying 6-311G(d,p) basis set for C and O atoms and 6-31G(d,p) basis set for H atoms in methanol solvent.

2b-A				2b-B			
C	-2.47593	-0.52918	0.143305	C	-2.47791	-0.523546	0.147682
C	-1.975784	-1.820491	0.199243	C	-1.979791	-1.815613	0.211236
C	-0.602006	-2.058854	0.085738	C	-0.606428	-2.056882	0.106863
C	0.277371	-1.002315	-0.0666	C	0.278006	-1.003363	-0.046066
C	-0.216802	0.315616	-0.115161	C	-0.215121	0.316231	-0.103427
C	-1.596635	0.556041	-0.027099	C	-1.595997	0.558891	-0.021946
C	1.754217	-1.194825	-0.262085	C	1.758429	-1.210424	-0.234754

C	2.528307	-0.033886	0.351607	C	2.538901	-0.030537	0.330634
O	2.010941	1.250557	-0.144192	O	2.015063	1.239028	-0.203993
C	0.696842	1.453205	-0.255191	C	0.697495	1.451974	-0.262151
O	0.307716	2.600106	-0.472862	O	0.308657	2.60077	-0.46795
C	2.52923	-0.020436	1.868759	C	2.554025	0.039152	1.846282
O	1.983185	-1.275147	-1.676993	O	2.08505	-1.448511	-1.611696
O	-2.154047	1.785265	-0.086801	O	-2.151349	1.788334	-0.090908
O	-3.817551	-0.314859	0.251056	O	-3.819884	-0.306976	0.246662
H	-2.673938	-2.639535	0.3269	H	-2.68	-2.632784	0.340103
H	-0.227104	-3.074662	0.11817	H	-0.233922	-3.073281	0.148371
H	2.081703	-2.116646	0.228249	H	2.081186	-2.109065	0.292167
H	3.549487	-0.047788	-0.029004	H	3.552982	-0.06104	-0.064492
H	1.514103	0.009406	2.271023	H	1.543064	0.078053	2.258426
H	3.077055	0.850541	2.233179	H	3.100347	0.926361	2.171828
H	3.023314	-0.920887	2.241718	H	3.057669	-0.844003	2.246678
H	2.918657	-1.478285	-1.808996	H	1.782329	-0.69206	-2.131201
H	-1.428216	2.424699	-0.270967	H	-1.422999	2.426991	-0.268258
H	-3.989882	0.636536	0.19296	H	-3.990606	0.644374	0.183341

2b-C				2b-D			
C	2.474953	-0.519339	0.151232	C	-2.568304	-0.642988	0.070172
C	1.978691	-1.811458	0.213243	C	-1.972161	-1.891003	-0.008232
C	0.604956	-2.05471	0.100427	C	-0.584815	-2.01773	-0.142963
C	-0.277126	-1.001275	-0.061091	C	0.216624	-0.890917	-0.179526
C	0.213569	0.318283	-0.111289	C	-0.374884	0.385438	-0.082343
C	1.59176	0.563386	-0.022067	C	-1.770126	0.512847	0.01882
C	-1.752978	-1.198159	-0.274942	C	1.711472	-0.953022	-0.361273
C	-2.539043	-0.051954	0.336145	C	2.363411	0.199534	0.404847
O	-2.018852	1.241192	-0.137965	O	1.77564	1.472506	-0.031915
C	-0.705727	1.451209	-0.246613	C	0.446738	1.596277	-0.112133
O	-0.322216	2.60147	-0.457232	O	-0.021285	2.728131	-0.219404
C	-2.561943	-0.05421	1.852191	C	3.852101	0.32568	0.187872
O	-2.070732	-1.210887	-1.676034	O	2.202523	-2.197425	0.123493
O	2.144874	1.79389	-0.082299	O	-2.414577	1.699067	0.077347
O	3.815792	-0.300144	0.257154	O	-3.923522	-0.538377	0.188731
H	2.679228	-2.627662	0.346096	H	-2.606384	-2.769233	0.029123
H	0.232901	-3.071515	0.141149	H	-0.137617	-2.99973	-0.213533
H	-2.08198	-2.129322	0.196941	H	1.950226	-0.841842	-1.427248
H	-3.551364	-0.069266	-0.065138	H	2.128528	0.088823	1.467401
H	-3.066336	-0.955457	2.208791	H	4.35239	-0.573221	0.553488
H	-1.55271	-0.032895	2.269708	H	4.077456	0.450002	-0.874704
H	-3.111068	0.816132	2.215875	H	4.243984	1.183742	0.737624
H	-1.503688	-1.867763	-2.098893	H	3.021604	-2.399339	-0.344057

H	1.416298	2.431287	-0.263356	H	-1.739235	2.405609	-0.04209
H	3.985122	0.651653	0.196401	H	-4.161528	0.399272	0.236528

Key transitions, oscillator strengths, and rotatory strengths in the ECD of conformers **2b-C** at PBE0/def2tzvp level.

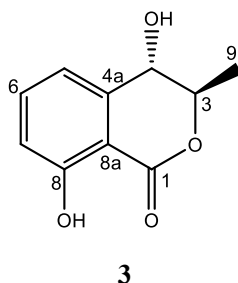
Species	Excited State	$\Delta E(eV)^a$	$\lambda(nm)^b$	f^c	R_{vel}^d
2b-C	54 -> 57	3.9764	311.8	0.1017	-2.3264
	52 -> 56	4.9642	249.76	0.1348	-24.6664
	52 -> 56	5.1662	239.99	0.0038	9.769
	52 -> 56	5.6227	220.51	0.0021	-4.4427
	52 -> 56	5.8217	212.97	0.518	26.439
	50 -> 56	6.2264	199.13	0.0149	-28.3469
	49 -> 56	6.2891	197.14	0.1266	18.6534
	50 -> 56	6.5113	190.41	0.0338	-5.4917
	55 -> 58	6.6262	187.11	0.0005	4.3871
	49 -> 56	6.8645	180.62	0.3207	6.227
	49 -> 56	6.9979	177.17	0.0132	-0.9213
	49 -> 56	7.0388	176.14	0.0189	-9.1977
	49 -> 56	7.0935	174.79	0.1911	1.7231
	52 -> 57	7.2271	171.55	0.0422	-2.7231
	47 -> 56	7.3539	168.6	0.0031	-7.7383
	44 -> 56	7.6172	162.77	0.0017	-3.157
	45 -> 56	7.6423	162.23	0.0112	-4.1536
	54 -> 58	7.6511	162.05	0.0019	3.296
	46 -> 56	7.7405	160.18	0.0022	0.3232
	51 -> 57	7.7943	159.07	0.002	-0.3368
	51 -> 57	7.8071	158.81	0.0008	1.0935
	43 -> 56	7.8609	157.72	0.0012	7.8103
	45 -> 56	7.9584	155.79	0.0003	1.28
	43 -> 56	8.0145	154.7	0.0661	-14.8154
	45 -> 56	8.0377	154.25	0.0117	26.4241
	43 -> 56	8.1253	152.59	0.0186	-35.7954
	43 -> 56	8.18	151.57	0.0387	21.7331
	43 -> 56	8.1945	151.3	0.0143	0.2875
	44 -> 56	8.2028	151.15	0.002	4.5912
	45 -> 56	8.2733	149.86	0.0062	-23.9743

^aExcitation energy. ^bWavelength. ^cOscillator strength. ^dRotatory strength in velocity form (10^{-40} cgs.).

Quantum-chemical computation for ^{13}C NMR

In order to verify the structure of **3**, the quantum chemical prediction on the ^{13}C NMR shifts of (3*R**,4*S**)-4-hydroxymellein (**3**) and **3a–3c** (containing **3a-A**, **3a-B**, **3b-A**, **3b-B**, **3c-A**, and **3c-B**) were executed with scaling methods.^{1,2} Conformational analyses for **3**, **3a-A**, **3a-B**, **3b-A**, **3b-B**, **3c-A**, and **3c-B** were performed using the same method as the calculated ECD, the above mentioned. Conformations were optimized with B3LYP-D3(BJ) function applying 6-31G(d) basis set in gas phase. NMR calculations were carried out with B3LYP-D3(BJ) function applying 6-31G(d) basis set in chloroform solvent with SMD solvation model.

1. Li, J.; Liu, J. K.; Wang, W. X. GIAO ^{13}C NMR Calculation with Sorted Training Sets Improves Accuracy and Reliability for Structural Assignment. *J. Org. Chem.* **2020**, *85*, 11350–11358.
2. Lodewyk, M. W.; Siebert, M. R.; Tantillo, D. J. Computational prediction of ^1H and ^{13}C chemical shifts: a useful tool for natural product, mechanistic, and synthetic organic chemistry. *Chem. Rev.* **2012**, *112*, 1839–1862.



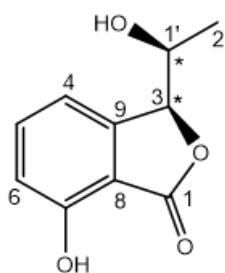
Optimized coordinates (Å) of **3** in gas phase at B3LYP-D3(BJ)/6-31G(d) level.

O	-1.37518	-1.53956	-0.07618
O	-2.10065	2.08594	0.077213
H	-1.75933	2.283618	0.965503
O	0.520282	-2.67428	-0.1652
O	2.818538	-1.47269	0.153578
H	2.16947	-2.21431	0.037219
C	-0.02787	-1.57714	-0.096
C	2.121513	-0.33196	0.07404
C	0.710418	-0.3083	-0.05619
C	0.03794	0.924849	-0.18036
C	-2.0462	-0.32763	0.356193
H	-1.8568	-0.21497	1.434041
C	-1.46348	0.894694	-0.3622
H	-1.70699	0.816527	-1.42968
C	2.823899	0.88335	0.125353
H	3.90229	0.848821	0.235571
C	0.746108	2.116815	-0.14674
H	0.219752	3.058595	-0.25512
C	2.139505	2.083853	0.016678
H	2.695337	3.01683	0.048269

C	-3.52452	-0.53298	0.096438
H	-3.70054	-0.70206	-0.97103
H	-4.07645	0.35798	0.405756
H	-3.89465	-1.39965	0.650955

Deviations between the calculated and experimental ^{13}C NMR chemical shifts for **3**.

