Supporting Information

Guaiane Sesquiterpenes from the Gorgonian *Echinogorgia flora* Collected in the South China Sea

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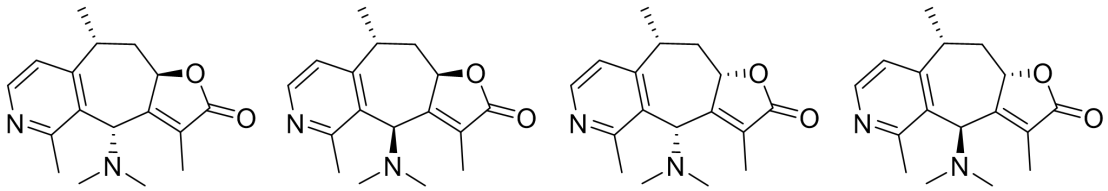


Fig. S1. The target structures of compound **1** for calculation.

Table S1. Stable conformers of compound **1** with (4*R*, 6*R*, 8*R*)-**1a**, (4*R*, 6*R*, 8*S*)-**1b**, (4*R*, 6*S*, 8*R*)-**1c** and (4*R*, 6*S*, 8*S*)-**1d** configurations, respectively.

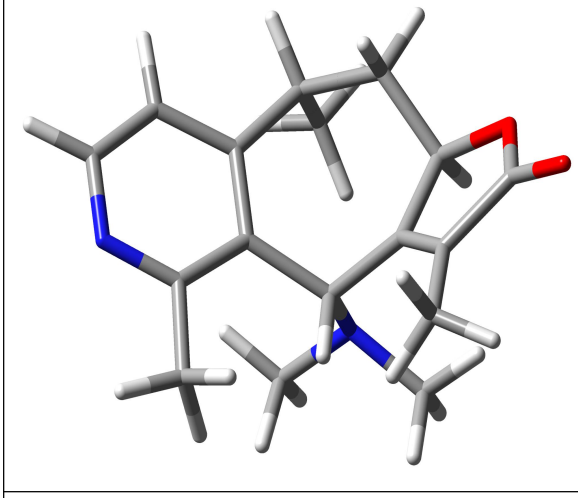
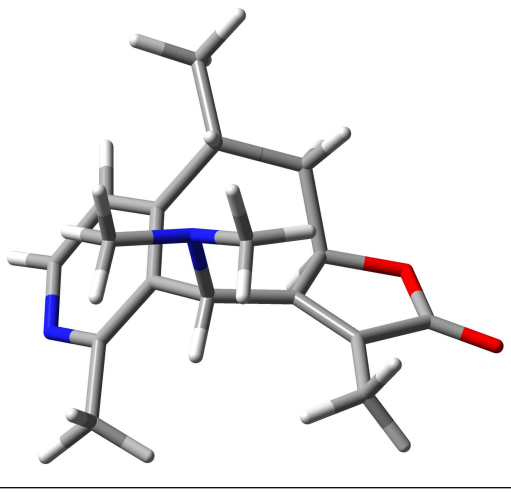
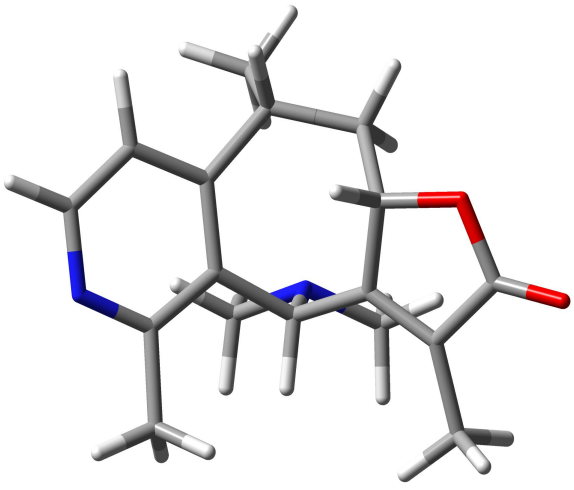
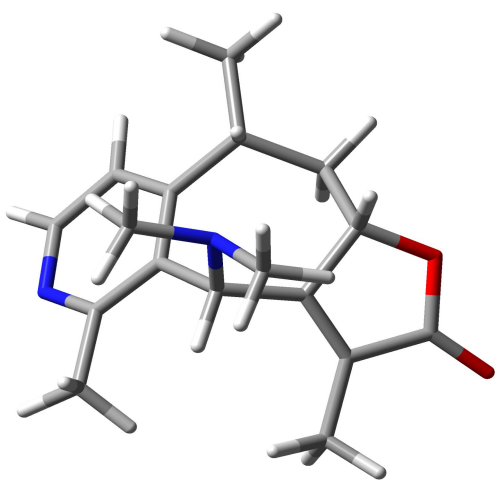
	
1a (99.85%)	**1b** (99.99%)
	
1c (99.99%)	**1d** (99.99%)

Table S2. Important thermodynamic parameters (a.u.) of the optimized compound **1** with simplified structures at B3LYP/6-31+G(d,p) level in the gas phase.

NO.	E+ZPE	G	NO.	E+ZPE	G
1a	-920.670050	-920.717362	**1b**	-920.666615	-920.713374
1c	-920.663978	-920.710861	**1d**	-920.673352	-920.720436

Table S3. Optimized *Z*-Matrixes of compound **1** with simplified structures in the Gas Phase (Å) at B3LYP/6-31+G(d,p) level.

1a				**1b**			
C	1.558967	1.069277	-0.539885	C	1.734230	0.816509	-0.080712
C	1.291596	-0.285838	-0.227453	C	1.258819	-0.470487	0.276978
C	0.095753	-0.746867	0.619686	C	-0.059257	-1.008665	-0.298187
C	-1.213518	-0.237927	0.066669	C	-1.206871	-0.129465	0.173454
C	-1.636128	1.203066	0.197717	C	-0.995244	1.310456	0.590210
C	-0.762007	2.193546	-0.574534	C	-0.361376	2.244984	-0.439670
C	0.717542	2.288002	-0.150892	C	0.957137	1.698555	-1.058513
C	-2.177962	-0.921851	-0.573492	C	-2.485413	-0.461814	0.428367
C	-3.297624	0.015952	-0.855935	C	-3.194504	0.754225	0.914237
O	-2.963073	1.251213	-0.361910	O	-2.297262	1.788914	0.965692
O	-4.353345	-0.210260	-1.396326	O	-4.353940	0.872703	1.228613
N	0.217706	-0.369104	2.053769	N	0.025087	-1.126586	-1.782082
C	-2.286282	-2.354045	-0.986692	C	-3.231273	-1.751441	0.313272
C	-0.853599	-0.967455	2.850933	C	1.091754	-2.044894	-2.178513
C	1.513783	-0.718375	2.635359	C	-1.226303	-1.517914	-2.424062
C	2.705515	1.336426	-1.300553	C	2.931104	1.242622	0.499867
C	3.519812	0.299778	-1.730327	C	3.595168	0.408747	1.394482
N	3.262979	-0.982405	-1.467445	N	3.150981	-0.797610	1.747733
C	2.176016	-1.273691	-0.735716	C	2.000603	-1.233400	1.202910
C	1.983408	-2.760985	-0.511161	C	1.570242	-2.608197	1.670669
C	0.910771	2.731266	1.313957	C	1.767347	2.853461	-1.659188
H	0.055590	-1.842388	0.545018	H	-0.243513	-2.010059	0.122842
H	-1.709493	1.499176	1.250016	H	-0.379903	1.323457	1.499641
H	-1.217772	3.184668	-0.468742	H	-0.177085	3.206012	0.054615
H	-0.820498	1.928659	-1.636462	H	-1.085274	2.430310	-1.240454
H	1.117354	3.103092	-0.765736	H	0.663951	1.031123	-1.873472
H	-1.557074	-2.989920	-0.478921	H	-3.900133	-1.865077	1.171264
H	-3.292892	-2.727025	-0.776319	H	-2.561627	-2.613068	0.261823
H	-2.133730	-2.457380	-2.067333	H	-3.865107	-1.761543	-0.580995
H	-0.765026	-0.624342	3.885594	H	0.904652	-3.086148	-1.853243
H	-1.833818	-0.664946	2.476539	H	2.049536	-1.723376	-1.766085
H	-0.818559	-2.073266	2.854028	H	1.175224	-2.045504	-3.269163
H	2.324676	-0.238947	2.085619	H	-1.576047	-2.523554	-2.124828
H	1.701615	-1.807451	2.655635	H	-2.014681	-0.797735	-2.203326
H	1.543630	-0.357432	3.667747	H	-1.073850	-1.528629	-3.507360
H	2.953031	2.360723	-1.563711	H	3.350441	2.212950	0.261537
H	4.411646	0.502869	-2.320833	H	4.530232	0.728449	1.851862
H	1.986759	-3.030226	0.549992	H	0.595297	-2.587781	2.170452
H	1.043513	-3.127128	-0.939085	H	2.312992	-2.974209	2.380170

H	2.806874	-3.281274	-1.000956	H	1.498128	-3.323293	0.843786
H	0.560325	1.968955	2.011709	H	2.677953	2.495417	-2.149337
H	1.969741	2.921142	1.516133	H	2.053262	3.595716	-0.905812
H	0.364402	3.663692	1.495606	H	1.165717	3.373264	-2.411520
1c				**1d**			
C	1.705674	0.925086	-0.336344	C	-1.623765	0.888487	-0.277636
C	1.285377	-0.423595	-0.266856	C	-1.212583	-0.459357	-0.150349
C	-0.003620	-0.837779	0.446452	C	0.001709	-0.860448	0.698727
C	-1.202378	-0.214918	-0.233033	C	1.246092	-0.206592	0.140695
C	-1.150360	1.194469	-0.765524	C	1.554562	1.255978	0.357410
C	-0.558189	2.183544	0.232967	C	0.514699	2.240678	-0.182350
C	0.994853	2.172596	0.215941	C	-0.894868	2.032052	0.429287
C	-2.436080	-0.709975	-0.429323	C	2.223032	-0.753320	-0.603792
C	-3.279070	0.378050	-0.999274	C	3.221608	0.306812	-0.905053
O	-2.507986	1.507161	-1.120575	O	2.807835	1.473842	-0.313088
O	-4.447511	0.345533	-1.299985	O	4.248176	0.220031	-1.534428
N	0.064666	-0.470473	1.891752	N	-0.162051	-0.533933	2.137303
C	-3.042773	-2.041398	-0.127097	C	2.432442	-2.139829	-1.121397
C	1.198915	-1.128540	2.543905	C	-1.414848	-1.047156	2.690913
C	-1.160497	-0.785685	2.625604	C	0.964376	-1.037841	2.922975
C	2.919859	1.175962	-0.992497	C	-2.722371	1.148417	-1.103030
C	3.649170	0.132926	-1.542368	C	-3.354801	0.099812	-1.760265
N	3.242986	-1.138638	-1.510159	N	-2.979244	-1.174029	-1.645022
C	2.084556	-1.413262	-0.891721	C	-1.929390	-1.454942	-0.854532
C	1.701052	-2.878872	-0.924529	C	-1.592260	-2.930794	-0.785619
C	1.552079	2.579749	1.594290	C	-1.667680	3.359167	0.432322
H	-0.115702	-1.929474	0.364915	H	0.136096	-1.946711	0.589702
H	-0.569692	1.230067	-1.698178	H	1.711346	1.458633	1.424685
H	-0.902555	3.190118	-0.024804	H	0.869753	3.250721	0.049105
H	-0.934173	1.957079	1.233920	H	0.475315	2.156856	-1.274218
H	1.288472	2.962711	-0.486625	H	-0.757326	1.724026	1.471997
H	-2.287832	-2.799364	0.093821	H	3.495481	-2.393298	-1.079995
H	-3.722846	-1.975295	0.729966	H	1.865913	-2.883727	-0.555885
H	-3.645508	-2.375143	-0.977235	H	2.132535	-2.212093	-2.173542
H	1.253202	-0.796616	3.584759	H	-1.490748	-0.739769	3.738049
H	1.111301	-2.231503	2.544944	H	-2.270626	-0.636231	2.153200
H	2.135450	-0.859109	2.053336	H	-1.481930	-2.150752	2.658340
H	-1.406565	-1.864007	2.616479	H	0.843815	-0.728942	3.965240
H	-2.010613	-0.236310	2.219394	H	1.908822	-0.630026	2.555879
H	-1.031323	-0.482273	3.668473	H	1.041779	-2.141182	2.900292
H	3.287432	2.194774	-1.079110	H	-3.089631	2.157936	-1.240425
H	4.595003	0.324446	-2.046285	H	-4.207719	0.292716	-2.409053
H	1.644915	-3.316266	0.078472	H	-2.324994	-3.471112	-1.385684

H	0.731856	-3.042774	-1.408176	H	-0.595449	-3.148842	-1.184336
H	2.463934	-3.414417	-1.490310	H	-1.627515	-3.319223	0.237829
H	2.641619	2.678047	1.570484	H	-1.739575	3.797665	-0.568947
H	1.280562	1.832647	2.343011	H	-2.681772	3.238175	0.825060
H	1.132070	3.544733	1.898511	H	-1.148322	4.083188	1.067029

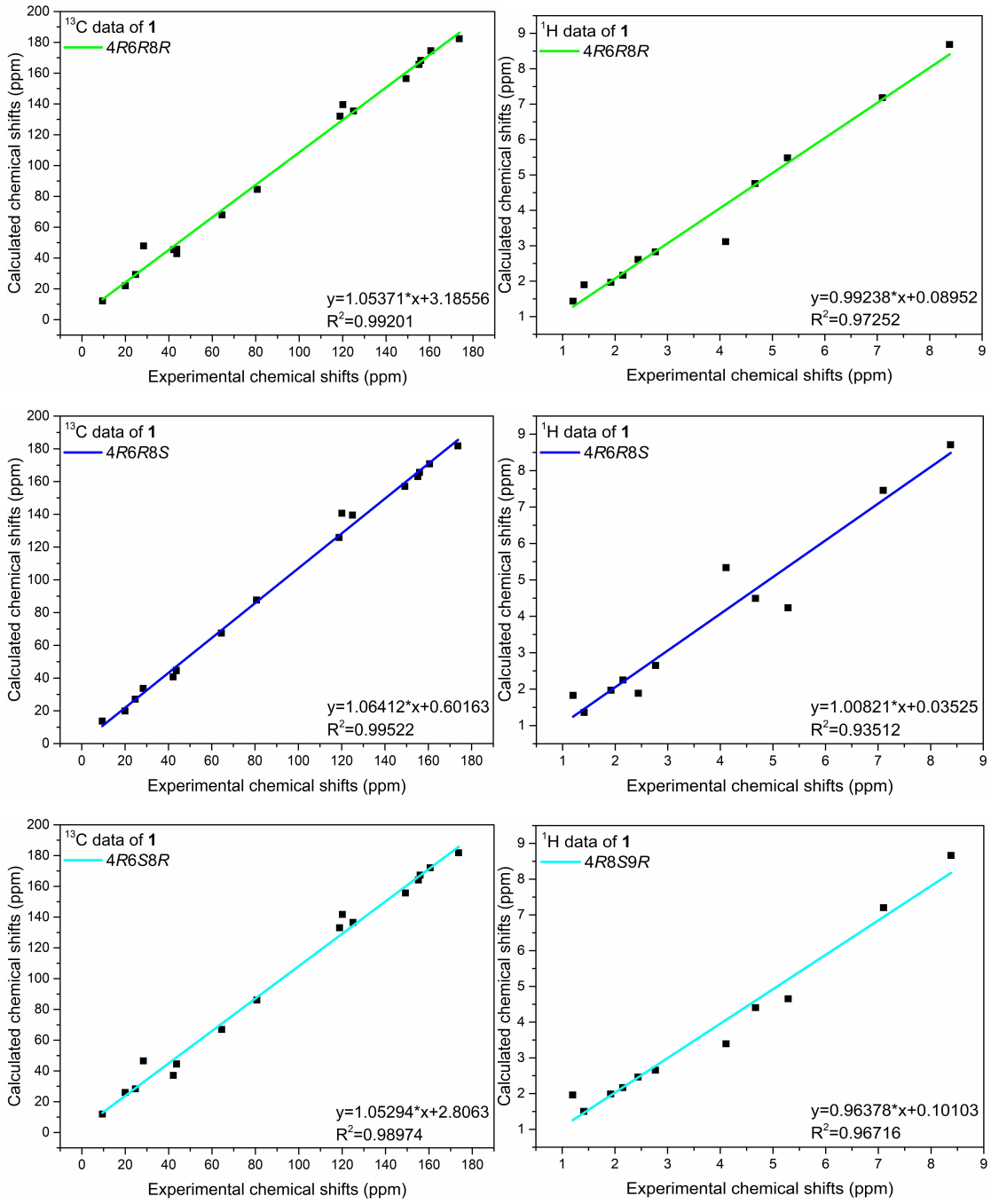


Fig. S2 The fitting lines of experimental and calculated NMR data of **1**.

Table S4 Chemical shifts of experimental and calculated NMR and spatial distance between H-4 and N-1'.

	Chemical shift (ppm)	Spatial distance (Å)
Expetl.	4.11	--
Calcd. For 4*R*6*R*8*R*	3.12	4.56
Calcd. For 4*R*6*R*8*S*	5.33	2.25
Calcd. For 4*R*6*S*8*R*	3.39	4.35
Calcd. For 4*R*6*S*8*S*	4.45	2.42

	A	B	C	D	E	F	G	H
1	Functional		Solvent?		Basis Set		Type of Data	
2	B3LYP		PCM		6-31+G(d,p)		Unscaled Shifts	
3								
12			DP4+	0.00%	0.00%	0.00%	100.00%	-
14	Nuclei	sp2?	xperimenta	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5
15	C	x	155.2	165.6309	163.031	164.0987	165.6045	
16	C	x	120.1	139.4987	140.6198	141.7372	139.2584	
17	C		64.5	67.9516	67.441	66.9533	69.3415	
18	C	x	160.6	174.5185	170.7675	172.0453	173.3425	
19	C		80.7	84.5074	87.6118	86.0367	86.2166	
20	C		42.2	45.3764	40.7453	37.0889	47.5415	
21	C		28.4	47.795	33.6546	46.5458	34.6522	
22	C	x	125	135.381	139.5042	136.5257	134.7425	
23	C	x	173.7	182.3171	181.7725	181.7933	181.9192	
24	C		9.5	12.1005	13.7195	11.9115	12.0503	
25	C		43.7	44.4804	46.60623745	44.3971	43.1678	
26	C		43.7	44.7492	42.48684755	44.5548	45.173	
27	C	x	118.8	132.0331	125.8288	133.0309	124.326	
28	C	x	149.2	156.4742	157.0274	155.6494	156.8612	
29	C	x	156	168.1975	165.5414	167.2391	166.3813	
30	C		24.7	29.3018	27.0638	28.358	28.5173	
31	C		20	21.9811	19.8791	26.0044	20.9726	
32								
33	H		4.67	4.76	4.49	4.41	4.71	
34	H		5.29	5.48	4.23	4.65	5.41	
35	H		2.44	2.61	1.89	2.46	2.40	
36	H		1.2	1.43	1.83	1.96	1.13	
37	H		4.11	3.12	5.33	3.39	4.45	
38	H		1.92	1.96	1.97	1.99	1.95	
39	H		2.15	2.16	2.25	2.17	2.14	
40	H	x	7.1	7.18	7.46	7.20	7.34	
41	H	x	8.38	8.68	8.71	8.66	8.57	
42	H		2.77	2.83	2.65	2.65	2.83	
43	H		1.41	1.90	1.36	1.50	1.39	
44								

Main | Detailed Results

	A	B	C	D	E	F	G	H
1	Functional		Solvent?		Basis Set		Type of Data	
2	B3LYP		PCM		6-31+G(d,p)		Unscaled Shifts	
3								
4			Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6
5	sDP4+ (H data)		0.00%	0.00%	0.00%	100.00%	-	-
6	sDP4+ (C data)		0.00%	0.05%	0.00%	99.95%	-	-
7	sDP4+ (all data)		0.00%	0.00%	0.00%	100.00%	-	-
8	uDP4+ (H data)		0.00%	0.00%	0.00%	100.00%	-	-
9	uDP4+ (C data)		0.00%	1.01%	0.00%	98.99%	-	-
10	uDP4+ (all data)		0.00%	0.00%	0.00%	100.00%	-	-
11	DP4+ (H data)		0.00%	0.00%	0.00%	100.00%	-	-
12	DP4+ (C data)		0.00%	0.00%	0.00%	100.00%	-	-
13	DP4+ (all data)		0.00%	0.00%	0.00%	100.00%	-	-

Main | Detailed Results

Fig. S3 Detailed DP4+ probability (calculated at PCM/b3lyp/6-311+G(d,p) level) for compound **1**. Isomer 1 is (4*R*, 6*R*, 8*R*)-**1a**, isomer 2 is (4*R*, 6*R*, 8*S*)-**1b**, isomer 3 is (4*R*, 6*S*, 8*R*)-**1c**, and isomer 4 is (4*R*, 6*S*, 8*S*)-**1d**.

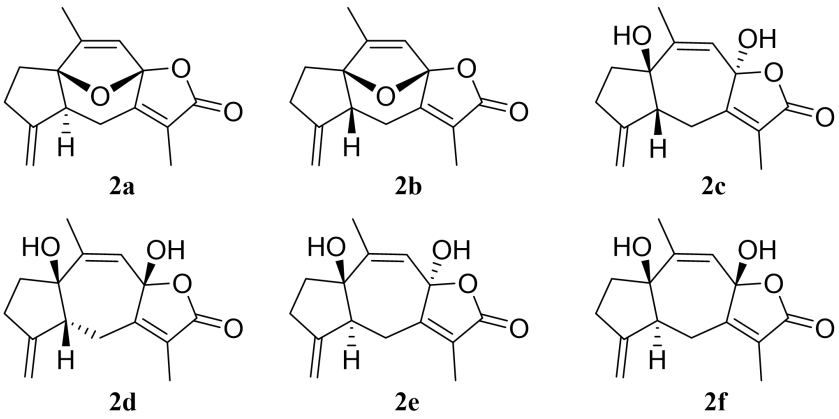


Fig. S4. The target structures of compound **2** for calculation.

Table S5. Stable conformers of compound **2** with (1*R*, 5*S*, 8*S*)-**2a** and (1*R*, 5*R*, 8*S*)-**2b** configurations, respectively.

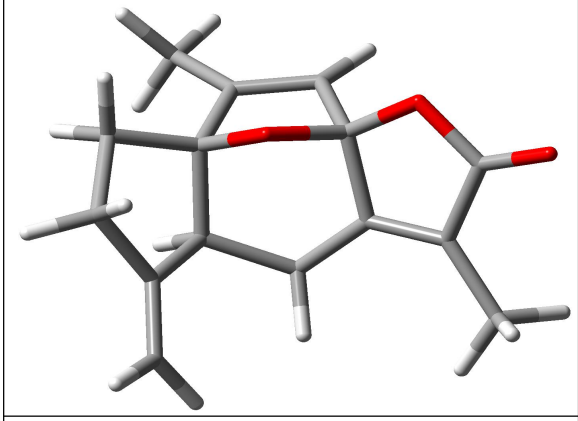
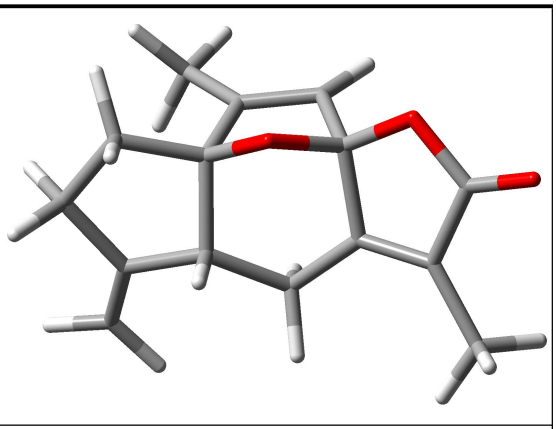
	
2a1 (100%)	**2b1** (100%)

Table S6. Important thermodynamic parameters (a.u.) of the optimized compound **2** with simplified structures at B3LYP/6-31+G(d,p) level in the gas phase.

conformations	E+ZPE	G	conformations	E+ZPE	G
2a1	-806.605191	-806.647421	**2b1**	-806.600672	-806.642066

Table S7. Optimized *Z*-Matrixes of compound **2** with simplified structures in the Gas Phase (Å) at B3LYP/6-31+G(d,p) level.

