

Discovery of Acylphloroglucinol-based Meroterpenoid Enantiomers as KSHV Inhibitors from *Hypericum japonicum*

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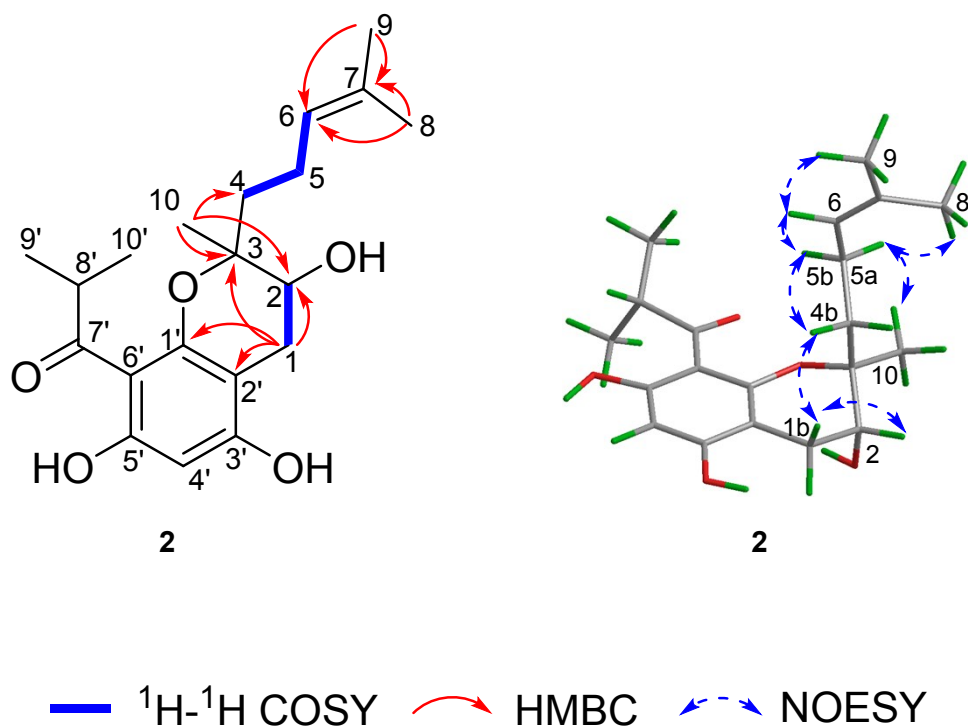


Figure S1. Key 2D NMR correlations of **2**.

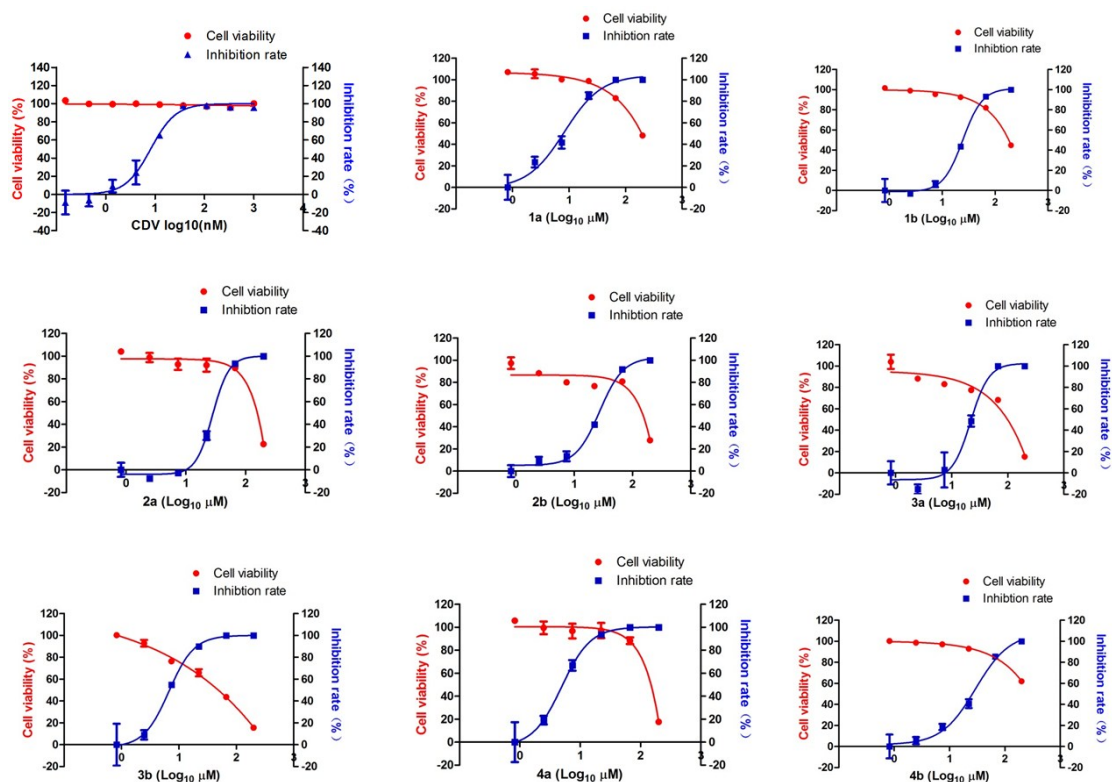


Figure S2. Effects on Human iSLK.219 cells viabilities and inhibition on lytic replication of KSHV infecting Vero cells of **1a/1b-4a/4b** were measured using CDV as positive control *in vitro*.

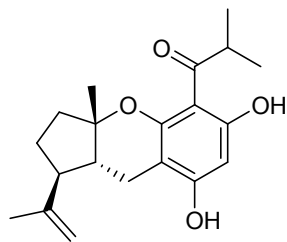
Extraction and Isolation

The whole herbs of *H. japonicum* (30 kg) were soaked in 95% EtOH at 25 °C and yielded a crude extract (0.75 kg) after removed the solvent under vacuum. The crude extract was suspended in water and sequentially partitioned with petroleum ether, chloroform, and ethyl acetate. The petroleum ether-soluble extract (400 g) was subsequently partitioned by silica gel column chromatography (3 kg, 20 × 120 cm; petroleum ether-acetone, 50:1→5:1) to afford seven fractions (Fr.1–Fr.7). Fr.6 was repeatedly chromatographed using silica gel CC (0.6 kg, 10 × 100 cm), eluting with a gradient of petroleum ether-EtoAc (30:1→3:1) to afford six subfractions (Fr.6.1–Fr.6.6). Fr.6.4 was subjected to MPLC (ODS, 1.5 × 20 cm, MeOH-H₂O, 30–90%) to obtain subfractions Fr.6.4.1–Fr.6.4.6. Fr.6.4.3 was partitioned by Sephadex LH-20 (2 × 150 cm, MeOH) and purified via semi-preparative HPLC (CH₃CN/H₂O 55:45). Finally, a second semi-preparative HPLC (MeOH/H₂O 53:47) was performed to yield three pairs of racemates, namely, **1** (4.00 mg), **2** (7.00 mg), and **3** (11.02 mg). Fr.6.4.2 was repurified by silica gel CC (CHCl₃/MeOH 40:1), Sephadex LH-20 (2 × 150 cm, CH₂Cl₂-MeOH, 1:1), and semi-preparative HPLC (CH₃CN/H₂O 70:30) to afford the pair of racemates **4** (3.51 mg).

Computational ECD details

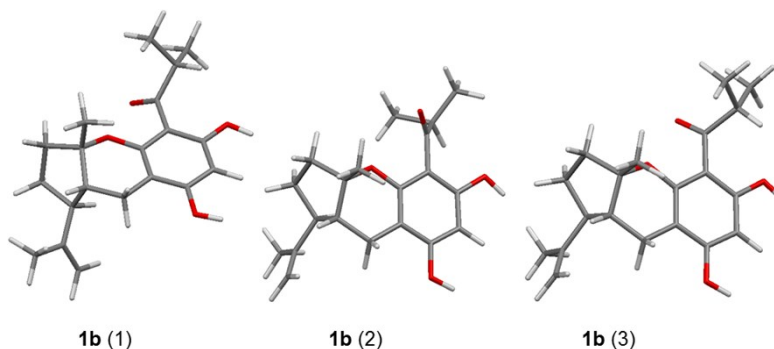
Conformational analyses were performed whereby both BALLOON and confab programs^{1,2} in order to confirm the stereochemistry structure of compounds **1b**, **2a/2b**, and **3b**. The BALLOON program explores conformational spaces with genetic algorithm, and synchronously, the confab program systematically generates diverse low energy conformations that are proposed to be close to crystal structures. The conformations generated by the above programs were assembled together 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 09 program.³ Duplicated conformations after geometry optimization were subsequently identified and disposed. Remaining conformations were further optimized at B3LYP/6-31G* level of theory in methanol solvent with IEFPCM3 solvation model using Gaussian 09 program,⁴ and 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 B3LYP/6-311++G** level of theory adopting methanol as solvent by the IEFPCM solvation model carried out in Gaussian 09 program. The ECD spectra data for each conformer were then simulated by using a Gaussian function with a bandwidth σ of 0.45 eV. Calculated spectra for each conformation were combined after Boltzmann weighting according to their population contribution.

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1b

Optimized geometries of predominant conformers for compound **1b** at the B3LYP/6-31G (d,p) level in methanol solution.



Important thermodynamic parameters (a.u.) and Boltzmann distributions of the optimized compound **1b** at B3LYP/6-31G(d,p) level in methanol solution.

Conformations	E+ZPE	G	%
1b (1)	-1078.253342	-1078.307663	75.62%
1b (2)	-1078.252215	-1078.305855	11.15%
1b (3)	-1078.252391	-1078.306017	13.23%

E+ZPE, G: total energy with zero point energy (ZPE) and Gibbs free energy in methanol solution at B3LYP/6-31G (d,p) level. %: Boltzmann distributions, using the relative Gibbs free energies as weighting factors.

Optimized Z-matrixes of compound **1b** in methanol solution (Å) at B3LYP/6-31G (d,p) level.

1b (1)				1b (2)			
C	-1.489183	2.856428	0.113342	C	-1.578917	2.833843	-0.354931
C	-1.775115	0.453837	-0.235691	C	-1.844508	0.456438	0.141581
C	0.374153	1.341035	0.593465	C	0.356313	1.540545	0.408164
C	-0.436027	0.268815	0.196848	C	-0.473094	0.415266	0.496404
C	-2.272325	1.767968	-0.272379	C	-2.37154	1.687218	-0.284564
C	-0.180955	2.62989	0.543522	C	-0.228777	2.746039	-0.011826
C	4.146206	0.920343	-2.13253	C	4.814028	0.456418	-0.806019
C	-2.617148	-0.706232	-0.669694	C	-2.714321	-0.759572	0.26191
C	4.058964	0.074203	-1.09753	C	3.82026	-0.287445	-1.307265
C	1.796192	1.131681	1.06228	C	1.828868	1.468037	0.741541
C	2.633817	-2.087147	-0.875478	C	2.516552	-2.207659	-0.199881
C	1.776276	-2.60081	0.311149	C	1.81427	-2.316067	1.179452

C	2.725196	-0.535692	-0.71027	C	2.572902	-0.679411	-0.537597
C	2.289647	-0.284905	0.759041	C	2.323491	0.019167	0.817777
C	1.207321	-1.350263	0.995672	C	1.309521	-0.905626	1.513469
C	5.28279	-0.292273	-0.288327	C	3.882323	-0.816443	-2.722287
C	0.792141	-1.552554	2.450105	C	1.094549	-0.642588	3.000945
C	-3.872313	-2.054235	0.992679	C	-4.927891	-1.631077	-0.608239
C	-5.068208	-1.191517	-1.080522	C	-2.711891	-2.39487	-1.601175
C	-3.995245	-0.898668	-0.023143	C	-3.495578	-1.221629	-0.973961
O	-2.196941	-1.535618	-1.467878	O	-2.751472	-1.417933	1.294259
O	0.01261	-1.015677	0.219074	O	0.014121	-0.808471	0.839987
O	-3.543582	1.945695	-0.743473	O	-3.707834	1.732003	-0.572458
O	0.632092	3.652949	0.934913	O	0.595891	3.831514	-0.067909
H	-1.887937	3.866948	0.062082	H	-2.012106	3.78526	-0.65467
H	5.094021	1.360763	-2.434223	H	5.693032	0.691762	-1.401726
H	3.27292	1.20007	-2.717659	H	4.800234	0.85789	0.202816
H	2.45682	1.865414	0.584609	H	2.407629	2.023017	-0.004952
H	1.866202	1.329068	2.141024	H	2.01943	1.974467	1.698511
H	3.625671	-2.549686	-0.860024	H	3.529208	-2.621515	-0.147198
H	2.186612	-2.337381	-1.842057	H	1.98313	-2.764495	-0.975672
H	0.967242	-3.270249	0.003526	H	0.984417	-3.029137	1.188531
H	2.395662	-3.145333	1.03236	H	2.523294	-2.629782	1.953002
H	1.963759	-0.08419	-1.356425	H	1.713923	-0.454113	-1.185992
H	3.12672	-0.524205	1.426066	H	3.244926	-0.016856	1.411935
H	5.213839	0.085298	0.740154	H	3.837434	-1.913448	-2.740573
H	5.413662	-1.379056	-0.212808	H	3.025541	-0.460563	-3.310734
H	6.189796	0.126004	-0.73494	H	4.800013	-0.505736	-3.230984
H	0.342191	-0.644107	2.864788	H	0.691515	0.361202	3.172685
H	1.661276	-1.814229	3.063076	H	2.040748	-0.729384	3.545564
H	0.058309	-2.362067	2.52689	H	0.386868	-1.368094	3.415684
H	-3.599201	-2.985155	0.483855	H	-4.920998	-2.415907	0.154874
H	-4.827765	-2.208207	1.506398	H	-5.455065	-2.010981	-1.490543
H	-3.109753	-1.844348	1.751839	H	-5.491759	-0.777477	-0.215936
H	-4.792434	-2.068459	-1.675212	H	-2.657032	-3.237369	-0.902929
H	-5.19214	-0.341221	-1.759971	H	-1.68858	-2.101854	-1.862931
H	-6.033999	-1.388647	-0.601722	H	-3.210913	-2.735533	-2.515128
H	-4.263243	0.011534	0.519221	H	-3.527104	-0.403135	-1.697657
H	-3.777516	2.886927	-0.692167	H	-3.943016	2.623684	-0.877417
H	0.158752	4.496294	0.845016	H	0.100229	4.597709	-0.400572
1b (3)							
C	-1.474666	2.864786	-0.055644				
C	-1.755525	0.445238	-0.267217				
C	0.372415	1.380947	0.564882				
C	-0.428443	0.286966	0.21207				

C	-2.249011	1.755337	-0.396407				
C	-0.178954	2.664415	0.422647				
C	4.987548	0.548235	-0.18498				
C	-2.587725	-0.738865	-0.650955				
C	4.102507	-0.035267	-1.002425				
C	1.780694	1.20065	1.083602				
C	2.66663	-2.137004	-0.630804				
C	1.77395	-2.570634	0.56117				
C	2.755045	-0.574558	-0.559847				
C	2.285989	-0.230174	0.871843				
C	1.194407	-1.277479	1.150324				
C	4.400283	-0.211025	-2.474211				
C	0.744947	-1.386058	2.604453				
C	-3.921218	-1.986452	1.029985				
C	-5.02943	-1.213568	-1.125442				
C	-3.990601	-0.881813	-0.045277				
O	-2.143887	-1.62374	-1.373623				
O	0.018465	-0.992939	0.325855				
O	-3.50619	1.905693	-0.912424				
O	0.624322	3.709537	0.773717				
H	-1.869726	3.870577	-0.178362				
H	5.945666	0.903021	-0.557731				
H	4.803028	0.697642	0.874614				
H	2.452778	1.911967	0.590787				
H	1.818379	1.452699	2.152851				
H	3.664872	-2.578986	-0.543235				
H	2.253849	-2.464843	-1.589098				
H	0.96873	-3.253415	0.273629				
H	2.369754	-3.07284	1.330973				
H	2.006692	-0.171664	-1.257369				
H	3.105041	-0.431897	1.573072				
H	4.373749	-1.270096	-2.762535				
H	3.645057	0.297264	-3.089233				
H	5.383769	0.189053	-2.739207				
H	0.287784	-0.452904	2.950504				
H	1.59903	-1.609542	3.252703				
H	0.007363	-2.188179	2.715334				
H	-3.641829	-2.944361	0.578092				
H	-4.897003	-2.103775	1.514409				
H	-3.184499	-1.747784	1.806017				
H	-4.747386	-2.124537	-1.663432				
H	-5.114714	-0.398071	-1.851792				
H	-6.014829	-1.371414	-0.672712				

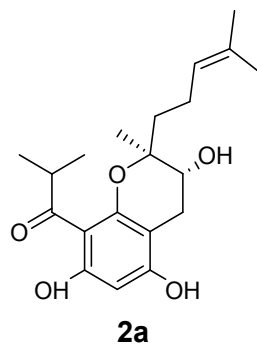
H	-4.265647	0.057566	0.440636				
H	-3.738806	2.848537	-0.924181				
H	0.154171	4.5455	0.620466				

Key transitions, oscillator strengths, and rotatory strengths in the ECD of conformers **1a (1)** at B3LYP /6-311++G(d,p) level.

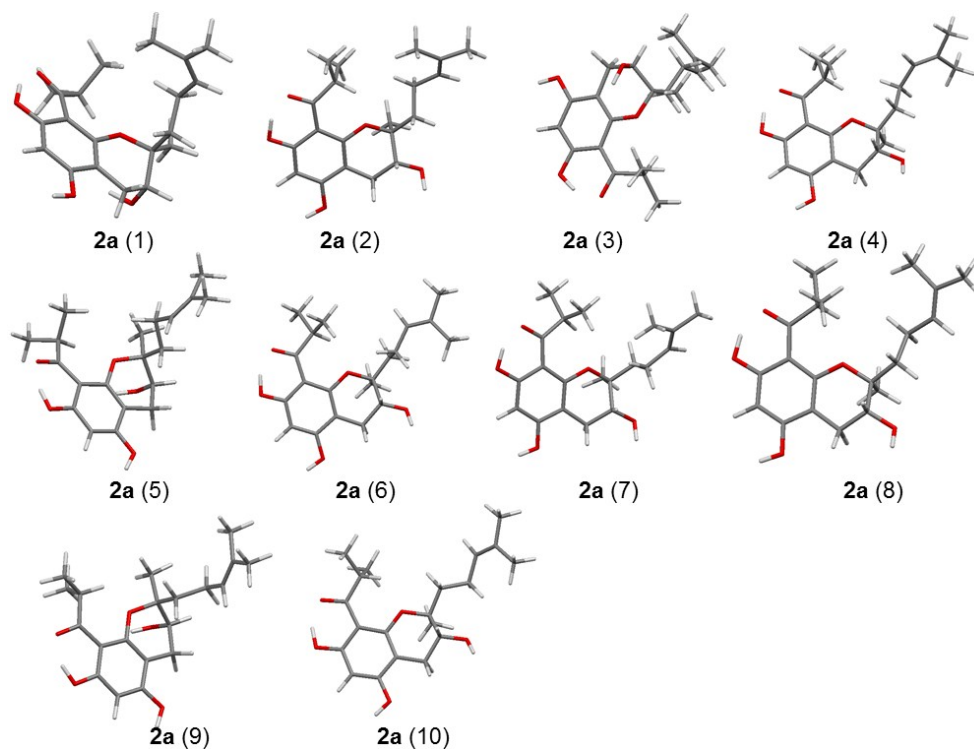
Species	Excited State	$\Delta E(eV)^a$	$\lambda(nm)^b$	f^c	R_{vel}^d
1b (1)	88 -> 90	4.0199	308.43	0.017	-59.9879
	86 -> 90	4.0793	303.93	0.0317	19.7563
	89 -> 90	4.3257	286.62	0.1875	55.8722
	86 -> 90	5.0648	244.79	0.0005	-1.0552
	89 -> 94	5.152	240.65	0.0046	4.9622
	89 -> 92	5.2619	235.63	0.0336	-6.8968
	88 -> 94	5.2929	234.24	0.0044	-2.5732
	89 -> 97	5.4901	225.83	0.0039	2.329
	89 -> 93	5.5531	223.27	0.0326	-13.8888
	89 -> 94	5.5813	222.14	0.0527	-6.6385
	88 -> 92	5.6373	219.93	0.0116	0.0207
	89 -> 96	5.6975	217.61	0.0223	-2.2737
	88 -> 93	5.724	216.6	0.0078	7.6239
	88 -> 97	5.7909	214.1	0.0013	3.5698
	88 -> 93	5.8259	212.81	0.0066	4.6942
	89 -> 98	5.8607	211.55	0.031	11.1585
	85 -> 90	5.9204	209.42	0.0045	21.5932
	88 -> 97	5.9321	209.01	0.0014	6.0943
	88 -> 97	5.9329	208.98	0.0293	-31.7962
	88 -> 97	5.9731	207.57	0.0017	3.7673
	88 -> 98	6.0005	206.62	0.0629	-25.1477
	86 -> 93	6.0342	205.47	0.0053	-1.7579
	89 -> 99	6.0538	204.8	0.0154	6.932
	88 -> 92	6.0926	203.5	0.0595	-12.2155
	89 -> 99	6.161	201.24	0.1501	87.088
	86 -> 92	6.1811	200.59	0.0271	9.9999
	87 -> 92	6.1844	200.48	0.0571	-19.4122
	84 -> 9	6.2138	199.53	0.0577	-115.5774
	88 ->100	6.2225	199.25	0.1151	-25.2682
	87 -> 91	6.2384	198.74	0.0899	4.1021
	89 ->101	6.2698	197.75	0.0387	9.2185
	89 -> 99	6.306	196.61	0.0558	-16.1767
	88 -> 99	6.323	196.09	0.0747	-12.4851
	89 ->101	6.3314	195.82	0.1566	45.7312
	87 -> 97	6.3943	193.9	0.0126	8.0745
	86 -> 98	6.4053	193.57	0.0202	-5.7307

	86 -> 94	6.4164	193.23	0.0032	0.2214
	86 -> 97	6.4219	193.07	0.0028	-1.9326
	88 ->101	6.4359	192.64	0.0363	-11.3067
	86 -> 93	6.5418	189.53	0.0005	1.455

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



Optimized geometries of predominant conformers for compound **2a** at the B3LYP/6-31G (d,p) level in methanol solution.



Important thermodynamic parameters (a.u.) and Boltzmann distributions of the optimized compound **2a** at B3LYP/6-31G(d,p) level in methanol solution.

Conformations	E+ZPE	G	%
2a (1)	-1154.665845	-1154.723759	18.10%
2a (2)	-1154.664538	-1154.723920	1.20%
2a (3)	-1154.666434	-1154.721195	21.47%
2a (4)	-1154.665194	-1154.721751	2.16%
2a (5)	-1154.665818	-1154.723254	10.61%

2a (6)	-1154.666594	-1154.723604	15.36%
2a (7)	-1154.666080	-1154.722340	4.03%
2a (8)	-1154.664929	-1154.721973	2.73%
2a (9)	-1154.666307	-1154.723578	14.95%
2a (10)	-1154.665295	-1154.723139	9.39%

E+ZPE, G: total energy with zero point energy (ZPE) and Gibbs free energy in methanol solution at B3LYP/6-31G (d,p) level. %: Boltzmann distributions, using the relative Gibbs free energies as weighting factors.

Optimized Z-matrixes of compound **2a** in methanol solution (Å) at B3LYP/6-31G (d,p) level.

2a (1)				2a (2)			
C	-2.093885	1.096032	-2.510522	C	4.257628	0.165307	-0.34937
C	-1.65391	-0.493694	-0.674791	C	2.000141	1.154788	-0.118603
C	-0.840294	1.846515	-0.544124	C	2.3121	-1.307269	-0.190852
C	-0.922854	0.554789	-0.022652	C	1.48255	-0.189501	-0.079197
C	-2.187088	-0.187822	-1.970364	C	3.42553	1.281755	-0.267139
C	-1.445558	2.094038	-1.793402	C	3.700415	-1.104729	-0.313101
C	3.961034	-0.402223	0.056486	C	-4.287022	-0.745182	0.233821
C	-1.958698	-1.809993	-0.101174	C	1.214698	2.395091	-0.02744
C	4.212539	-1.075631	-1.077963	C	-5.07221	0.129163	-0.415849
C	-0.126038	2.960556	0.18874	C	1.759451	-2.710722	-0.212404
C	0.175043	2.566455	1.637327	C	0.259137	-2.705936	-0.482257
C	0.731254	1.125291	1.69683	C	-0.454985	-1.640585	0.375709
C	5.549073	-0.944902	-1.771405	C	-6.491487	-0.237115	-0.785202
C	3.242161	-2.003924	-1.76821	C	-4.65935	1.518756	-0.836853
C	0.906814	0.657017	3.139024	C	-0.28174	-1.888634	1.876183
C	-0.64421	-3.079743	1.615989	C	-0.901283	3.744017	-0.32612
C	-3.153028	-2.790155	1.873693	C	-0.529443	2.324982	1.744269
C	2.703209	-0.392891	0.886531	C	-2.856935	-0.582904	0.685052
C	2.027583	0.994235	0.868789	C	-1.929397	-1.562275	-0.061583
C	-1.844848	-2.140544	1.387805	C	-0.289823	2.447423	0.222177
O	-2.409136	-2.719652	-0.836337	O	1.793724	3.505155	-0.110985
O	-0.297655	0.232314	1.145095	O	0.13382	-0.337999	0.042463
O	-2.818778	-1.110884	-2.711996	O	4.033249	2.475759	-0.325947
O	-1.335376	3.362119	-2.265812	O	4.462602	-2.22556	-0.401033
O	-0.98019	2.715567	2.465002	O	-0.332655	-3.969461	-0.189381
H	-2.526179	1.288894	-3.487556	H	5.328182	0.315032	-0.448213
H	4.755335	0.24134	0.441037	H	-4.717642	-1.721545	0.467361
H	0.800555	3.236922	-0.331097	H	2.268992	-3.29787	-0.985661
H	-0.746459	3.862927	0.199982	H	1.949819	-3.229119	0.737079
H	0.917035	3.247575	2.063776	H	0.082738	-2.43913	-1.535577
H	6.04745	-1.921011	-1.855473	H	-7.210301	0.462149	-0.33502
H	5.426582	-0.572006	-2.798119	H	-6.644178	-0.178773	-1.87219
H	6.221465	-0.264095	-1.239578	H	-6.751067	-1.249136	-0.458438

H	3.049257	-1.663253	-2.794963	H	-4.77499	1.642169	-1.922574
H	3.667643	-3.013484	-1.85386	H	-5.307307	2.27399	-0.37043
H	2.280142	-2.087312	-1.257447	H	-3.625086	1.759407	-0.581266
H	1.130411	-0.411753	3.177922	H	-0.776095	-1.107228	2.458116
H	-0.002518	0.849378	3.711388	H	0.774783	-1.896508	2.158124
H	1.734017	1.201112	3.607423	H	-0.716395	-2.855203	2.145966
H	-0.765682	-4.005354	1.042344	H	-0.486293	4.62493	0.17139
H	-0.569745	-3.341067	2.677447	H	-1.984821	3.735277	-0.163141
H	0.297006	-2.608358	1.316302	H	-0.720859	3.848341	-1.401603
H	-3.355534	-3.721045	1.336376	H	-0.048388	3.155357	2.274338
H	-4.009223	-2.120795	1.730757	H	-0.135639	1.385587	2.142144
H	-3.076502	-3.015776	2.94311	H	-1.602904	2.362332	1.959283
H	1.989657	-1.14528	0.53869	H	-2.507404	0.443014	0.546904
H	2.962862	-0.659358	1.919642	H	-2.811598	-0.786293	1.763578
H	1.819011	1.255524	-0.173357	H	-1.945788	-1.318882	-1.131642
H	2.73413	1.747951	1.242204	H	-2.331932	-2.576953	0.031103
H	-1.677725	-1.223864	1.950867	H	-0.756874	1.594636	-0.268852
H	-2.757235	-1.964706	-2.189495	H	3.293503	3.154961	-0.258982
H	-1.788579	3.430043	-3.122865	H	5.396028	-1.974849	-0.503997
H	-1.657899	2.100713	2.137291	H	0.087734	-4.627419	-0.76617
2a (3)				2a (4)			
C	-2.064135	2.813502	-0.895382	C	4.35329	-0.401055	-0.016062
C	-2.250542	0.375195	-0.527324	C	2.288008	0.962151	0.003715
C	-0.385638	1.677933	0.474758	C	2.178271	-1.517197	-0.079595
C	-1.054848	0.471397	0.262896	C	1.548031	-0.272173	-0.037258
C	-2.73887	1.606533	-1.084883	C	3.72123	0.842459	-0.001073
C	-0.906089	2.839508	-0.129477	C	3.585559	-1.556901	-0.052672
C	4.020641	-1.236553	-0.767192	C	-4.090438	0.435688	-0.409974
C	-2.987439	-0.860248	-0.835731	C	1.717823	2.316057	0.070942
C	4.947689	-0.466378	-1.359329	C	-5.380766	0.258652	-0.082529
C	0.850512	1.763981	1.342089	C	1.394642	-2.802804	-0.181822
C	1.01069	0.516595	2.214431	C	-0.050532	-2.540961	-0.595482
C	0.76302	-0.753581	1.375283	C	-0.646296	-1.359019	0.19635
C	5.651227	-0.935573	-2.612063	C	-6.481314	0.710875	-1.014583
C	5.386826	0.893783	-0.872898	C	-5.871778	-0.379172	1.19489
C	0.760162	-2.01406	2.236662	C	-0.660728	-1.610621	1.706193
C	-3.023316	-3.324194	-1.386368	C	-0.320934	2.64179	-1.332653
C	-3.158162	-2.524168	1.01809	C	-0.055574	3.949743	0.825538
C	3.212806	-0.952725	0.4735	C	-2.858151	0.054329	0.36987
C	1.701811	-0.890867	0.157597	C	-2.034548	-1.016048	-0.373912
C	-2.56384	-2.256674	-0.38289	C	0.222766	2.618884	0.11363
O	-4.04731	-0.796797	-1.503375	O	2.480385	3.312482	0.07437
O	-0.615485	-0.670211	0.865256	O	0.189892	-0.184994	-0.079688

O	-3.855742	1.658946	-1.825333	O	4.526125	1.915145	0.020768
O	-0.216111	3.987709	0.09208	O	4.148803	-2.792601	-0.077467
O	0.143593	0.560337	3.349419	O	-0.876741	-3.680293	-0.367912
H	-2.465024	3.714386	-1.349498	H	5.438287	-0.438218	-0.005482
H	3.798408	-2.198924	-1.232962	H	-3.881003	0.906923	-1.372879
H	1.745951	1.909135	0.722478	H	1.869767	-3.470131	-0.910735
H	0.792339	2.638332	1.998316	H	1.397228	-3.345598	0.773087
H	2.019299	0.481943	2.634365	H	-0.077419	-2.258981	-1.659308
H	5.491245	-0.232093	-3.441258	H	-7.123784	-0.132277	-1.305565
H	6.738231	-0.988422	-2.457784	H	-7.137767	1.443621	-0.524251
H	5.304428	-1.923506	-2.931565	H	-6.08379	1.167019	-1.926911
H	6.462495	0.894472	-0.648166	H	-6.5023	0.321783	1.759565
H	5.235499	1.648791	-1.656636	H	-6.503914	-1.249863	0.971701
H	4.857681	1.229141	0.022029	H	-5.066234	-0.711162	1.853978
H	0.523107	-2.891496	1.627031	H	-1.05285	-0.739435	2.236763
H	0.025212	-1.926258	3.038757	H	0.344373	-1.8106	2.087601
H	1.743368	-2.164716	2.692163	H	-1.292283	-2.474079	1.933678
H	-4.113513	-3.357586	-1.466156	H	0.174954	3.426943	-1.915554
H	-2.670718	-4.308402	-1.058324	H	-1.395739	2.854658	-1.322567
H	-2.617808	-3.134949	-2.386507	H	-0.169086	1.683541	-1.836613
H	-4.253147	-2.481428	0.98406	H	0.398971	4.79103	0.295139
H	-2.803092	-1.796528	1.753023	H	0.335195	3.946291	1.849035
H	-2.867145	-3.523433	1.360621	H	-1.137355	4.116907	0.875669
H	3.397246	-1.753404	1.203393	H	-2.240374	0.950747	0.513418
H	3.537995	-0.021734	0.947569	H	-3.122035	-0.305308	1.368453
H	1.408639	-1.806807	-0.371169	H	-1.889059	-0.703798	-1.416279
H	1.520695	-0.064848	-0.538603	H	-2.608106	-1.94797	-0.405125
H	-1.477998	-2.287947	-0.300782	H	-0.278156	1.815077	0.651714
H	-4.199857	0.714468	-1.85613	H	3.910423	2.710866	0.034447
H	-0.670417	4.729189	-0.342093	H	5.11689	-2.707238	-0.078053
H	-0.769705	0.522313	3.018843	H	-0.523913	-4.406738	-0.906579
2a (5)				2a (6)			
C	2.771371	-1.74893	-1.747691	C	4.027156	-1.058338	-0.776186
C	2.005914	0.331636	-0.662659	C	2.373991	0.695153	-0.222587
C	1.108554	-1.869958	0.047027	C	1.767871	-1.711275	-0.102621
C	1.119821	-0.476582	0.125866	C	1.432698	-0.361977	0.028141
C	2.791039	-0.356833	-1.645505	C	3.681031	0.288366	-0.661657
C	1.954223	-2.485122	-0.898837	C	3.082225	-2.03554	-0.490847
C	-3.549769	0.264346	-1.177913	C	-3.971826	0.770963	-0.416383
C	2.224858	1.77368	-0.497598	C	2.13455	2.132349	-0.025373
C	-4.880703	0.424055	-1.260609	C	-5.253135	0.471002	-0.684404
C	0.22522	-2.714158	0.938641	C	0.755971	-2.808663	0.132317
C	-0.340261	-1.885533	2.094553	C	-0.665007	-2.250048	0.131492

