Supporting Information for

Clausoxamine, an alkaloid possessing a 1,3-oxazine-4-one ring from the seeds of *Clausena lansium* and the anti-obesity effect of lansiumamide B

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Table S1. Effect of lansiumamide B on liver lipid profile [a]

	RD	HFD	HFD + LB
cholesterol (mmol L^{-1})	0.77 ± 0.02	0.94 ± 0.02#	0.82 ± 0.01*
HDL (mmol L^{-1})	1.22 ± 0.18	0.33 ± 0.09#	0.60 ± 0.08*
LDL (mmol L^{-1})	0.38 ± 0.06	0.72 ± 0.04#	0.51 ± 0.02*

[a] Data are shown as mean ± S.D., $n = 6$, #$p < 0.05$ RD vs. HFD group of mice.*$p < 0.05$, HFD + LB vs. HFD group of mice

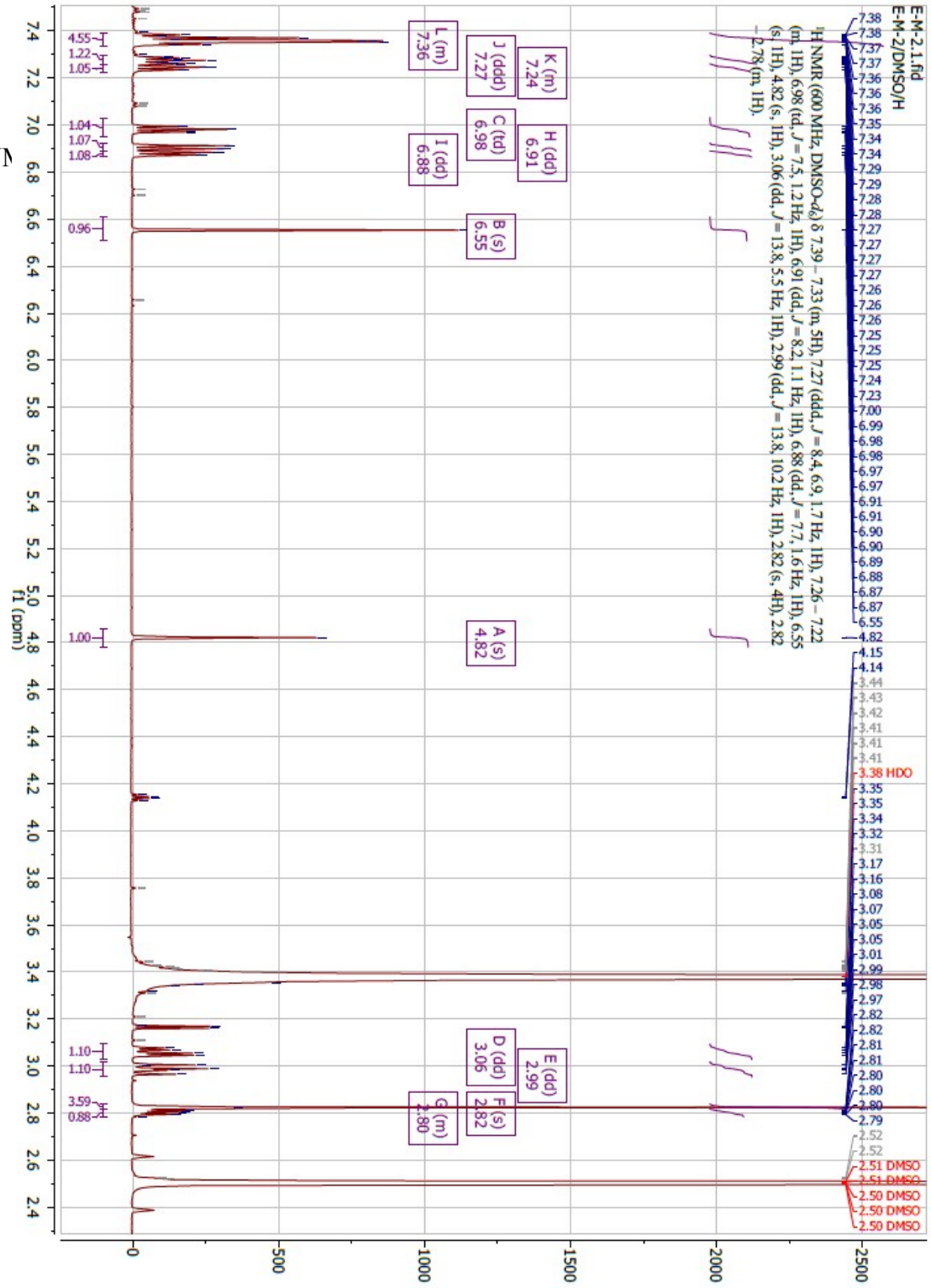

Figure S1. ^{1}H NM

Figure S2. ^{13}C NMR spectrum of *clausoxamine* (**1**) in DMSO-d_6

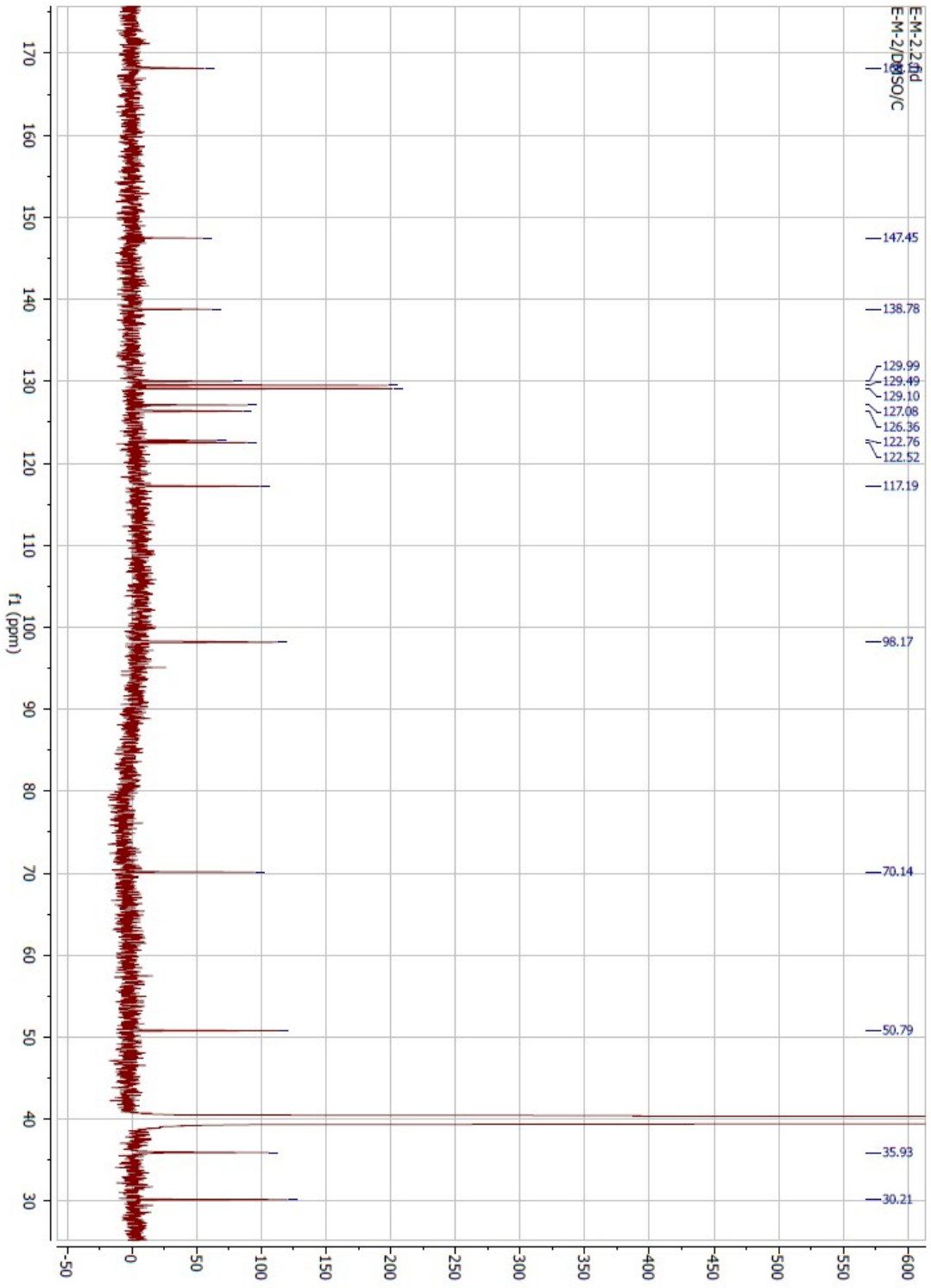

Figure S3. DEPT-135 spectrum of *clausoxamine* (**1**) in DMSO-d_6

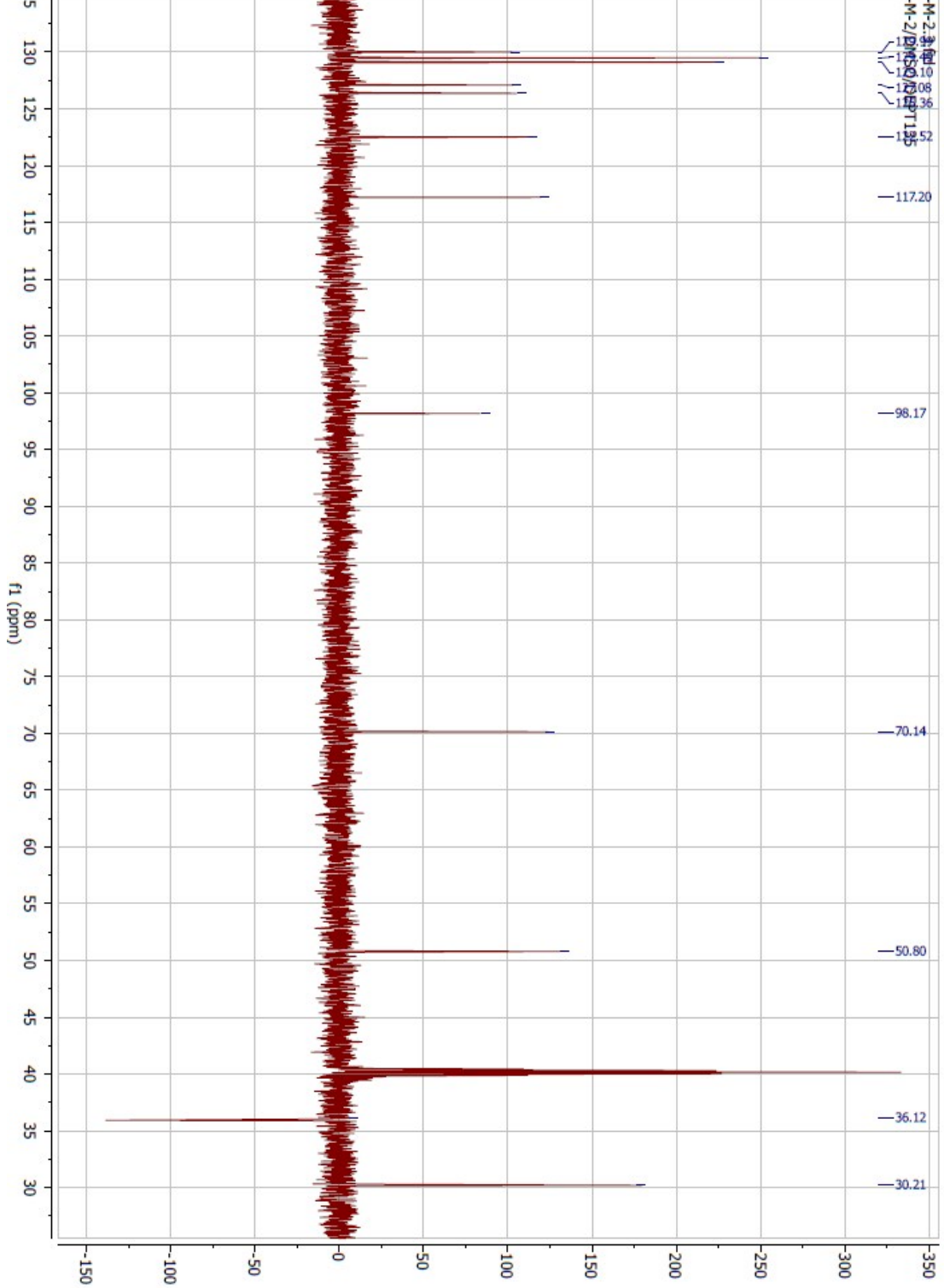