2a1				**2b1**			
C	-1.478349	-0.514769	-0.223943	C	-1.160734	-0.616712	-0.543077
C	-1.401156	0.706664	0.750932	C	-1.151928	0.940744	-0.420980
C	-0.016518	0.842626	1.455138	C	-0.039036	1.454740	0.514807
C	1.091636	0.247899	0.635340	C	1.192076	0.622782	0.264289
C	0.718212	-0.919727	-0.255292	C	0.972583	-0.864074	0.005778
C	0.058592	-2.073440	0.477561	C	0.172736	-1.502742	1.120958
C	-1.257542	-1.843817	0.497976	C	-1.117390	-1.321382	0.826527

C	2.372686	0.567908	0.414736	C	2.497188	0.890241	0.134424
C	2.897679	-0.380878	-0.607188	C	3.185711	-0.390614	-0.196095
O	1.873739	-1.241949	-0.987290	O	2.239186	-1.406007	-0.261543
C	-2.721531	-0.233099	-1.059574	C	-2.384790	-0.868840	-1.425287
C	-2.635106	1.287419	-1.321567	C	-3.408617	0.219011	-0.978873
C	-1.874332	1.861309	-0.127662	C	-2.605334	1.261800	-0.191749
C	-1.681722	3.157711	0.109528	C	-3.107887	2.223186	0.582732
O	4.001228	-0.453203	-1.081152	O	4.356280	-0.594855	-0.384171
C	-2.347376	-2.623355	1.160114	C	-2.318831	-1.656714	1.651831
C	3.236275	1.660691	0.955486	C	3.270512	2.164725	0.234115
O	-0.326544	-0.433584	-1.095950	O	0.101028	-0.990933	-1.125259
H	-2.159741	0.555506	1.533383	H	-0.895132	1.269370	-1.440346
H	0.194502	1.887901	1.698351	H	0.160075	2.519424	0.357626
H	-0.061828	0.307433	2.412272	H	-0.353666	1.336828	1.559861
H	0.612215	-2.875142	0.950644	H	0.611865	-1.913243	2.021896
H	-2.732017	-0.832551	-1.972987	H	-2.084770	-0.721893	-2.467246
H	-3.616293	-0.479727	-0.476546	H	-2.774136	-1.886213	-1.337966
H	-3.617977	1.751348	-1.448985	H	-4.202071	-0.203453	-0.354236
H	-2.066259	1.472102	-2.239080	H	-3.903635	0.672425	-1.844599
H	-1.124917	3.513921	0.971662	H	-2.467576	2.917159	1.119630
H	-2.075212	3.920798	-0.556143	H	-4.179388	2.360842	0.700207
H	-1.950940	-3.494622	1.687271	H	-2.031237	-2.180646	2.567004
H	-2.894250	-2.007329	1.885566	H	-2.868158	-0.750968	1.934311
H	-3.084488	-2.973204	0.427487	H	-3.018071	-2.296116	1.100227
H	4.090349	1.244442	1.501192	H	4.024759	2.097353	1.025660
H	2.681444	2.316199	1.630984	H	2.619676	3.016186	0.446744
H	3.649358	2.263962	0.140550	H	3.811945	2.360397	-0.697394

	A	B	C	D	E	F	G	H	I
1	Functional		Solvent?		Basis Set		Type of Data		
2	B3LYP		PCM		6-311+G(d,p)		Unscaled Shifts		
3									
12			DP4+	99.89%	0.11%	0.00%	0.00%	0.00%	0.00%
14	Nuclei	sp2?	xperimenta	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6
15	C		95.75	103.16	99.95	92.05	92.32	88.99	89.20
16	C		42.13	48.36	54.14	66.54	57.04	52.38	57.85
17	C		22.45	27.81	27.64	36.25	35.62	29.93	31.36
18	C	x	154.25	166.72	167.37	168.42	170.85	170.27	169.70
19	C		108.89	114.98	116.56	109.35	108.82	109.76	109.69
20	C	x	125.10	133.77	133.82	128.71	131.05	132.87	132.93
21	C	x	148.04	161.77	160.67	160.38	162.13	161.05	166.25
22	C	x	120.56	128.59	129.89	133.02	131.87	134.73	132.75
23	C	x	172.63	181.83	181.69	180.08	180.69	179.64	180.17
24	C		30.47	34.80	33.32	41.74	39.55	41.70	40.52
25	C		30.39	35.95	34.89	32.64	35.90	34.85	35.84
26	C	x	150.29	165.38	162.15	170.00	170.65	168.31	168.52
27	C	x	107.60	111.36	110.47	113.90	111.37	111.02	110.93
28	C		13.37	14.68	16.96	27.73	24.72	24.50	24.53
29	C		8.69	10.54	10.82	11.08	10.95	10.85	11.19
30									
31	H		2.46	2.74	2.79	2.52	3.54	2.65	3.68
32	H		2.91	3.10	3.09	2.85	2.81	3.00	2.91
33	H		2.67	2.82	2.32	2.73	2.46	2.78	3.10
34	H	x	5.78	5.89	5.98	6.04	6.00	6.06	6.05
35	H		2.60	1.88	2.04	2.19	2.10	1.82	2.03
36	H		2.67	1.98	2.10	2.26	1.72	2.01	1.89
37	H		1.99	2.74	2.57	2.71	2.45	2.84	2.51
38	H		1.96	2.81	2.92	2.64	2.95	2.58	2.94
39	H	x	4.93	5.28	5.12	5.48	5.36	5.33	5.39
40	H	x	5.07	5.40	5.13	5.34	5.25	5.19	5.22
41	H		1.89	2.00	1.93	2.01	2.03	2.03	1.89
42	H		1.79	1.78	1.84	1.86	1.82	1.84	1.89

	A	B	C	D	E	F	G	H
1	Functional		Solvent?		Basis Set		Type of Data	
2	B3LYP		PCM		6-311+G(d,p)		Unscaled Shifts	
3								
4			Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6
5	sDP4+ (H data)		3.02%	0.51%	65.08%	0.01%	31.38%	0.00%
6	sDP4+ (C data)		90.60%	9.40%	0.00%	0.00%	0.00%	0.00%
7	sDP4+ (all data)		98.27%	1.73%	0.00%	0.00%	0.00%	0.00%
8	uDP4+ (H data)		0.11%	0.07%	98.82%	0.01%	0.98%	0.00%
9	uDP4+ (C data)		91.07%	8.93%	0.00%	0.00%	0.00%	0.00%
10	uDP4+ (all data)		94.01%	5.99%	0.00%	0.00%	0.00%	0.00%
11	DP4+ (H data)		0.01%	0.00%	99.52%	0.00%	0.47%	0.00%
12	DP4+ (C data)		98.99%	1.01%	0.00%	0.00%	0.00%	0.00%
13	DP4+ (all data)		99.89%	0.11%	0.00%	0.00%	0.00%	0.00%

Fig. S5. Detailed DP4+ probability (calculated at PCM/b3lyp/6-311+G(d,p) level) for compound **2**. Isomer 1 is (1*R*, 5*S*, 8*S*)-**2a**, isomer 2 is (1*R*, 5*R*, 8*S*)-**2b**, isomer 3 is (1*R*, 5*R*, 8*R*)-**2c**, isomer 4 is (1*R*, 5*R*, 8*S*)-**2d**, isomer 5 is (1*R*, 5*S*, 8*R*)-**2e**, isomer 6 is (1*R*, 5*S*, 8*S*)-**2f**.

Table S8. Stable conformers of compound **3** with (1*S*, 4*R*, 8*R*, 10*R*)-**3a** and(1*R*, 4*S*, 8*S*, 10*S*)-**3b** configurations, respectively.

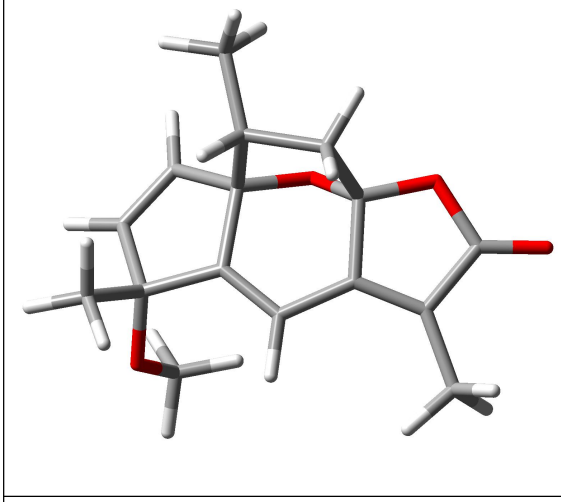
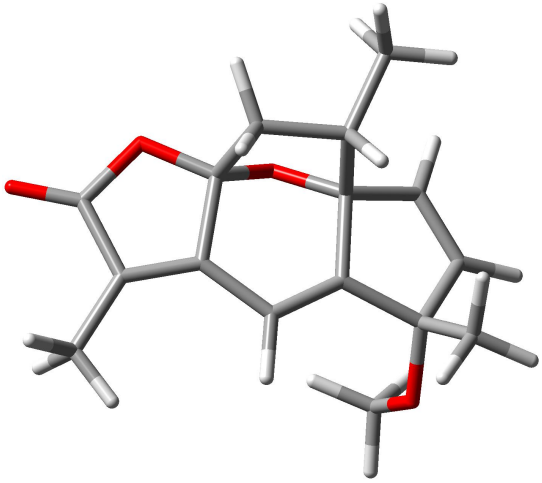
	
3a1 (99.38%)	**3b1** (99.38%)

Table S9. Important thermodynamic parameters (a.u.) of the optimized compound **3** with simplified structures at B3LYP/6-31+G(d,p) level in the gas phase.

NO.	E+ZPE	G	NO.	E+ZPE	G
3a1	-921.104802	-921.149688	**3b1**	-921.104802	-921.149688

Table S10. Optimized *Z*-Matrixes of compound **3** with simplified structures in the Gas Phase (Å) at B3LYP/6-31+G(d,p) level.

3a1				**3b1**			
C	-0.834277	0.982343	-0.329107	C	0.834277	0.982343	-0.329107
C	-1.069920	-0.364933	0.351658	C	1.069920	-0.364933	0.351658
C	-0.034303	-1.135482	0.733374	C	0.034303	-1.135482	0.733374
C	1.290009	-0.633095	0.431029	C	-1.290009	-0.633095	0.431029
C	1.362772	0.781877	-0.118538	C	-1.362772	0.781877	-0.118538
C	1.019570	1.887487	0.908759	C	-1.019570	1.887487	0.908759
C	-0.499401	2.112087	0.712574	C	0.499401	2.112087	0.712574
C	2.514806	-1.189883	0.361241	C	-2.514806	-1.189883	0.361241
C	3.401027	-0.218305	-0.328911	C	-3.401027	-0.218305	-0.328911
O	2.661629	0.917522	-0.642373	O	-2.661629	0.917522	-0.642373
C	-2.092736	1.148006	-1.135185	C	2.092736	1.148006	-1.135185
C	-3.022336	0.250942	-0.792561	C	3.022336	0.250942	-0.792561
C	-2.548759	-0.730968	0.274271	C	2.548759	-0.730968	0.274271
C	-0.823312	3.518106	0.198497	C	0.823312	3.518106	0.198497
O	4.564644	-0.322466	-0.620429	O	-4.564644	-0.322466	-0.620429
C	3.015957	-2.537698	0.761622	C	-3.015957	-2.537698	0.761622
C	-3.286448	-0.539654	1.607879	C	3.286448	-0.539654	1.607879
O	0.367626	0.931612	-1.133000	O	-0.367626	0.931612	-1.133000

O	-2.777021	-2.102933	-0.057838	O	2.777021	-2.102933	-0.057838
C	-2.333129	-2.528877	-1.340980	C	2.333129	-2.528877	-1.340980
H	-0.181534	-2.141576	1.116402	H	0.181534	-2.141576	1.116402
H	1.594203	2.778704	0.644143	H	-1.594203	2.778704	0.644143
H	1.292696	1.595213	1.925327	H	-1.292696	1.595213	1.925327
H	-1.051865	1.930551	1.639865	H	1.051865	1.930551	1.639865
H	-2.214055	1.947986	-1.856602	H	2.214055	1.947986	-1.856602
H	-4.032251	0.205472	-1.188747	H	4.032251	0.205472	-1.188747
H	-0.463997	4.273448	0.904773	H	0.463997	4.273448	0.904773
H	-1.900593	3.665379	0.072832	H	1.900593	3.665379	0.072832
H	-0.334205	3.699726	-0.764159	H	0.334205	3.699726	-0.764159
H	2.231575	-3.139051	1.227052	H	-2.231575	-3.139051	1.227052
H	3.403268	-3.079653	-0.108012	H	-3.403268	-3.079653	-0.108012
H	3.848979	-2.445464	1.467188	H	-3.848979	-2.445464	1.467188
H	-4.354369	-0.731368	1.468751	H	4.354369	-0.731368	1.468751
H	-2.901336	-1.248682	2.345670	H	2.901336	-1.248682	2.345670
H	-3.157007	0.476634	1.988404	H	3.157007	0.476634	1.988404
H	-2.552365	-3.597348	-1.395659	H	2.552365	-3.597348	-1.395659
H	-2.863481	-2.015247	-2.152607	H	2.863481	-2.015247	-2.152607
H	-1.255793	-2.376320	-1.479226	H	1.255793	-2.376320	-1.479226

Table S11. Stable conformers of compound **4** with (1*R*, 5*S*, 8*S*, 10*R*)-**4a** and (1*S*, 5*R*, 8*R*, 10*S*)-**4b** configurations, respectively.

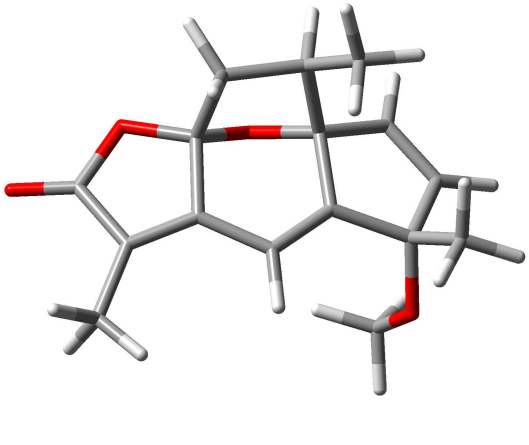
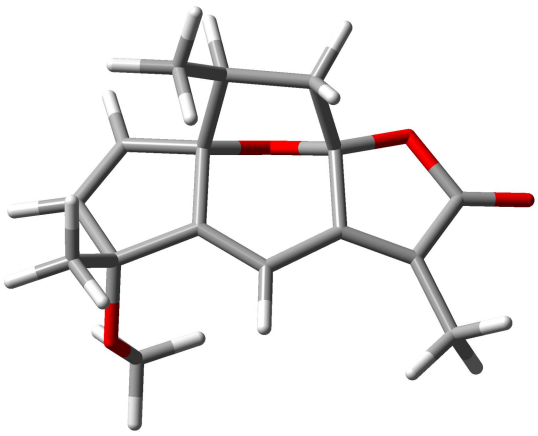
	
4a1 (99.26%)	**4b1** (99.26%)

Table S12. Important thermodynamic parameters (a.u.) of the optimized compound **4** at B3LYP/6-31+G(d,p) level in the gas phase.

NO.	E+ZPE	G	NO.	E+ZPE	G
4a1	-921.103880	-921.148568	**4b1**	-921.103880	-921.148568

Table S13. Optimized *Z*-Matrixes of compound **4** with simplified structures in the Gas Phase (Å) at B3LYP/6-31+G(d,p) level.

4a1				**4b1**			
C	0.819684	0.977039	-0.587258	C	-0.819684	0.977039	-0.587258
C	1.062314	-0.233212	0.314844	C	-1.062314	-0.233212	0.314844
C	0.025681	-0.910136	0.846250	C	-0.025681	-0.910136	0.846250
C	-1.302082	-0.456543	0.487804	C	1.302082	-0.456543	0.487804
C	-1.378394	0.823125	-0.329264	C	1.378394	0.823125	-0.329264
C	-1.028036	2.103543	0.468169	C	1.028036	2.103543	0.468169
C	0.472778	2.309031	0.162586	C	-0.472778	2.309031	0.162586
C	-2.529012	-1.010544	0.543485	C	2.529012	-1.010544	0.543485
C	-3.420143	-0.191985	-0.318242	C	3.420143	-0.191985	-0.318242
O	-2.681181	0.853896	-0.860591	O	2.681181	0.853896	-0.860591
C	2.069894	1.006411	-1.419472	C	-2.069894	1.006411	-1.419472
C	2.993405	0.152458	-0.967477	C	-2.993405	0.152458	-0.967477
C	2.519183	-0.684514	0.215892	C	-2.519183	-0.684514	0.215892
C	1.337175	2.671152	1.366535	C	-1.337175	2.671152	1.366535
O	-4.586953	-0.347933	-0.571480	O	4.586953	-0.347933	-0.571480
C	-3.029597	-2.249398	1.208849	C	3.029597	-2.249398	1.208849
C	3.342664	-0.439563	1.487065	C	-3.342664	-0.439563	1.487065
O	-0.390111	0.765657	-1.359734	O	0.390111	0.765657	-1.359734
O	2.644235	-2.095957	-0.002120	O	-2.644235	-2.095957	-0.002120
C	2.105075	-2.605554	-1.216646	C	-2.105075	-2.605554	-1.216646
H	0.170853	-1.849334	1.373307	H	-0.170853	-1.849334	1.373307
H	-1.644962	2.924959	0.097991	H	1.644962	2.924959	0.097991
H	-1.229875	1.977821	1.535636	H	1.229875	1.977821	1.535636
H	0.571388	3.097784	-0.592385	H	-0.571388	3.097784	-0.592385
H	2.189977	1.701836	-2.243911	H	-2.189977	1.701836	-2.243911
H	3.995395	0.035643	-1.369274	H	-3.995395	0.035643	-1.369274
H	2.391903	2.762650	1.087400	H	-2.391903	2.762650	1.087400
H	1.022976	3.632349	1.785470	H	-1.022976	3.632349	1.785470
H	1.253431	1.920176	2.158524	H	-1.253431	1.920176	2.158524
H	-2.240054	-2.755402	1.769276	H	2.240054	-2.755402	1.769276
H	-3.437080	-2.946947	0.469096	H	3.437080	-2.946947	0.469096
H	-3.848199	-2.012773	1.897529	H	3.848199	-2.012773	1.897529
H	3.316505	0.609729	1.785697	H	-3.316505	0.609729	1.785697
H	4.381359	-0.733066	1.310058	H	-4.381359	-0.733066	1.310058
H	2.947833	-1.052046	2.302373	H	-2.947833	-1.052046	2.302373
H	2.222133	-3.690209	-1.164941	H	-2.222133	-3.690209	-1.164941
H	2.643597	-2.231538	-2.096336	H	-2.643597	-2.231538	-2.096336
H	1.041352	-2.364808	-1.332822	H	-1.041352	-2.364808	-1.332822

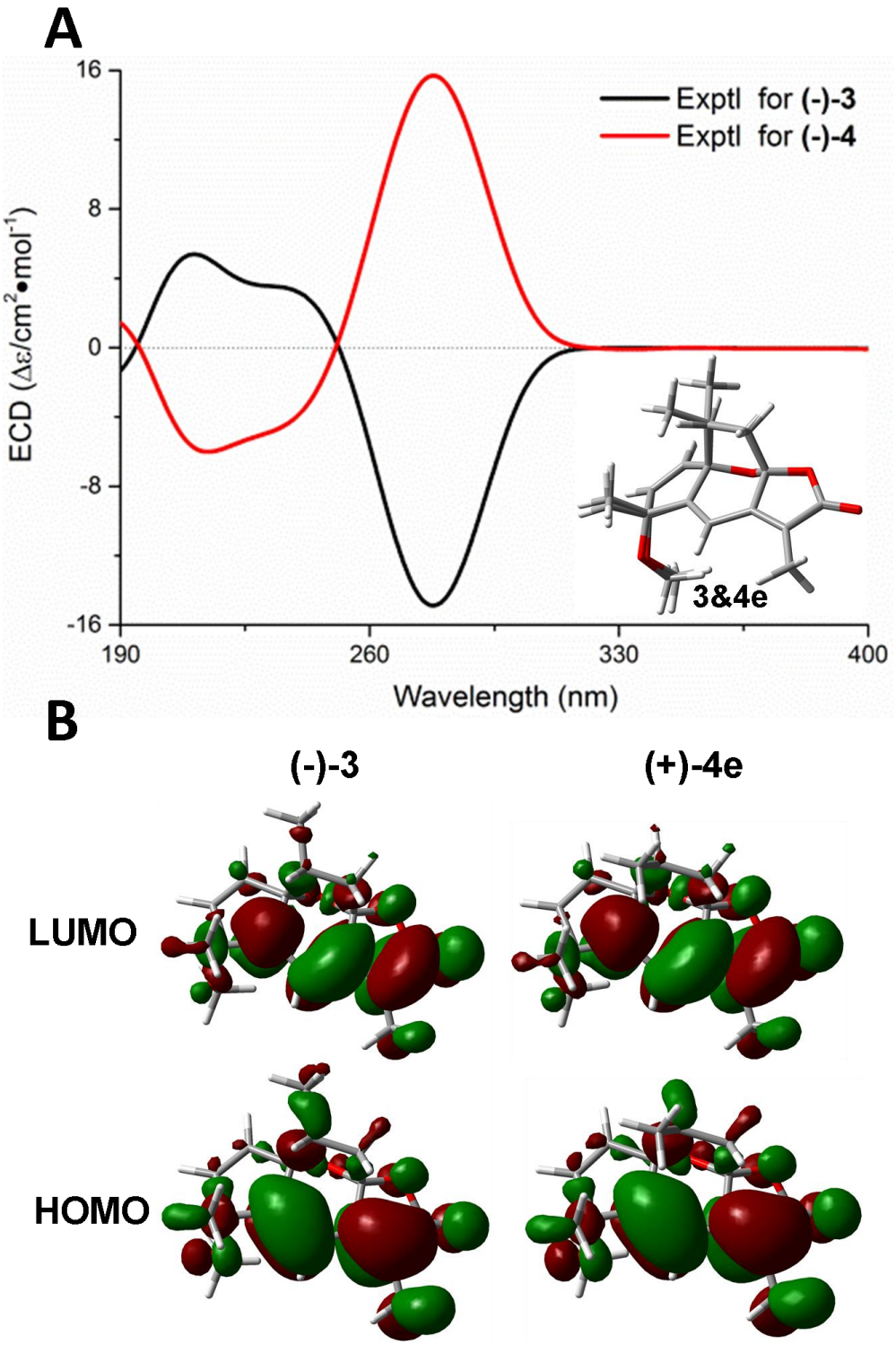


Fig. S6 (**A**) Experimental ECD spectra of **3-4**; (**B**) optimal conformations and MOs of **3** and **4e** (the enantiomer of **4**).