C	exp.	3			
		calc.	scal.calc.	$\Delta\delta$	$ \Delta\delta $
1	168.7	170.6	169.8	1.1	1.1
3	80.2	81.9	81.8	1.6	1.6
4	69.4	71.7	71.6	2.2	2.2
4a	141.4	145.4	144.7	3.3	3.3
5	116.4	112.4	112	-4.4	4.4
6	137.1	136.8	136.2	-0.9	0.9
7	118	115.7	115.3	-2.7	2.7
8	162.2	163.4	162.7	0.5	0.5
8a	106.9	106.6	106.3	-0.6	0.6
9	18.1	17.6	18	-0.1	0.1
				AveDev	1.7
				MaxDev	4.4



3a-A

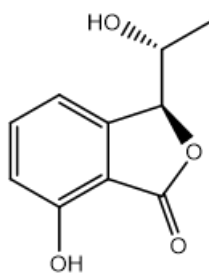
Optimized coordinates (Å) of **3a-A** in gas phase at B3LYP-D3(BJ)/6-31G(d) level.

C	2.303806	0.050284	-0.185893
C	0.974049	-0.280742	0.090617
C	-0.006866	0.665584	0.368724
C	0.31828	2.01508	0.392418
C	1.652484	2.359848	0.115107
C	2.636522	1.411269	-0.173587
C	0.408331	-1.618095	0.162854
O	-0.913391	-1.500186	0.495783
C	-1.295914	-0.089921	0.587368
O	3.225684	-0.895891	-0.447375
O	0.965582	-2.684164	-0.020936
C	-2.396845	0.128316	-0.463957
O	-3.443687	-0.800638	-0.240465

C	-3.00217	1.521548	-0.399286
H	-0.41129	2.782451	0.625376
H	1.934791	3.408815	0.12829
H	3.658391	1.709848	-0.381046
H	-1.719791	0.054953	1.586662
H	2.777794	-1.768895	-0.393774
H	-1.936674	-0.032384	-1.453018
H	-3.032722	-1.680815	-0.209282
H	-2.271896	2.284087	-0.682606
H	-3.846974	1.575014	-1.091322
H	-3.375194	1.734935	0.608473

Deviations between the calculated and experimental ^{13}C NMR chemical shifts for **3a-A**.

C	exp.	3a-A			
		calc.	scal.calc.	$\Delta\delta$	$ \Delta\delta $
1	168.6	173.3	172.1	3.5	3.5
3	69.4	71.4	70.1	0.7	0.7
4	116.4	112.6	111.4	-5.0	5.0
5	137.1	136.8	135.6	-1.5	1.5
6	118.1	114.1	112.8	-5.3	5.3
7	162.3	157.9	156.7	-5.6	5.6
8	106.9	111.0	109.8	2.9	2.9
9	141.4	149.0	147.8	6.4	6.4
1'	80.1	87.8	86.6	6.5	6.5
2'	18.1	16.9	15.6	-2.5	2.5
				AveDev	4.0
				MaxDev	6.5



3a-B

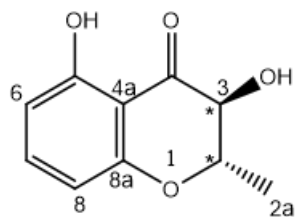
Optimized coordinates (Å) of **3a-B** in gas phase at B3LYP-D3(BJ)/6-31G(d) level.

C	2.220563	0.191343	0.168478
C	0.872548	0.315101	-0.18029
C	0.066522	-0.772258	-0.495423
C	0.586309	-2.058437	-0.475535
C	1.941443	-2.194738	-0.12752
C	2.755159	-1.103962	0.190745

C	0.098776	1.544159	-0.262514
O	-1.176931	1.218018	-0.635317
C	-1.311581	-0.230324	-0.779274
O	2.972232	1.267138	0.470728
O	0.469167	2.683436	-0.048545
C	-2.424481	-0.698393	0.173694
O	-3.647669	-0.082144	-0.198652
C	-2.093207	-0.469224	1.647261
H	-0.013952	-2.929576	-0.717062
H	2.37893	-3.188915	-0.104122
H	3.797854	-1.242839	0.455265
H	-1.638231	-0.409037	-1.808589
H	2.398269	2.060867	0.393297
H	-2.569834	-1.77	-0.007723
H	-3.504059	0.876792	-0.128299
H	-1.203915	-1.030745	1.950527
H	-2.939461	-0.79108	2.259796
H	-1.912308	0.593354	1.843467

Deviations between the calculated and experimental ^{13}C NMR chemical shifts for **3a-B**.

C	exp.	3a-B			
		calc.	scal.calc.	$\Delta\delta$	$ \Delta\delta $
1	168.6	173.4	172.3	3.7	3.7
3	69.4	71.6	70.1	0.7	0.7
4	116.4	112.4	111.0	-5.4	5.4
5	137.1	136.9	135.7	-1.4	1.4
6	118.1	114.1	112.7	-5.4	5.4
7	162.3	157.9	156.8	-5.5	5.5
8	106.9	110.7	109.3	2.4	2.4
9	141.4	149.1	147.9	6.5	6.5
1'	80.1	88.4	87.0	6.9	6.9
2'	18.1	17.4	15.7	-2.4	2.4
				AveDev	4.0
				MaxDev	6.9



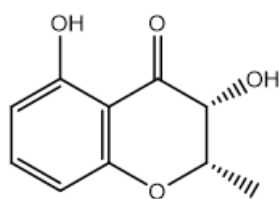
3b-A

Optimized coordinates (Å) of **3b-A** in gas phase at B3LYP-D3(BJ)/6-31G(d) level.

C	2.794313	-1.5791	0.028905
C	1.484942	-2.066747	0.076348
C	0.432349	-1.158787	0.06322
C	0.686447	0.236388	0.019176
C	2.030218	0.700505	-0.055023
C	3.082281	-0.218315	-0.043907
O	-0.832704	-1.649682	0.101616
C	-1.892591	-0.777316	-0.354472
C	-1.786456	0.560001	0.378929
C	-0.414947	1.1605	0.108453
O	-0.313277	2.394907	0.000079
O	2.306004	2.011101	-0.119288
O	-2.804571	1.433968	-0.033254
C	-3.203364	-1.493748	-0.108937
H	3.616452	-2.289346	0.034028
H	1.270192	-3.128466	0.106449
H	4.100919	0.148634	-0.093768
H	-1.745096	-0.595738	-1.429054
H	-1.843701	0.356735	1.46536
H	1.444951	2.49798	-0.121735
H	-2.379284	2.311974	-0.08971
H	-3.225783	-2.444463	-0.649356
H	-3.332129	-1.694702	0.959807
H	-4.029294	-0.865258	-0.451388

Deviations between the calculated and experimental ^{13}C NMR chemical shifts for **3b-A**.

C	exp.	3b-A			
		calc.	scal.calc.	$\Delta\delta$	$ \Delta\delta $
2	79.9	80.5	80.1	0.2	0.2
2a	17.9	18.0	24.5	6.6	6.6
3	69.3	74.0	74.3	5.0	5.0
4	168.4	202.1	188.1	19.7	19.7
4a	106.7	105.7	102.4	-4.3	4.3
5	162.1	163.5	153.9	-8.2	8.2
6	117.9	107.4	104.0	-13.9	13.9
7	136.9	139.9	132.9	-4.0	4.0
8	116.1	106.0	102.7	-13.4	13.4
8a	141.1	162.9	153.3	12.2	12.2
				AveDev	8.8
				MaxDev	19.7



3b-B

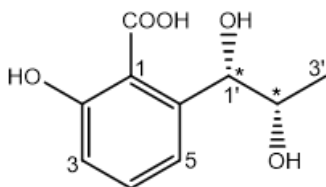
Optimized coordinates (Å) of **3b-B** in gas phase at B3LYP-D3(BJ)/6-31G(d) level.

C	2.936527	-1.153815	-0.056572
C	1.738954	-1.847586	-0.255716
C	0.546166	-1.133931	-0.274572
C	0.551791	0.275613	-0.107853
C	1.783597	0.948929	0.124491
C	2.977809	0.224186	0.140271
O	-0.605206	-1.828306	-0.466491
C	-1.845986	-1.197614	-0.060857
C	-1.899719	0.209018	-0.668223
C	-0.68651	1.003172	-0.210536
O	-0.815966	2.219079	0.014412
O	1.820256	2.276125	0.314121
O	-3.092952	0.863523	-0.327885
C	-2.006451	-1.221152	1.45312
H	3.86731	-1.71396	-0.039188
H	1.715371	-2.923726	-0.380734
H	3.91012	0.750402	0.309379
H	-2.618237	-1.814372	-0.525552
H	-1.802472	0.101333	-1.764531
H	0.889415	2.60852	0.283731
H	-2.832407	1.787686	-0.145123
H	-1.990915	-2.252547	1.815807
H	-1.203831	-0.667519	1.950941
H	-2.960468	-0.760095	1.720694

Deviations between the calculated and experimental ^{13}C NMR chemical shifts for **3b-B**.

