Supporting Information

Sarcaglarone A, a lindenane−monoterpene heterodimer from the seeds of *Sarcandra glabra*

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I Supplementary figures

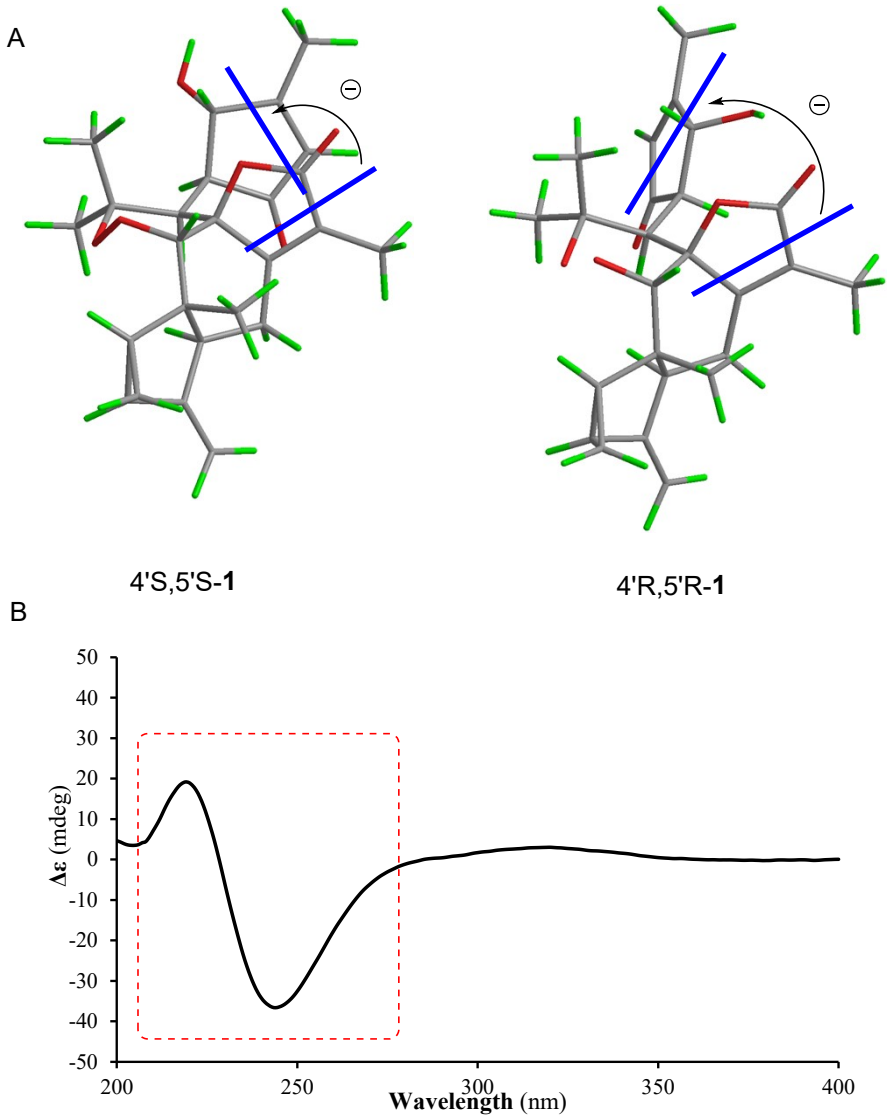


Fig. S1. The stereoview of 4'S,5'S-**1** and 4'R,5'R-**1**, and bold lines denote the electric transition dipole of the coupling chromophores (A); ECD curve of **1** (B).

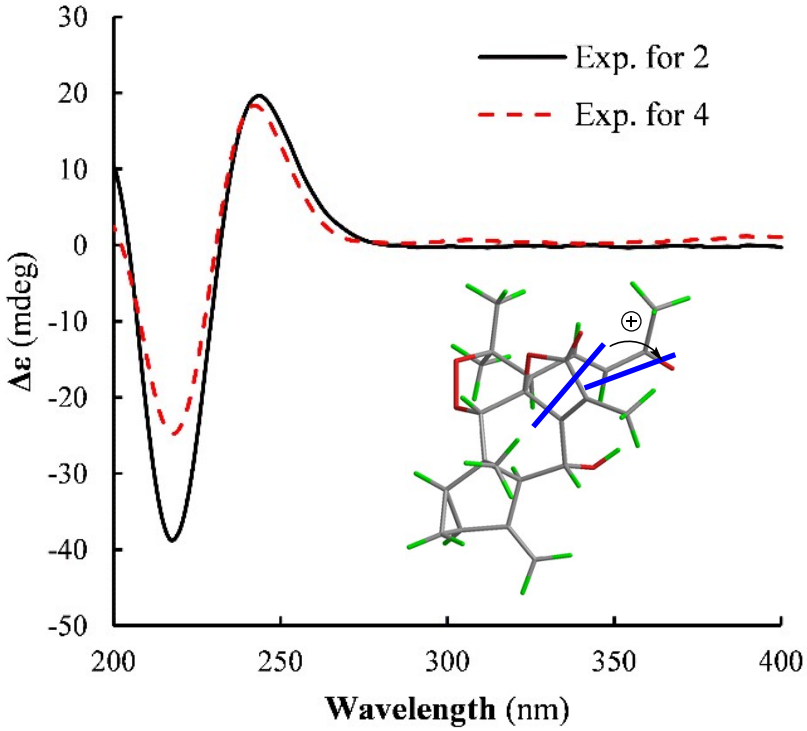


Fig. S2. ECD spectra of **2** and **4**.

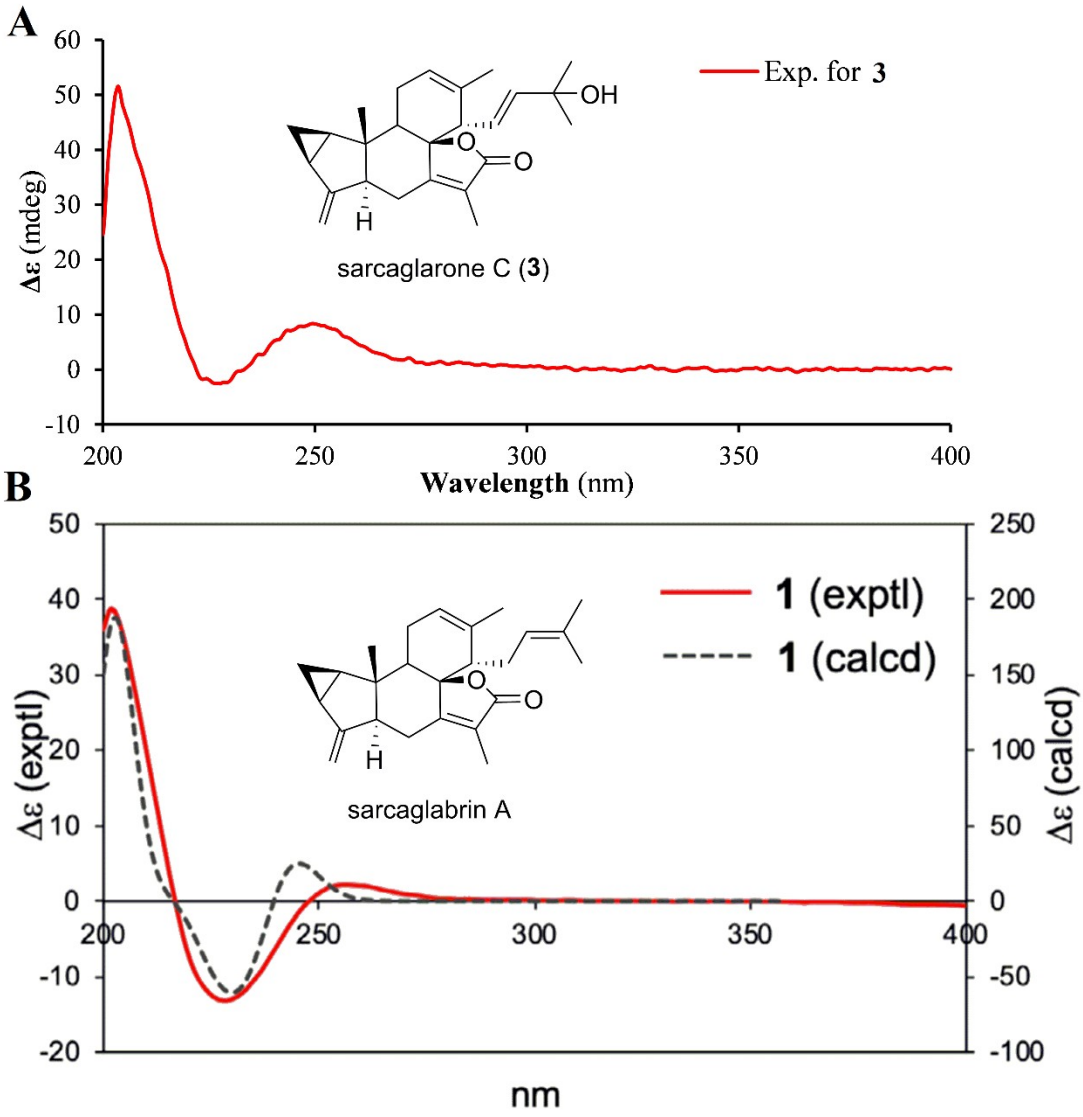


Fig. S3. ECD spectra of sarcaglarone C (**3**) **(A)** and sarcaglabrin A **(B)**[1].

References

[1] X. R. Yang, N. Tanaka, D. Tsuji, F. L. Lu, X. J. Yan, K. Itoh, D. P. Li, Y. Kashiwada, Tetrahedron Lett. 61 (2020) 151916.

II ECD Computational details of compound 1.

The initial conformational analysis of the compound **1** was executed by employing Monte Carlo searching algorithm via the MMFF94 molecular mechanics force field [1], with the aid of the SPARTAN'16 program package, leading to afford a panel of relatively favored conformations in an energy range of 3 kcal/mol above the global minimum. The force field minimum energy conformers thus obtained were subsequently optimized by applying the density functional theory (DFT) with the B3LYP/6-31G(d) level in vacuum, implemented in the Gaussian 09 software package [2]. Harmonic vibrational frequencies were also performed to confirm no imaginary frequencies of the finally optimized conformers. These predominant conformers were subjected to theoretical calculation of ECD by utilizing Time-dependent density functional theory (TDDFT) calculations at the B3LYP/6-311g (2d, p) level in MeOH using the Polarizable Continuum Model (PCM) solvent model. The energies, oscillator strengths, and rotational strengths of each conformers were carried out with Gaussian 09 software package. The oretical calculations of ECD spectra for each conformer were then approximated by the Gaussian distribution. The final ECD spectrum of the individual conformers was summed up on the basis of Boltzmann-weighed population contribution by the SpecDisv1.64 [3].

Table S1. Energy analyses of conformers (1*R*,3*S*,5*S*,8*S*,9*S*,10*S*,4′*S*,5′*S*,6′*S*)-**1**

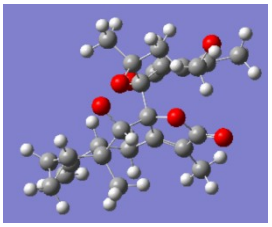
NO.	3D comformers	Free energy		
		E (Hartree)	ΔE (Kcal/mol)	Boltzmann distribution
4′*S*,5′*S* -1		-1460.850915	0	100%

Table S2. Energy analyses of conformers (1*R*,3*S*,5*S*,8*S*,9*S*,10*S*,4′*R*,5′*R*,6′*S*)-**1**a-b

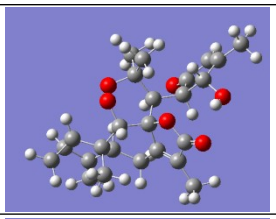
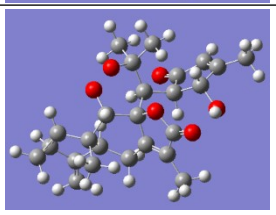
NO.	3D comformers	Free energy		
		E (Hartree)	ΔE (Kcal/mol)	Boltzmann distribution
4′*R*,5′*R*-1a		-1420.401883	0.0000	97.09%
4′*R*,5′*R*-1b		-1420.398571	2.0780	2.90%

Table S3. Cartesian coordinates of low-energy conformers of 1 optimized at B3LYP/6-31G(d) level in gas phase

Atom	Conformers (4′*S*,5′*S*)-**1**			Conformers (4′*R*,5′*R*)-**1**a			Conformers (4′*R*,5′*R*)-**1**b		
	X	Y	Z	X	Y	Z	X	Y	Z
C	2.69961	-0.73613	-0.57367	-2.72932	0.14755	-0.57856	-2.78853	0.10104	-0.53884
C	2.48413	-0.41997	0.93955	-2.43058	-0.06202	0.93802	-2.46434	0.02721	0.98681
C	1.23621	-1.08177	1.52639	-1.6033	1.07475	1.54753	-1.53394	1.14646	1.46307
C	0.15041	-1.05267	0.48404	-0.57525	1.50409	0.53451	-0.53349	1.42644	0.37542
C	0.17189	-0.02822	-0.64548	-0.1406	0.53089	-0.55038	-0.18706	0.34819	-0.64063
C	1.58333	-0.02457	-1.38356	-1.39688	0.10515	-1.40053	-1.49165	-0.23196	-1.32589
C	4.12796	-0.17139	-0.8128	-3.714	-1.01565	-0.86184	-3.913	-0.96485	-0.66872
C	4.82692	-0.09091	0.53636	-4.34983	-1.41071	0.46339	-4.52708	-1.16455	0.70914
C	3.8482	-0.58737	1.57086	-3.7482	-0.51951	1.52311	-3.79103	-0.25158	1.65727
C	-0.82376	-1.95494	0.24293	0.01778	2.69726	0.32729	0.08398	2.57459	0.03579
C	-1.46494	-1.6076	-1.04744	0.87582	2.57412	-0.87404	0.84738	2.32357	-1.20705
O	-0.84192	-0.50153	-1.55385	0.73579	1.31233	-1.38482	0.61418	1.04532	-1.6144
C	5.31614	-1.05126	-0.52235	-5.18754	-0.79804	-0.63496	-5.33854	-0.55286	-0.40894
O	1.99184	1.30828	-1.61437	-1.1536	-1.07909	-2.12682	-1.38636	-1.63733	-1.41815
O	0.91807	1.90282	-2.36152	-0.74798	-2.121	-1.21452	-0.14013	-1.8711	-2.09301
C	-0.04385	2.43181	-1.42473	0.65185	-1.92047	-0.90884	0.89679	-1.97152	-1.09086
C	-0.1773	1.43283	-0.21894	0.68126	-0.67097	0.03131	0.68371	-0.8077	-0.04368
C	2.62745	-2.24452	-0.89246	-3.37699	1.52659	-0.83902	-3.27582	1.49419	-0.98927
O	-2.37971	-2.14609	-1.6172	1.62299	3.37904	-1.37168	1.59945	3.05996	-1.80175
C	-1.23842	-3.17036	1.00462	-0.07484	3.98335	1.07988	0.10782	3.91284	0.69429
C	-1.28707	2.58119	-2.30404	1.4495	-1.82524	-2.21767	2.15393	-1.89142	-1.96061
C	0.45595	3.79413	-0.92715	1.00575	-3.21471	-0.16956	0.78363	-3.35113	-0.42925
C	-1.44581	1.66452	0.63609	2.02937	-0.21344	0.6407	1.92058	-0.29366	0.74482
C	4.12881	-1.03501	2.79893	-4.25007	-0.24047	2.73035	-4.20623	0.17814	2.85319
C	-2.839	1.01467	0.39992	0.12267	-1.0104	0.91586	0.06527	-1.254	0.74917
C	-3.44426	0.94153	1.79352	-1.81631	-0.97708	0.96842	-1.91808	-0.92723	1.09609
C	-2.51445	1.14013	2.75152	3.30426	0.09293	-0.19438	3.17494	0.35329	0.08849
C	-1.21086	1.44695	2.14559	4.42111	-0.6295	0.5506	4.35319	-0.311	0.79254
O	-0.13557	1.53965	2.70573	3.96175	-1.33514	1.60514	3.9577	-1.26304	1.66258
C	-4.89459	0.64643	1.96175	2.50527	-1.18198	1.74458	2.49032	-1.36362	1.69962
O	-3.7074	1.72428	-0.45934	1.78	-1.69001	2.57546	1.81828	-2.11908	2.37192
H	2.32034	0.67229	0.97323	5.83303	-0.46194	0.10608	5.74071	0.15331	0.51053
H	0.92316	-0.53996	2.43348	3.65219	1.46256	-0.24921	3.26114	1.7557	0.29848
H	1.42994	-2.12595	1.82091	1.82793	0.72321	1.18845	1.54671	0.48791	1.42788
H	1.42763	-0.52223	-2.35515	-1.1051	0.7277	2.47082	-1.02324	0.84277	2.39475
H	4.24206	0.62691	-1.54708	-2.22933	1.93441	1.8358	-2.0897	2.06781	1.70124
H	5.46662	0.75715	0.80088	-1.4661	0.84512	-2.21244	-1.53169	0.19411	-2.34257
H	6.2521	-0.78714	-1.02346	-3.40073	-1.77278	-1.58201	-3.73129	-1.81719	-1.32451
H	5.19053	-2.12367	-0.36197	-4.52635	-2.45976	0.72161	-4.81142	-2.1576	1.07149
H	0.63	1.71238	0.47326	-5.86808	-1.47556	-1.15917	-6.1165	-1.1853	-0.84665
H	3.21048	-2.83827	-0.17418	-5.5876	0.20851	-0.49962	-5.61166	0.50227	-0.34826

H	1.59906	-2.62877	-0.86998	-4.18737	1.73885	-0.12725	-4.02797	1.90239	-0.29911
H	3.03256	-2.43528	-1.89815	-2.64939	2.34669	-0.75364	-2.459	2.22563	-1.04784
H	-0.5748	-3.36696	1.85816	-3.79931	1.56062	-1.85545	-3.73385	1.42561	-1.9879
H	-2.26567	-3.05686	1.39005	-0.82172	3.93546	1.88472	-0.61873	3.98335	1.51615
H	-1.25064	-4.0557	0.34874	0.90022	4.23956	1.52663	1.11297	4.10627	1.10573
H	-2.09102	3.10423	-1.77002	-0.3335	4.81306	0.40246	-0.09507	4.71373	-0.03412
H	-1.02233	3.17169	-3.19454	2.51394	-2.03302	-2.03917	3.05935	-2.07709	-1.36587
H	-1.63859	1.59615	-2.6406	1.07248	-2.59173	-2.91104	2.09316	-2.67559	-2.73029
H	0.53306	4.49728	-1.76987	1.35505	-0.8459	-2.70203	2.2251	-0.92137	-2.46926
H	-0.22314	4.22989	-0.17817	0.79717	-4.07014	-0.82924	0.86434	-4.13032	-1.20225
H	1.45092	3.68715	-0.47081	2.07224	-3.23553	0.09321	1.56279	-3.51511	0.32572
H	-1.66017	2.74694	0.582	0.4241	-3.3263	0.75511	-0.19228	-3.45566	0.06583
H	3.34166	-1.34659	3.49137	-3.71717	0.39649	3.4424	-3.58294	0.81937	3.48305
H	5.15896	-1.09088	3.16194	-5.20913	-0.65272	3.05635	-5.18322	-0.10831	3.25239
H	-2.74716	-0.02544	0.05138	3.23373	-0.31879	-1.21365	3.23381	0.13834	-0.98756
H	-2.6637	1.07575	3.83063	4.55711	-1.93407	2.29667	4.60173	-1.87961	2.29231
H	-5.18805	0.604	3.01983	6.5395	-1.01754	0.73838	6.49122	-0.38978	1.10155
H	-5.48854	1.41847	1.44653	5.953	-0.79352	-0.94023	5.97967	0.03665	-0.56123
H	-5.15471	-0.31165	1.47903	6.08946	0.60984	0.12091	5.81302	1.2312	0.72911
H	-3.57568	1.40526	-1.36076	3.18743	1.90338	-0.97658	3.08118	2.22681	-0.52871
C	-5.10514	-4.56841	-1.65743	-2.72932	0.14755	-0.57856	-2.78853	0.10104	-0.53884
H	-5.5903	-4.62399	-0.67157	-2.43058	-0.06202	0.93802	-2.46434	0.02721	0.98681
H	-4.72849	-5.56464	-1.93201	-1.6033	1.07475	1.54753	-1.53394	1.14646	1.46307
H	-5.84238	-4.24237	-2.4056	-0.57525	1.50409	0.53451	-0.53349	1.42644	0.37542
H	-4.27151	-3.85296	-1.62512	-0.1406	0.53089	-0.55038	-0.18706	0.34819	-0.64063

References

[1] Halgren TA. *J Comput Chem*, 1999, **20**, 730-748.