C	-0.862241	-0.527042	1.571987	C	-0.742694	-0.965976	0.975247
C	-5.622731	0.062768	-2.526818	C	-6.331838	1.523495	-0.569357
C	-5.760092	0.960466	-0.156764	C	-5.75318	-0.886904	-1.115623
C	-1.305942	0.375082	2.720996	C	-0.317661	-1.182884	2.432109
C	0.604156	3.470674	0.382169	C	-0.115121	3.05232	-0.583551
C	2.989026	3.405335	1.246741	C	1.170042	3.97854	1.399183
C	-2.63564	0.558274	-0.016473	C	-2.762624	-0.126705	-0.466844
C	-1.967781	-0.72742	0.513393	C	-2.130636	-0.304628	0.928505
C	1.801447	2.567907	0.738883	C	0.857856	2.723918	0.569978
O	2.854784	2.411308	-1.373961	O	3.017746	2.959189	-0.358037
O	0.273653	0.182546	0.966408	O	0.164516	0.004414	0.35861
O	3.596451	0.299567	-2.494763	O	4.638723	1.177611	-0.963547
O	1.904425	-3.841099	-0.946795	O	3.367108	-3.35995	-0.58828
O	0.627834	-1.712606	3.130648	O	-1.612031	-3.172381	0.663126
H	3.394478	-2.230905	-2.494682	H	5.032844	-1.315645	-1.093622
H	-3.041291	-0.14191	-2.055079	H	-3.754147	1.795778	-0.107198
H	-0.590818	-3.169383	0.362688	H	0.850809	-3.575654	-0.645618
H	0.80001	-3.546141	1.358691	H	0.940258	-3.318391	1.087806
H	-1.168552	-2.419566	2.569122	H	-0.93477	-1.980733	-0.898927
H	-6.387831	-0.701814	-2.33125	H	-6.852251	1.662513	-1.52758
H	-6.154778	0.93379	-2.934881	H	-7.099849	1.223957	0.15775
H	-4.949753	-0.31853	-3.301465	H	-5.927502	2.492107	-0.258221
H	-6.277082	1.873527	-0.483436	H	-6.520342	-1.252848	-0.419219
H	-6.546021	0.234892	0.094496	H	-6.235982	-0.826715	-2.101051
H	-5.214081	1.193926	0.760108	H	-4.965838	-1.641922	-1.173325
H	-1.506678	1.389212	2.366818	H	-0.465973	-0.263046	3.006649
H	-0.532133	0.415973	3.489917	H	0.735842	-1.46623	2.508648
H	-2.222238	-0.022264	3.170835	H	-0.921115	-1.976832	2.880811
H	0.873113	4.163177	-0.423211	H	0.32709	3.794421	-1.258508
H	0.305053	4.059659	1.256269	H	-1.045108	3.468631	-0.18061
H	-0.259832	2.8825	0.057624	H	-0.364971	2.160344	-1.165175
H	3.325353	4.114467	0.485186	H	1.620373	4.762569	0.784293
H	3.839044	2.769605	1.520286	H	1.860377	3.754321	2.220249
H	2.68813	3.96809	2.137398	H	0.243195	4.369125	1.833969
H	-1.847349	1.247771	-0.349603	H	-3.01657	-1.106242	-0.881927
H	-3.172884	1.063779	0.790402	H	-2.015672	0.318748	-1.138943
H	-1.550123	-1.275128	-0.338528	H	-2.803912	-0.901203	1.553123
H	-2.736744	-1.377368	0.951196	H	-2.037833	0.674578	1.415521
H	1.494619	1.880082	1.524962	H	0.3859	1.981185	1.211175
H	3.454831	1.273682	-2.301394	H	4.217697	2.080291	-0.824028
H	2.522299	-4.165545	-1.623326	H	4.287409	-3.473871	-0.879526
H	1.381277	-1.229185	2.752212	H	-1.586476	-3.969296	0.109277
2a (7)				2a (8)			

C	4.015677	-0.229195	-0.95459	C	4.285672	0.25253	-0.114948
C	2.024166	1.015393	-0.189965	C	1.998849	1.188404	0.025122
C	2.036137	-1.466711	-0.218429	C	2.365477	-1.261047	-0.143006
C	1.384779	-0.253841	0.014547	C	1.509728	-0.16463	-0.023085
C	3.352656	0.978432	-0.734334	C	3.427406	1.348063	-0.017473
C	3.364516	-1.42706	-0.685542	C	3.753658	-1.027657	-0.179786
C	-4.207405	-0.669961	-0.271512	C	-4.259079	-0.885475	0.209614
C	1.46738	2.326892	0.167694	C	1.179248	2.407062	0.113008
C	-4.880828	0.318464	-0.8821	C	-5.12288	0.088531	-0.118635
C	1.338663	-2.792076	-0.018973	C	1.842627	-2.672476	-0.250693
C	-0.175726	-2.60311	0.029391	C	0.344246	-2.695096	-0.538163
C	-0.549064	-1.428656	0.950965	C	-0.402141	-1.665287	0.335177
C	-6.349584	0.538715	-0.600972	C	-6.500674	-0.248265	-0.641225
C	-4.289545	1.280127	-1.884519	C	-4.847397	1.568094	-0.003175
C	-0.050348	-1.619388	2.38809	C	-0.232194	-1.932707	1.832591
C	-0.982899	2.802576	0.074102	C	-0.766157	2.293857	-1.445015
C	0.40885	3.684642	2.005208	C	-0.922502	3.698368	0.663863
C	-2.757172	-1.055915	-0.413484	C	-2.852586	-0.772741	0.742544
C	-2.058144	-1.128933	0.958064	C	-1.875247	-1.606071	-0.109574
C	0.210113	2.527418	1.013164	C	-0.344703	2.422873	0.0369
O	2.054861	3.372002	-0.200622	O	1.738576	3.526062	0.205587
O	0.077596	-0.22798	0.392358	O	0.160361	-0.346519	0.022366
O	4.03065	2.098168	-1.029149	O	4.012057	2.554195	0.035949
O	3.963991	-2.629606	-0.884281	O	4.541353	-2.129223	-0.285249
O	-0.853815	-3.759565	0.512218	O	-0.218729	-3.97897	-0.277702
H	5.029586	-0.20831	-1.341851	H	5.357066	0.426204	-0.139243
H	-4.768154	-1.296092	0.426402	H	-4.601139	-1.915242	0.082263
H	1.598409	-3.477101	-0.834571	H	2.377147	-3.20653	-1.045563
H	1.671317	-3.278775	0.907976	H	2.033305	-3.235198	0.673173
H	-0.526951	-2.351637	-0.980751	H	0.170151	-2.409964	-1.587025
H	-6.529614	1.550983	-0.212109	H	-7.283112	0.173151	0.005655
H	-6.945614	0.451595	-1.520489	H	-6.660594	0.183598	-1.639402
H	-6.739878	-0.179994	0.126772	H	-6.660342	-1.329209	-0.708444
H	-4.807203	1.195985	-2.850362	H	-4.954086	2.060423	-0.979907
H	-4.426007	2.318359	-1.55156	H	-5.579645	2.045036	0.663183
H	-3.223699	1.120965	-2.062301	H	-3.850766	1.794594	0.382197
H	-0.416665	-0.806657	3.023303	H	-0.720949	-1.151705	2.42013
H	1.042205	-1.625515	2.439171	H	0.823106	-1.953611	2.117519
H	-0.419144	-2.568181	2.787715	H	-0.676603	-2.897917	2.091641
H	-0.80654	3.711237	-0.512935	H	-0.376743	3.136142	-2.029112
H	-1.896734	2.945845	0.661388	H	-1.858793	2.304511	-1.523376
H	-1.149291	1.970287	-0.615838	H	-0.403075	1.36363	-1.890057
H	0.600055	4.627055	1.484692	H	-0.595409	4.593355	0.127017

H	1.250837	3.492626	2.679989	H	-0.617368	3.804517	1.710499
H	-0.493366	3.802422	2.61567	H	-2.017074	3.658612	0.631205
H	-2.702752	-2.046165	-0.887875	H	-2.524044	0.269564	0.789318
H	-2.218686	-0.363169	-1.067227	H	-2.839894	-1.150426	1.774818
H	-2.541688	-1.901807	1.566081	H	-1.892303	-1.23896	-1.143436
H	-2.197948	-0.179453	1.489299	H	-2.230732	-2.6419	-0.141232
H	0.003744	1.614482	1.569678	H	-0.726596	1.554288	0.572318
H	3.402865	2.85389	-0.819894	H	3.256861	3.212953	0.12391
H	4.860584	-2.492417	-1.233505	H	5.473924	-1.858393	-0.323831
H	-0.649266	-4.491504	-0.0919	H	0.220654	-4.613846	-0.866075
2a (9)				2a (10)			
C	2.88147	-2.116748	-1.338818	C	4.14518	-1.357368	-0.337597
C	2.317204	0.149053	-0.523819	C	2.611227	0.572466	-0.131972
C	0.939736	-1.818567	0.118622	C	1.740828	-1.75305	-0.132301
C	1.207231	-0.449165	0.164016	C	1.534394	-0.376687	-0.040188
C	3.15553	-0.749951	-1.268537	C	3.931266	0.019794	-0.265844
C	1.788869	-2.633931	-0.655335	C	3.060251	-2.222456	-0.277551
C	-4.082793	-0.377086	-0.93871	C	-4.510862	0.666712	0.373275
C	2.647286	1.582804	-0.553247	C	2.475943	2.036132	-0.133044
C	-5.123217	0.41432	-1.24595	C	-5.611537	0.490576	-0.375733
C	-0.208027	-2.434474	0.88837	C	0.587942	-2.724425	-0.089576
C	-0.745237	-1.474645	1.951917	C	-0.748085	-2.017355	-0.310648
C	-0.906193	-0.061015	1.355749	C	-0.837469	-0.735667	0.540842
C	-5.780634	0.328117	-2.604149	C	-6.582726	1.626999	-0.599552
C	-5.738756	1.436789	-0.321289	C	-6.001129	-0.802404	-1.051119
C	-1.307402	0.961207	2.416316	C	-0.717908	-1.005664	2.042809
C	1.961454	4.013622	-0.589855	C	1.24146	4.107197	-0.880789
C	2.318139	2.793835	1.606617	C	0.73132	3.022826	1.355214
C	-3.293057	-0.43622	0.34411	C	-3.433591	-0.331812	0.711327
C	-1.828625	0.002568	0.119997	C	-2.058759	0.138879	0.19178
C	1.833212	2.671473	0.144291	C	1.141212	2.780167	-0.114084
O	3.669345	1.968732	-1.169143	O	3.504931	2.753966	-0.147706
O	0.434662	0.373667	0.930171	O	0.283438	0.123522	0.133152
O	4.233089	-0.323598	-1.943397	O	5.023276	0.796114	-0.333149
O	1.482694	-3.956298	-0.684726	O	3.209936	-3.570403	-0.349874
O	0.098107	-1.449961	3.105419	O	-1.840249	-2.866923	0.032536
H	3.53625	-2.752814	-1.926645	H	5.161361	-1.725587	-0.43942
H	-3.735602	-1.068288	-1.709479	H	-4.352522	1.660389	0.799065
H	-1.016238	-2.729152	0.204997	H	0.723392	-3.496331	-0.856947
H	0.119451	-3.353513	1.384887	H	0.549669	-3.254842	0.871711
H	-1.711785	-1.827974	2.320195	H	-0.825082	-1.706552	-1.363687
H	-6.846799	0.077585	-2.511417	H	-6.693477	1.846671	-1.670918
H	-5.734997	1.294336	-3.126063	H	-7.58618	1.367714	-0.233003

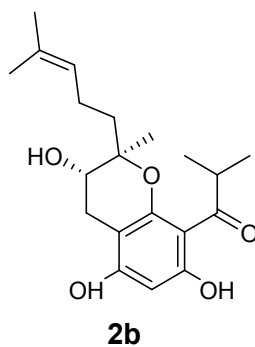
H	-5.307479	-0.426056	-3.24108	H	-6.263209	2.544574	-0.095026
H	-5.71143	2.434592	-0.780499	H	-6.974985	-1.1539	-0.68215
H	-6.798927	1.208515	-0.143874	H	-6.118929	-0.65112	-2.133135
H	-5.242665	1.501715	0.649796	H	-5.276088	-1.605455	-0.901
H	-1.347897	1.965221	1.982678	H	-0.871954	-0.080974	2.60798
H	-0.594298	0.956776	3.242706	H	0.270503	-1.399413	2.296548
H	-2.295337	0.718642	2.819184	H	-1.466401	-1.737385	2.357743
H	2.994059	4.373782	-0.591428	H	1.976087	4.777706	-0.426467
H	1.335626	4.762475	-0.091667	H	0.266275	4.6067	-0.874418
H	1.630776	3.934038	-1.631349	H	1.532085	3.945459	-1.924895
H	3.377083	3.075976	1.637262	H	1.479306	3.641495	1.864796
H	2.190838	1.856209	2.154505	H	0.62527	2.083185	1.904441
H	1.744128	3.570549	2.124003	H	-0.228664	3.55	1.391887
H	-3.753991	0.181839	1.119831	H	-3.384036	-0.43667	1.804744
H	-3.311769	-1.469794	0.718421	H	-3.655376	-1.323093	0.31422
H	-1.820887	1.039741	-0.236364	H	-1.853023	1.138618	0.595302
H	-1.395241	-0.600713	-0.685837	H	-2.101189	0.24641	-0.899527
H	0.785753	2.372356	0.160519	H	0.379669	2.156874	-0.580867
H	4.27117	0.668923	-1.785727	H	4.685083	1.739847	-0.253096
H	2.138039	-4.429536	-1.224332	H	4.150842	-3.786932	-0.461012
H	0.941843	-1.04768	2.838417	H	-1.792818	-3.64676	-0.544038

Key transitions, oscillator strengths, and rotatory strengths in the ECD of conformers **2a** (3) at B3LYP /6-311++G(d,p) level.

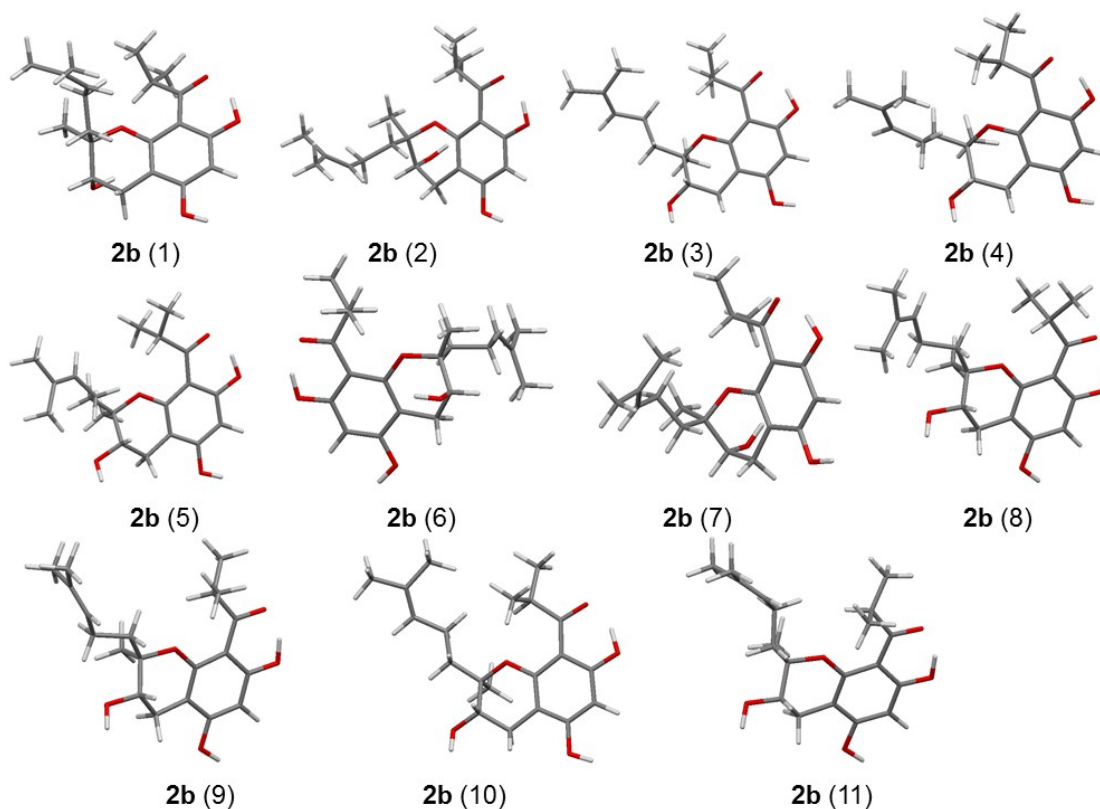
Species	Excited State	$\Delta E(eV)^a$	$\lambda(nm)^b$	f^c	R_{vel}^d
2a (3)	92 -> 97	3.7469	330.9	0.0712	11.6899
	91 ->106	4.1588	298.12	0.0014	3.0508
	94 -> 97	4.316	287.27	0.0513	16.2671
	93 -> 95	4.4985	275.61	0.3459	8.166
	94 -> 99	5.2052	238.19	0.0058	0.0829
	93 -> 97	5.2535	236	0.0032	4.7223
	93 -> 97	5.4987	225.48	0.1074	-9.7329
	93 ->100	5.5233	224.47	0.0101	5.7499
	94 -> 99	5.5875	221.9	0.0272	-13.6235
	92 -> 97	5.6153	220.8	0.0354	-19.1975
	93 -> 96	5.6392	219.86	0.0003	1.0407
	89 -> 95	5.7168	216.88	0.0095	1.6304
	94 -> 99	5.7663	215.01	0.0193	1.2329
	93 -> 97	5.8327	212.57	0.1117	-110.0444
	93 -> 96	5.9076	209.87	0.0131	-14.4686
	93 -> 99	5.9297	209.09	0.0473	-1.0213
	93 -> 98	5.9471	208.48	0.0451	39.8988
	94 -> 99	5.9861	207.12	0.0117	8.8114

	94 ->101	6.0176	206.04	0.0114	10.1219
	93 ->100	6.034	205.48	0.0002	0.0822
	92 -> 97	6.0734	204.14	0.0077	3.5274
	92 -> 98	6.0761	204.05	0.0059	8.5484
	93 ->100	6.1107	202.9	0.0032	-0.4824
	93 ->101	6.1488	201.64	0.0035	-6.4037
	94 ->103	6.2123	199.58	0.0137	9.378
	94 ->105	6.2245	199.19	0.0359	40.7268
	94 ->102	6.2422	198.62	0.0098	10.5549
	91 -> 99	6.2706	197.72	0.0007	-2.1583
	93 -> 96	6.3124	196.41	0.2346	204.466
	92 -> 98	6.3457	195.38	0.0583	17.0626
	93 ->101	6.3749	194.49	0.1572	-139.9957
	92 ->100	6.4185	193.17	0.0082	-0.957
	93 ->103	6.4277	192.89	0.0554	-13.8562
	93 ->103	6.4408	192.5	0.0133	21.335
	94 ->110	6.4684	191.68	0.0971	70.286
	93 ->103	6.4772	191.42	0.0278	-57.4108
	84 -> 95	6.5113	190.42	0.0234	-16.8602
	93 ->105	6.5568	189.09	0.0147	-14.5178
	93 ->104	6.6013	187.82	0.012	-15.2854
	94 ->111	6.6096	187.58	0.0023	-3.2513

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



Optimized geometries of predominant conformers for compound **2b** at the B3LYP/6-31G (d,p) level in methanol solution.



Important thermodynamic parameters (a.u.) and Boltzmann distributions of the optimized compound **2b** at B3LYP/6-31G(d,p) level in methanol solution.

Conformations	E+ZPE	G	%
2b (1)	-1154.665820	-1154.723263	9.26%
2b (2)	-1154.666309	-1154.723587	13.05%
2b (3)	-1154.664541	-1154.721202	1.04%
2b (4)	-1154.666078	-1154.722336	3.47%
2b (5)	-1154.666733	-1154.724088	22.19%
2b (6)	-1154.666434	-1154.723920	18.57%
2b (7)	-1154.666457	-1154.723650	13.95%
2b (8)	-1154.665296	-1154.723141	8.14%
2b (9)	-1154.665294	-1154.722958	6.71%
2b (10)	-1154.664872	-1154.721693	1.76%
2b (11)	-1154.665193	-1154.721746	1.86%

E+ZPE, G: total energy with zero point energy (ZPE) and Gibbs free energy in methanol solution at B3LYP/6-31G (d,p) level. %: Boltzmann distributions, using the relative Gibbs free energies as weighting factors.

Optimized Z-matrixes of compound **2b** in methanol solution (Å) at B3LYP/6-31G (d,p) level.

2b (1)				2b (2)			
C	-2.773941	-1.747107	-1.747337	C	-2.881704	-2.116066	-1.33936
C	-2.006461	0.332773	-0.662341	C	-2.317028	0.149453	-0.523838
C	-1.110105	-1.869586	0.046351	C	-0.94006	-1.818641	0.118343
C	-1.120311	-0.476214	0.125482	C	-1.207245	-0.449176	0.163993

C	-2.792653	-0.355012	-1.644804	C	-3.155443	-0.749224	-1.268869
C	-1.956773	-2.483989	-0.899131	C	-1.789308	-2.633651	-0.655842
C	3.551354	0.261698	-1.176998	C	4.082786	-0.37728	-0.938873
C	-2.224353	1.774903	-0.496894	C	-2.6469	1.583277	-0.55288
C	4.882106	0.422692	-1.260224	C	5.122936	0.414538	-1.245981
C	-0.226847	-2.714562	0.937294	C	0.207554	-2.434957	0.887963
C	0.338924	-1.886603	2.093514	C	0.745131	-1.47547	1.95165
C	0.861967	-0.528374	1.571459	C	0.906344	-0.061766	1.355806
C	5.624107	0.060969	-2.526324	C	5.780156	0.329058	-2.604321
C	5.761319	0.96106	-0.15719	C	5.738288	1.436901	-0.321085
C	1.305835	0.373211	2.720799	C	1.307686	0.960218	2.416525
C	-2.985052	3.407656	1.248021	C	-2.318015	2.793649	1.607232
C	-0.60093	3.470107	0.381249	C	-1.960546	4.013981	-0.588775
C	2.637107	0.555961	-0.015738	C	3.293125	-0.436933	0.343965
C	1.967746	-0.729313	0.513203	C	1.828683	0.001932	0.119987
C	-1.798947	2.568797	0.739161	C	-1.832728	2.67161	0.144973
O	-2.854836	2.413013	-1.372522	O	-3.668886	1.969487	-1.168699
O	-0.273108	0.182257	0.96536	O	-0.434567	0.37326	0.930422
O	-3.598202	0.302068	-2.493408	O	-4.232809	-0.322517	-1.943901
O	-1.907901	-3.839998	-0.947342	O	-1.483467	-3.956101	-0.685433
O	-0.629313	-1.713393	3.129458	O	-0.098004	-1.450868	3.105289
H	-3.397836	-2.228479	-2.494055	H	-3.536545	-2.751879	-1.927394
H	3.043065	-0.14587	-2.05367	H	3.735709	-1.068301	-1.709854
H	-0.801788	-3.546589	1.357036	H	-0.120118	-3.353993	1.384356
H	0.588984	-3.169722	0.361003	H	1.015659	-2.729764	0.204521
H	1.166806	-2.421243	2.568112	H	1.711667	-1.829112	2.319656
H	6.155237	0.932121	-2.935311	H	5.734255	1.295521	-3.12577
H	6.389981	-0.702725	-2.330306	H	6.846386	0.078688	-2.511908
H	4.95127	-0.321633	-3.300449	H	5.307032	-0.424883	-3.241548
H	6.548484	0.236819	0.09404	H	6.798893	1.209655	-0.144978
H	6.276747	1.874714	-0.484677	H	5.709379	2.435075	-0.77941
H	5.215498	1.194265	0.759855	H	5.243153	1.500458	0.650579
H	1.507481	1.387255	2.366899	H	1.348456	1.964282	1.983036
H	2.221647	-0.024894	3.170955	H	2.295503	0.717366	2.819504
H	0.531738	0.414554	3.489407	H	0.594469	0.955831	3.242819
H	-3.321141	4.117225	0.486773	H	-3.377011	3.075612	1.637696
H	-2.682733	3.970028	2.138443	H	-1.744275	3.570385	2.124903
H	-3.835643	2.772999	1.522278	H	-2.19066	1.855979	2.155026
H	-0.869693	4.162665	-0.424154	H	-2.993033	4.374506	-0.590269
H	0.262153	2.880848	0.056276	H	-1.629894	3.934691	-1.630302
H	-0.300504	4.059089	1.254902	H	-1.334477	4.76245	-0.090319
H	3.174578	1.06045	0.791615	H	3.31182	-1.47063	0.717939
H	1.849655	1.246495	-0.348732	H	3.754065	0.18087	1.119884

H	2.735889	-1.380233	0.951014	H	1.395254	-0.60124	-0.68589
H	1.549862	-1.276219	-0.339123	H	1.82098	1.039144	-0.23625
H	-1.492181	1.880644	1.524979	H	-0.785352	2.372243	0.161443
H	-3.456014	1.276046	-2.299719	H	-4.270996	0.669916	-1.785862
H	-2.526208	-4.163914	-1.623738	H	-2.13894	-4.429097	-1.225107
H	-1.383016	-1.230663	2.750647	H	-0.941784	-1.048573	2.838417
2b (3)				2b (4)			
C	-4.257667	0.16543	-0.349073	C	-4.015691	-0.228885	-0.954441
C	-2.000118	1.154829	-0.118642	C	-2.024015	1.015549	-0.189971
C	-2.312164	-1.307219	-0.190788	C	-2.036161	-1.466581	-0.218677
C	-1.482583	-0.189465	-0.079276	C	-1.384744	-0.25377	0.01449
C	-3.425516	1.281852	-0.267068	C	-3.352597	0.978671	-0.734045
C	-3.700494	-1.104624	-0.312794	C	-3.364552	-1.426829	-0.685698
C	4.287051	-0.745496	0.233603	C	4.207226	-0.669911	-0.271194
C	-1.214602	2.39509	-0.027649	C	-1.46709	2.327025	0.167798
C	5.072216	0.129144	-0.415705	C	4.880631	0.318305	-0.882113
C	-1.759565	-2.710688	-0.212507	C	-1.338771	-2.792012	-0.019271
C	-0.259244	-2.705991	-0.482377	C	0.175613	-2.603167	0.029279
C	0.454928	-1.640569	0.37549	C	0.548892	-1.428873	0.95107
C	6.491402	-0.237055	-0.785457	C	6.349347	0.538816	-0.600949
C	4.659355	1.519045	-0.83575	C	4.289331	1.279497	-1.884961
C	0.28171	-1.888533	1.875973	C	0.049978	-1.619854	2.388072
C	0.529463	2.324843	1.744213	C	-0.408035	3.684785	2.005026
C	0.901461	3.743999	-0.326096	C	0.983243	2.802448	0.07372
C	2.857045	-0.583422	0.685163	C	2.757029	-1.055954	-0.413149
C	1.92934	-1.562333	-0.061868	C	2.057981	-1.129228	0.958373
C	0.289942	2.447391	0.222127	C	-0.209655	2.527531	1.012979
O	-1.793539	3.505169	-0.111479	O	-2.054555	3.372179	-0.200409
O	-0.133816	-0.338019	0.042126	O	-0.07766	-0.22806	0.392601
O	-4.033179	2.475886	-0.325937	O	-4.030691	2.098452	-1.028599
O	-4.462743	-2.225432	-0.400527	O	-3.96411	-2.629324	-0.884494
O	0.33244	-3.969534	-0.189337	O	0.853587	-3.759704	0.512061
H	-5.32823	0.315185	-0.447783	H	-5.029688	-0.207843	-1.341455
H	4.717629	-1.722024	0.466539	H	4.767971	-1.295765	0.42697
H	-1.949916	-3.229178	0.736924	H	-1.671537	-3.278801	0.907585
H	-2.269179	-3.29774	-0.985787	H	-1.59847	-3.47693	-0.834971
H	-0.082805	-2.439309	-1.535711	H	0.526967	-2.351583	-0.98078
H	6.644009	-0.177942	-1.872415	H	6.945377	0.4523	-1.520523
H	7.210358	0.461783	-0.334834	H	6.52914	1.550952	-0.211618
H	6.750875	-1.249348	-0.459452	H	6.73988	-0.180113	0.12645
H	5.30719	2.273972	-0.368657	H	4.426474	2.317914	-1.552866
H	4.775104	1.643287	-1.921353	H	4.806498	1.194327	-2.850979
H	3.625054	1.759427	-0.580071	H	3.223316	1.120715	-2.06211

H	0.775872	-1.106955	2.457839	H	0.416288	-0.807319	3.023535
H	0.71662	-2.854961	2.145865	H	0.418634	-2.568783	2.7875
H	-0.774806	-1.896662	2.157924	H	-1.042581	-1.62589	2.439
H	0.048099	3.155011	2.274336	H	-0.598293	4.627472	1.484652
H	1.60289	2.362528	1.959346	H	0.494023	3.801822	2.615869
H	0.135909	1.385289	2.141958	H	-1.250443	3.493346	2.679444
H	0.486461	4.62492	0.17138	H	0.806701	3.710789	-0.513764
H	0.721091	3.848321	-1.401591	H	1.149776	1.969848	-0.615802
H	1.984987	3.735221	-0.163084	H	1.897089	2.946245	0.660862
H	2.811904	-0.787538	1.763563	H	2.218482	-0.363201	-1.066847
H	2.507501	0.442592	0.547759	H	2.702683	-2.046165	-0.887639
H	2.331721	-2.577106	0.030398	H	2.197778	-0.179907	1.489882
H	1.945666	-1.318501	-1.131825	H	2.54143	-1.902289	1.566224
H	0.756965	1.59461	-0.268953	H	-0.003289	1.614619	1.569542
H	-3.293353	3.155049	-0.259275	H	-3.402962	2.854181	-0.819568
H	-5.396164	-1.974691	-0.503433	H	-4.860707	-2.492092	-1.2337
H	-0.086518	-4.627187	-0.767505	H	0.649143	-4.49156	-0.092199
2b (5)				2b (6)			
C	-4.068577	-0.948209	-0.729478	C	2.064134	2.813503	-0.895379
C	-2.351088	0.7465	-0.186027	C	2.250541	0.375195	-0.527325
C	-1.802318	-1.676894	-0.166075	C	0.385638	1.677932	0.47476
C	-1.435857	-0.342854	0.024524	C	1.054848	0.471396	0.262896
C	-3.691434	0.384159	-0.557179	C	2.738868	1.606534	-1.084884
C	-3.131419	-1.955322	-0.539193	C	0.906089	2.839508	-0.129473
C	3.963572	0.743228	-0.34535	C	-4.020643	-1.236552	-0.76719
C	-2.030939	2.177635	-0.079447	C	2.987439	-0.860247	-0.835735
C	5.227684	0.441369	-0.683813	C	-4.947689	-0.466376	-1.35933
C	-0.811377	-2.804636	0.005183	C	-0.850512	1.763978	1.342091
C	0.617659	-2.268903	0.023469	C	-1.010688	0.516591	2.214433
C	0.722667	-1.046837	0.951525	C	-0.76302	-0.753583	1.375282
C	6.337694	1.449785	-0.495086	C	-5.651229	-0.935574	-2.612062
C	5.67757	-0.875182	-1.270682	C	-5.386821	0.893788	-0.872904
C	0.308649	-1.358565	2.39452	C	-0.760162	-2.014064	2.236659
C	-0.460084	2.8521	1.740312	C	3.158158	-2.524162	1.018091
C	-0.434411	4.094161	-0.472245	C	3.023323	-3.324195	-1.386365
C	2.729014	-0.114493	-0.450568	C	-3.212807	-0.952723	0.473501
C	2.119379	-0.402601	0.93605	C	-1.701812	-0.890867	0.157597
C	-0.636903	2.733448	0.210364	C	2.563841	-2.256673	-0.382892
O	-2.941569	3.028454	-0.224202	O	4.047307	-0.796795	-1.503382
O	-0.174989	-0.02106	0.417932	O	0.615485	-0.670213	0.865253
O	-4.646636	1.303915	-0.759768	O	3.855739	1.658948	-1.825336
O	-3.444398	-3.267465	-0.697501	O	0.216111	3.987709	0.092087
O	1.556964	-3.238434	0.478686	O	-0.14359	0.560333	3.34942

H	-5.093631	-1.170495	-1.009339	H	2.465023	3.714388	-1.349494
H	3.783855	1.735478	0.074402	H	-3.798413	-2.198926	-1.232956
H	-0.998887	-3.363825	0.931751	H	-0.792339	2.638329	1.99832
H	-0.92382	-3.525115	-0.813964	H	-1.745951	1.909133	0.722481
H	0.878402	-1.934666	-0.990331	H	-2.019297	0.481938	2.634368
H	7.121018	1.055471	0.167617	H	-6.738233	-0.988418	-2.457783
H	6.829559	1.679685	-1.450869	H	-5.491242	-0.232099	-3.44126
H	5.970171	2.388164	-0.06748	H	-5.304433	-1.92351	-2.931558
H	6.137014	-0.721687	-2.257164	H	-5.235493	1.648792	-1.656645
H	6.451188	-1.333425	-0.639049	H	-6.46249	0.894481	-0.648171
H	4.867807	-1.599103	-1.386835	H	-4.857674	1.229148	0.022021
H	0.482605	-0.48582	3.031678	H	-0.523103	-2.891498	1.627026
H	0.900472	-2.194455	2.777959	H	-1.743368	-2.164723	2.692157
H	-0.749642	-1.625158	2.463378	H	-0.025212	-1.926263	3.038756
H	-1.202198	3.541299	2.160034	H	4.253143	-2.481425	0.984063
H	0.537009	3.244004	1.970478	H	2.867138	-3.523425	1.360625
H	-0.567343	1.882704	2.234851	H	2.803088	-1.796518	1.75302
H	-1.144358	4.838771	-0.101883	H	4.11352	-3.357585	-1.466149
H	-0.559491	4.019489	-1.558287	H	2.617818	-3.134954	-2.386506
H	0.580812	4.454542	-0.272289	H	2.670725	-4.308403	-1.058319
H	1.981721	0.409214	-1.063945	H	-3.537994	-0.021729	0.947568
H	2.949097	-1.057576	-0.958854	H	-3.397248	-1.753399	1.203396
H	2.048039	0.533278	1.504873	H	-1.520695	-0.064847	-0.538602
H	2.794091	-1.058815	1.495971	H	-1.408642	-1.806807	-0.37117
H	0.109824	2.034475	-0.164031	H	1.477999	-2.287947	-0.300788
H	-4.206605	2.189866	-0.578262	H	4.199854	0.71447	-1.856135
H	-4.376129	-3.349659	-0.961544	H	0.670417	4.729189	-0.342085
H	1.507563	-3.997247	-0.124886	H	0.769707	0.522307	3.018842
2b (7)				2b (8)			
C	-2.431552	-0.514445	-2.44276	C	-4.145228	-1.35719	-0.337525
C	-1.578953	0.795766	-0.526172	C	-2.611158	0.572573	-0.13205
C	-1.154419	-1.648786	-0.691834	C	-1.740891	-1.752989	-0.132379
C	-1.004353	-0.426261	-0.033993	C	-1.534368	-0.376641	-0.040296
C	-2.294679	0.700043	-1.768493	C	-3.931218	0.019968	-0.26584
C	-1.872095	-1.665193	-1.904358	C	-3.060351	-2.222334	-0.277514
C	3.909913	-0.145749	-0.131419	C	4.510902	0.666444	0.373522
C	-1.498669	2.115423	0.122303	C	-2.475788	2.036249	-0.133139
C	4.188879	0.673165	-1.15869	C	5.611471	0.490548	-0.3757
C	-0.587586	-2.936047	-0.133674	C	-0.588076	-2.724438	-0.089699
C	-0.172067	-2.775523	1.330482	C	0.748031	-2.017476	-0.310666
C	0.592488	-1.446277	1.526191	C	0.837435	-0.735779	0.540799
C	5.441895	0.478073	-1.981114	C	6.582659	1.627029	-0.599235
C	3.332205	1.836544	-1.597741	C	6.000932	-0.802178	-1.05165

