

Supplementary materials for

**Four New Highly Oxygenated Eremophilane Sesquiterpenes
from an Endophytic Fungus *Boeremia exigua* Isolated from
*Fritillaria hupehensis***

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Quantum chemical calculation

The initial conformational analysis of the compound **1-4** were executed by employing Monte Carlo searching algorithm via the MMFF94 molecular mechanics force field, 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 M06-2X/def2-SVP level in vacuum, implemented in the Gaussian 09 software package. 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 M06-2X/def2-SVP 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-weighted population contribution by the SpecDisv1.71. Gauge Independent Atomic Orbital (GIAO) calculations of their ^1H and ^{13}C NMR chemical shifts using density functional theory (DFT) at the mPW1PW91/6-311+G(d,p) level with the PCM model in methanol. The calculated NMR data of these conformers were averaged according to the Boltzmann distribution theory and their relative Gibbs free energy. The ^1H and ^{13}C NMR chemical shifts for TMS were also calculated by the same procedures and used as the reference. After calculation, the experimental and calculated data were evaluated by the improved probability DP4+ method.

1 NMR computational details for compound 1

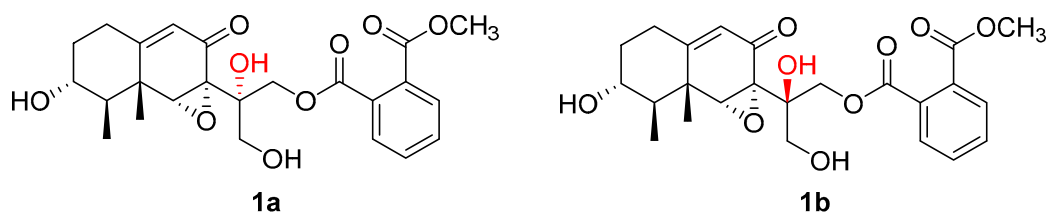


Table S1. DP4+ analysis results of **1a** (Isomer 1) and **1b** (Isomer 2).

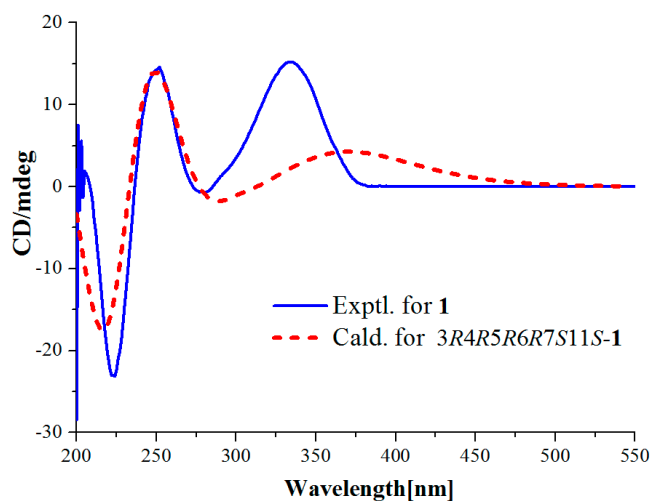
Functional mPW1PW91		Solvent? PCM	Basis Set 6-311+G(d,p)		Type of Data Unscaled Shifts		
		DP4+	100.00%	0.00%	–	–	–
Nuclei	sp2?	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5
C	x	121.8	122.3	121.4			
C		73.9	72.5	73.3			
C		69.2	69.0	67.3			
C		65.6	62.9	64.6			
C		11.6	12.9	11.8			
C		18.3	19.0	19.4			
C		36.2	38.1	37.9			
C	x	169.5	166.7	166.3			
C	x	134.3	134.5	132.7			
C	x	129.7	131.0	131.1			
C	x	132.9	132.6	131.7			
C	x	132.8	131.6	132.5			
C	x	130.3	130.4	129.7			
C	x	132.3	132.4	134.5			
C	x	168.9	168.7	169.8			
C		71.1	70.4	70.5			
C		53.5	53.8	53.2			
C		45.9	45.8	47.3			
C		42.2	43.5	43.9			
C	x	166.5	171.4	171.8			
C		31.6	32.8	33.2			
C		63.9	61.3	61.3			
C		62.9	61.4	60.6			
C	x	195.5	195.2	194.7			
H		2.03	1.88	2.36			
H		1.27	1.19	1.48			
H		3.44	3.52	3.77			
H		1.63	1.65	1.92			
H		2.41	2.11	2.53			
H		2.24	2.61	2.86			
H		3.8	3.74	4.63			
H	x	5.61	5.57	6.17			
H		4.64	4.37	5.21			
H		4.59	4.78	4.37			
H		4.19	3.63	5.18			
H		3.76	3.45	3.80			
H		1.16	1.34	1.91			
H		0.64	1.23	1.14			
H	x	7.6	7.74	8.51			
H	x	7.61	7.64	8.33			
H	x	7.62	7.62	8.42			
H	x	7.77	7.93	8.38			
H		3.85	3.84	4.66			

Functional mPW1PW91		Solvent? PCM	Basis Set 6-311+G(d,p)		Type of Data Unscaled Shifts		
		Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6
sDP4+ (H data)		94.72%	5.28%	–	–	–	–
sDP4+ (C data)		99.27%	0.73%	–	–	–	–
sDP4+ (all data)		99.96%	0.04%	–	–	–	–
uDP4+ (H data)		100.00%	0.00%	–	–	–	–
uDP4+ (C data)		68.40%	31.60%	–	–	–	–
uDP4+ (all data)		100.00%	0.00%	–	–	–	–
DP4+ (H data)		100.00%	0.00%	–	–	–	–
DP4+ (C data)		99.66%	0.34%	–	–	–	–
DP4+ (all data)		100.00%	0.00%	–	–	–	–

Table S2. Experimental and calculated ^{13}C NMR chemical shifts of **1a** and **1b**.

Num.	Exp.	1a	1b	Num.	Exp.	1a	1b
1	121.8	122.3	121.4	15	168.9	168.7	169.8
2	73.9	72.5	73.3	16	71.1	70.4	70.5
3	69.2	69.0	67.3	17	53.5	53.8	53.2
4	65.6	62.9	64.6	18	45.9	45.8	47.3
5	11.6	12.9	11.8	19	42.2	43.5	43.9
6	18.3	19.0	19.4	20	166.5	171.4	171.8
7	36.2	38.1	37.9	21	31.6	32.8	33.2
8	169.5	166.7	166.3	22	63.9	61.3	61.3
9	134.3	134.5	132.7	23	62.9	61.4	60.6
10	129.7	131.0	131.1	24	195.5	195.2	194.7
11	132.9	132.6	131.7	R ²		0.9991	0.9988
12	132.8	131.6	132.5	MAE		2.6428	3.3397
13	130.3	130.4	129.7	RMSD		1.6257	1.8275
14	132.3	132.4	134.5				

2 ECD computational details of compound **1**

Figure S1. Experimental ECD spectra and calculated ECD spectra of **1**.Table S3. Important thermodynamic parameters of the M06-2X/def2-SVP optimized conformers of **1a** in the gas phase

Conformers	E ^a (Hartree)	C ^b (Hartree)	G ^c (kcal/mol)
1a_1	-1606.598579	0.442916	-1007867.497250
1a_2	-1606.598449	0.442945	-1007867.397478
1a_3	-1606.59598	0.442534	-1007866.106076
1a_4	-1606.59598	0.442543	-1007866.100366
1a_5	-1606.595358	0.442541	-1007865.711126

^aElectronic energy; ^bThermal correction to Gibbs free energy ; ^cGibbs free energy (E + C).

Table S4. Conformational analysis of the M06-2X/def2-SVP optimized conformers of **1a** in the gas phase (T=298.15 K)

Conformers	ΔG (kcal/mol) ^a	Population ^b
1a_1	0.000000	47.99%
1a_2	0.099773	40.55%
1a_3	1.391802	4.57%
1a_4	1.397449	4.53%
1a_5	1.786501	2.35%

^aThe relative Gibbs free energy; ^bThe Boltzmann distribution of each conformer.

3 ECD computational details of compound **2**

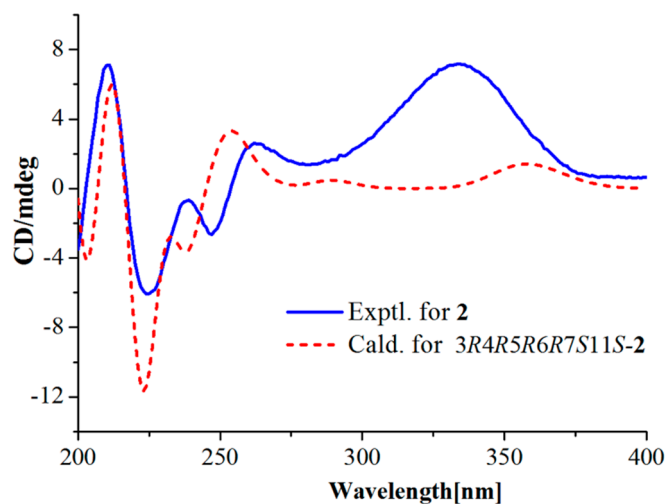


Figure S2. Experimental ECD spectra and calculated ECD spectra of **2**.

Table S5. Important thermodynamic parameters of the M06-2X/def2-SVP optimized conformers of **2** in the gas phase

Conformers	E ^a (Hartree)	C ^b (Hartree)	G ^c (kcal/mol)
2_1	-1454.115283	0.404613	-912207.806683
2_2	-1454.115638	0.405111	-912207.716573
2_3	-1454.115283	0.404840	-912207.663800
2_4	-1454.114912	0.404576	-912207.596720
2_5	-1454.114626	0.404514	-912207.456536
2_6	-1454.114230	0.404397	-912207.281149
2_7	-1454.114175	0.404669	-912207.076395

^aElectronic energy; ^bThermal correction to Gibbs free energy ; ^cGibbs free energy (E + C).

Table S6. Conformational analysis of the M06-2X/def2-SVP optimized conformers of **2** in the gas phase (T=298.15 K)

Conformers	ΔG (kcal/mol) ^a	Population ^b
2_1	0.000000	21.73%
2_2	0.090110	18.66%
2_3	0.142883	17.07%
2_4	0.209963	15.24%
2_5	0.350147	12.03%
2_6	0.525534	8.94%
2_7	0.730288	6.33%

^aThe relative Gibbs free energy; ^bThe Boltzmann distribution of each conformer.