[2] Frisch MJ, Trucks GW, Schlegel H B, Scuseria GE, Robb MA, Cheeseman JR, Scalmani G, Barone V, Mennucci B, Petersson GA, Nakatsuji H, Caricato M, Li X, Hratchian H P, Izmaylov AF, Bloino J, Zheng G, Sonnenberg JL, Hada M, Ehara M, Toyota K, Fukuda R, Hasegawa J, Ishida M, Nakajima T, Honda Y, Kitao O, Nakai H, Vreven T, Montgomery Jr JA, Peralta JE, Ogliaro F, Bearpark M, Heyd JJ, Brothers E, Kudin KN, Staroverov VN, Kobayashi R, Normand J, Raghavachari K, Rendell A, Burant JC, Iyengar SS, Tomasi J, Cossi M, Rega N, Millam JM, Klene M, Knox JE, Cross J B, Bakken V, Adamo C, Jaramillo J, Gomperts R, Stratmann RE, Yazyev O, Austin AJ, Cammi R, Pomelli C, Ochterski JW, Martin RL, Morokuma K, Zakrzewski VG, Voth GA, Salvador P, Dannenberg JJ, Dapprich S, Daniels AD, Farkas Ö, Foresman JB, Ortiz JV, Cioslowski J, Fox DJ, Gaussian 09, Rev. C 01; Gaussian, Inc., Wallingford CT, 2009.

[3] Bruhn T, Schaumloffel A, Hemberger Y, Bringmann G. *Chirality*, 2013, **25**, 243-24.