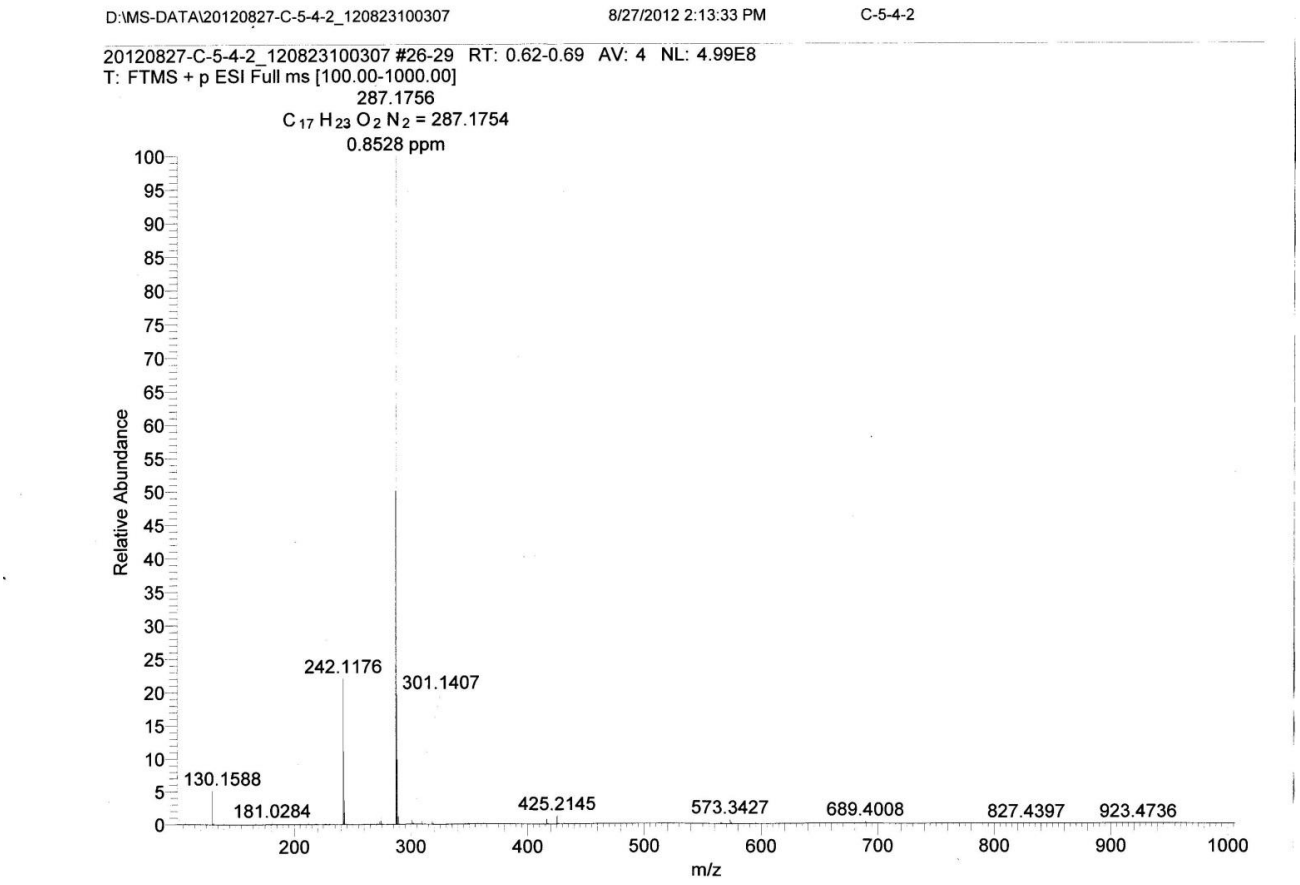


Fig. S7. HRESIMS spectrum of compound **1**.

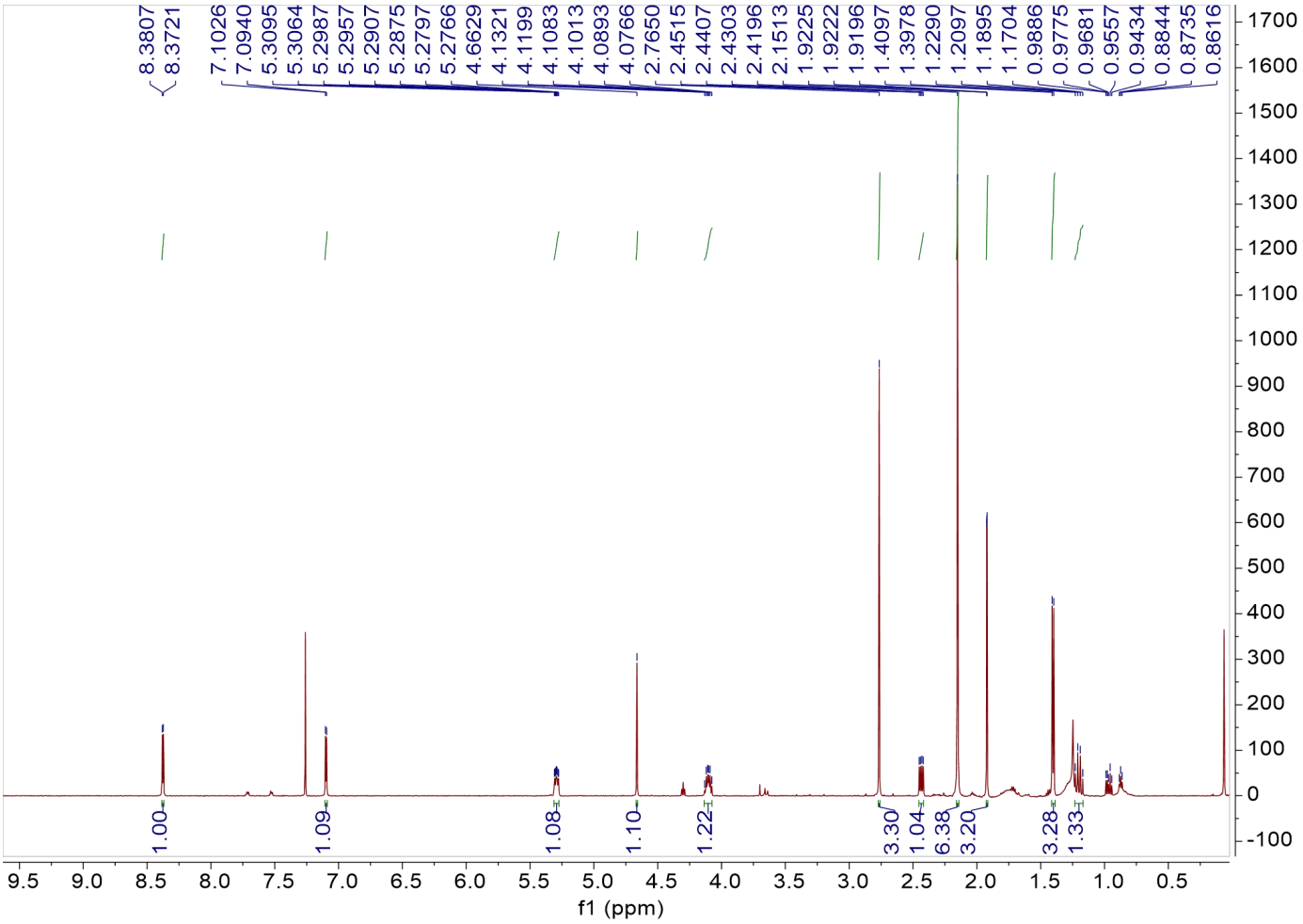


Fig. S8. ^{1}H NMR spectrum of compound **1** in $CDCl_3$.

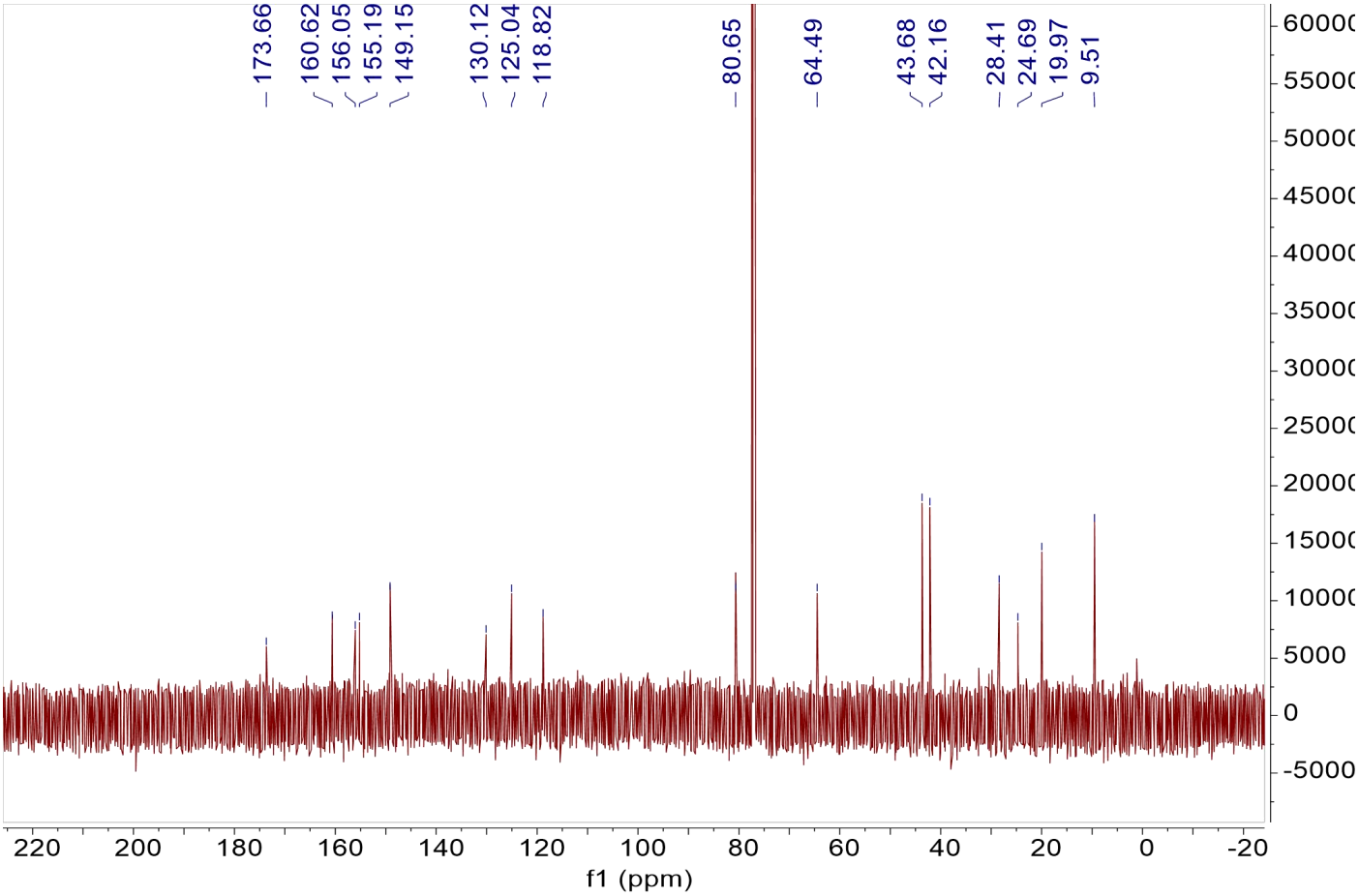


Fig. S9. ^{13}C NMR spectrum of compound **1** in $CDCl_3$.

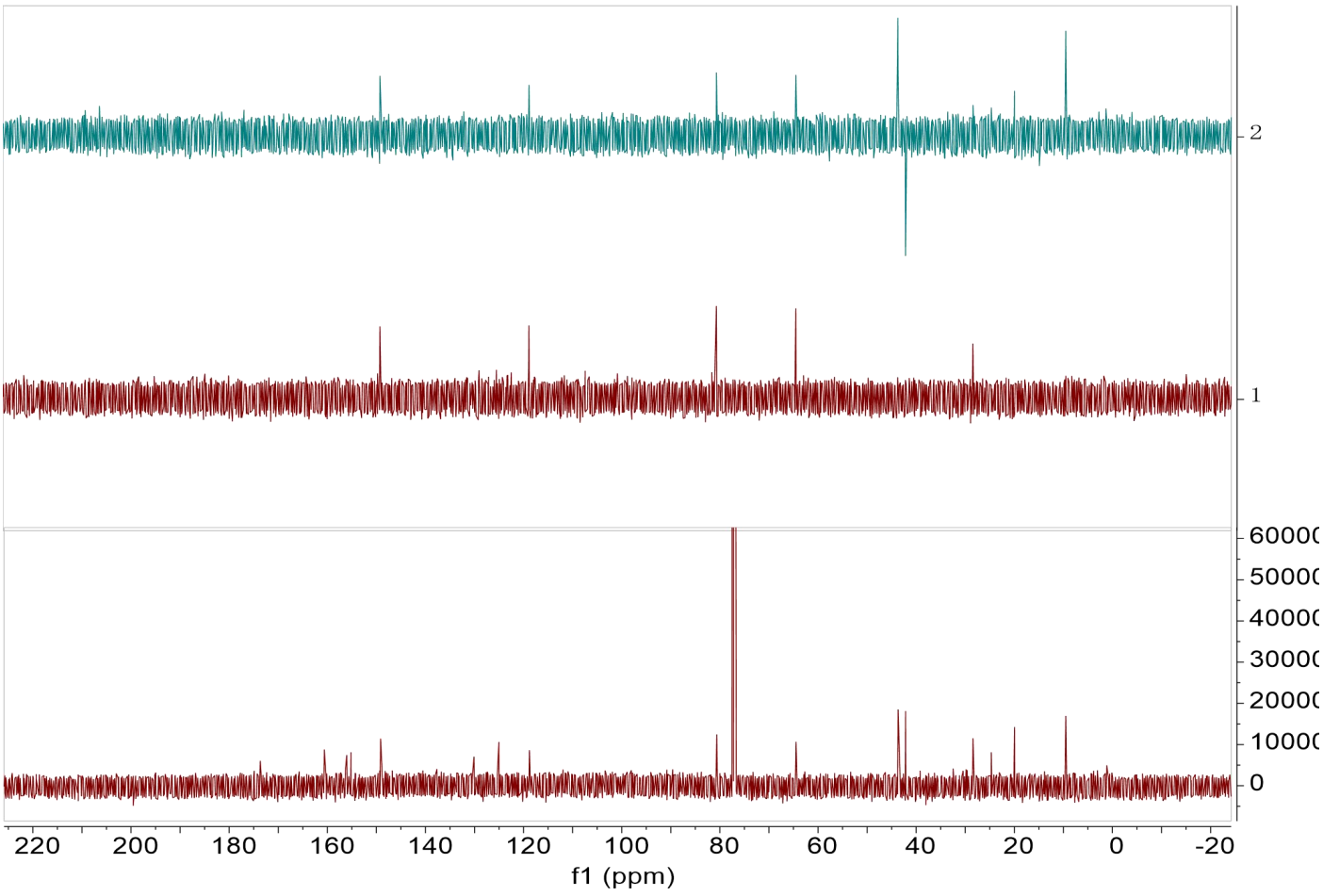


Fig. S10. ^{13}C and DEPT spectrum of compound **1** in $CDCl_3$.

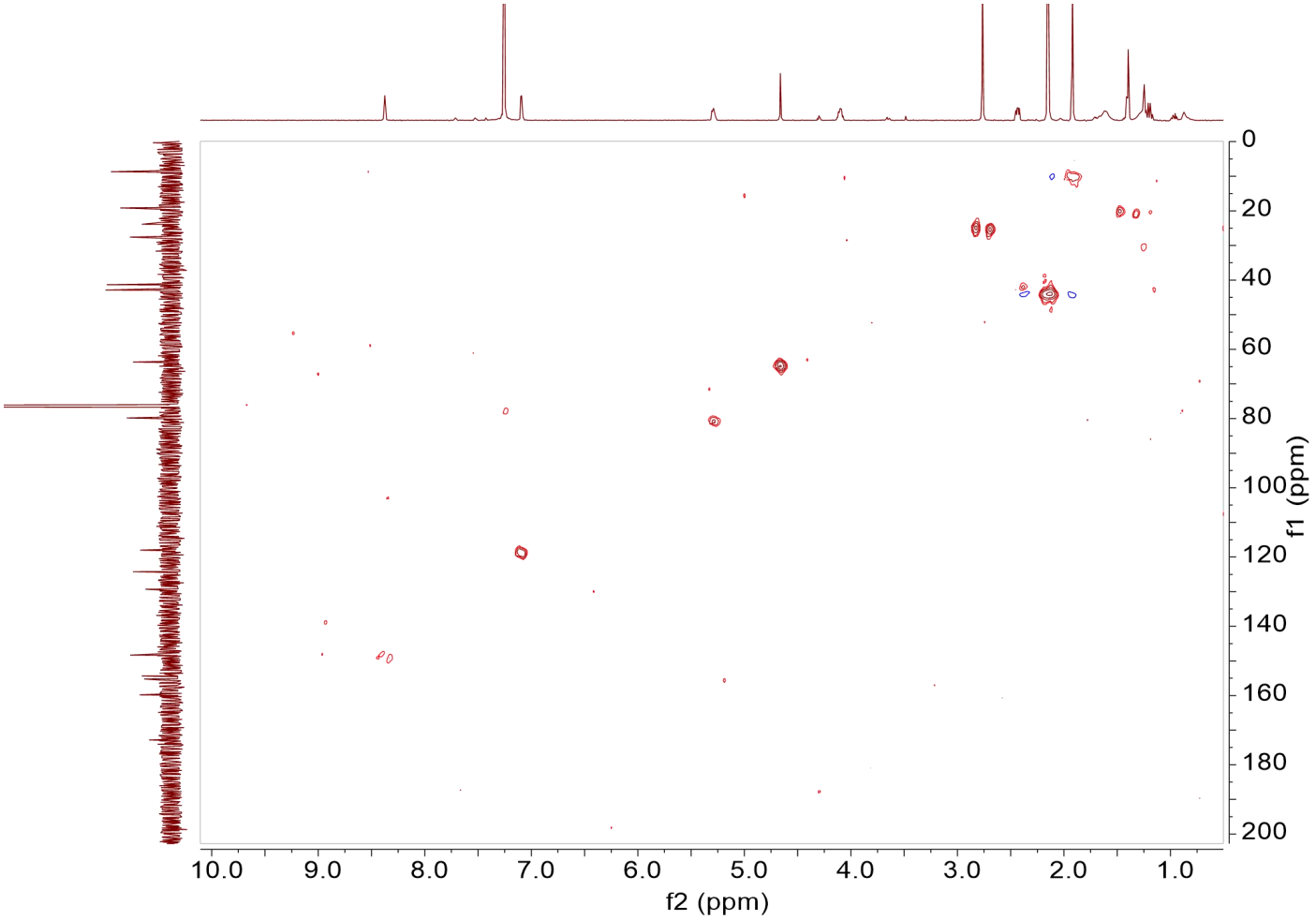


Fig. S11. HSQC spectrum of compound **1** in $CDCl_3$.

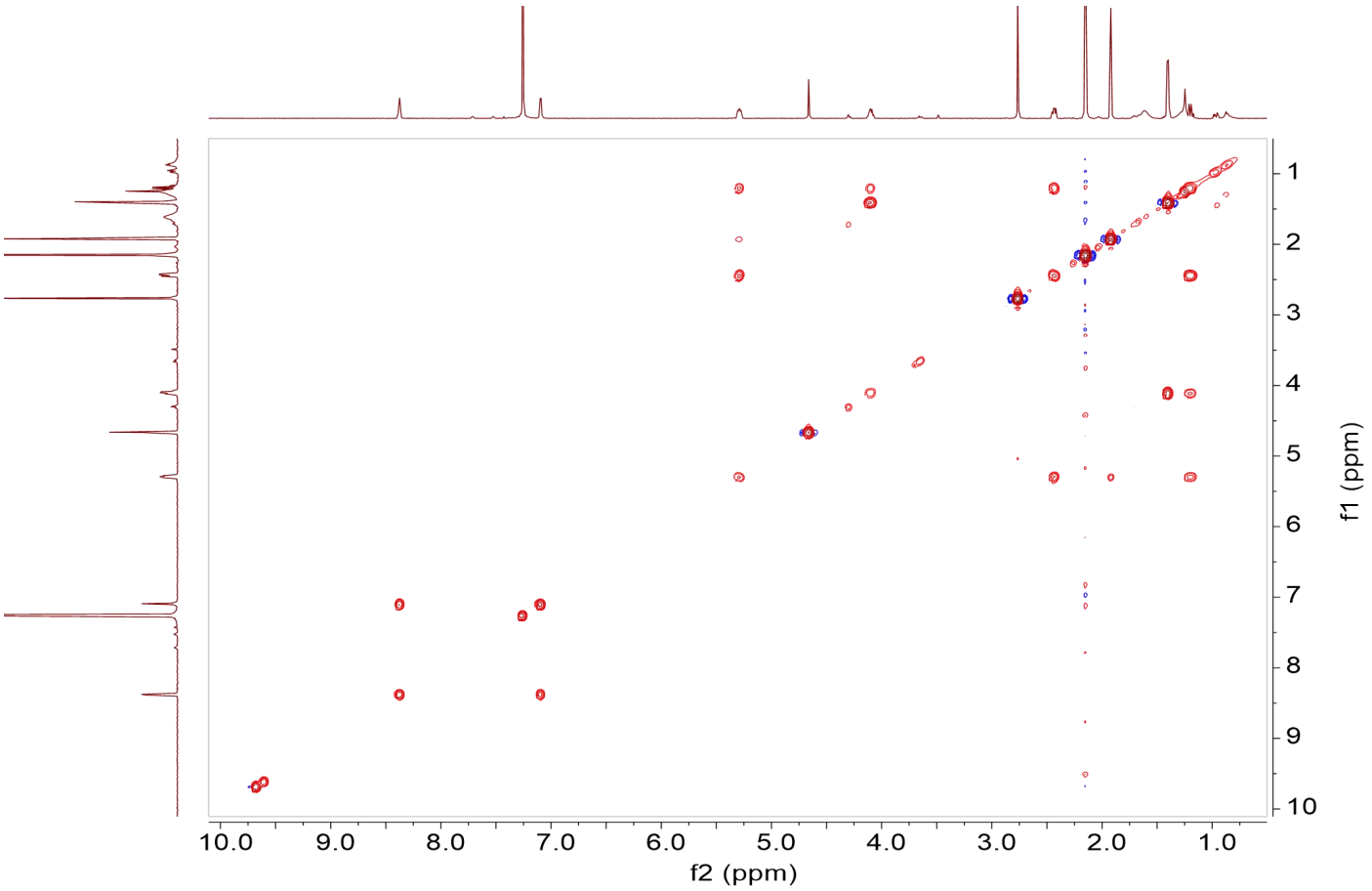


Fig. S12. ^{1}H-^{1}H-COSY spectrum of compound **1** in $CDCl_3$.