4 ECD computational details of compound **3**

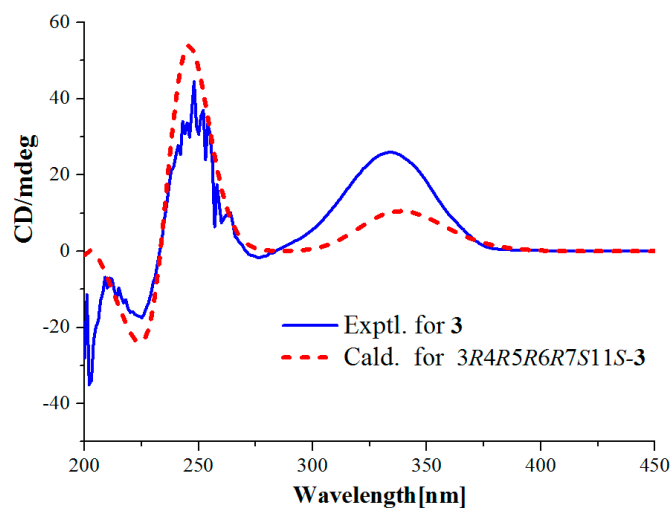


Figure S3. Experimental ECD spectra and calculated ECD spectra of **3**.

Table S7. Important thermodynamic parameters of the M06-2X/def2-SVP optimized conformers of **3** in the gas phase

Conformers	E ^a (Hartree)	C ^b (Hartree)	G ^c (kcal/mol)
3_1	-1454.121572	0.405281	-912211.333689
3_2	-1454.121054	0.405538	-912210.847311
3_3	-1454.117371	0.405032	-912208.853922
3_4	-1454.117396	0.405106	-912208.823237
3_5	-1454.116985	0.404891	-912208.700310

^aElectronic energy; ^bThermal correction to Gibbs free energy ; ^cGibbs free energy (E + C).

Table S8. Conformational analysis of the M06-2X/def2-SVP optimized conformers of **3** in the gas phase (T=298.15 K)

Conformers	ΔG (kcal/mol) ^a	Population ^b
3_1	0.000000	67.52%
3_2	0.486378	29.69%
3_3	2.479767	1.02%
3_4	2.510452	0.97%
3_5	2.633379	0.79%

^aThe relative Gibbs free energy; ^bThe Boltzmann distribution of each conformer.

5 ECD computational details of compound **4**

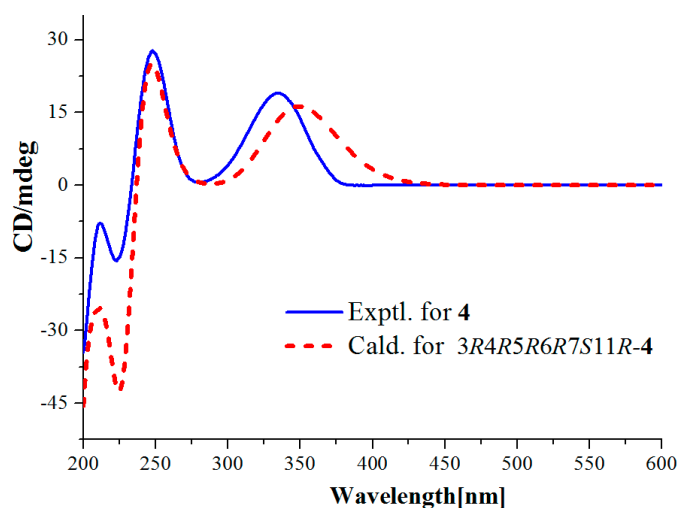


Figure S4. Experimental ECD spectra and calculated ECD spectra of **4**.

Table S9. Important thermodynamic parameters of the M06-2X/def2-SVP optimized conformers of **4** in the gas phase

Conformers	E ^a (Hartree)	C ^b (Hartree)	G ^c (kcal/mol)
4_1	-1111.065458	0.324859	-696993.057969
4_2	-1111.065133	0.324707	-696992.949599
4_3	-1111.061775	0.324333	-696991.077318
4_4	-1111.061525	0.324398	-696990.879529
4_5	-1111.061126	0.325496	-696989.939781
4_6	-1111.058664	0.323275	-696989.788866

^aElectronic energy; ^bThermal correction to Gibbs free energy ; ^cGibbs free energy (E + C).

Table S10. Conformational analysis of the M06-2X/def2-SVP optimized conformers of **4** in the gas phase (T=298.15 K)

Conformers	ΔG (kcal/mol) ^a	Population ^b
4_1	0.000000	52.56%
4_2	0.108370	43.77%
4_3	1.980650	1.85%
4_4	2.178439	1.33%
4_5	3.118188	0.27%
4_6	3.269102	0.21%

^aThe relative Gibbs free energy; ^bThe Boltzmann distribution of each conformer.

Table S11. Cartesian coordinates for the low-energy optimized conformers of **1-4** at M06-2X/def2-SVP level.

Conformer 1a_1							
C	3.813507	-2.167609	1.672918	C	-0.17331	-1.812801	-2.600849
C	4.137678	-2.014072	0.194551	O	1.455004	3.825742	-1.175527
C	3.075336	-1.184588	-0.530326	H	4.596367	-2.763237	2.170226
C	2.820246	0.204901	0.136454	H	2.866455	-2.723197	1.762109
C	2.648075	0.034432	1.6392	H	5.113317	-1.492316	0.096363
C	3.690018	-0.797845	2.335704	H	2.12925	-1.745179	-0.417978
C	1.566643	0.765918	-0.502885	H	3.444206	-0.890163	3.401706
C	0.478136	1.419105	0.247573	H	4.663476	-0.280695	2.272913
C	0.651241	1.513818	1.743047	H	1.670516	1.097119	-1.540589
C	1.658893	0.617246	2.336711	H	1.608595	0.523532	3.423783
O	0.021852	2.303343	2.413142	H	-2.475791	3.015593	-0.565427
O	0.362169	0.091133	-0.235474	H	-1.786789	3.06384	1.09709
C	-0.396858	2.453321	-0.46871	H	0.526931	4.086188	0.616187
C	-1.793077	2.524202	0.141707	H	-0.449447	4.575477	-0.796653
C	0.275049	3.828088	-0.421287	H	-1.007365	1.311001	-1.940317
O	-0.474561	2.120783	-1.83399	H	3.446084	-2.108574	-2.440647
C	3.417668	-1.097272	-2.017393	H	4.410701	-0.647965	-2.169671
C	3.950684	1.216986	-0.123395	H	2.685641	-0.504348	-2.582328
O	4.188841	-3.265708	-0.451582	H	3.707447	2.176929	0.353401
O	-2.213434	1.182439	0.365349	H	4.917986	0.865846	0.262047
C	-3.512193	0.898127	0.26672	H	4.059163	1.403805	-1.200864
C	-3.754861	-0.579024	0.395461	H	4.860331	-3.804964	-0.020848
O	-4.381824	1.717243	0.169166	H	-5.372392	-0.201376	1.746442
C	-4.775087	-0.973274	1.259189	H	-5.806638	-2.623263	2.18695
C	-5.010778	-2.325553	1.503002	H	-4.403649	-4.350728	1.067834
C	-4.226528	-3.291569	0.877131	H	-2.621225	-3.651354	-0.528393

C	-3.222716	-2.905545	-0.009319	H	0.289559	-0.831738	-2.436532
C	-2.987629	-1.553027	-0.266117	H	0.580082	-2.60603	-2.566925
C	-2.022015	-1.167798	-1.34165	H	-0.690249	-1.810129	-3.570369
O	-2.117734	-0.160569	-2.002835	H	1.208415	3.47908	-2.044112
O	-1.092776	-2.089426	-1.553252				

Conformer 1a_2							
C	3.820279	-2.168969	1.681244	C	-0.209963	-1.731348	-2.676541
C	4.122762	-2.039706	0.195929	O	1.457617	3.835284	-1.156868
C	3.0617	-1.195807	-0.528184	H	4.607445	-2.767514	2.161345
C	2.818644	0.199691	0.132106	H	2.867506	-2.714835	1.801483
C	2.651941	0.033026	1.635728	H	5.105157	-1.550849	0.073665
C	3.700845	-0.792119	2.330137	H	2.10193	-1.736972	-0.408855
C	1.568585	0.770349	-0.506282	H	3.465579	-0.873756	3.399414
C	0.478392	1.417653	0.246594	H	4.674072	-0.277135	2.252756
C	0.647227	1.501876	1.743597	H	1.676038	1.108721	-1.541486
C	1.660311	0.610119	2.334567	H	1.613341	0.517306	3.421869
O	0.010539	2.28241	2.41713	H	-2.478628	3.007567	-0.558723
O	0.362267	0.09353	-0.247693	H	-1.78741	3.070854	1.101975
C	-0.395282	2.458411	-0.461789	H	0.529798	4.08137	0.636793
C	-1.79154	2.524781	0.150341	H	-0.446398	4.583297	-0.771501
C	0.277691	3.832192	-0.402816	H	-1.021084	1.34014	-1.945441
O	-0.471703	2.137065	-1.830233	H	3.452141	-2.130845	-2.432438
C	3.396962	-1.117078	-2.016807	H	4.38031	-0.649963	-2.17539
C	3.959951	1.197418	-0.134732	H	2.651339	-0.547014	-2.587317
O	4.265344	-3.304851	-0.407372	H	3.736967	2.156454	0.353664
O	-2.203215	1.181868	0.382999	H	4.927172	0.829099	0.234473
C	-3.501573	0.891251	0.301666	H	4.056959	1.39249	-1.211743
C	-3.732049	-0.589159	0.417858	H	3.439567	-3.78711	-0.276664
O	-4.377393	1.705562	0.223726	H	-5.321062	-0.244075	1.810941
C	-4.729614	-1.003802	1.298066	H	-5.728781	-2.675492	2.222408
C	-4.950673	-2.361491	1.525464	H	-4.34206	-4.375487	1.043344
C	-4.175212	-3.312331	0.866166	H	-2.601359	-3.639248	-0.582146
C	-3.194308	-2.905597	-0.036528	H	0.256758	-0.756118	-2.488512
C	-2.97358	-1.547571	-0.276074	H	0.544318	-2.524357	-2.691284
C	-2.034916	-1.136084	-1.364631	H	-0.749865	-1.694715	-3.632622
O	-2.150754	-0.116928	-2.00374	H	1.21045	3.501397	-2.030203
O	-1.102663	-2.046118	-1.616734				

Conformer 1a_3							
C	-4.23733	-2.292152	-0.640628	C	4.074632	1.447555	2.375053
C	-3.92598	-2.209531	0.848999	O	-1.28349	3.917138	0.807963