C	0.89191	-1.192509	3.001678	C	0.717746	-1.005734	2.042762
C	-1.902913	1.951975	2.582145	C	-0.731225	3.022641	1.355321
C	-0.462185	3.829374	1.666677	C	-1.241118	4.107327	-0.880592
C	2.723267	-0.118659	0.797213	C	3.433609	-0.332149	0.711317
C	1.85734	-1.387289	0.644948	C	2.058809	0.138686	0.191832
C	-0.880895	2.363116	1.497476	C	-1.141004	2.780203	-0.114048
O	-2.004178	3.113148	-0.444451	O	-3.504722	2.754134	-0.147877
O	-0.324377	-0.361876	1.146515	O	-0.283364	0.123477	0.132961
O	-2.865913	1.767197	-2.345907	O	-5.023218	0.796326	-0.333128
O	-1.985092	-2.872855	-2.514495	O	-3.210091	-3.570282	-0.349778
O	-1.303051	-2.857367	2.199653	O	1.840098	-2.867125	0.032625
H	-2.97888	-0.534405	-3.380039	H	-5.161443	-1.725341	-0.439261
H	4.618442	-0.952082	0.070343	H	4.352661	1.659967	0.799706
H	-1.334511	-3.734414	-0.193188	H	-0.549891	-3.254951	0.871541
H	0.266417	-3.275048	-0.734613	H	-0.72355	-3.496266	-0.857152
H	0.475687	-3.604715	1.62947	H	0.82514	-1.706709	-1.363713
H	5.197179	0.307532	-3.039043	H	7.58618	1.36755	-0.233009
H	6.07701	1.374827	-1.952486	H	6.69319	1.847151	-1.670533
H	6.035989	-0.370734	-1.627574	H	6.263278	2.544404	-0.094258
H	2.417906	1.950037	-1.010883	H	6.118337	-0.650531	-2.133659
H	3.895288	2.777956	-1.531525	H	6.974946	-1.153708	-0.683137
H	3.04347	1.724327	-2.651909	H	5.276012	-1.605339	-0.90154
H	1.266597	-0.177971	3.15793	H	0.871746	-0.081021	2.607909
H	1.652674	-1.898904	3.350903	H	1.466221	-1.737442	2.357763
H	-0.010209	-1.33231	3.599983	H	-0.270676	-1.39949	2.296448
H	-2.816163	2.552848	2.497434	H	-1.479259	3.641212	1.86495
H	-1.475922	2.122346	3.576626	H	0.228751	3.549824	1.392165
H	-2.173379	0.895402	2.505946	H	-0.625193	2.08291	1.904399
H	-1.322378	4.502898	1.614985	H	-1.975746	4.777822	-0.426254
H	0.250195	4.134869	0.892646	H	-1.531664	3.945728	-1.924743
H	0.01919	3.95962	2.642337	H	-0.265906	4.606773	-0.874084
H	3.088555	-0.049305	1.830578	H	3.655396	-1.323342	0.31399
H	2.103308	0.766032	0.624522	H	3.38403	-0.437274	1.804708
H	2.46419	-2.272883	0.877175	H	2.10124	0.246303	-0.899468
H	1.568577	-1.477441	-0.407047	H	1.853147	1.138412	0.59543
H	-0.003686	1.726237	1.607345	H	-0.379469	2.156906	-0.58084
H	-2.654828	2.542646	-1.741661	H	-4.685	1.74003	-0.253151
H	-2.511937	-2.778742	-3.325848	H	-4.151007	-3.786782	-0.460889
H	-1.883079	-2.105051	1.993875	H	1.791889	-3.647582	-0.54305
2b (9)				2b (10)			
C	-4.323037	-0.88575	-0.038442	C	4.14518	-1.357368	-0.337597
C	-2.501581	0.786584	-0.061061	C	2.611227	0.572466	-0.131972
C	-1.998387	-1.644704	-0.030535	C	1.740828	-1.75305	-0.132301

C	-1.578345	-0.314955	-0.051148	C	1.534394	-0.376687	-0.040188
C	-3.896925	0.442154	-0.083807	C	3.931266	0.019794	-0.265844
C	-3.38152	-1.906735	-0.00567	C	3.060251	-2.222456	-0.277551
C	4.545606	-0.300993	-0.655179	C	-4.510862	0.666712	0.373275
C	-2.14696	2.212414	-0.011303	C	2.475943	2.036132	-0.133044
C	5.568396	0.37218	-0.103269	C	-5.611537	0.490576	-0.375733
C	-1.008077	-2.781828	-0.067825	C	0.587942	-2.724425	-0.089576
C	0.376473	-2.309388	-0.509631	C	-0.748085	-2.017355	-0.310648
C	0.7728	-1.007917	0.216139	C	-0.837469	-0.735667	0.540842
C	6.627728	1.012885	-0.97051	C	-6.582726	1.626999	-0.599552
C	5.782825	0.56114	1.379505	C	-6.001129	-0.802404	-1.051119
C	0.825303	-1.161689	1.738146	C	-0.717908	-1.005664	2.042809
C	-0.722954	4.060135	0.951094	C	1.24146	4.107197	-0.880789
C	-0.097729	2.940955	-1.239404	C	0.73132	3.022826	1.355214
C	3.399238	-1.002864	0.026778	C	-3.433591	-0.331812	0.711327
C	2.049503	-0.358753	-0.355474	C	-2.058759	0.138879	0.19178
C	-0.724774	2.744448	0.158478	C	1.141212	2.780167	-0.114084
O	-3.048887	3.078844	-0.111693	O	3.504931	2.753966	-0.147706
O	-0.255214	-0.011862	-0.118387	O	0.283438	0.123522	0.133152
O	-4.858872	1.376058	-0.130377	O	5.023276	0.796114	-0.333149
O	-3.741405	-3.21586	0.032557	O	3.209936	-3.570403	-0.349874
O	1.364512	-3.300329	-0.237212	O	-1.840249	-2.866923	0.032536
H	-5.388356	-1.094673	-0.038599	H	5.161361	-1.725587	-0.43942
H	4.51578	-0.352597	-1.746027	H	-4.352522	1.660389	0.799065
H	-0.917019	-3.259722	0.917209	H	0.723392	-3.496331	-0.856947
H	-1.362416	-3.562446	-0.751844	H	0.549669	-3.254842	0.871711
H	0.355273	-2.07947	-1.585752	H	-0.825082	-1.706552	-1.363687
H	6.682834	2.096098	-0.791551	H	-6.693477	1.846671	-1.670918
H	7.624557	0.611467	-0.738929	H	-7.58618	1.367714	-0.233003
H	6.436026	0.853239	-2.036486	H	-6.263209	2.544574	-0.095026
H	6.747343	0.134175	1.688119	H	-6.974985	-1.1539	-0.68215
H	5.826025	1.630519	1.628825	H	-6.118929	-0.65112	-2.133135
H	5.002963	0.105144	1.993737	H	-5.276088	-1.605455	-0.901
H	1.175391	-0.232875	2.199733	H	-0.871954	-0.080974	2.60798
H	1.507594	-1.969685	2.014707	H	0.270503	-1.399413	2.296548
H	-0.161656	-1.395028	2.148092	H	-1.466401	-1.737385	2.357743
H	-1.280469	4.842914	0.429509	H	1.976087	4.777706	-0.426467
H	0.308833	4.402736	1.087544	H	0.266275	4.6067	-0.874418
H	-1.170406	3.9308	1.943022	H	1.532085	3.945459	-1.924895
H	-0.678314	3.66671	-1.820831	H	1.479306	3.641495	1.864796
H	-0.054098	2.001134	-1.796568	H	0.62527	2.083185	1.904441
H	0.923836	3.32422	-1.138321	H	-0.228664	3.55	1.391887
H	3.384935	-2.056642	-0.272725	H	-3.384036	-0.43667	1.804744

H	3.521044	-0.988078	1.114033	H	-3.655376	-1.323093	0.31422
H	1.953909	-0.330176	-1.448966	H	-1.853023	1.138618	0.595302
H	2.053407	0.68483	-0.01796	H	-2.101189	0.24641	-0.899527
H	-0.131436	2.005403	0.695228	H	0.379669	2.156874	-0.580867
H	-4.373988	2.256449	-0.161727	H	4.685083	1.739847	-0.253096
H	-4.710689	-3.287113	0.024355	H	4.150842	-3.786932	-0.461012
H	1.122528	-4.096041	-0.738239	H	-1.792818	-3.64676	-0.544038
2b (11)							
C	-4.353333	-0.400778	-0.016612				
C	-2.287939	0.962236	0.003796				
C	-2.178395	-1.517136	-0.079397				
C	-1.548046	-0.272172	-0.036913				
C	-3.721155	0.842685	-0.001396				
C	-3.585701	-1.55669	-0.052997				
C	4.090238	0.435606	-0.410084				
C	-1.717628	2.316093	0.071091				
C	5.380645	0.258668	-0.082899				
C	-1.394829	-2.802797	-0.181361				
C	0.05028	-2.540981	-0.595231				
C	0.646259	-1.35922	0.196677				
C	6.480976	0.710984	-1.015162				
C	5.871949	-0.379137	1.194414				
C	0.661043	-1.611131	1.706467				
C	0.055793	3.949752	0.825676				
C	0.32128	2.64149	-1.332359				
C	2.858145	0.054077	0.369971				
C	2.034387	-1.016155	-0.373852				
C	-0.222568	2.618842	0.11388				
O	-2.48012	3.312588	0.074498				
O	-0.189915	-0.185035	-0.078704				
O	-4.525966	1.915439	0.020282				
O	-4.14906	-2.792339	-0.078025				
O	0.876503	-3.680364	-0.367949				
H	-5.438336	-0.437839	-0.006331				
H	3.880574	0.906861	-1.37293				
H	-1.397315	-3.345399	0.773657				
H	-1.870001	-3.470268	-0.910104				
H	0.076966	-2.258863	-1.659027				
H	7.137494	1.443749	-0.524948				
H	7.123428	-0.132132	-1.306293				
H	6.083244	1.167124	-1.927401				
H	6.503932	-1.249912	0.971114				
H	6.502698	0.321795	1.758861				

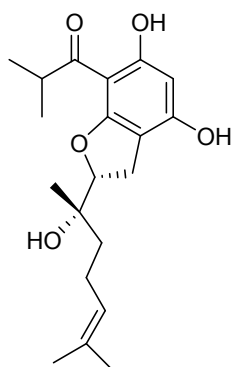
H	5.06655	-0.710988	1.85375				
H	1.053083	-0.739941	2.237092				
H	1.292813	-2.474495	1.9337				
H	-0.343956	-1.811365	2.088019				
H	-0.398585	4.791051	0.295149				
H	1.137583	4.116828	0.875941				
H	-0.335137	3.946443	1.849116				
H	-0.17468	3.426398	-1.915527				
H	0.169632	1.683068	-1.836044				
H	1.396038	2.854563	-1.322185				
H	3.122272	-0.305793	1.368409				
H	2.240373	0.950442	0.513892				
H	2.607926	-1.94808	-0.405369				
H	1.888657	-0.703694	-1.416121				
H	0.278269	1.815085	0.65212				
H	-3.910185	2.71111	0.03424				
H	-5.117137	-2.706877	-0.078818				
H	0.523863	-4.40659	-0.907034				

Key transitions, oscillator strengths, and rotatory strengths in the ECD of conformers **2b** (5) at B3LYP /6-311++G(d,p) level.

Species	Excited State	$\Delta E(eV)^a$	$\lambda(nm)^b$	f^c	R_{vel}^d
2b (5)	92 -> 97	3.7269	332.67	0.076	5.1071
	91 ->108	4.1589	298.12	0.0011	-0.2518
	91 -> 95	4.2772	289.87	0.0188	-4.1331
	84 -> 95	4.4623	277.85	0.3639	6.7243
	94 -> 99	5.2236	237.36	0.003	-0.6586
	89 -> 95	5.4583	227.15	0.0631	1.2971
	93 -> 98	5.4769	226.37	0.0051	-2.6545
	94 -> 98	5.5539	223.24	0.0055	-0.1919
	94 -> 99	5.5662	222.74	0.0101	-3.9368
	94 -> 97	5.5937	221.65	0.0272	6.4633
	92 -> 97	5.6289	220.26	0.0131	3.5137
	94 -> 99	5.6495	219.46	0.0044	-4.4822
	94 ->100	5.7884	214.2	0.2025	61.3966
	94 ->100	5.822	212.96	0.0047	-7.9166
	94 ->101	5.8463	212.07	0.0792	-41.1861
	93 -> 99	5.8861	210.64	0.0046	-3.7936
	93 ->100	5.9038	210.01	0.021	-8.0402
	87 -> 95	5.9134	209.67	0.0128	-21.5855
	93 -> 97	5.952	208.31	0.0274	-6.0836
	93 -> 97	5.9661	207.82	0.0268	2.7626
	93 ->101	6.0398	205.28	0.036	-0.0051

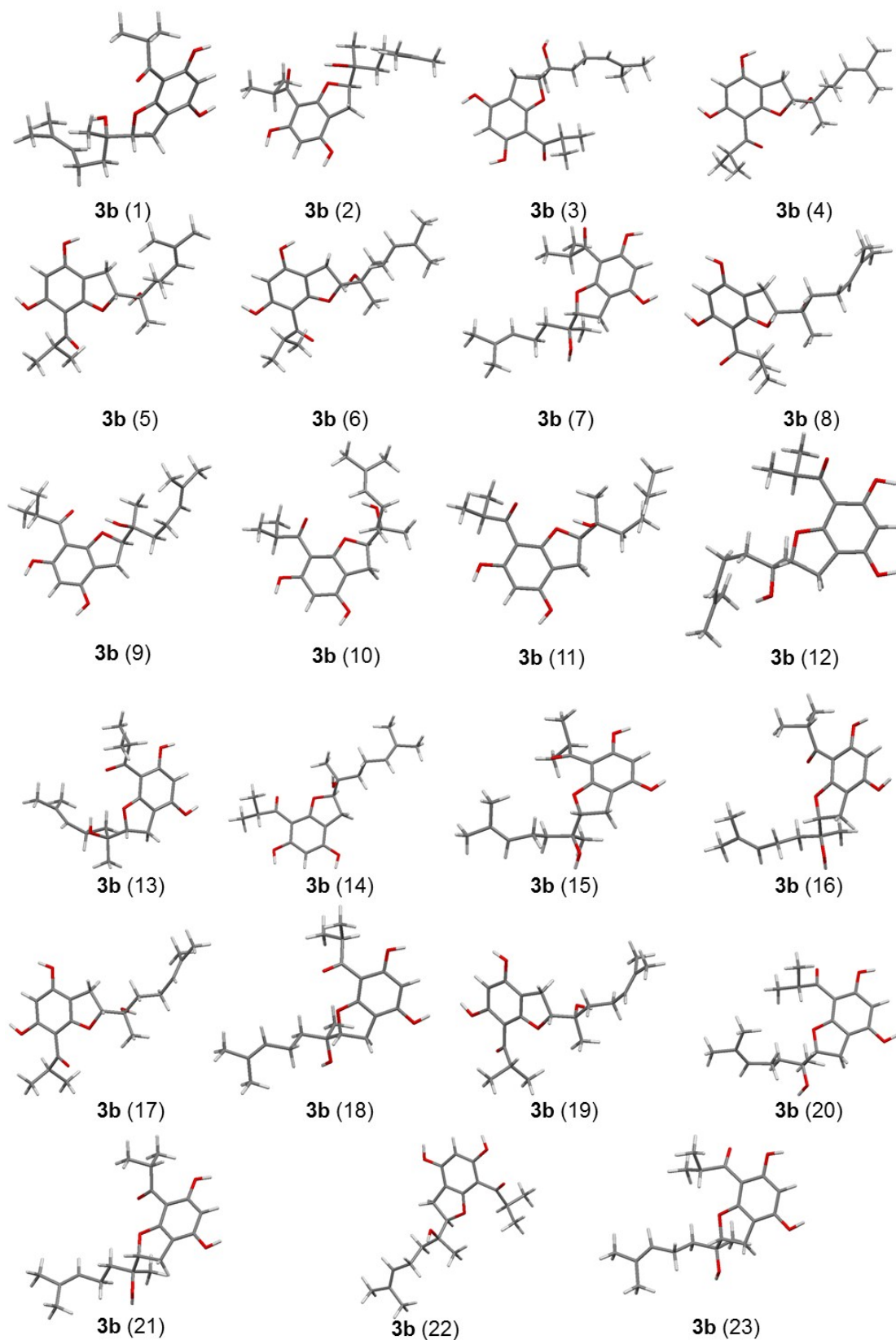
	93 ->100	6.0558	204.74	0.0027	11.3979
	93 ->100	6.0647	204.44	0.0437	5.1613
	94 ->102	6.1164	202.71	0.0003	-0.8966
	94 ->103	6.1368	202.03	0.0159	-2.3557
	94 ->104	6.1608	201.25	0.0197	10.3733
	94 ->105	6.256	198.19	0.0293	25.3519
	94 ->104	6.2947	196.97	0.1071	-12.3992
	94 ->105	6.3085	196.54	0.0269	-19.2831
	91 -> 97	6.3101	196.48	0.0697	3.1114
	93 ->107	6.3561	195.06	0.117	-32.8891
	94 ->105	6.3806	194.31	0.0836	-18.3998
	86 -> 95	6.416	193.24	0.0175	-16.5408
	94 ->106	6.4229	193.04	0.1149	-17.0325
	91 -> 99	6.4407	192.5	0.0133	45.8503
	93 ->103	6.4605	191.91	0.0585	61.9068
	92 ->105	6.4858	191.16	0.031	-26.9348
	94 ->114	6.4903	191.03	0.0948	-30.2598
	93 ->106	6.5273	189.95	0.0063	10.1916
	93 ->105	6.5396	189.59	0.0192	12.5553

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



3b

Optimized geometries of predominant conformers for compound **3b** at the B3LYP/6-31G (d,p) level in methanol solution.



Important thermodynamic parameters (a.u.) and Boltzmann distributions of the optimized compound **3b** at B3LYP/6-31G(d,p) level in methanol solution.

Conformations	E+ZPE	G	%
3b (1)	-1154.651026	-1154.709271	2.71%
3b (2)	-1154.652849	-1154.711691	35.14%
3b (3)	-1154.649200	-1154.708913	1.86%
3b (4)	-1154.651495	-1154.710475	9.70%
3b (5)	-1154.651179	-1154.710562	10.63%
3b (6)	-1154.651071	-1154.709747	4.49%
3b (7)	-1154.648744	-1154.708680	1.45%
3b (8)	-1154.649054	-1154.708471	1.16%
3b (9)	-1154.649967	-1154.709170	2.44%
3b (10)	-1154.649569	-1154.708504	1.20%
3b (11)	-1154.650086	-1154.708437	1.12%
3b (12)	-1154.650153	-1154.708681	1.45%
3b (13)	-1154.649131	-1154.708671	1.44%
3b (14)	-1154.649662	-1154.708576	1.30%
3b (15)	-1154.649867	-1154.710090	6.45%
3b (16)	-1154.649849	-1154.708931	1.89%
3b (17)	-1154.649875	-1154.709039	2.12%
3b (18)	-1154.649701	-1154.709618	3.91%
3b (19)	-1154.649182	-1154.709043	2.13%
3b (20)	-1154.649396	-1154.708644	1.40%
3b (21)	-1154.649366	-1154.708570	1.29%
3b (22)	-1154.649210	-1154.708434	1.12%
3b (23)	-1154.649407	-1154.709542	3.61%

E+ZPE, G: total energy with zero point energy (ZPE) and Gibbs free energy in methanol solution at B3LYP/6-31G (d,p) level. %: Boltzmann distributions, using the relative Gibbs free energies as weighting factors.

Optimized Z-matrixes of compound **2b** in methanol solution (Å) at B3LYP/6-31G (d,p) level.

3b (1)				3b (2)			
C	3.160313	2.29046	0.892372	C	2.915794	2.752421	0.102459
C	2.665022	0.080692	-0.089364	C	2.871899	0.285767	0.131627
C	1.034283	1.941004	-0.194174	C	0.837778	1.612855	-0.350673
C	1.429037	0.638864	-0.486688	C	1.495954	0.402505	-0.159062
C	3.524718	0.974344	0.603794	C	3.555673	1.523093	0.271128
C	1.900461	2.772824	0.505518	C	1.548214	2.799855	-0.20889
C	-4.863988	0.299618	0.412904	C	-5.617112	-0.611135	-0.488236
C	2.99631	-1.335187	-0.404857	C	3.503156	-1.053034	0.2841
C	-5.322988	-0.762053	1.102715	C	-6.588299	-0.002372	0.211745
C	-0.374272	2.159008	-0.675834	C	-0.618694	1.348159	-0.626689
C	-0.67434	0.82114	-1.404294	C	-0.615282	-0.181058	-0.862823
C	-5.586153	-0.660422	2.587521	C	-7.829727	0.513593	-0.479162
C	-5.643262	-2.111241	0.505516	C	-6.567348	0.22675	1.704011
C	5.156475	-2.587055	-0.076449	C	4.925104	-2.417193	-1.252743
C	2.998918	-3.423522	0.970167	C	5.835867	-1.675935	1.000334

C	-2.024852	-1.299645	-1.603413	C	-1.52514	-2.491885	-0.430043
C	-4.57578	0.417463	-1.064321	C	-4.316129	-1.186056	0.008568
C	-3.172239	0.97613	-1.394256	C	-3.102416	-0.491914	-0.643907
C	3.822016	-2.183486	0.575141	C	4.942076	-1.298672	-0.194237
C	-1.966649	0.1002	-0.969665	C	-1.727563	-0.991044	-0.161631
O	2.56002	-1.866893	-1.424115	O	2.856959	-1.997115	0.734176
O	0.47344	-0.053728	-1.149998	O	0.669423	-0.663636	-0.335488
O	4.766827	0.520322	0.940776	O	4.871746	1.477595	0.626388
O	1.483766	4.038033	0.779999	O	0.87425	3.968538	-0.375004
O	-1.88731	-0.014555	0.45829	O	-1.662764	-0.734473	1.248989
H	3.861633	2.944311	1.405173	H	3.475626	3.675415	0.234585
H	-4.697208	1.221556	0.974504	H	-5.76655	-0.707344	-1.566207
H	-1.065033	2.313743	0.159908	H	-1.242298	1.6105	0.236809
H	-0.469449	3.014737	-1.352235	H	-1.003395	1.888368	-1.496612
H	-0.70551	0.961074	-2.490154	H	-0.61293	-0.409313	-1.935375
H	-5.340614	0.330857	2.98112	H	-7.805815	0.327703	-1.557787
H	-6.642276	-0.8656	2.810959	H	-8.734603	0.040982	-0.071364
H	-5.001545	-1.406073	3.14343	H	-7.949129	1.594879	-0.321115
H	-5.422666	-2.18011	-0.561971	H	-5.657876	-0.138	2.18666
H	-6.708327	-2.34335	0.642748	H	-7.42425	-0.267616	2.182783
H	-5.085291	-2.904319	1.020983	H	-6.663965	1.297569	1.93101
H	5.765067	-1.707637	-0.310574	H	4.313318	-2.140628	-2.1195
H	4.975557	-3.141258	-1.004145	H	4.519089	-3.341794	-0.830631
H	5.73155	-3.229116	0.600538	H	5.942803	-2.614912	-1.60765
H	2.062678	-3.142284	1.466564	H	5.890979	-0.858854	1.72702
H	3.572297	-4.051358	1.661497	H	6.85329	-1.897695	0.65867
H	2.749556	-4.018756	0.086193	H	5.441796	-2.564215	1.506139
H	-2.08803	-1.241147	-2.696495	H	-1.641307	-2.723646	-1.495122
H	-2.899329	-1.850213	-1.243067	H	-2.253454	-3.08049	0.133871
H	-1.131083	-1.86746	-1.335535	H	-0.522131	-2.80352	-0.123253
H	-4.734775	-0.533591	-1.580997	H	-4.22844	-1.107833	1.095434
H	-5.301514	1.119695	-1.501065	H	-4.291898	-2.258123	-0.232057
H	-3.070183	1.96066	-0.920596	H	-3.174151	0.583519	-0.443875
H	-3.117499	1.14117	-2.478029	H	-3.15199	-0.614227	-1.734239
H	4.033248	-1.600057	1.473292	H	5.333599	-0.387724	-0.650954
H	5.247482	1.219812	1.413471	H	5.222638	2.38162	0.684116
H	2.175981	4.511269	1.271065	H	1.481074	4.717399	-0.251008
H	-2.766832	-0.296801	0.769797	H	-0.769771	-0.997479	1.531893
3b (3)				3b (4)			
C	-4.41381	-0.744021	0.45974	C	3.071022	2.660175	-0.184958
C	-2.534757	0.83138	0.185028	C	2.858652	0.209772	0.010256
C	-2.286517	-1.582569	-0.310747	C	0.868805	1.685276	-0.0173
C	-1.786551	-0.287731	-0.231844	C	1.468185	0.430479	0.07593

C	-3.882186	0.545501	0.546749	C	3.641813	1.390836	-0.111919
C	-3.613059	-1.814865	0.035675	C	1.67758	2.811613	-0.135534
C	4.855152	-0.329336	-0.388213	C	-5.257921	0.387437	-0.480435
C	-1.973319	2.207733	0.269009	C	3.409562	-1.171173	0.078381
C	5.608486	0.584089	0.245547	C	-6.473266	-0.173646	-0.587451
C	-1.198309	-2.522531	-0.752578	C	-0.62715	1.526915	0.110533
C	0.008116	-1.561347	-0.921459	C	-0.784279	-0.003331	-0.050957
C	6.646401	1.383433	-0.508326	C	-7.721623	0.67667	-0.533003
C	5.521493	0.911004	1.717089	C	-6.734381	-1.649509	-0.769954
C	0.323364	3.165356	-0.142342	C	4.307297	-2.739533	-1.649995
C	-1.650432	3.823228	-1.60079	C	5.808023	-1.920068	0.229175
C	0.972093	-1.878473	1.422156	C	-1.738367	-2.221525	0.695756
C	3.773399	-1.213641	0.175904	C	-3.906958	-0.281354	-0.504304
C	2.402255	-0.918611	-0.466377	C	-3.172793	-0.117757	0.842818
C	-0.980849	2.688243	-0.801266	C	4.658499	-1.557453	-0.728135
C	1.265293	-1.895135	-0.083155	C	-1.749702	-0.701964	0.928309
O	-2.328912	2.992916	1.143841	O	2.833845	-2.037717	0.73348
O	-0.463703	-0.224134	-0.555005	O	0.550342	-0.568126	0.18615
O	-4.670958	1.581836	0.939984	O	4.998111	1.246882	-0.111551
O	-4.076128	-3.090061	-0.051462	O	1.187535	4.07832	-0.204098
O	1.589341	-3.22755	-0.521005	O	-1.317639	-0.422111	2.269288
H	-5.455288	-0.915545	0.722495	H	3.697262	3.544555	-0.258777
H	5.023023	-0.457852	-1.459729	H	-5.218339	1.470508	-0.345853
H	-0.992203	-3.311545	-0.022181	H	-0.984528	1.853047	1.095418
H	-1.433462	-3.023529	-1.697925	H	-1.199875	2.062138	-0.654548
H	0.309789	-1.502064	-1.971682	H	-1.04201	-0.256978	-1.085002
H	7.648566	1.230175	-0.083485	H	-7.488836	1.738137	-0.400627
H	6.681281	1.112959	-1.568561	H	-8.313098	0.568398	-1.4531
H	6.442965	2.461307	-0.437039	H	-8.376232	0.364443	0.292916
H	6.48493	0.724541	2.211837	H	-7.36744	-2.030903	0.043153
H	4.756712	0.338292	2.246786	H	-5.824217	-2.252873	-0.796606
H	5.303145	1.97822	1.861339	H	-7.287476	-1.831504	-1.701895
H	0.115902	3.960742	0.581285	H	3.964422	-3.597991	-1.064103
H	1.012946	3.556948	-0.898608	H	5.188746	-3.041703	-2.226587
H	0.825718	2.345901	0.383675	H	3.514892	-2.47303	-2.359239
H	-2.568574	3.481163	-2.092692	H	6.688481	-2.241041	-0.339097
H	-0.969111	4.19147	-2.376002	H	5.508863	-2.740081	0.891405
H	-1.90768	4.657802	-0.940347	H	6.095053	-1.062906	0.846644
H	0.722937	-0.868743	1.761765	H	-2.036308	-2.48012	-0.325776
H	1.848132	-2.214795	1.987453	H	-2.429945	-2.706015	1.392631
H	0.142831	-2.546287	1.673901	H	-0.735265	-2.626001	0.863389
H	4.039405	-2.261963	-0.02948	H	-3.99796	-1.342324	-0.753796
H	3.712097	-1.113369	1.263394	H	-3.307541	0.174438	-1.306386

H	2.512756	-0.953172	-1.558708	H	-3.762322	-0.600288	1.632015
H	2.095799	0.102708	-0.211898	H	-3.125838	0.946582	1.105035
H	-0.753433	1.867428	-1.48415	H	4.969561	-0.710814	-1.34337
H	-5.576071	1.253618	1.06958	H	5.41365	2.118867	-0.214894
H	-5.006692	-3.121415	0.226534	H	0.21806	4.057778	-0.149271
H	2.248875	-3.587298	0.092823	H	-0.397312	-0.733458	2.326889
3b (5)				3b (6)			
C	2.536017	2.824747	0.257941	C	3.033681	2.696412	-0.043538
C	2.702728	0.413295	-0.238999	C	2.838708	0.248119	-0.284996
C	0.519719	1.498038	0.202658	C	0.841829	1.685621	0.000905
C	1.298347	0.388634	-0.121697	C	1.446084	0.445144	-0.19636
C	3.291362	1.694288	-0.049168	C	3.611839	1.439973	-0.215414
C	1.145285	2.724716	0.40604	C	1.643174	2.820341	0.087743
C	-5.398794	-0.820081	-0.137329	C	-5.299866	0.446894	-0.221078
C	3.46245	-0.828846	-0.553047	C	3.407229	-1.119468	-0.444434
C	-6.178881	0.217221	-0.481797	C	-6.520911	-0.091858	-0.369796
C	-0.915223	1.061743	0.373371	C	-0.641387	1.485337	0.19707
C	-0.868634	-0.375223	-0.198796	C	-0.810467	0.012081	-0.241935
C	-7.623943	0.273127	-0.042201	C	-7.76078	0.706145	-0.0375
C	-5.736786	1.398008	-1.31265	C	-6.79836	-1.49108	-0.864989
C	5.907561	-1.116843	-1.074495	C	5.791224	-1.824708	-0.845366
C	4.832829	-2.38324	0.84698	C	4.499911	-2.69228	1.162802
C	-1.389133	-2.843305	-0.017725	C	-1.718591	-2.318288	0.12503
C	-3.947286	-1.059506	-0.465796	C	-3.955715	-0.180675	-0.489082
C	-3.08591	-1.127317	0.812644	C	-3.120089	-0.298794	0.802543
C	4.855976	-1.066903	0.048514	C	4.737913	-1.493231	0.226555
C	-1.593549	-1.461184	0.622662	C	-1.698708	-0.875206	0.654473
O	2.958915	-1.708551	-1.248077	O	2.788551	-1.985772	-1.058546
O	0.551875	-0.741961	-0.247603	O	0.537993	-0.567823	-0.225335
O	4.638666	1.799248	-0.234083	O	4.960647	1.323072	-0.380881
O	0.472844	3.858448	0.740299	O	1.146821	4.070119	0.290179
O	-1.048054	-1.467449	1.95189	O	-1.158911	-0.862381	1.985565
H	3.012659	3.793261	0.377276	H	3.650548	3.589774	-0.016251
H	-5.852024	-1.604762	0.472366	H	-5.248625	1.471361	0.153768
H	-1.207331	1.049337	1.430782	H	-0.926117	1.613462	1.24906
H	-1.639067	1.676898	-0.172219	H	-1.26922	2.147828	-0.408548
H	-1.219308	-0.38885	-1.236461	H	-1.148996	-0.041666	-1.282215
H	-7.903907	-0.599116	0.557121	H	-7.517792	1.714185	0.31346
H	-7.820187	1.175241	0.554348	H	-8.417416	0.798234	-0.914173
H	-8.298735	0.323506	-0.908413	H	-8.354249	0.206525	0.74115
H	-4.688219	1.350164	-1.615526	H	-7.37845	-2.053563	-0.120373
H	-5.885162	2.335095	-0.758309	H	-5.894632	-2.063224	-1.087098
H	-6.346647	1.479173	-2.223137	H	-7.411925	-1.463771	-1.77623

H	5.659701	-1.905624	-1.79335	H	5.441596	-2.643034	-1.484569
H	6.898742	-1.330074	-0.658254	H	6.729862	-2.135267	-0.372489
H	5.961071	-0.163472	-1.609947	H	5.999931	-0.955816	-1.477733
H	4.105709	-2.343114	1.666519	H	5.43856	-2.98215	1.648185
H	5.820193	-2.576803	1.280978	H	4.1199	-3.551359	0.601161
H	4.568259	-3.223932	0.198018	H	3.774341	-2.450351	1.948354
H	-1.77143	-2.879728	-1.043138	H	-2.116222	-2.373367	-0.8938
H	-1.908067	-3.604164	0.574264	H	-2.34228	-2.940048	0.775446
H	-0.324534	-3.094659	-0.051255	H	-0.706789	-2.735474	0.110494
H	-3.861732	-2.01172	-1.007747	H	-4.068095	-1.164513	-0.953233
H	-3.566378	-0.286004	-1.140617	H	-3.418053	0.444885	-1.217088
H	-3.495565	-1.89286	1.484176	H	-3.650907	-0.942149	1.514964
H	-3.165739	-0.175849	1.351629	H	-3.046027	0.686697	1.279225
H	5.10508	-0.247654	0.725593	H	5.095683	-0.649283	0.819555
H	4.914686	2.716526	-0.072277	H	5.369816	2.201108	-0.307237
H	-0.477718	3.669253	0.802739	H	0.177684	4.033247	0.342486
H	-0.093123	-1.626166	1.85277	H	-0.243236	-1.182863	1.910087
3b (7)				3b (8)			
C	-4.468556	-1.11221	-0.065149	C	3.230456	2.669104	0.412066
C	-2.777415	0.677788	-0.218481	C	3.001927	0.233034	0.083002
C	-2.142958	-1.715079	-0.287647	C	1.114227	1.782733	-0.327981
C	-1.827931	-0.360711	-0.300513	C	1.668418	0.508481	-0.280958
C	-4.129007	0.242437	-0.108476	C	3.772764	1.38161	0.426933
C	-3.473991	-2.096662	-0.161697	C	1.895683	2.874113	0.033474
C	4.685249	0.636524	0.35292	C	-4.767623	-0.627271	0.327531
C	-2.421632	2.121771	-0.285866	C	3.595408	-1.13211	0.069842
C	5.878259	0.525016	-0.253482	C	-5.843956	-0.035253	0.871876
C	-0.888353	-2.531641	-0.435759	C	-0.329425	1.685719	-0.741201
C	0.192493	-1.43046	-0.598853	C	-0.415001	0.22012	-1.225982
C	6.669915	1.756781	-0.62841	C	-6.1739	-0.236167	2.333638
C	6.548107	-0.778583	-0.616423	C	-6.814067	0.859953	0.138045
C	-1.519012	3.645781	1.472892	C	3.403042	-3.059929	1.649485
C	-0.195446	3.241889	-0.659348	C	2.586973	-3.288861	-0.745935
C	0.91309	-1.355956	1.851406	C	-1.563725	-2.026348	-1.283228
C	3.744152	-0.455648	0.792246	C	-4.286087	-0.549668	-1.098784
C	2.413753	-0.406693	0.012122	C	-2.916139	0.144281	-1.296095
C	-1.134764	2.621417	0.388547	C	2.736293	-2.344867	0.460052
C	1.376395	-1.488616	0.39525	C	-1.658013	-0.579584	-0.772935
O	-3.15898	2.936441	-0.834409	O	4.776688	-1.311463	-0.214455
O	-0.49125	-0.143323	-0.457348	O	0.777268	-0.448213	-0.677921
O	-5.097756	1.19112	0.004066	O	5.061742	1.192094	0.817938
O	-3.752218	-3.427282	-0.140704	O	1.32149	4.105452	0.000582
O	1.91718	-2.801279	0.15431	O	-1.708403	-0.56912	0.660934