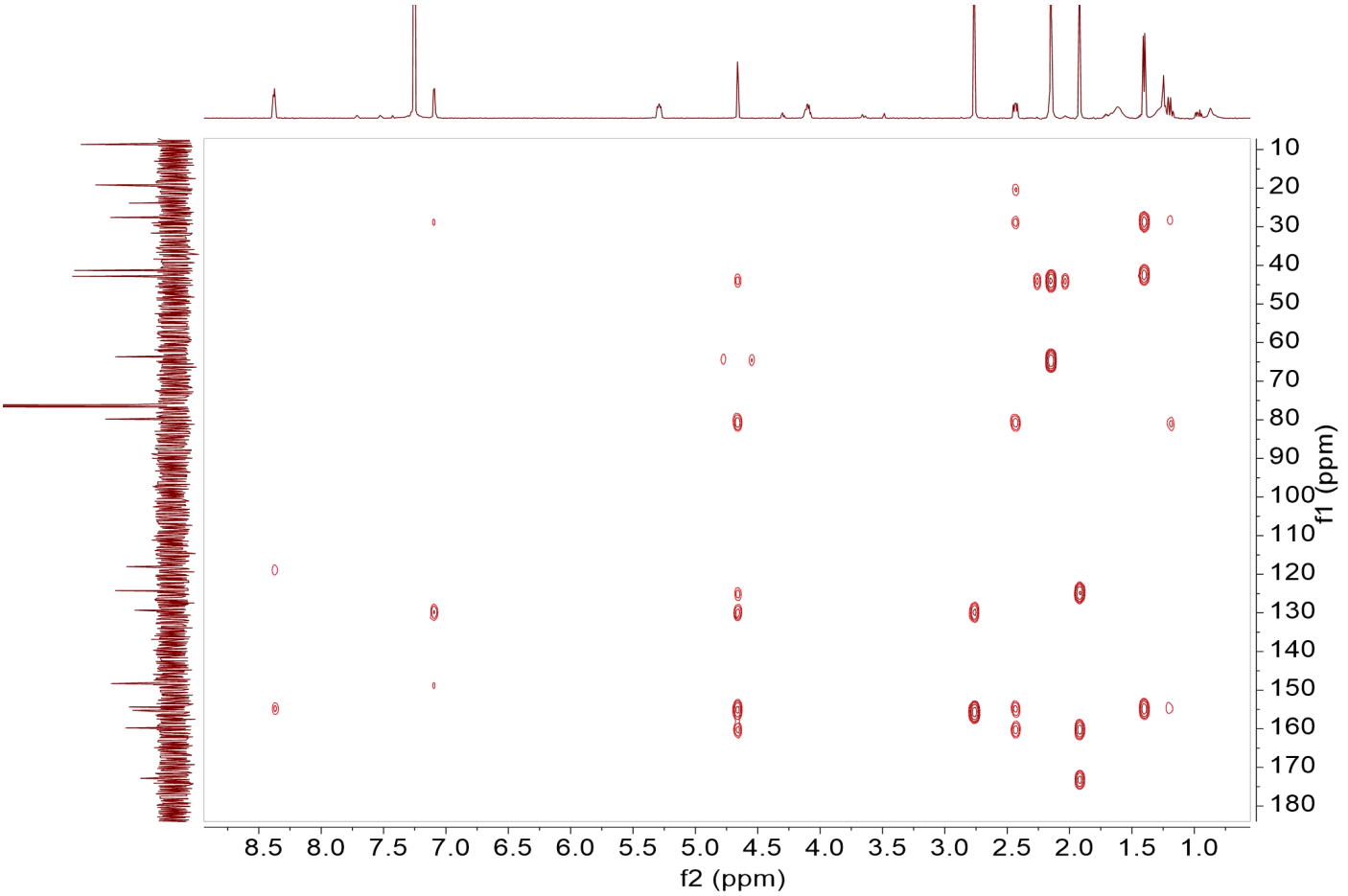


Fig. S13. HMBC spectrum of compound **1** in $CDCl_3$.

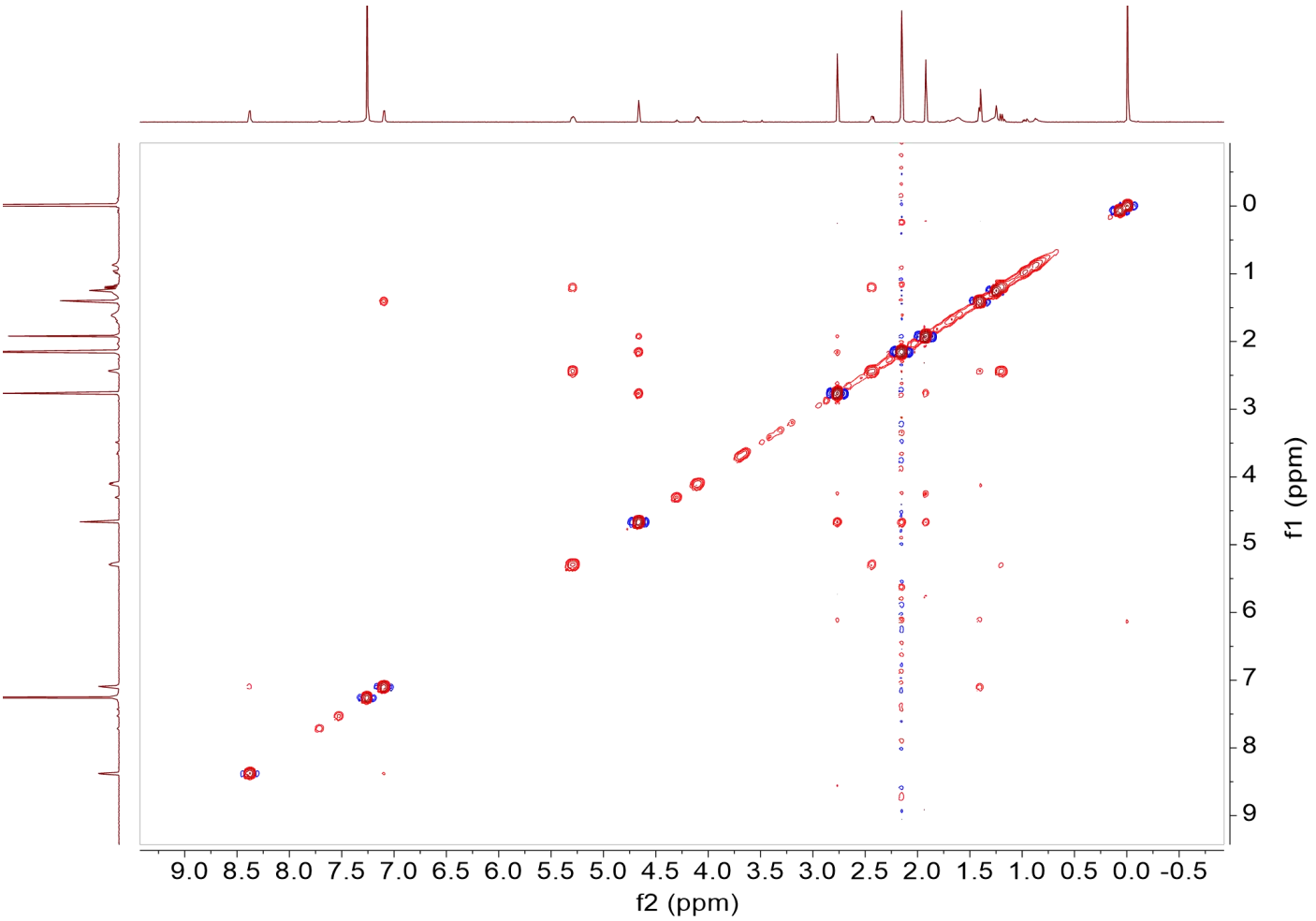


Fig. S14. NOESY spectrum of compound **1** in $CDCl_3$.

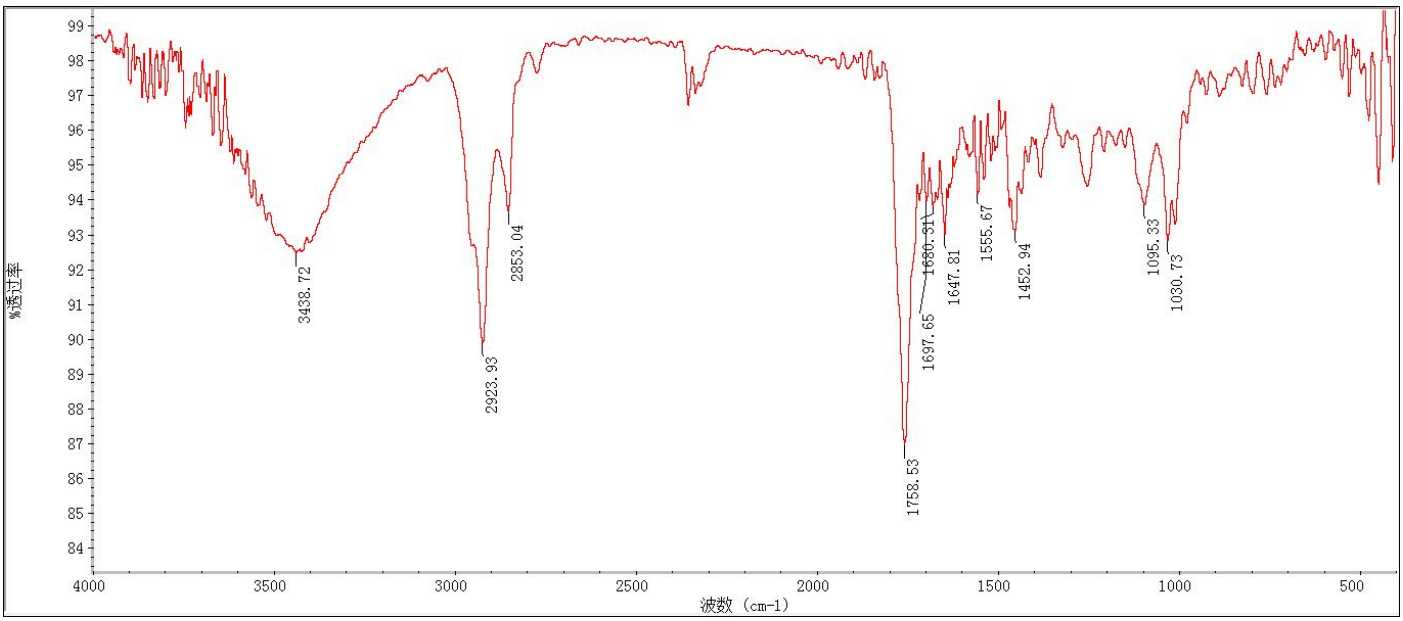


Fig. S15. IR spectrum of compound **1**.

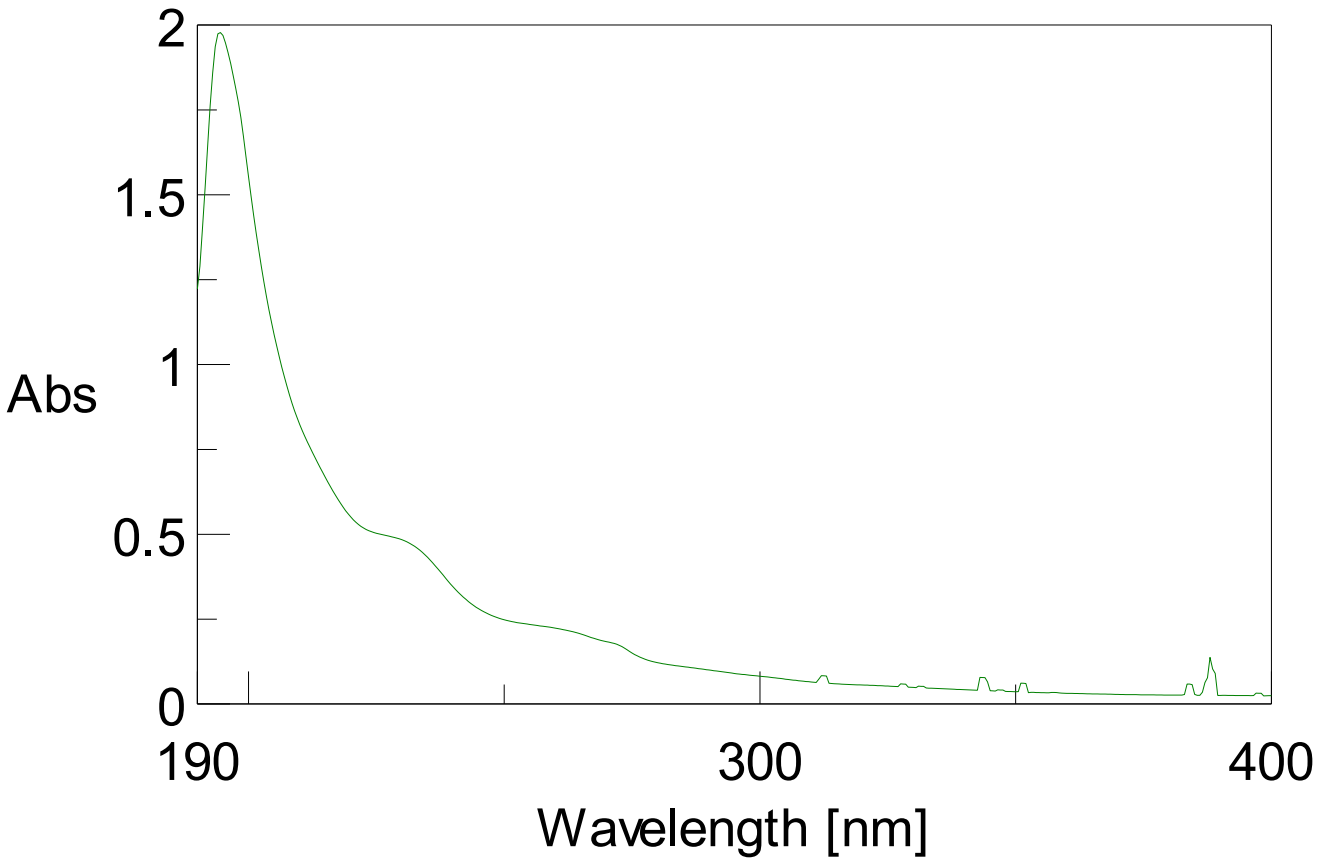


Fig. S16. UV spectrum of compound **1**.

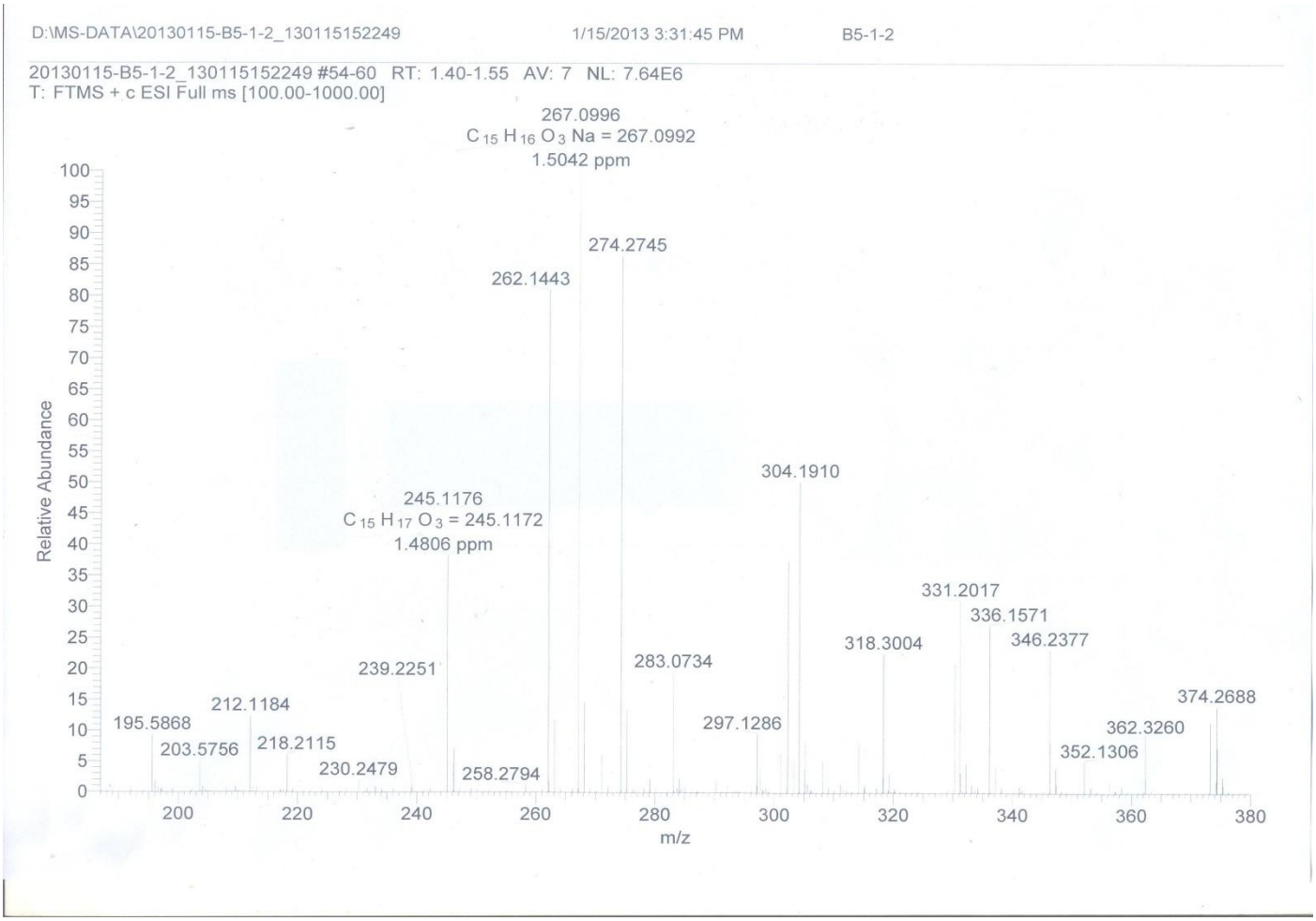


Fig. S17. HRESIMS spectrum of compound **2**.

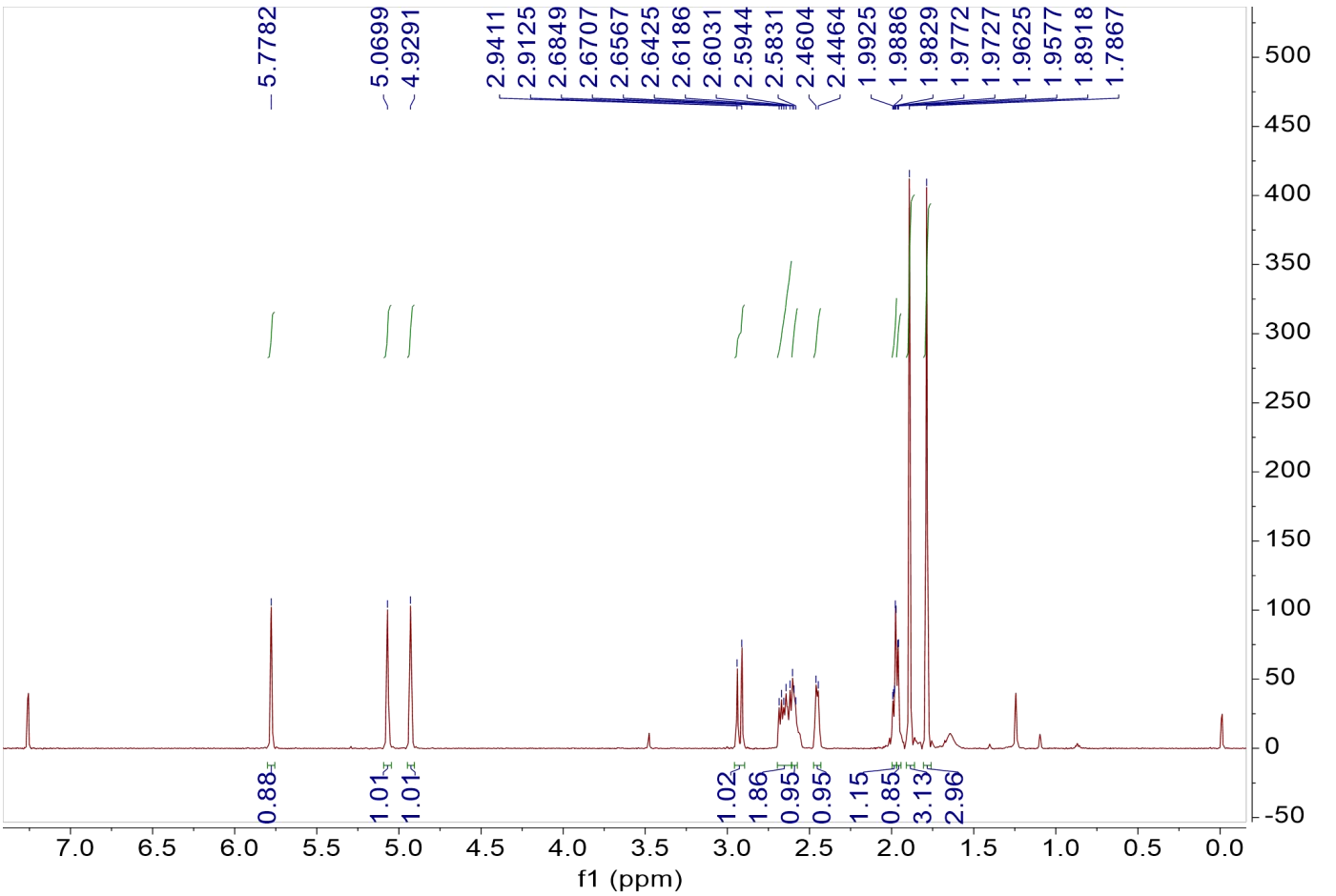


Fig. S18. ^{1}H NMR spectrum of compound **2** in $CDCl_3$.

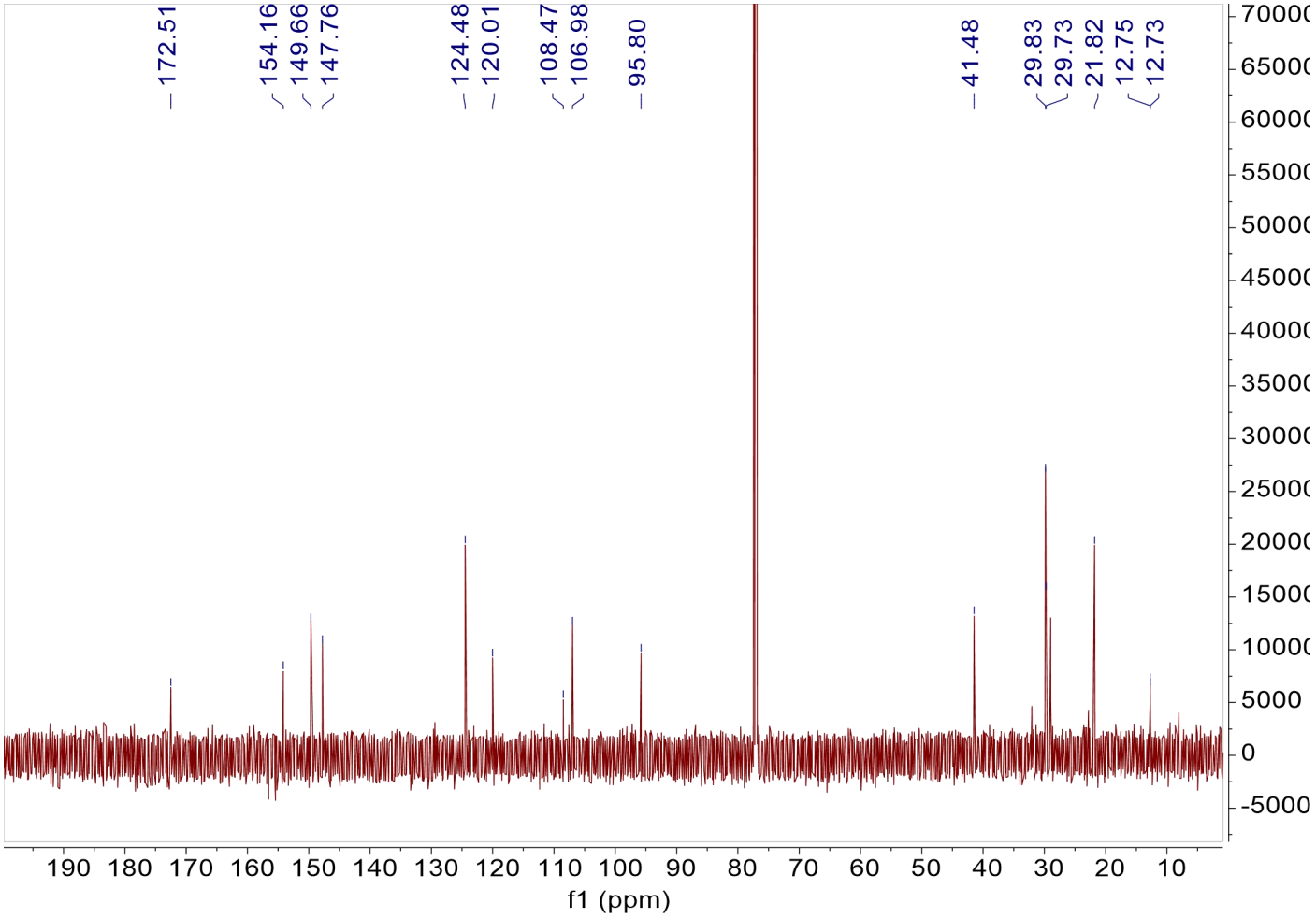


Fig. S19. ^{13}C NMR spectrum of compound **2** in $CDCl_3$.