C	-2.65116	-1.388793	1.095458	H	-5.163807	-2.865055	-0.788559
C	-2.740411	0.046307	0.484173	H	-3.42118	-2.85298	-1.129942
C	-3.120646	-0.075407	-0.983254	H	-4.770171	-1.728493	1.37277
C	-4.343284	-0.905199	-1.272686	H	-1.845896	-1.887581	0.522425
C	-1.380402	0.684872	0.670881	H	-4.497721	-0.976328	-2.357531
C	-0.646076	1.377832	-0.40422	H	-5.227439	-0.391356	-0.857935
C	-1.319132	1.454343	-1.755614	H	-1.160787	1.014965	1.691086
C	-2.447125	0.532105	-1.97362	H	-2.779993	0.453433	-3.010797
O	-0.98551	2.265767	-2.590224	H	2.3376	3.10051	-0.726134
O	-0.300421	0.064903	0.020512	H	1.309981	2.394307	-2.035705
C	0.401069	2.436633	-0.051149	H	-0.591169	4.062455	-1.098552
C	1.608289	2.321212	-0.983069	H	0.586152	4.558392	0.155259
C	-0.214605	3.836964	-0.094475	H	1.106862	1.351268	1.433433
O	0.819912	2.271689	1.284365	H	-2.967548	-0.8513	3.192623
C	-2.251786	-1.40772	2.569245	H	-1.246834	-0.991391	2.7231
C	-3.755192	0.960535	1.193659	H	-2.248119	-2.444006	2.928066
O	-3.833104	-3.497725	1.411632	H	-3.696505	1.971238	0.763503
O	2.271345	1.078118	-0.740665	H	-4.786811	0.597433	1.097684
C	1.951982	0.028141	-1.513044	H	-3.522492	1.040046	2.264822
C	2.631222	-1.227451	-1.061797	H	-3.105047	-3.957068	0.974907
O	1.242568	0.09483	-2.477273	H	2.229865	-2.129229	-2.956734
C	2.698479	-2.274765	-1.982645	H	3.406728	-4.269823	-2.385281
C	3.354237	-3.458533	-1.658427	H	4.470049	-4.522507	-0.14637
C	3.948669	-3.599949	-0.405308	H	4.329935	-2.676831	1.50997
C	3.87556	-2.56402	0.524302	H	5.044192	1.953239	2.357956
C	3.209762	-1.379999	0.206454	H	3.270043	2.12978	2.066553
C	3.06442	-0.329962	1.26969	H	3.853628	1.068972	3.381769
O	2.059479	-0.168381	1.917283	H	-0.937103	3.604184	1.654711
O	4.173276	0.369364	1.448287				

Conformer 1a_4							
C	4.236731	2.292667	-0.640771	C	-4.074409	-1.448108	2.374917
C	3.926052	2.209587	0.84897	O	1.283696	-3.917074	0.807576
C	2.651519	1.388515	1.09582	H	5.162951	2.86592	-0.788943
C	2.740616	-0.046364	0.483991	H	3.420195	2.853313	-1.129641
C	3.120476	0.075787	-0.983516	H	4.770592	1.728573	1.372202
C	4.3429	0.905852	-1.273062	H	1.845851	1.887385	0.52342
C	1.380633	-0.684979	0.670802	H	4.497145	0.977149	-2.357921
C	0.646136	-1.37774	-0.404321	H	5.227222	0.392133	-0.858507
C	1.319072	-1.454112	-1.755771	H	1.16116	-1.015281	1.690966
C	2.446837	-0.531619	-1.973866	H	2.779487	-0.452677	-3.011091
O	0.98554	-2.265607	-2.590351	H	-2.337541	-3.100392	-0.726332

O	0.300574	-0.064887	0.02068	H	-1.309938	-2.394034	-2.035838
C	-0.400995	-2.436567	-0.051289	H	0.591063	-4.062405	-1.09882
C	-1.608235	-2.321067	-0.983191	H	-0.586049	-4.558327	0.155171
C	0.21467	-3.836897	-0.094682	H	-1.106922	-1.351302	1.433306
O	-0.819858	-2.271692	1.284226	H	1.248462	0.989925	2.724303
C	2.253068	1.406869	2.569861	H	2.249054	2.443049	2.928976
C	3.755586	-0.960812	1.19291	H	2.969573	0.850705	3.192612
O	3.833145	3.497599	1.412016	H	3.697033	-1.971307	0.762259
O	-2.271308	-1.078004	-0.740639	H	4.787132	-0.597465	1.097055
C	-1.951997	-0.027924	-1.512887	H	3.522973	-1.040918	2.264048
C	-2.631431	1.227539	-1.061579	H	3.104219	3.956587	0.97636
O	-1.242391	-0.094425	-2.476995	H	-2.230026	2.129564	-2.956404
C	-2.698744	2.274925	-1.98234	H	-3.407238	4.269922	-2.384862
C	-3.35469	3.458582	-1.658069	H	-4.470776	4.52226	-0.146007
C	-3.949251	3.5998	-0.404995	H	-4.330577	2.676462	1.510161
C	-3.876093	2.563789	0.524526	H	-5.043947	-1.95383	2.357978
C	-3.210112	1.379893	0.206638	H	-3.853148	-1.069636	3.381616
C	-3.064593	0.329729	1.26973	H	-3.26984	-2.130229	2.066135
O	-2.059581	0.16825	1.917244	H	0.937448	-3.604169	1.654399
O	-4.17332	-0.369789	1.448298				

Conformer 1a_5							
C	-4.23545	-2.273248	-0.649264	C	4.094781	1.421301	2.369255
C	-3.950828	-2.167586	0.843825	O	-1.26174	3.915517	0.816606
C	-2.667083	-1.373722	1.094699	H	-5.170478	-2.832433	-0.817672
C	-2.734453	0.057835	0.473225	H	-3.416875	-2.85361	-1.103723
C	-3.103304	-0.066148	-0.997079	H	-4.794144	-1.64275	1.340027
C	-4.325898	-0.892651	-1.296692	H	-1.871136	-1.897896	0.536884
C	-1.368779	0.682424	0.665959	H	-4.464251	-0.973835	-2.382978
C	-0.628679	1.37813	-0.403589	H	-5.212798	-0.368218	-0.900754
C	-1.296295	1.462092	-1.756915	H	-1.150607	1.008301	1.687736
C	-2.422891	0.540285	-1.983261	H	-2.748151	0.461094	-3.022796
O	-0.960046	2.277712	-2.586511	H	2.362692	3.090442	-0.707666
O	-0.289819	0.06184	0.016224	H	1.335692	2.396755	-2.024456
C	0.420539	2.432317	-0.042847	H	-0.563382	4.064978	-1.087625
C	1.630347	2.316187	-0.971305	H	0.611794	4.552707	0.171565
C	-0.190513	3.834763	-0.083275	H	1.117878	1.340147	1.44121
O	0.834246	2.261911	1.293526	H	-2.251569	-2.43143	2.917553
C	-2.28369	-1.391428	2.572822	H	-3.019025	-0.856702	3.193187
C	-3.739739	0.994242	1.168185	H	-1.291299	-0.950203	2.737879
O	-3.774529	-3.445339	1.412028	H	-3.643454	2.006715	0.748892
O	2.285553	1.068349	-0.733395	H	-4.778771	0.661319	1.046261

C	1.962784	0.02429	-1.51301	H	-3.528222	1.057025	2.244992
C	2.625077	-1.239845	-1.061468	H	-4.572358	-3.960947	1.254883
O	1.261348	0.102524	-2.482242	H	2.21493	-2.135383	-2.957399
C	2.679238	-2.287862	-1.982354	H	3.356379	-4.294041	-2.38261
C	3.315186	-3.481736	-1.656203	H	4.40693	-4.564118	-0.139756
C	3.902384	-3.632874	-0.400877	H	4.289903	-2.71709	1.516501
C	3.84219	-2.596223	0.528755	H	5.06708	1.921497	2.345174
C	3.196836	-1.401583	0.208694	H	3.291984	2.107655	2.065131
C	3.065604	-0.349758	1.271947	H	3.878031	1.045854	3.378099
O	2.066122	-0.179316	1.925447	H	-0.919696	3.593492	1.661797
O	4.181205	0.341236	1.443856				

Conformer 2_1							
O	0.852007	-2.795104	-1.238511	C	3.868586	-1.091705	-0.393751
C	1.559303	-1.876972	-0.879395	C	3.021285	-1.917002	-1.031824
C	0.982271	-0.640265	-0.234222	H	-0.374286	-2.684259	0.962963
C	-0.480714	-0.655608	0.213174	H	-1.77047	-1.727766	1.540324
C	-0.689013	-1.693638	1.316238	H	-0.167474	-0.463734	2.682705
O	0.072966	-1.369869	2.447713	H	-0.836841	1.258444	0.118596
O	-0.796168	0.580458	0.811044	H	-1.086256	-0.250371	-1.826994
C	-1.386695	-0.909474	-0.999151	H	-1.316393	-1.955022	-1.313613
O	-2.750175	-0.668122	-0.668872	H	-4.631901	2.811236	-0.851328
C	-3.207189	0.583088	-0.798821	H	-7.063695	3.088313	-0.26855
C	-4.651338	0.704451	-0.444507	H	-8.395045	1.102061	0.456918
C	-5.240593	1.966077	-0.531074	H	-6.996678	-2.097245	0.701176
C	-6.588812	2.108342	-0.206175	H	-4.915121	-1.386158	0.019273
C	-7.339674	1.009923	0.198805	H	1.493778	0.883752	1.230884
C	-6.743644	-0.254322	0.283431	H	3.080375	-1.307245	2.218318
O	-7.518618	-1.287521	0.681424	H	4.731188	-0.622153	2.180902
C	-5.39537	-0.407821	-0.039698	H	3.353308	0.38026	2.686701
O	-2.526507	1.506013	-1.171404	H	3.771749	1.582583	-0.875393
C	1.922095	0.278689	0.427281	H	4.320564	3.4229	0.688881
O	1.397093	0.574372	-0.846025	H	4.156664	2.348515	2.081449
C	3.411452	0.02259	0.534578	H	2.729096	2.7366	1.082069
C	3.671052	-0.408252	1.990462	H	6.072401	0.933127	1.017202
C	4.140405	1.34725	0.141858	H	5.971112	2.625145	-1.225182
C	3.806486	2.525791	1.053753	H	7.110429	-0.04785	-0.999474
C	5.662856	1.17648	0.021292	H	5.666901	0.3466	-1.956145
O	6.290093	2.382071	-0.347166	H	5.575409	-2.0533	-1.26464
C	6.017526	0.058075	-0.949278	H	5.77663	-1.580338	0.427329
C	5.357096	-1.257087	-0.540833	H	3.394806	-2.734142	-1.652858