H	-5.511005	-1.402578	0.043749	H	3.849281	3.516533	0.69832
H	4.318851	1.64623	0.550635	H	-4.146696	-1.234845	0.983536
H	-0.691124	-3.17208	0.430131	H	-1.00004	1.856416	0.109966
H	-0.913546	-3.187701	-1.312314	H	-0.604871	2.387387	-1.533868
H	0.604703	-1.44466	-1.612724	H	-0.317612	0.164658	-2.316336
H	6.859266	1.789979	-1.710679	H	-7.174242	-0.675208	2.457434
H	6.151842	2.6786	-0.345051	H	-5.451119	-0.892012	2.829647
H	7.656062	1.755777	-0.142839	H	-6.190024	0.722653	2.871318
H	5.961004	-1.65938	-0.346517	H	-6.859916	1.849526	0.613984
H	7.526329	-0.86093	-0.122512	H	-7.832291	0.448879	0.185903
H	6.744242	-0.822665	-1.696728	H	-6.561828	1.007835	-0.914552
H	-2.058071	4.489724	1.03052	H	3.480963	-2.400576	2.52191
H	-0.618978	4.028661	1.96691	H	4.411406	-3.391179	1.382024
H	-2.160098	3.196507	2.240504	H	2.814517	-3.937161	1.940689
H	0.11956	2.49752	-1.398292	H	2.067492	-2.795578	-1.574172
H	0.702632	3.643451	-0.17633	H	2.012248	-4.178725	-0.465033
H	-0.69823	4.060332	-1.185981	H	3.571927	-3.612766	-1.099614
H	0.503635	-0.360055	2.045354	H	-1.602333	-2.065701	-2.377912
H	1.753548	-1.509764	2.536974	H	-2.38882	-2.623349	-0.886252
H	0.149632	-2.100473	2.095923	H	-0.625111	-2.487083	-0.960786
H	4.203674	-1.441976	0.668017	H	-4.237891	-1.562963	-1.521186
H	3.544738	-0.33386	1.866311	H	-5.007958	-0.007493	-1.718143
H	2.637787	-0.520265	-1.056489	H	-2.960152	1.137935	-0.836112
H	1.953934	0.581461	0.135491	H	-2.774063	0.300362	-2.37388
H	-0.624285	1.781937	0.865502	H	1.744263	-2.006599	0.767225
H	-5.950897	0.750251	0.151229	H	5.432538	2.046377	1.095096
H	-4.71121	-3.561118	-0.058926	H	1.972611	4.778052	0.261017
H	2.556118	-2.99121	0.859133	H	-0.876095	-0.969912	0.96609
3b (9)				3b (10)			
C	3.734177	2.14284	0.312069	C	3.604425	-1.646069	-0.783532
C	2.800646	-0.085186	-0.198532	C	2.193872	0.248875	-0.067469
C	1.374808	1.938985	-0.148062	C	1.394082	-2.089785	0.076333
C	1.561995	0.575189	-0.348911	C	1.210272	-0.719026	0.233445
C	3.889756	0.767542	0.126915	C	3.401964	-0.276863	-0.599026
C	2.46558	2.730544	0.194358	C	2.595554	-2.559413	-0.442267
C	-5.333926	0.19676	-0.348958	C	-3.479533	0.82752	-1.345605
C	2.907994	-1.559023	-0.384749	C	1.925221	1.694938	0.158541
C	-6.074084	-0.815488	0.132091	C	-4.253884	1.726417	-0.714123
C	-0.091313	2.261989	-0.258902	C	0.147691	-2.818493	0.50344
C	-0.657774	0.942165	-0.834298	C	-0.693773	-1.666116	1.111096
C	-6.993498	-1.599608	-0.775739	C	-3.998142	3.208108	-0.868164
C	-6.085437	-1.266846	1.572843	C	-5.423128	1.383352	0.176307
C	4.955734	-3.023276	-0.429523	C	2.640192	3.306598	1.93248

C	3.082768	-3.460788	1.229025	C	3.311223	3.695246	-0.48628
C	-2.299544	-0.966782	-0.795353	C	-2.964052	-2.730751	1.187675
C	-4.400916	1.120078	0.394216	C	-3.578095	-0.678888	-1.356887
C	-3.070494	1.436377	-0.327668	C	-2.28759	-1.381244	-0.869491
C	3.881549	-2.385541	0.469714	C	3.049489	2.642127	0.605279
C	-1.944266	0.394124	-0.175905	C	-2.166596	-1.530543	0.669975
O	2.173842	-2.143874	-1.178333	O	0.783698	2.138572	0.050322
O	0.397494	-0.063139	-0.642875	O	-0.005401	-0.418763	0.757987
O	5.129737	0.204371	0.201338	O	4.363561	0.613449	-0.977057
O	2.248512	4.057063	0.396199	O	2.735412	-3.9019	-0.602634
O	-1.712068	0.244229	1.232986	O	-2.708575	-0.391632	1.355263
H	4.601747	2.758906	0.53799	H	4.539252	-2.002026	-1.21052
H	-5.433183	0.423027	-1.413342	H	-2.664422	1.218541	-1.959364
H	-0.524193	2.47793	0.725598	H	-0.353337	-3.300178	-0.345599
H	-0.304745	3.111211	-0.914607	H	0.340754	-3.599802	1.245386
H	-0.807252	1.023507	-1.91739	H	-0.680315	-1.711215	2.205553
H	-8.035525	-1.54091	-0.430424	H	-3.141513	3.410998	-1.518821
H	-6.956885	-1.236731	-1.808054	H	-4.875955	3.717289	-1.290634
H	-6.729831	-2.666807	-0.779229	H	-3.807529	3.679416	0.106158
H	-5.377452	-0.722375	2.201882	H	-5.55049	0.309792	0.325787
H	-5.850252	-2.337817	1.64516	H	-6.356909	1.785218	-0.241336
H	-7.086544	-1.141552	2.009124	H	-5.300863	1.847932	1.164173
H	5.628718	-3.649288	0.167508	H	2.481716	2.562572	2.721983
H	5.557608	-2.258765	-0.931334	H	1.71319	3.875337	1.81012
H	4.488341	-3.653629	-1.194091	H	3.426515	3.992196	2.26784
H	2.338005	-3.011295	1.89633	H	4.081391	4.40167	-0.156103
H	3.758742	-4.070508	1.838966	H	2.396397	4.259255	-0.699414
H	2.559112	-4.118645	0.528386	H	3.654258	3.227292	-1.414651
H	-2.514611	-0.868705	-1.865692	H	-2.575659	-3.672037	0.786153
H	-3.181155	-1.386853	-0.307669	H	-4.014372	-2.63963	0.893588
H	-1.464491	-1.665474	-0.681871	H	-2.921075	-2.772932	2.281412
H	-4.916423	2.083402	0.53092	H	-4.441625	-1.032743	-0.786518
H	-4.179843	0.751594	1.399729	H	-3.747694	-0.996424	-2.396148
H	-2.698288	2.387531	0.069043	H	-1.424516	-0.820099	-1.248507
H	-3.256749	1.595633	-1.398113	H	-2.230298	-2.379238	-1.319145
H	4.373298	-1.733832	1.194237	H	3.964822	2.069281	0.76567
H	5.779782	0.886105	0.438425	H	5.135206	0.130852	-1.316654
H	3.083422	4.493638	0.633713	H	3.613006	-4.098213	-0.970712
H	-0.974029	-0.382845	1.322514	H	-2.384641	0.403138	0.898889
3b (11)				3b (12)			
C	3.406353	2.339798	0.549706	C	-3.829367	-2.115886	0.437886
C	2.712667	-0.003504	0.207833	C	-2.941029	0.134598	-0.049591
C	1.16484	1.881733	-0.216606	C	-1.518643	-1.886405	-0.216675

C	1.455904	0.522592	-0.159563	C	-1.714045	-0.512244	-0.303718
C	3.67838	0.970719	0.577269	C	-4.007649	-0.735225	0.318856
C	2.142572	2.800181	0.149078	C	-2.58187	-2.696436	0.165513
C	-5.093006	0.330135	0.319998	C	4.802176	0.60518	-0.571934
C	2.950471	-1.472438	0.199164	C	-3.140446	1.602941	-0.189755
C	-5.850797	-0.671974	0.79366	C	5.713234	0.161398	0.315012
C	-0.270607	2.064156	-0.633281	C	-0.100493	-2.224654	-0.587986
C	-0.633037	0.638928	-1.11198	C	0.46492	-0.835785	-0.986357
C	-6.307921	-0.677974	2.234525	C	6.881097	-0.684172	-0.138722
C	-6.327004	-1.85631	-0.013589	C	5.698993	0.459122	1.795112
C	4.125257	-2.984795	-1.407552	C	-2.514304	3.473262	1.341974
C	4.955082	-2.779241	0.984949	C	-1.5793	3.39685	-1.01935
C	-2.174513	-1.353871	-1.179226	C	1.557294	-0.263264	1.249525
C	-4.569327	0.5325	-1.078475	C	3.595421	1.482023	-0.337162
C	-3.109589	1.028851	-1.161731	C	2.277401	0.909305	-0.905896
C	4.318519	-2.041306	-0.206091	C	-2.010398	2.567867	0.202358
C	-2.001292	0.082	-0.659255	C	1.762443	-0.401492	-0.266032
O	2.033847	-2.251311	0.452978	O	-4.209769	2.06967	-0.573893
O	0.402305	-0.243219	-0.554022	O	-0.591593	0.142136	-0.715019
O	4.890665	0.520873	1.011286	O	-5.216108	-0.178634	0.603215
O	1.82264	4.120563	0.106836	O	-2.35869	-4.034513	0.254967
O	-2.039379	0.090146	0.77458	O	2.658183	-1.488978	-0.551539
H	4.169902	3.048953	0.861292	H	-4.664931	-2.742691	0.74141
H	-4.830149	1.127983	1.0166	H	4.952286	0.326307	-1.617395
H	-0.895534	2.364441	0.216847	H	0.459596	-2.672535	0.239541
H	-0.405549	2.802591	-1.428837	H	-0.039494	-2.926901	-1.425957
H	-0.546352	0.562867	-2.202612	H	0.647355	-0.792876	-2.064938
H	-5.948166	0.199513	2.78159	H	6.89593	-1.649857	0.384816
H	-7.405088	-0.696467	2.30316	H	6.853447	-0.87825	-1.2155
H	-5.951573	-1.576268	2.758789	H	7.834283	-0.190208	0.095665
H	-7.425259	-1.878051	-0.05612	H	4.838125	1.051372	2.113109
H	-6.01941	-2.798345	0.461432	H	6.606706	1.008159	2.080878
H	-5.956175	-1.86039	-1.041427	H	5.705791	-0.47264	2.37639
H	3.705442	-2.454697	-2.270567	H	-2.790101	2.888775	2.227626
H	3.448008	-3.805057	-1.149763	H	-3.393547	4.04104	1.021133
H	5.088418	-3.411358	-1.709533	H	-1.731167	4.181393	1.63501
H	5.911907	-3.223828	0.688456	H	-0.8085	4.122426	-0.735597
H	4.296402	-3.582468	1.333423	H	-2.43496	3.944989	-1.428274
H	5.141221	-2.096695	1.820437	H	-1.170096	2.756977	-1.808531
H	-2.223493	-1.378984	-2.274186	H	0.897488	0.576859	1.488159
H	-3.093893	-1.788535	-0.779348	H	2.516166	-0.094473	1.749155
H	-1.332837	-1.978026	-0.863611	H	1.125975	-1.17516	1.673507
H	-4.69163	-0.369199	-1.686071	H	3.475016	1.724534	0.7229

H	-5.178789	1.305598	-1.572837	H	3.76582	2.442922	-0.845444
H	-3.023213	1.971598	-0.6079	H	2.407183	0.723251	-1.980718
H	-2.898067	1.263958	-2.213203	H	1.496573	1.672462	-0.809143
H	4.977689	-1.223185	-0.503059	H	-1.151689	1.997561	0.562121
H	5.462149	1.279033	1.216691	H	-5.815761	-0.876807	0.914503
H	2.592571	4.652207	0.368999	H	-3.175453	-4.485998	0.525629
H	-1.286872	-0.454682	1.065095	H	3.549163	-1.199958	-0.280248
3b (13)				3b (14)			
C	-3.108745	-1.541997	1.534467	C	3.264186	2.58646	0.201608
C	-2.11327	0.194079	0.0904	C	2.937917	0.184227	-0.260191
C	-1.235104	-2.120932	0.12801	C	1.038744	1.770779	-0.252823
C	-1.206605	-0.805599	-0.322106	C	1.569916	0.496065	-0.423339
C	-3.067183	-0.231397	1.052925	C	3.76956	1.294697	0.044612
C	-2.191456	-2.494836	1.066383	C	1.886881	2.823025	0.070997
C	4.016341	0.783674	0.273288	C	-5.529373	0.242107	0.507255
C	-2.008182	1.577321	-0.449523	C	3.423247	-1.214771	-0.40851
C	4.24318	1.871545	1.028853	C	-6.696374	-0.216346	0.026174
C	-0.154462	-2.916417	-0.555684	C	-0.457159	1.716672	-0.399271
C	0.533029	-1.835214	-1.431877	C	-0.687049	0.230486	-0.791136
C	4.602824	3.191474	0.385224	C	-7.889173	0.702339	-0.106429
C	4.172495	1.91981	2.536717	C	-6.953339	-1.636446	-0.417869
C	-3.316775	2.827028	-2.17483	C	5.769042	-2.134069	-0.370256
C	-3.24997	3.661513	0.22351	C	4.021431	-2.957706	1.278988
C	2.893564	-2.674039	-1.565255	C	-1.647227	-2.037913	-0.235695
C	3.65005	-0.605985	0.7311	C	-4.235386	-0.503297	0.708457
C	2.229225	-1.077271	0.328189	C	-3.109012	0.058872	-0.18301
C	-3.267652	2.422691	-0.689764	C	4.551963	-1.747316	0.488177
C	2.01713	-1.492174	-1.146351	C	-1.702304	-0.535998	0.079632
O	-0.913293	2.038302	-0.76706	O	2.883132	-1.984105	-1.200733
O	-0.238067	-0.59958	-1.251587	O	0.619477	-0.425994	-0.709091
O	-3.927717	0.705839	1.5434	O	5.112837	1.068325	0.12856
O	-2.187396	-3.784451	1.494631	O	1.334441	4.054043	0.241021
O	2.358592	-0.416132	-2.037793	O	-1.299627	-0.302797	1.439779
H	-3.844457	-1.81808	2.286331	H	3.941047	3.411082	0.412913
H	4.090993	0.899101	-0.806324	H	-5.484064	1.297476	0.784707
H	0.537623	-3.382712	0.15431	H	-0.96277	1.962821	0.540364
H	-0.56176	-3.723787	-1.174751	H	-0.837458	2.396246	-1.169014
H	0.457242	-2.072914	-2.496609	H	-0.998887	0.142526	-1.837082
H	4.647529	3.115574	-0.706034	H	-8.234572	0.753089	-1.148676
H	3.87104	3.970193	0.643593	H	-8.740221	0.332188	0.482634
H	5.577268	3.554663	0.742236	H	-7.661639	1.719949	0.226957
H	3.904181	0.964009	2.992791	H	-7.762696	-2.086281	0.17401
H	3.434867	2.666106	2.863523	H	-6.07751	-2.284027	-0.334647

H	5.136659	2.235629	2.959506	H	-7.289315	-1.656834	-1.463862
H	-3.366624	1.948535	-2.828868	H	5.4868	-2.885201	-1.116198
H	-2.427913	3.404398	-2.447591	H	6.560253	-2.556176	0.259843
H	-4.20305	3.441975	-2.367591	H	6.177856	-1.263127	-0.892693
H	-3.268741	3.375702	1.280228	H	3.689337	-3.747552	0.59791
H	-4.124472	4.29144	0.025061	H	3.174677	-2.680105	1.917756
H	-2.348713	4.256946	0.040852	H	4.810686	-3.362666	1.922377
H	2.726047	-3.54295	-0.921061	H	-2.334121	-2.595839	0.410293
H	3.951563	-2.404051	-1.507777	H	-0.636452	-2.419154	-0.075098
H	2.676721	-2.959748	-2.60012	H	-1.934557	-2.23353	-1.27484
H	4.391138	-1.320147	0.345635	H	-3.931525	-0.397144	1.760607
H	3.715225	-0.675458	1.821725	H	-4.365655	-1.573915	0.525572
H	1.517257	-0.278518	0.56961	H	-3.060481	1.144546	-0.031691
H	1.967845	-1.931716	0.964691	H	-3.372499	-0.100719	-1.236608
H	-4.153108	1.828197	-0.456911	H	4.852803	-0.970396	1.193572
H	-4.523221	0.291575	2.189351	H	5.567505	1.89786	0.349493
H	-2.894544	-3.916246	2.14801	H	2.025954	4.6928	0.481476
H	1.745858	0.310833	-1.82859	H	-1.763528	-0.944889	1.9994
3b (15)				3b (16)			
C	-4.029083	-1.144732	-0.493821	C	-4.044863	-1.143645	-0.379209
C	-2.24088	0.542907	-0.272121	C	-2.265344	0.507922	0.06262
C	-1.727462	-1.869697	-0.494097	C	-1.738281	-1.840861	-0.517169
C	-1.337955	-0.538781	-0.376981	C	-1.357873	-0.548287	-0.169631
C	-3.612417	0.180197	-0.353162	C	-3.635019	0.148884	-0.046267
C	-3.081886	-2.177984	-0.553687	C	-3.091405	-2.143759	-0.622721
C	4.822711	0.053177	0.035374	C	4.825328	0.065197	0.028706
C	-1.741391	1.933384	-0.093138	C	-1.776818	1.868569	0.418882
C	5.227447	1.164803	-0.600344	C	5.195516	1.271321	-0.431754
C	-0.5107	-2.75469	-0.51763	C	-0.513756	-2.688455	-0.734264
C	0.635461	-1.72072	-0.353024	C	0.627328	-1.675353	-0.447366
C	6.477701	1.892834	-0.162489	C	6.460401	1.93183	0.066801
C	4.522692	1.795444	-1.777436	C	4.434723	2.078945	-1.455889
C	-3.027606	4.097811	-0.132337	C	-1.523359	3.961563	-0.924198
C	-1.611937	3.466188	1.879274	C	-3.066707	3.925158	1.092807
C	0.701324	-1.823417	2.201088	C	0.83425	-2.20874	2.043368
C	3.616046	-0.806353	-0.238909	C	3.612268	-0.752571	-0.330825
C	2.638967	-0.816238	0.95406	C	2.691042	-0.971925	0.886803
C	-2.526753	2.94496	0.756225	C	-2.508254	3.118656	-0.092884
C	1.519793	-1.884141	0.903853	C	1.581368	-2.036085	0.713348
O	-0.660161	2.273697	-0.569211	O	-0.746748	2.009444	1.074758
O	0.011537	-0.398502	-0.314429	O	-0.008638	-0.397102	-0.134107
O	-4.532837	1.186884	-0.338979	O	-4.561636	1.108655	0.239143
O	-3.428999	-3.486549	-0.676418	O	-3.43174	-3.416446	-0.958696

O	2.081773	-3.197137	0.730731	O	2.144453	-3.290307	0.290639
H	-5.089669	-1.37204	-0.572053	H	-5.105698	-1.376539	-0.431987
H	5.429955	-0.286662	0.877598	H	5.471097	-0.401131	0.776417
H	-0.507311	-3.500434	0.283317	H	-0.467361	-3.55653	-0.069099
H	-0.411422	-3.304047	-1.460627	H	-0.44894	-3.072929	-1.758264
H	1.282993	-1.7263	-1.232525	H	1.224359	-1.509738	-1.347078
H	7.208587	1.951256	-0.981553	H	7.15685	2.128579	-0.760711
H	6.251108	2.930023	0.122647	H	6.242898	2.907245	0.524706
H	6.960896	1.403853	0.689632	H	6.979052	1.315698	0.808419
H	4.259001	2.838564	-1.554252	H	4.159665	3.060238	-1.044802
H	3.607789	1.273666	-2.066985	H	3.519577	1.59227	-1.800887
H	5.185166	1.826373	-2.653881	H	5.062761	2.278719	-2.335367
H	-2.184962	4.588112	-0.632348	H	-0.666196	4.266243	-0.315471
H	-3.548983	4.846343	0.475206	H	-2.022119	4.863212	-1.297057
H	-3.722109	3.736286	-0.897485	H	-1.146307	3.402168	-1.788414
H	-0.724851	3.95176	1.460912	H	-2.258588	4.210814	1.775261
H	-1.278106	2.653185	2.534814	H	-3.805458	3.344372	1.654518
H	-2.150296	4.196205	2.494142	H	-3.553052	4.839619	0.734494
H	1.359991	-1.98142	3.063348	H	1.539639	-2.509093	2.827329
H	-0.072318	-2.596594	2.22564	H	0.062015	-2.980814	1.975564
H	0.224956	-0.84545	2.320136	H	0.366896	-1.269867	2.355857
H	3.100072	-0.475969	-1.145573	H	3.054152	-0.284383	-1.147431
H	3.940845	-1.840154	-0.421729	H	3.934096	-1.737971	-0.695684
H	2.178661	0.172629	1.061855	H	2.226044	-0.02222	1.175149
H	3.210433	-0.990977	1.877407	H	3.307498	-1.284866	1.742419
H	-3.389638	2.450127	1.205837	H	-3.339167	2.815285	-0.732819
H	-5.425924	0.807783	-0.387357	H	-5.453327	0.739421	0.128476
H	-4.396899	-3.568205	-0.704366	H	-4.399159	-3.495972	-1.004724
H	2.647105	-3.374768	1.500512	H	2.749976	-3.585965	0.990353
3b (17)				3b (18)			
C	2.885016	2.727335	0.260349	C	-4.025956	-1.577587	-0.33455
C	2.884079	0.299076	-0.18648	C	-2.504136	0.366642	-0.306297
C	0.824189	1.657449	-0.394482	C	-1.642223	-1.954432	-0.354411
C	1.511203	0.450847	-0.487036	C	-1.452542	-0.575689	-0.357429
C	3.547463	1.501422	0.179149	C	-3.807947	-0.198728	-0.314669
C	1.510727	2.803919	-0.01285	C	-2.936667	-2.461785	-0.341344
C	-5.578859	-0.726693	-0.335172	C	4.450379	1.056224	-0.503305
C	3.536934	-1.035667	-0.268381	C	-2.214569	1.825542	-0.252184
C	-6.52441	-0.04917	0.335941	C	5.792692	1.067037	-0.45999
C	-0.63323	1.432219	-0.690273	C	-0.308505	-2.65142	-0.345054
C	-0.654035	-0.074891	-1.06801	C	0.67503	-1.450276	-0.346801
C	-7.833731	0.308448	-0.329221	C	6.553508	2.372921	-0.43752
C	-6.408047	0.413354	1.768457	C	6.667854	-0.163119	-0.433733

C	5.981314	-1.606679	-0.068738	C	-3.800319	3.772474	-0.422714
C	4.264849	-2.708897	1.443867	C	-2.281038	3.510413	1.596235
C	-1.393546	-2.432912	-0.554484	C	0.932584	-1.317673	2.192156
C	-4.219198	-1.169415	0.140649	C	3.517762	-0.127061	-0.52359
C	-3.087571	-0.522223	-0.684436	C	2.605127	-0.153993	0.719195
C	4.663481	-1.418887	0.704404	C	-3.12617	2.777278	0.538427
C	-1.65272	-0.944385	-0.278829	C	1.659646	-1.373127	0.841223
O	3.142934	-1.875355	-1.075779	O	-1.205493	2.281614	-0.786152
O	0.704972	-0.575258	-0.849056	O	-0.1379	-0.234588	-0.354655
O	4.891899	1.437649	0.403302	O	-4.866293	0.660909	-0.354434
O	0.809096	3.96573	0.071568	O	-3.086839	-3.812727	-0.343821
O	-1.409106	-0.649588	1.107066	O	2.399234	-2.601905	0.724577
H	3.440225	3.624615	0.523282	H	-5.042168	-1.964003	-0.361486
H	-5.798308	-0.99621	-1.370579	H	3.944755	2.024451	-0.514943
H	-1.258799	1.630536	0.1863	H	-0.169662	-3.294754	0.529548
H	-1.004678	2.054969	-1.510782	H	-0.158083	-3.282592	-1.227773
H	-0.852415	-0.211585	-2.136147	H	1.251431	-1.436804	-1.27467
H	-8.684855	-0.123104	0.216335	H	7.181607	2.44907	0.461435
H	-7.99021	1.396437	-0.333618	H	7.235067	2.448426	-1.296701
H	-7.877743	-0.046095	-1.364029	H	5.882855	3.23797	-0.458367
H	-6.530134	1.50351	1.832271	H	7.350127	-0.170693	-1.295271
H	-5.453602	0.154675	2.232422	H	6.102246	-1.097558	-0.445858
H	-7.209535	-0.02255	2.381032	H	7.304212	-0.164693	0.462244
H	5.864877	-2.374794	-0.841489	H	-3.044104	4.339962	-0.976547
H	6.779443	-1.923354	0.612467	H	-4.420593	4.48175	0.137076
H	6.294629	-0.674883	-0.550209	H	-4.441891	3.254882	-1.1432
H	4.102081	-3.526431	0.734756	H	-1.478467	4.083642	1.121834
H	3.343775	-2.571488	2.022435	H	-1.825242	2.807206	2.303294
H	5.058902	-3.004468	2.138806	H	-2.910774	4.201978	2.167205
H	-2.07697	-3.061504	0.026745	H	1.665795	-1.308631	3.007417
H	-0.368775	-2.693405	-0.280994	H	0.283345	-2.186326	2.336528
H	-1.543249	-2.669983	-1.613799	H	0.32766	-0.409646	2.276514
H	-4.075817	-0.928696	1.19894	H	2.897722	-0.063483	-1.429434
H	-4.156965	-2.263517	0.053577	H	4.062862	-1.073123	-0.58593
H	-3.17738	0.566246	-0.585254	H	2.000097	0.759947	0.757022
H	-3.23438	-0.754609	-1.747821	H	3.239778	-0.139537	1.616475
H	4.799012	-0.620532	1.436583	H	-3.901963	2.201057	1.045792
H	5.218308	2.318672	0.650061	H	-5.695077	0.154304	-0.344025
H	1.399998	4.685722	0.348345	H	-4.031933	-4.03784	-0.327108
H	-1.86925	-1.319101	1.637008	H	3.041673	-2.623246	1.452945
3b (19)				3b (20)			
C	2.992191	2.8528	0.076718	C	-4.351583	-0.453098	-0.364581
C	3.02723	0.38812	0.171685	C	-2.35854	0.915472	0.129268

C	0.971497	1.632885	-0.422694	C	-2.167121	-1.46478	-0.528379
C	1.666918	0.451187	-0.192443	C	-1.611989	-0.24562	-0.155851
C	3.665871	1.652564	0.317633	C	-3.770108	0.757487	0.021757
C	1.636717	2.845501	-0.285138	C	-3.549384	-1.571381	-0.635249
C	-5.434936	-0.757546	-0.340406	C	4.61356	-0.554408	-0.081666
C	3.754561	-0.889072	0.407196	C	-1.742549	2.209829	0.530557
C	-6.422783	0.071921	0.033283	C	5.125775	0.626434	-0.465033
C	-0.470126	1.321866	-0.716957	C	-1.078825	-2.487382	-0.711325
C	-0.462603	-0.230949	-0.757736	C	0.196279	-1.649934	-0.42316
C	-7.662635	0.225021	-0.81755	C	6.506052	1.050435	-0.0182
C	-6.422169	0.911403	1.288197	C	4.423333	1.629629	-1.348183
C	3.127584	-3.334376	0.34342	C	0.640118	2.907285	0.974505
C	4.721282	-2.341674	-1.368231	C	-0.684715	3.920609	-0.942516
C	-1.26935	-2.432582	0.18299	C	0.411214	-2.306933	2.036875
C	-4.128127	-1.040889	0.354746	C	3.269867	-1.151909	-0.409854
C	-2.92191	-0.60989	-0.505165	C	2.393007	-1.313752	0.848538
C	3.470936	-2.096647	-0.499622	C	-0.417511	2.650689	-0.111146
C	-1.532881	-0.921594	0.108874	C	1.127157	-2.189157	0.684319
O	4.626527	-0.982257	1.26688	O	-2.297764	2.965313	1.323868
O	0.872506	-0.646216	-0.312549	O	-0.254869	-0.309619	-0.042991
O	4.985178	1.666032	0.651676	O	-4.553269	1.844039	0.259863
O	0.930782	3.986234	-0.508366	O	-4.065188	-2.775251	-0.999228
O	-1.410675	-0.335488	1.415413	O	1.481165	-3.493623	0.191824
H	3.522195	3.79762	0.173693	H	-5.432974	-0.52714	-0.455227
H	-5.568521	-1.302223	-1.277561	H	5.232272	-1.177665	0.568074
H	-1.133013	1.694132	0.071338	H	-1.177427	-3.338276	-0.029457
H	-0.813555	1.743476	-1.667153	H	-1.053408	-2.898947	-1.72602
H	-0.562949	-0.597125	-1.784788	H	0.779285	-1.528808	-1.339071
H	-8.565707	-0.046587	-0.252812	H	7.162714	1.231489	-0.881015
H	-7.798494	1.269326	-1.13252	H	6.467035	1.994981	0.542749
H	-7.622609	-0.398983	-1.71617	H	6.980702	0.296227	0.617768
H	-6.522104	1.97681	1.038654	H	4.335142	2.597671	-0.835357
H	-5.519151	0.79096	1.890784	H	3.420441	1.317455	-1.648404
H	-7.285413	0.660909	1.920347	H	5.005505	1.817431	-2.261278
H	3.939264	-3.557337	1.043822	H	0.284858	3.662369	1.683867
H	2.978198	-4.207394	-0.301838	H	1.571183	3.268053	0.522992
H	2.210191	-3.179246	0.922315	H	0.866052	1.992048	1.532834
H	5.590877	-2.555604	-0.737836	H	-1.069975	4.723352	-0.305302
H	4.956271	-1.470017	-1.990286	H	-1.416823	3.734221	-1.737089
H	4.556651	-3.196829	-2.033302	H	0.242885	4.265819	-1.412709
H	-2.02467	-2.929686	0.801378	H	1.093811	-2.733158	2.78155
H	-0.287772	-2.622721	0.622766	H	-0.463941	-2.960201	1.973149
H	-1.301147	-2.889306	-0.812511	H	0.090566	-1.325312	2.398811

H	-4.078828	-0.532109	1.322794	H	2.74715	-0.547621	-1.157603
H	-4.067645	-2.119237	0.560241	H	3.414437	-2.146174	-0.854914
H	-3.000834	0.470067	-0.677667	H	2.09797	-0.325995	1.221451
H	-2.98564	-1.09172	-1.490049	H	2.997974	-1.771426	1.644861
H	2.6297	-1.868798	-1.156847	H	-0.055723	1.866059	-0.778484
H	5.304397	2.583276	0.626804	H	-5.475866	1.614458	0.060001
H	1.504781	4.758133	-0.371001	H	-5.035014	-2.721872	-1.027409
H	-1.932619	-0.874519	2.030189	H	2.066349	-3.903002	0.850473
3b (21)				3b (22)			
C	-4.06917	-1.599625	0.142965	C	-3.43739	2.607187	-0.06803
C	-2.573182	0.359456	0.032545	C	-3.095669	0.165767	-0.131232
C	-1.738373	-1.932612	-0.389575	C	-1.227284	1.722442	0.326198
C	-1.544953	-0.560578	-0.264885	C	-1.744123	0.443621	0.151685
C	-3.850472	-0.224152	0.243807	C	-3.929738	1.312264	-0.250438
C	-3.008805	-2.458979	-0.18285	C	-2.078129	2.815666	0.211364
C	4.753958	1.027712	0.521473	C	5.419238	0.483432	-0.259462
C	-2.282391	1.815703	0.133703	C	-3.626375	-1.213779	-0.320853
C	5.969802	1.116364	-0.041807	C	6.573003	-0.065801	0.153574
C	-0.439477	-2.593672	-0.76394	C	0.258759	1.641313	0.543382
C	0.535534	-1.386677	-0.790591	C	0.49561	0.106018	0.58826
C	6.625956	2.461905	-0.251161	C	7.719726	0.805629	0.612015
C	6.79625	-0.05714	-0.510518	C	6.859276	-1.547333	0.206729
C	-2.661804	3.700179	-1.461319	C	-2.832786	-3.61218	-0.153283
C	-3.76076	3.731619	0.829613	C	-4.28312	-2.567319	1.6535
C	1.199001	-1.51965	1.670193	C	1.564251	-1.955297	-0.409537
C	3.932523	-0.203881	0.804186	C	4.168583	-0.20303	-0.744165
C	2.617905	-0.209368	-0.002837	C	2.960464	0.107182	0.163333
C	-3.307513	2.852779	-0.349148	C	-3.157439	-2.329119	0.624266
C	1.703715	-1.437038	0.224056	C	1.597132	-0.421333	-0.351722
O	-1.191717	2.205799	0.545723	O	-4.486827	-1.458465	-1.161438
O	-0.262526	-0.192451	-0.519516	O	-0.785496	-0.517141	0.239027
O	-4.869383	0.607156	0.607188	O	-5.253351	1.112243	-0.498224
O	-3.164806	-3.804064	-0.304234	O	-1.54387	4.055545	0.37636
O	2.393067	-2.646159	-0.143499	O	1.295426	0.126519	-1.64543
H	-5.059623	-2.00545	0.335447	H	-4.11261	3.45641	-0.145506
H	4.268488	1.962755	0.80931	H	5.350885	1.573291	-0.240586
H	-0.11925	-3.357273	-0.048332	H	0.814045	2.103723	-0.279444
H	-0.488622	-3.081476	-1.744046	H	0.581611	2.120824	1.473231
H	0.962738	-1.250523	-1.78859	H	0.723412	-0.227553	1.605918
H	7.589231	2.51803	0.275348	H	8.003338	0.571925	1.647937
H	6.845508	2.632814	-1.314602	H	8.616509	0.632575	0.000372
H	5.996161	3.28451	0.102576	H	7.471818	1.870589	0.55859
H	7.029701	0.039059	-1.579982	H	7.721194	-1.797013	-0.42764