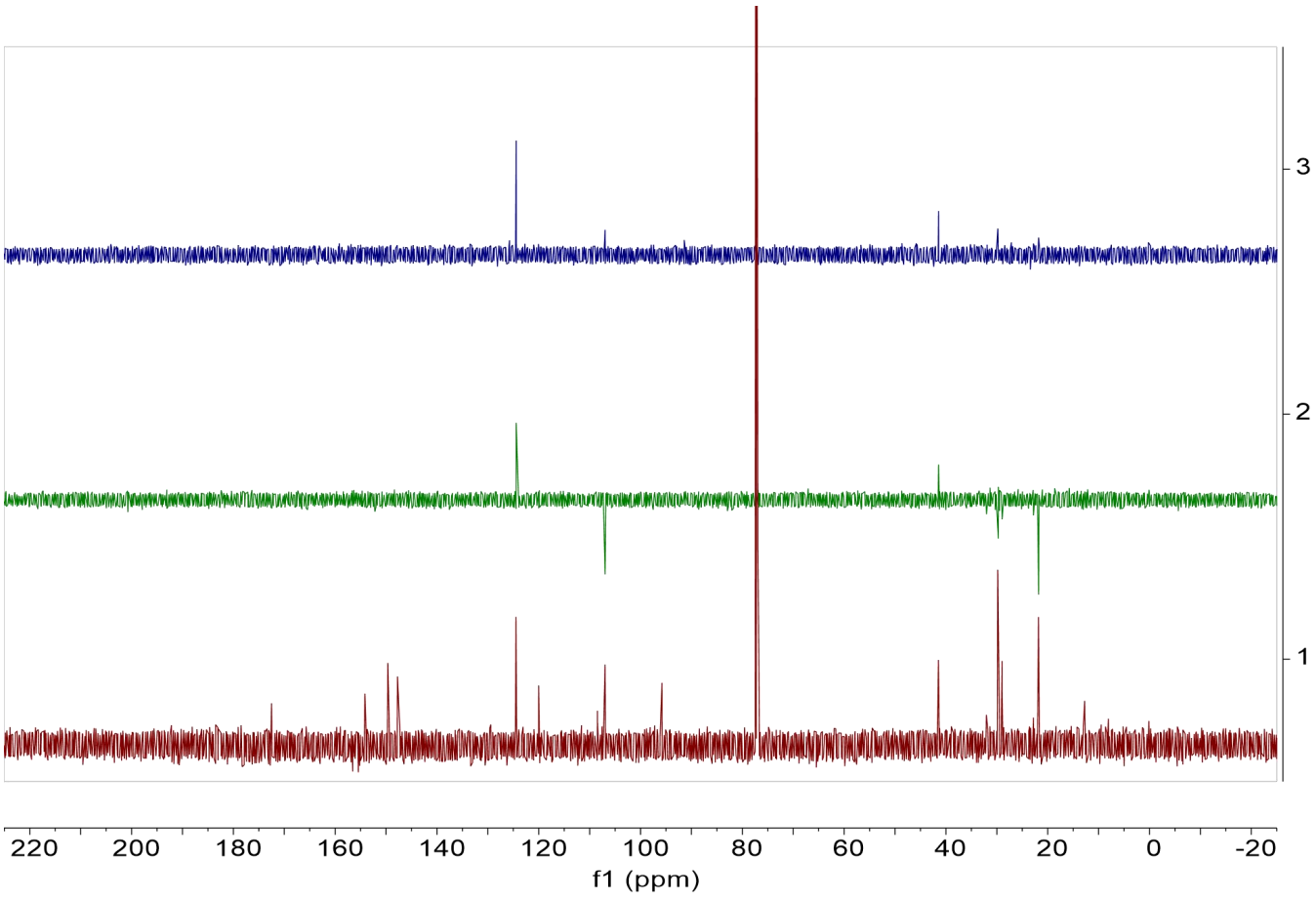


Fig. S20. ^{13}C and DEPT spectrum of compound **2** in $CDCl_3$.

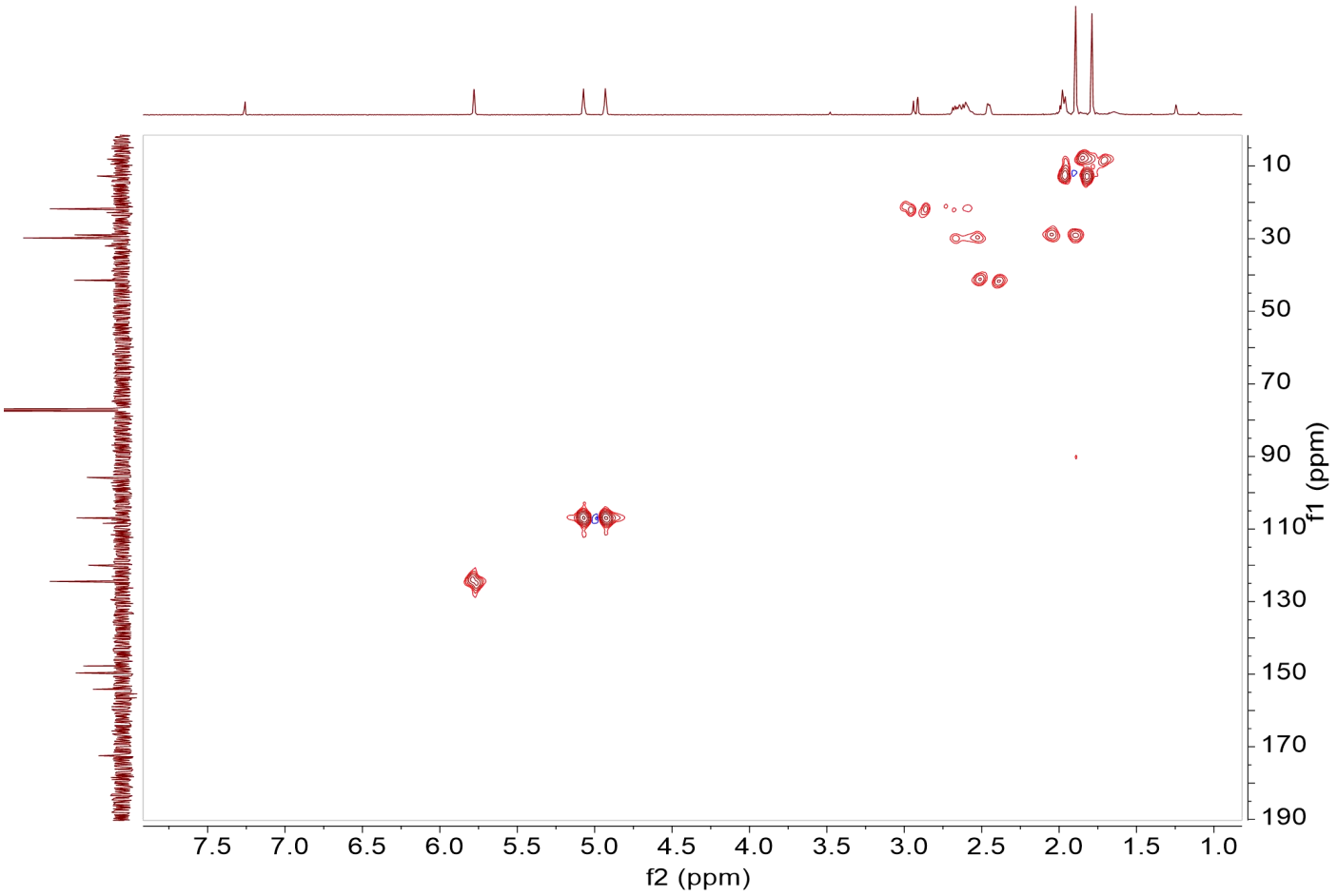


Fig. S21. HSQC spectrum of compound **2** in $CDCl_3$.

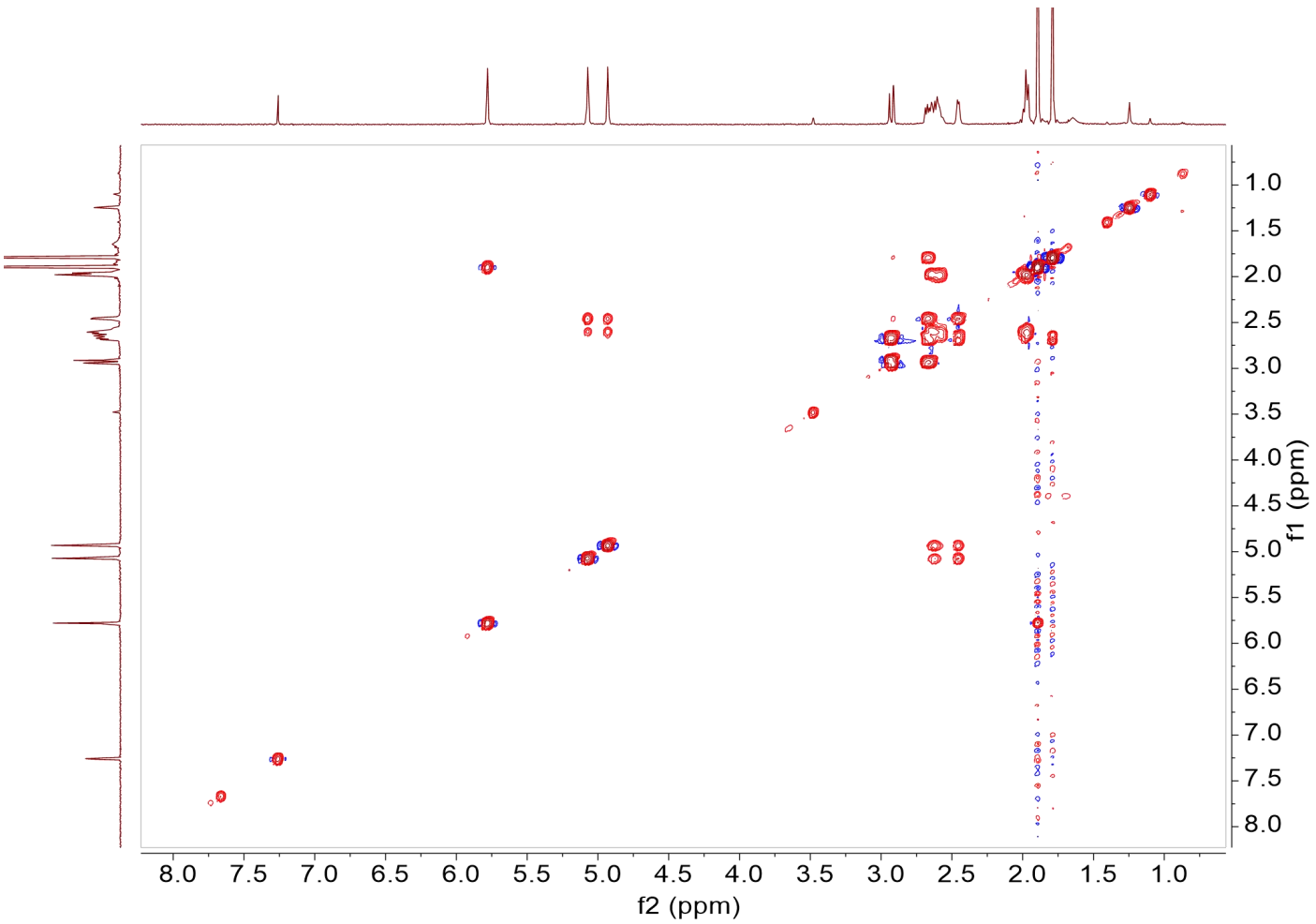


Fig. S22. ^{1}H-^{1}H-COSY spectrum of compound **2** in $CDCl_3$.

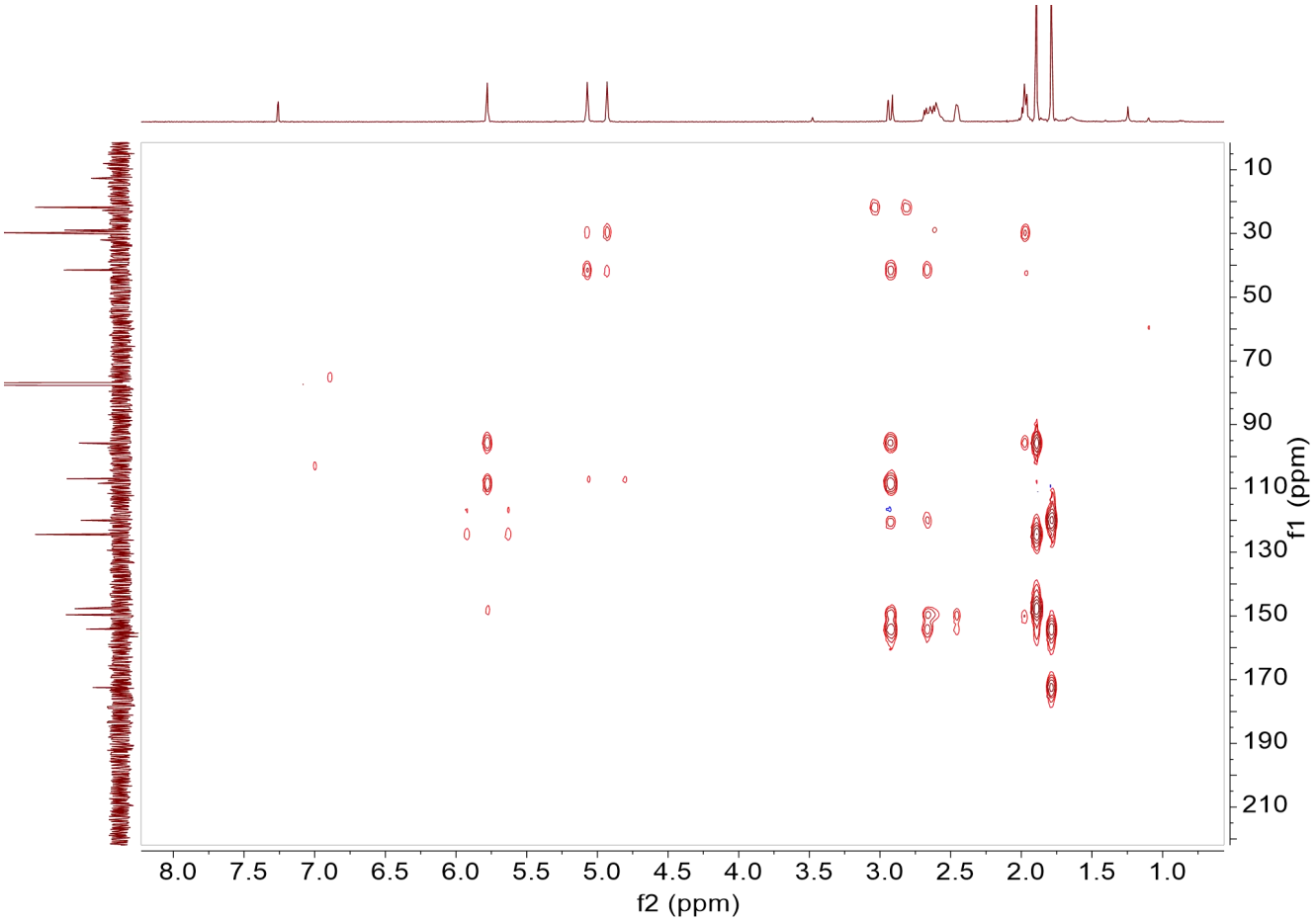


Fig. S23. NOESY spectrum of compound **2** in $CDCl_3$.

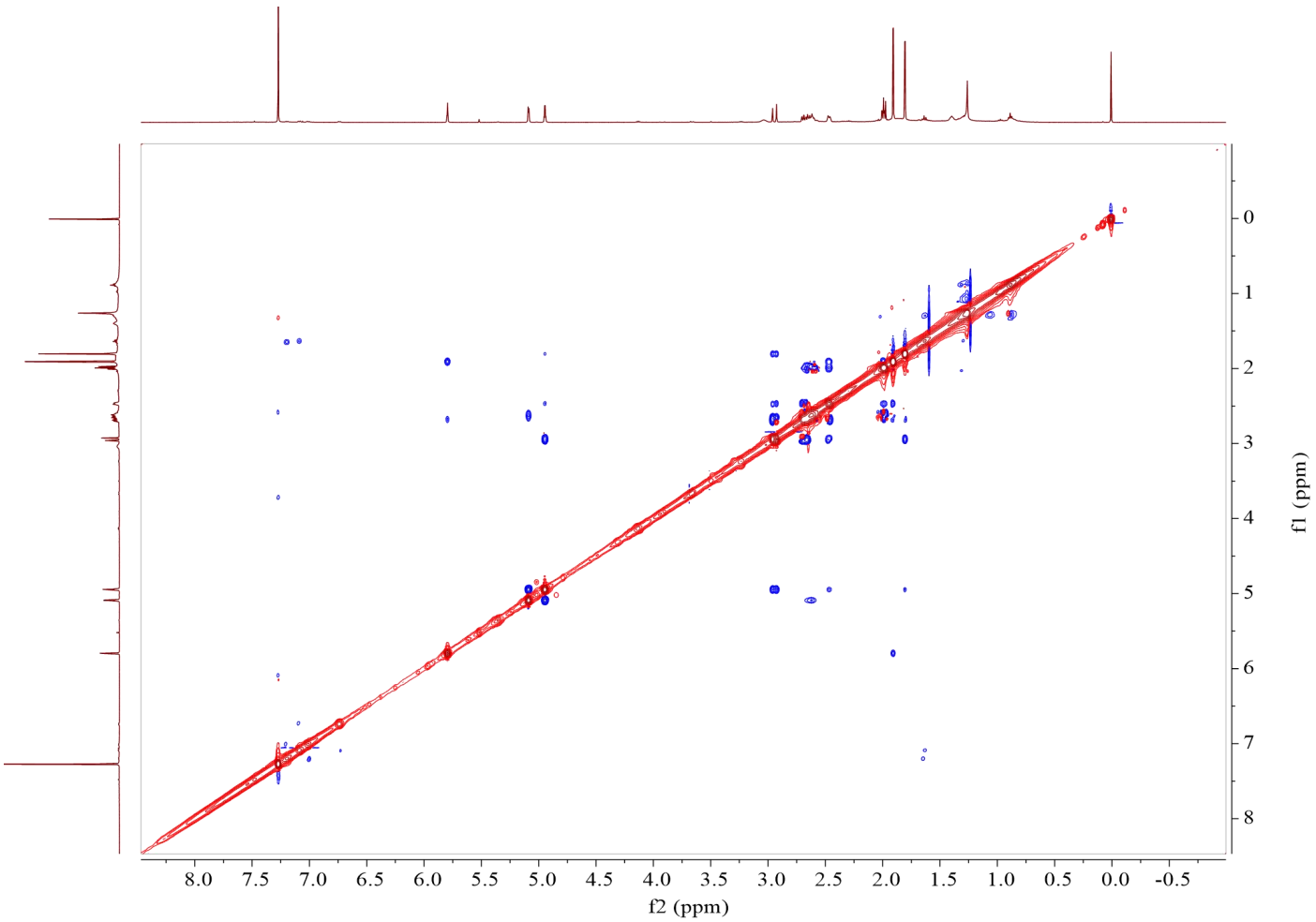


Fig. S24. HMBC spectrum of compound **2** in $CDCl_3$.

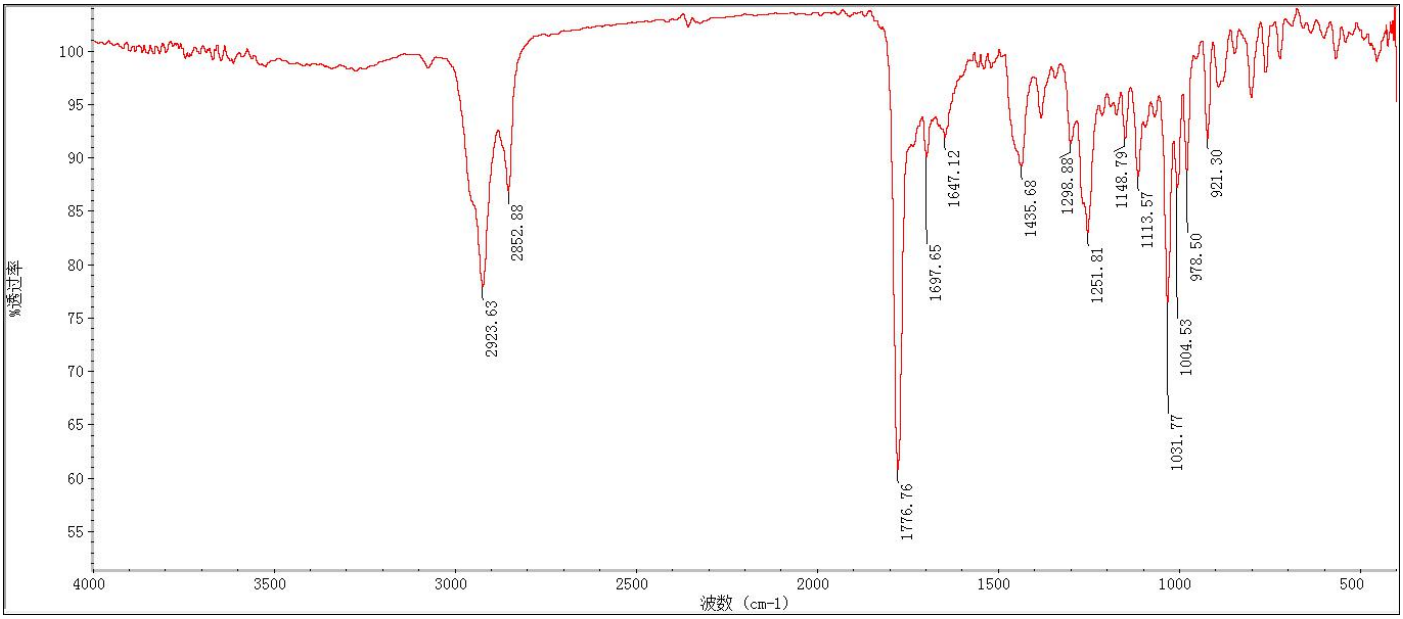


Fig. S25. IR spectrum of compound **2**.