III Original spectra of compounds 1–3

3.1 NMR ($CDCl_3$, DMSO-d_6), MS, IR, UV and CD spectra of compound 1

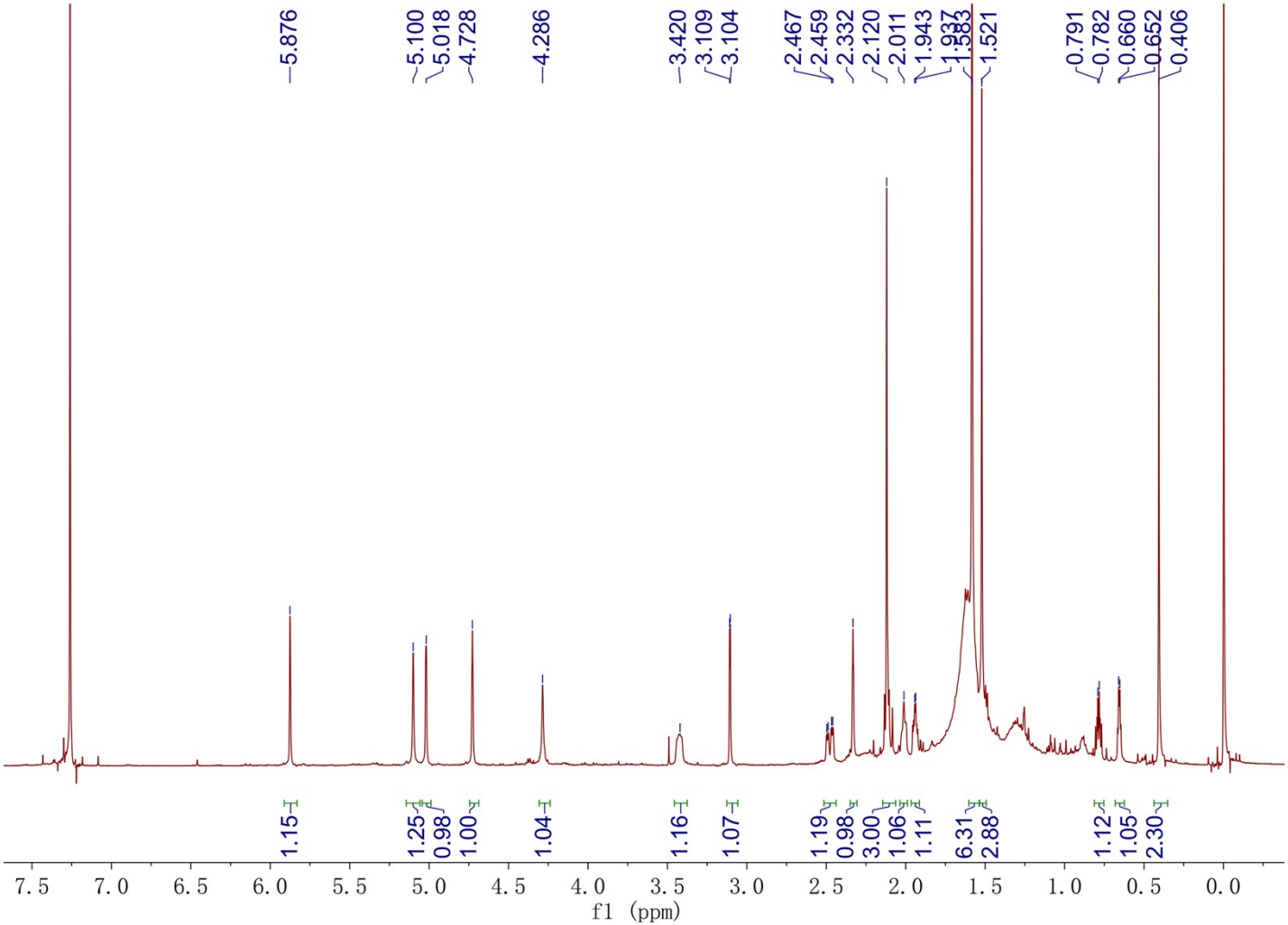


Figure S3.1.1 ^{1}H NMR (600 MHz; $CDCl_3$) spectrum of **1**

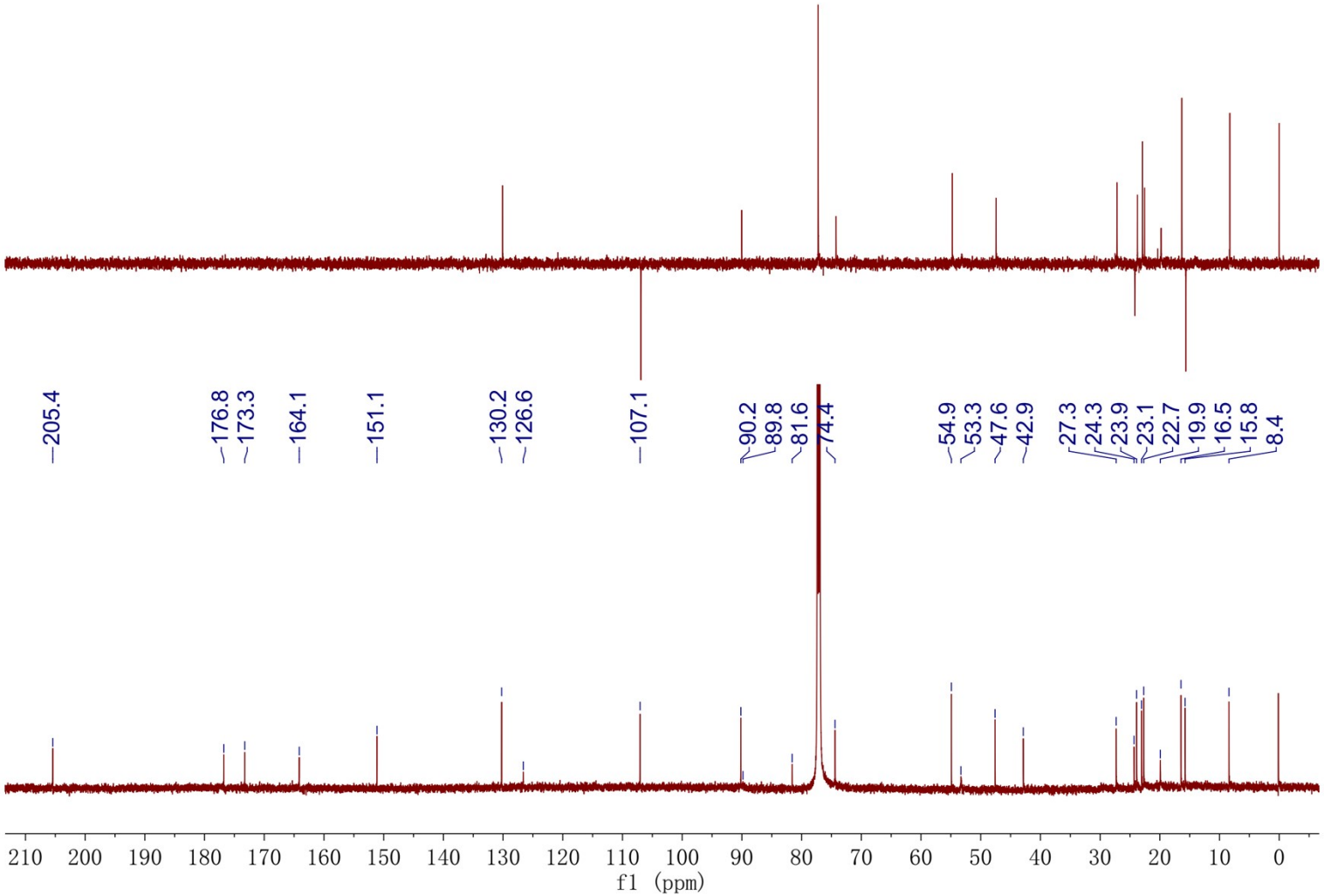


Figure S3.2 ^{13}C NMR (150 MHz; $CDCl_3$) spectrum of **1**

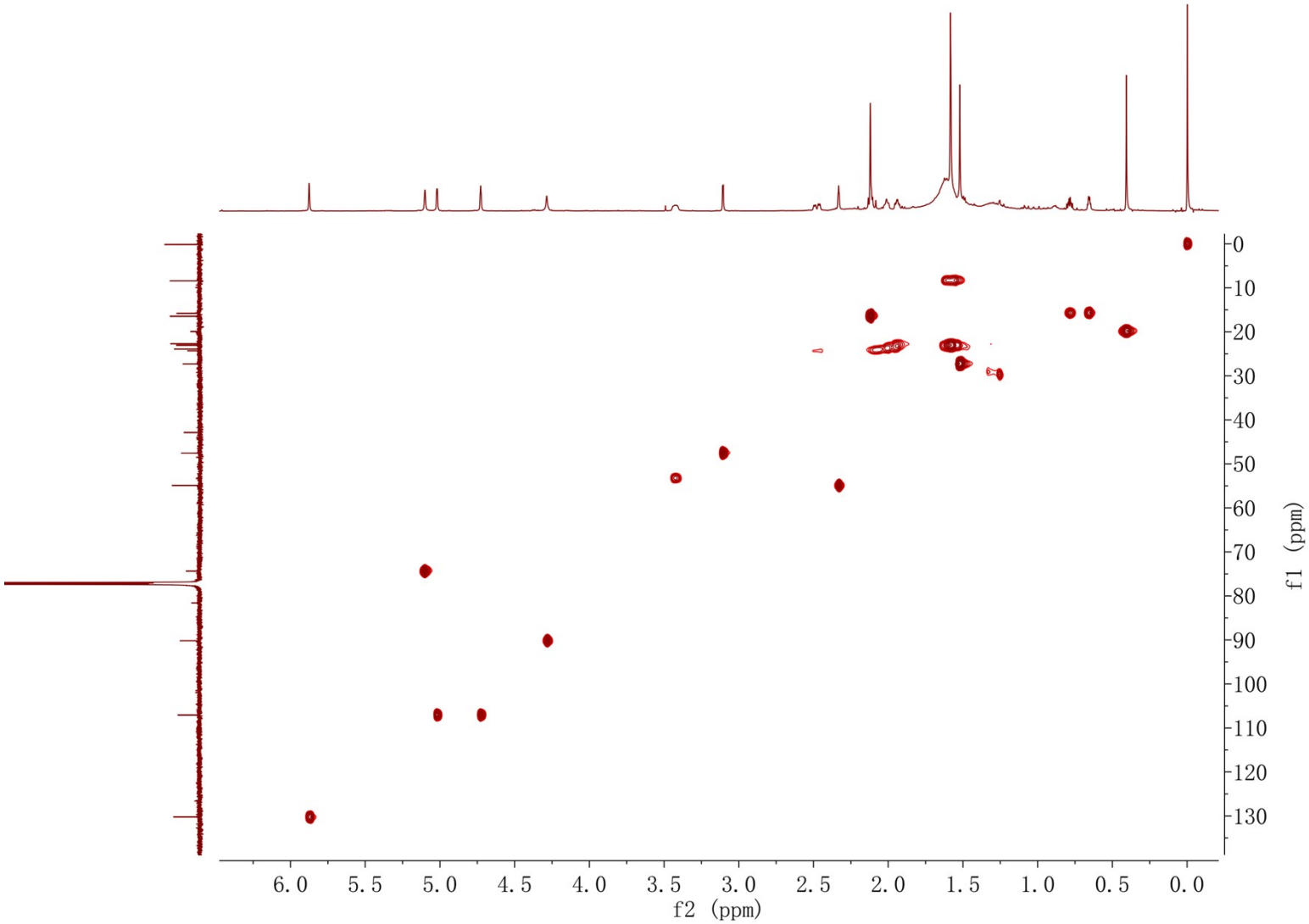


Figure S3.1.3 HSQC (^{1}H: 600 MHz, ^{13}C: 150 MHz; $CDCl_3$) spectrum of **1**

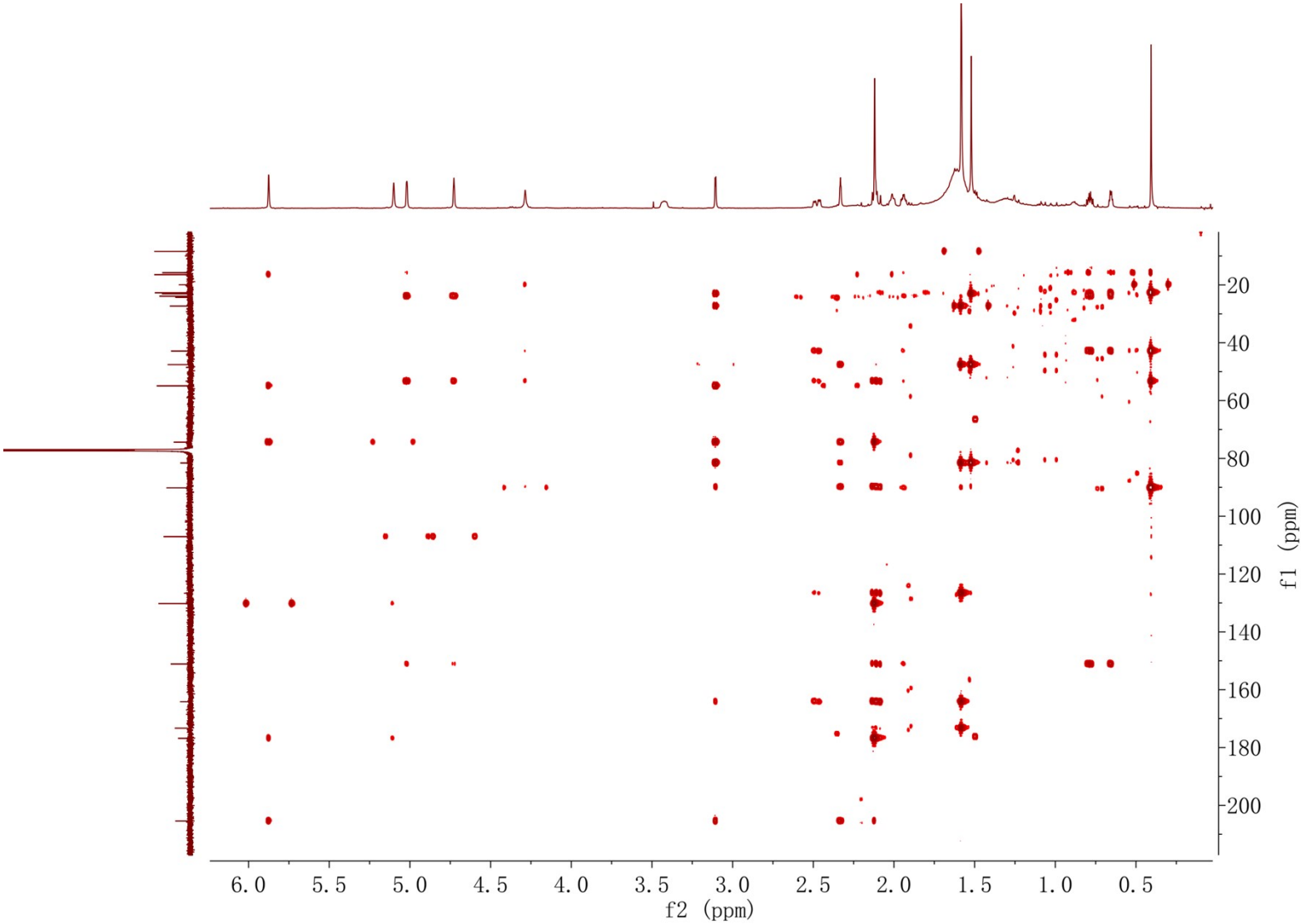


Figure S3.1.4 HMBC (^{1}H: 600 MHz, ^{13}C: 150 MHz; $CDCl_3$) spectrum of **1**

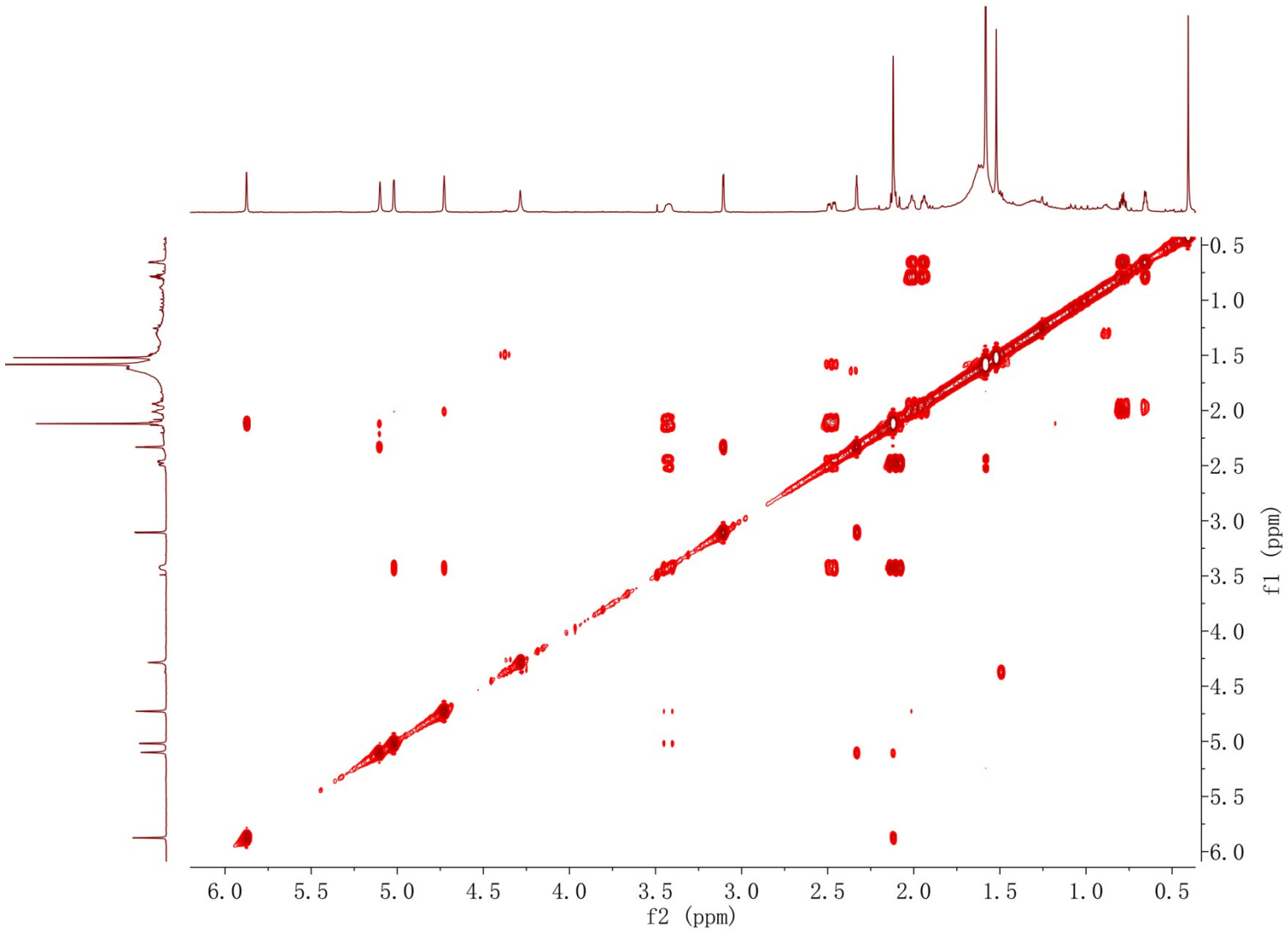


Figure S3.1.5 ^{1}H-^{1}H COSY (600 MHz; $CDCl_3$) spectrum of **1**

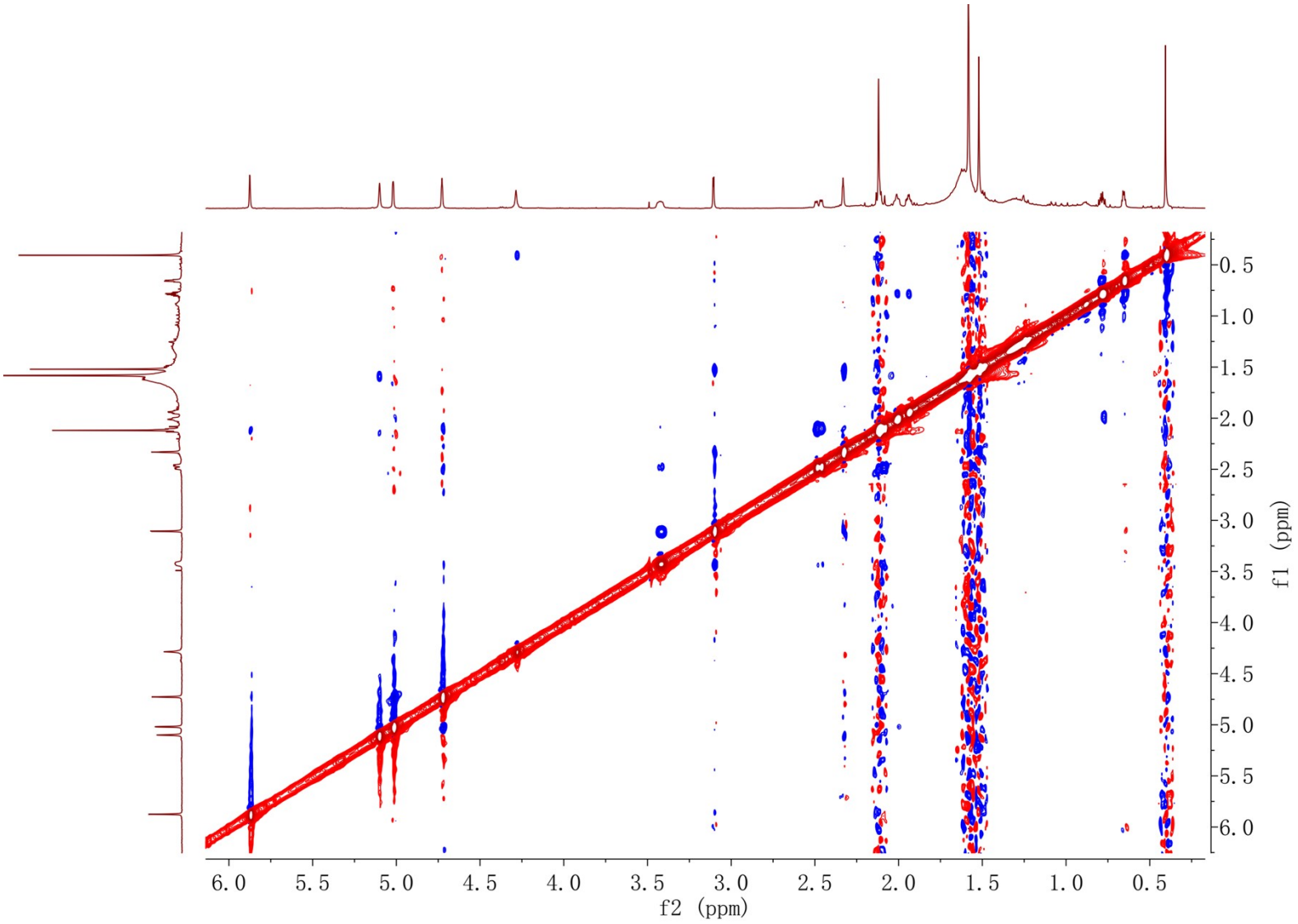


Figure S3.1.6 ROESY (600 MHz; $CDCl_3$) spectrum of **1**

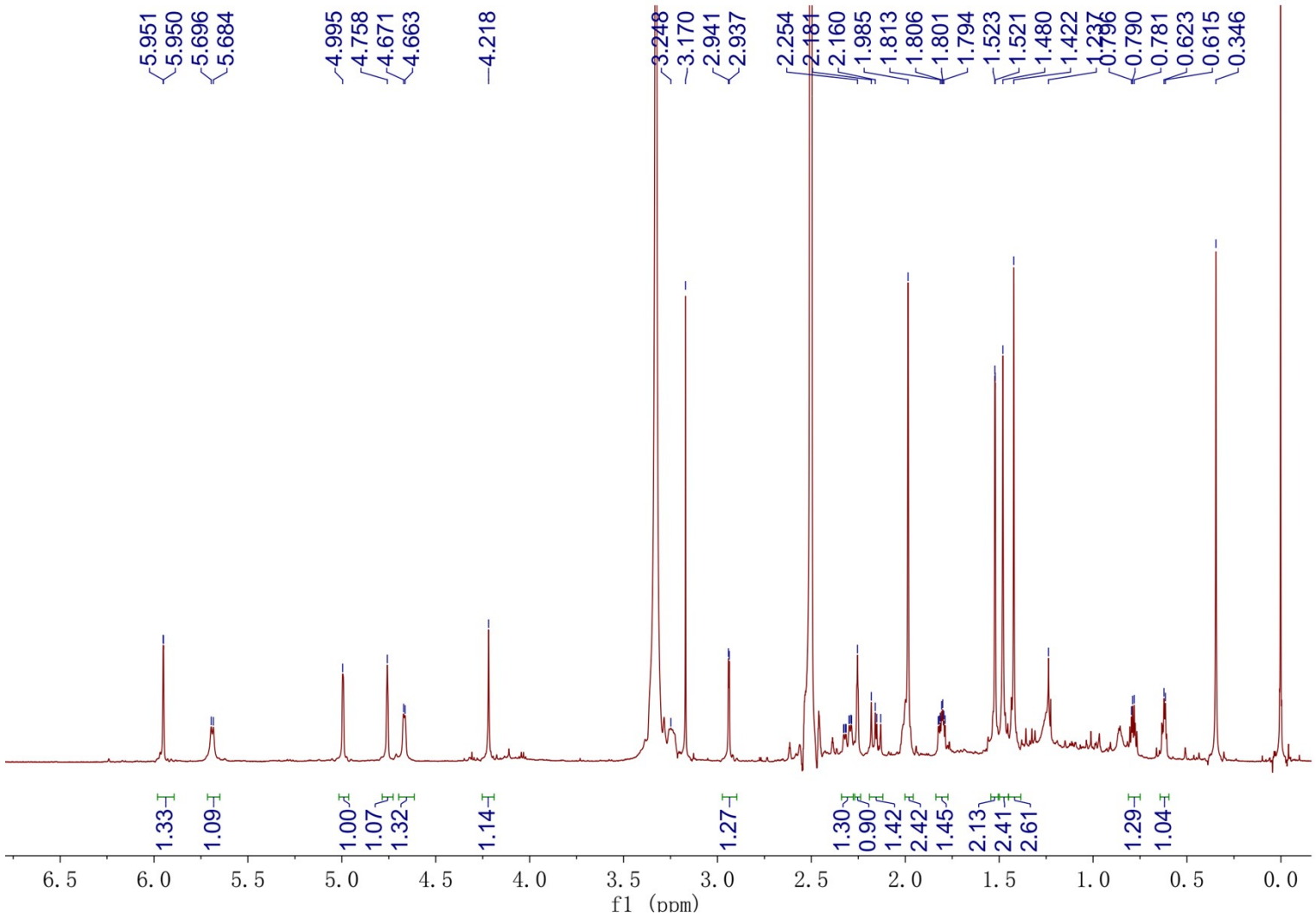


Figure S3.1.7 ^{1}H NMR (600 MHz; DMSO-d_6) spectrum of **1**

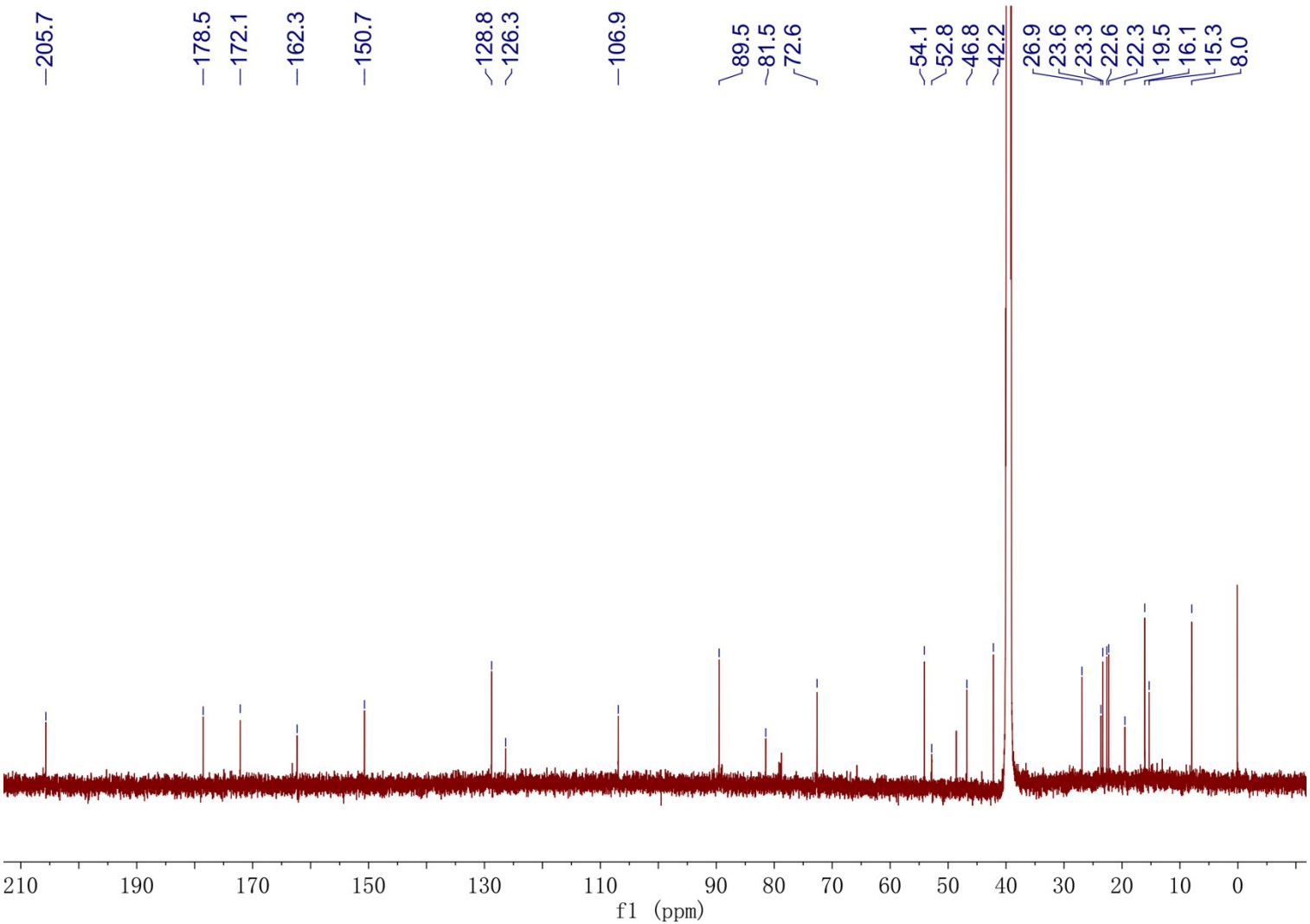