H	6.306573	-1.021947	-0.359866	H	6.017827	-2.166038	-0.113581
H	7.761648	-0.083494	0.013923	H	7.130855	-1.849813	1.227598
H	-1.767469	4.208689	-1.087776	H	-3.700356	-3.938235	-0.735764
H	-3.369286	4.457509	-1.817378	H	-2.557066	-4.417155	0.537111
H	-2.369447	3.082148	-2.318451	H	-1.996924	-3.458328	-0.845515
H	-2.898873	4.228731	1.288089	H	-5.201081	-2.892221	1.151497
H	-4.265106	3.135075	1.596846	H	-4.50807	-1.657749	2.222471
H	-4.459004	4.502258	0.483803	H	-3.984255	-3.345557	2.364561
H	2.03772	-1.636464	2.365004	H	2.3262	-2.333708	-1.099718
H	0.534345	-2.377287	1.811198	H	0.586955	-2.298418	-0.756353
H	0.659527	-0.608863	1.946739	H	1.760814	-2.392649	0.575726
H	4.500023	-1.113473	0.580492	H	3.942545	0.158827	-1.758509
H	3.703324	-0.231332	1.878945	H	4.318661	-1.283589	-0.821862
H	2.870288	-0.171608	-1.070639	H	2.890056	1.19594	0.279175
H	2.044574	0.698844	0.218995	H	3.146741	-0.304854	1.1636
H	-4.178648	2.338391	-0.759355	H	-2.265719	-1.998094	1.159982
H	-5.686128	0.091314	0.709229	H	-5.710578	1.968634	-0.462823
H	-4.092705	-4.042398	-0.141702	H	-2.235986	4.728001	0.262799
H	3.020774	-2.854858	0.566028	H	1.83817	-0.34136	-2.299125
3b (23)							
C	-4.348624	-1.106434	-0.171801				
C	-2.652823	0.666558	0.084182				
C	-2.018799	-1.665617	-0.457312				
C	-1.704046	-0.336494	-0.197441				
C	-4.004812	0.220092	0.101466				
C	-3.353572	-2.055576	-0.448132				
C	4.352912	0.731738	-0.232481				
C	-2.289803	2.082629	0.364951				
C	5.688657	0.595836	-0.265736				
C	-0.757266	-2.453099	-0.684978				
C	0.337772	-1.371542	-0.47699				
C	6.591449	1.774669	0.016906				
C	6.420245	-0.687425	-0.578366				
C	-0.089775	3.305658	0.541111				
C	-1.750839	3.853157	-1.302298				
C	0.649728	-1.814897	2.020305				
C	3.293599	-0.311653	-0.476135				
C	2.41351	-0.532403	0.770968				
C	-1.146293	2.741363	-0.422238				
C	1.345513	-1.646399	0.66206				
O	-2.923548	2.759089	1.170436				
O	-0.358799	-0.115111	-0.19292				
O	-4.977361	1.139263	0.346716				

O	-3.635394	-3.359776	-0.708348				
O	1.952164	-2.886121	0.255351				
H	-5.39521	-1.402384	-0.170909				
H	3.958826	1.720818	0.01168				
H	-0.642497	-3.290303	0.010256				
H	-0.70407	-2.87345	-1.695489				
H	0.893663	-1.210615	-1.402911				
H	7.252892	1.570048	0.870693				
H	7.249054	1.983419	-0.838937				
H	6.021828	2.683217	0.23748				
H	7.063196	-0.561172	-1.460691				
H	5.752961	-1.531186	-0.76813				
H	7.086588	-0.963037	0.250832				
H	-0.547783	4.016236	1.237206				
H	0.696938	3.826163	-0.016447				
H	0.380235	2.507351	1.126341				
H	-2.25043	4.604327	-0.681742				
H	-2.485494	3.451236	-2.009931				
H	-0.962031	4.348377	-1.879527				
H	1.391874	-2.063777	2.787909				
H	-0.089887	-2.620465	1.997417				
H	0.150977	-0.889719	2.32515				
H	2.662859	0.023781	-1.31217				
H	3.727946	-1.268552	-0.779039				
H	1.915093	0.405093	1.046245				
H	3.067289	-0.789474	1.616356				
H	-0.674755	2.000691	-1.071022				
H	-5.84363	0.712704	0.239328				
H	-4.595646	-3.502395	-0.663996				
H	2.602318	-3.126646	0.935917				

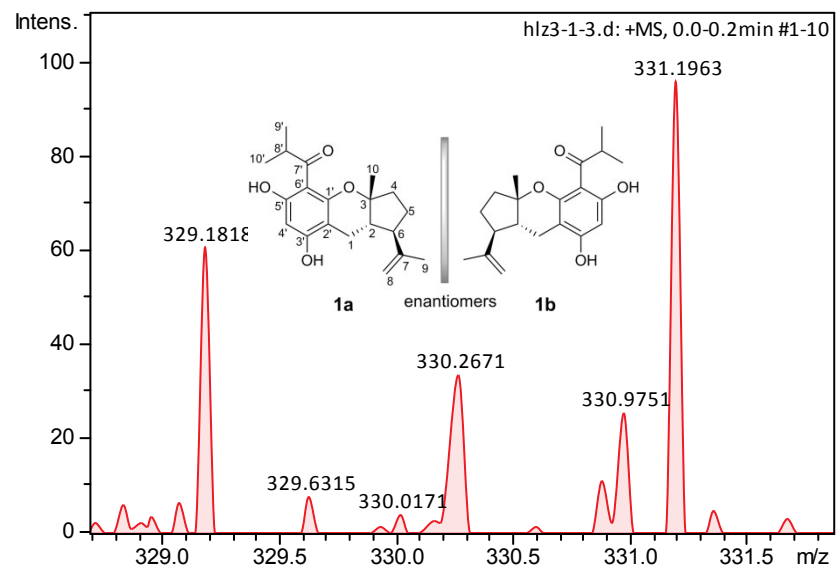
Key transitions, oscillator strengths, and rotatory strengths in the ECD of conformers **3b** (2) at B3LYP /6-311++G(d,p) level.

Species	Excited State	$\Delta E(eV)^a$	$\lambda(nm)^b$	f^c	R_{vel}^d
3b (2)	94 -> 95	3.918700	316.39	0.0305	-75.8784
	91 ->106	3.937700	314.86	0.0308	53.8871
	93 -> 95	4.528300	273.8	0.3085	40.2122
	94 -> 95	4.620700	268.32	0.0115	-0.367
	94 ->104	5.112700	242.5	0.0023	-1.5119
	92 -> 97	5.387300	230.14	0.0899	14.9736
	93 -> 96	5.478400	226.31	0.0012	-1.3631
	93 -> 98	5.484200	226.08	0.005	-9.8991
	92 -> 96	5.513300	224.88	0.0283	13.2656

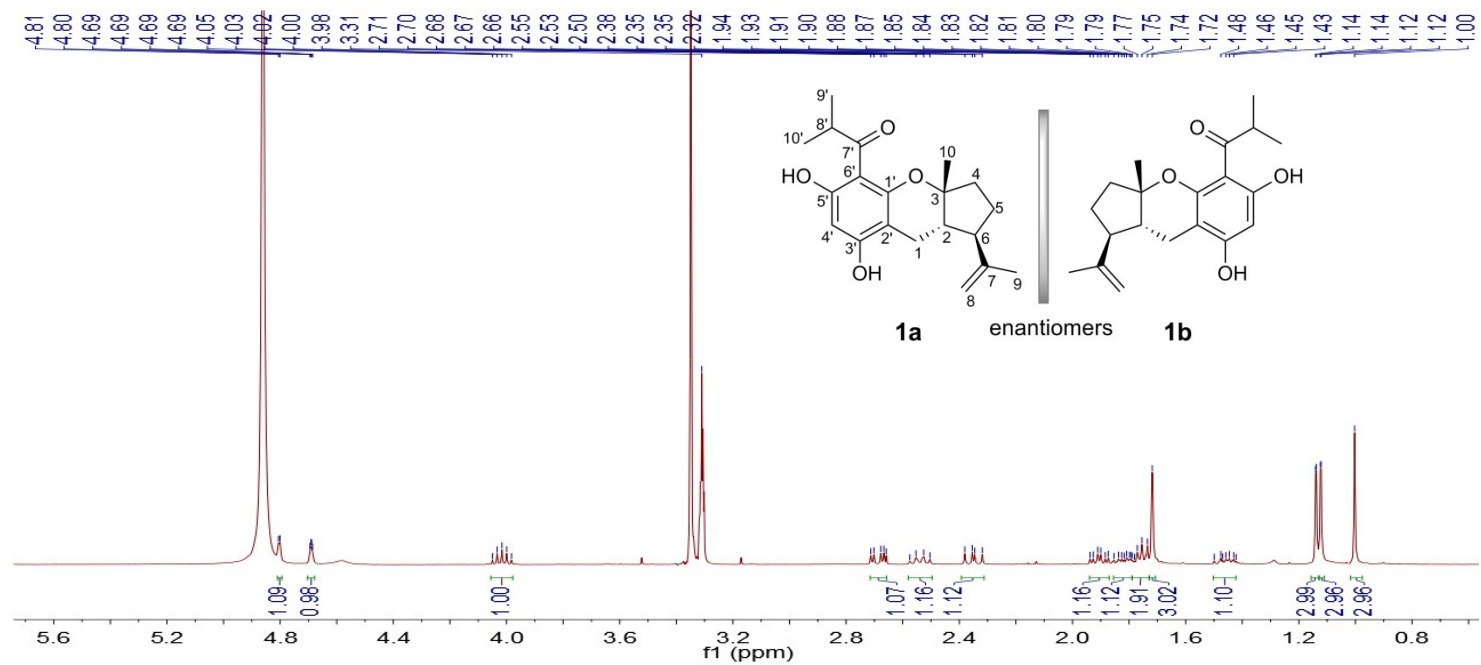
	94 -> 98	5.520600	224.58	0.0927	1.4995
	94 -> 96	5.555800	223.16	0.0171	1.65
	94 -> 97	5.664500	218.88	0.023	-0.0083
	93 -> 96	5.783600	214.37	0.0029	-5.345
	93 -> 97	5.811700	213.33	0.0045	-0.5347
	93 -> 99	5.867800	211.29	0.0002	-0.7141
	92 -> 99	5.872700	211.12	0.0006	-0.2906
	92 ->100	5.895400	210.31	0.0057	4.8729
	92 -> 98	5.906800	209.9	0.0048	-2.7276
	91 -> 97	5.917100	209.54	0.0137	-0.5534
	94 ->102	5.971800	207.62	0.0504	-42.6022
	91 -> 99	5.972500	207.59	0.004	-3.7499
	89 -> 95	5.981000	207.3	0.011	-10.7148
	94 ->101	6.009900	206.3	0.0104	-3.0651
	94 ->102	6.035900	205.41	0.0003	-2.7403
	93 ->101	6.073300	204.15	0.0798	-4.896
	94 ->103	6.089400	203.61	0.006	11.9507
	93 ->102	6.128200	202.32	0.0403	10.4256
	92 -> 97	6.162500	201.19	0.0472	9.4553
	92 ->100	6.200500	199.96	0.0721	3.0761
	93 ->101	6.238400	198.74	0.0833	-20.8478
	92 ->106	6.258400	198.11	0.0245	6.1696
	92 ->102	6.321300	196.14	0.0684	31.3548
	94 ->106	6.349800	195.26	0.1312	-41.1168
	91 ->100	6.367200	194.72	0.1481	-2.2898
	92 ->101	6.393300	193.93	0.0191	-7.9926
	91 -> 98	6.404700	193.58	0.0041	11.0496
	92 ->104	6.407900	193.49	0.0043	-4.4652
	93 ->104	6.421300	193.08	0.0702	20.2539
	91 ->104	6.446100	192.34	0.0119	25.4312
	92 ->104	6.463700	191.82	0.0074	-15.6493

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

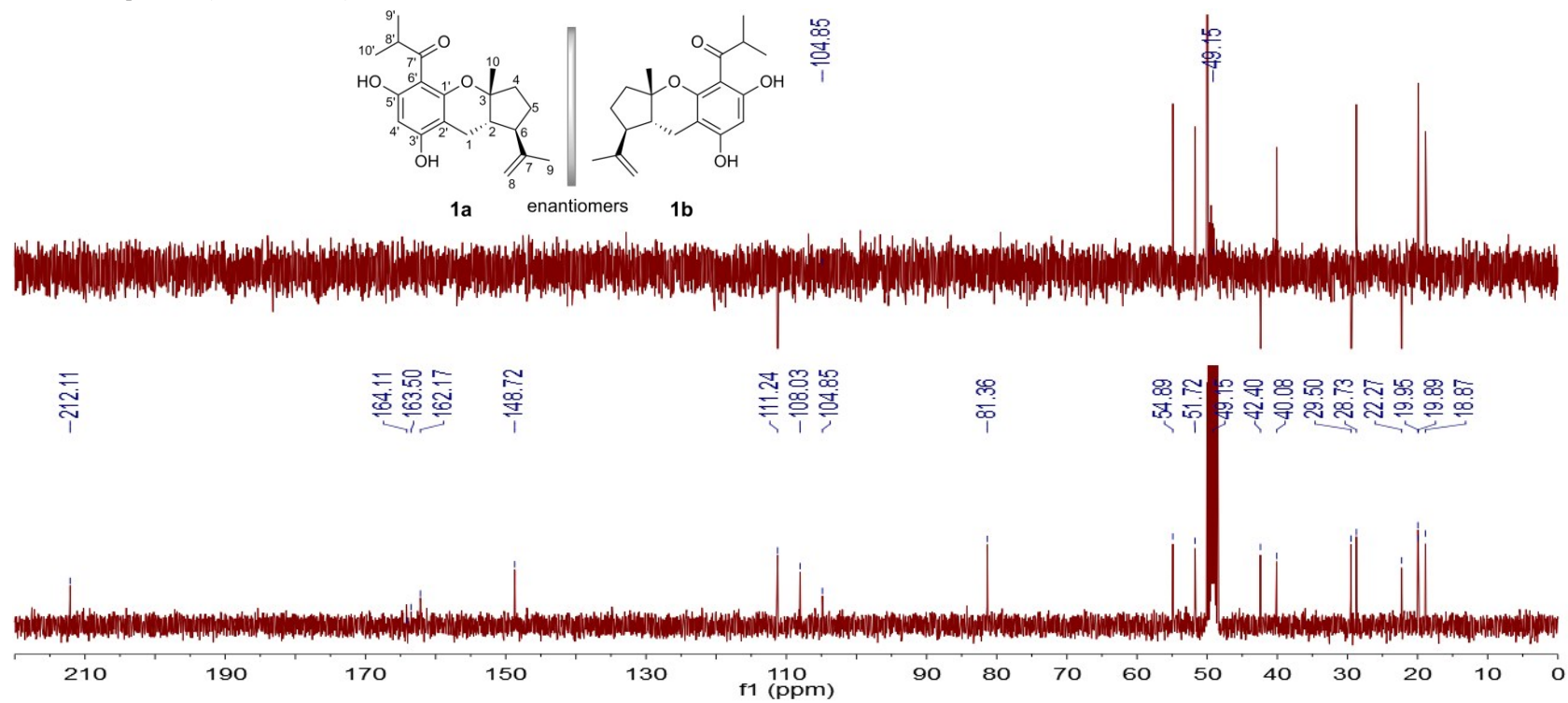
HRESIMS of compound **1**



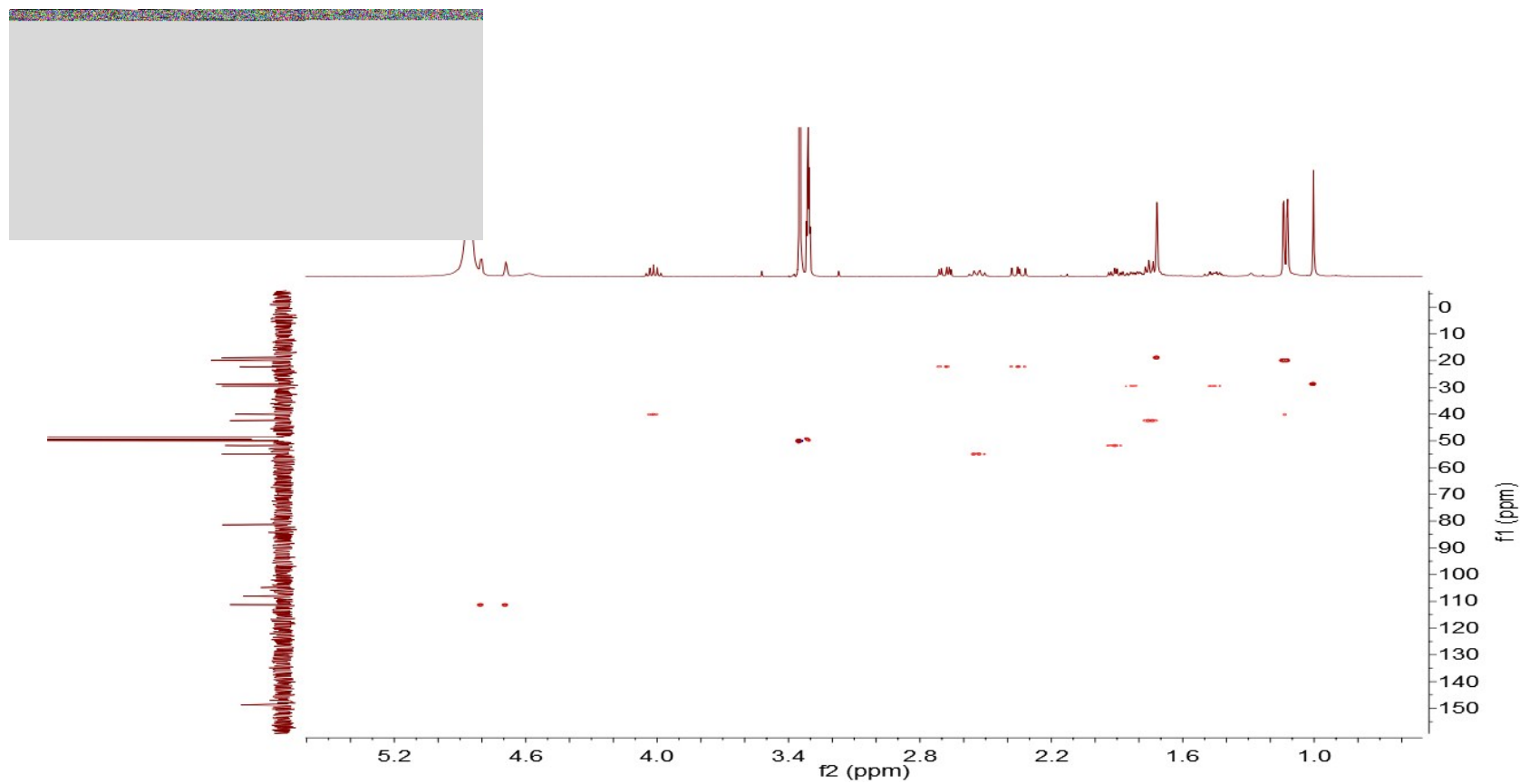
¹H NMR of compound **1** (in methanol-*d*₄)



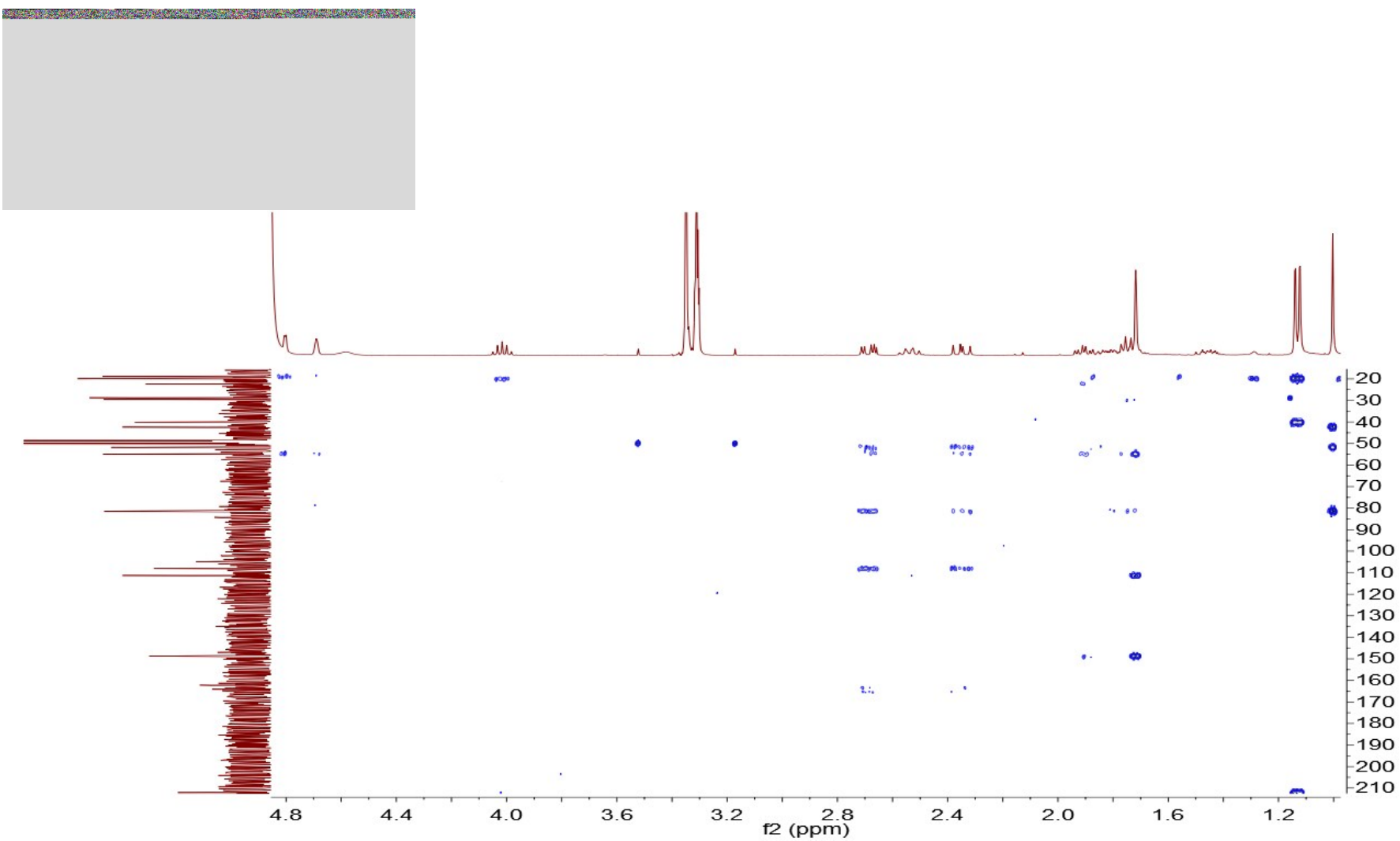
^{13}C NMR of compound **1** (in methanol- d_4)



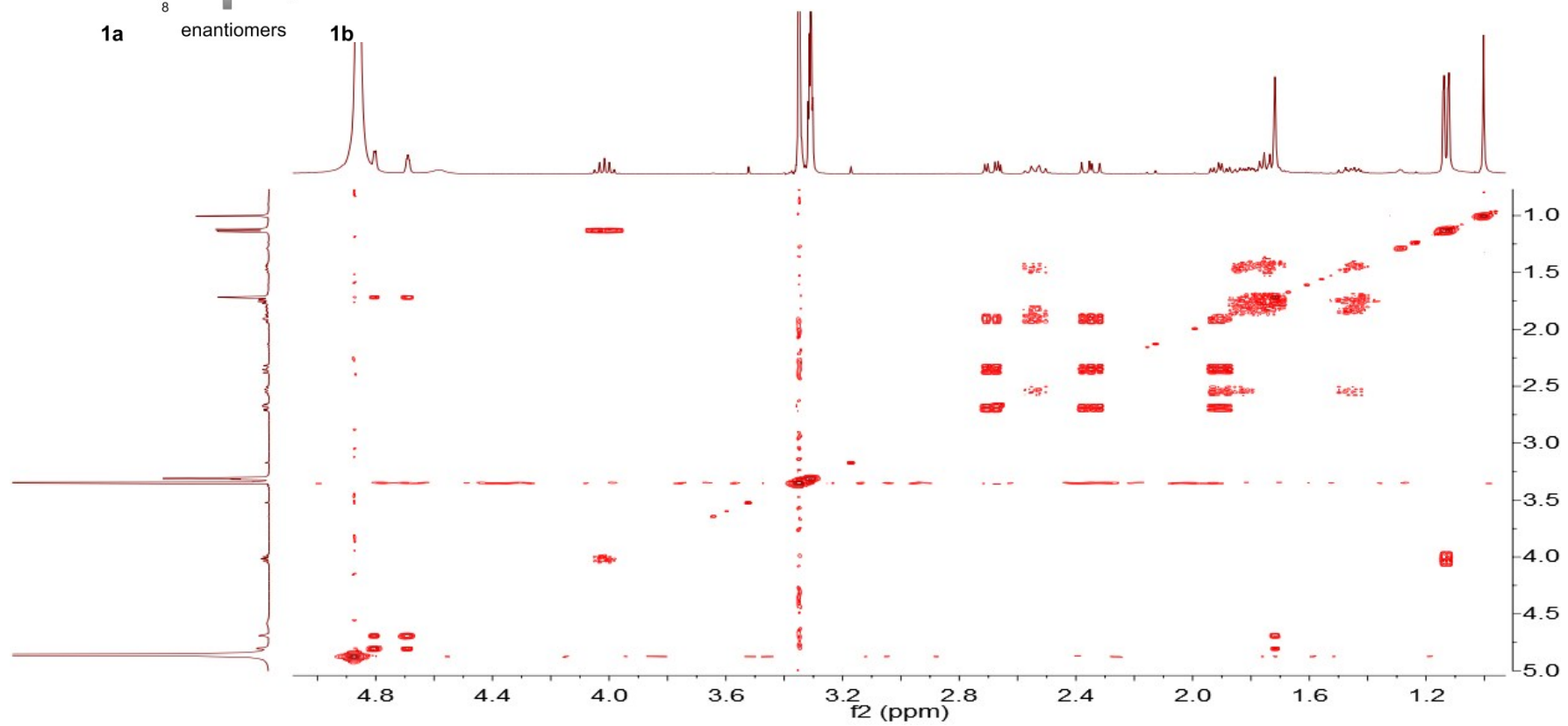
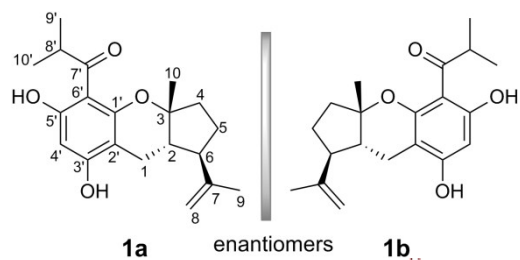
HSQC of compound **1** (in methanol-*d*₄)



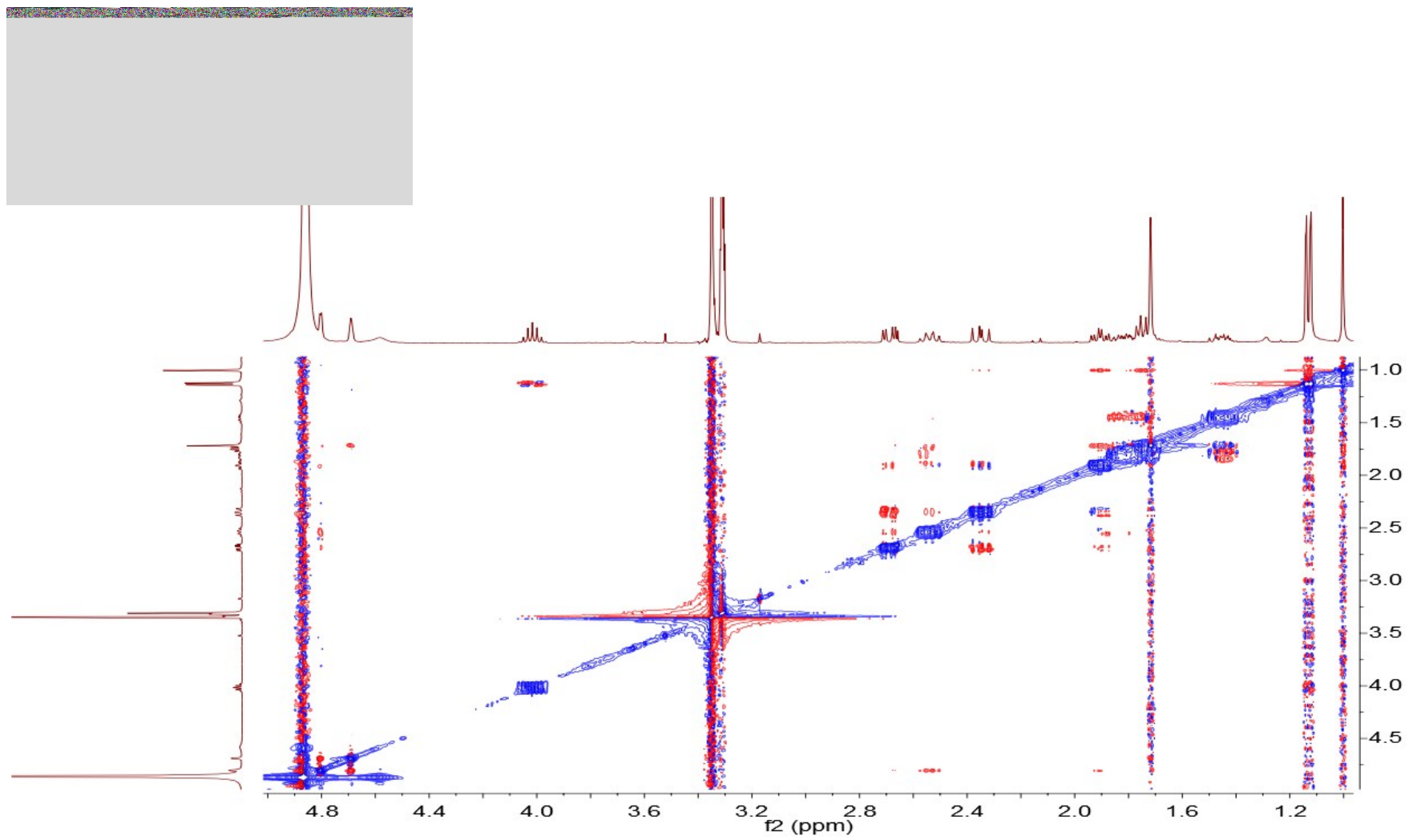
HMBC of compound 1 (in methanol-*d*₄)



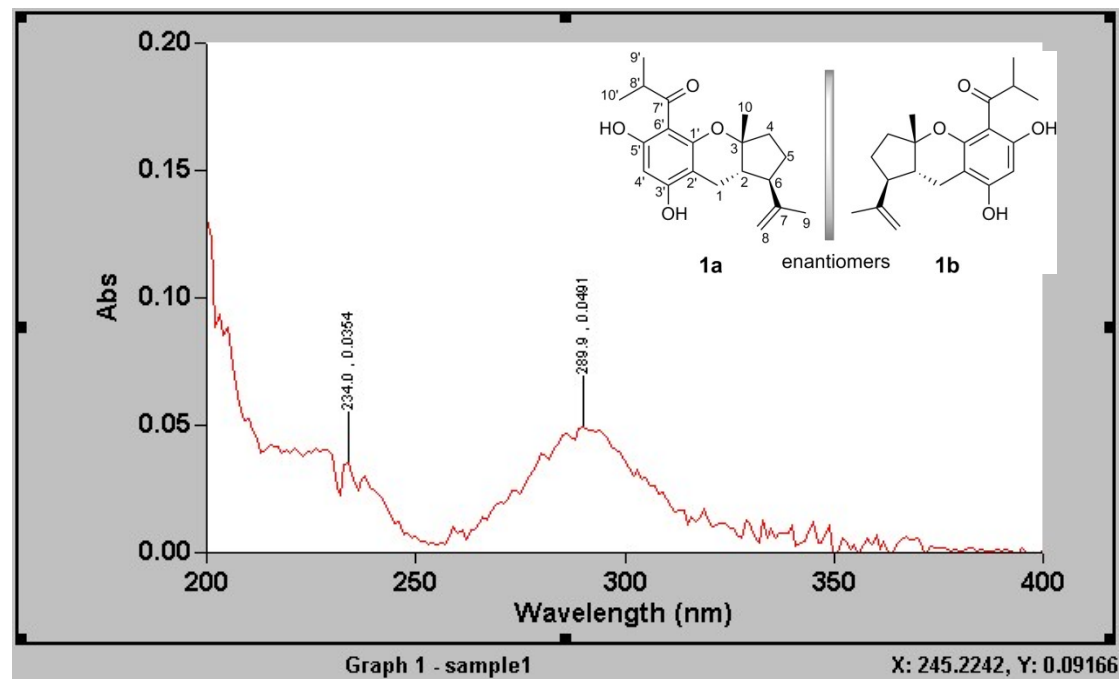
^1H - ^1H COSY of compound **1** (in methanol- d_4)