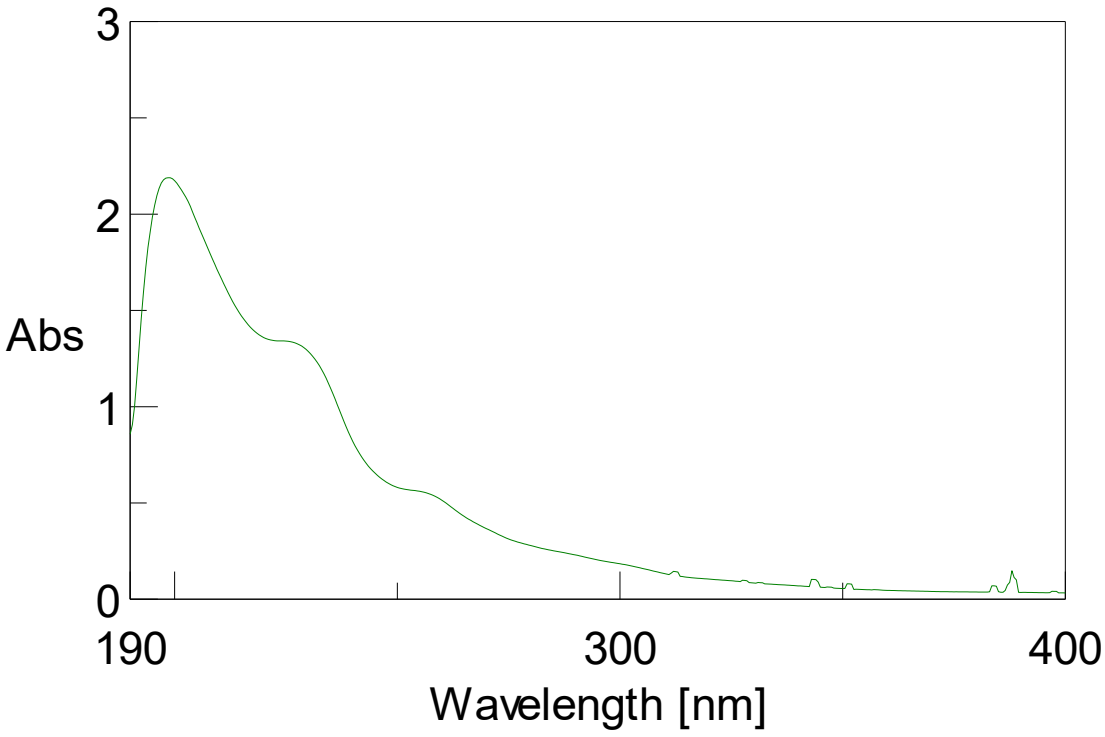


Fig. S26. UV spectrum of compound **2**.

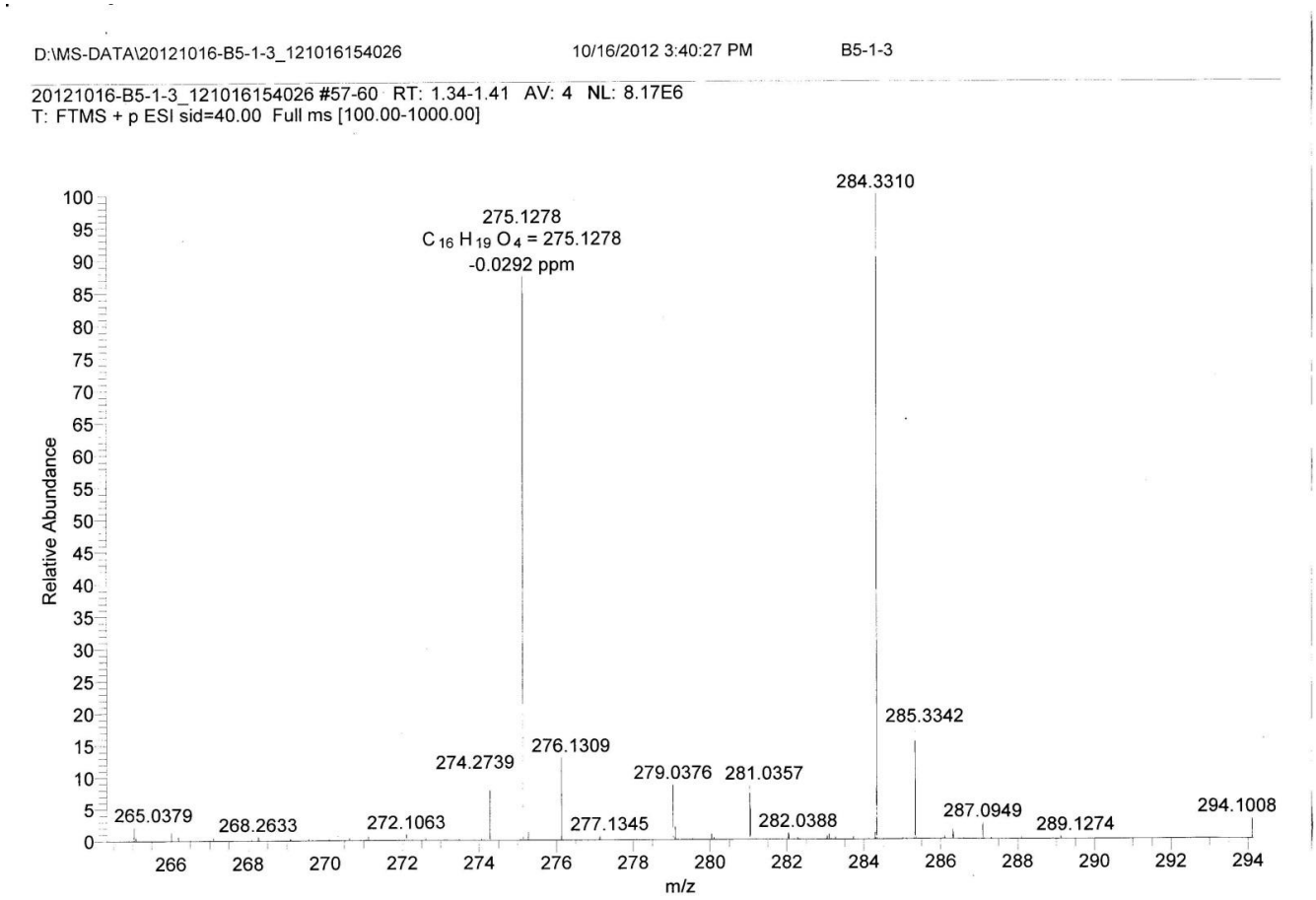


Fig. S27. HRESIMS spectrum of compound **3**.

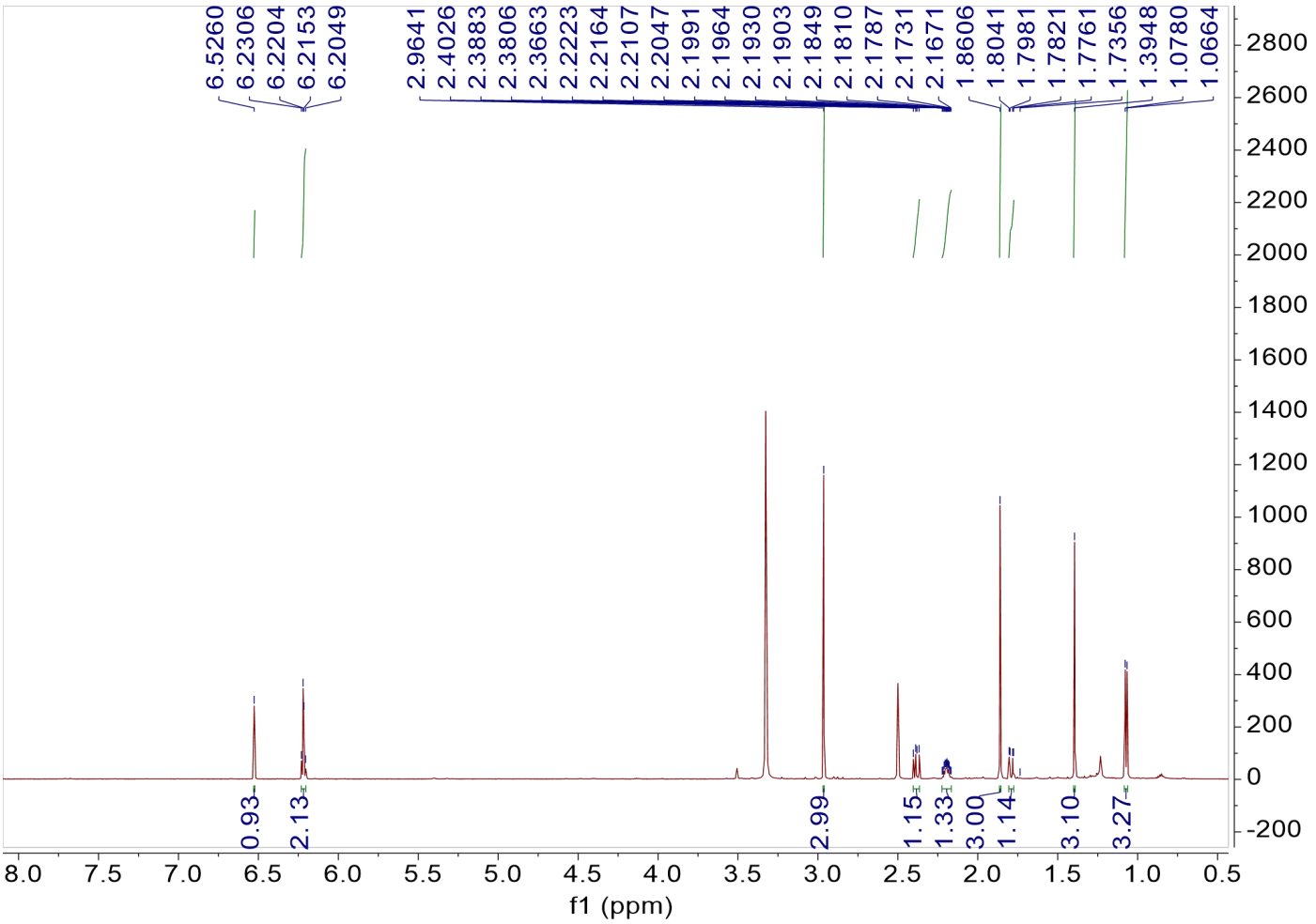


Fig. S28. ^{1}H NMR spectrum of compound **3** in DMSO.

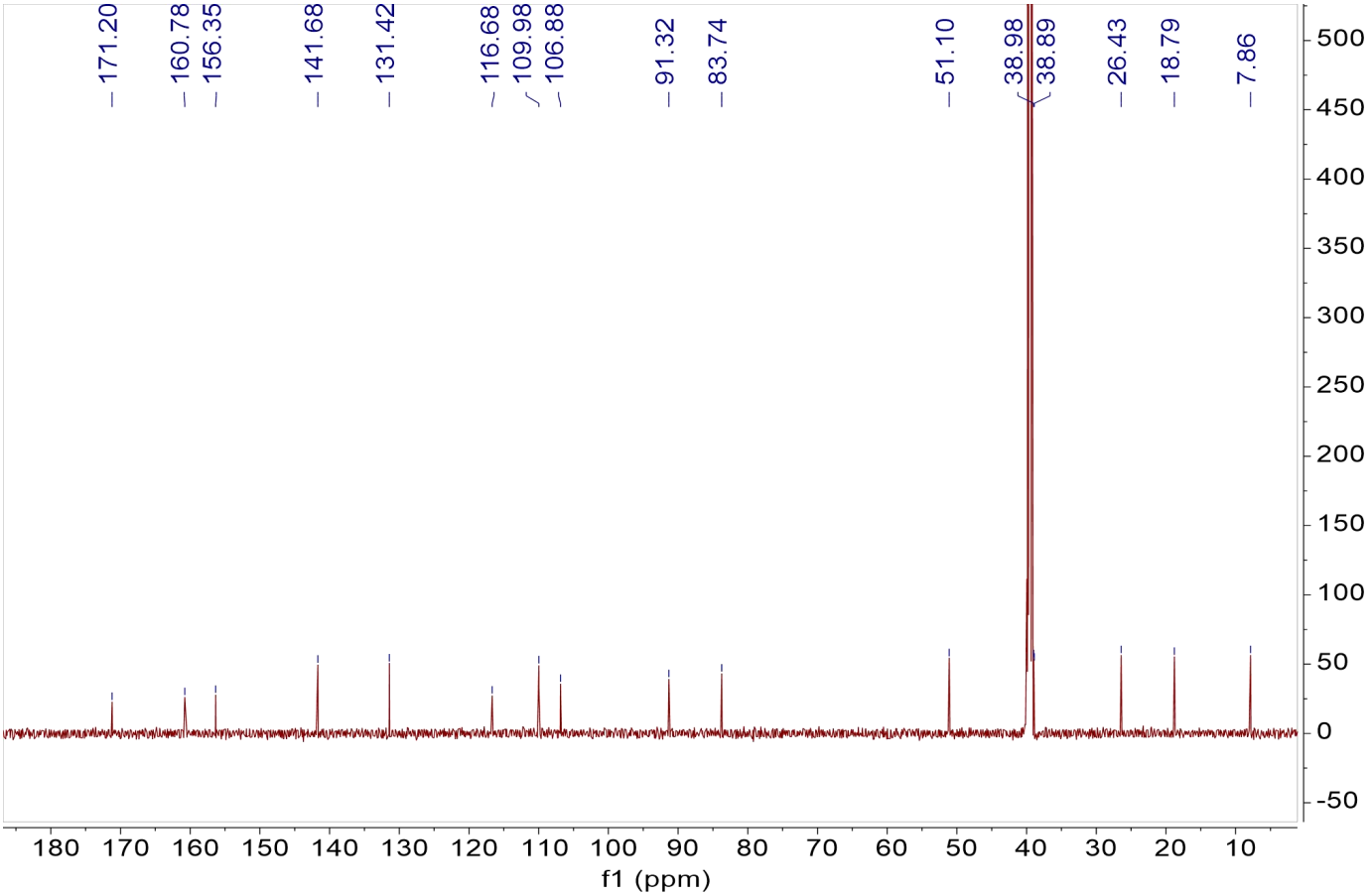


Fig. S29. ^{13}C NMR spectrum of compound **3** in DMSO.

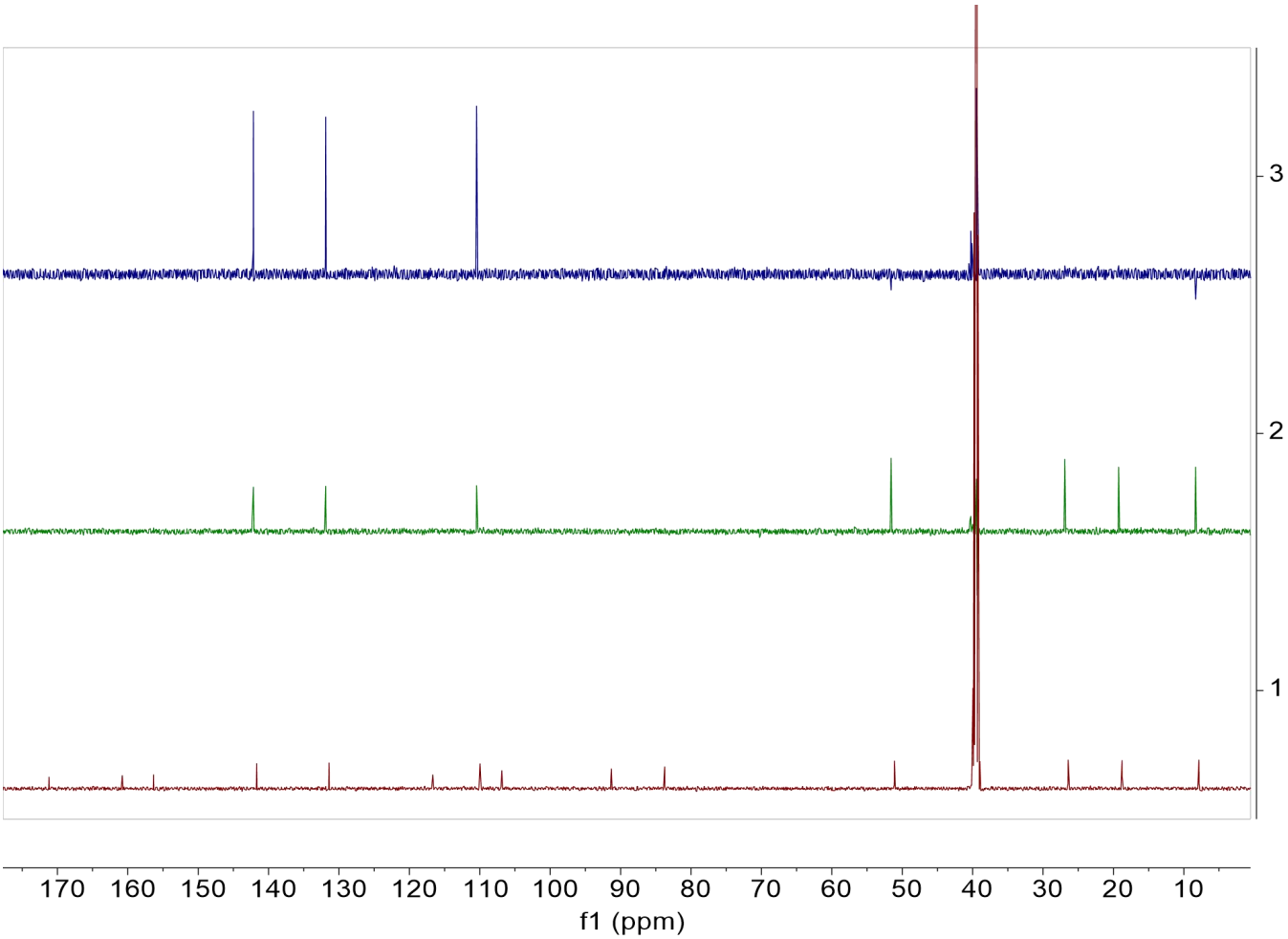


Fig. S30. ^{13}C and DEPT spectrum of compound **3** in DMSO.

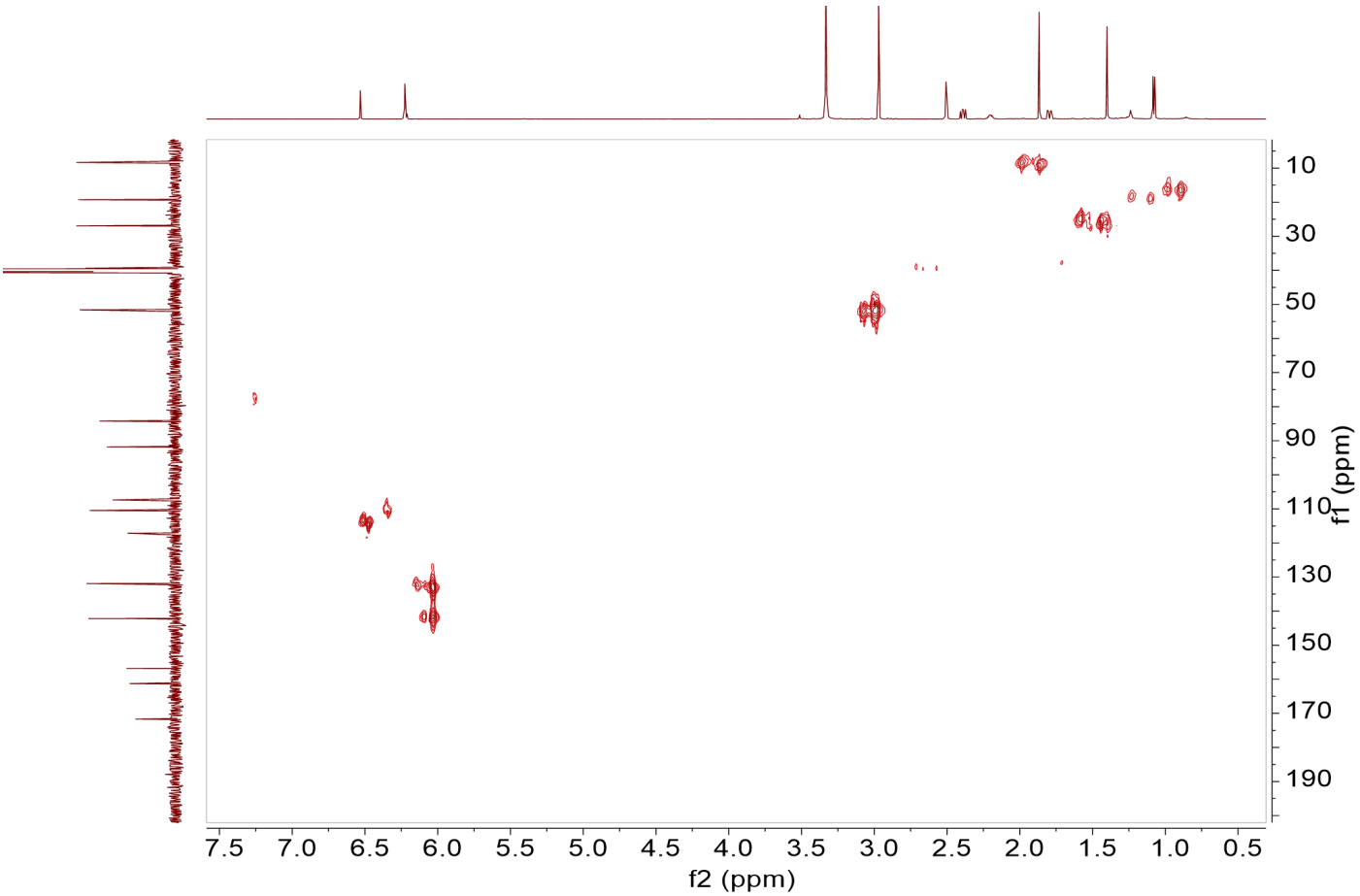


Fig. S31. HSQC spectrum of compound **3** in DMSO.

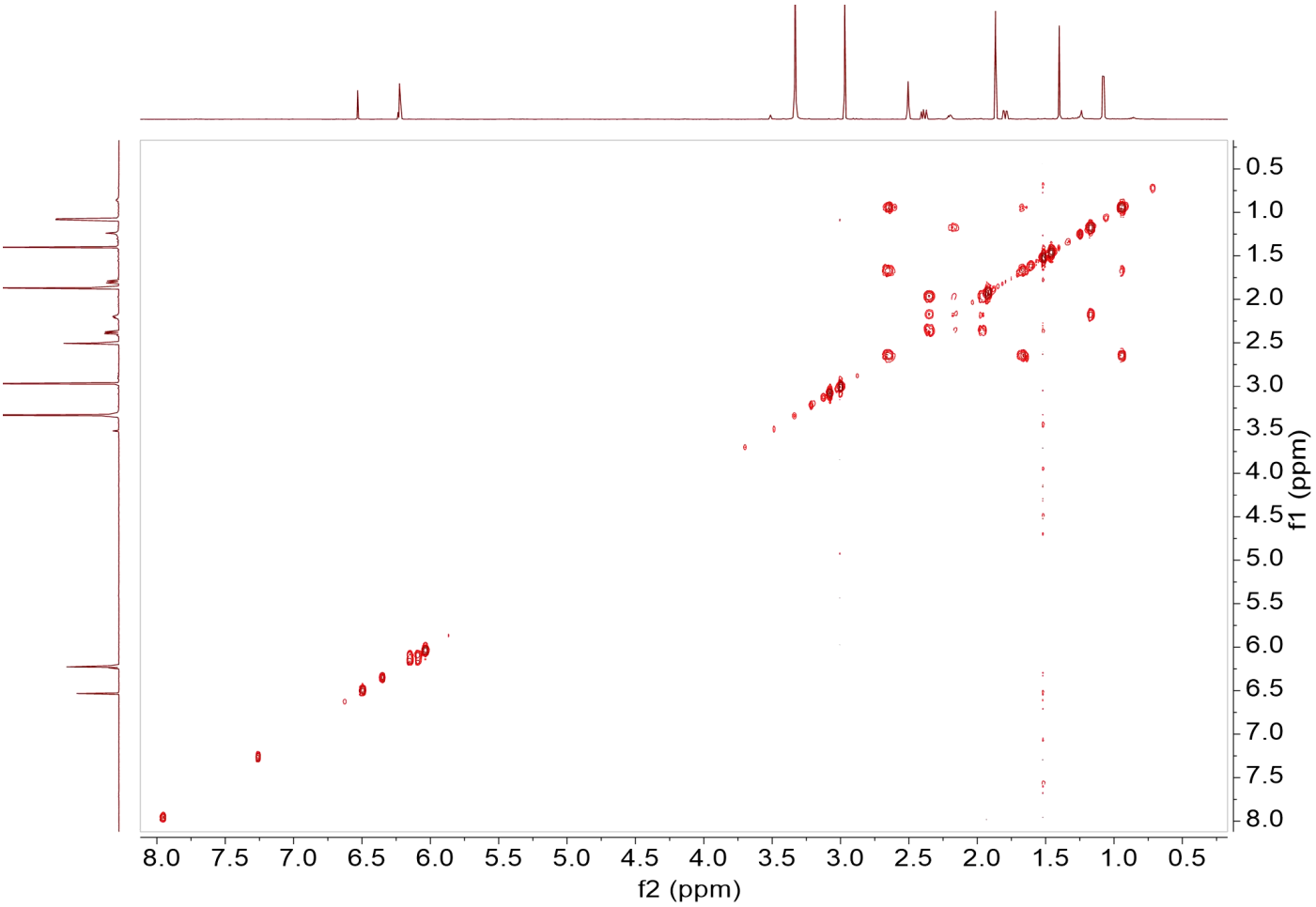


Fig. S32. ^{1}H-^{1}H-COSY spectrum of compound **3** in DMSO.