Figure S3.1.8 ^{13}C NMR (150 MHz; DMSO-d_6) spectrum of **1**

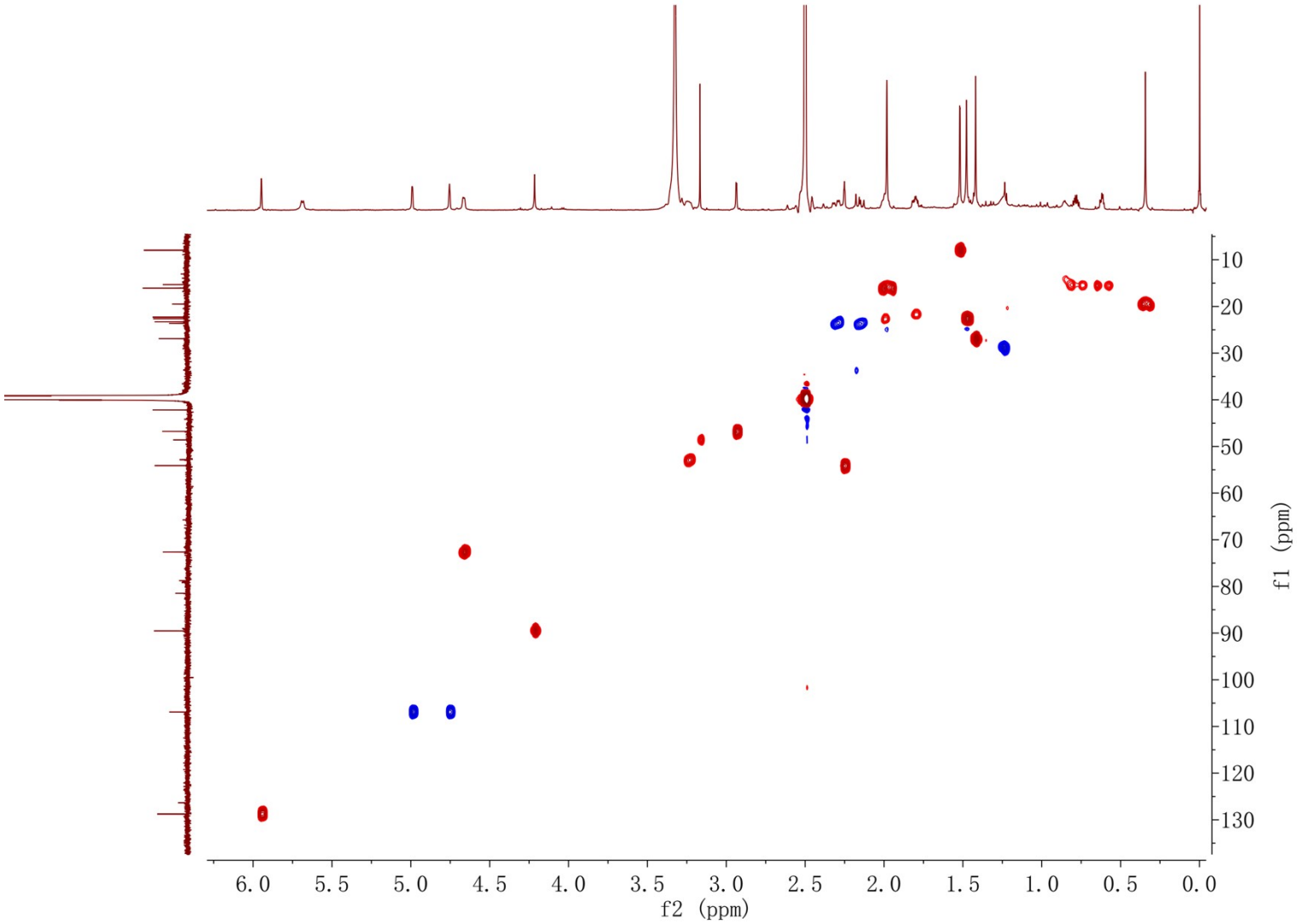


Figure S3.1.9 HSQC (^{1}H: 600 MHz, ^{13}C: 150 MHz; DMSO-d_6) spectrum of **1**

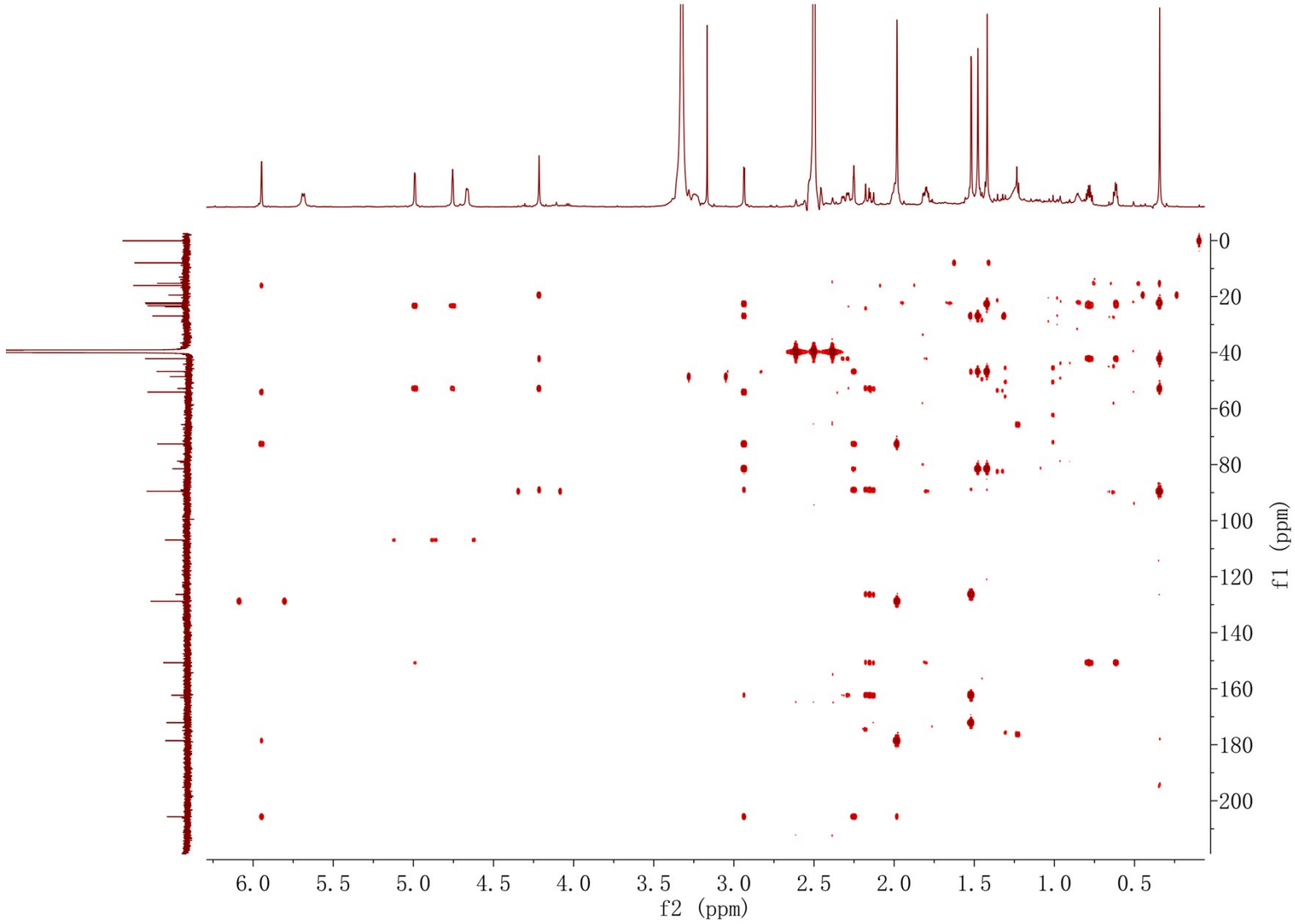


Figure S3.1.10 HMBC (^{1}H: 600 MHz, ^{13}C: 150 MHz; DMSO-d_6) spectrum of **1**

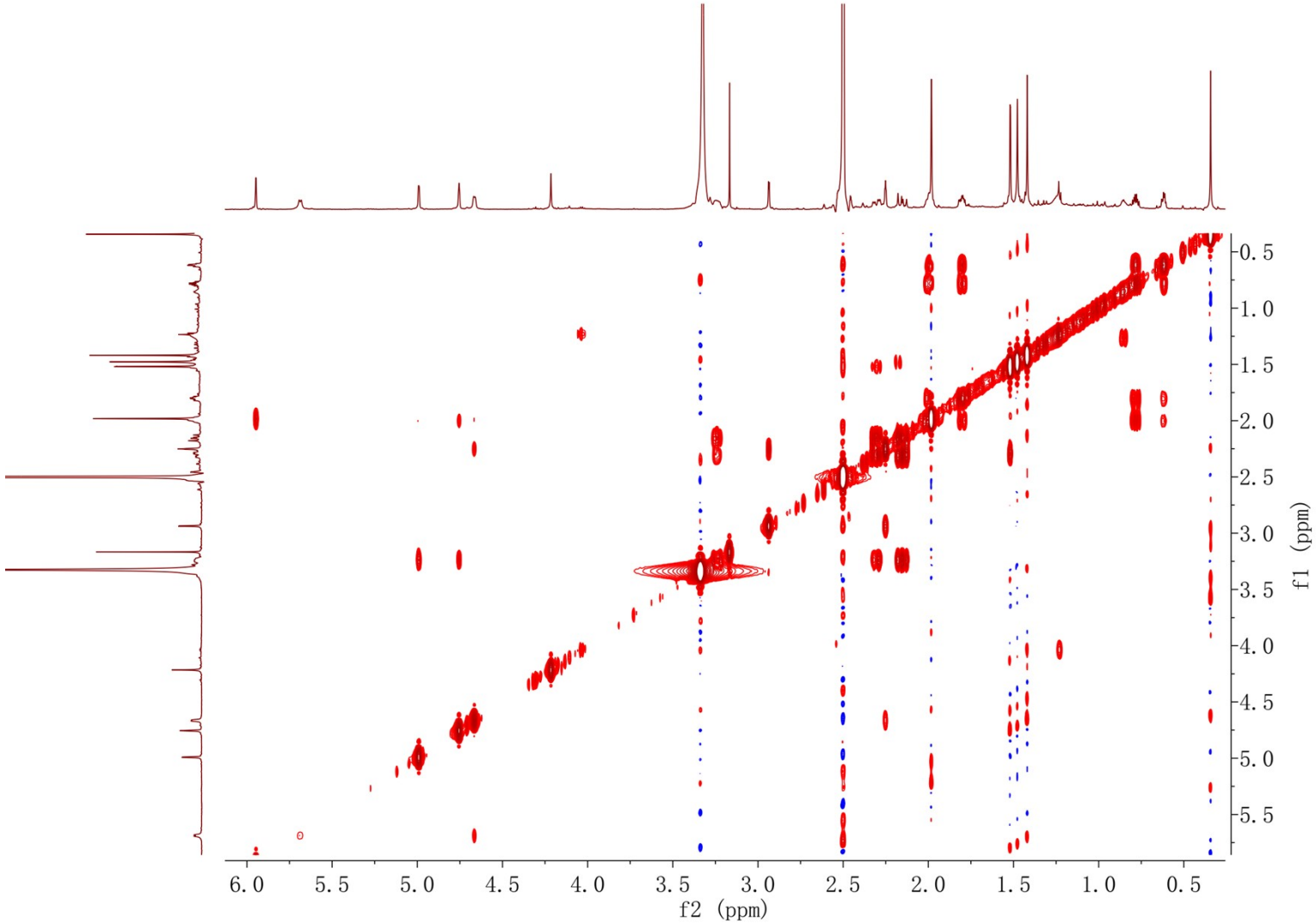


Figure S3.1.11 ^{1}H-^{1}H COSY (600 MHz; DMSO-d_6) spectrum of **1**

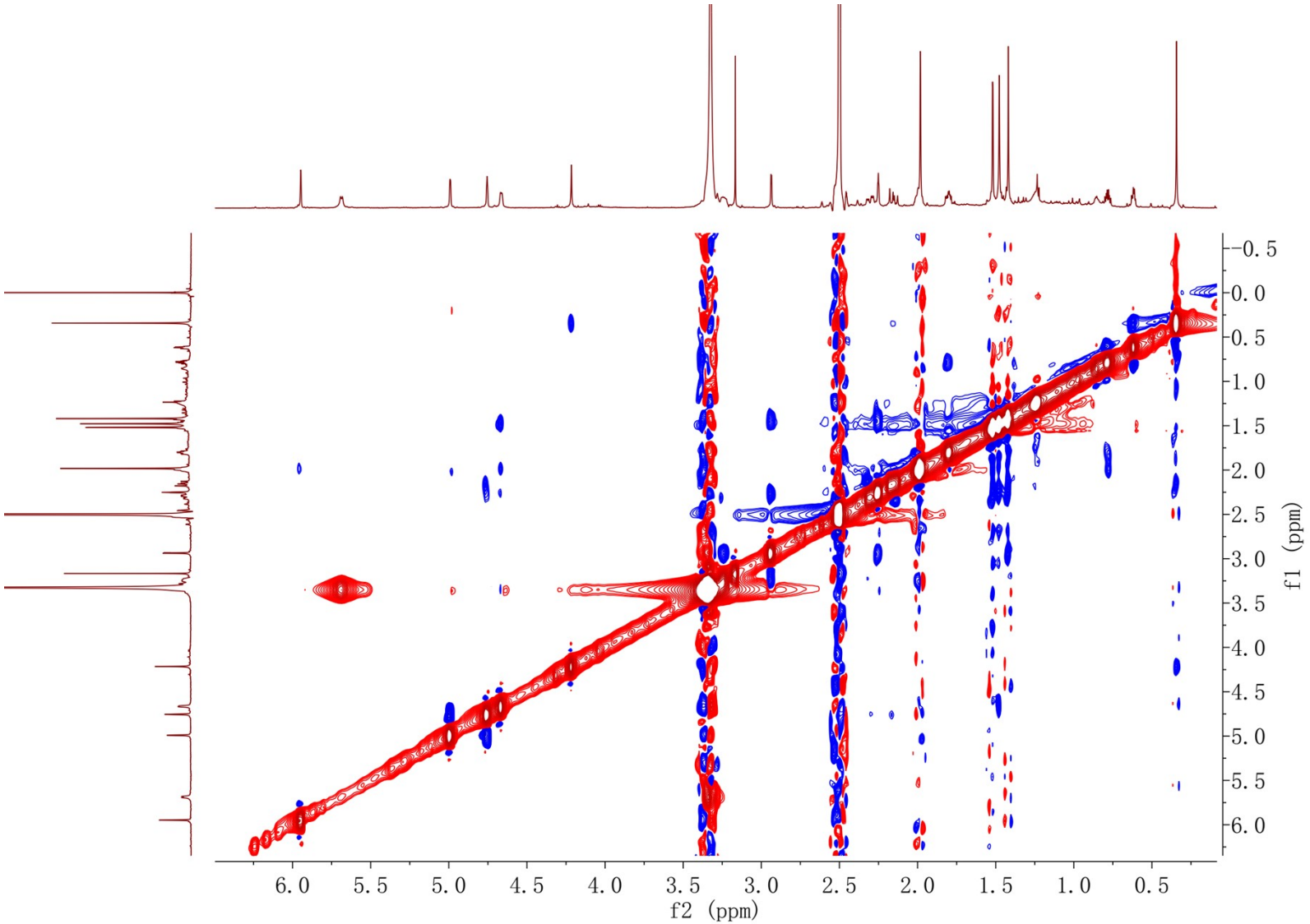
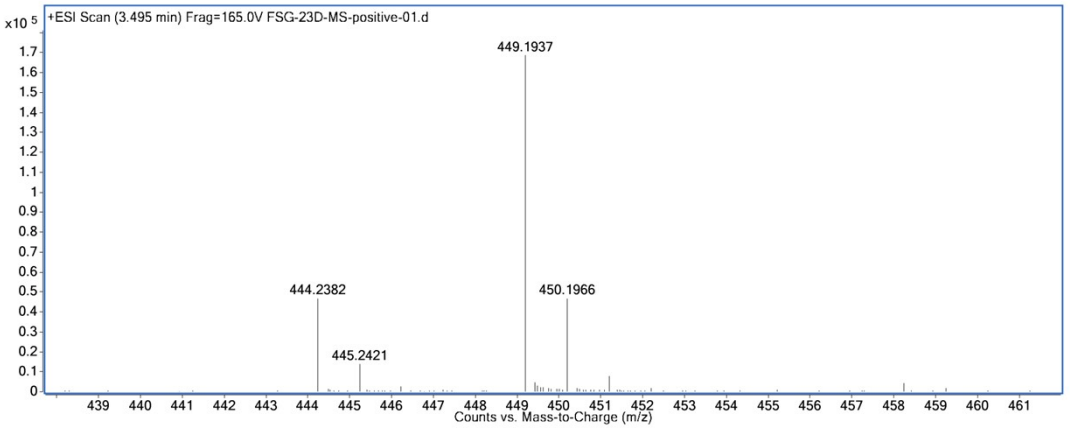


Figure S3.1.12 ROESY (600 MHz; DMSO-d_6) spectrum of **1**



Elemental Composition Calculator

Target m/z:	449.1937	**Result type:**	Positive ions	**Species:**	$[M+Na]^+$
Elements:		C (0-80); H (0-120); O (0-30); Na (0-5)			
Ion Formula		**Calculated m/z**		**PPM Error**	
C25H30NaO6		449.1935		-0.63	

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Figure S3.1.13 HRESIMS spectrum of **1**