Figure S4. ^{1}H–^{1}H COSY spectrum of *clausoxamine* (**1**) in DMSO-d_6

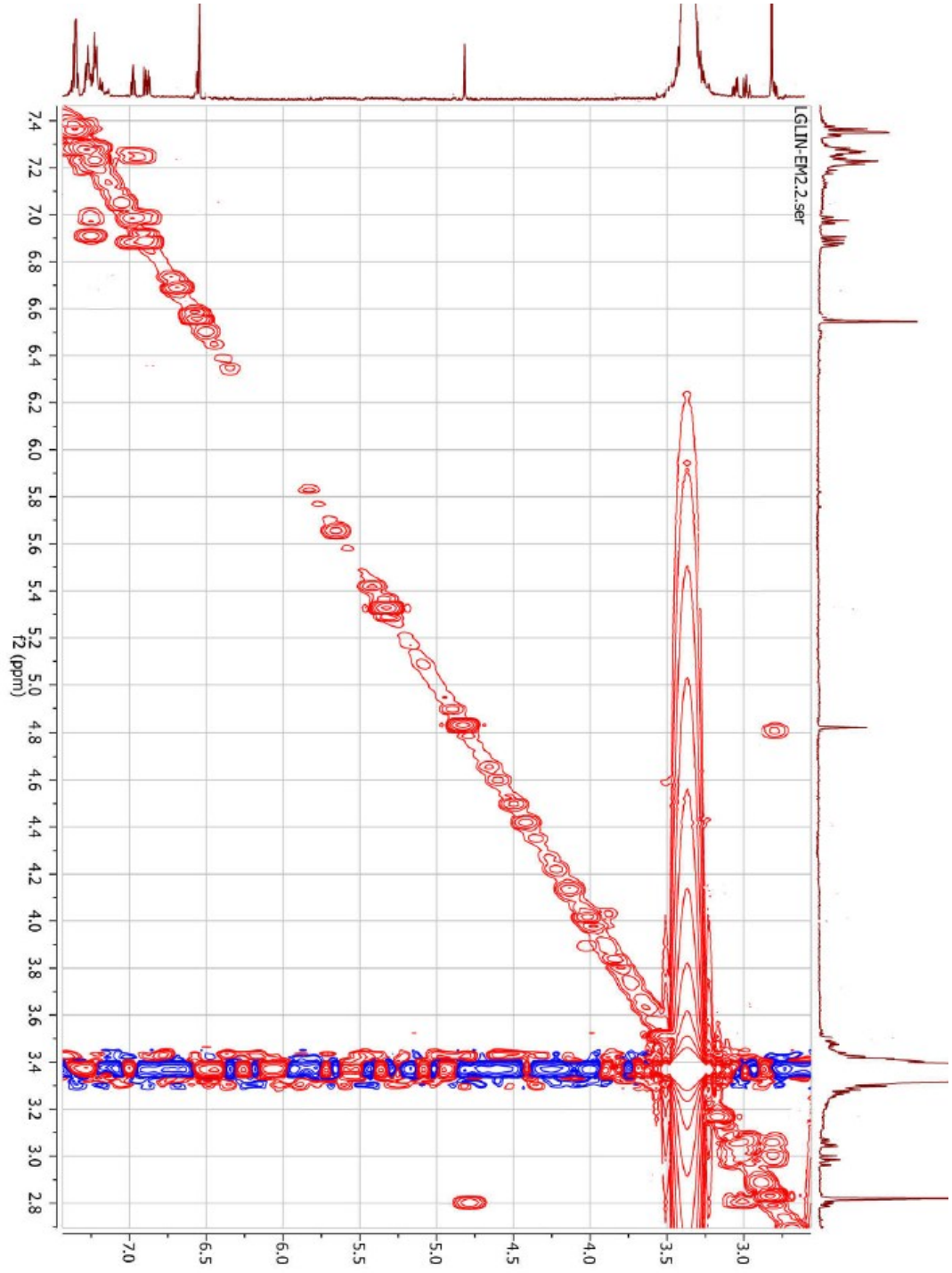
LGLIN-EM2.2.ser
f2 (ppm)
7.4
7.2
7.0
6.8
6.6
6.4
6.2
6.0
5.8
5.6
5.4
5.2
5.0
4.8
4.6
4.4
4.2
4.0
3.8
3.6
3.4
3.2
3.0
2.8
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0