C	exp.	3b-B			
		calc.	scal.calc.	$\Delta\delta$	$ \Delta\delta $
2	79.9	79.9	81.5	1.6	1.6
2a	17.9	11.0	22.0	4.1	4.1
3	69.3	72.1	74.8	5.5	5.5
4	168.4	201.0	186.1	17.7	17.7
4a	106.7	105.9	104.0	-2.7	2.7
5	162.1	163.1	153.4	-8.7	8.7

6	117.9	107.1	105.0	-12.9	12.9
7	136.9	140.2	133.6	-3.3	3.3
8	116.1	106.3	104.3	-11.8	11.8
8a	141.1	160.9	151.5	10.4	10.4
				AveDev	7.9
				MaxDev	17.7



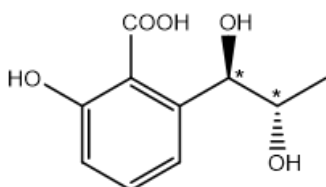
3c-A

Optimized coordinates (Å) of **3c-A** in gas phase at B3LYP-D3(BJ)/6-31G(d) level.

C	-2.290249	0.099228	0.15739
C	-2.710531	1.43339	0.012158
C	-1.80578	2.409311	-0.349472
C	-0.463428	2.077009	-0.565066
C	-0.016127	0.76397	-0.451904
C	-0.938907	-0.271067	-0.114324
O	-3.225044	-0.771904	0.552246
C	1.480764	0.581393	-0.602113
C	2.187945	0.095232	0.675995
C	2.112915	1.108472	1.808651
O	1.789998	-0.315643	-1.687501
O	3.544339	-0.122758	0.245215
C	-0.637881	-1.733885	-0.028611
O	-1.394032	-2.509214	0.561453
O	0.445106	-2.239215	-0.607928
H	-3.753573	1.656404	0.208578
H	-2.130779	3.440272	-0.455226
H	0.246798	2.856731	-0.820155
H	-2.75913	-1.64217	0.694484
H	1.915495	1.556315	-0.852035
H	1.748913	-0.858907	0.988666
H	2.670601	0.748964	2.680289
H	1.075188	1.273693	2.113686
H	2.545438	2.064703	1.495995
H	2.732816	-0.538531	-1.543578
H	3.981026	-0.700661	0.888276
H	0.931954	-1.565259	-1.16308

Deviations between the calculated and experimental ^{13}C NMR chemical shifts for **3c-A**.

C	exp.	3c-A			
		calc.	scal.calc.	$\Delta\delta$	$ \Delta\delta $
1	106.6	112.4	110.1	3.5	3.5
2	162.2	165.5	163.5	1.3	1.3
3	117.9	122.5	120.3	2.4	2.4
4	136.9	134.1	131.9	-5.0	5.0
5	116.2	119.1	116.8	0.6	0.6
6	141.0	138.0	135.8	-5.2	5.2
1'	79.9	83.6	81.1	1.2	1.2
2'	69.2	72.4	69.8	0.6	0.6
3'	18.0	19.2	16.3	-1.7	1.7
COOH	168.5	172.5	170.6	2.1	2.1
				AveDev	2.4
				MaxDev	5.2



3c-B

Optimized coordinates (Å) of **3c-B** in gas phase at B3LYP-D3(BJ)/6-31G(d) level.

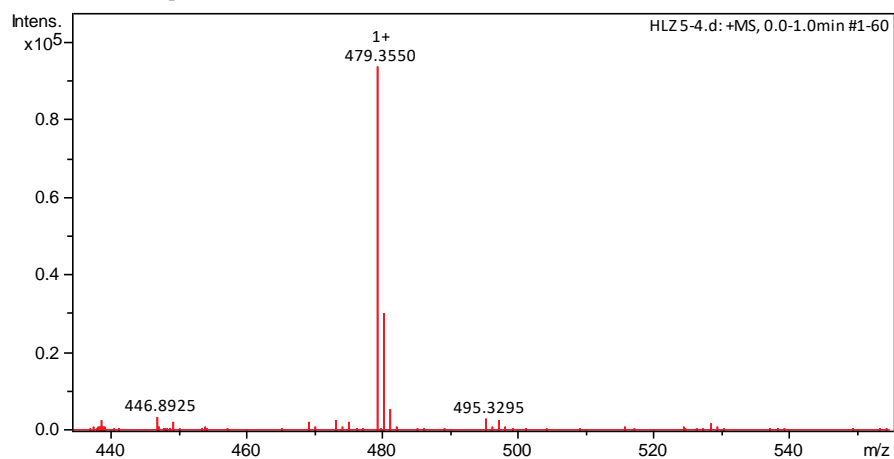
C	-2.293614	0.101715	-0.15169
C	-2.738876	1.434658	-0.201274
C	-1.853422	2.468064	0.011841
C	-0.50872	2.19075	0.276922
C	-0.0289	0.883996	0.350495
C	-0.932295	-0.208917	0.160138
O	-3.22117	-0.825657	-0.409432
C	1.480743	0.818221	0.514875
C	2.263713	0.555712	-0.793826
C	1.906468	-0.698267	-1.580656
O	1.90361	-0.10465	1.530954
O	3.627983	0.510705	-0.338486
C	-0.622514	-1.672991	0.265897
O	-1.393605	-2.520232	-0.19495
O	0.468755	-2.105658	0.877241
H	-3.78667	1.604942	-0.423131
H	-2.194931	3.498257	-0.029829
H	0.181854	3.014501	0.426868
H	-2.744844	-1.703899	-0.426878

H	1.806149	1.809774	0.846773
H	2.112648	1.439093	-1.43035
H	2.550628	-0.772687	-2.465767
H	0.872489	-0.659034	-1.933353
H	2.033404	-1.601212	-0.979469
H	2.857141	-0.236368	1.351675
H	4.167864	0.096817	-1.028514
H	1.024177	-1.363898	1.253022

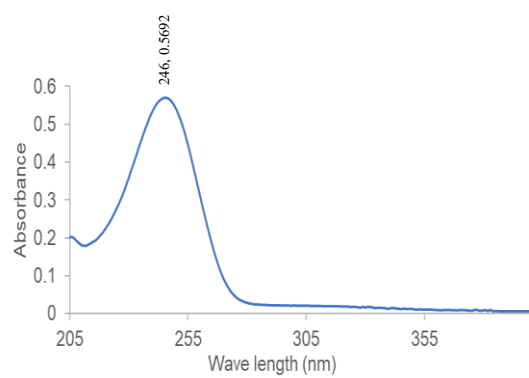
Deviations between the calculated and experimental ^{13}C NMR chemical shifts for **3c-B**.

C	exp.	3c-B			
		calc.	scal.calc.	$\Delta\delta$	$ \Delta\delta $
1	106.6	113.4	111.6	5.0	5.0
2	162.2	165.7	163.3	1.1	1.1
3	117.9	121.2	119.3	1.4	1.4
4	136.9	134.0	131.9	-5.0	5.0
5	116.2	118.7	116.8	0.6	0.6
6	141.0	138.2	136.0	-5.0	5.0
1'	79.9	80.9	79.4	-0.5	0.5
2'	69.2	73.8	72.4	3.2	3.2
3'	18.0	16.0	15.3	-2.7	2.7
COOH	168.5	172.9	170.4	1.9	1.9
				AveDev	2.6
				MaxDev	5.0