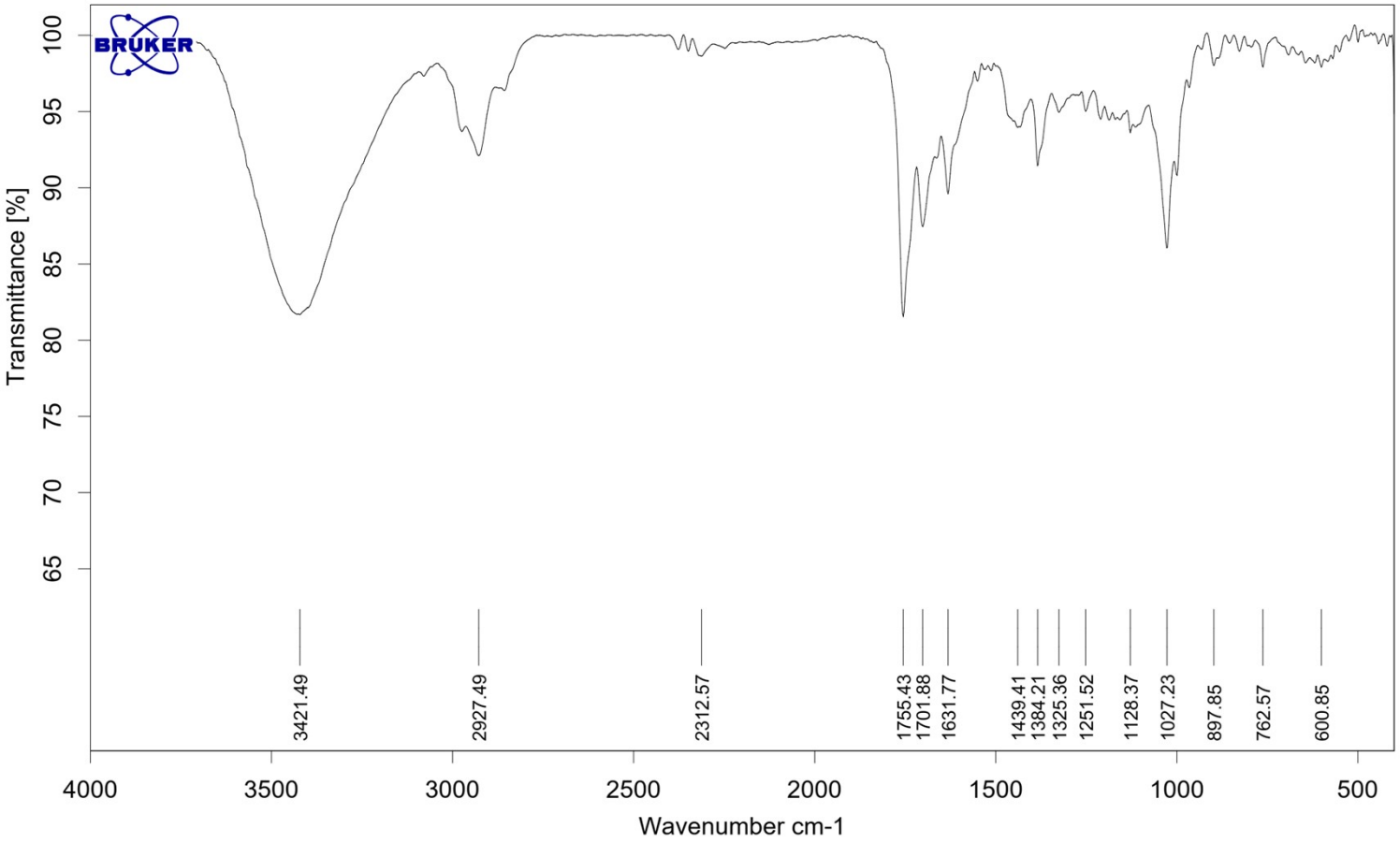


Figure S3.1.14 IR spectrum of **1**

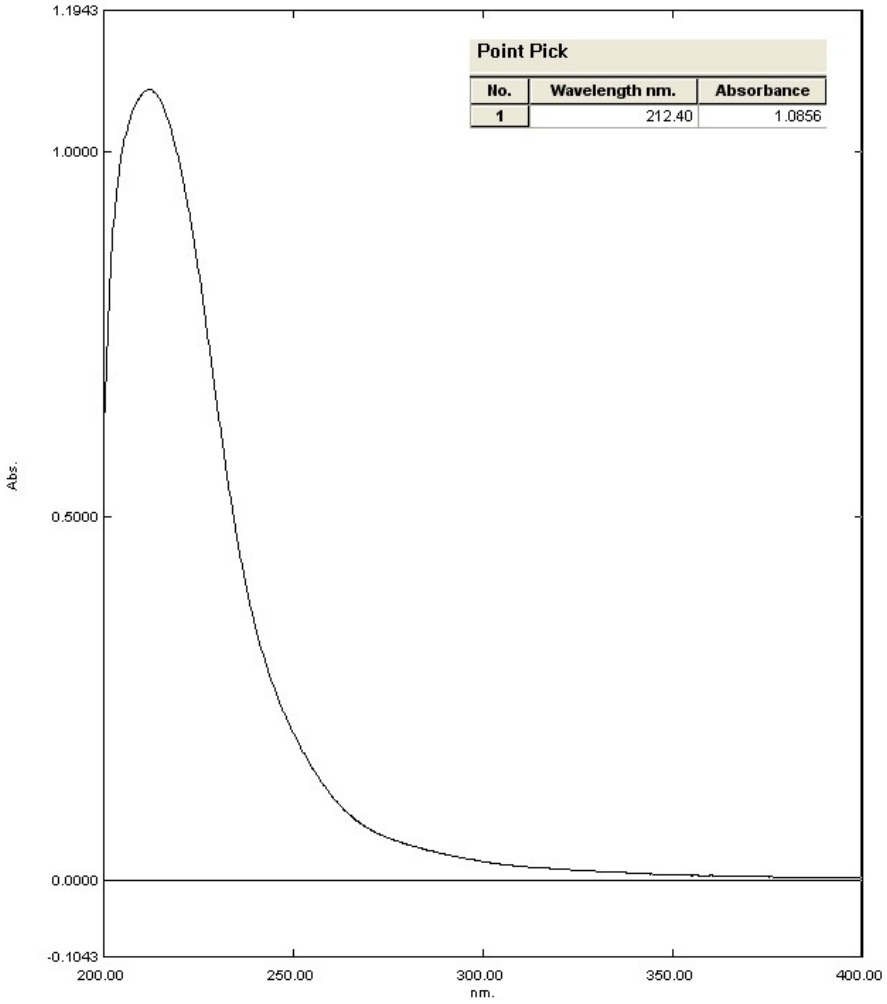


Figure S3.1.15 UV spectrum of **1**

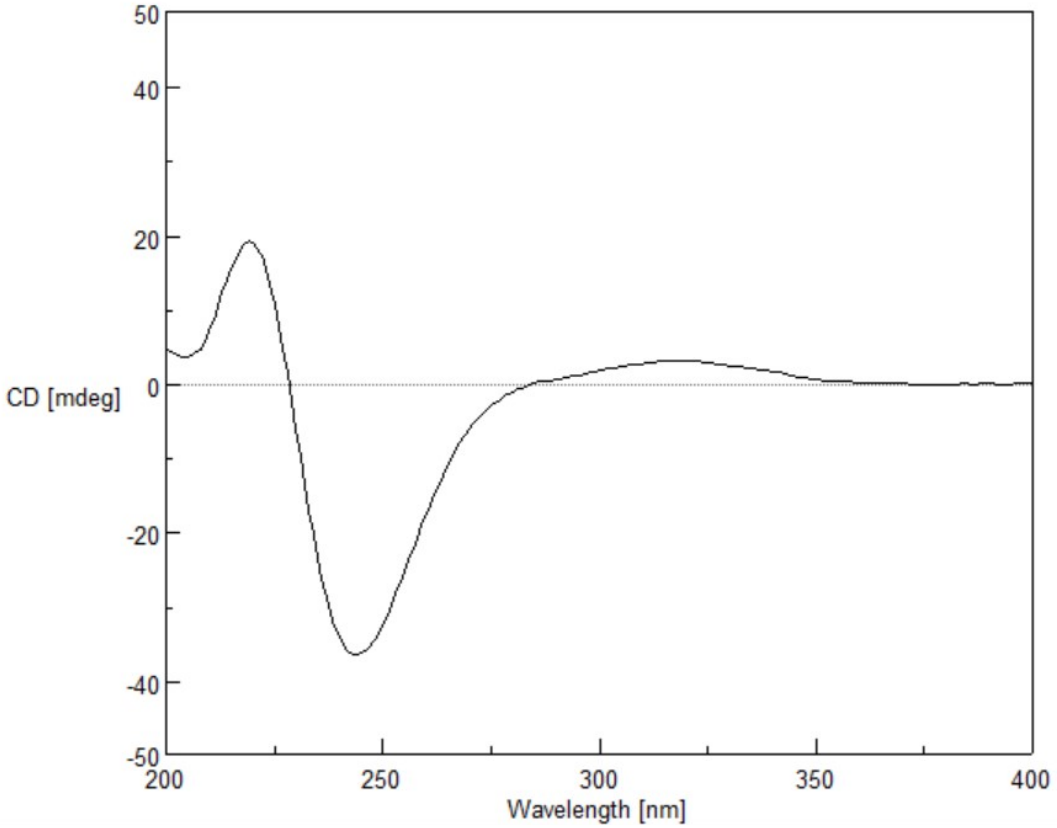


Figure S3.1.16 CD spectrum of **1**

3.2 NMR ($CDCl_3$), MS, IR, UV and CD spectra of compound 2

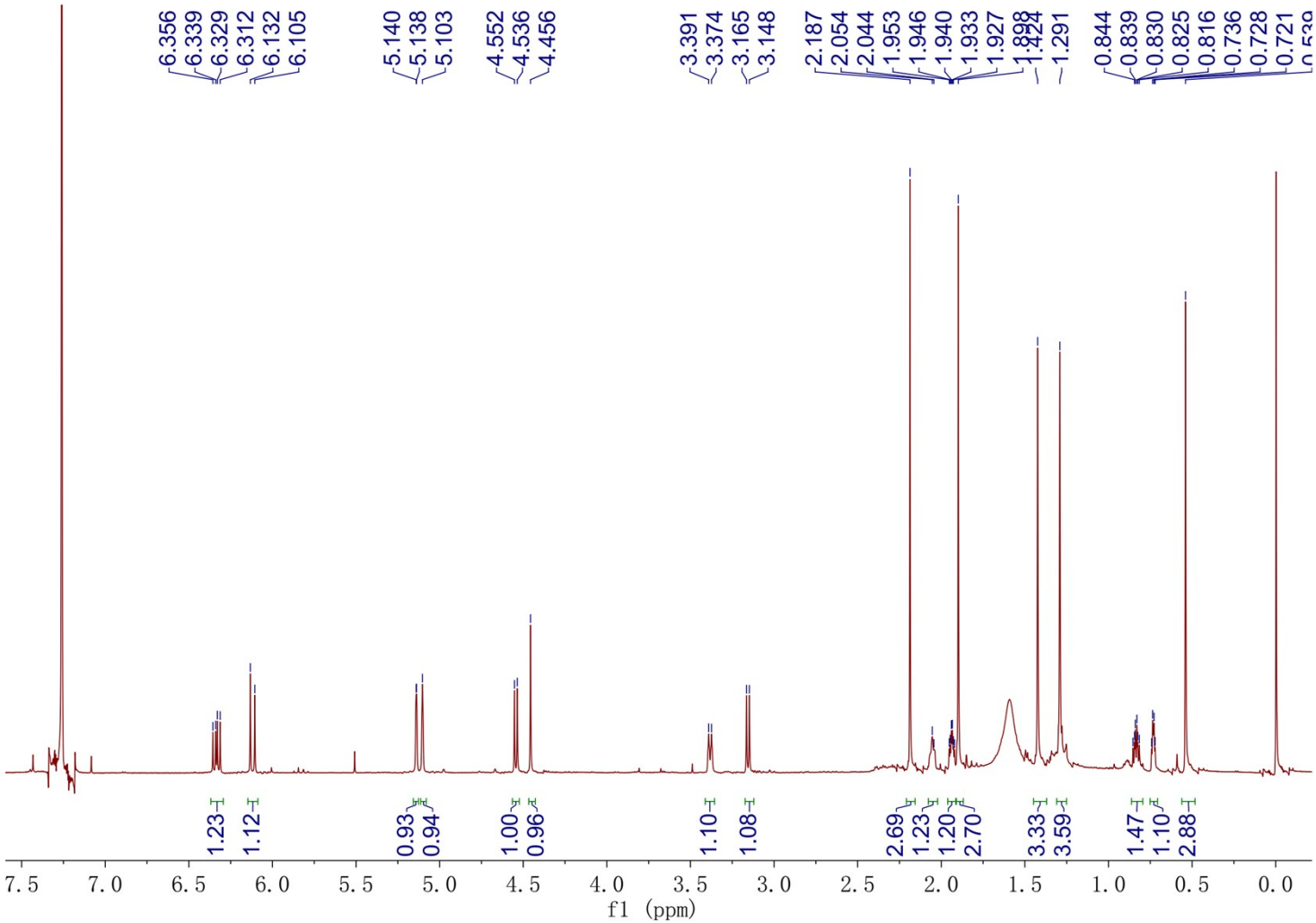


Figure S3.2.1 ^{1}H NMR (500 MHz; $CDCl_3$) spectrum of **2**

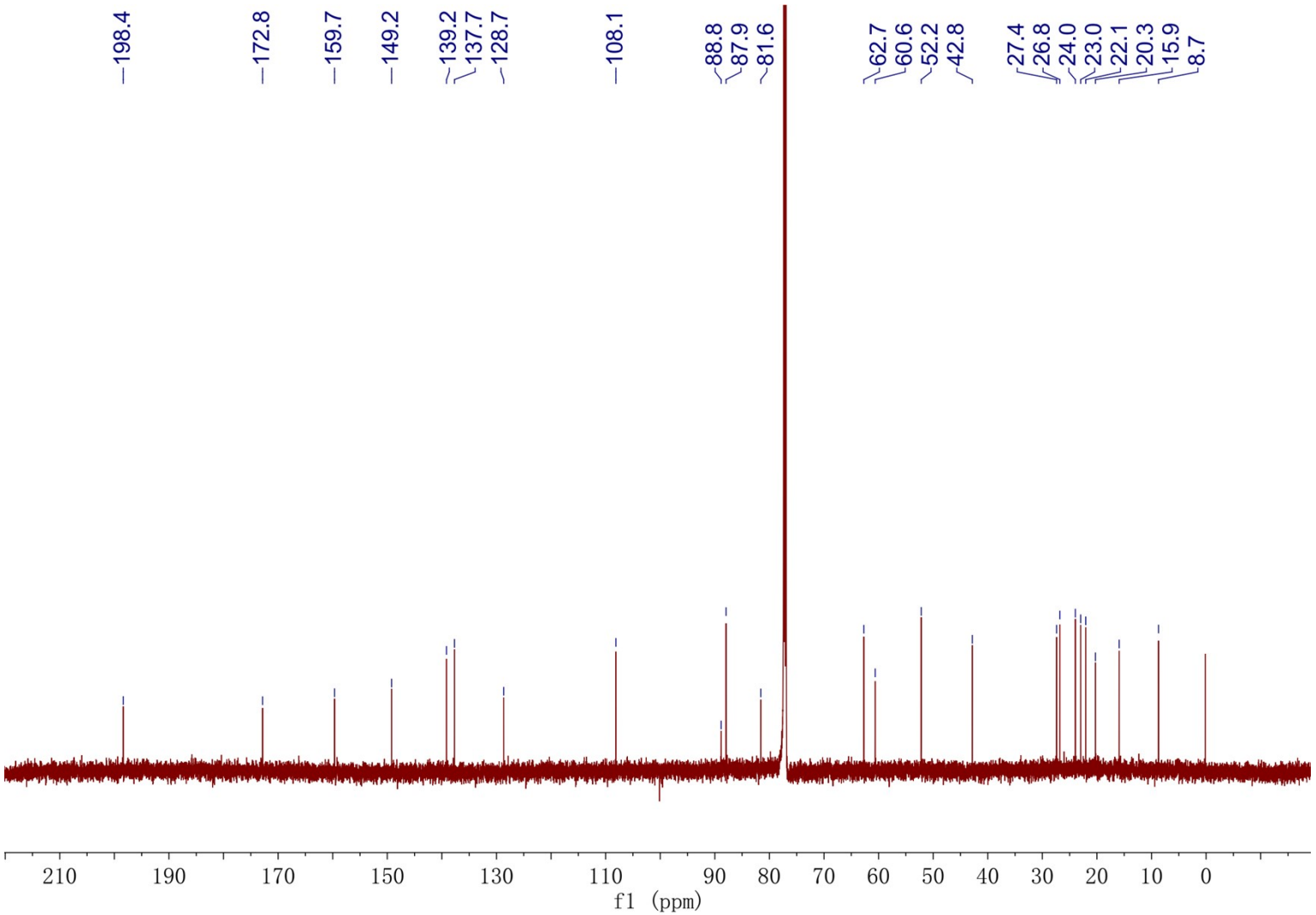


Figure S3.2.2 ^{13}C NMR (125 MHz; $CDCl_3$) spectrum of **2**

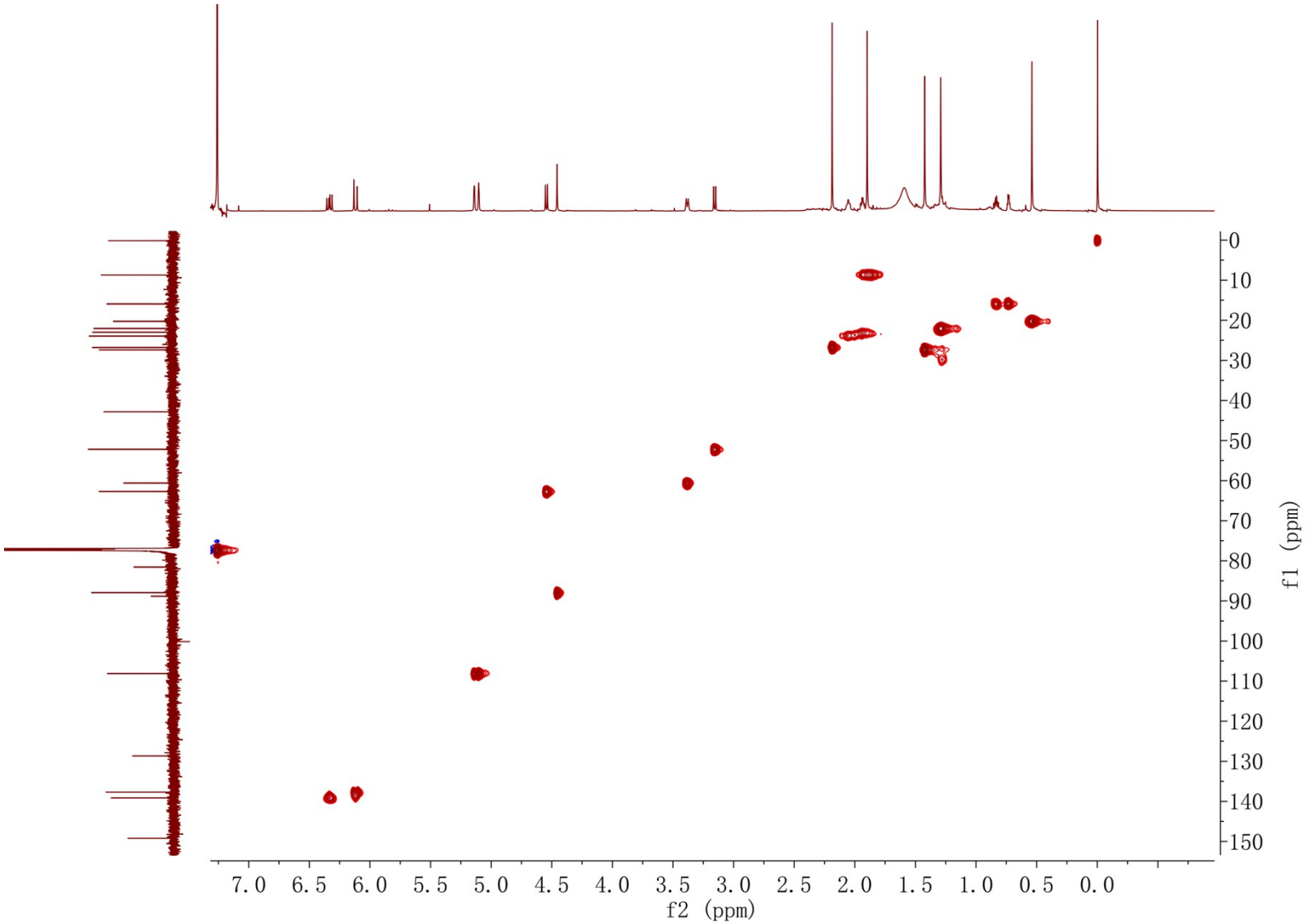


Figure S3.2.3 HSQC (^{1}H: 600 MHz, ^{13}C: 150 MHz; $CDCl_3$) spectrum of **2**

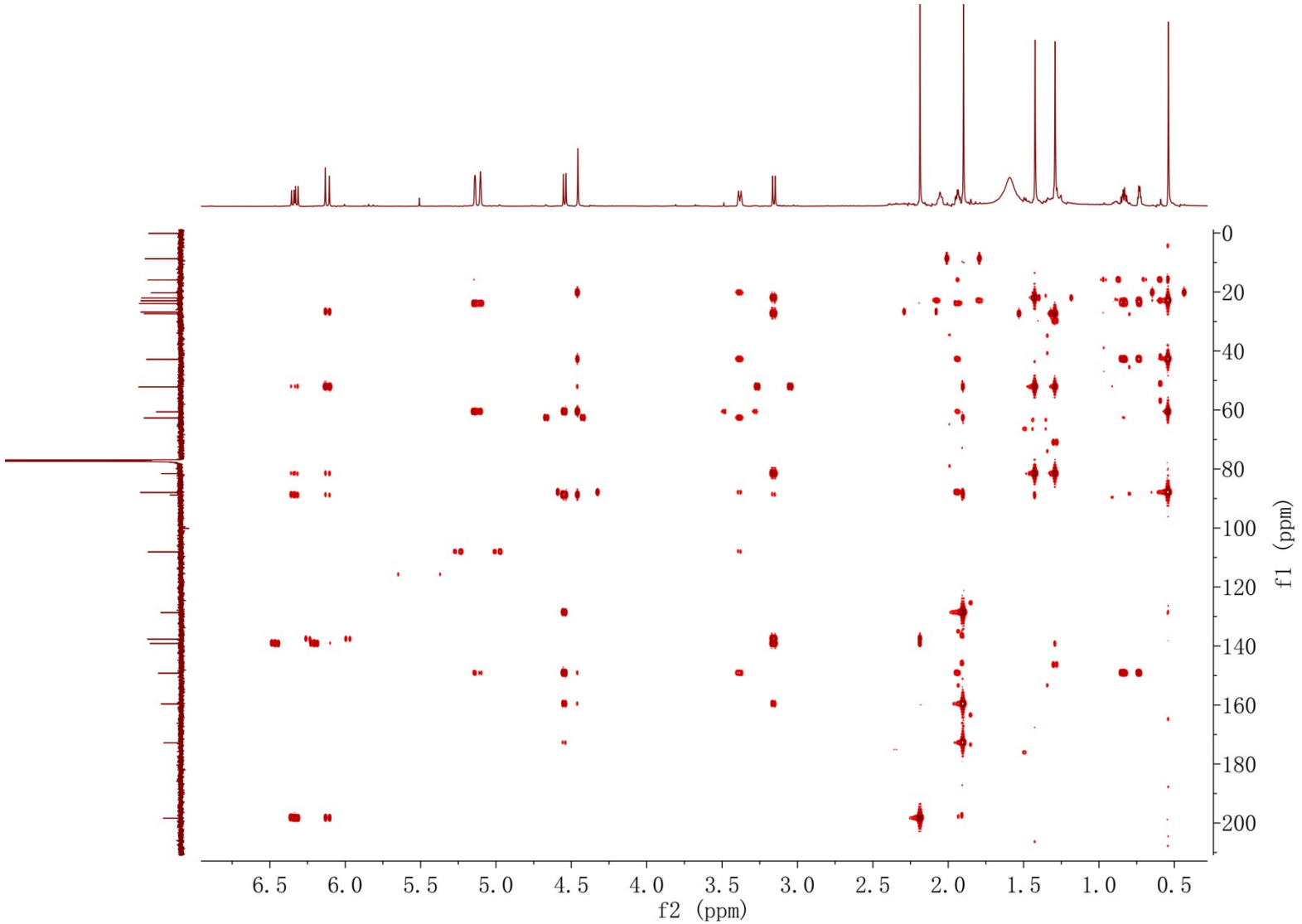