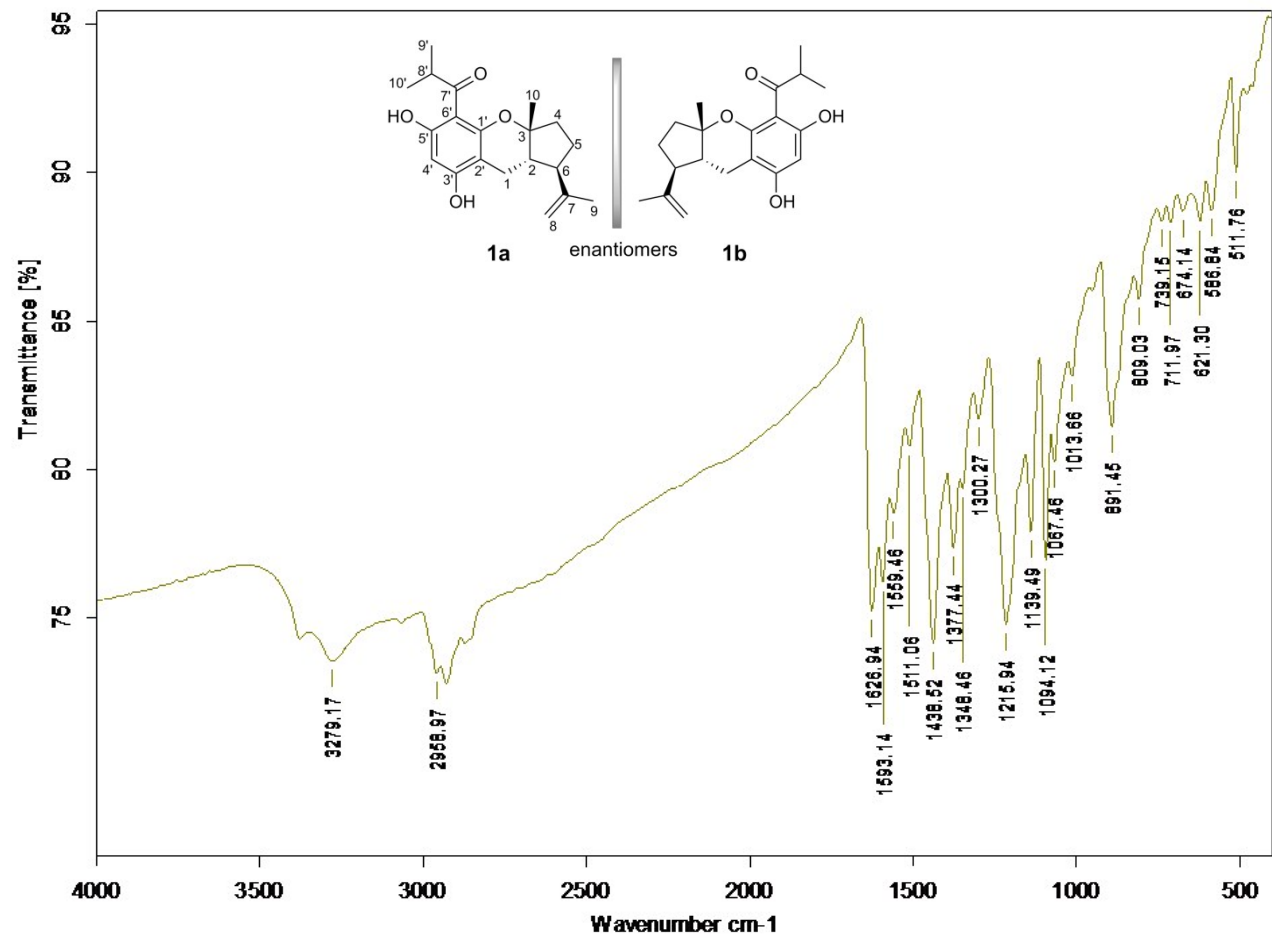
NOESY of compound **1** (in methanol-*d*₄)



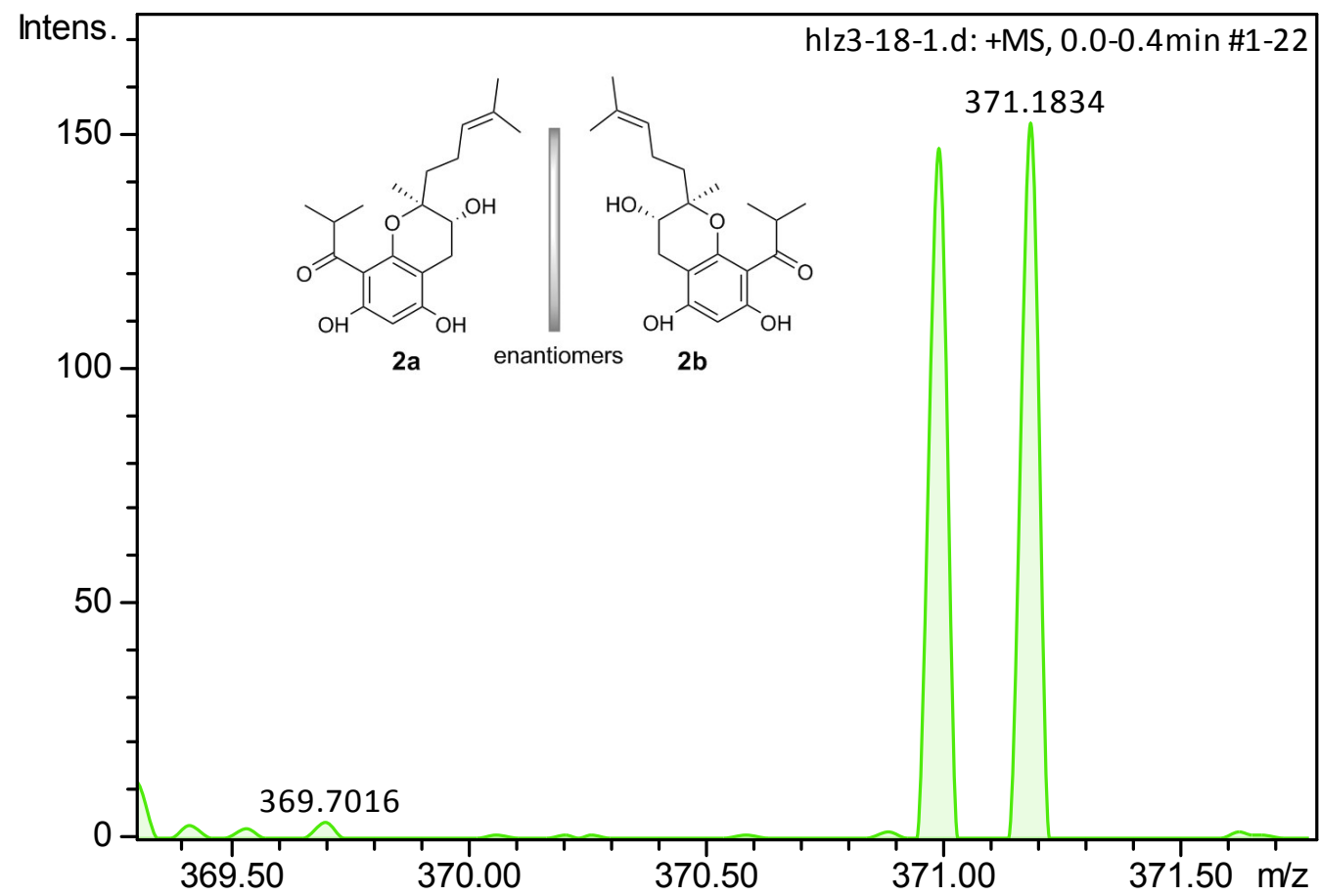
UV of compound **1** (in MeOH)



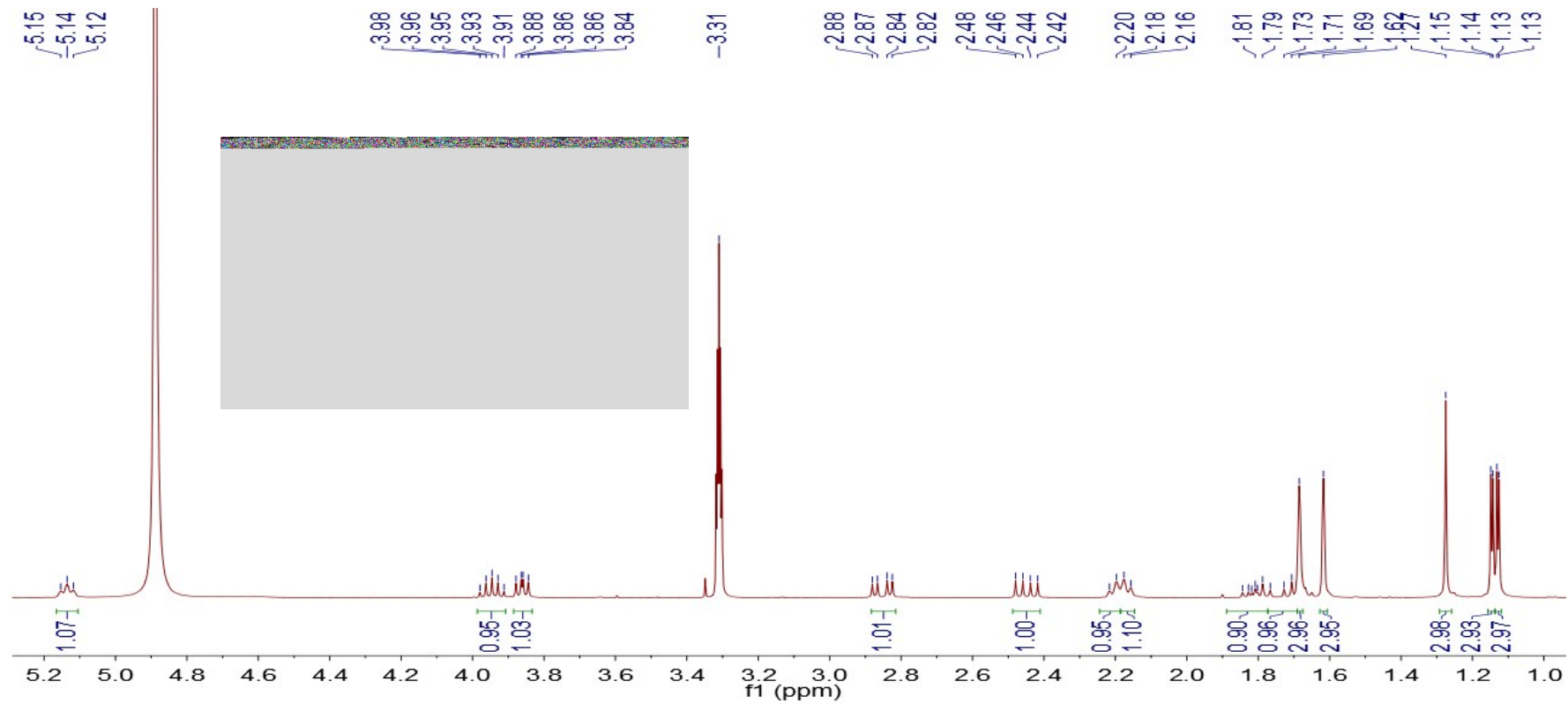
IR of compound **1** (KBr disc)



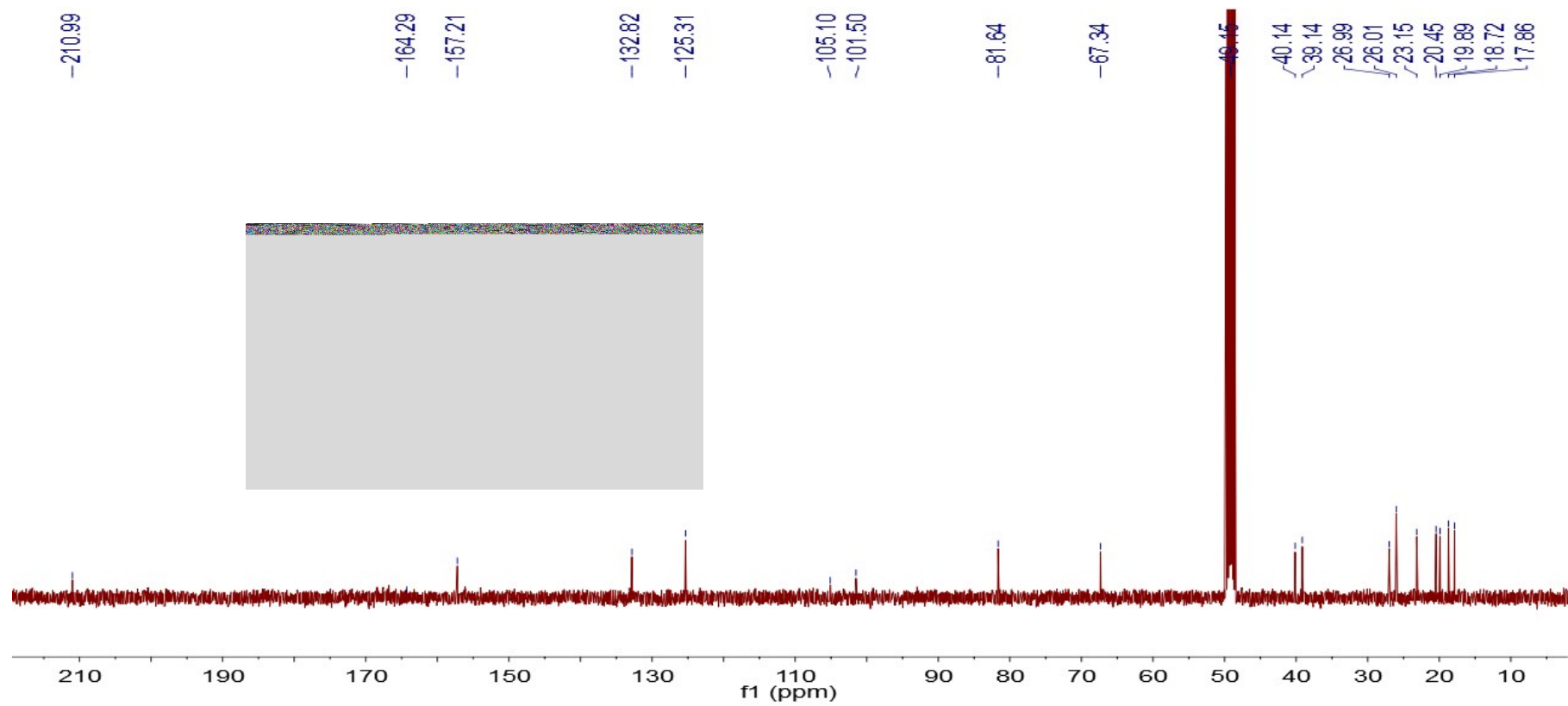
HRESIMS of compound 2

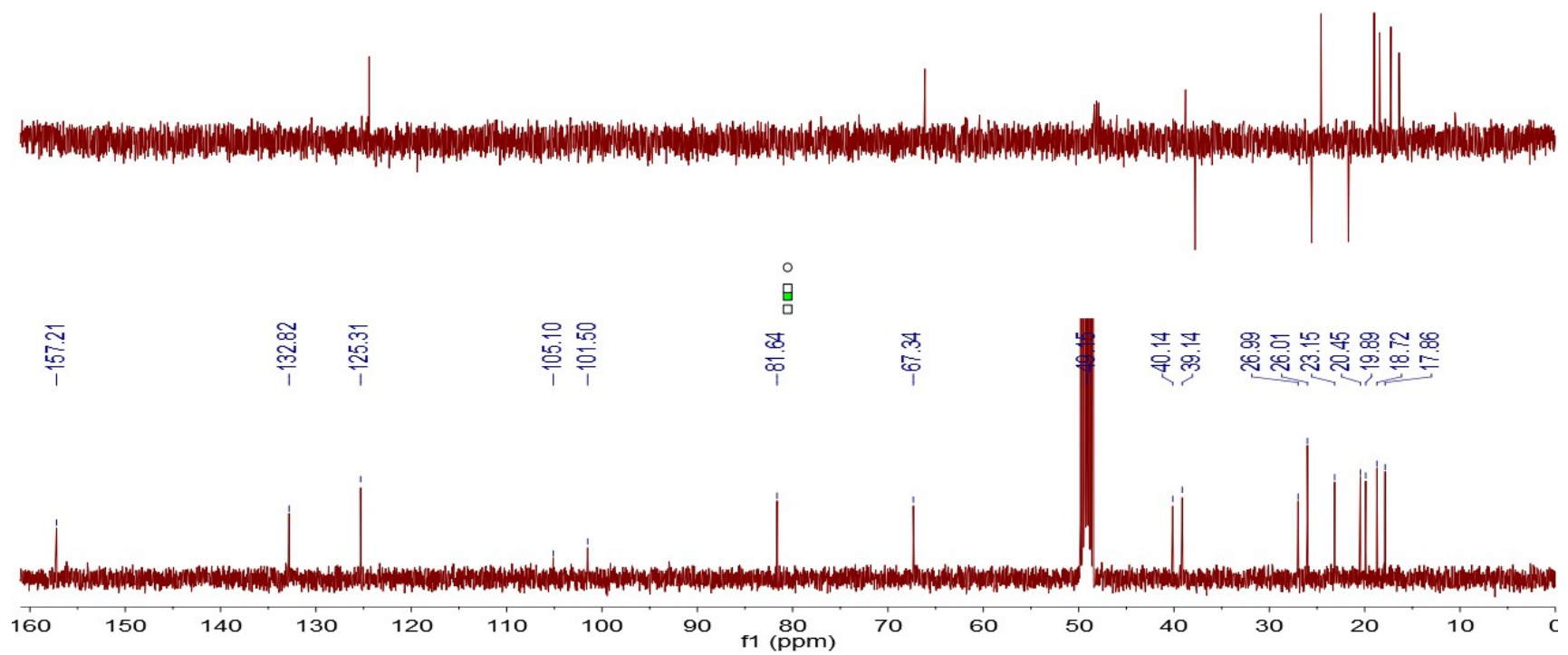


^1H NMR of compound **2** (in methanol- d_4)

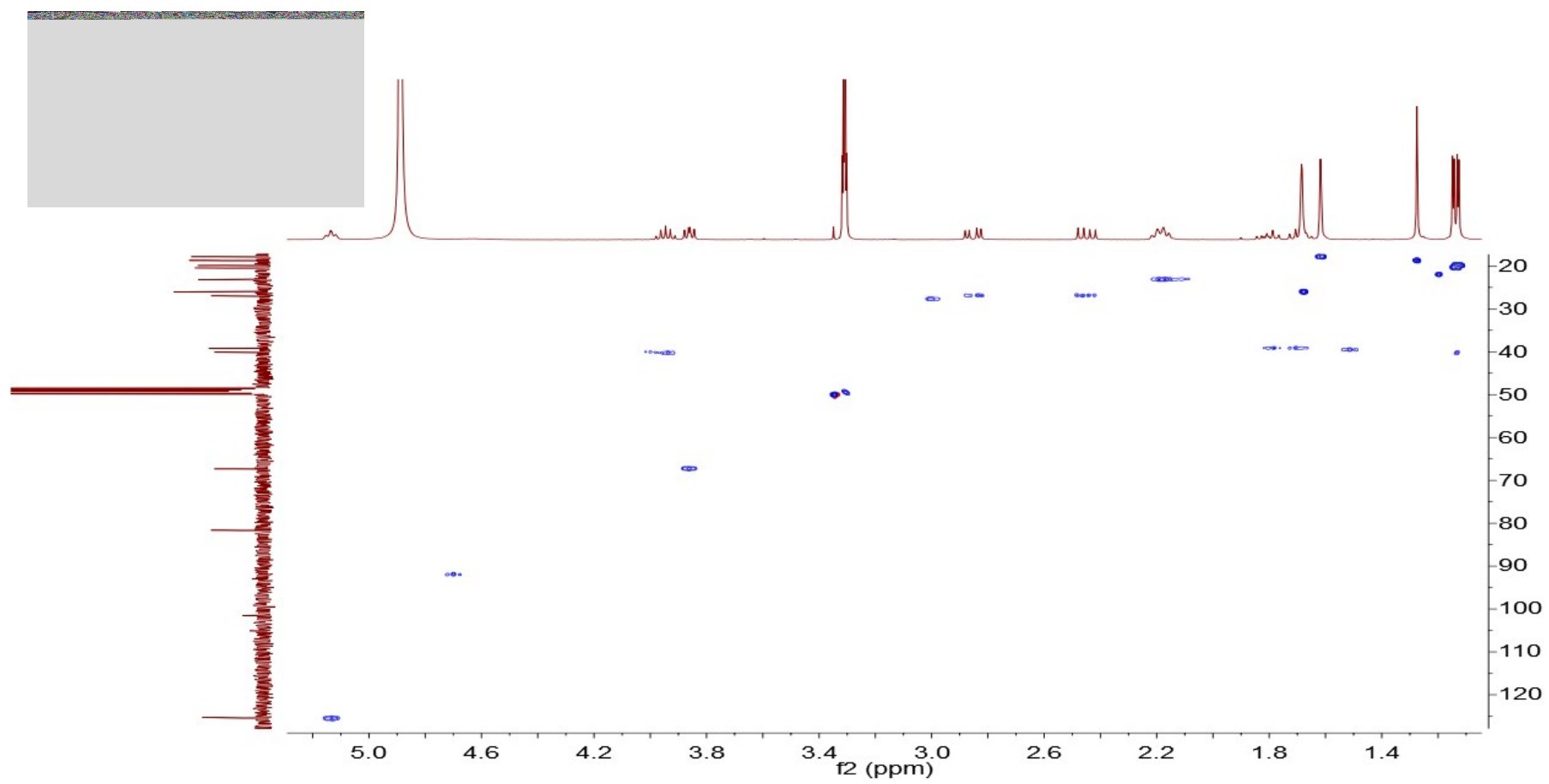


^{13}C NMR of compound **2** (in methanol- d_4)

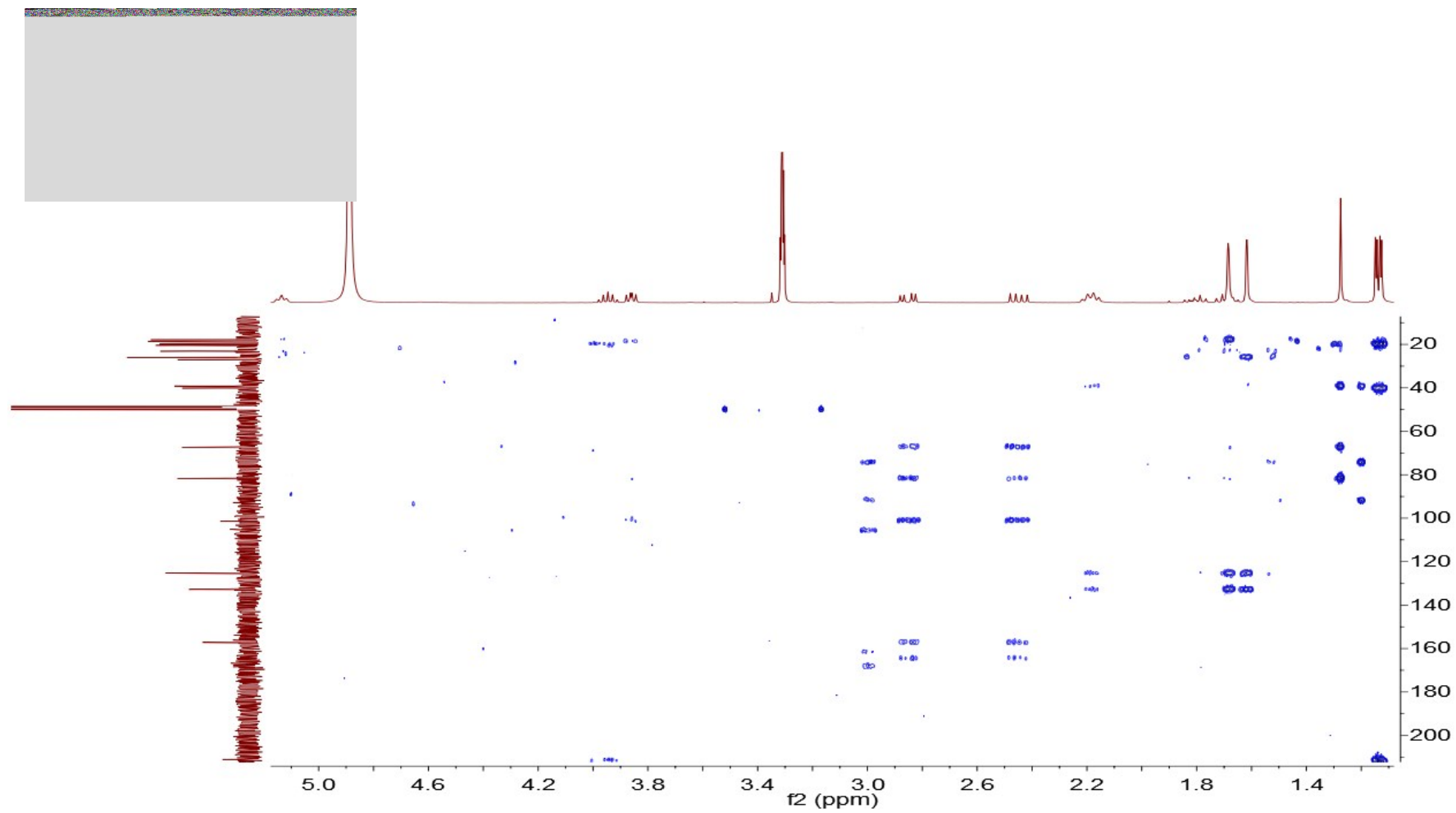




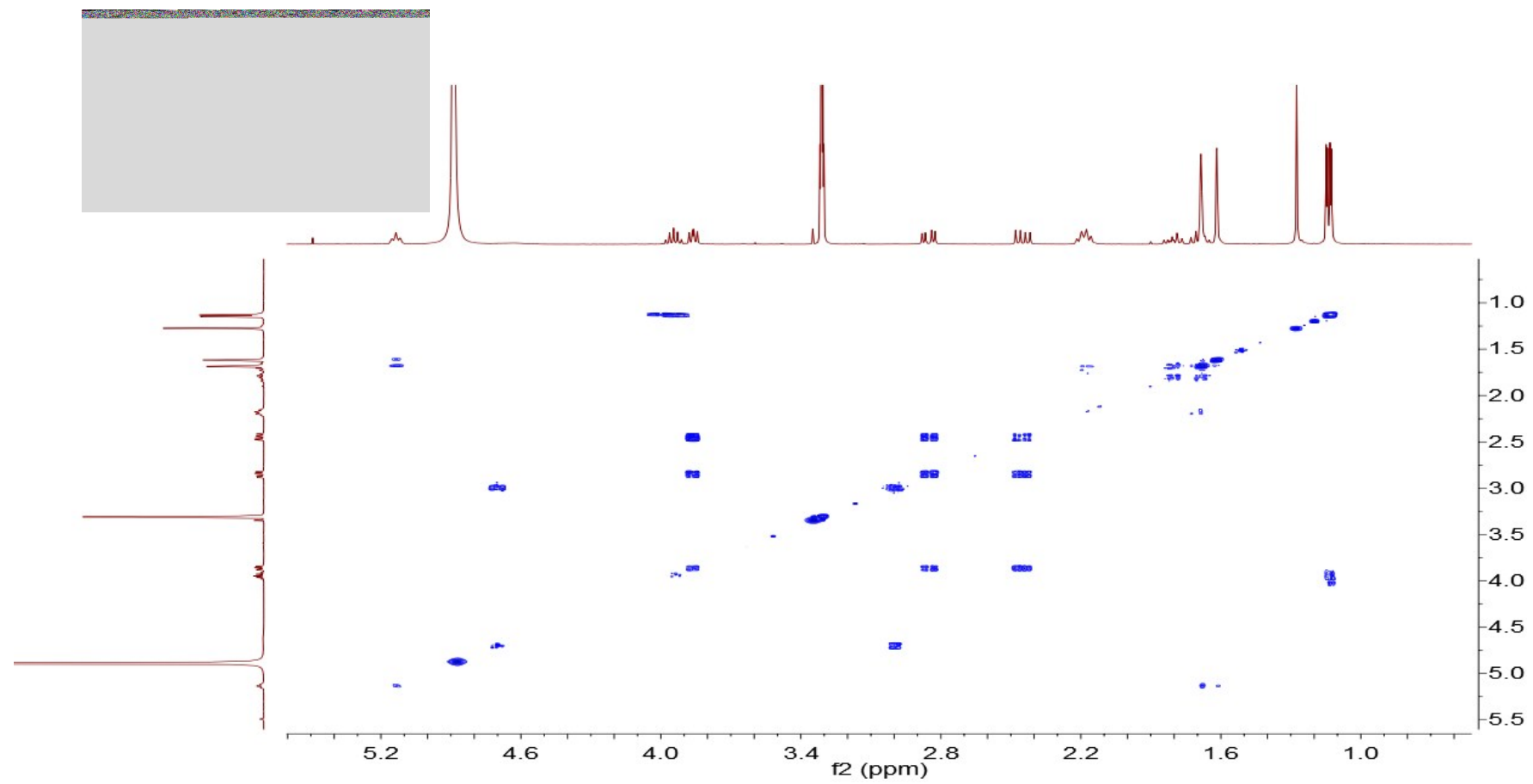
HSQC of compound 2 (in methanol- d_4)



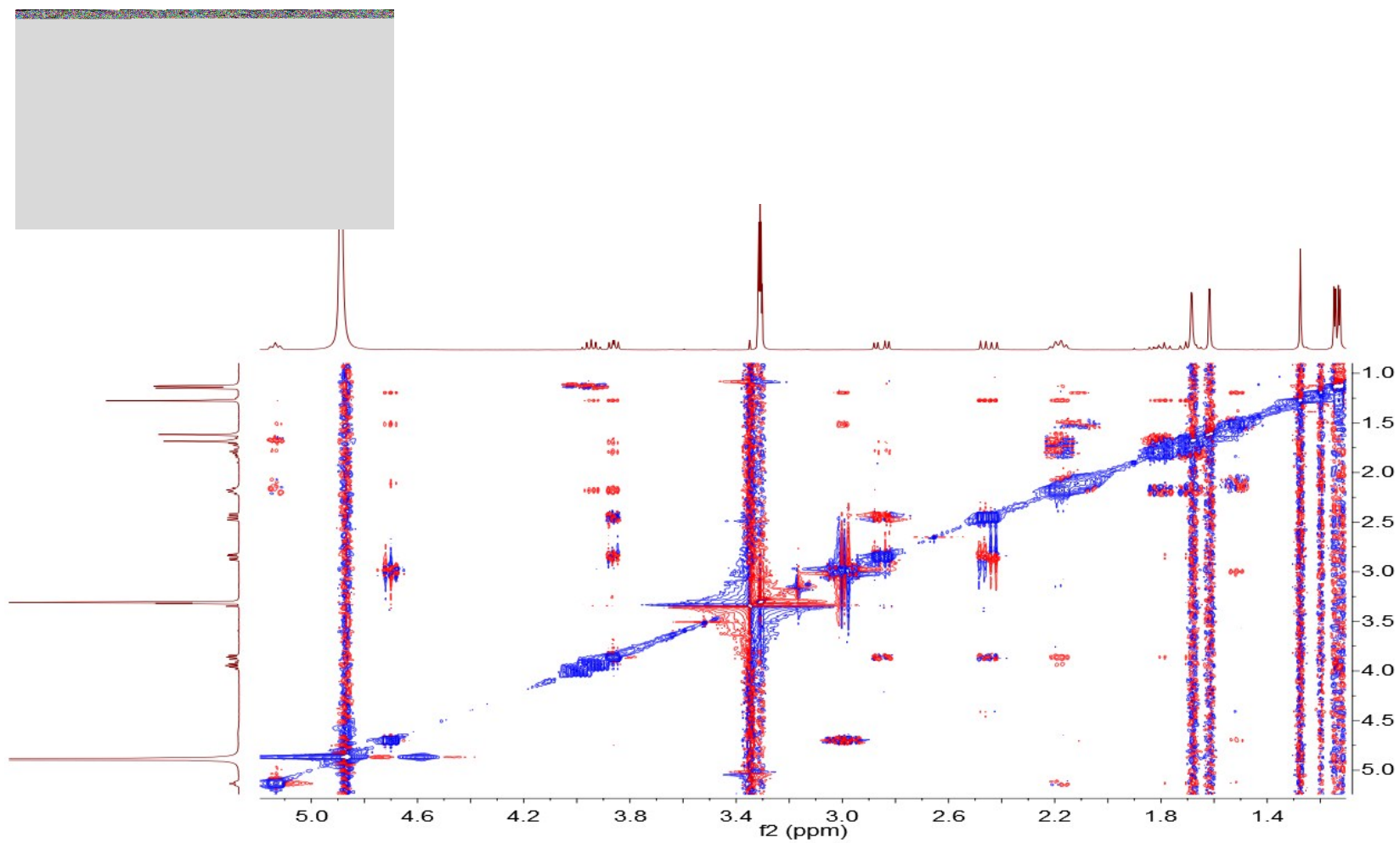
HMBC of compound 2 (in methanol- d_4)



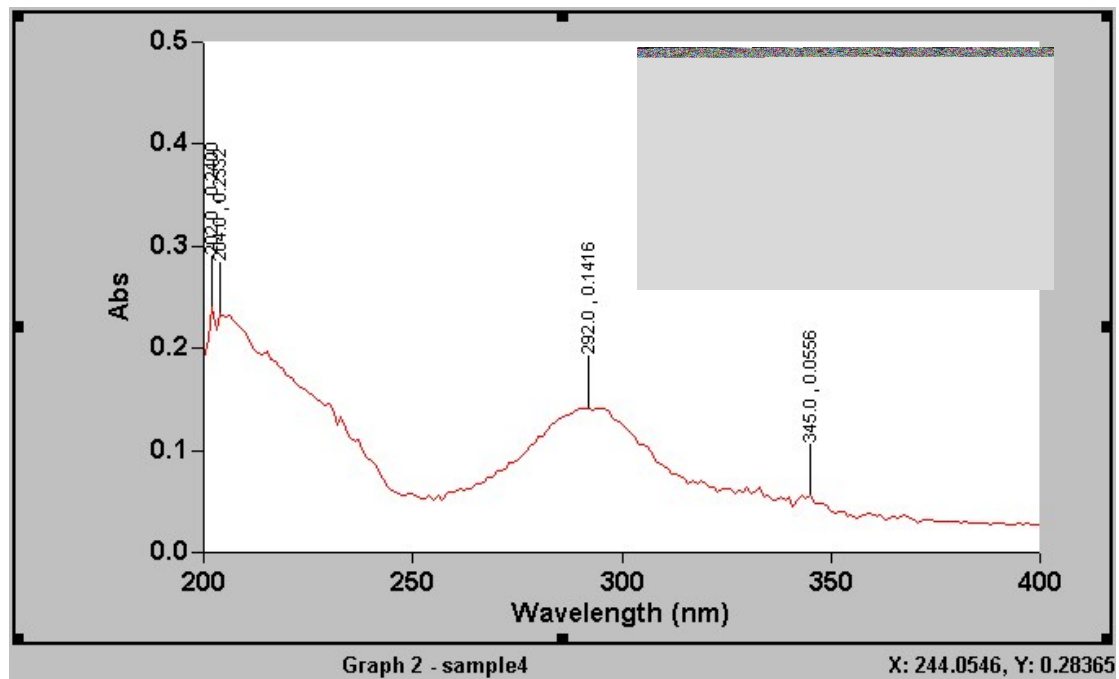
^1H - ^1H COSY of compound 2 (in methanol- d_4)