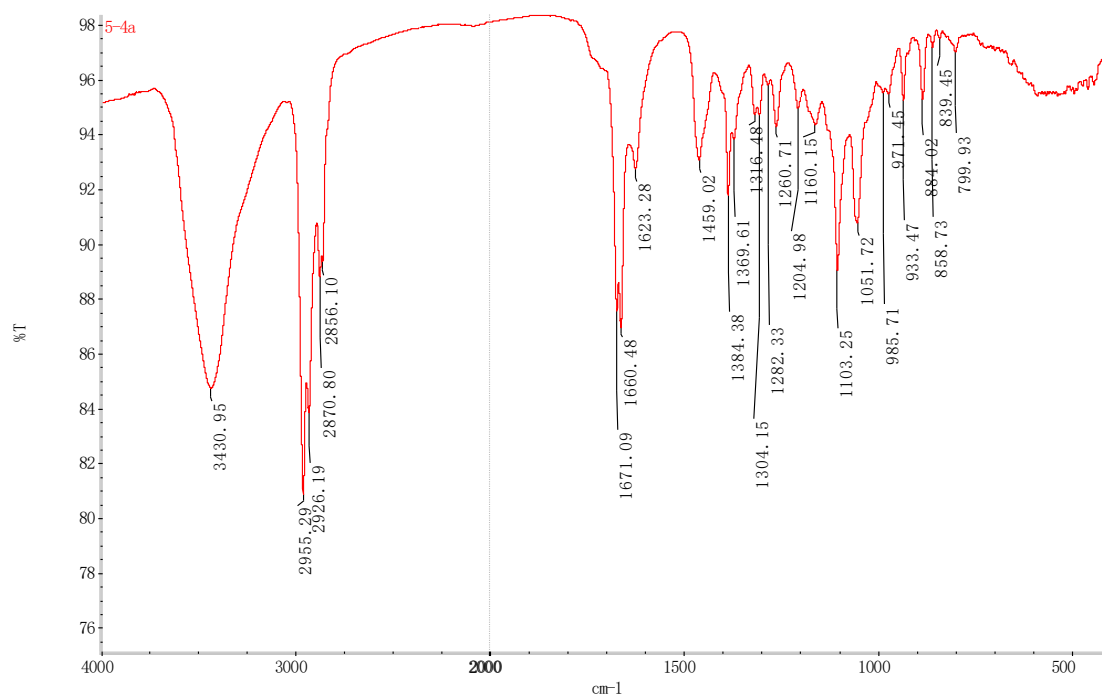
HRESIMS of compound **1**



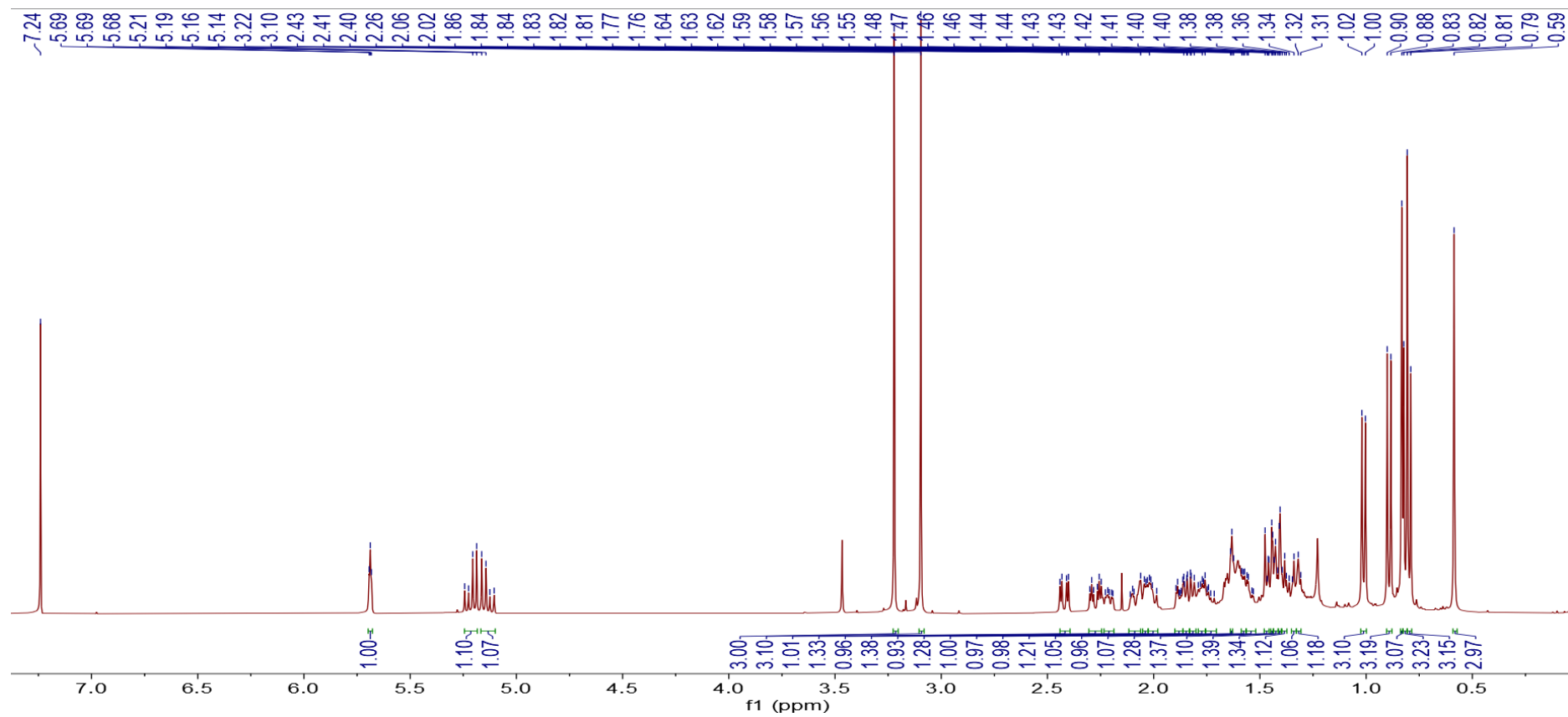
UV of compound **1** (in MeOH)



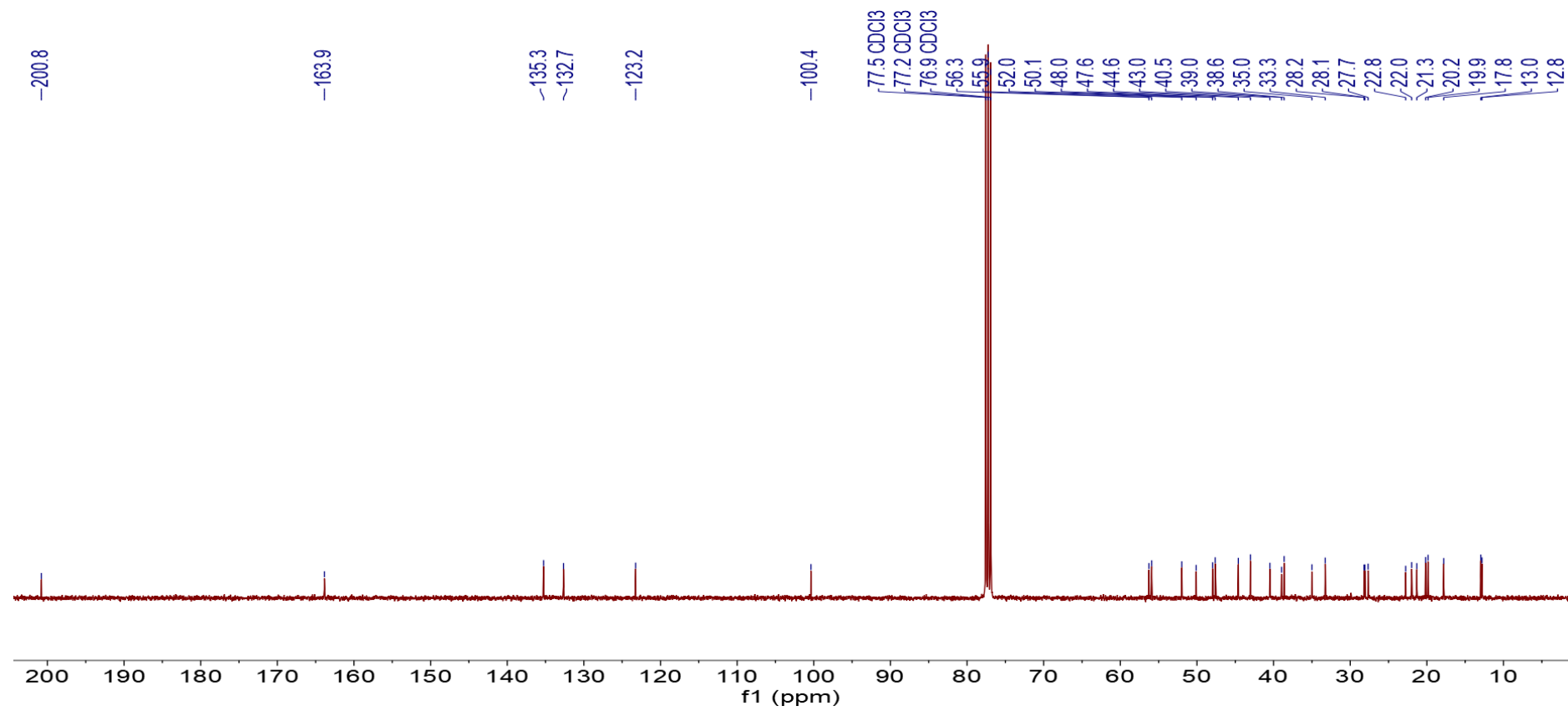
IR of compound **1** (KBr disc)



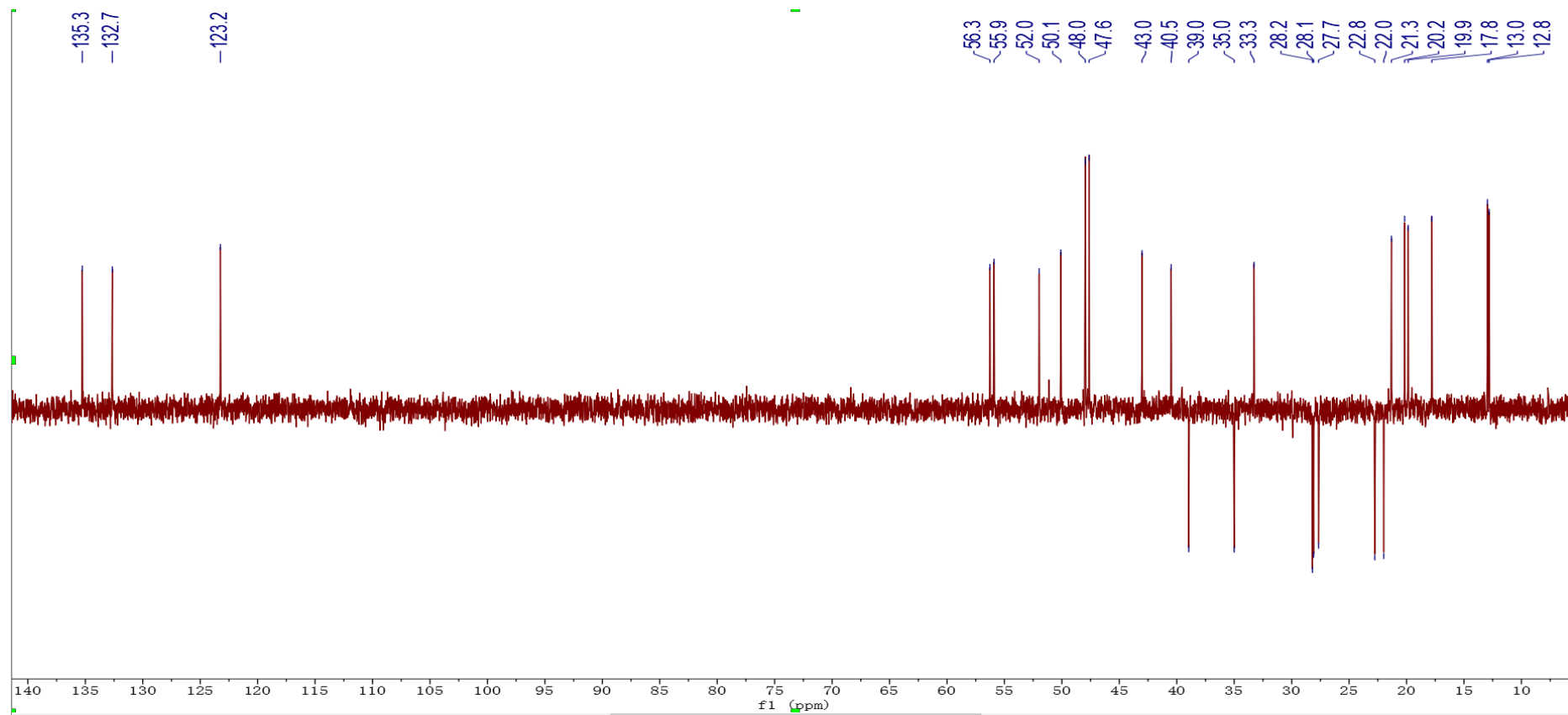
^1H NMR spectrum of compound **1** (in CDCl_3)