Figure S3.2.4 HMBC (^{1}H: 600 MHz, ^{13}C: 150 MHz; $CDCl_3$) spectrum of **2**

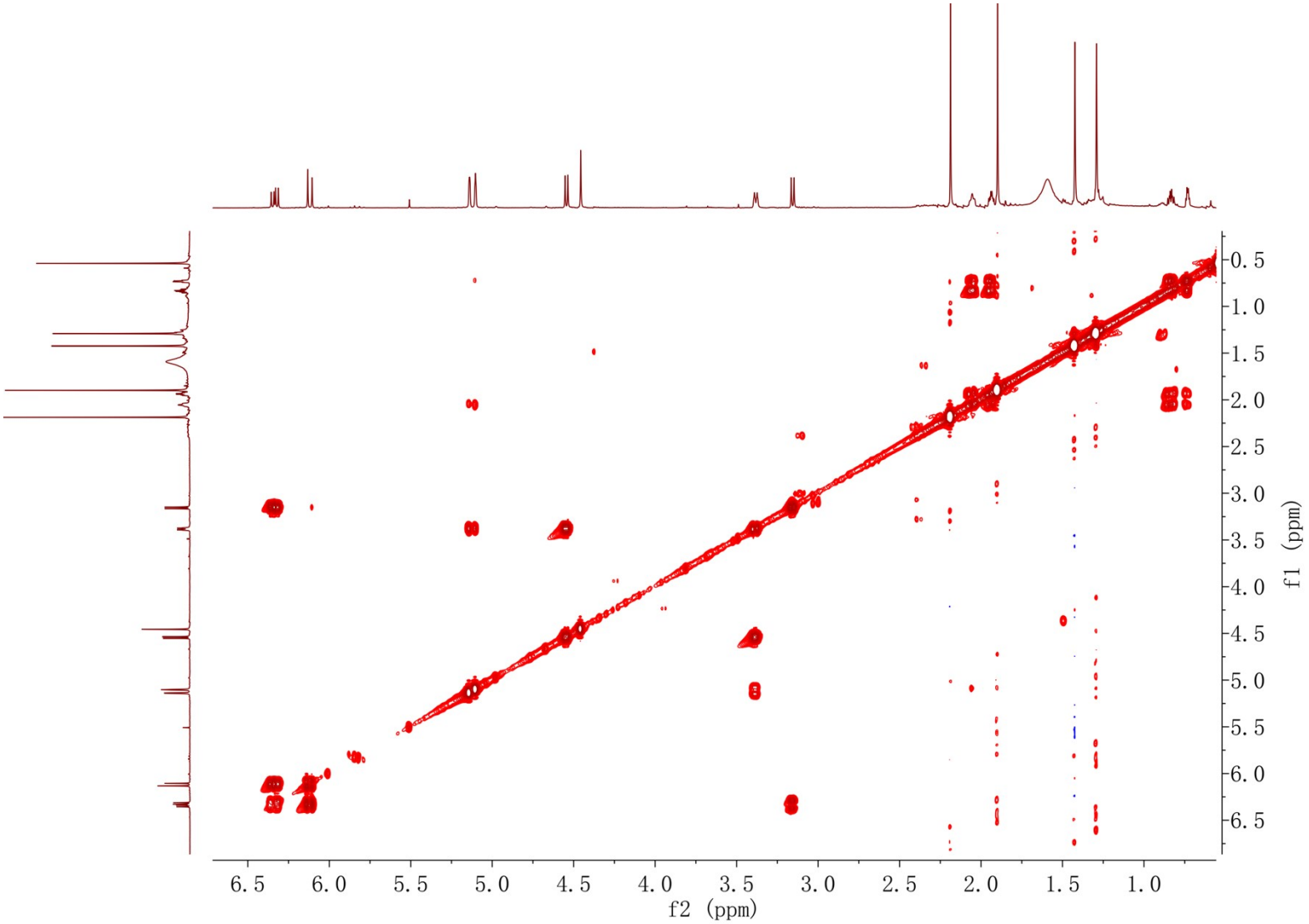


Figure S3.2.5 ^{1}H-^{1}H COSY (600 MHz; $CDCl_3$) spectrum of **2**

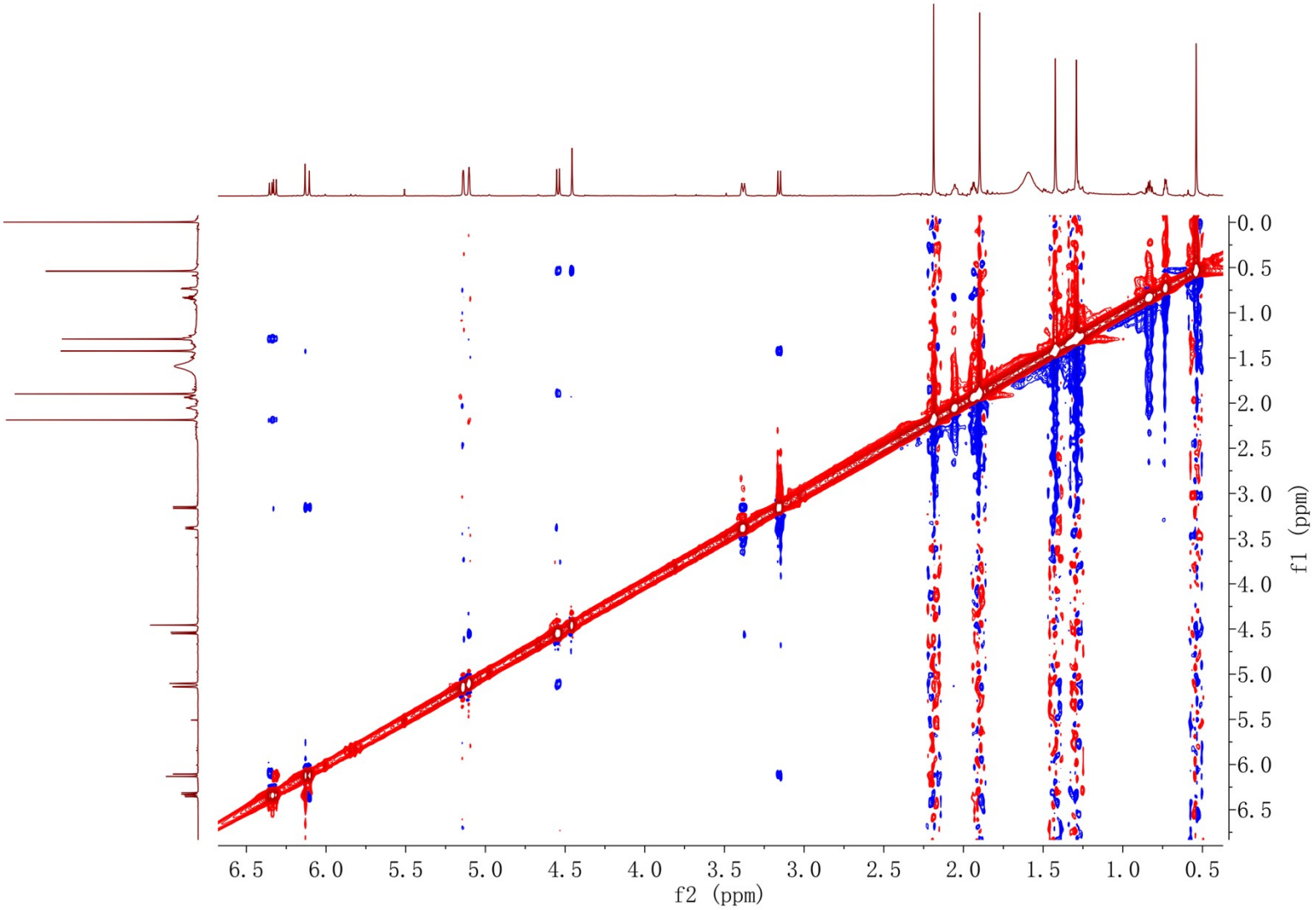
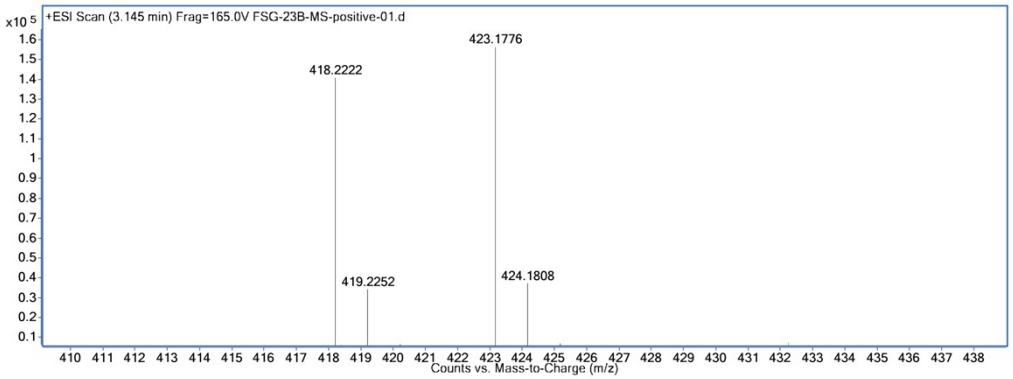


Figure S3.2.6 ROESY (600 MHz; $CDCl_3$) spectrum of **2**



Elemental Composition Calculator

Target m/z:	423.1776	**Result type:**	Positive ions	**Species:**	$[M+Na]^+$
Elements:		C (0-80); H (0-120); O (0-30); Na (0-5)			
Ion Formula		**Calculated m/z**		**PPM Error**	
C23H28NaO6		423.1778		0.53	

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Figure S3.2.7 HRESIMS spectrum of **2**