Conformer 2_2							
O	1.069423	-2.910431	-1.186459	C	3.942784	-0.947313	-0.407844
C	1.701176	-1.931839	-0.847314	C	3.158953	-1.84892	-1.02338
C	1.03099	-0.742237	-0.203552	H	-0.123611	-2.876962	1.045789
C	-0.417499	-0.877298	0.26988	H	-1.587324	-2.036465	1.63515
C	-0.517027	-1.911917	1.39108	H	-0.083937	-0.622575	2.733552
O	0.233555	-1.505946	2.5038	H	-0.924815	0.999886	0.15331
O	-0.828455	0.337059	0.854731	H	-1.088621	-0.561428	-1.766327
C	-1.319807	-1.226776	-0.921403	H	-1.171249	-2.268893	-1.218714
O	-2.692104	-1.090934	-0.569036	H	-4.804057	-1.96401	0.202168
C	-3.253081	0.11301	-0.711931	H	-7.226867	-1.826465	0.818469
C	-4.69519	0.121784	-0.328949	H	-8.441518	0.346046	0.61855
C	-5.349597	-1.025254	0.122446	H	-6.873124	3.266118	-0.511713
C	-6.699766	-0.939944	0.463427	H	-4.827942	2.212707	-0.800161
C	-7.386375	0.264409	0.355955	H	1.434137	0.834721	1.2387
C	-6.723839	1.4116	-0.099165	H	4.805799	-0.370259	2.145747
O	-7.436998	2.555978	-0.185521	H	3.354248	0.514902	2.664268
C	-5.374988	1.337505	-0.441801	H	3.221947	-1.196021	2.221022
O	-2.660673	1.083447	-1.116678	H	3.607264	1.700652	-0.919201
C	1.899468	0.260485	0.433056	H	2.50085	2.790331	1.03759
O	1.329776	0.497137	-0.833647	H	3.968105	2.535068	2.02214
C	3.406962	0.134934	0.516106	H	4.024505	3.602075	0.615193
C	3.727968	-0.252168	1.971886	H	5.986349	1.278532	0.940505
C	4.01154	1.512198	0.094262	H	5.703946	2.923495	-1.321131
C	3.591693	2.669897	0.997262	H	7.072293	0.363256	-1.081672
C	5.540978	1.471995	-0.050905	H	5.584701	0.618787	-2.017924
O	6.055399	2.722119	-0.444964	H	5.711588	-1.770273	-1.296841
C	5.975276	0.375238	-1.01385	H	5.899086	-1.259806	0.385756
C	5.437398	-0.986457	-0.578541	H	3.590762	-2.638427	-1.642381

Conformer 2_3							
O	1.066391	-2.925277	-1.157341	C	3.939088	-0.9483	-0.41535
C	1.697671	-1.940802	-0.834311	C	3.154069	-1.856128	-1.01996
C	1.029305	-0.744098	-0.202652	H	-0.128069	-2.864562	1.069669
C	-0.418904	-0.872712	0.273277	H	-1.590407	-2.015598	1.650633
C	-0.519919	-1.895452	1.405083	H	-0.081606	-0.590846	2.73076
O	0.231278	-1.479095	2.513678	H	-0.917591	1.00548	0.138293
O	-0.828707	0.347952	0.845729	H	-1.091248	-0.575089	-1.765035
C	-1.321884	-1.23304	-0.914193	H	-1.173251	-2.277793	-1.202148

O	-2.693928	-1.094267	-0.561863	H	-4.80432	-1.95995	0.221994
C	-3.255288	0.10822	-0.715821	H	-7.2259	-1.816452	0.8422
C	-4.696624	0.12058	-0.329246	H	-8.440926	0.354149	0.624252
C	-5.350092	-1.022011	0.13457	H	-6.874267	3.263196	-0.536806
C	-6.699517	-0.933374	0.477621	H	-4.830235	2.20676	-0.820229
C	-7.386352	0.269956	0.360173	H	1.43533	0.84833	1.220802
C	-6.724705	1.412661	-0.107244	H	4.794	-0.394483	2.139091
O	-7.437845	2.556402	-0.202882	H	3.362184	0.524807	2.653519
C	-5.376627	1.335159	-0.452191	H	3.192562	-1.185064	2.216638
O	-2.664621	1.074468	-1.13232	H	3.622148	1.71363	-0.925407
C	1.899641	0.265781	0.420656	H	2.510575	2.770323	1.067348
O	1.328052	0.48766	-0.846956	H	4.011765	2.554625	2.008187
C	3.40679	0.137035	0.507223	H	4.001088	3.605569	0.581184
C	3.719075	-0.253285	1.964353	H	5.973077	1.241221	0.94484
C	4.014001	1.513308	0.087545	H	6.914629	2.729027	-0.576754
C	3.601841	2.671857	0.993576	H	7.063229	0.349353	-1.108457
C	5.537416	1.462969	-0.052295	H	5.569211	0.64292	-2.024316
O	5.955398	2.734048	-0.493111	H	5.702036	-1.767475	-1.319462
C	5.964153	0.377484	-1.030851	H	5.899757	-1.264297	0.364439
C	5.432568	-0.986583	-0.596253	H	3.583848	-2.648274	-1.636976

Conformer 2_4							
O	0.848425	-2.81153	-1.206752	C	3.865183	-1.091799	-0.400157
C	1.555494	-1.886371	-0.8653	C	3.01646	-1.924099	-1.026971
C	0.980427	-0.641792	-0.234344	H	-0.379337	-2.669751	0.988256
C	-0.482208	-0.650265	0.21429	H	-1.773728	-1.703735	1.554429
C	-0.692229	-1.674469	1.329761	H	-0.164701	-0.427234	2.677899
O	0.070305	-1.338454	2.457389	H	-0.828076	1.264321	0.097716
O	-0.796524	0.59319	0.797305	H	-1.089125	-0.266739	-1.829512
C	-1.388776	-0.917355	-0.994705	H	-1.318225	-1.966194	-1.298041
O	-2.752051	-0.673176	-0.665771	H	-4.636612	2.802391	-0.884848
C	-3.209822	0.576338	-0.809305	H	-7.066861	3.084883	-0.297732
C	-4.653095	0.700936	-0.451725	H	-8.394306	1.10673	0.456687
C	-5.243689	1.960896	-0.552078	H	-6.992025	-2.088076	0.736125
C	-6.590974	2.10613	-0.224649	H	-4.913565	-1.383846	0.03885
C	-7.339679	1.012239	0.196386	H	1.495124	0.899093	1.210817
C	-6.742272	-0.250303	0.294819	H	4.715719	-0.641955	2.175811
O	-7.51503	-1.279294	0.708169	H	3.358045	0.39035	2.676542
C	-5.394915	-0.406728	-0.03072	H	3.051572	-1.293464	2.213492
O	-2.531379	1.49508	-1.195296	H	3.789141	1.595279	-0.880665
C	1.922438	0.284972	0.413672	H	2.736467	2.718028	1.109796

O	1.395421	0.564666	-0.861476	H	4.198923	2.364494	2.069765
C	3.411031	0.025729	0.526045	H	4.299975	3.429023	0.656644
C	3.660348	-0.407157	1.983466	H	6.054799	0.896483	1.023634
C	4.143156	1.349046	0.136109	H	7.150396	2.316578	-0.457692
C	3.816429	2.527875	1.050839	H	7.101385	-0.060164	-1.023493
C	5.658679	1.168024	0.022267	H	5.654927	0.372831	-1.960156
O	6.193634	2.403354	-0.392849	H	5.567188	-2.048841	-1.285338
C	6.007627	0.062015	-0.963971	H	5.777146	-1.584097	0.408113
C	5.352918	-1.256004	-0.556679	H	3.388166	-2.744216	-1.645151

Conformer 2_5							
O	0.861303	-2.798055	-1.242474	C	3.873071	-1.089881	-0.390263
C	1.565834	-1.879009	-0.880899	C	3.028514	-1.916661	-1.029861
C	0.985262	-0.643636	-0.236414	H	-0.365378	-2.688326	0.965233
C	-0.477935	-0.662081	0.210175	H	-1.764669	-1.735834	1.539986
C	-0.683541	-1.697858	1.315893	H	-0.16963	-0.464382	2.682009
O	0.077874	-1.368414	2.446588	H	-0.836852	1.250697	0.109144
O	-0.796417	0.575351	0.804113	H	-1.083874	-0.2665	-1.832167
C	-1.383814	-0.921801	-1.001081	H	-1.314085	-1.968828	-1.310553
O	-2.74686	-0.679296	-0.670783	H	-4.62492	2.79992	-0.870615
C	-3.204655	0.569139	-0.805248	H	-7.054084	3.087001	-0.284772
C	-4.649266	0.692516	-0.448383	H	-8.387123	1.130197	0.453077
C	-5.235633	1.959073	-0.543198	H	-8.335187	-1.116946	0.881143
C	-6.578866	2.107573	-0.217512	H	-4.934885	-1.400294	0.036594
C	-7.331177	1.008858	0.197728	H	1.491256	0.881416	1.228974
C	-6.73959	-0.254632	0.289921	H	4.730139	-0.616579	2.185483
O	-7.421653	-1.352211	0.685859	H	3.349833	0.384328	2.687919
C	-5.390177	-0.41376	-0.035868	H	3.080117	-1.303933	2.221009
O	-2.526896	1.492532	-1.183271	H	3.771593	1.583049	-0.874992
C	1.922283	0.277163	0.426247	H	2.722612	2.737097	1.078744
O	1.398892	0.571734	-0.848045	H	4.149065	2.35382	2.08151
C	3.411992	0.024273	0.536283	H	4.313287	3.426809	0.687836
C	3.669988	-0.404443	1.993071	H	6.070106	0.941067	1.02279
C	4.138898	1.349906	0.143257	H	5.968634	2.63017	-1.22172
C	3.800581	2.528959	1.052866	H	7.114115	-0.040278	-0.990585
C	5.661905	1.18224	0.025798	H	5.671585	0.349964	-1.950562
O	6.287383	2.388728	-0.343173	H	5.58355	-2.049233	-1.256489
C	6.020869	0.063362	-0.942669	H	5.780516	-1.573919	0.435345
C	5.362228	-1.252638	-0.534009	H	3.404633	-2.733418	-1.649857