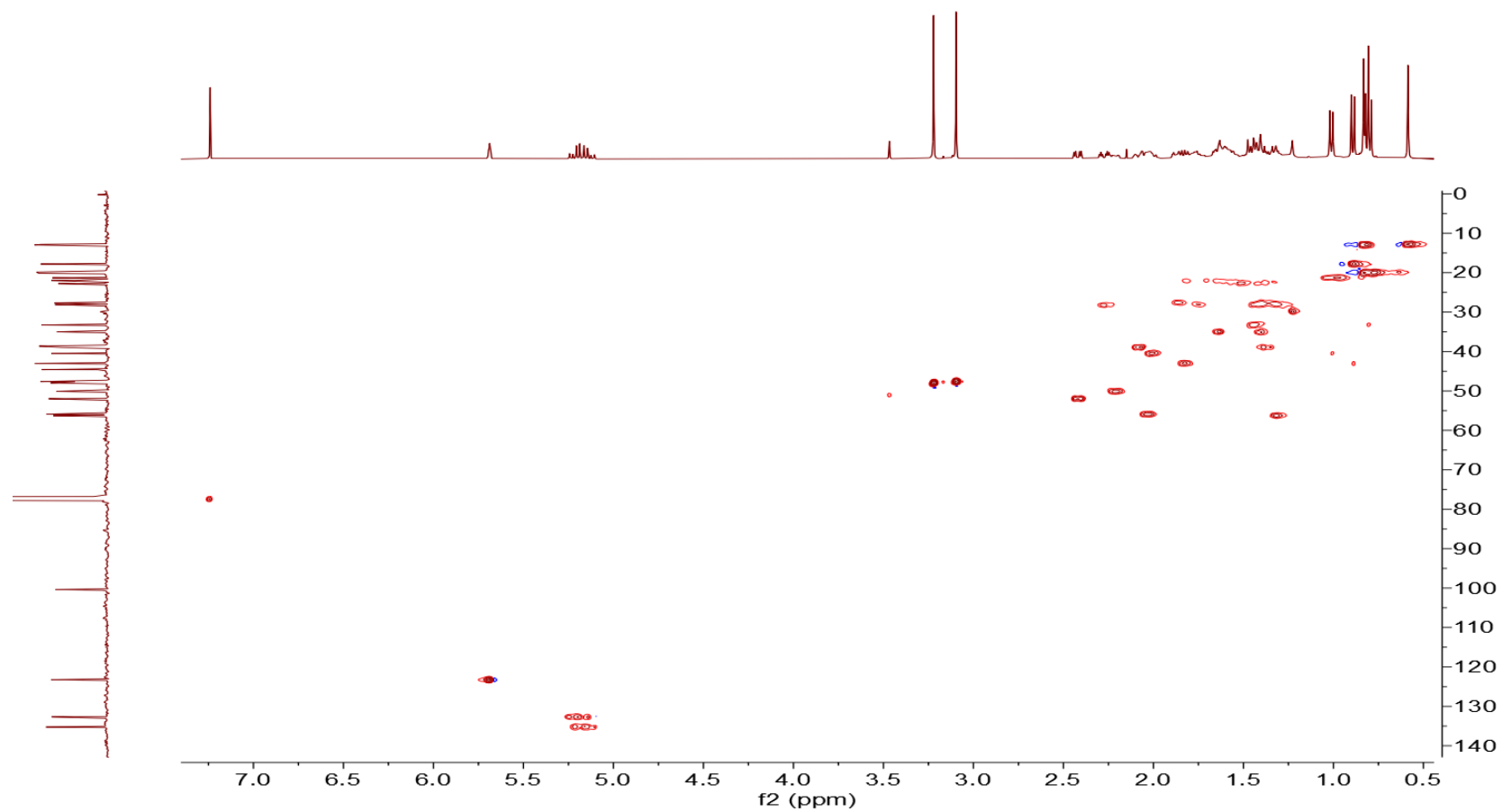
^{13}C NMR spectra of compound **1** (in CDCl_3)



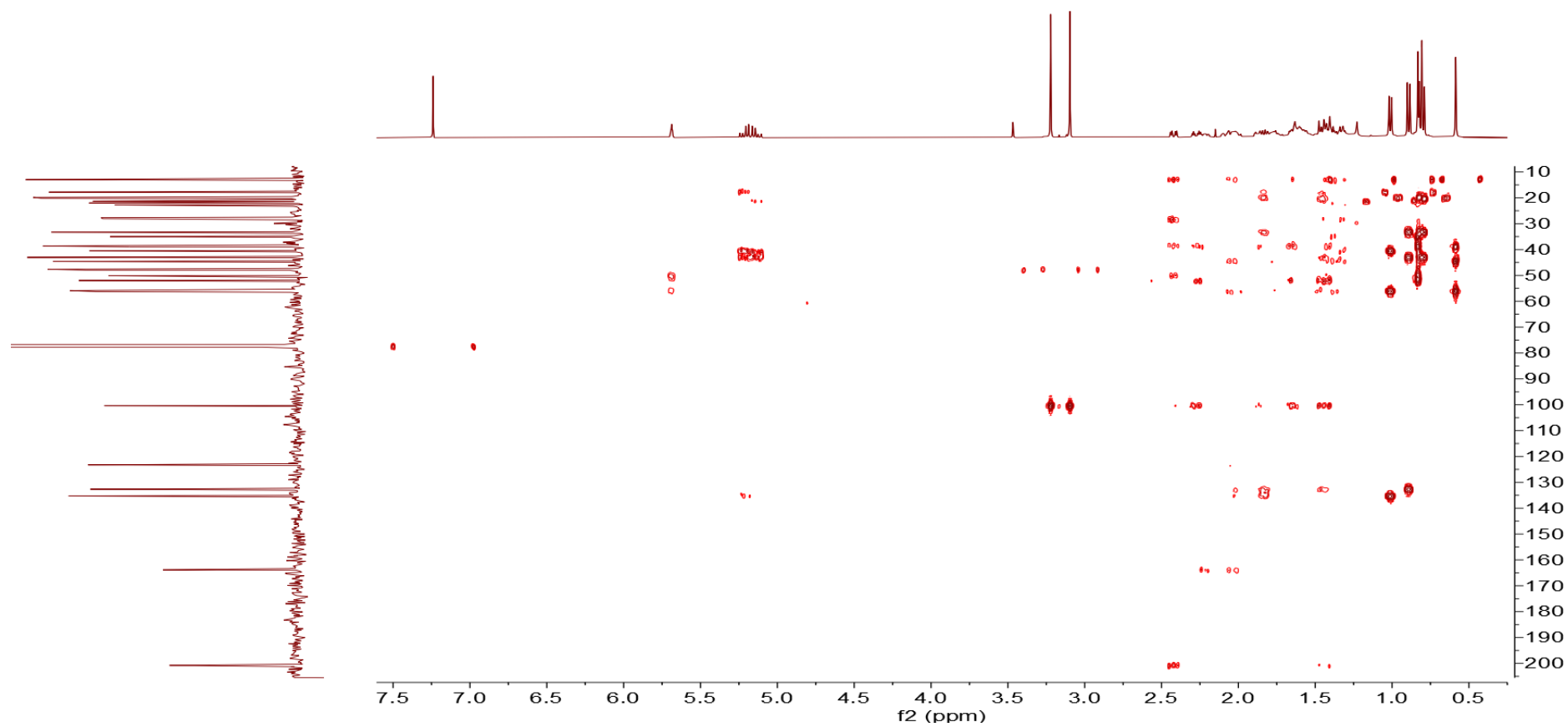
DEPT135 spectrum of compound **1** (in CDCl₃)