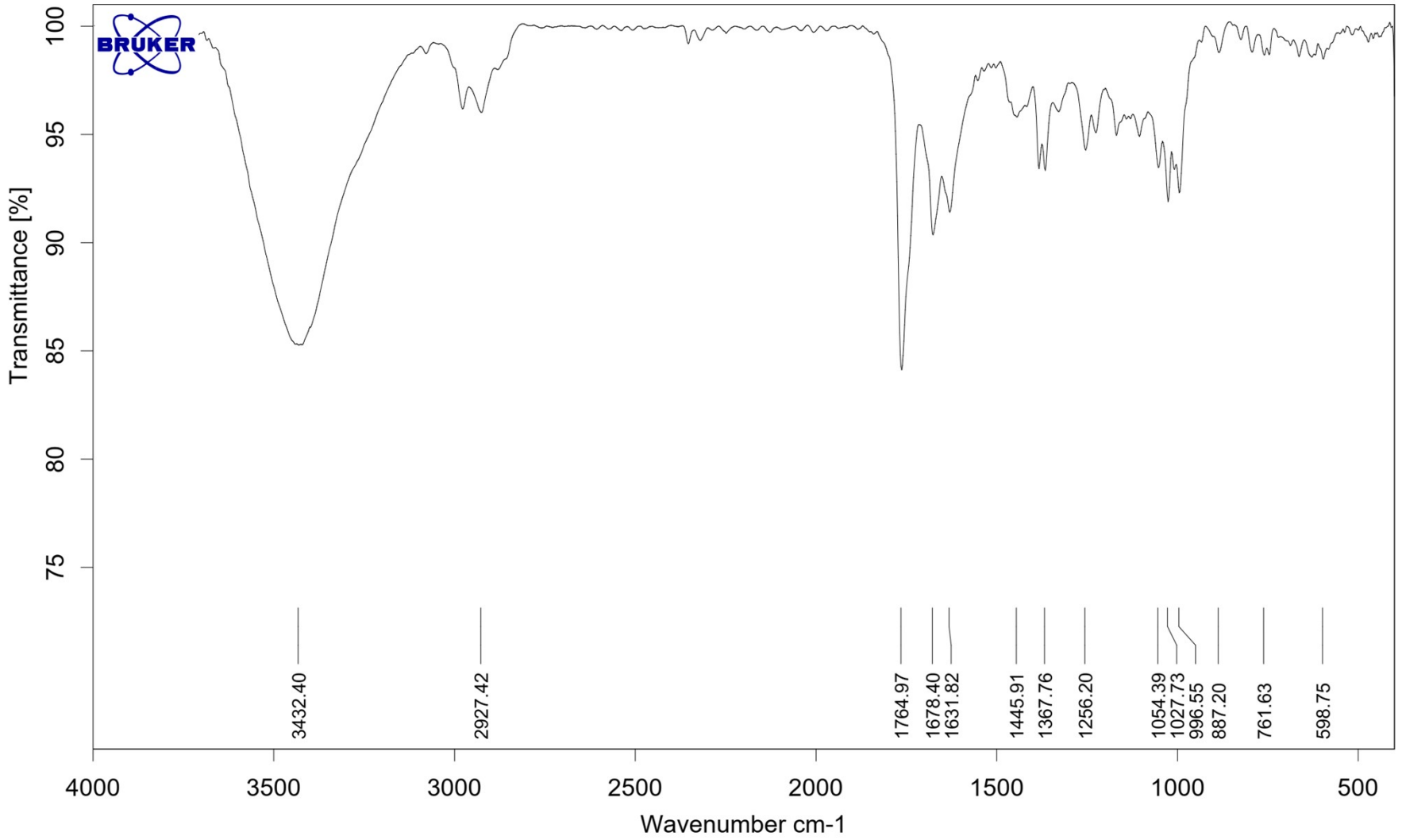


Figure S3.2.8 IR spectrum of **2**

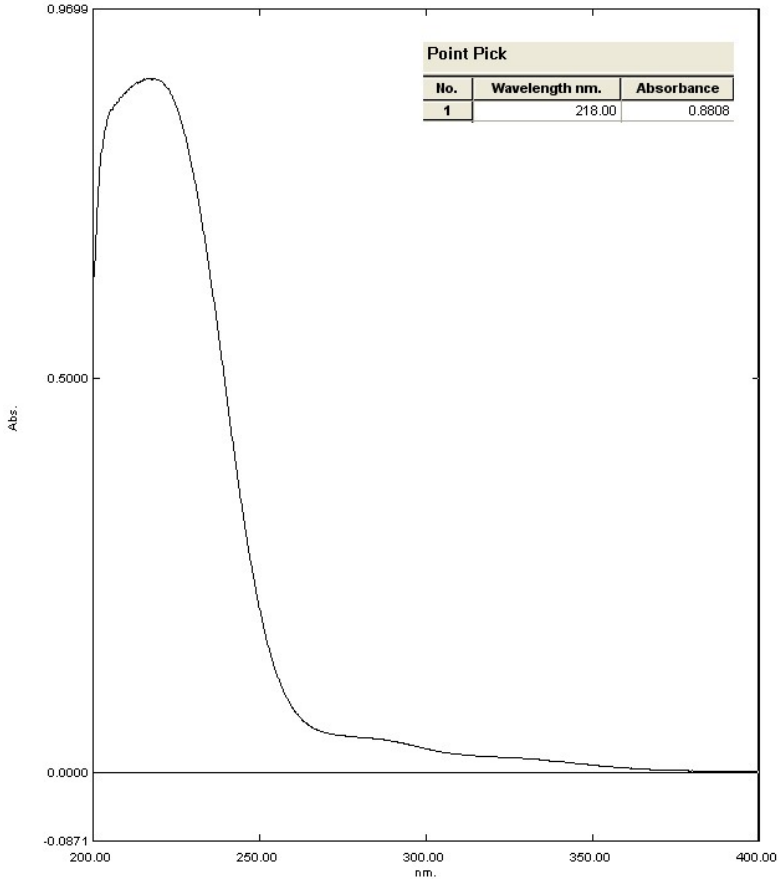


Figure S3.2.9 UV spectrum of **2**

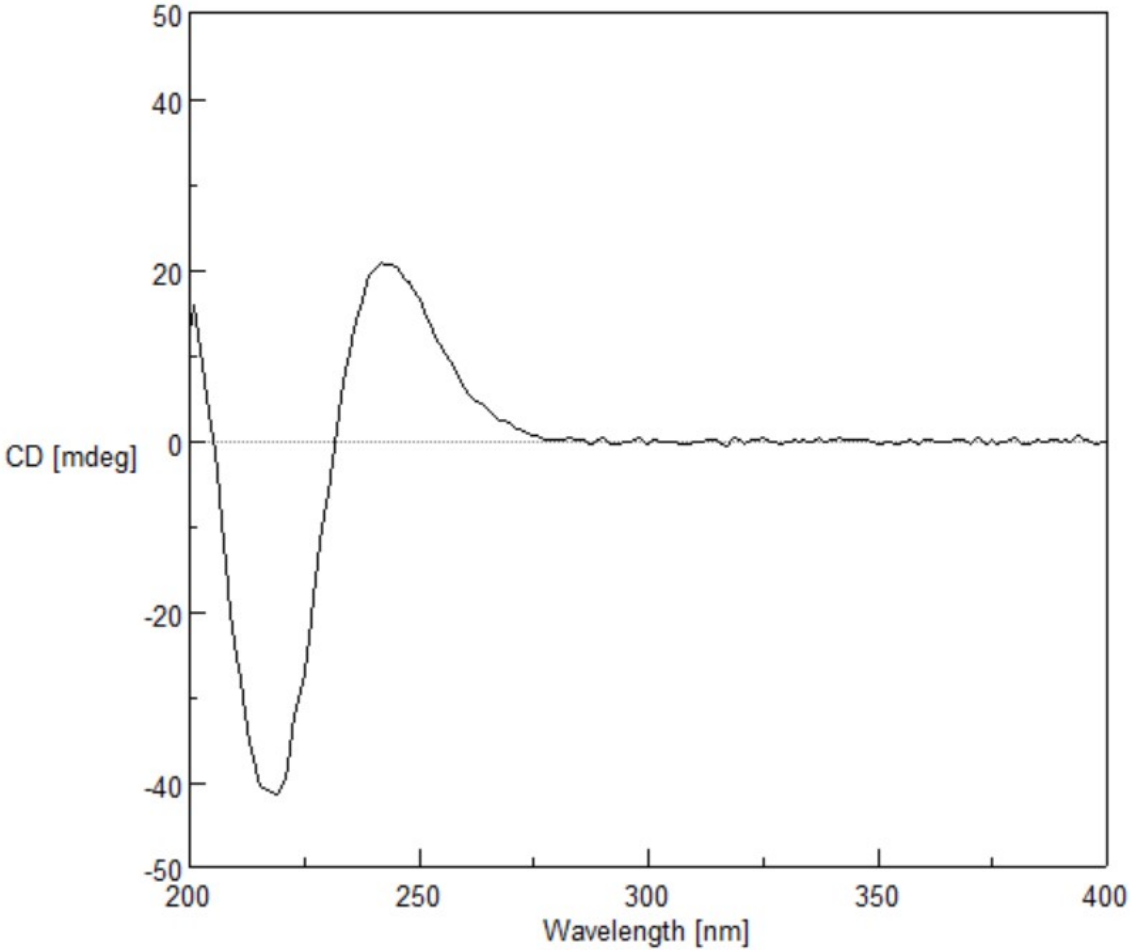


Figure S3.2.10 CD spectrum of **2**

3.3 NMR ($CDCl_3$), MS, IR, UV and CD spectra of compound 3

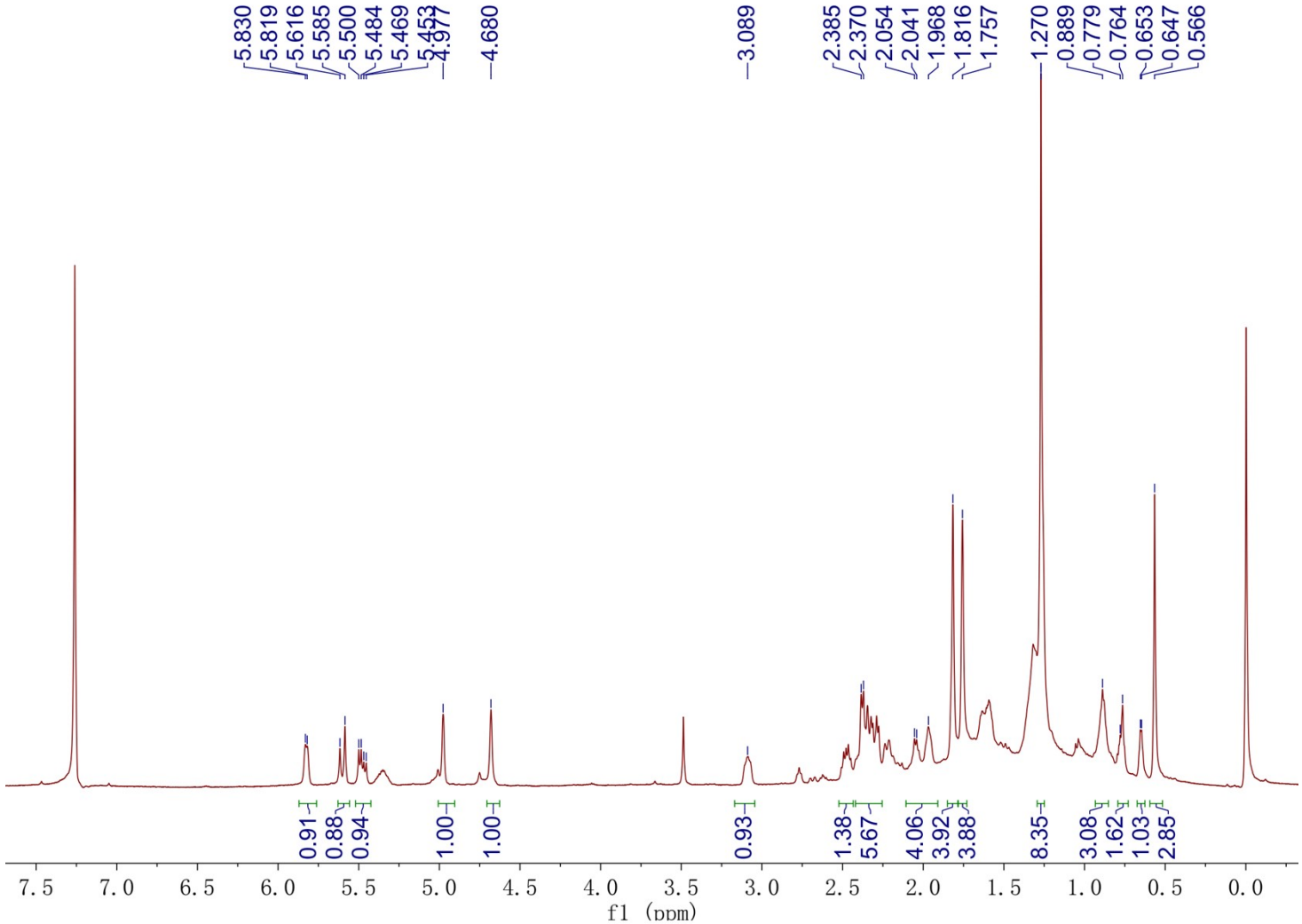


Figure S3.3.1 ^{1}H NMR (600 MHz; $CDCl_3$) spectrum of **3**

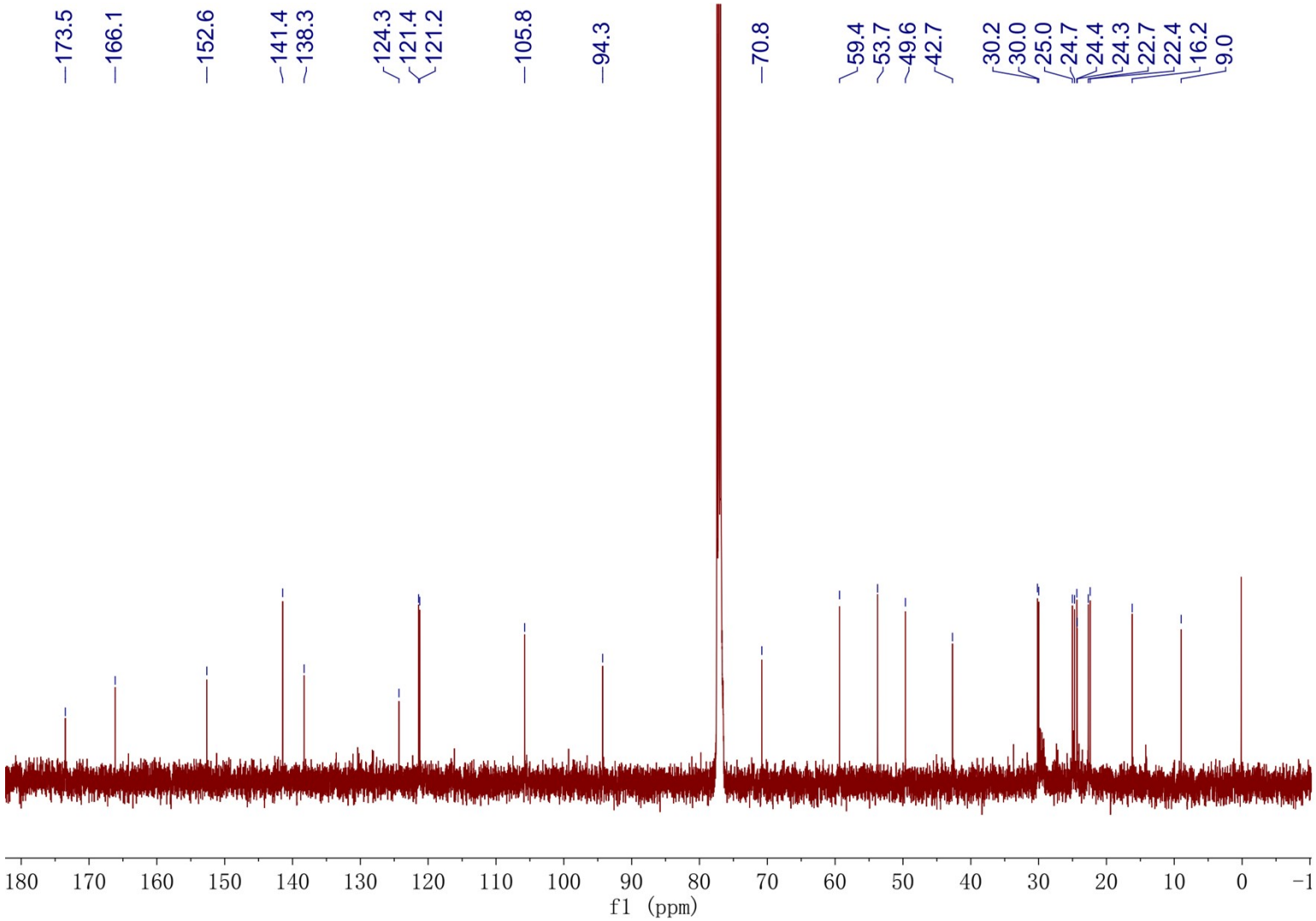


Figure S3.3.2 ^{13}C NMR (150 MHz; $CDCl_3$) spectrum of **3**

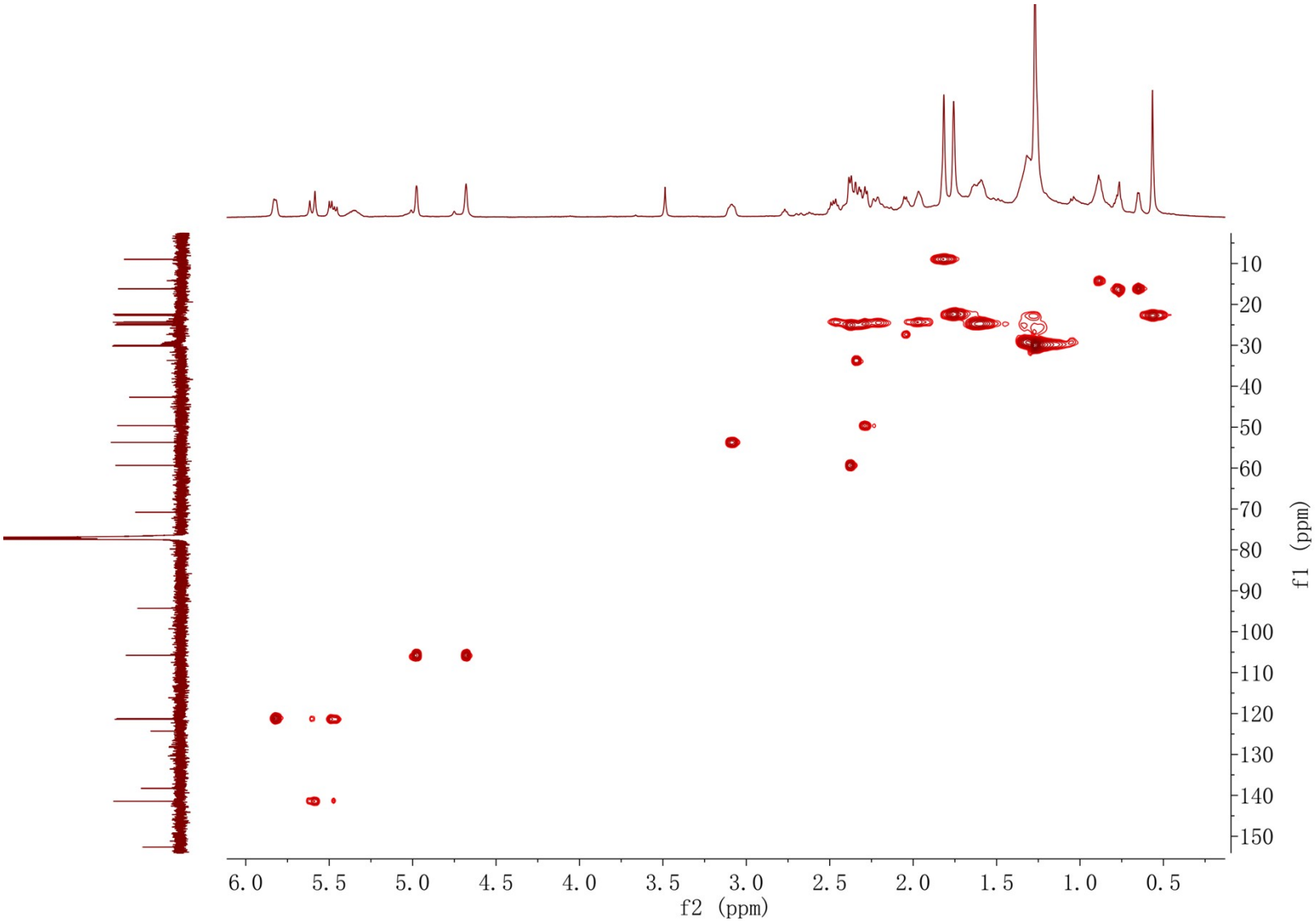


Figure S3.3.3 HSQC (^{1}H: 600 MHz, ^{13}C: 150 MHz; $CDCl_3$) spectrum of **3**

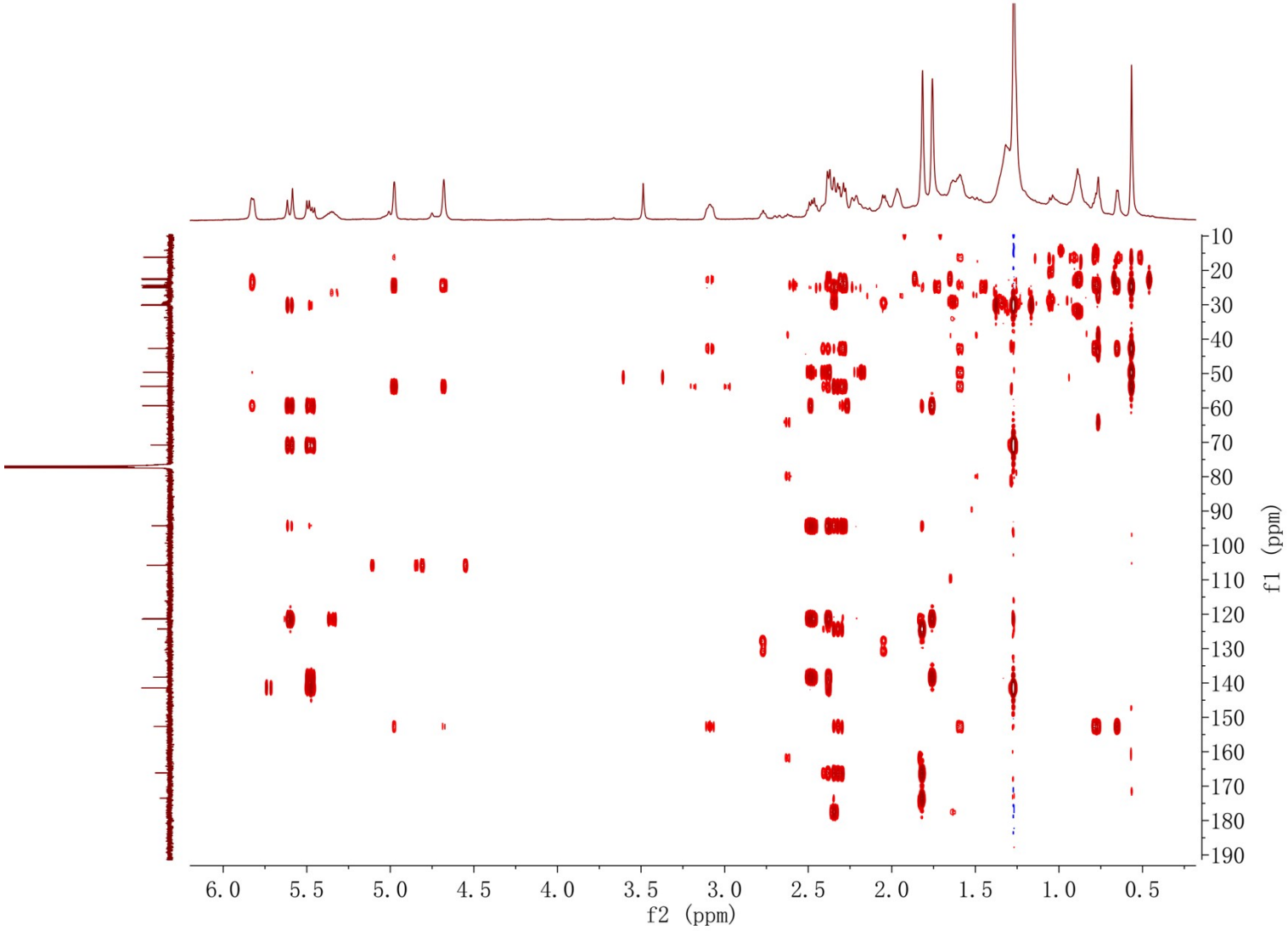


Figure S3.3.4 HMBC (^{1}H: 600 MHz, ^{13}C: 150 MHz; $CDCl_3$) spectrum of **3**

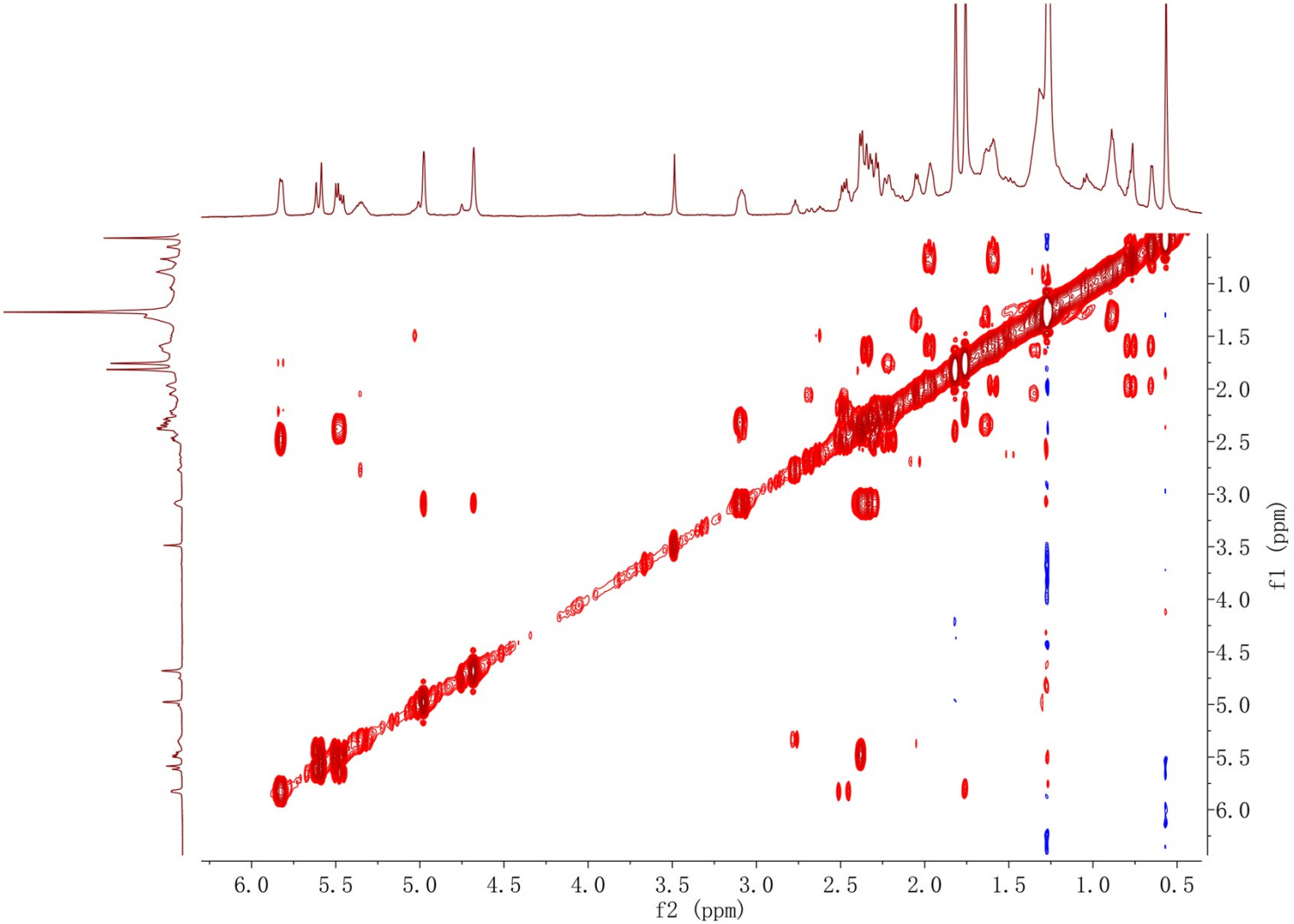