Conformer 2_6							
O	0.857803	-2.814772	-1.210462	C	3.869632	-1.089693	-0.397002
C	1.562061	-1.888487	-0.866905	C	3.023728	-1.923619	-1.025272
C	0.983388	-0.645158	-0.236893	H	-0.369888	-2.673543	0.99096
C	-0.479443	-0.656829	0.210932	H	-1.767634	-1.711725	1.554197
C	-0.686471	-1.678384	1.329456	H	-0.166988	-0.426992	2.676868
O	0.075406	-1.336144	2.456166	H	-0.828296	1.256359	0.087096
O	-0.797032	0.588171	0.789449	H	-1.086866	-0.284027	-1.835087
C	-1.385903	-0.930456	-0.996767	H	-1.315754	-1.98084	-1.294631
O	-2.748771	-0.68512	-0.667823	H	-4.630057	2.789583	-0.907996
C	-3.20746	0.561455	-0.816473	H	-7.057511	3.08296	-0.317652
C	-4.651117	0.688432	-0.456081	H	-8.386185	1.135584	0.452598
C	-5.238985	1.953002	-0.566581	H	-8.330699	-1.104781	0.912182
C	-6.581181	2.104974	-0.238241	H	-4.933053	-1.397496	0.059339
C	-7.331039	1.011589	0.195179	H	1.492419	0.897205	1.208205
C	-6.73793	-0.249906	0.303075	H	3.05019	-1.290219	2.21555
O	-7.417718	-1.342358	0.717182	H	4.713888	-0.637078	2.180314
C	-5.389583	-0.41251	-0.025361	H	3.35402	0.394171	2.677568
O	-2.532002	1.480303	-1.20867	H	3.789108	1.596531	-0.879781
C	1.922507	0.283668	0.41214	H	2.730008	2.718245	1.107798
O	1.397174	0.561901	-0.864105	H	4.191642	2.369337	2.070645
C	3.411392	0.027573	0.52752	H	4.292593	3.432881	0.656723
C	3.658604	-0.403609	1.985793	H	6.052185	0.903619	1.029835
C	4.141646	1.351938	0.137904	H	7.148459	2.323814	-0.451725
C	3.810568	2.530891	1.050889	H	7.105166	-0.052169	-1.014427
C	5.657747	1.173819	0.027434	H	5.659669	0.377028	-1.954404
O	6.191619	2.409897	-0.387206	H	5.57539	-2.044242	-1.277715
C	6.011002	0.06778	-0.957238	H	5.78099	-1.577551	0.415757
C	5.358046	-1.251196	-0.550186	H	3.398111	-2.743331	-1.642393

Conformer 2_7							
O	1.066907	-2.928581	-1.142664	C	3.941702	-0.951448	-0.409637
C	1.698994	-1.942942	-0.824642	C	3.155693	-1.861254	-1.009945
C	1.031913	-0.741803	-0.20019	H	-0.129987	-2.854747	1.079698
C	-0.416973	-0.865196	0.275307	H	-1.592174	-2.001242	1.654811
C	-0.52106	-1.883794	1.410611	H	-0.081076	-0.572816	2.728991
O	0.228679	-1.463919	2.518958	H	-0.918941	1.012716	0.134828
O	-0.824074	0.357897	0.844119	H	-1.087792	-0.571852	-1.763789
C	-1.319681	-1.227676	-0.911627	H	-1.171059	-2.273242	-1.196812
O	-2.691853	-1.087356	-0.561099	H	-4.795303	-1.95702	0.212096
C	-3.251704	0.116655	-0.718979	H	-7.217197	-1.825202	0.828893

C	-4.695184	0.128668	-0.335441	H	-8.440365	0.320196	0.619421
C	-5.345207	-1.021498	0.126133	H	-8.270615	2.521696	0.019636
C	-6.691576	-0.940724	0.466787	H	-4.854738	2.225291	-0.819647
C	-7.382441	0.264793	0.349759	H	1.439303	0.85807	1.214494
C	-6.726561	1.410087	-0.113379	H	3.192188	-1.173622	2.222757
O	-7.348225	2.602487	-0.246225	H	4.795163	-0.386318	2.142764
C	-5.375318	1.33887	-0.457356	H	3.3645	0.538153	2.651159
O	-2.658292	1.080178	-1.134898	H	3.629532	1.708432	-0.933411
C	1.90348	0.270209	0.418164	H	2.517907	2.777095	1.052798
O	1.333631	0.48566	-0.85108	H	4.017975	2.563844	1.996123
C	3.410349	0.139419	0.506918	H	4.010062	3.607382	0.563666
C	3.720643	-0.244067	1.966297	H	5.977917	1.241175	0.94139
C	4.02017	1.512595	0.08088	H	6.923646	2.719675	-0.586996
C	3.609052	2.676438	0.980571	H	7.068517	0.337847	-1.106776
C	5.543608	1.458969	-0.05724	H	5.575657	0.629391	-2.025242
O	5.964413	2.727144	-0.503688	H	5.703894	-1.777763	-1.30871
C	5.969405	0.368111	-1.030199	H	5.901414	-1.266803	0.372891
C	5.435266	-0.992946	-0.589428	H	3.584665	-2.65722	-1.622608

Conformer 3_1							
C	-2.673459	3.308165	1.029953	O	5.533303	3.18304	0.388325
C	-3.049825	3.031357	-0.419329	O	-2.557989	-3.577603	-0.373049
C	-2.30635	1.801754	-0.963801	H	-3.234155	4.18189	1.391275
C	-2.511182	0.527242	-0.083731	H	-1.599872	3.56504	1.067904
C	-2.222549	0.874325	1.369202	H	-4.136313	2.845223	-0.479801
C	-2.932838	2.08641	1.908831	H	-1.225875	2.030218	-0.882533
C	-1.569362	-0.536089	-0.611366	H	-2.624281	2.269932	2.946517
C	-0.714682	-1.365822	0.252905	H	-4.017814	1.885516	1.927661
C	-0.74905	-1.096133	1.736676	H	-1.860561	-1.000204	-1.557637
C	-1.412903	0.147706	2.158373	H	-1.272557	0.409599	3.209514
O	-0.270468	-1.872264	2.536382	H	1.565726	-3.82602	-0.391646
O	-0.189097	-0.285144	-0.505888	H	1.020615	-3.552111	1.308741
C	-0.298699	-2.759315	-0.222727	H	-1.464458	-3.728271	1.334324
C	1.096928	-3.117654	0.307424	H	-0.917683	-4.800515	0.013667
C	-1.323204	-3.797295	0.247848	H	0.462272	-2.407334	-1.975551
O	-0.349201	-2.818443	-1.628609	H	-3.705873	1.361358	-2.579638
C	-2.638643	1.588405	-2.43901	H	-2.04607	0.778345	-2.884496
C	-3.931596	-0.059331	-0.181873	H	-2.429535	2.510306	-2.994612
O	-2.827996	4.166359	-1.223166	H	-3.993244	-0.976997	0.420574
O	1.933129	-1.975313	0.47813	H	-4.700118	0.644807	0.164382
C	2.411379	-1.376193	-0.613959	H	-4.163515	-0.332169	-1.2207

C	3.235874	-0.187068	-0.299367	H	-1.883778	4.365334	-1.197963
O	2.189579	-1.771956	-1.736612	H	3.656986	0.156413	-2.375951
C	3.821886	0.515972	-1.359456	H	5.058404	2.204438	-1.925163
C	4.590928	1.642491	-1.116787	H	4.33869	1.735704	2.288413
C	4.779202	2.082523	0.200607	H	2.958696	-0.290304	1.834695
C	4.191319	1.386051	1.263699	H	5.595273	3.381625	1.329422
C	3.423236	0.255492	1.013308	H	-2.369501	-3.519188	-1.320033

Conformer 3_2							
C	-2.727142	3.277302	1.024645	O	5.546093	3.222035	0.380061
C	-3.123322	2.9788	-0.414738	O	-2.514562	-3.596027	-0.373133
C	-2.350245	1.77729	-0.963555	H	-3.302461	4.13741	1.404416
C	-2.520336	0.501078	-0.079326	H	-1.663019	3.562066	1.030551
C	-2.230505	0.854498	1.371966	H	-4.207771	2.741786	-0.448119
C	-2.954433	2.057386	1.914401	H	-1.281075	2.045317	-0.893487
C	-1.558225	-0.542596	-0.609735	H	-2.635029	2.252275	2.946695
C	-0.695794	-1.364857	0.254252	H	-4.035224	1.835781	1.949563
C	-0.73464	-1.09851	1.738238	H	-1.841309	-1.008811	-1.557339
C	-1.410916	0.138411	2.160368	H	-1.270483	0.403442	3.210706
O	-0.249715	-1.871021	2.537803	H	1.610463	-3.8009	-0.392654
O	-0.182002	-0.275939	-0.500476	H	1.063451	-3.531934	1.307958
C	-0.264142	-2.752938	-0.223038	H	-1.418081	-3.73724	1.333334
C	1.13526	-3.096869	0.306537	H	-0.860509	-4.801152	0.010301
C	-1.276825	-3.802854	0.246675	H	0.491719	-2.390269	-1.975758
O	-0.314514	-2.811894	-1.628916	H	-3.75904	1.341344	-2.575276
C	-2.688606	1.556456	-2.436565	H	-2.107479	0.734006	-2.874267
C	-3.925291	-0.124139	-0.167629	H	-2.459688	2.471061	-2.995529
O	-2.839907	4.074272	-1.254371	H	-3.950857	-1.056354	0.414904
O	1.960682	-1.946872	0.476591	H	-4.70823	0.549339	0.206114
C	2.434402	-1.345035	-0.61633	H	-4.165445	-0.380291	-1.208982
C	3.255444	-0.153427	-0.303303	H	-3.334195	4.83763	-0.938168
O	2.212197	-1.742127	-1.738476	H	3.664979	0.195834	-2.38127
C	3.834357	0.553361	-1.364832	H	5.061888	2.247266	-1.933333
C	4.601224	1.681579	-1.123703	H	4.363872	1.768444	2.282648
C	4.794094	2.119816	0.193536	H	2.988013	-0.261016	1.831764
C	4.213266	1.419715	1.258089	H	5.605475	3.422757	1.320831
C	3.447396	0.287402	1.00927	H	-2.326271	-3.528432	-1.31961