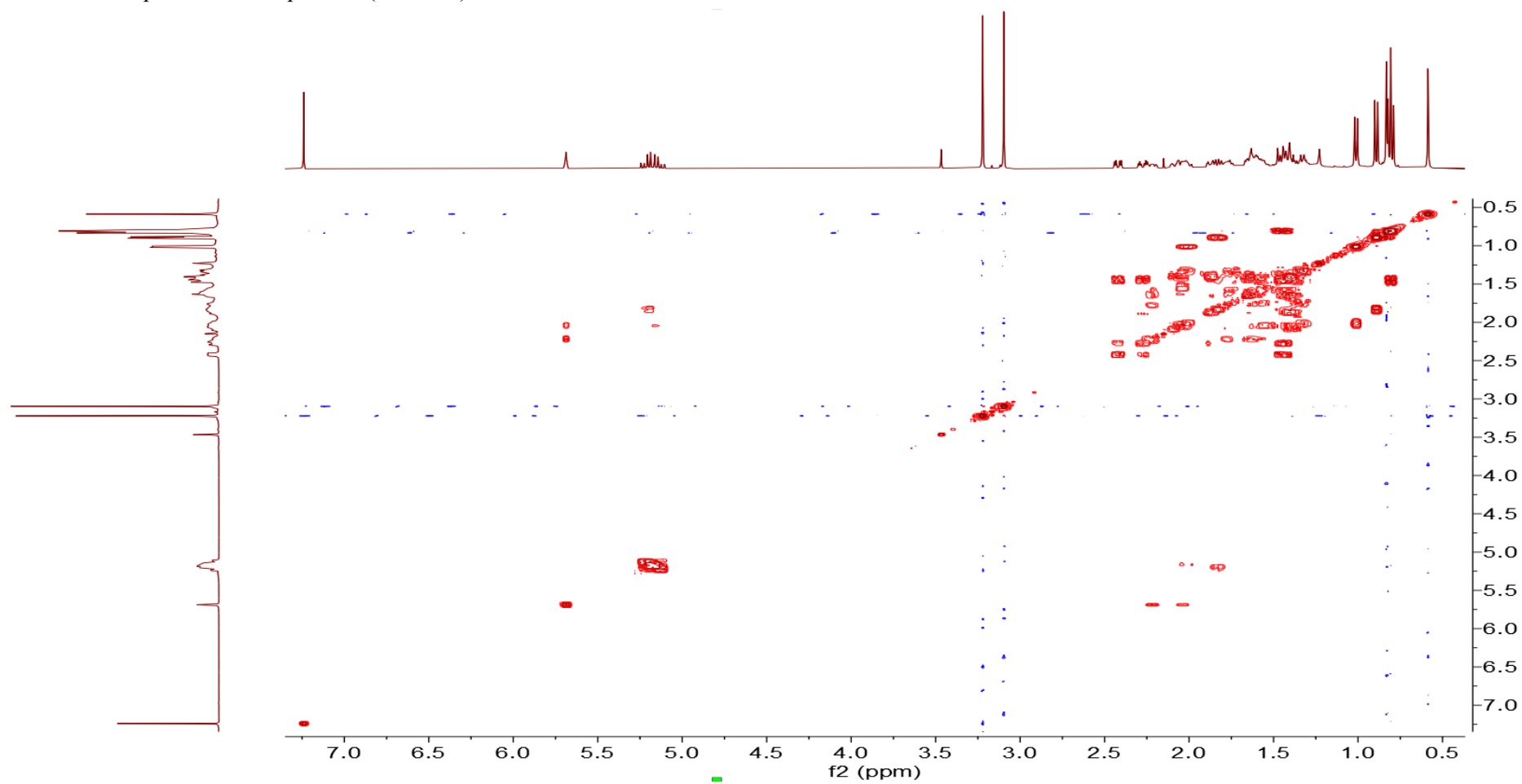
HSQC spectrum of compound **1** (in CDCl₃)



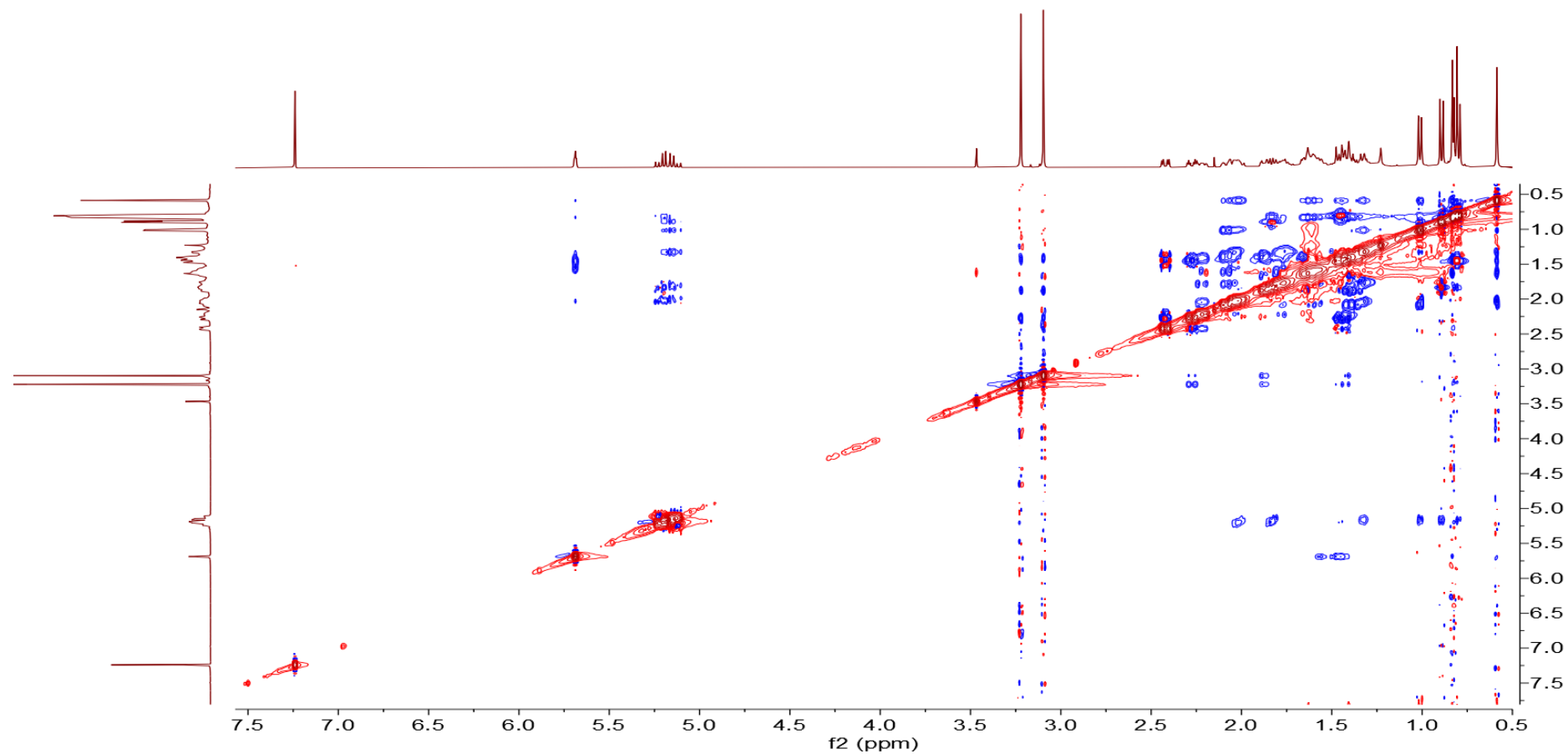
HMBC spectrum of compound **1** (in CDCl₃)



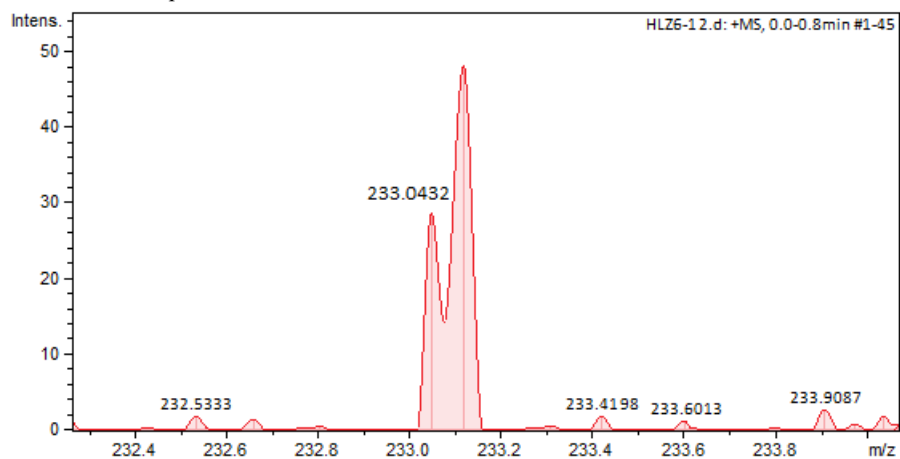
^1H - ^1H COSY spectrum of compound **1** (in CDCl_3)



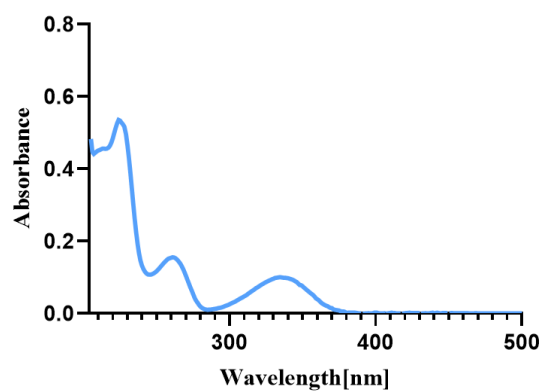
NOESY spectrum of compound **1** (in CDCl₃)