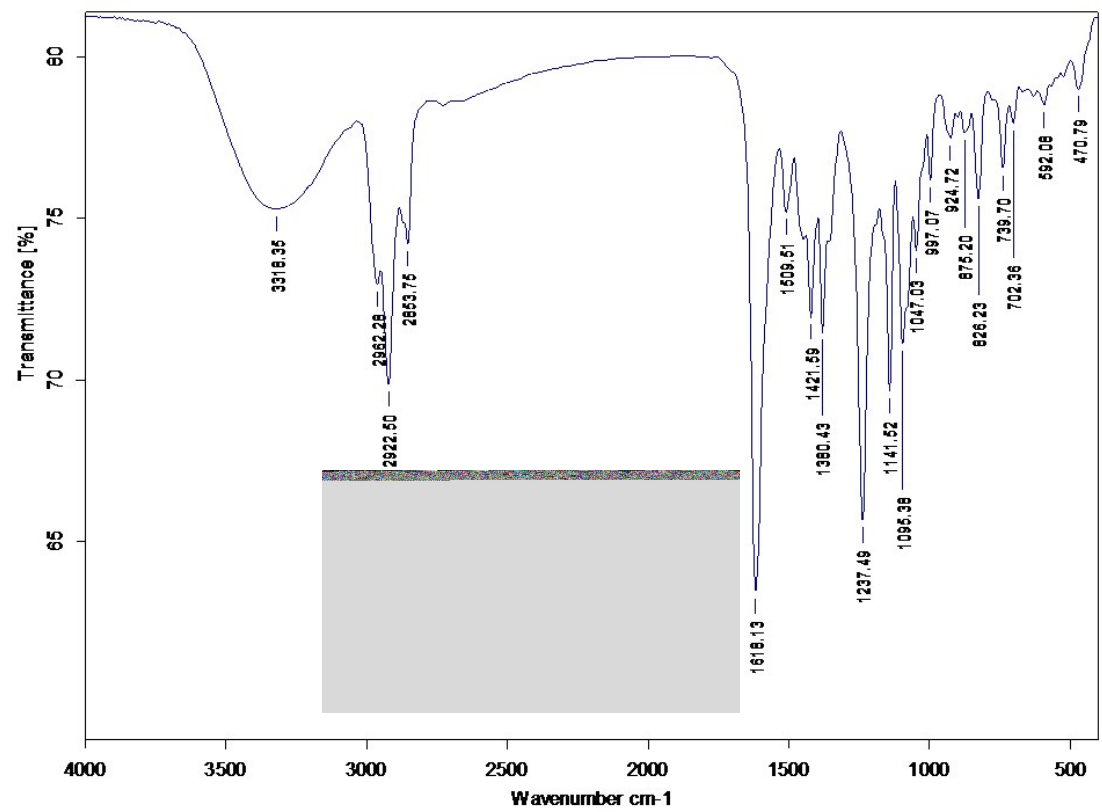
NOESY of compound 2 (in methanol-*d*₄)



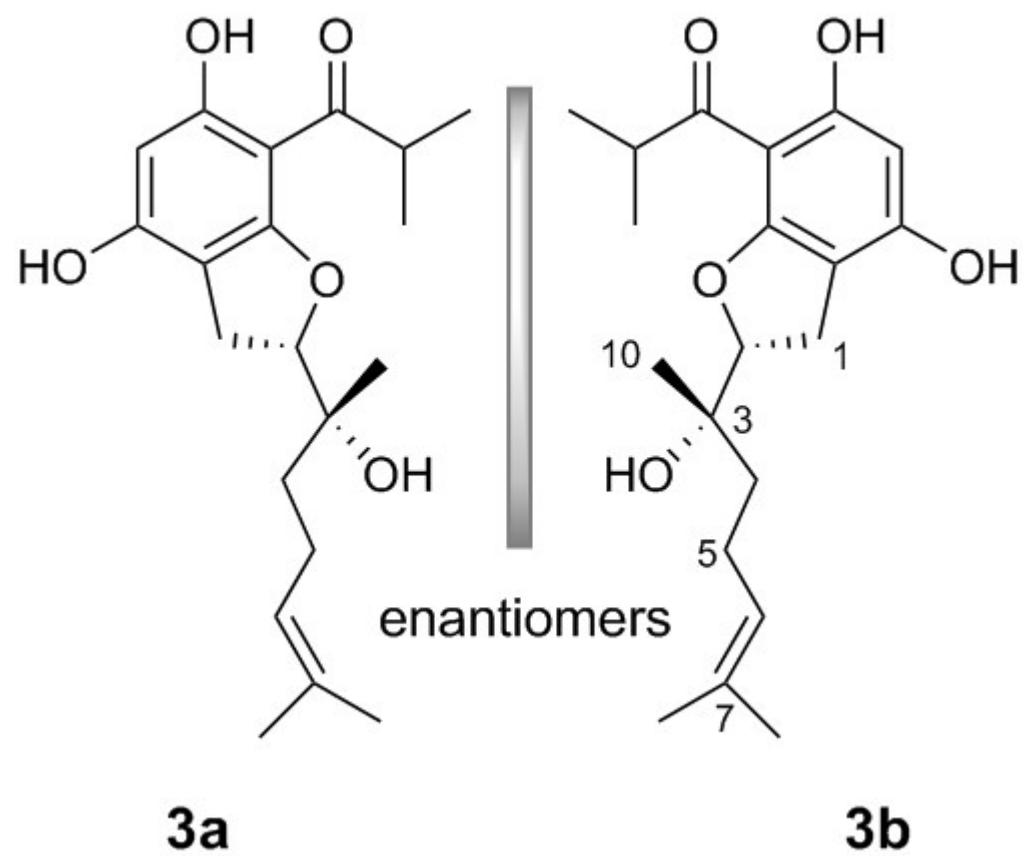
UV of compound 2(in MeOH)

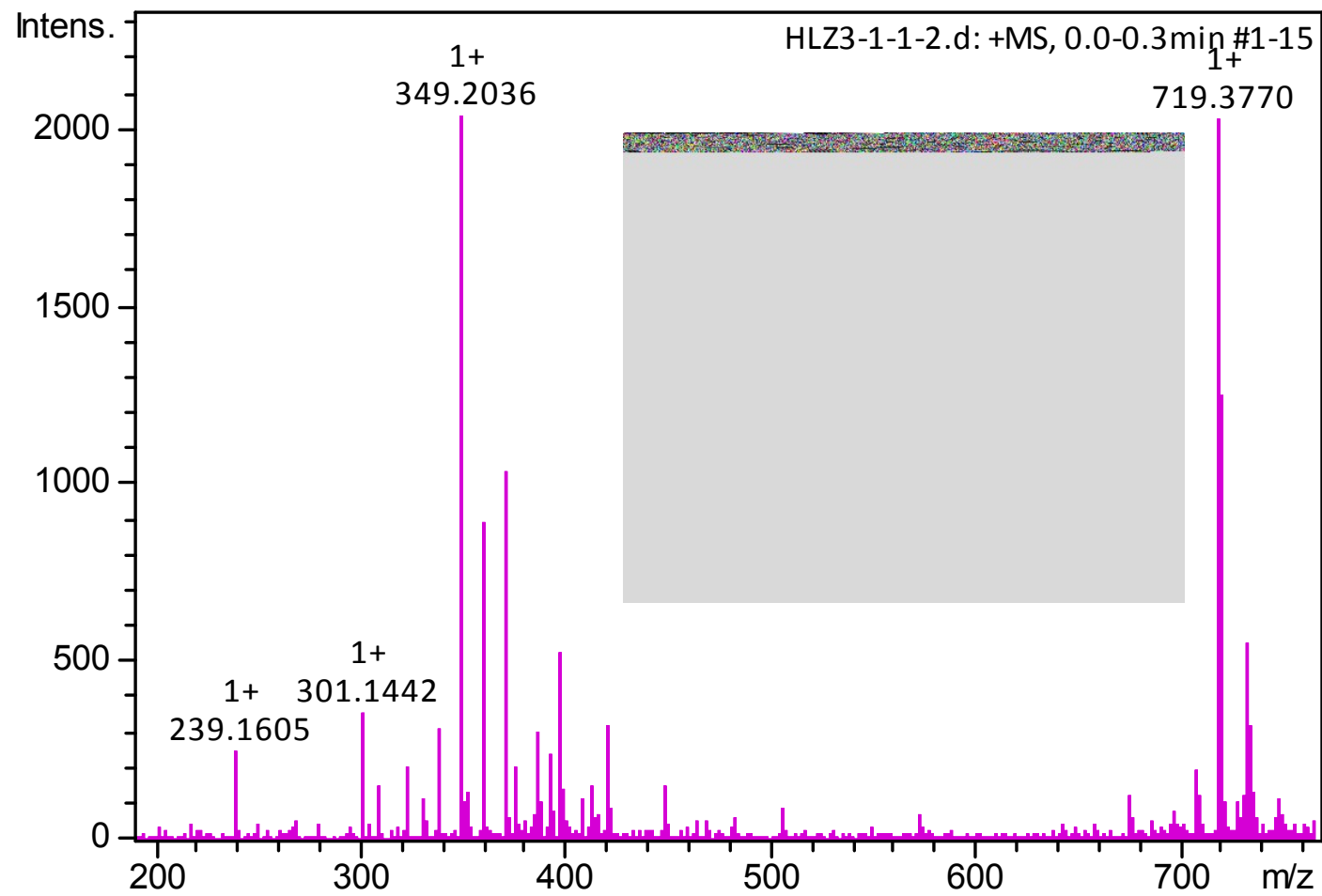


IR of compound 2(KBr disc)

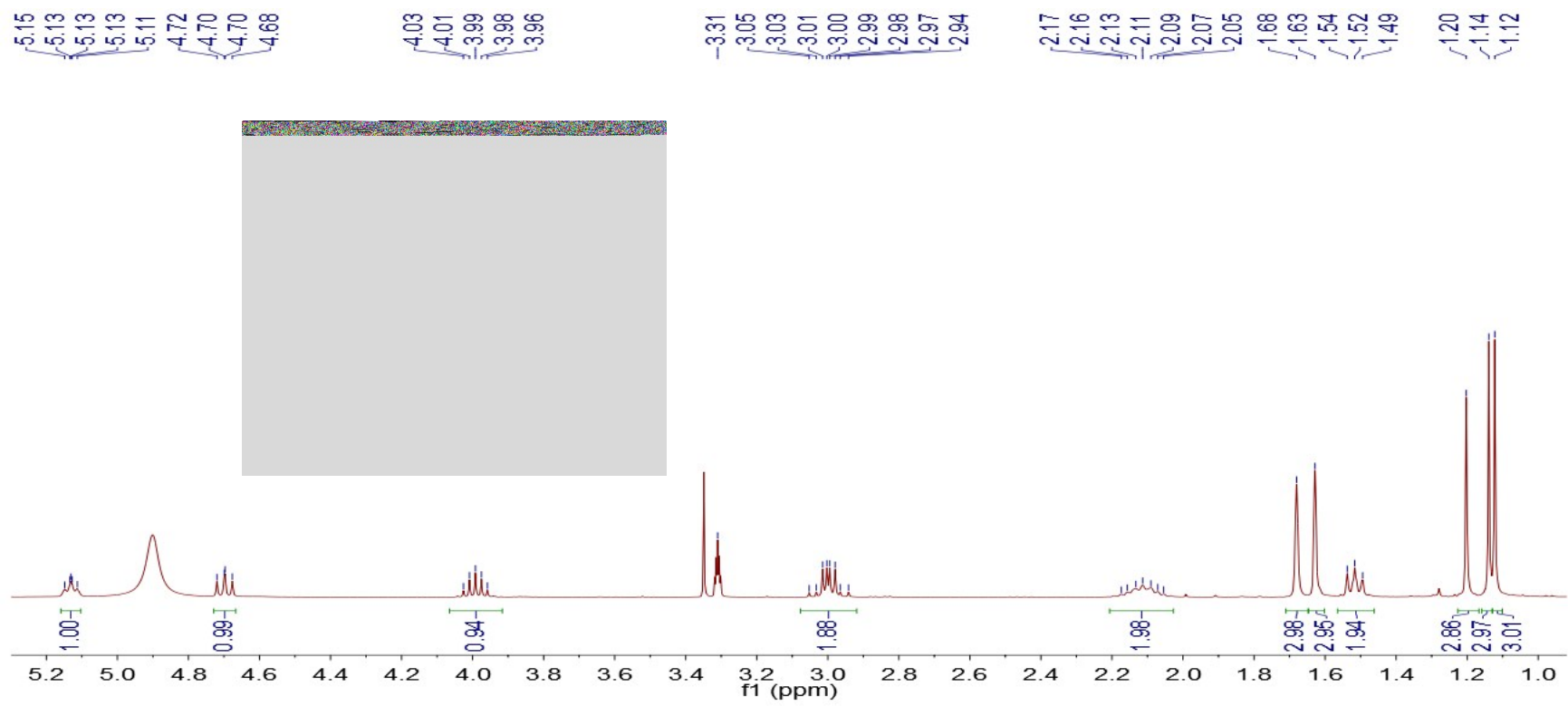


HRESIMS of compound 3

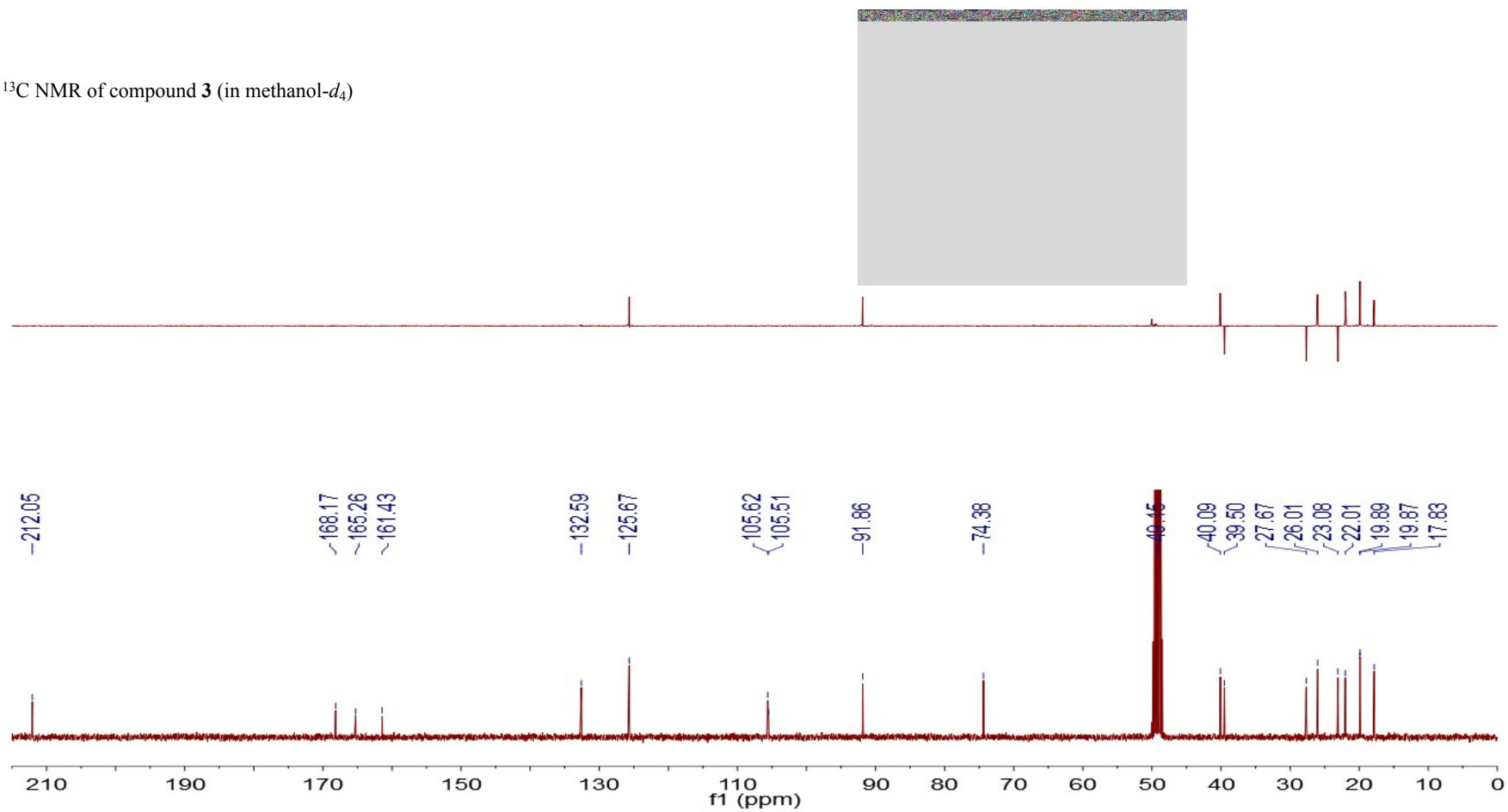




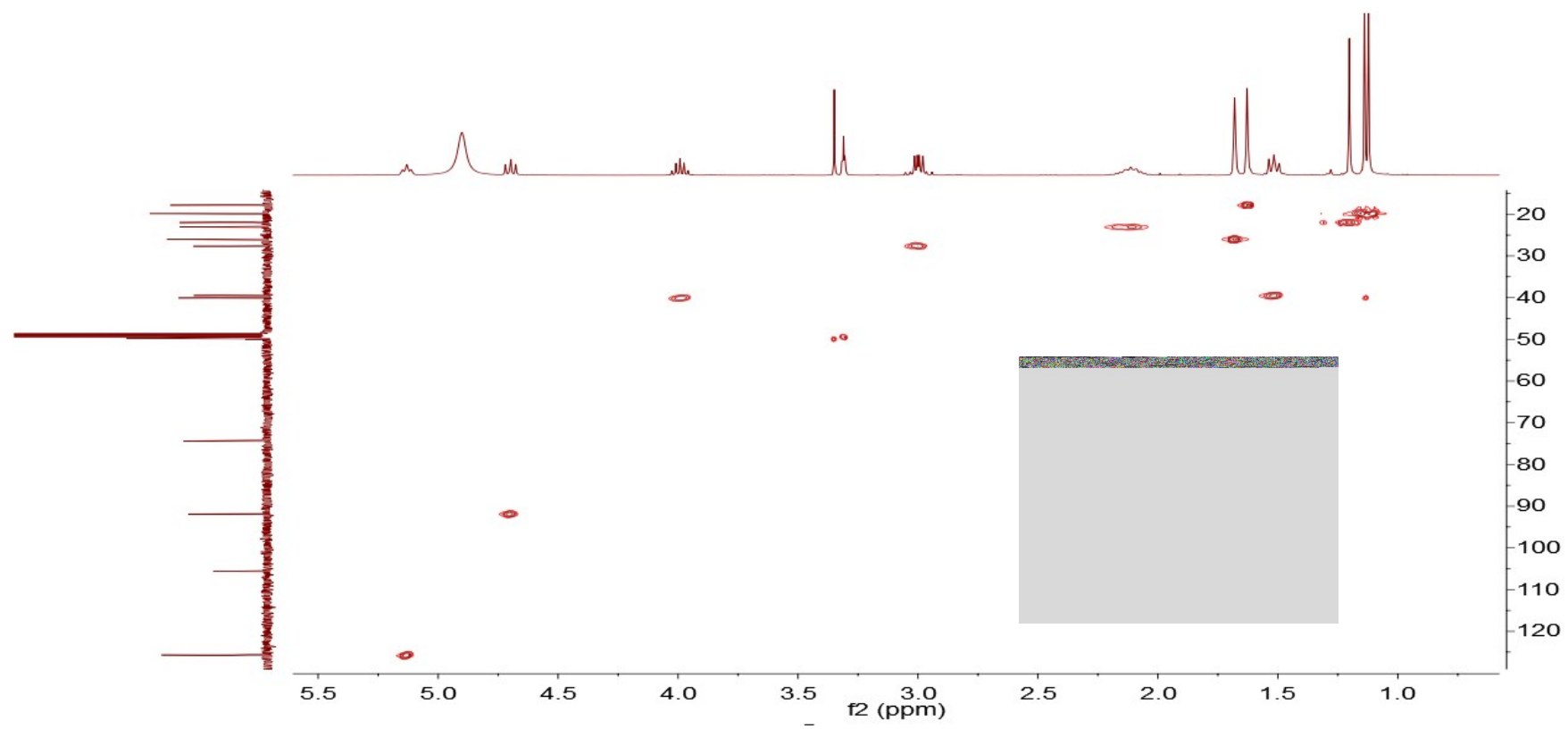
^1H NMR of compound **3** (in methanol- d_4)



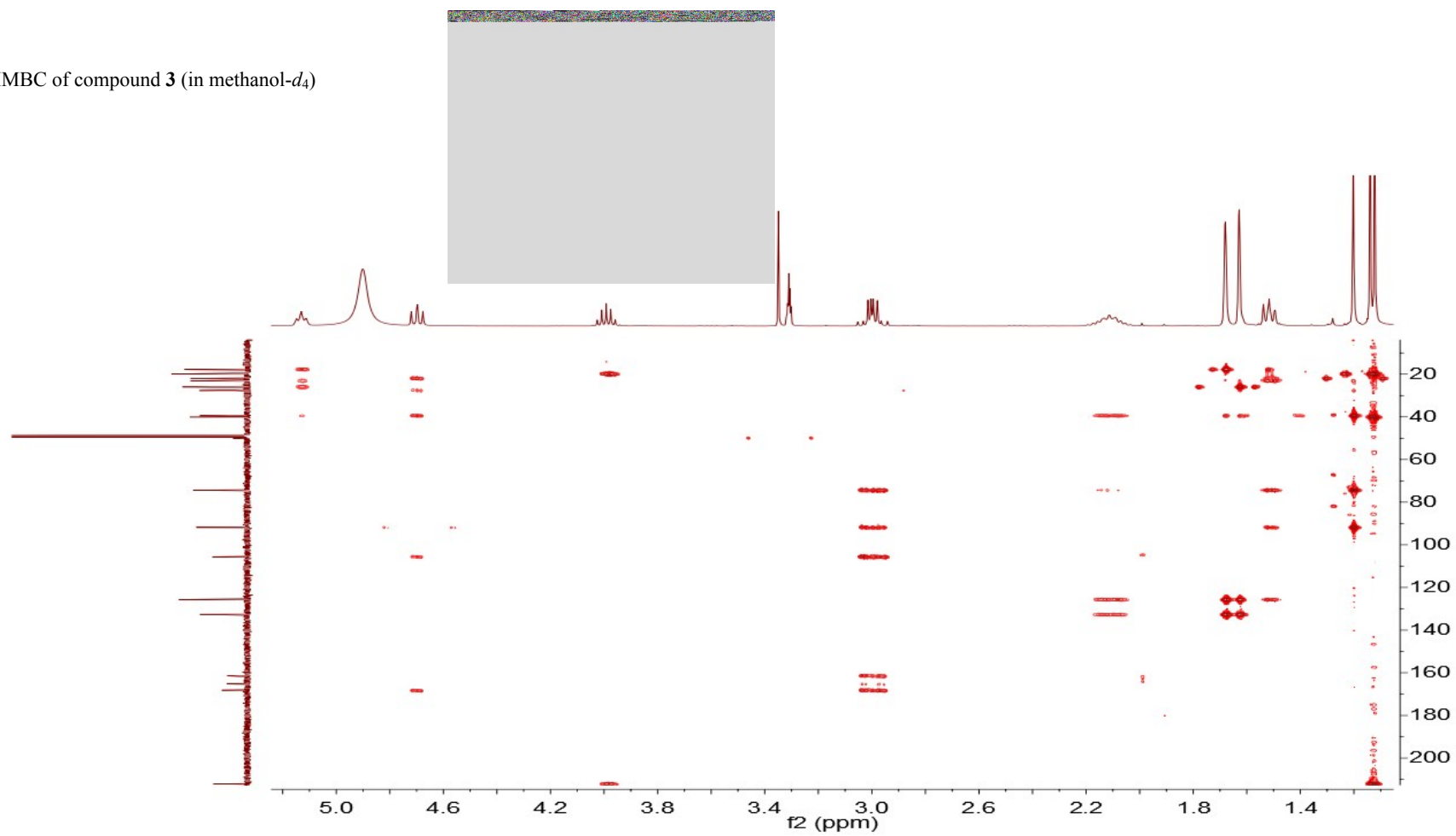
^{13}C NMR of compound **3** (in methanol- d_4)



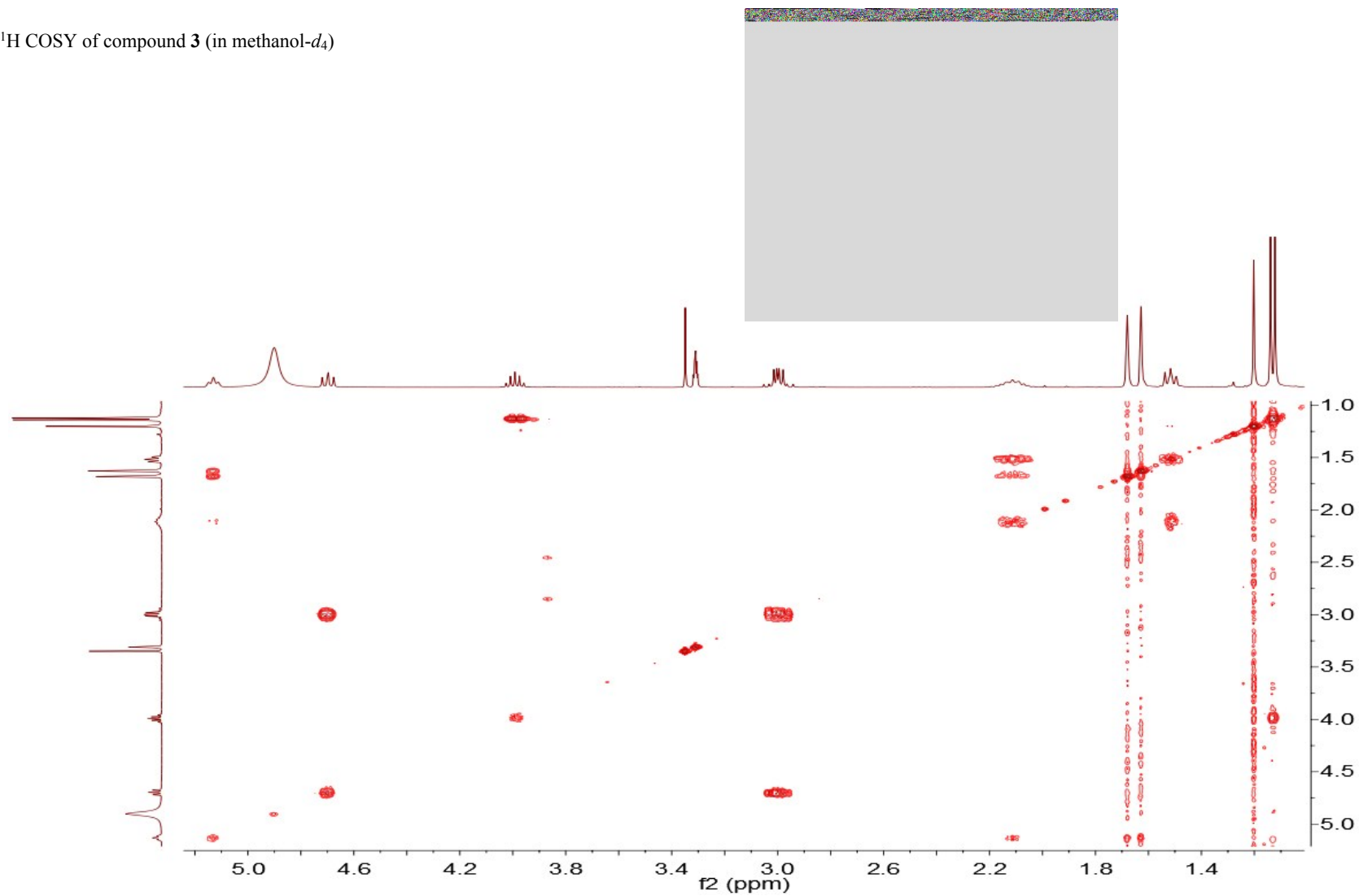
HSQC of compound 3 (in methanol-*d*₄)



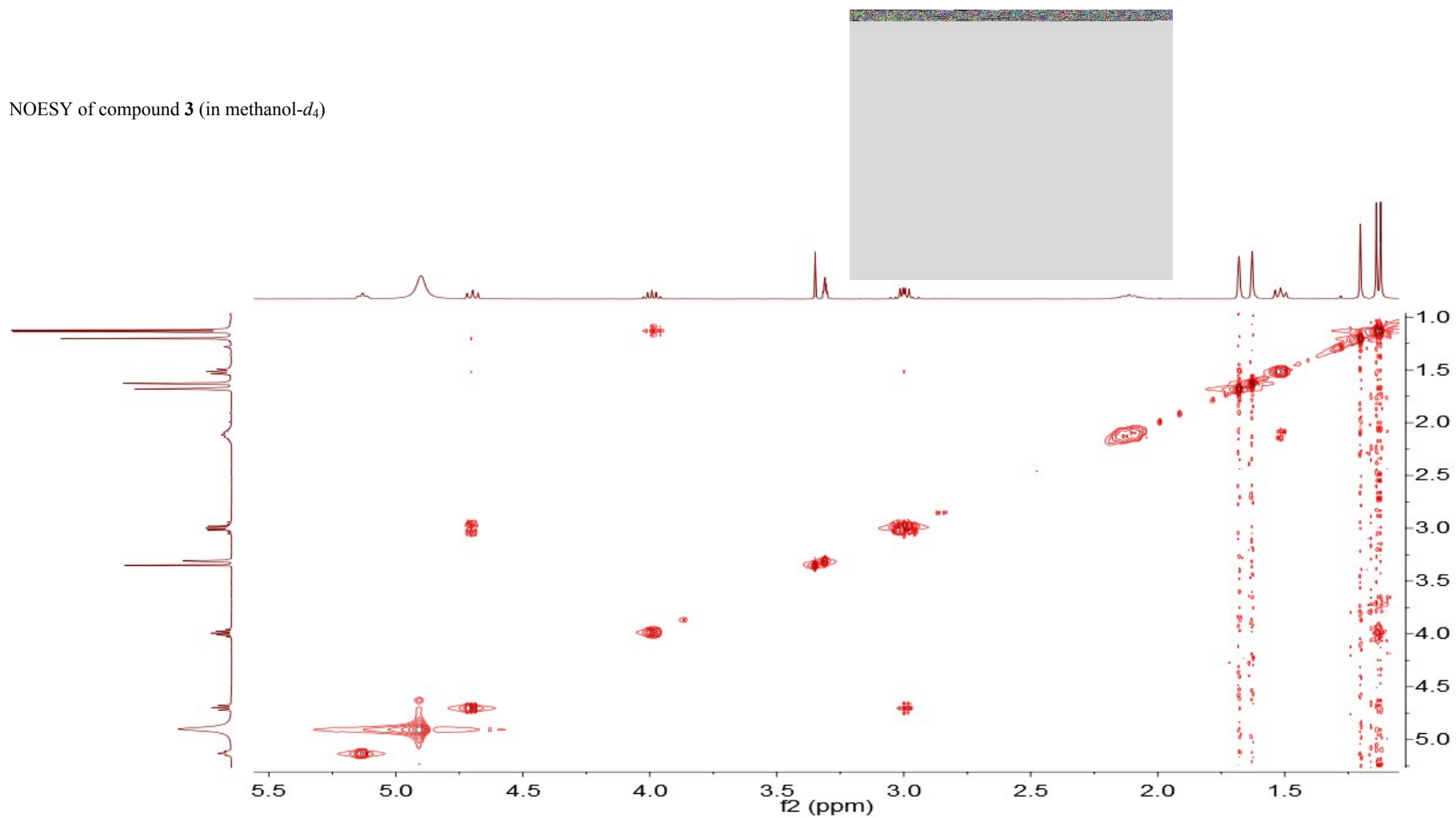
HMBC of compound 3 (in methanol- d_4)



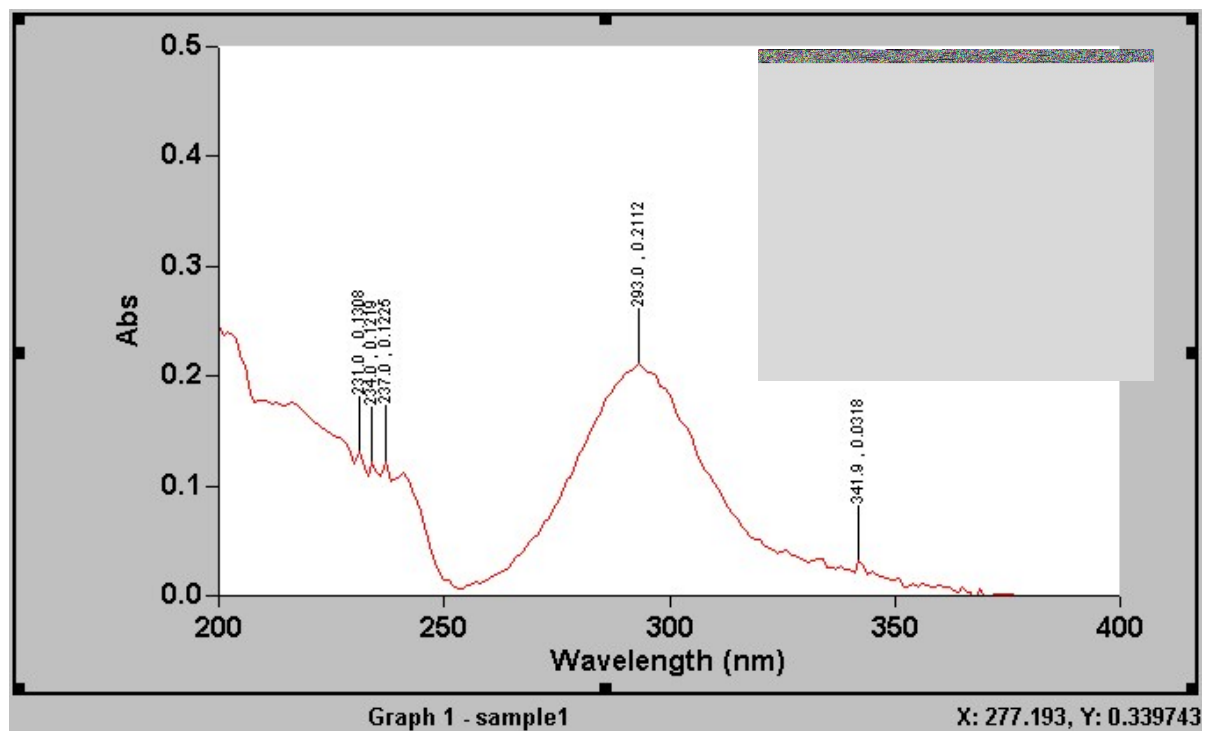
^1H - ^1H COSY of compound **3** (in methanol- d_4)