Conformer 3_3							
C	6.058903	0.183854	-0.967845	O	-8.64961	0.773017	0.443007

C	5.656399	1.335991	-0.057138	O	0.192906	-1.334753	2.530259
C	4.128089	1.44396	0.061893	H	7.155366	0.124803	-1.017758
C	3.461498	0.111	0.530035	H	5.692892	0.40158	-1.986968
C	3.965332	-1.029238	-0.34062	H	6.07927	1.165606	0.948289
C	5.459427	-1.135787	-0.486287	H	3.746228	1.606135	-0.96472
C	1.961689	0.294017	0.418077	H	5.711127	-1.958988	-1.167862
C	1.061309	-0.698645	-0.189746	H	5.895798	-1.387812	0.495487
C	1.691234	-1.939576	-0.774588	H	1.508762	0.919859	1.191676
C	3.153653	-1.922746	-0.931141	H	3.561235	-2.753724	-1.511073
O	1.025678	-2.905406	-1.084824	H	-1.180026	-2.157568	-1.193479
O	1.420262	0.499735	-0.865696	H	-1.028445	-0.469277	-1.784317
C	-0.397983	-0.754976	0.267273	H	-0.197986	-2.739198	1.112841
C	-1.296964	-1.103198	-0.9263	H	-1.634669	-1.819828	1.649383
C	-0.556486	-1.747822	1.419071	H	-0.86637	1.128969	0.083717
O	-0.762592	0.493405	0.809304	H	4.10102	2.548749	1.944365
C	3.743013	2.654457	0.909505	H	2.657357	2.818578	0.929205
C	3.745776	-0.228715	2.005164	H	4.216851	3.552179	0.494965
O	6.227607	2.546897	-0.49343	H	3.196812	-1.139648	2.284258
O	-2.668646	-0.910256	-0.601484	H	4.815135	-0.384485	2.200496
C	-3.184348	0.312418	-0.786205	H	3.39519	0.580971	2.660113
C	-4.627418	0.379623	-0.447328	H	5.892945	2.728752	-1.380389
O	-2.541026	1.249946	-1.193548	H	-4.709063	2.46639	-0.943494
C	-5.283765	1.609206	-0.590223	H	-7.160641	2.675609	-0.39293
C	-6.630688	1.728934	-0.289223	H	-7.252071	-1.492954	0.657948
C	-7.342627	0.609125	0.16218	H	-4.830291	-1.69114	0.110843
C	-6.692634	-0.622709	0.306326	H	-9.02845	-0.060843	0.743231
C	-5.34135	-0.734876	0.001817	H	-0.086962	-0.429166	2.71928

Conformer 3_4							
C	6.057584	0.191945	-0.970176	O	-8.653281	0.648201	0.473502
C	5.652948	1.343946	-0.060245	O	0.199137	-1.334538	2.533039
C	4.124463	1.448602	0.05945	H	7.154155	0.135212	-1.02046
C	3.461086	0.114586	0.529065	H	5.690729	0.408148	-1.98933
C	3.966822	-1.025109	-0.341209	H	6.076712	1.17544	0.945114
C	5.461078	-1.128639	-0.487515	H	3.741734	1.609049	-0.967115
C	1.960805	0.294264	0.41812	H	5.714166	-1.951701	-1.16874
C	1.062168	-0.700526	-0.188639	H	5.898454	-1.379217	0.494176
C	1.694314	-1.940237	-0.773651	H	1.507063	0.919312	1.191877
C	3.156677	-1.920524	-0.930905	H	3.565619	-2.750962	-1.510654
O	1.030553	-2.907358	-1.083481	H	-1.178644	-2.167821	-1.185988
O	1.417931	0.498444	-0.865365	H	-1.029092	-0.481201	-1.78211

C	-0.39649	-0.76001	0.269981	H	-0.19027	-2.742253	1.118473
C	-1.296085	-1.11276	-0.921879	H	-1.628528	-1.82602	1.655704
C	-0.550948	-1.751332	1.423643	H	-0.868126	1.122389	0.082908
O	-0.763664	0.488595	0.809916	H	4.095557	2.554829	1.941043
C	3.737101	2.65898	0.906181	H	2.651089	2.82075	0.926032
C	3.747166	-0.223481	2.004218	H	4.208986	3.557341	0.490781
O	6.221205	2.555787	-0.497952	H	3.200324	-1.135364	2.284351
O	-2.667689	-0.920094	-0.596323	H	4.816996	-0.37683	2.198885
C	-3.184848	0.300842	-0.783914	H	3.395279	0.585867	2.658891
C	-4.627919	0.36695	-0.444367	H	5.886337	2.73549	-1.385267
O	-2.543216	1.238553	-1.194364	H	-4.831671	-1.703319	0.120536
C	-5.344784	-0.748334	0.009329	H	-7.271047	-1.491956	0.6682
C	-6.693066	-0.638803	0.313445	H	-7.142403	2.67024	-0.403524
C	-7.343339	0.593525	0.165239	H	-4.708518	2.450747	-0.946658
C	-6.631642	1.711078	-0.289011	H	-8.987361	1.541015	0.331139
C	-5.281506	1.593461	-0.59099	H	-0.084845	-0.43046	2.722945

Conformer 3_5							
C	-3.6856563	3.12944699	-3.057654	O	4.99516989	-5.2533028	5.77387385
C	-2.6464934	4.03089438	-2.3962828	O	1.95465975	-0.9474846	-1.8312765
C	-1.7850212	3.26176965	-1.3681527	H	-4.2510616	3.70146419	-3.8036753
C	-1.1214875	1.97213608	-1.9780573	H	-4.4250448	2.80827593	-2.3115856
C	-2.1939873	1.1609315	-2.7213721	H	-2.0051775	4.48384606	-3.1612446
C	-3.0420129	1.91945332	-3.7146972	H	-2.4582222	2.94702288	-0.5562146
C	-0.437107	1.18855446	-0.8638235	H	-3.8319367	1.28379336	-4.133249
C	-0.6810311	-0.3021603	-0.671354	H	-2.4241175	2.2355426	-4.5629935
C	-1.6768958	-0.9757863	-1.5484142	H	0.51590718	1.61008717	-0.5700242
C	-2.4181182	-0.1494557	-2.5236225	H	-3.1826055	-0.6902514	-3.0726157
O	-1.9054113	-2.1768144	-1.4613067	H	-0.8178154	-2.8976608	0.54135513
O	-1.283066	0.69899753	0.18550701	H	-0.9208877	-1.6085175	1.72453238
C	0.39873219	-1.1379444	0.03015852	H	0.66652794	-2.5423163	-1.6580273
C	-0.230631	-2.1258372	1.04600107	H	2.02314775	-2.5011353	-0.5166206
C	1.25688033	-1.8916806	-1.007651	H	0.92228779	-0.031652	1.57801736
O	1.32837024	-0.2526194	0.71172947	H	-0.1113537	4.67729318	-1.4568809
C	-0.7767041	4.22509658	-0.7148326	H	-0.1632295	3.7209904	0.03716019
C	-0.0163345	2.32530869	-3.0083861	H	-1.2952202	5.04113399	-0.1998156
O	-3.330566	5.09818771	-1.7390545	H	0.38861033	1.41644455	-3.4714299
O	0.76907336	-2.8310756	1.81301105	H	-0.3772958	2.97223783	-3.8134772
C	1.21383595	-2.1911555	2.92332462	H	0.83062264	2.83532101	-2.5357321
C	2.20775393	-3.0212467	3.65471834	H	-3.8499543	5.57677221	-2.4076114
O	0.86641462	-1.0746742	3.27971829	H	2.1527368	-4.7400553	2.32539517

C	2.58177199	-4.3012706	3.22253411	H	3.81368917	-6.0301308	3.61632145
C	3.52127663	-5.0374515	3.94851592	H	4.15827616	-2.8002	6.44128425
C	4.08350867	-4.4972135	5.09989185	H	2.50268763	-1.4976732	5.16570426
C	3.72384343	-3.2287905	5.54340407	H	5.30352427	-4.7559879	6.54930997
C	2.78417237	-2.490476	4.81882777	H	2.38096494	-0.3389822	-1.1931607

Conformer 4_1							
C	1.937348	-0.553228	-2.071236	H	2.816218	-0.946315	-2.599989
C	2.374039	0.068302	-0.754853	H	1.480582	0.233313	-2.692778
C	1.195029	0.617401	0.049127	H	2.927819	-0.680427	-0.164011
C	0.108134	-0.476119	0.306843	H	0.70396	1.376042	-0.584624
C	-0.240066	-1.158185	-1.009309	H	0.571302	-2.105808	-2.752946
C	0.926069	-1.668591	-1.810726	H	1.423126	-2.477341	-1.248255
C	-1.090082	0.229525	0.916903	H	-0.9933	0.522403	1.96784
C	-2.474895	0.015061	0.456586	H	-1.698177	-1.871579	-2.378148
C	-2.694535	-0.912549	-0.707326	H	-5.310032	1.5262	1.559427
C	-1.499515	-1.336062	-1.447354	H	-4.604399	1.495793	-0.07436
O	-3.809704	-1.291264	-1.008898	H	-3.04871	-1.418718	2.739561
O	3.254098	1.166924	-1.005536	H	-4.777577	-0.769296	2.975473
O	-1.739326	1.183017	0.116956	H	-5.465913	-0.67638	-0.185371
C	-3.636877	0.238655	1.38258	H	5.316575	2.751526	-0.60107
C	-4.893796	0.864217	0.786982	H	6.370922	1.859373	-1.753698
C	-3.774208	-0.615327	2.567787	H	4.884789	2.70765	-2.317826
O	-3.260867	0.695637	2.665298	H	2.243699	0.595744	1.965019
O	-5.870212	-0.076652	0.45872	H	0.860353	1.721998	1.910941
C	4.540544	0.876159	-1.269836	H	2.364143	2.118399	1.062613
C	5.340267	2.12777	-1.50465	H	-0.212706	-2.316825	1.420273
O	4.967464	-0.244639	-1.303453	H	1.494144	-2.045588	0.998923
C	1.686479	1.297243	1.325789	H	0.741117	-1.099382	2.300263
C	0.566674	-1.548078	1.31235				

Conformer 4_2							
C	1.926264	-0.607352	-2.140065	H	2.809607	-0.988587	-2.670175
C	2.358565	0.034547	-0.832149	H	1.451388	0.164846	-2.766051
C	1.174193	0.570232	-0.027251	H	2.928697	-0.698246	-0.236942
C	0.109434	-0.540341	0.248133	H	0.665661	1.312611	-0.666446
C	-0.234798	-1.243614	-1.059103	H	0.585241	-2.190709	-2.798937
C	0.937377	-1.73838	-1.862841	H	1.453516	-2.532888	-1.297011
C	-1.097933	0.150776	0.858009	H	-1.000339	0.455459	1.905557
C	-2.480048	-0.093437	0.403851	H	-1.685593	-2.008725	-2.405345