Figure S3.3.5 ^{1}H-^{1}H COSY (600 MHz; $CDCl_3$) spectrum of **3**

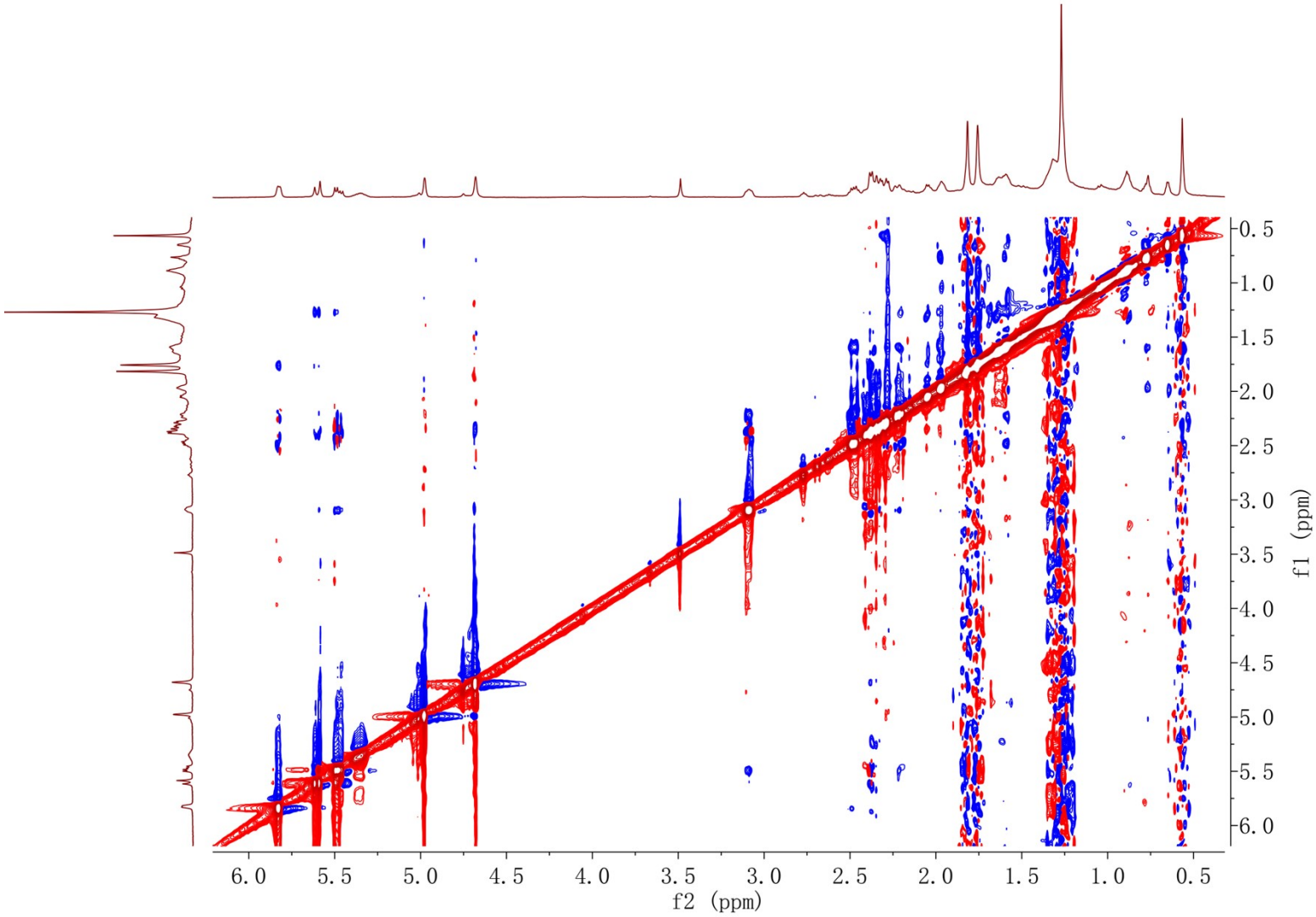
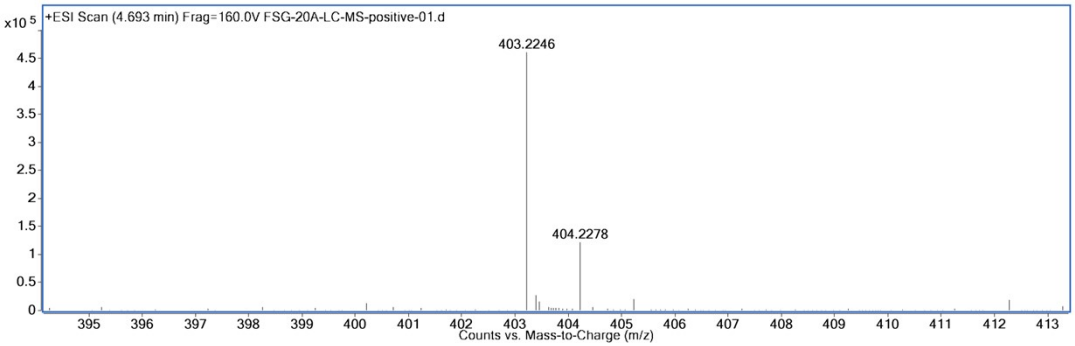


Figure S3.3.6 ROESY (600 MHz; $CDCl_3$) spectrum of **3**



Elemental Composition Calculator

Target m/z:	403.2246	**Result type:**	Positive ions	**Species:**	$[M+Na]^+$
Elements:		C (0-80); H (0-120); O (0-30); Na (0-5)			
Ion Formula		**Calculated m/z**		**PPM Error**	
C25H32NaO3		403.2244		-0.63	

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Figure S3.3.7 HRESIMS spectrum of **3**

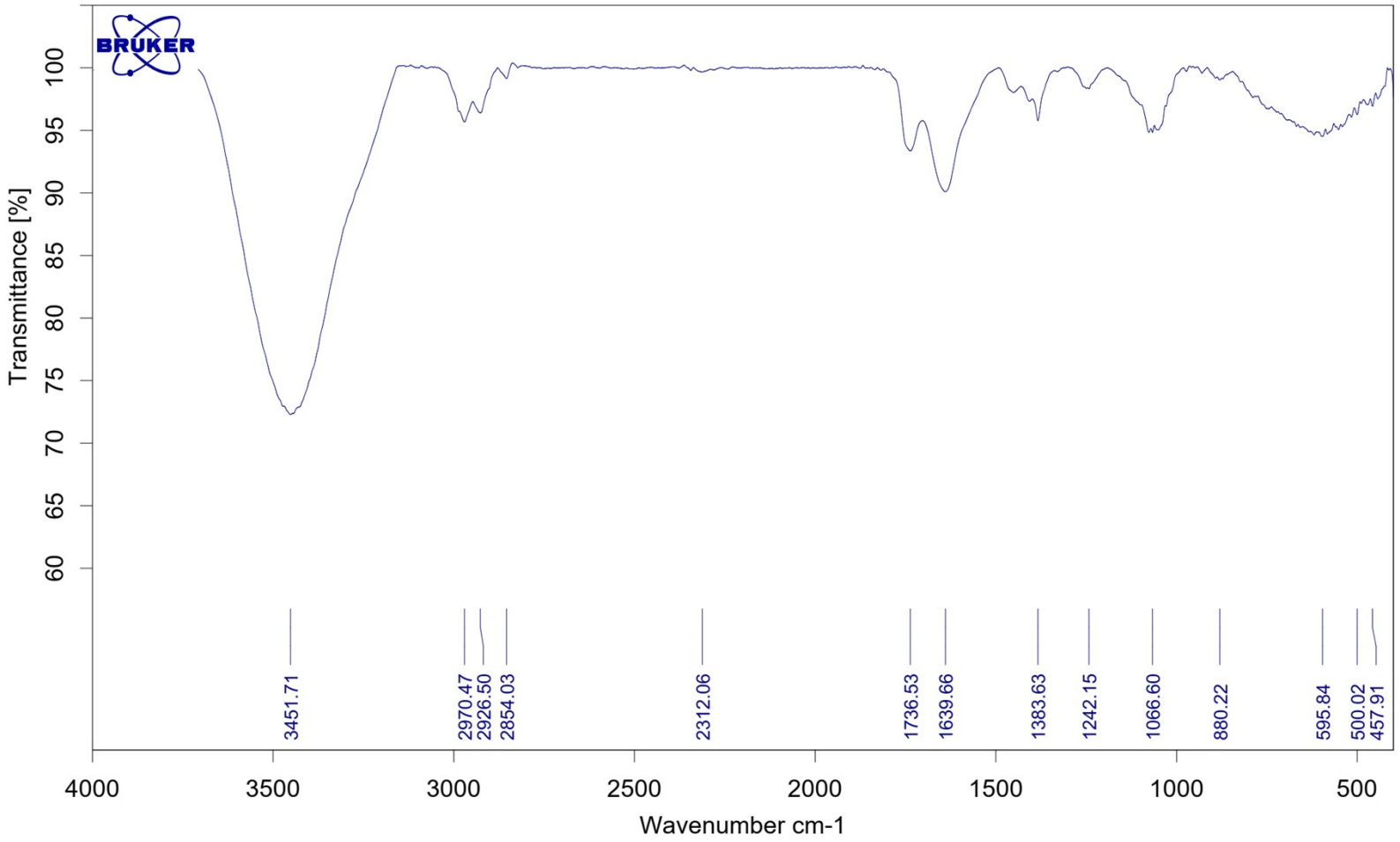

Figure S3.3.8 IR spectrum of **3**

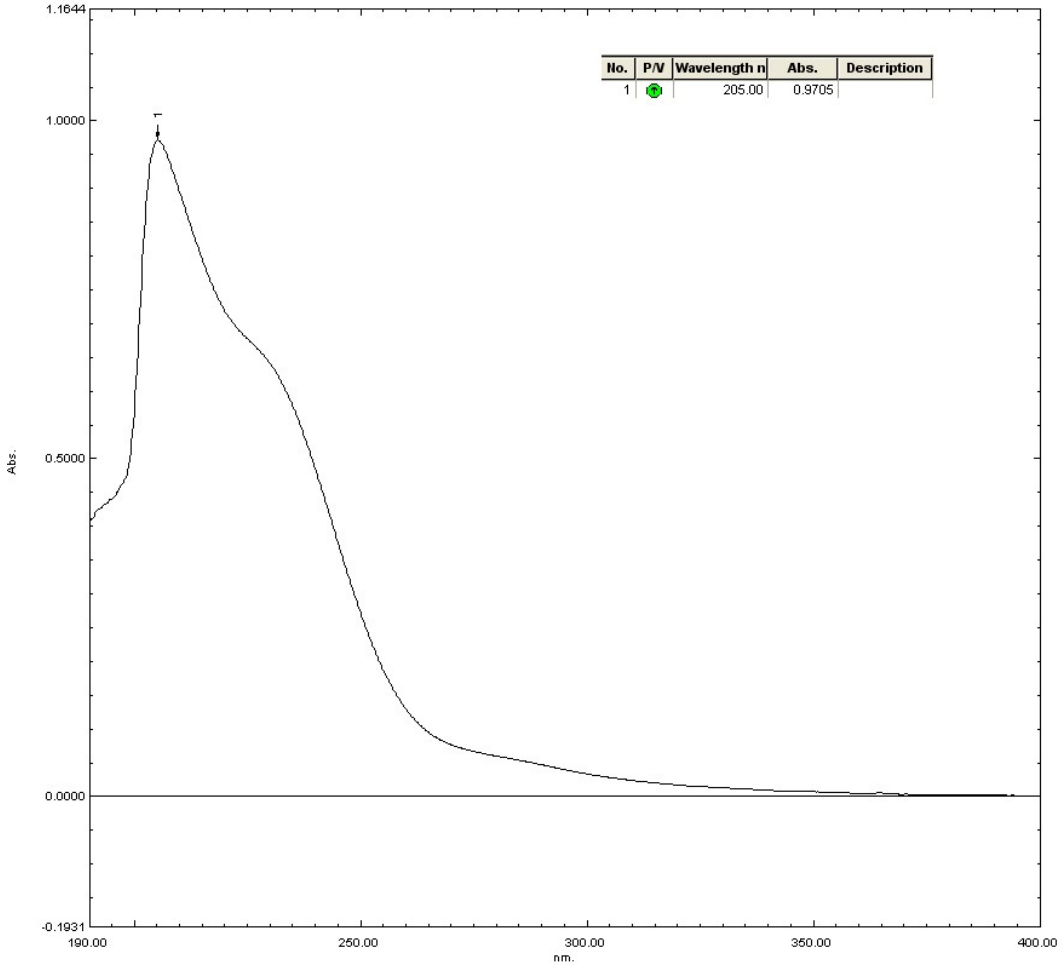

Figure S3.3.9 UV spectrum of **3**

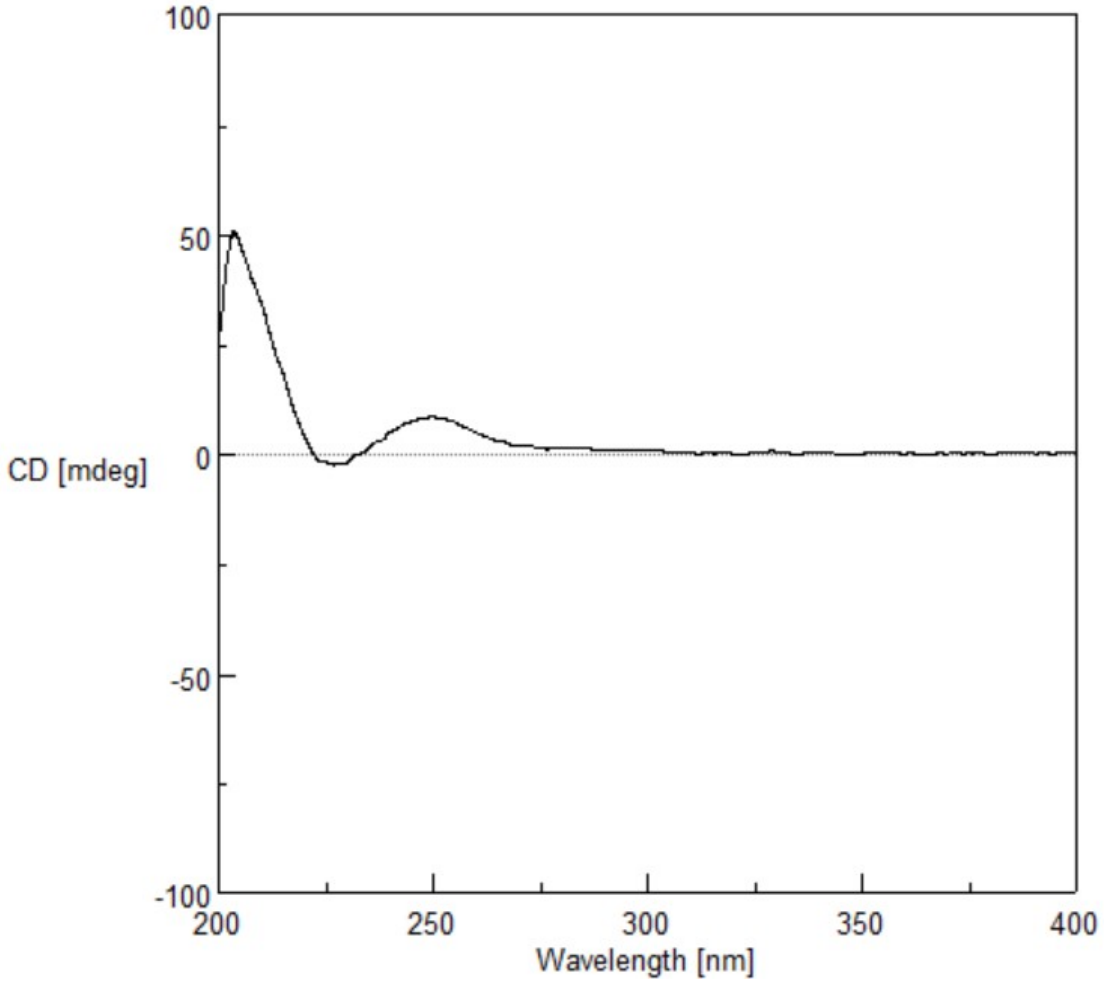

Figure S3.3.10 CD spectrum of **3**