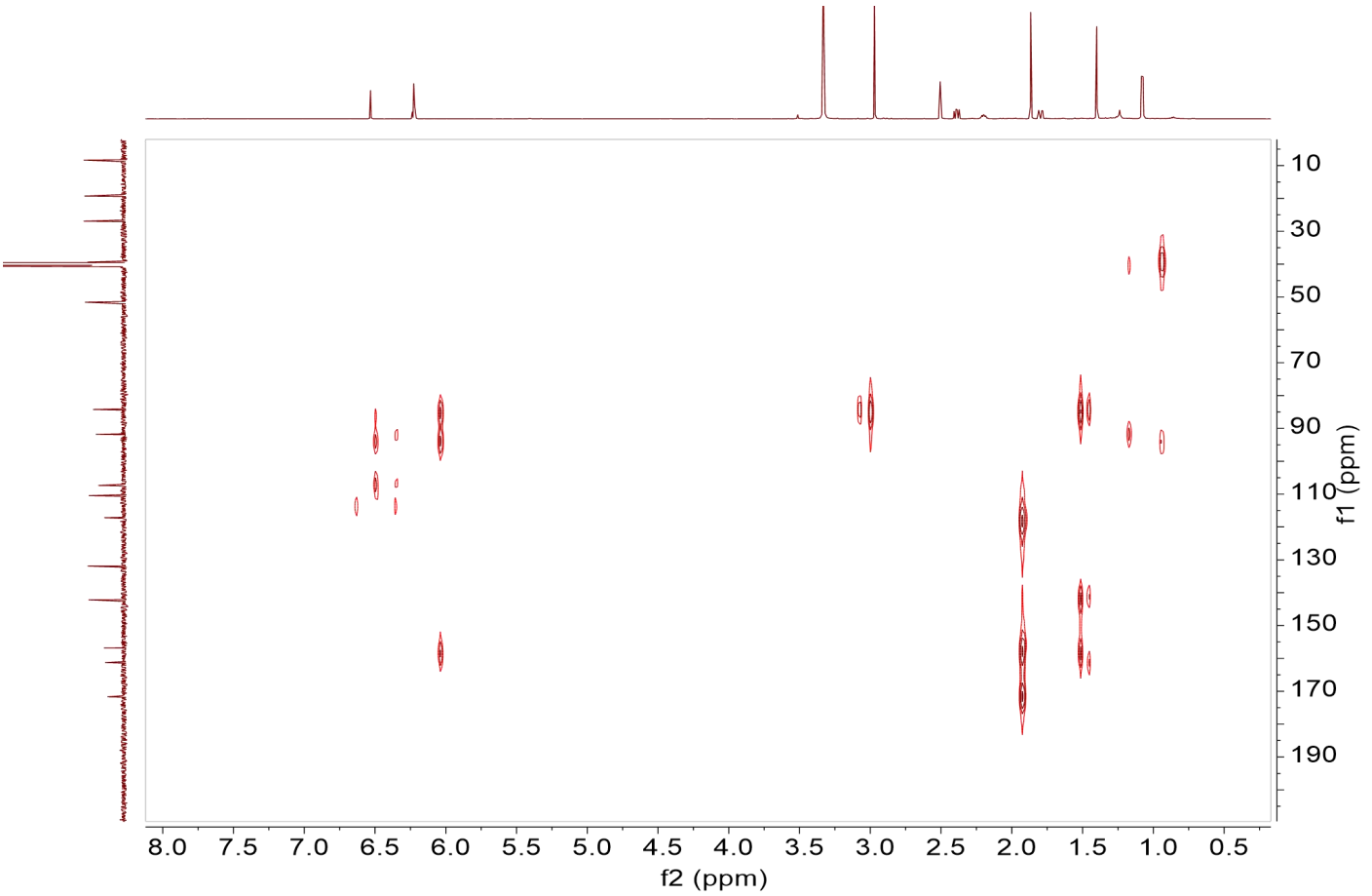


Fig. S33. HMBC spectrum of compound **3** in DMSO.

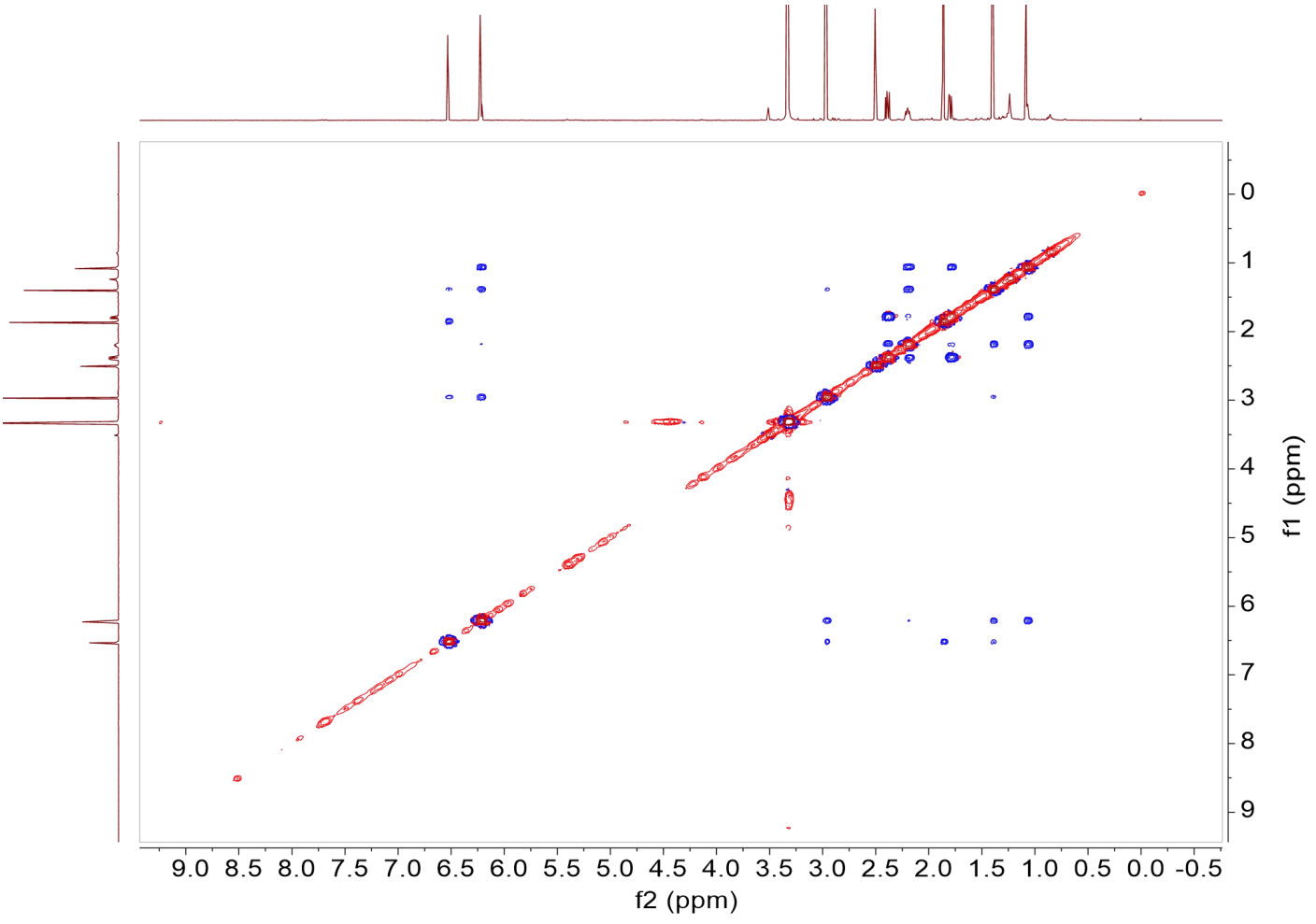


Fig. S34. NOESY spectrum of compound **3** in DMSO.

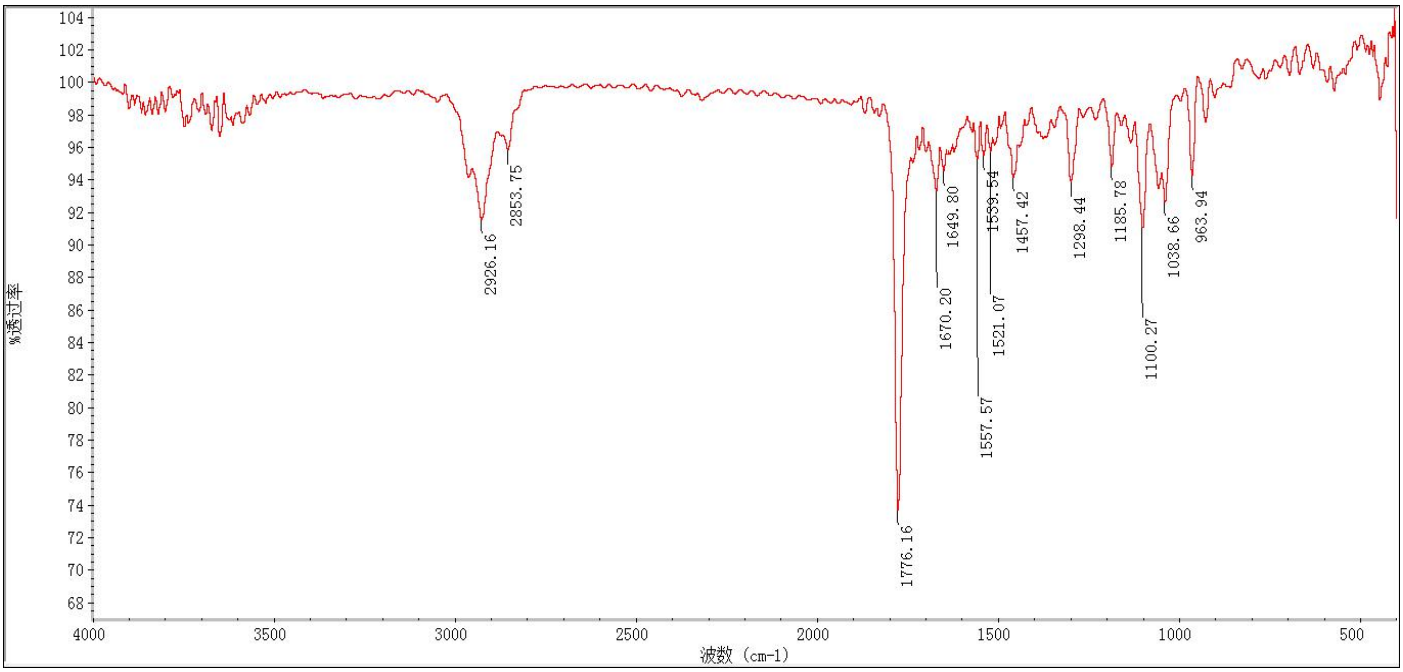


Fig. S35. IR spectrum of compound **3**.

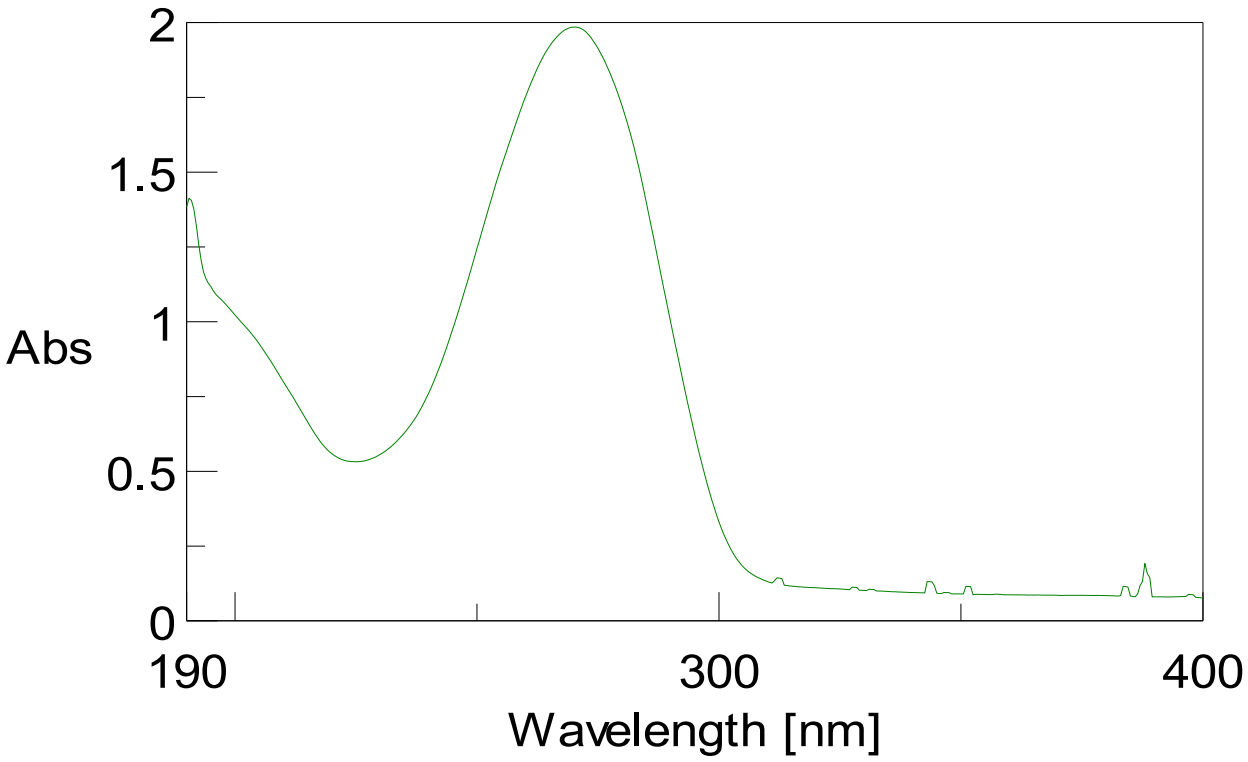


Fig. S36. UV spectrum of compound **3**.

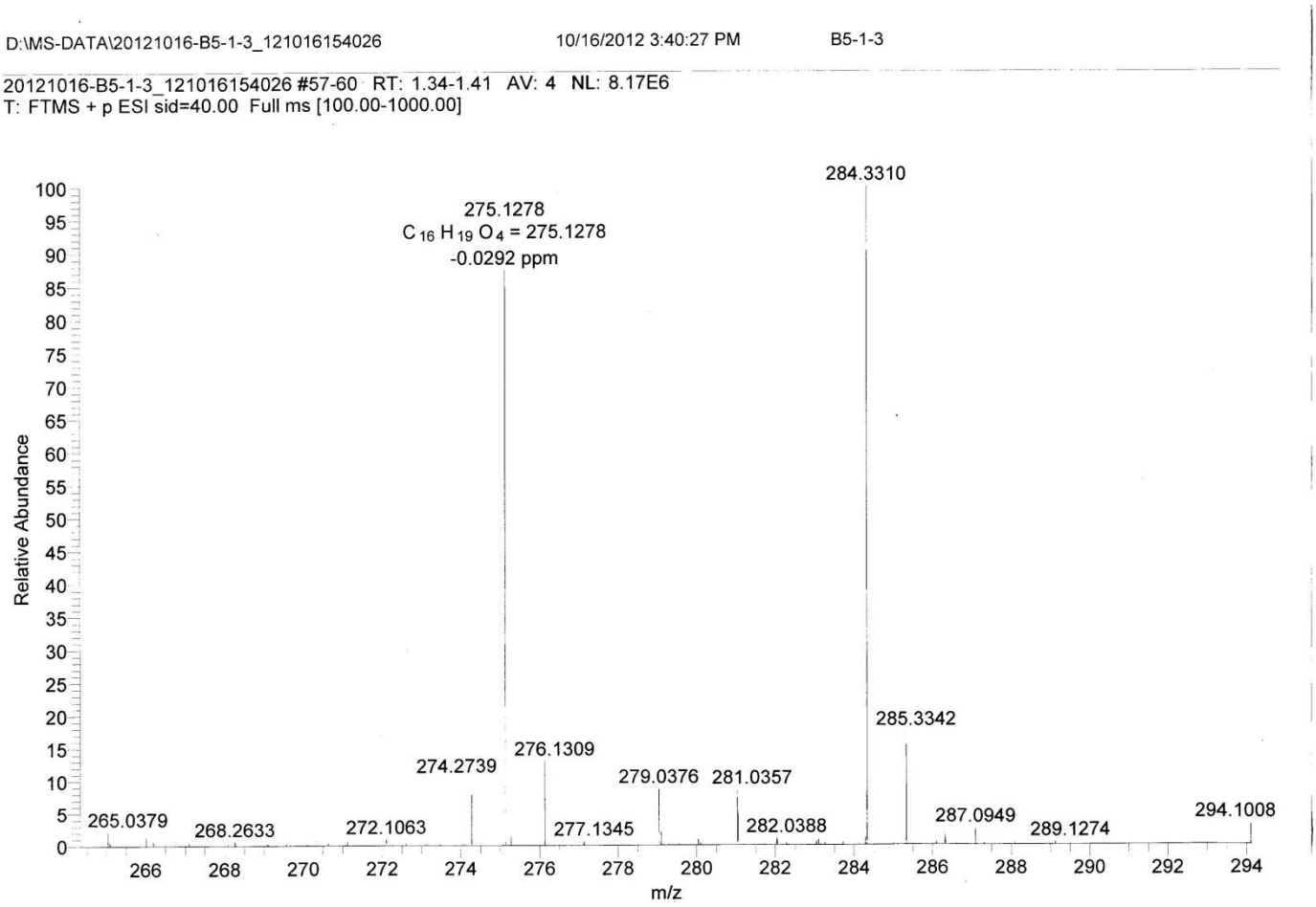


Fig. S37. HRESIMS spectrum of compound **4**.

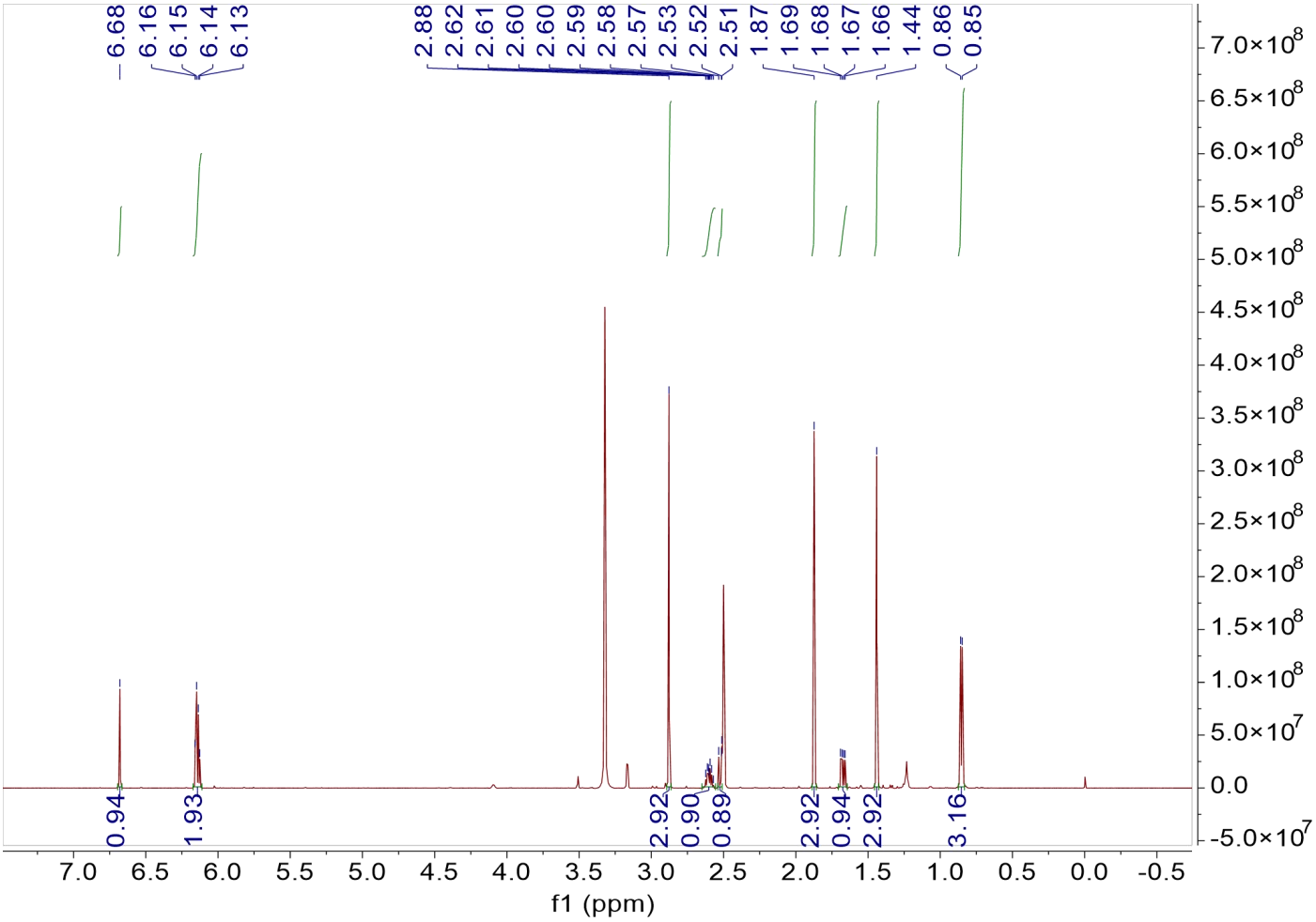


Fig. S38. ^{1}H NMR spectrum of compound **4** in DMSO.