C	-2.695188	-1.060453	-0.731847	H	-4.406814	1.815638	0.295372
C	-1.492702	-1.455852	-1.483315	H	-5.299556	0.297344	-0.008791
O	-3.798213	-1.491281	-0.983244	H	-3.131639	-1.613212	2.614946
O	3.217726	1.146603	-1.097869	H	-4.848891	-0.920962	2.84808
O	-1.766688	1.083462	0.049009	H	-5.256285	1.584351	2.497915
C	-3.637931	0.121657	1.3323	H	5.25699	2.770688	-0.715418
C	-4.812824	0.901251	0.767968	H	6.316347	1.889458	-1.871469
C	-3.834886	-0.78756	2.462608	H	4.810045	2.707284	-2.427744
O	-3.287177	0.509539	2.647014	H	2.237944	0.589851	1.880474
O	-5.74785	1.18905	1.76549	H	0.830737	1.685536	1.826902
C	4.508199	0.877231	-1.363552	H	2.319038	2.106026	0.962956
C	5.283296	2.141237	-1.61502	H	-0.171656	-2.372399	1.385366
O	4.956915	-0.235333	-1.385919	H	1.526828	-2.077277	0.947809
C	1.66108	1.273075	1.238824	H	0.768309	-1.129427	2.24478
C	0.593613	-1.591721	1.263143				

Conformer 4_3							
C	1.776101	0.705461	-2.146369	H	2.566486	0.663189	-2.90811
C	2.288912	0.098805	-0.851138	H	1.526981	1.762516	-1.961422
C	1.23238	0.106497	0.254026	H	2.637915	-0.929673	-1.043223
C	-0.081802	-0.613628	-0.191075	H	0.949406	1.161346	0.413684
C	-0.522112	-0.073286	-1.547077	H	0.12929	0.392819	-3.53534
C	0.535713	-0.051101	-2.617368	H	0.822762	-1.088178	-2.862717
C	-1.114234	-0.342536	0.88987	H	-0.987617	-0.893035	1.828127
C	-2.49411	0.094065	0.593712	H	-2.056067	0.652398	-2.82096
C	-2.886547	0.255854	-0.850669	H	-5.310928	0.927087	0.881161
C	-1.776622	0.326526	-1.816657	H	-5.158126	0.787332	2.663247
O	-4.049189	0.279692	-1.184446	H	-3.43916	-2.363746	1.444548
O	3.401795	0.855877	-0.367097	H	-4.96691	-1.745163	2.300196
O	-1.500393	0.996866	1.058031	H	-3.185561	2.189719	2.216147
C	-3.601421	-0.15897	1.577236	H	6.62201	1.286142	-0.811215
C	-4.605448	0.965275	1.721406	H	5.385662	2.537744	-0.423202
C	-3.95485	-1.533604	1.940188	H	5.741906	1.267465	0.757958
O	-3.156998	-0.740576	2.790991	H	2.185256	-1.471351	1.425799
O	-3.989935	2.221998	1.683593	H	1.084901	-0.434458	2.372774
C	4.600238	0.614305	-0.926913	H	2.666559	0.179088	1.862919
C	5.666364	1.481856	-0.316444	H	-0.852894	-2.592871	-0.656475
O	4.769497	-0.195597	-1.795894	H	0.886455	-2.426129	-0.987946
C	1.817019	-0.442216	1.554619	H	0.314574	-2.573295	0.687466
C	0.082742	-2.140508	-0.295938				

Conformer 4_4							
C	1.655531	-0.106838	-2.346121	H	2.412468	-0.422087	-3.077074
C	2.236597	-0.198414	-0.944931	H	1.395063	0.944594	-2.546918
C	1.228545	0.206242	0.131262	H	2.598686	-1.224776	-0.7667
C	-0.08612	-0.63396	0.040061	H	0.930302	1.245748	-0.089752
C	-0.598117	-0.618613	-1.395888	H	-0.044772	-0.904712	-3.447017
C	0.410004	-0.985008	-2.451234	H	0.704772	-2.039983	-2.317485
C	-1.077893	-0.006785	1.003485	H	-0.907171	-0.197939	2.068043
C	-2.47692	0.28046	0.641275	H	-2.193595	-0.384375	-2.77527
C	-2.931422	-0.027946	-0.762942	H	-4.759287	1.810552	0.72924
C	-1.868282	-0.334583	-1.733821	H	-5.15463	1.535548	2.447636
O	-4.107702	-0.035895	-1.046375	H	-3.7301	-1.855257	1.769941
O	3.352402	0.687321	-0.822778	H	-5.126668	-0.929924	2.568257
O	-1.485898	1.308926	0.710806	H	-2.694806	2.6832	1.695907
C	-3.544228	0.35099	1.696282	H	6.541721	0.936351	-1.544324
C	-4.326175	1.645295	1.733066	H	5.299479	2.241191	-1.566468
C	-4.100436	-0.912509	2.188786	H	5.73457	1.476029	-0.029926
O	-3.173407	-0.175184	2.952727	H	2.260821	-0.832766	1.75142
O	-3.53704	2.717752	2.166339	H	1.180776	0.474221	2.305945
C	4.531006	0.262242	-1.312373	H	2.726849	0.865171	1.534673
C	5.605763	1.293363	-1.105164	H	-0.829367	-2.654255	0.353149
O	4.677458	-0.806691	-1.837167	H	0.889137	-2.605055	-0.103016
C	1.87792	0.171197	1.513666	H	0.394144	-2.146458	1.54057
C	0.110021	-2.09638	0.48021				

Conformer 4_5							
C	1.887005	-0.858749	-2.194085	H	2.702727	-1.312311	-2.775791
C	2.45131	-0.227643	-0.929752	H	1.414518	-0.081834	-2.810014
C	1.358058	0.428671	-0.074386	H	2.935464	-1.015307	-0.330304
C	0.265892	-0.616386	0.330059	H	0.83659	1.162498	-0.707213
C	-0.216816	-1.333838	-0.924095	H	0.402549	-2.370878	-2.69442
C	0.856399	-1.91905	-1.803046	H	1.363521	-2.730991	-1.253294
C	-0.851812	0.154442	1.010505	H	-0.655897	0.479243	2.038073
C	-2.277717	-0.028747	0.679653	H	-1.810359	-2.039186	-2.137245
C	-2.626779	-0.988074	-0.425179	H	-4.956791	1.614757	1.970831
C	-1.514287	-1.481033	-1.24656	H	-4.394843	1.513759	0.285017
O	-3.775422	-1.33693	-0.617321	H	-2.699672	-1.369605	3.050369
O	3.544198	0.656963	-1.203039	H	-4.379006	-0.651127	3.410724
O	-1.53824	1.100243	0.23469	H	-5.331047	-0.630674	0.315872
C	-3.346966	0.265697	1.693474	H	5.408366	1.926733	-2.462466
C	-4.629423	0.917252	1.186958	H	4.457139	3.446795	-2.652061

C	-3.409971	-0.546022	2.914092	H	4.966594	2.865933	-1.027988
O	-2.846575	0.747778	2.923538	H	2.590438	0.48704	1.73258
O	-5.659812	0.001219	0.972187	H	1.204783	1.613225	1.758522
C	3.345722	1.78566	-1.904319	H	2.621229	1.972855	0.76903
C	4.627654	2.564473	-2.028504	H	-0.040506	-2.370638	1.576622
O	2.285532	2.120416	-2.355753	H	1.622151	-2.239345	0.965357
C	1.971987	1.159006	1.118128	H	1.074453	-1.174322	2.27834
C	0.767659	-1.661969	1.342213				

Conformer 4_6							
C	1.655469	-0.362157	-2.352597	H	2.463114	-0.754686	-2.985216
C	2.221313	0.044109	-1.003271	H	1.235102	0.532182	-2.839558
C	1.147136	0.596102	-0.065529	H	2.723256	-0.823332	-0.542373
C	-0.028875	-0.413531	0.134229	H	0.703737	1.470048	-0.574552
C	-0.504034	-0.930236	-1.219449	H	0.122333	-1.707225	-3.115134
C	0.569243	-1.416156	-2.155736	H	1.02956	-2.324394	-1.729426
C	-1.132674	0.328669	0.86513	H	-0.915985	0.57218	1.913111
C	-2.558619	0.185362	0.524787	H	-2.096916	-1.462955	-2.516755
C	-2.907791	-0.694492	-0.65151	H	-3.039675	-0.848836	3.257141
C	-1.80026	-1.023121	-1.562167	H	-4.798014	-0.706307	2.989223
O	-4.029064	-1.124872	-0.808027	H	-3.36782	2.548411	1.665556
O	3.195693	1.077154	-1.174129	H	-4.34113	1.813211	3.07437
O	-1.810887	1.337956	0.168277	H	-4.323518	-2.046764	1.053925
C	-3.615057	0.352879	1.578479	H	5.425618	2.399453	-0.718413
C	-3.824451	-0.845322	2.484115	H	6.323896	1.559665	-2.031288
C	-3.934388	1.701606	2.062861	H	4.904213	2.606621	-2.398129
O	-4.768642	1.036735	1.14241	H	2.316816	0.244637	1.744396
O	-3.728001	-2.070867	1.816571	H	1.040814	1.473982	1.943136
C	4.430645	0.701143	-1.551444	H	2.509508	1.857532	1.031735
C	5.339706	1.891456	-1.688287	H	-0.528314	-2.277387	1.126144
O	4.740581	-0.441901	-1.742984	H	1.169916	-2.208602	0.580864
C	1.78148	1.065175	1.243357	H	0.65733	-1.291509	2.014
C	0.347636	-1.621615	1.01216				