Figure S5. HSQC sp

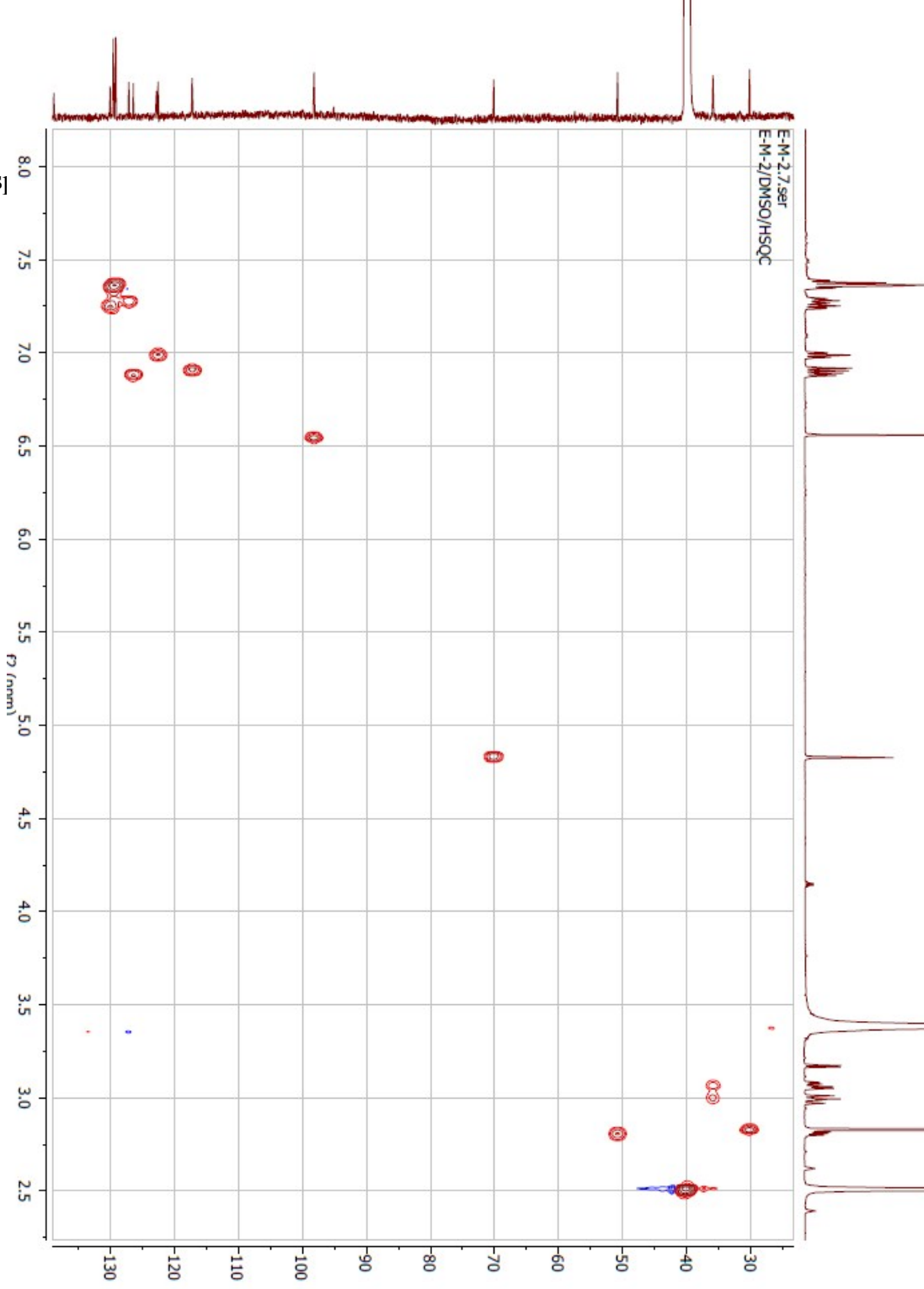

Figure S6. HMBC spectrum of *clausoxamine* (**1**) in DMSO-d_6

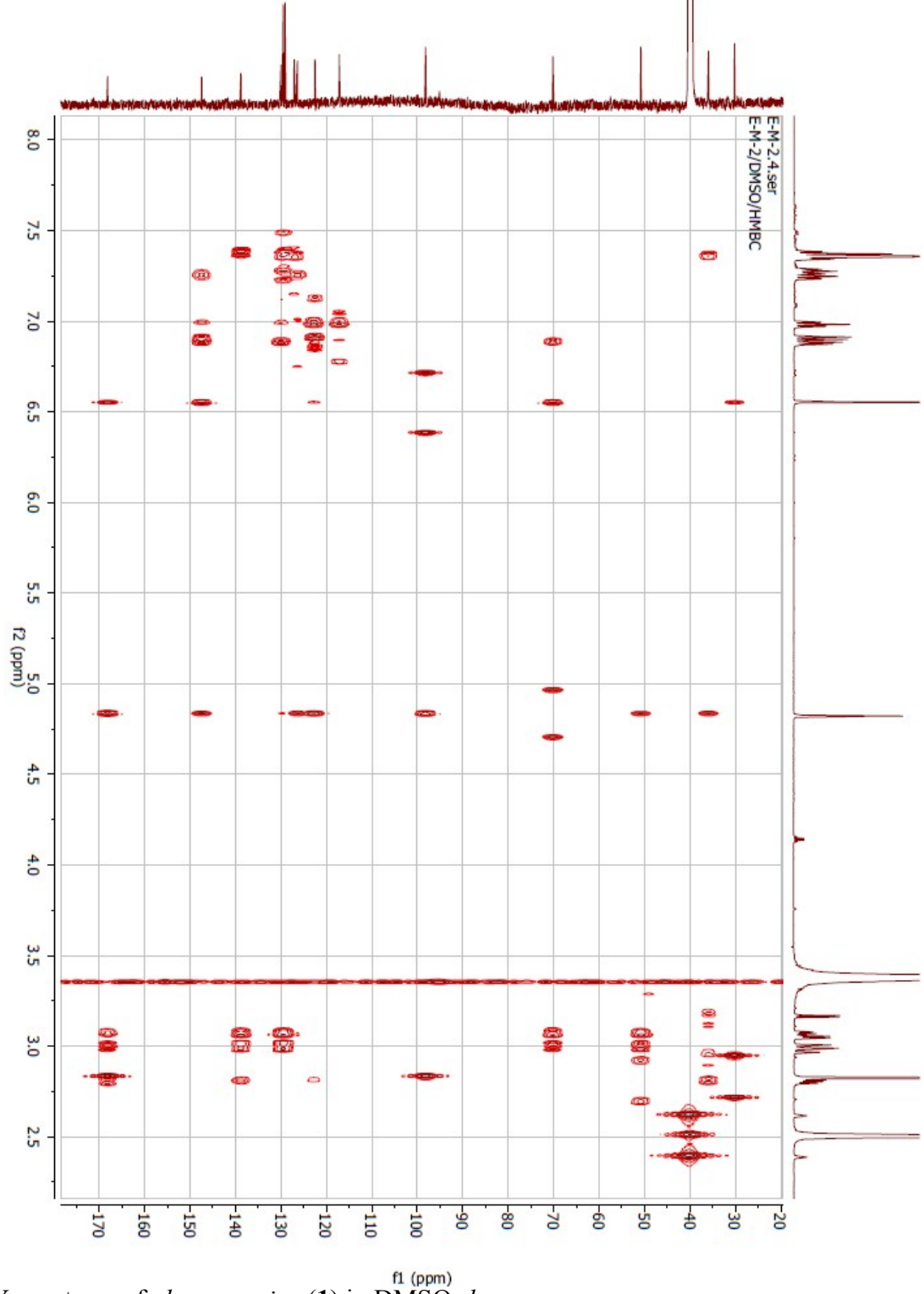