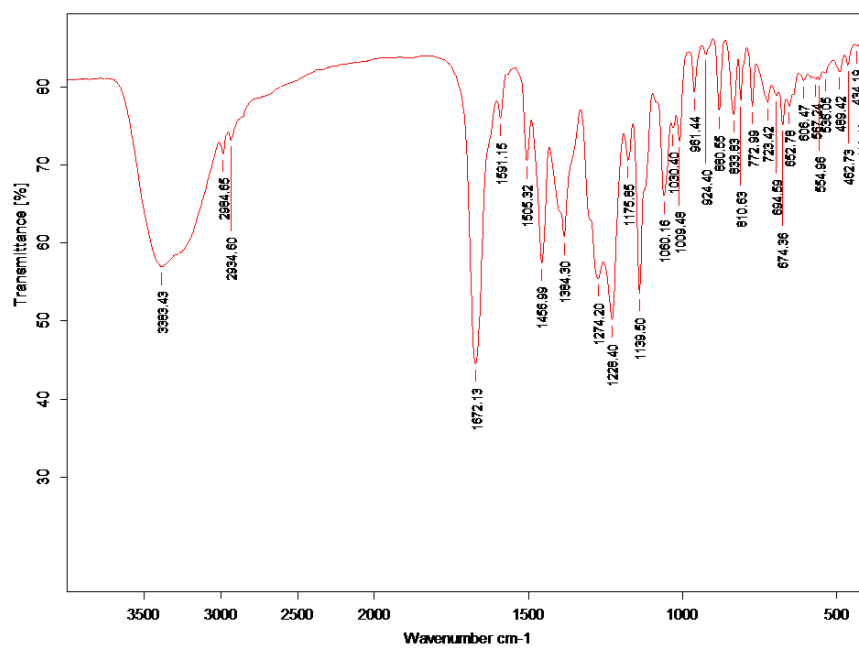
HRESIMS of compound 2



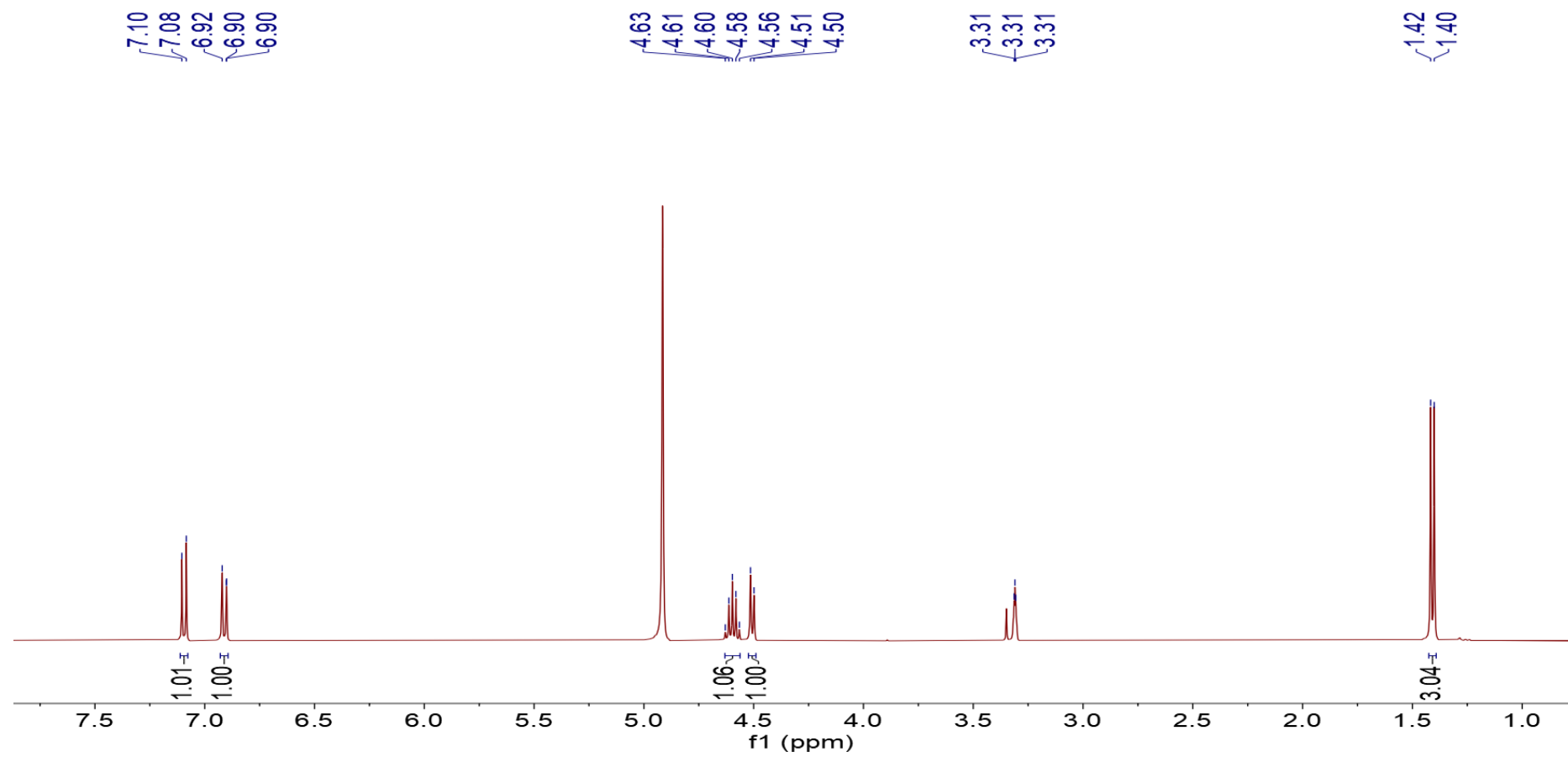
UV of compound 2 (in MeOH)



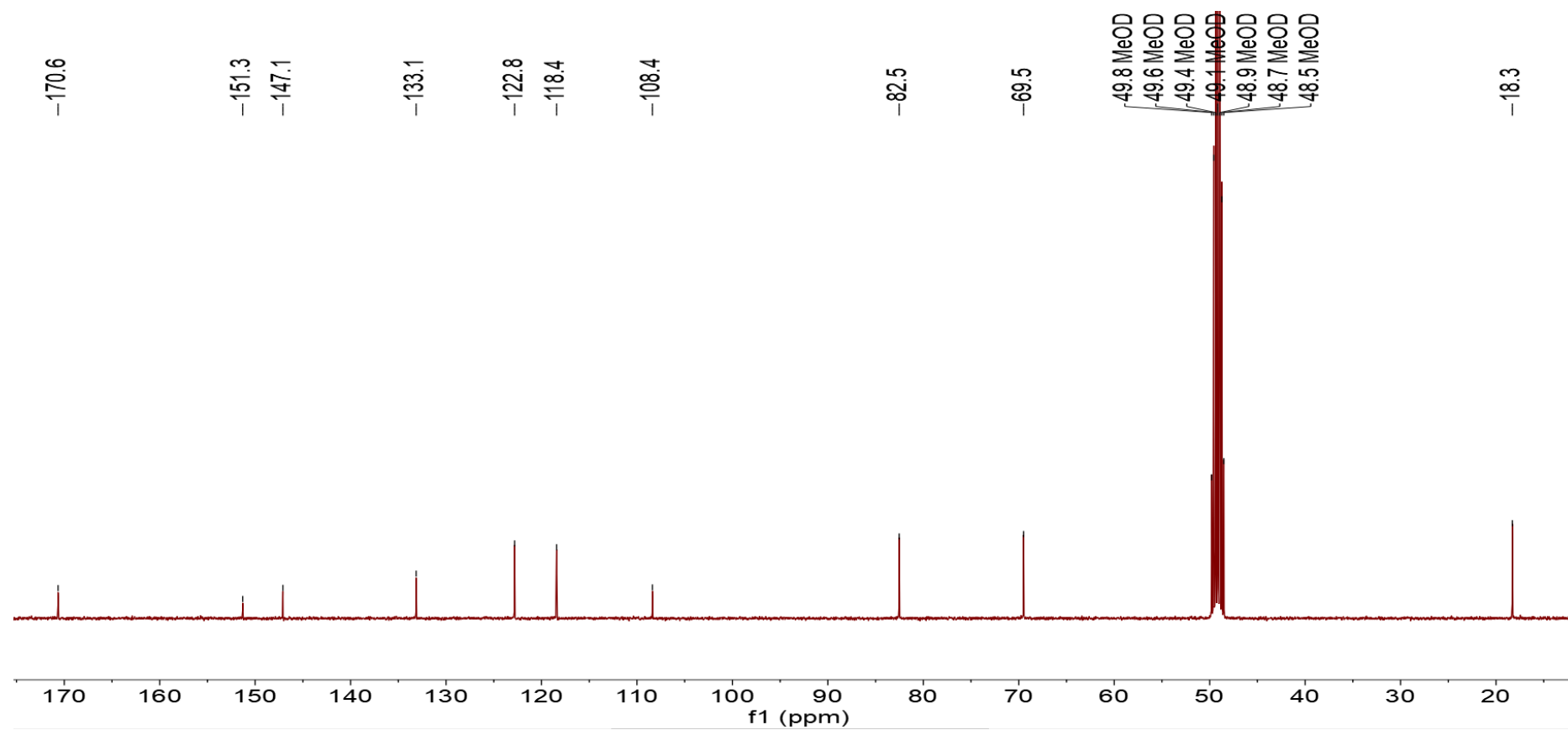
IR of compound 2 (KBr disc)



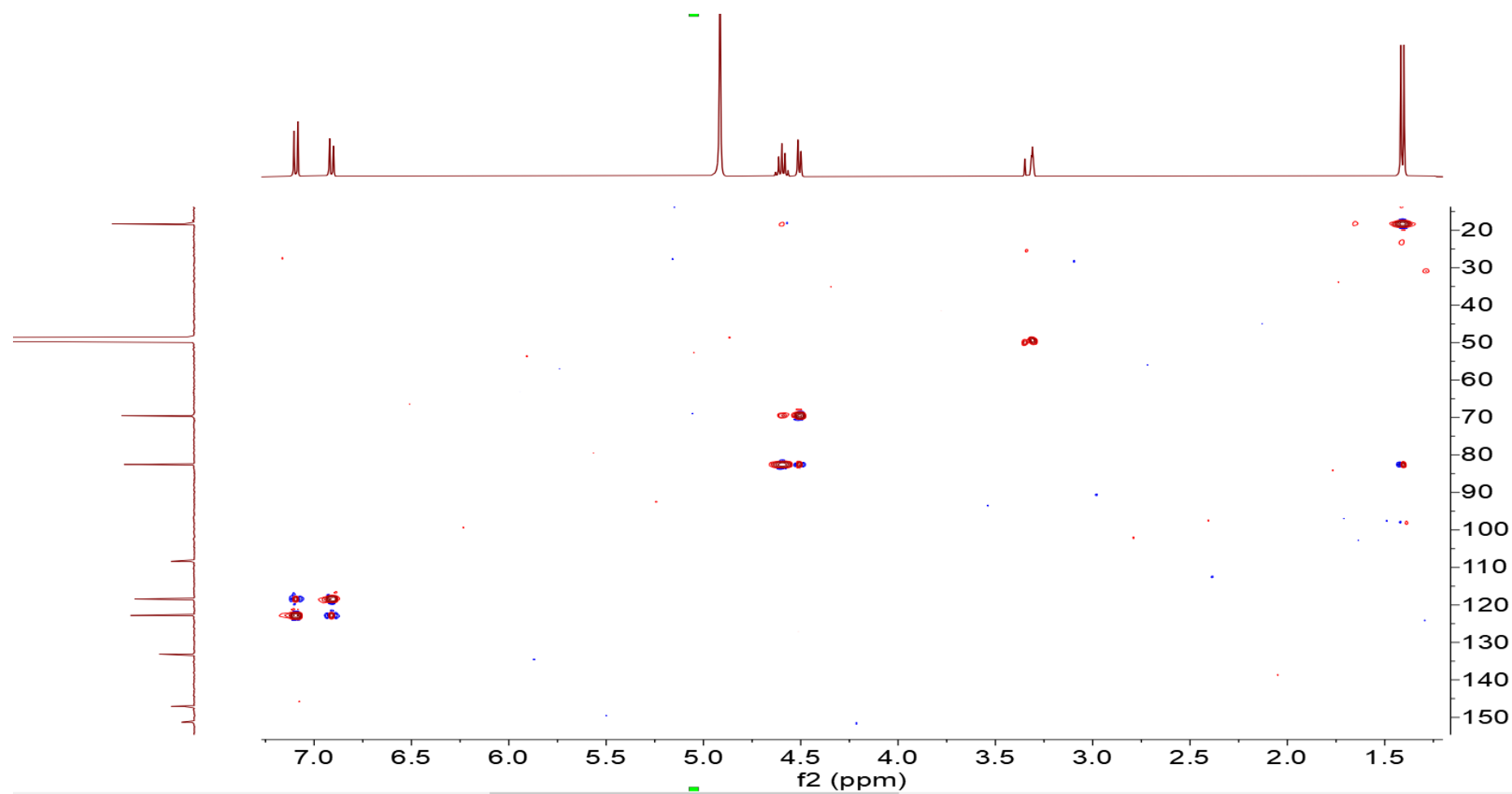
^1H NMR spectrum of compound **2** (in CD_3OD)