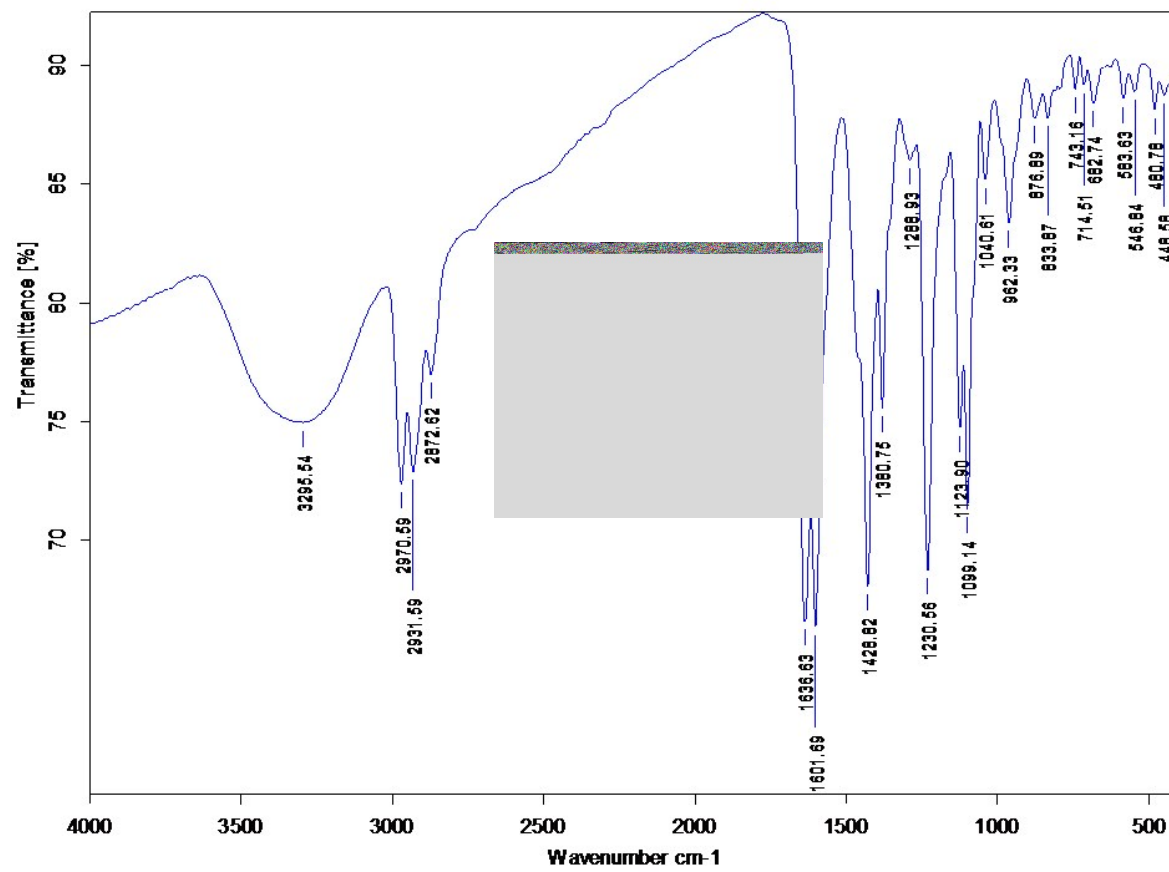
NOESY of compound 3 (in methanol-*d*₄)



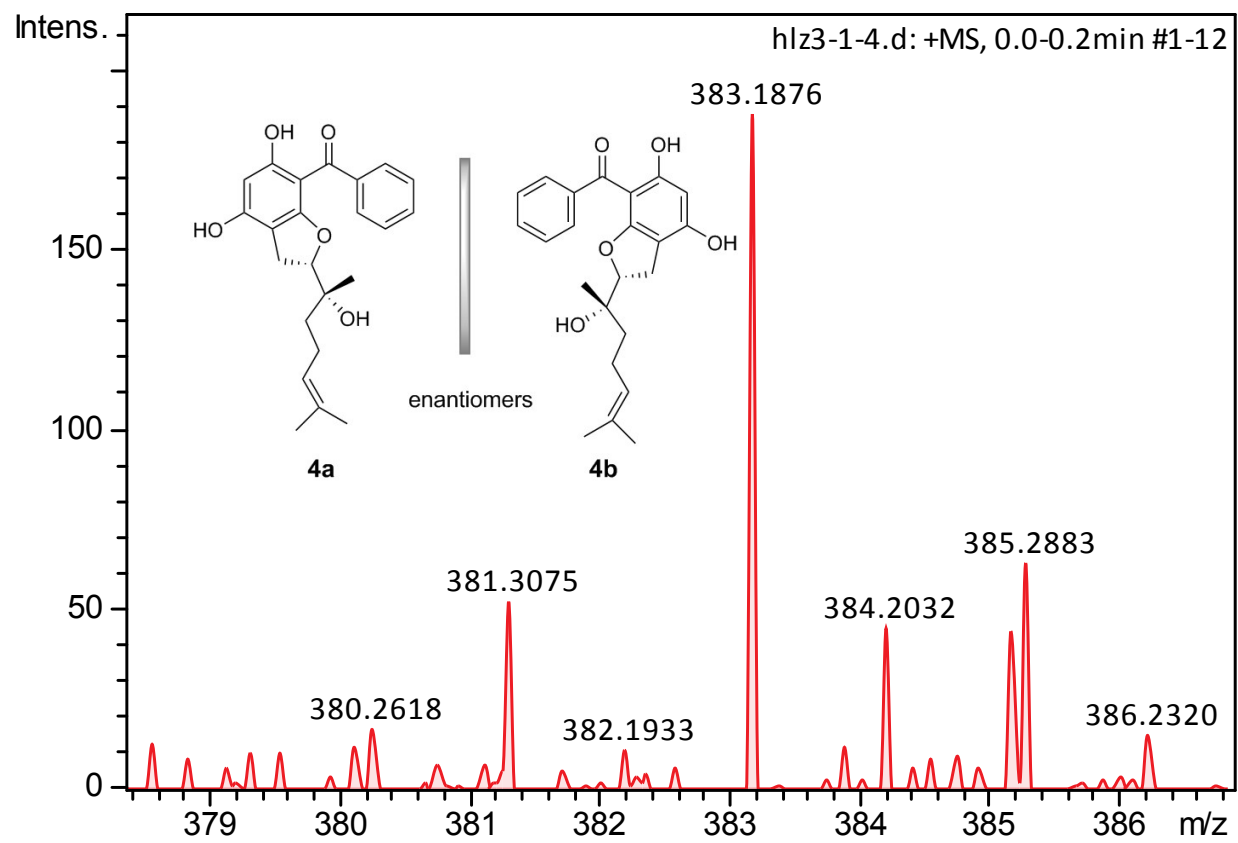
UV of compound 3(in MeOH)



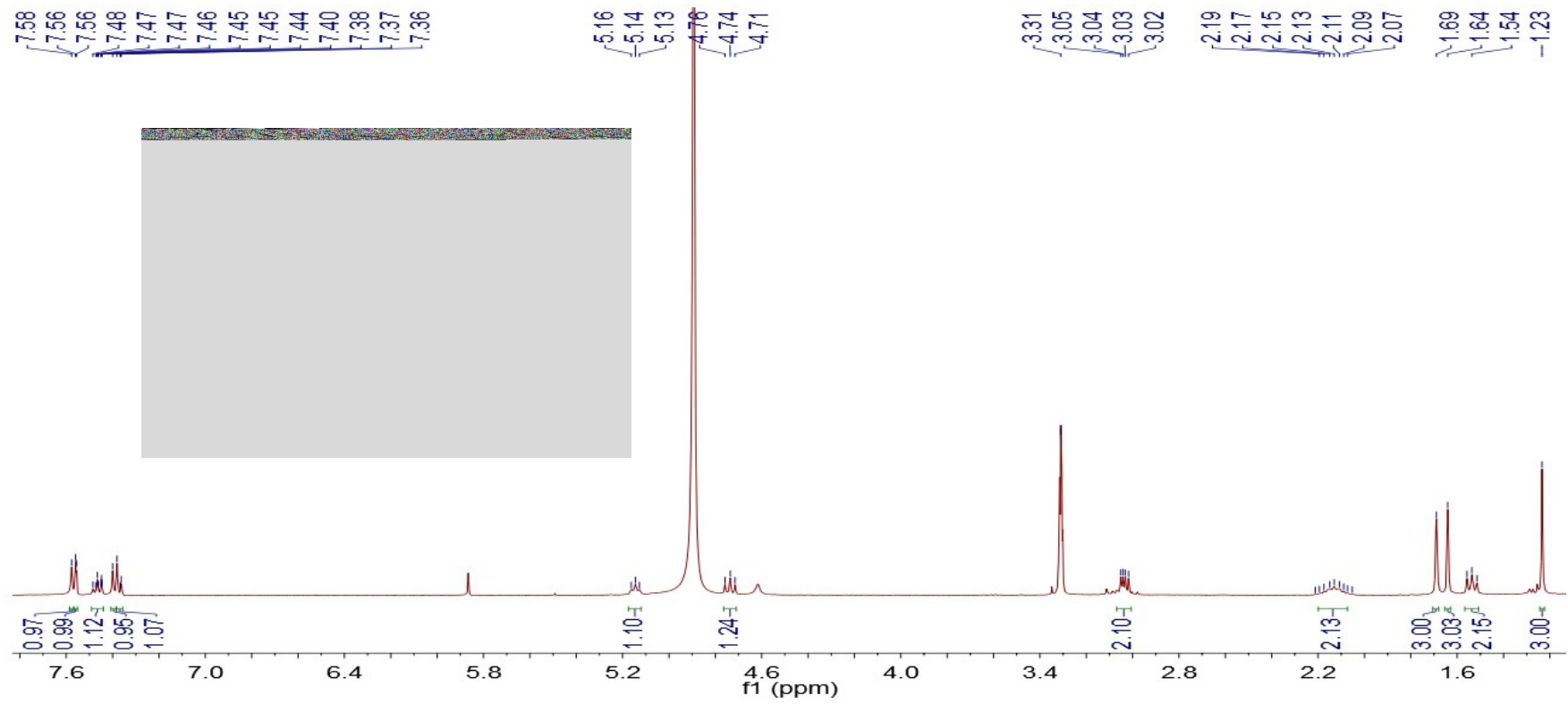
IR of compound 3 (KBr disc)



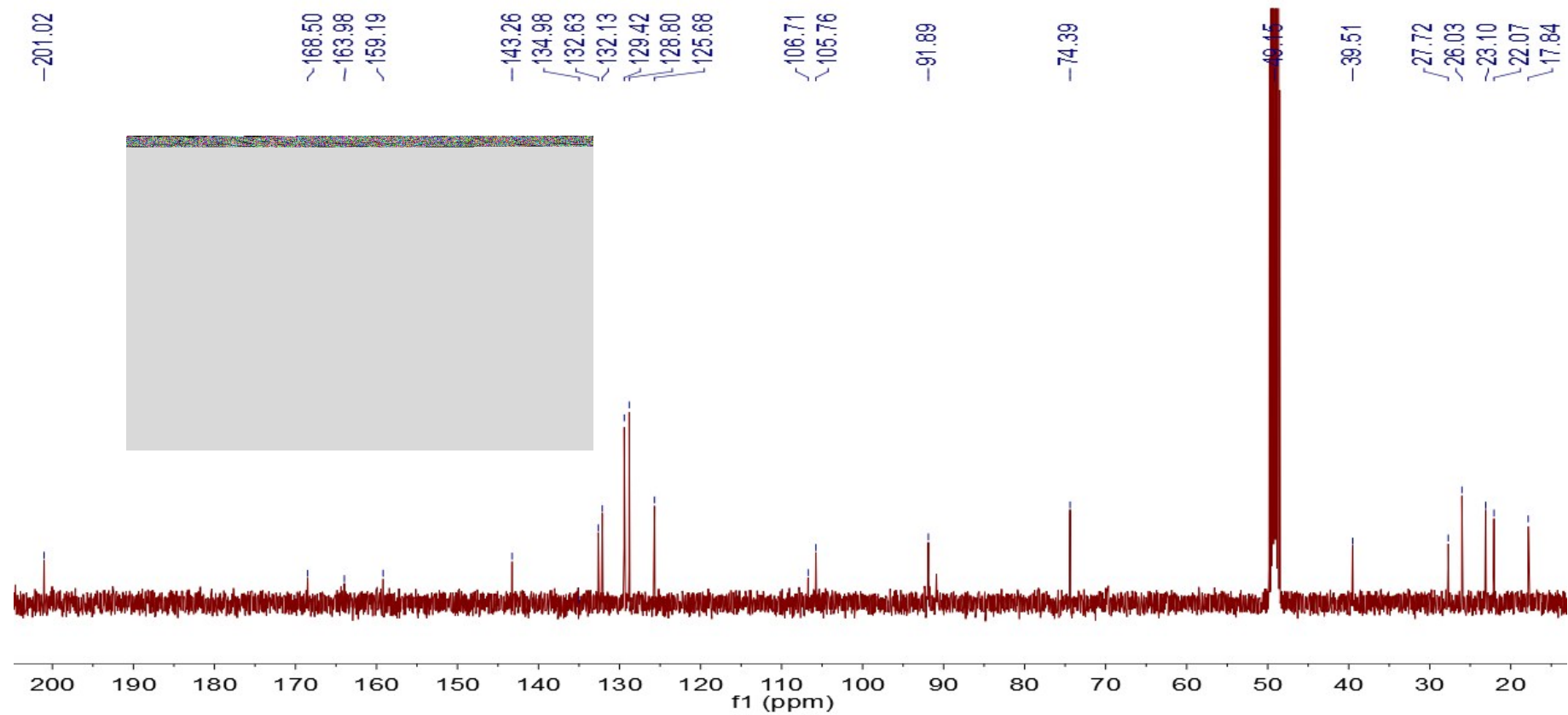
HRESIMS of compound 4

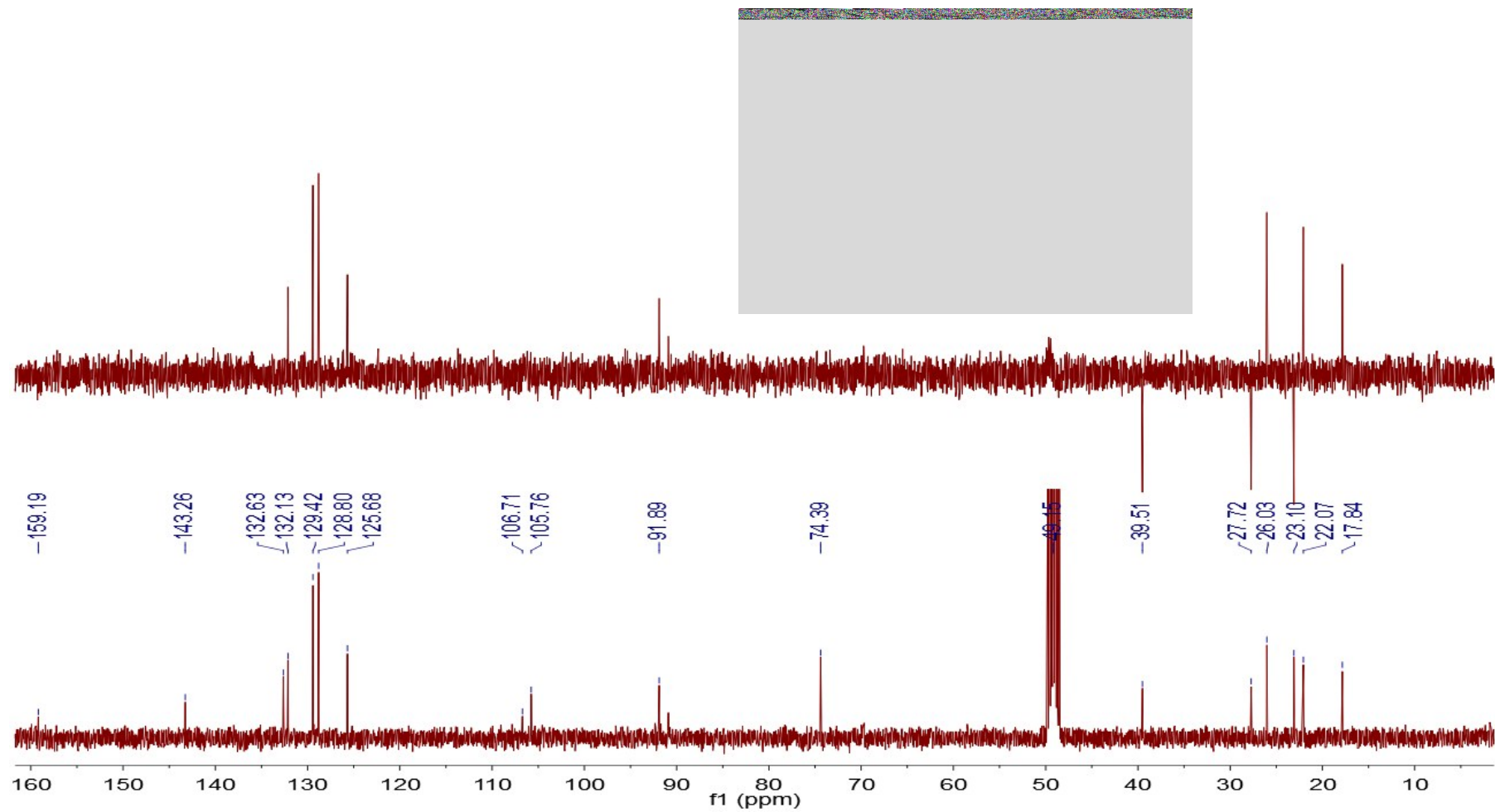


¹H NMR of compound 4 (in methanol-d₄)

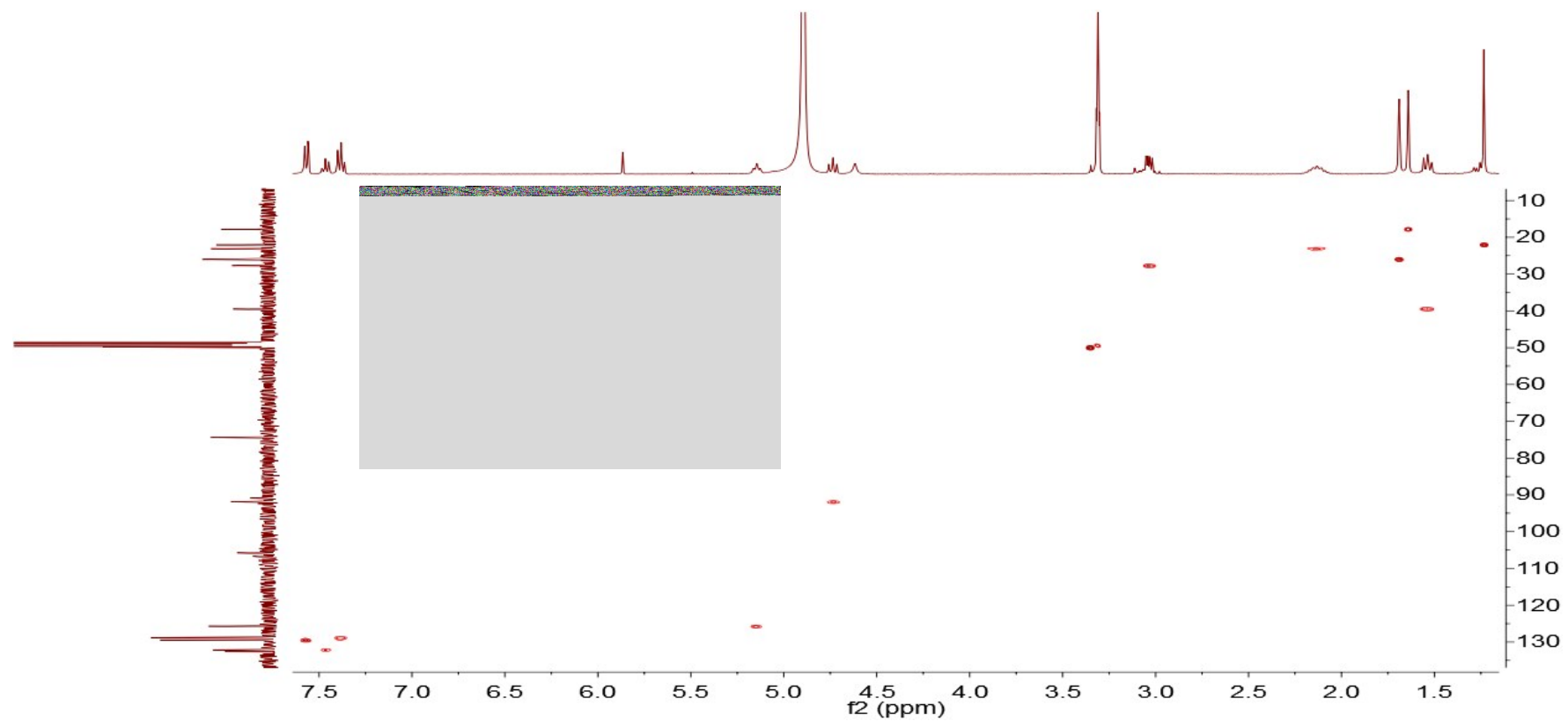


^{13}C NMR of compound **4** (in methanol- d_4)

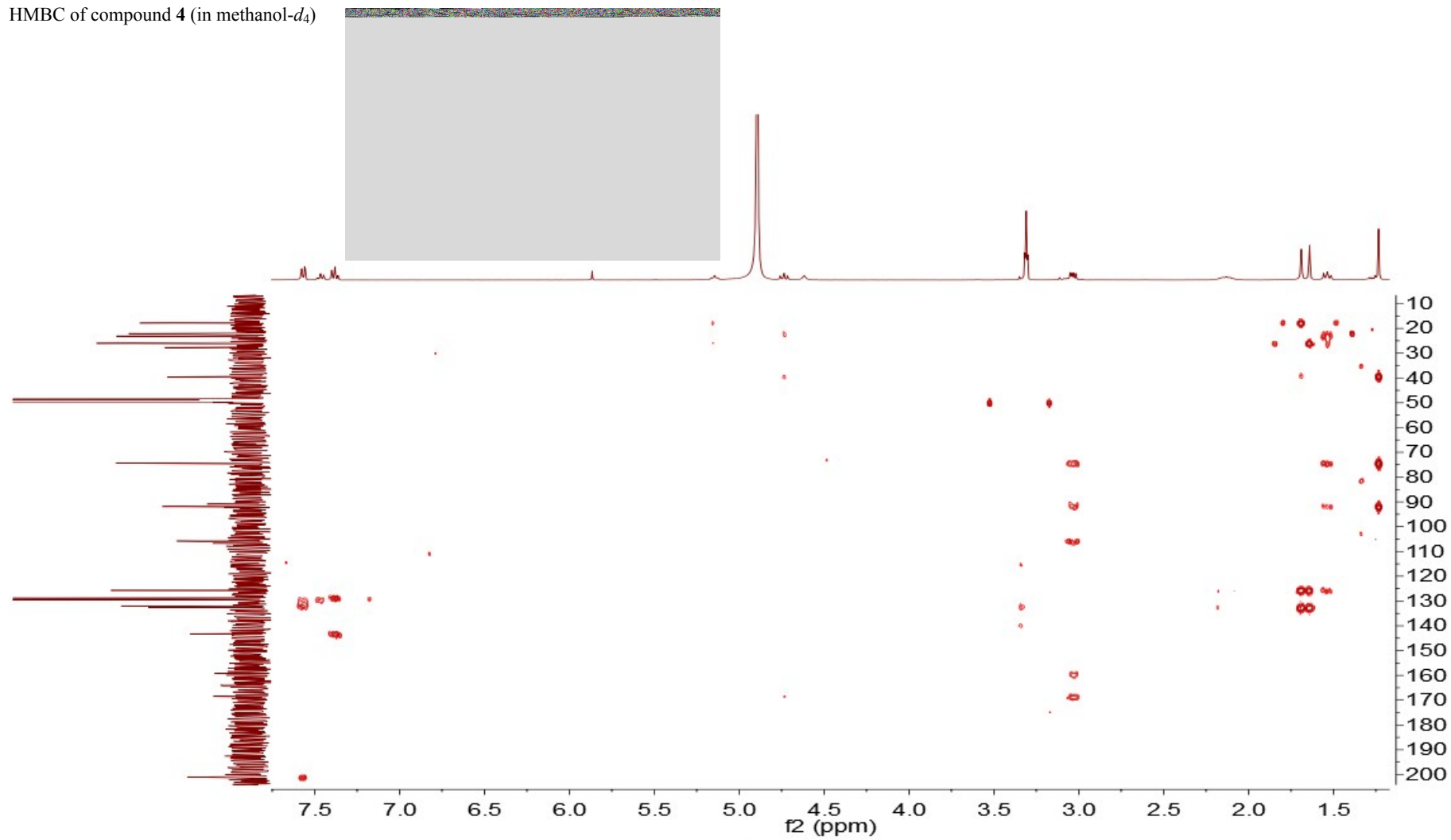




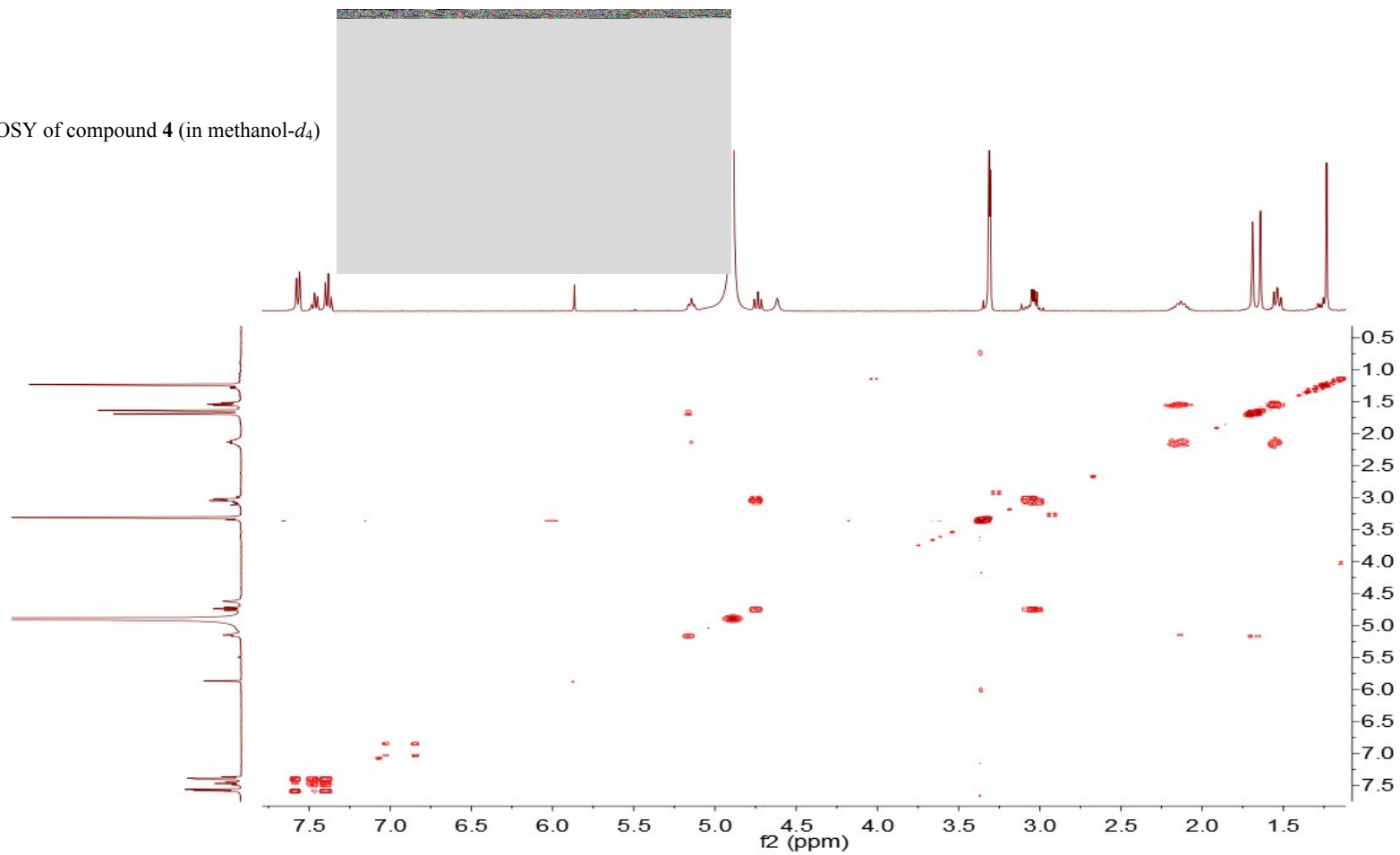
HSQC of compound 4 (in methanol-*d*₄)



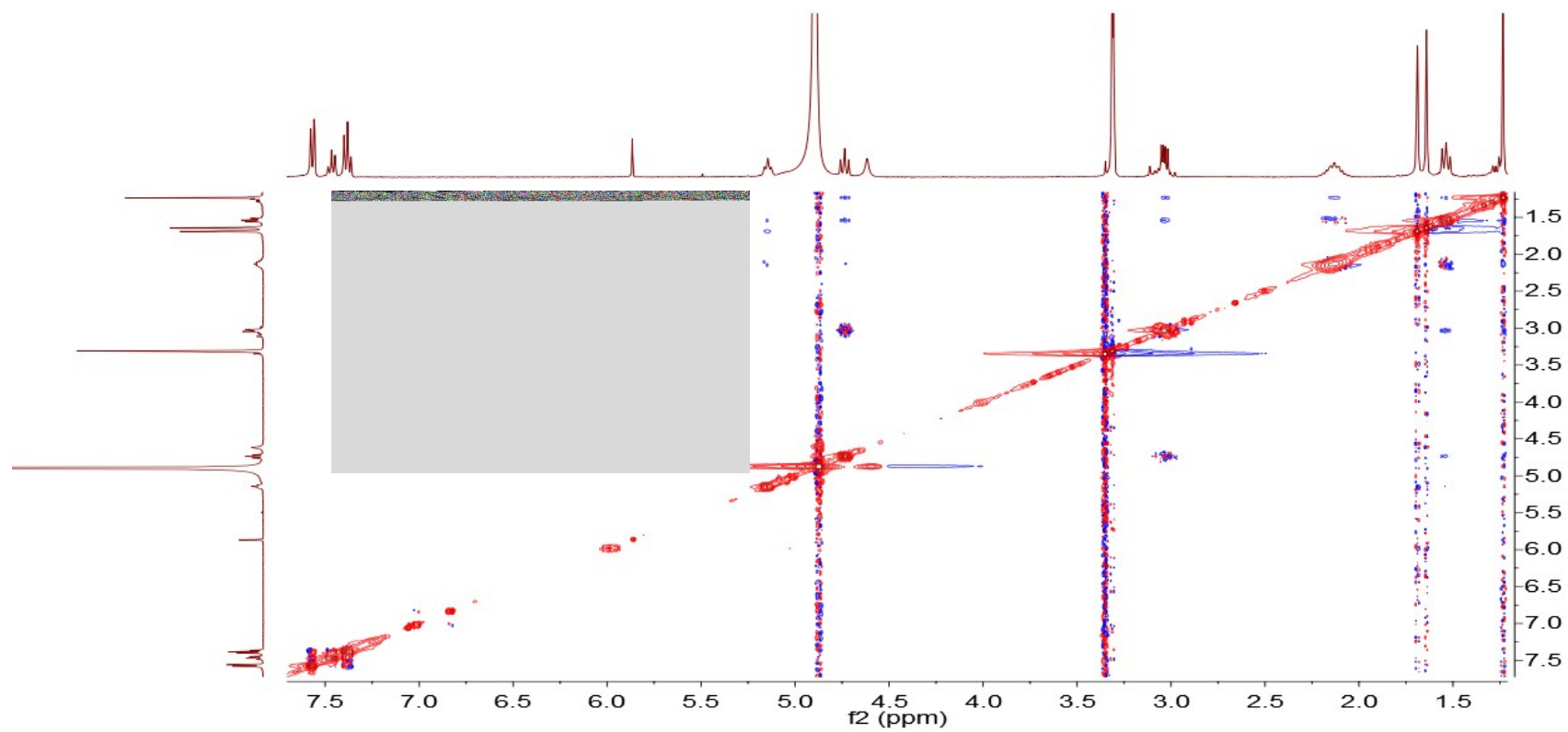
HMBC of compound 4 (in methanol- d_4)



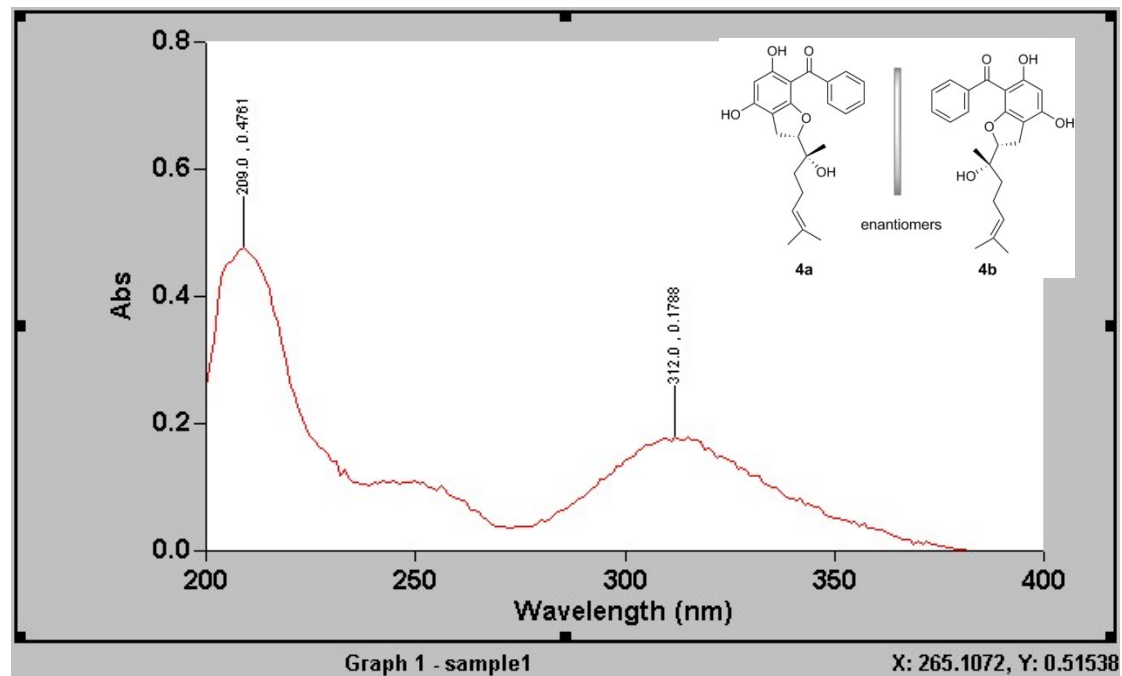
^1H - ^1H COSY of compound **4** (in methanol- d_4)



NOESY of compound 4 (in methanol-*d*₄)



UV of compound 4 (in MeOH)



IR of compound 4 (KBr disc)