Figure S7. ROESY spectrum of *clausoxamine* (**1**) in DMSO-d_6

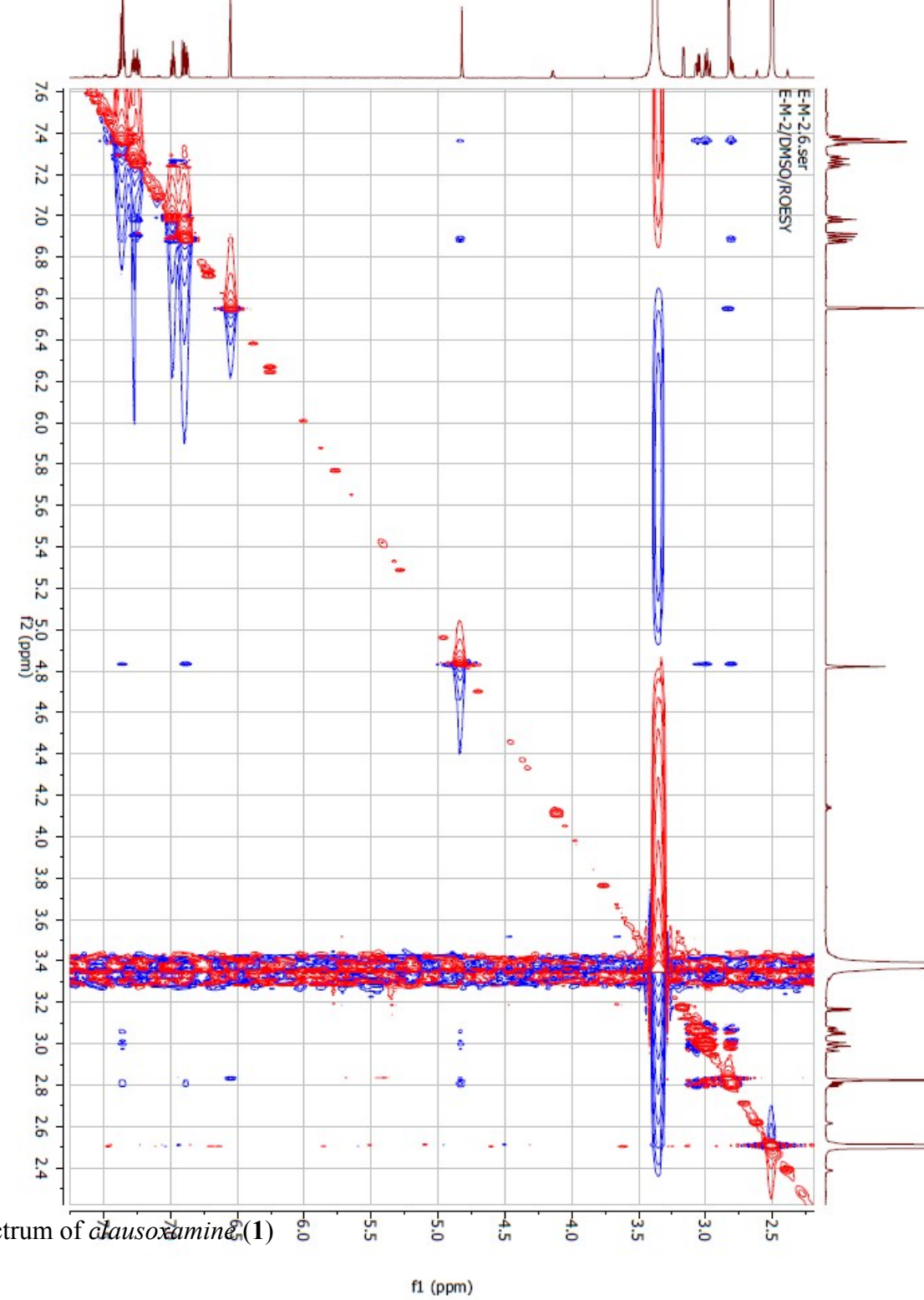

Figure S8. IR spectrum of *clausoxamine* (**1**)

Figure S9. HRESIMS spectrum of *clausoxamine* (**1**)