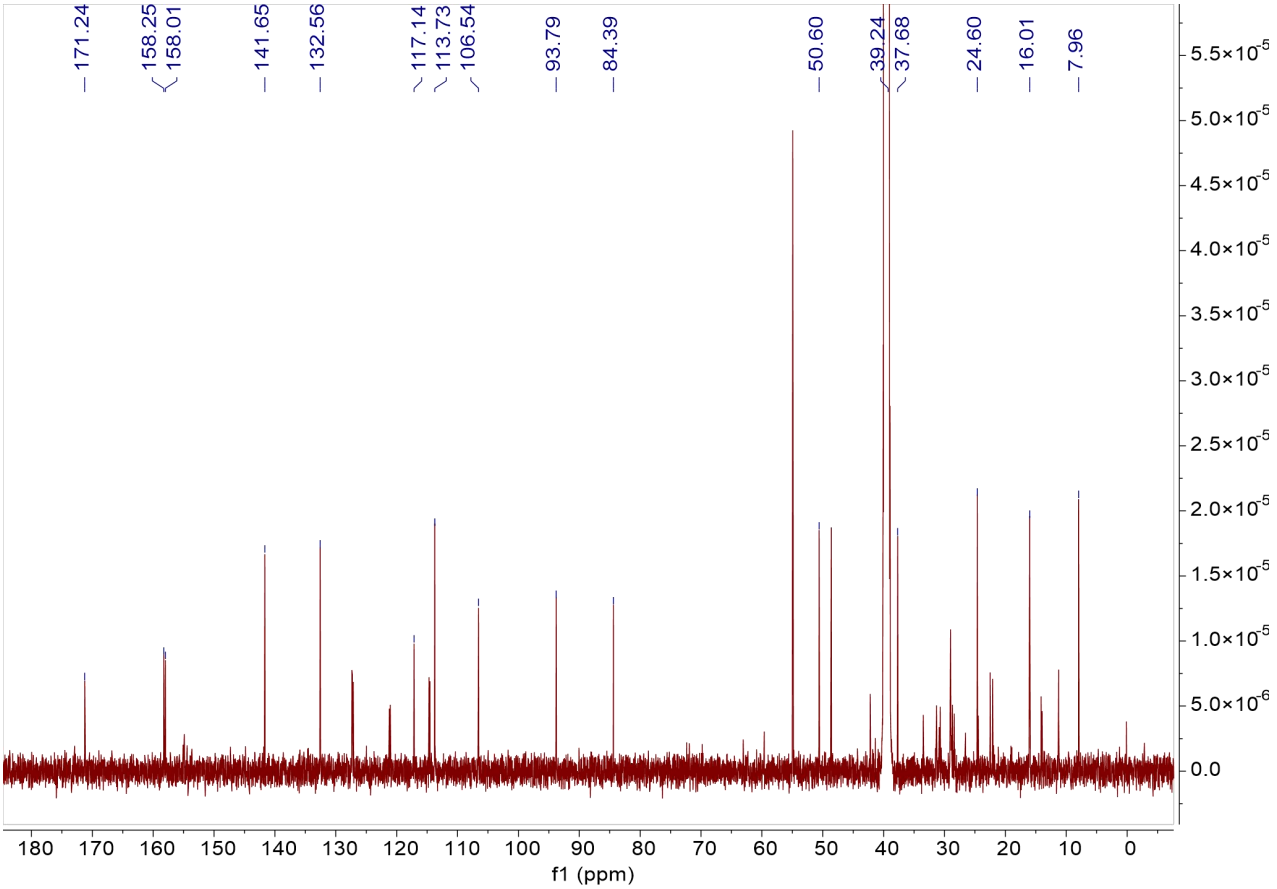


Fig. S39. ^{13}C NMR spectrum of compound **4** in DMSO.

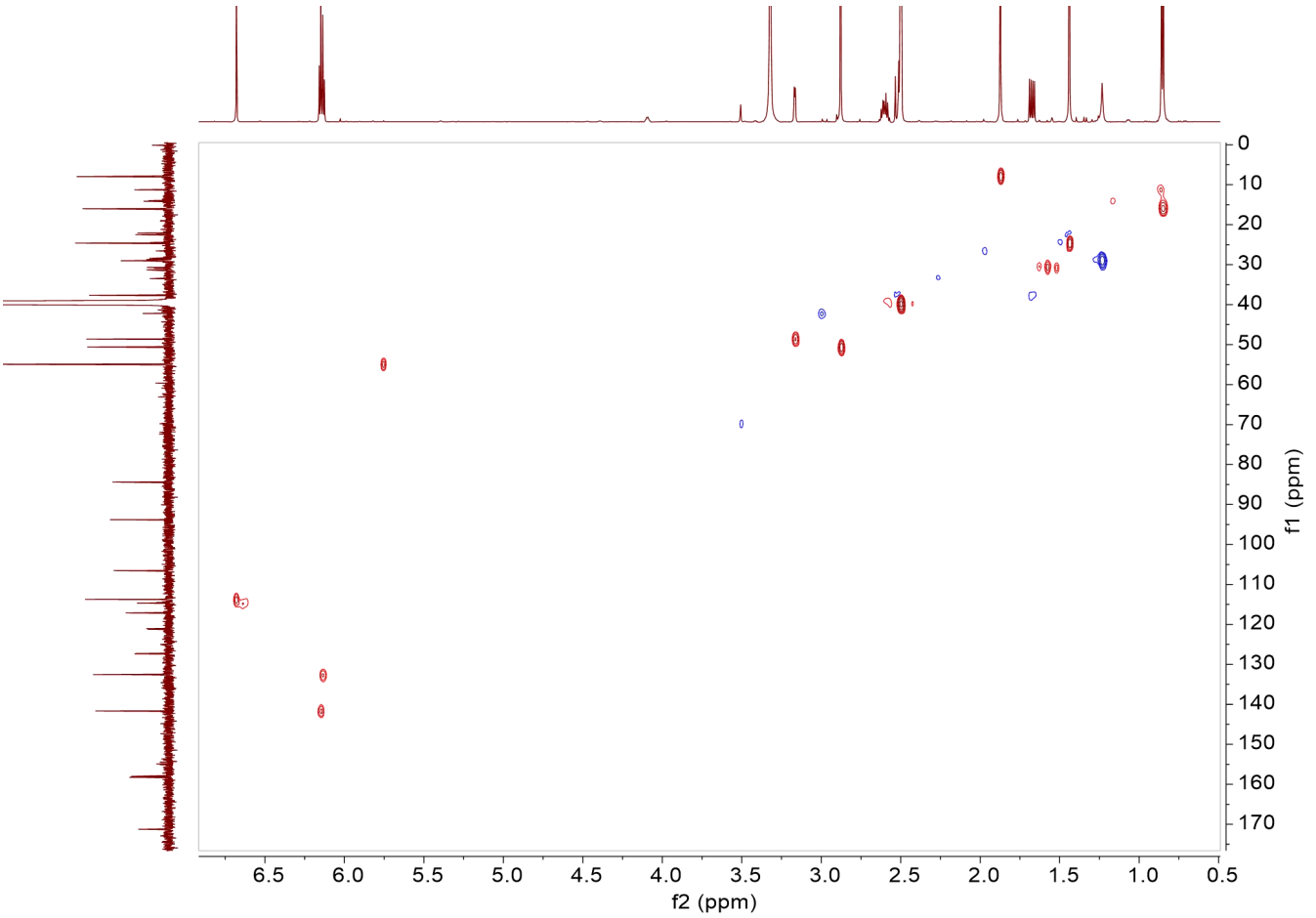


Fig. S40. HSQC spectrum of compound **4** in DMSO.

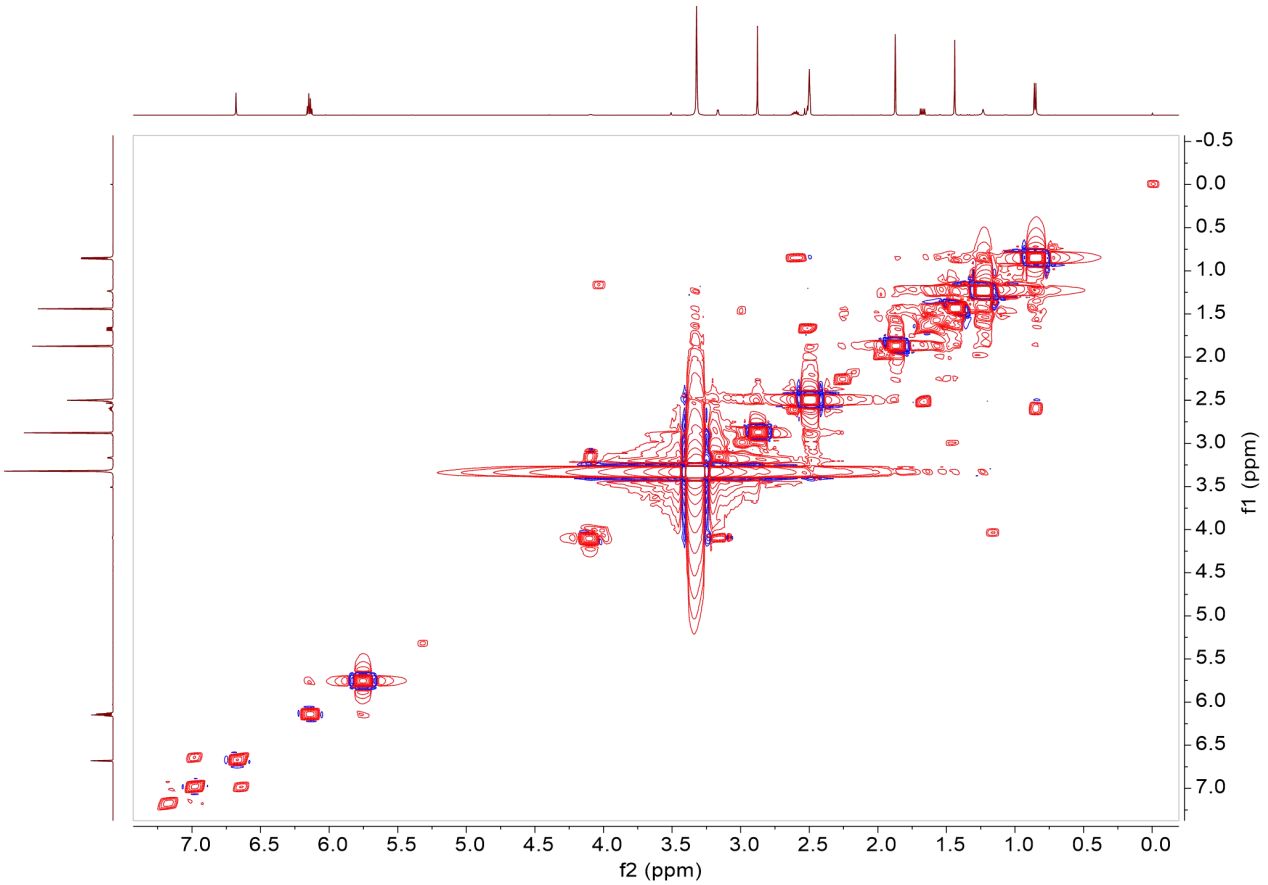


Fig. S41. ^{1}H-^{1}H-COSY NMR spectrum of compound **4** in DMSO.

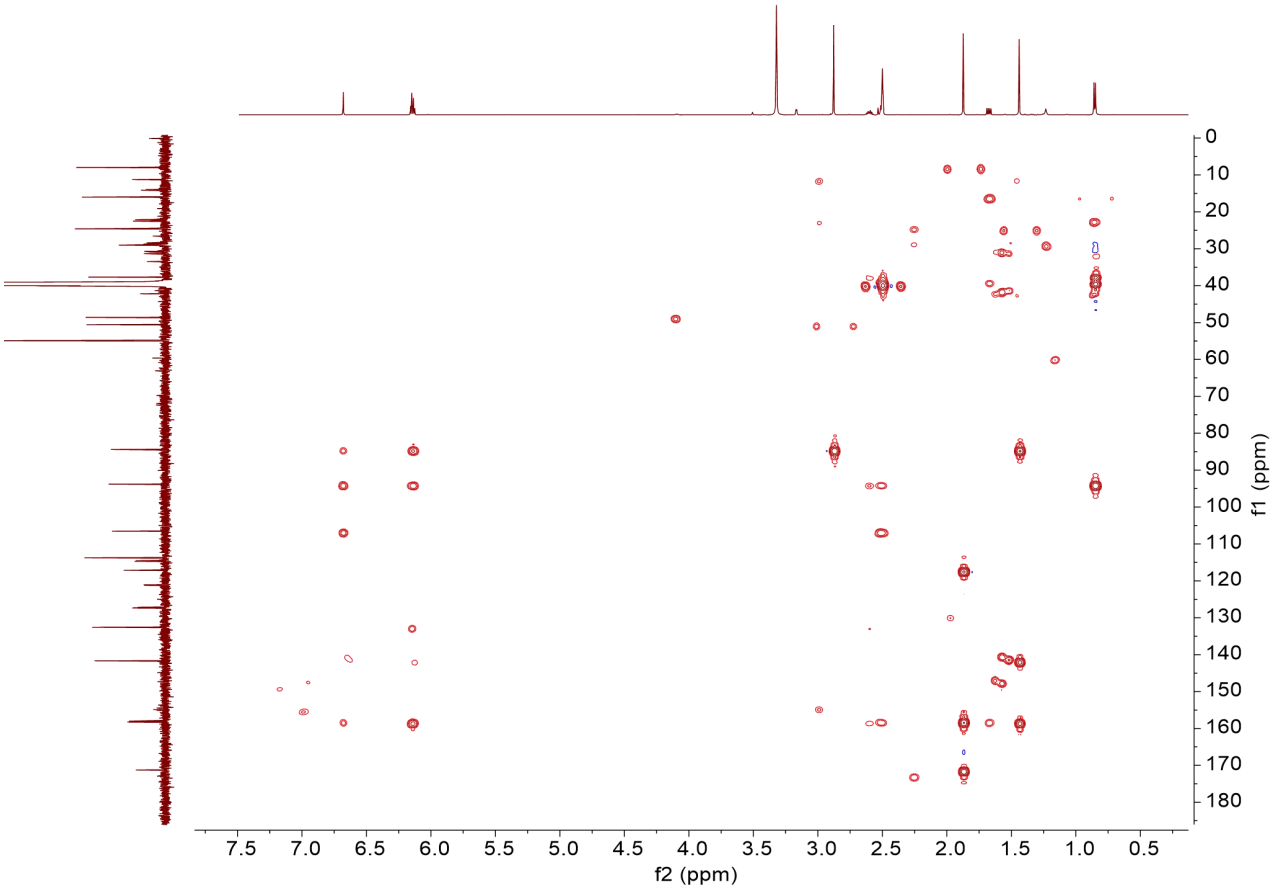


Fig. S42. HMBC NMR spectrum of compound **4** in DMSO.

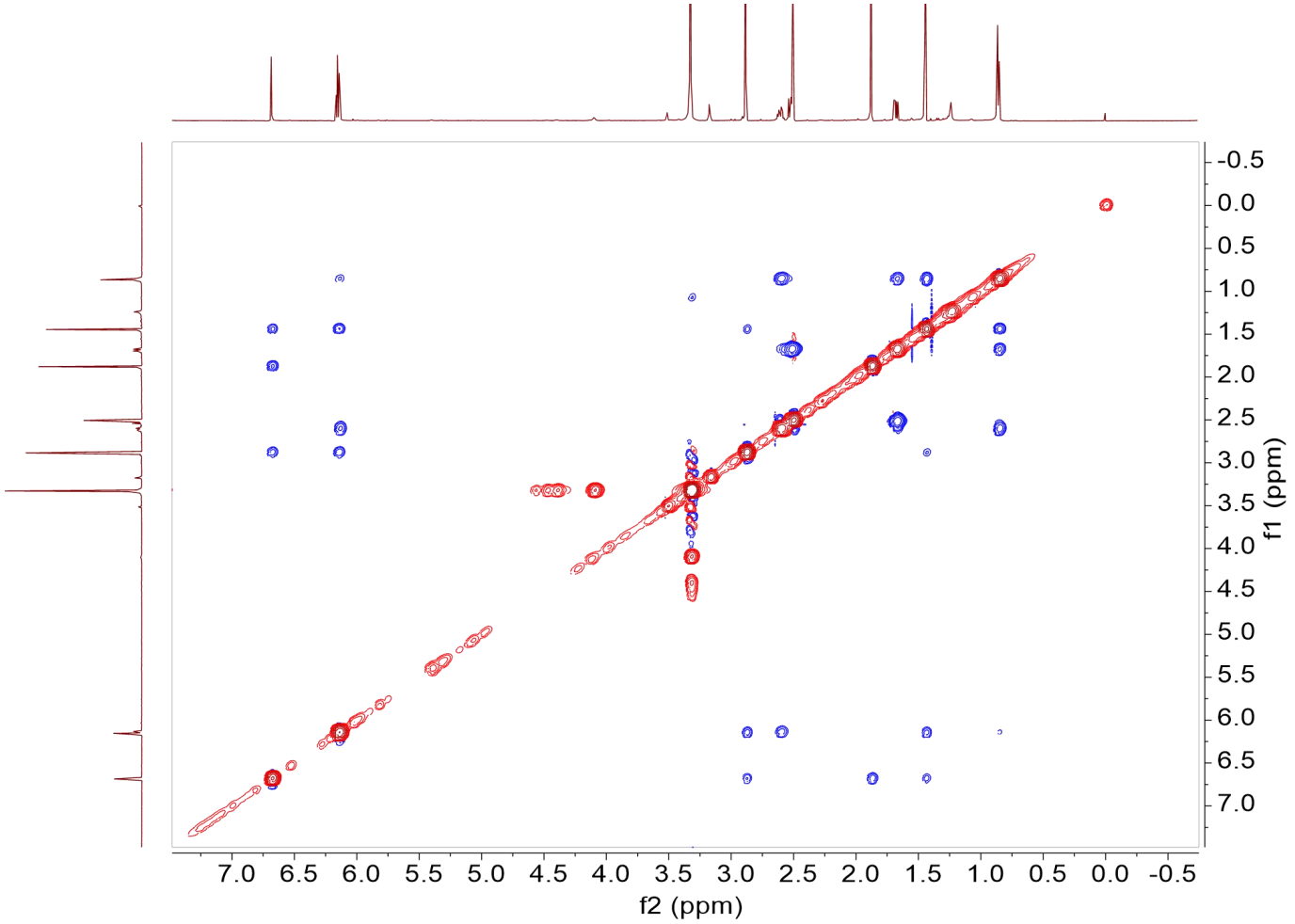


Fig. S43 NOESY spectrum of compound **4** in $CDCl_3$.

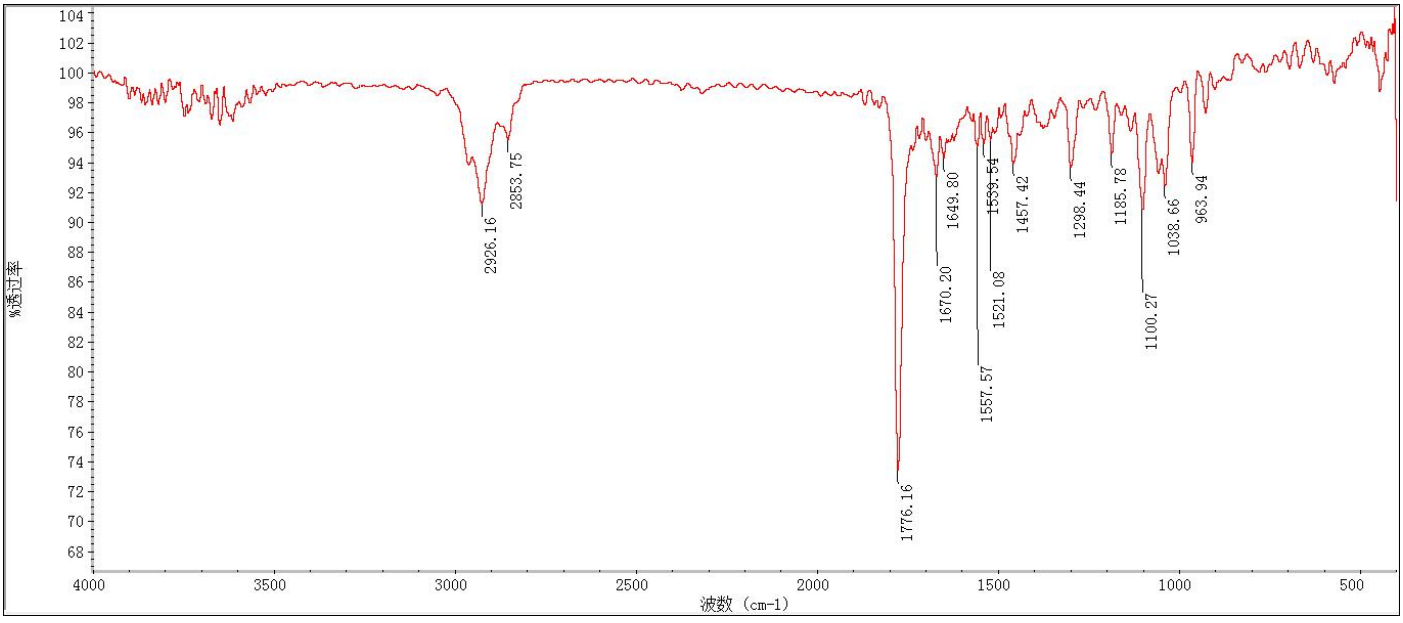


Fig. S44. IR spectrum of compound **4**.

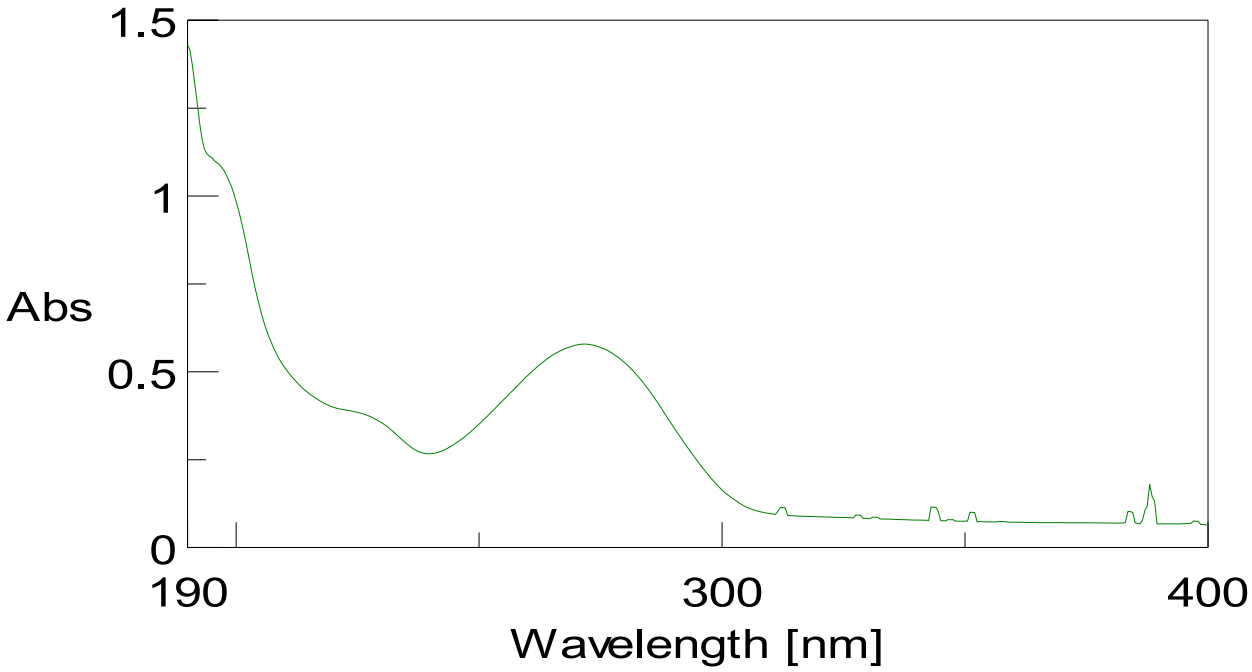


Fig. S45. UV spectrum of compound **4**.