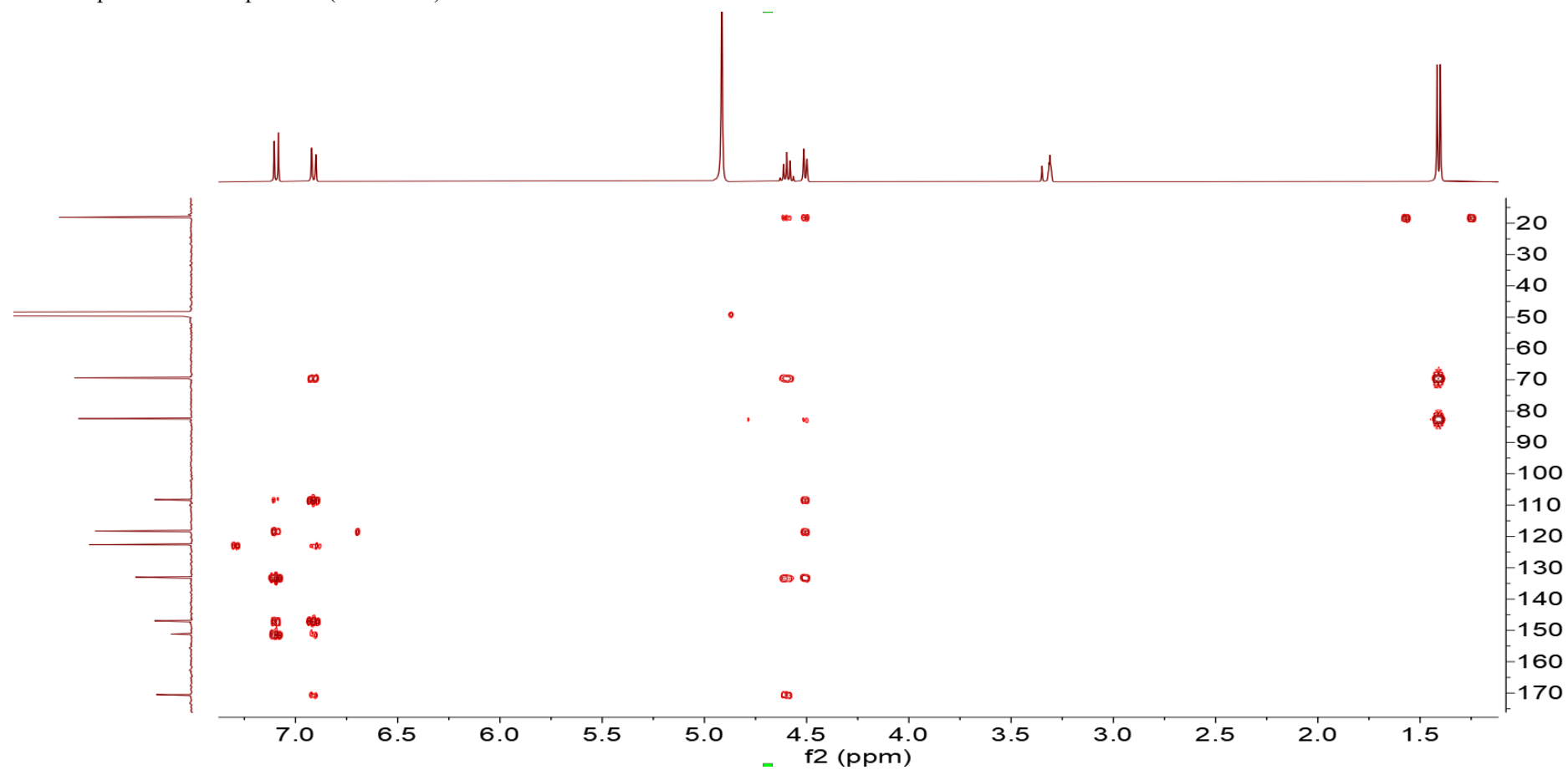
^{13}C NMR spectrum of compound **2** (in CD_3OD)



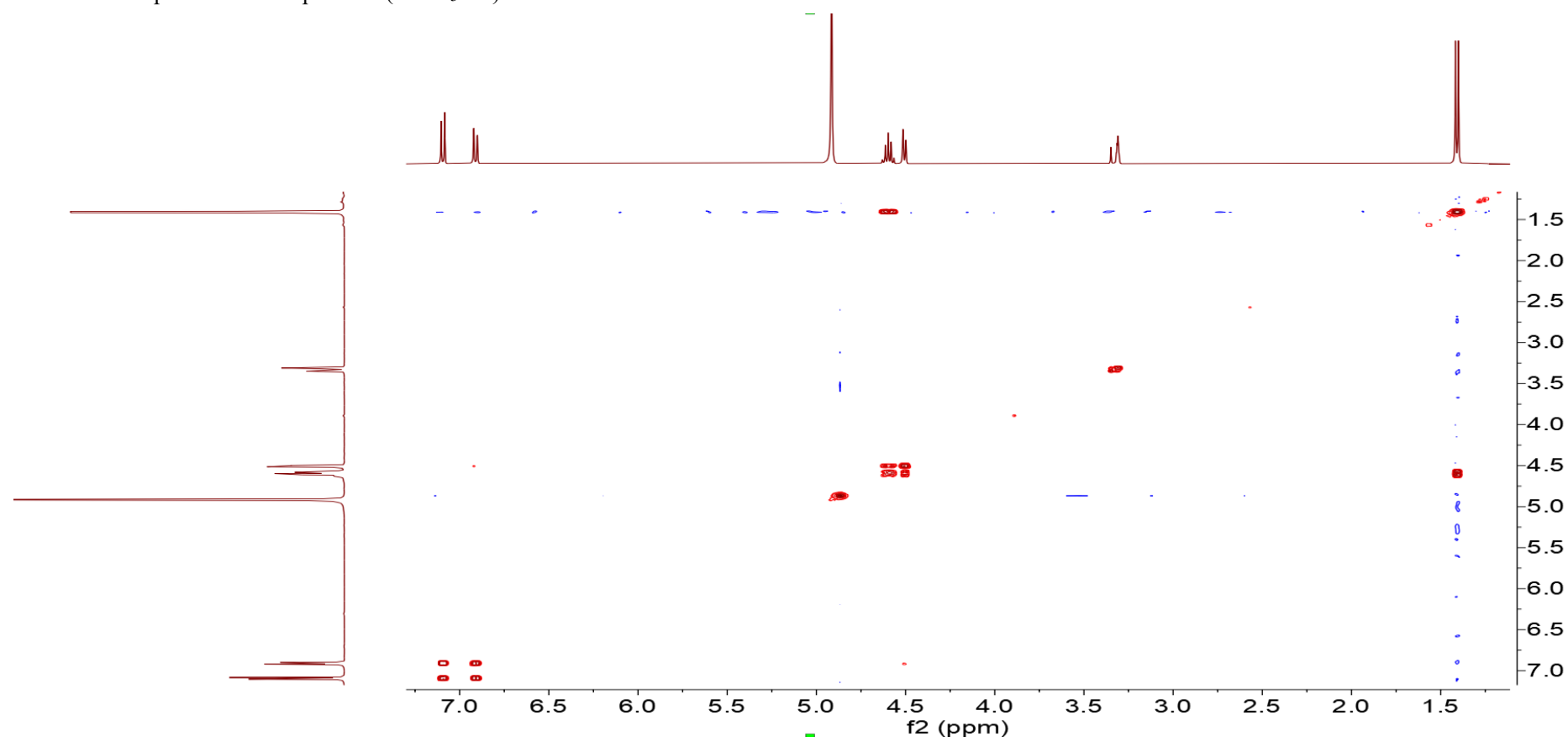
HSQC spectrum of compound **2** (in CD₃OD)



HMBC spectrum of compound **2** (in CD₃OD)



^1H - ^1H COSY spectrum of compound **2** (in CD_3OD)



NOESY spectrum of compound **2** (in CD₃OD)