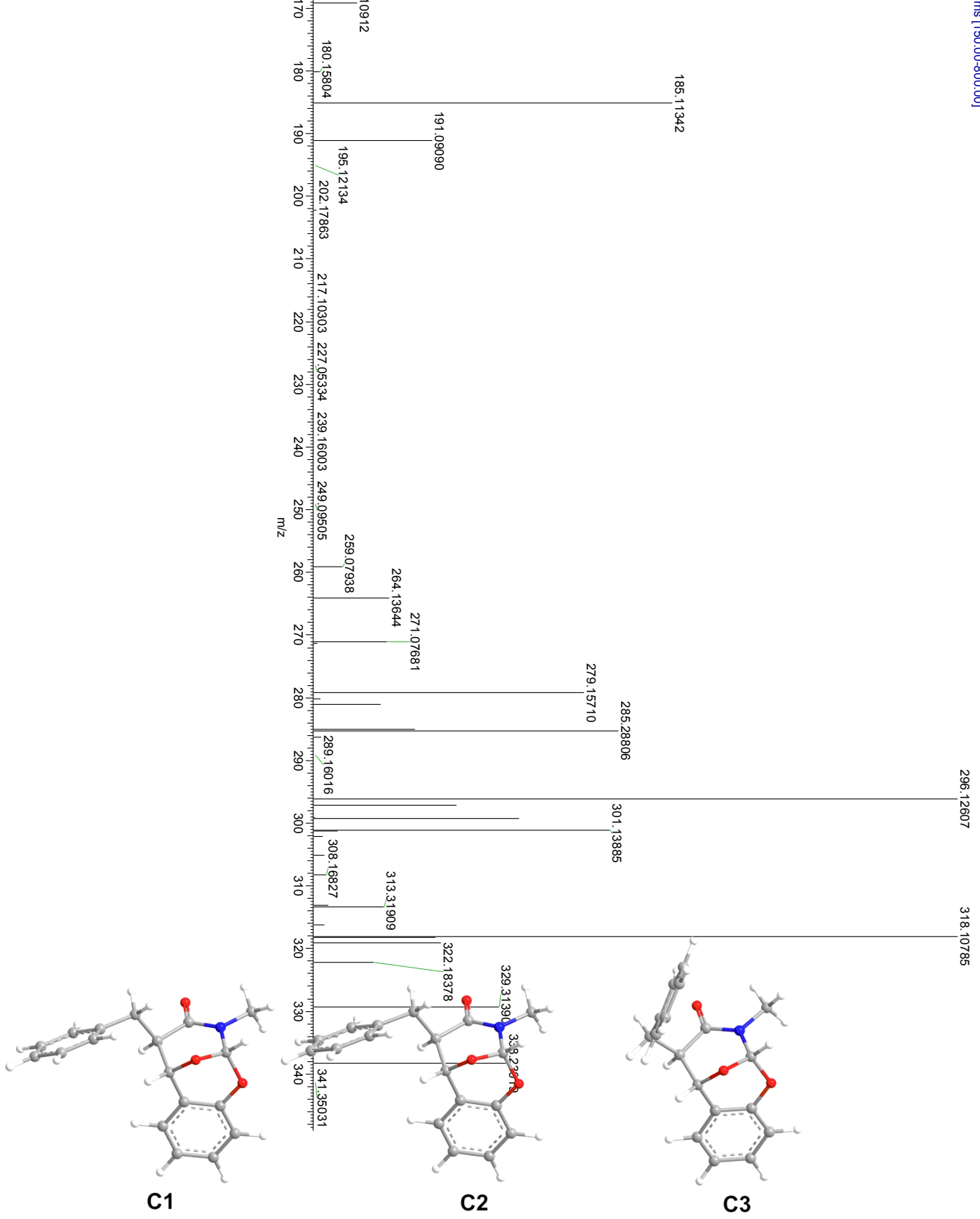

Figure S10. B3LYP/6-311+G(d) optimized lowest energy 3D conformers of **1**.

ECD simulation:

ECD spectrum of each conformation is simulated according to the overlapping Gaussian functions expressed as:

$$\Delta\varepsilon(E)=\frac{1}{2.296\times10^{-39}\sqrt{\pi}\sigma}\sum_{i}^{A}\Delta E_i R_i e^{[-(E-\Delta Ei)^2/\sigma^2]}$$

Where σ is half the bandwidth at 1/e peak height and expressed in energy units. The parameters ΔE_i and R_i are the excitation energies and rotational strengths for the transition *i*, respectively.

The above function is converted to Δε, λ (wavelength) correlations as:

$$\Delta\varepsilon(\lambda)=\frac{1}{2.296\times10^{-39}\sqrt{\pi}\sigma}\sum_{i}^{A}\Delta E_i R_i e^{[-(1240/\lambda-\Delta Ei)^2/\sigma^2]}$$

and then simulation were accomplished by using the Excel 2003 and the Origin 7.0 software.

To get the final spectra, all the simulated spectra of conformations of each compound were averaged according to their energy and the Boltzmann distribution theory expressed as:

$$\frac{N_i^*}{N}=\frac{g_i e^{-\varepsilon_i/k_B T}}{\sum g_i e^{-\varepsilon_i/k_B T}}$$

Energy analysis for 1

conf.	Gibbs free energy (298.15 K)		
	G (Hartree)	ΔG (Kcal/mol)	Boltzmann Distribution
C1	-976.353416	0	0.499
C2	-976.353410	0.003765	0.496
C3	-976.349110	2.702058	0.005

ECD Data for 1：

State	**C1**		**C2**		**C3**	
	Excitation energies(eV)	Rotatory Strengths *	Excitation energies(eV)	Rotatory Strengths *	Excitation energies(eV)	Rotatory Strengths *
1	4.8892	5.1463	4.8891	5.1667	4.8797	6.0616
2	5.1777	-11.2253	5.1777	-11.2774	5.1751	1.4114

3	5.1932	-3.4154	5.1931	-3.4079	5.2309	-22.791
4	5.3712	-2.9113	5.371	-2.8961	5.3994	2.5861
5	5.4431	-0.3083	5.4431	-0.3082	5.4409	-6.428
6	5.5002	7.1271	5.5	7.1283	5.5168	30.7853
7	5.564	3.1864	5.564	3.1893	5.5797	10.5141
8	5.6079	2.3472	5.6079	2.3493	5.6393	-6.0291
9	5.7236	22.1421	5.7235	22.1372	5.6473	-2.4219
10	5.8161	-8.0254	5.8161	-7.994	5.6733	-5.4163
11	5.8239	-4.6048	5.8239	-4.696	5.7482	13.0391
12	5.8357	39.6298	5.8357	39.6085	5.7576	12.1201
13	5.8665	0.2875	5.8664	0.3468	5.7919	12.9807
14	5.8872	-1.1507	5.8872	-1.1396	5.8158	-4.3759
15	5.9061	-7.0823	5.906	-7.0427	5.8283	16.1267
16	5.9353	-10.7497	5.9352	-10.7531	5.8839	-11.4601
17	5.9498	8.8242	5.9497	8.8258	5.9413	26.7683
18	5.9819	-8.5895	5.9819	-8.6122	5.9666	-0.5667
19	6.0115	13.3089	6.0114	13.3397	5.9812	15.8684
20	6.0679	-36.3779	6.0679	-36.3578	6.009	-5.84
21	6.1467	-10.9679	6.1466	-10.8343	6.0438	-5.923
22	6.1591	-27.7993	6.1592	-28.0546	6.0878	-13.788
23	6.1744	44.2445	6.1743	44.434	6.1001	-11.0318
24	6.1826	58.4163	6.1826	58.2875	6.1154	10.6846
25	6.1975	-11.9345	6.1974	-11.8617	6.1554	-6.1979
26	6.223	-14.9876	6.223	-14.9393	6.1633	6.5516
27	6.2439	-8.9178	6.2438	-8.9214	6.1945	27.3276
28	6.2479	0.0691	6.2479	0.1298	6.2142	9.5963
29	6.2637	-29.1537	6.2637	-29.4067	6.2177	-28.1346
30	6.274	-14.8736	6.2739	-14.8344	6.2479	-0.5677
31	6.3052	8.156	6.3051	8.1349	6.2733	10.4512
32	6.3511	-28.2074	6.3512	-28.0671	6.2991	-6.5973
33	6.3644	11.0731	6.3644	10.946	6.3061	-5.9372
34	6.3962	24.9054	6.3962	24.9235	6.3128	-21.465
35	6.4445	-8.3494	6.4446	-8.2651	6.3137	-16.6253
36	6.4652	-35.0764	6.4652	-34.9835	6.3747	106.2558
37	6.4689	-14.846	6.4688	-14.9416	6.412	1.3543
38	6.4862	10.3948	6.4863	9.6227	6.4402	-28.4802
39	6.4909	-44.7469	6.4909	-44.6833	6.4497	32.2536
40	6.4992	74.5544	6.4992	75.2042	6.4572	20.7581
41	6.5316	15.0792	6.5314	15.1539	6.4681	-3.6809
42	6.5449	-21.2063	6.5449	-21.2386	6.4851	-22.6107
43	6.5632	20.0046	6.5631	19.8138	6.4976	84.3425
44	6.571	6.7935	6.571	6.5663	6.5	44.7682
45	6.5953	30.0162	6.5953	30.3114	6.5257	-107.316

46	6.6225	-16.7908	6.6225	-16.5709	6.5721	-5.287
47	6.6331	111.2125	6.6331	111.3005	6.5759	1.5406
48	6.6542	-164.8094	6.6541	-164.905	6.6016	-105.556
49	6.7046	2.4209	6.7047	2.4853	6.6202	1.9077
50	6.7141	115.6556	6.7142	115.0028	6.6798	41.0684
51	6.7278	-115.6985	6.7279	-114.905	6.682	-63.3628
52	6.7633	7.4172	6.7632	7.4806	6.7019	-12.3537
53	6.7772	33.854	6.7772	33.3828	6.7131	-20.8768
54	6.7986	68.1323	6.7986	67.5366	6.7176	-2.3911
55	6.8106	-22.2608	6.8106	-21.8094	6.7507	-13.0372
56	6.8246	45.672	6.8245	46.2103	6.7526	-60.563
57	6.8415	-43.6915	6.8416	-43.8353	6.7681	33.5111
58	6.8646	42.246	6.8646	42.1274	6.7839	1.8371
59	6.8784	13.075	6.8784	13.0462	6.7983	-87.0675
60	6.8928	-9.2864	6.8927	-9.2302	6.8119	35.4018

* R(velocity) 10**-40 erg-esu-cm