Spectroscopic data

Figure S5. ^1H NMR spectrum of **1** in CD_3OD

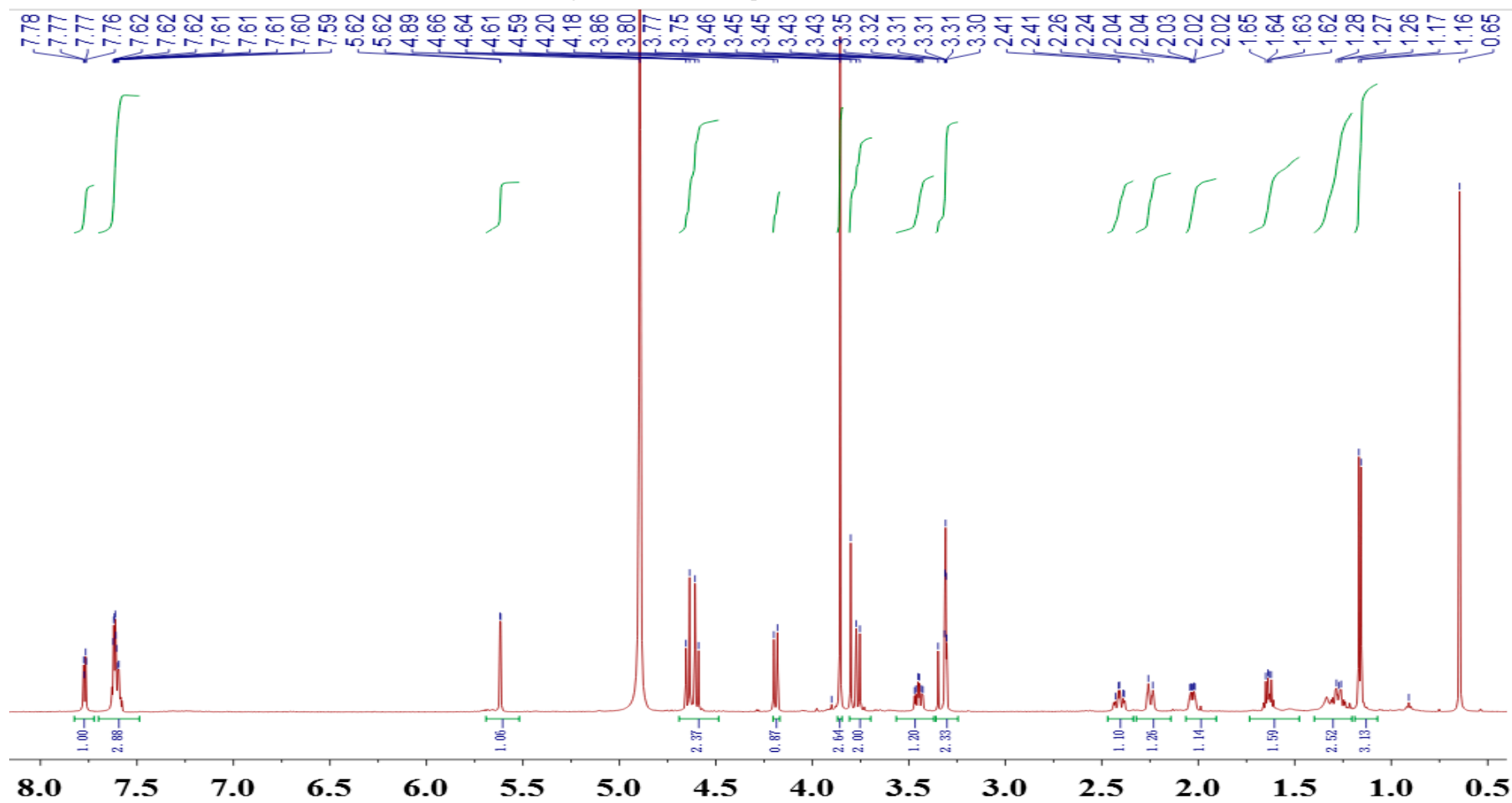


Figure S6 ^{13}C NMR spectrum of **1** in CD_3OD

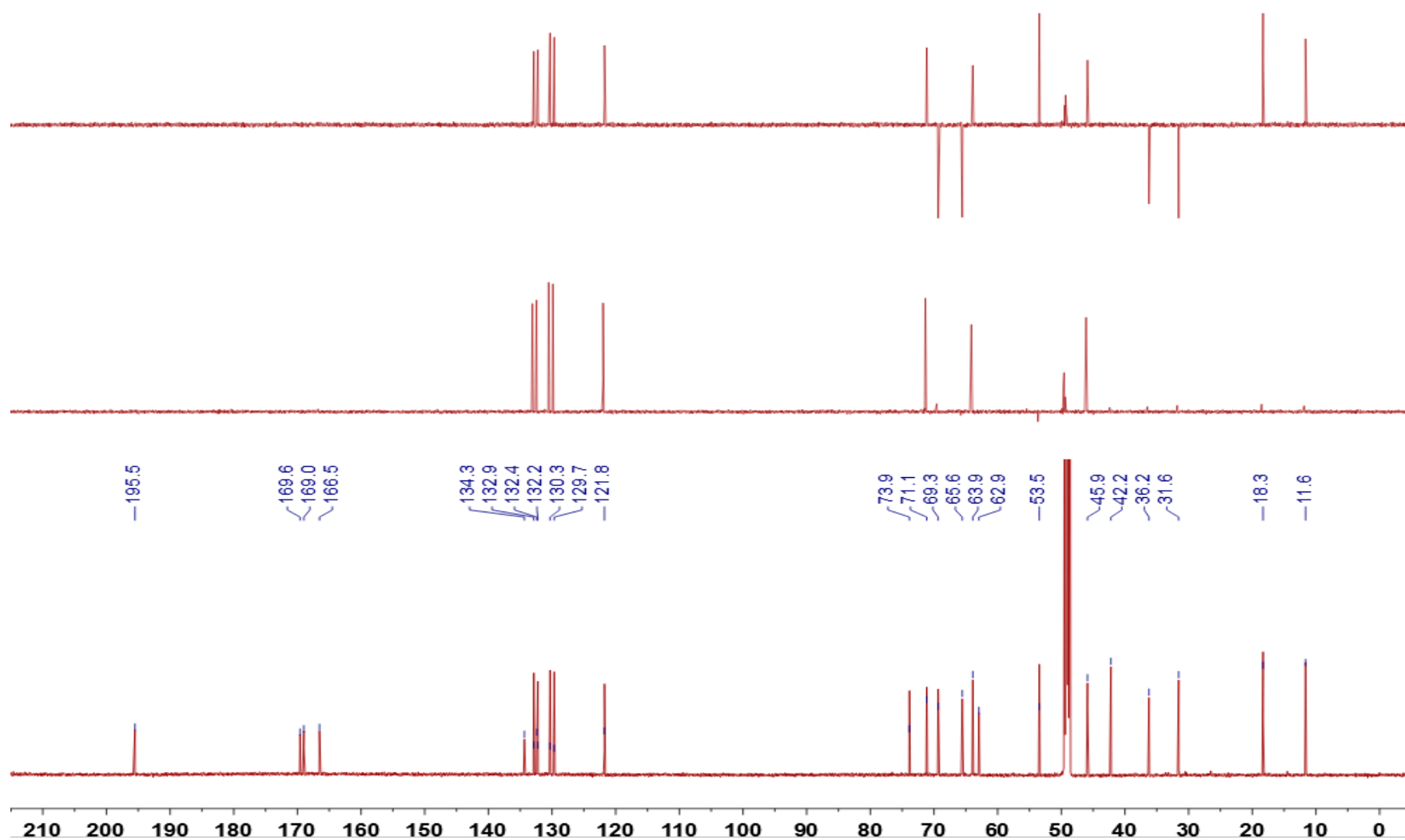


Figure S7 HSQC spectrum of **1** in CD₃OD

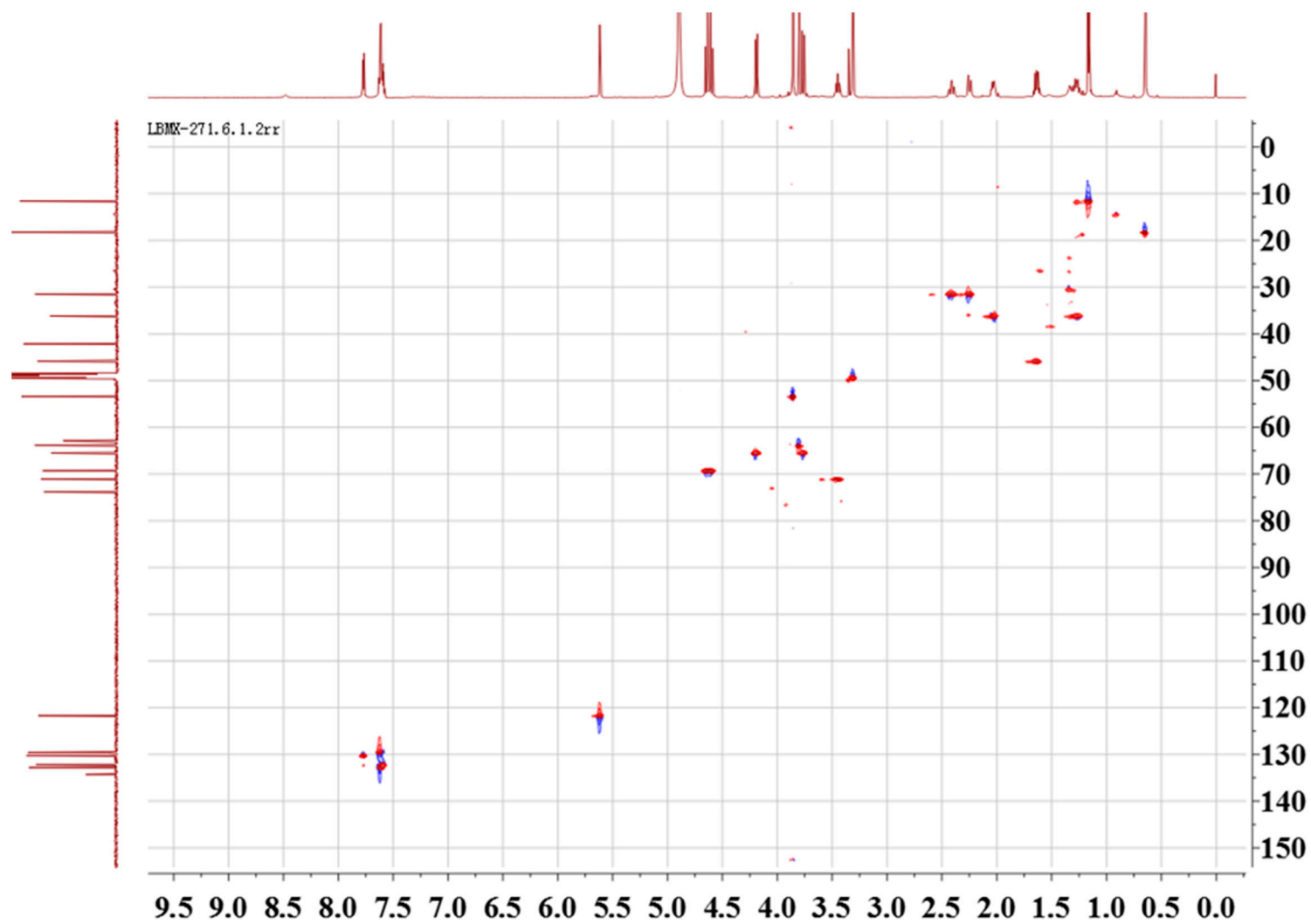


Figure S8 HMBC spectrum of **1** in CD₃OD

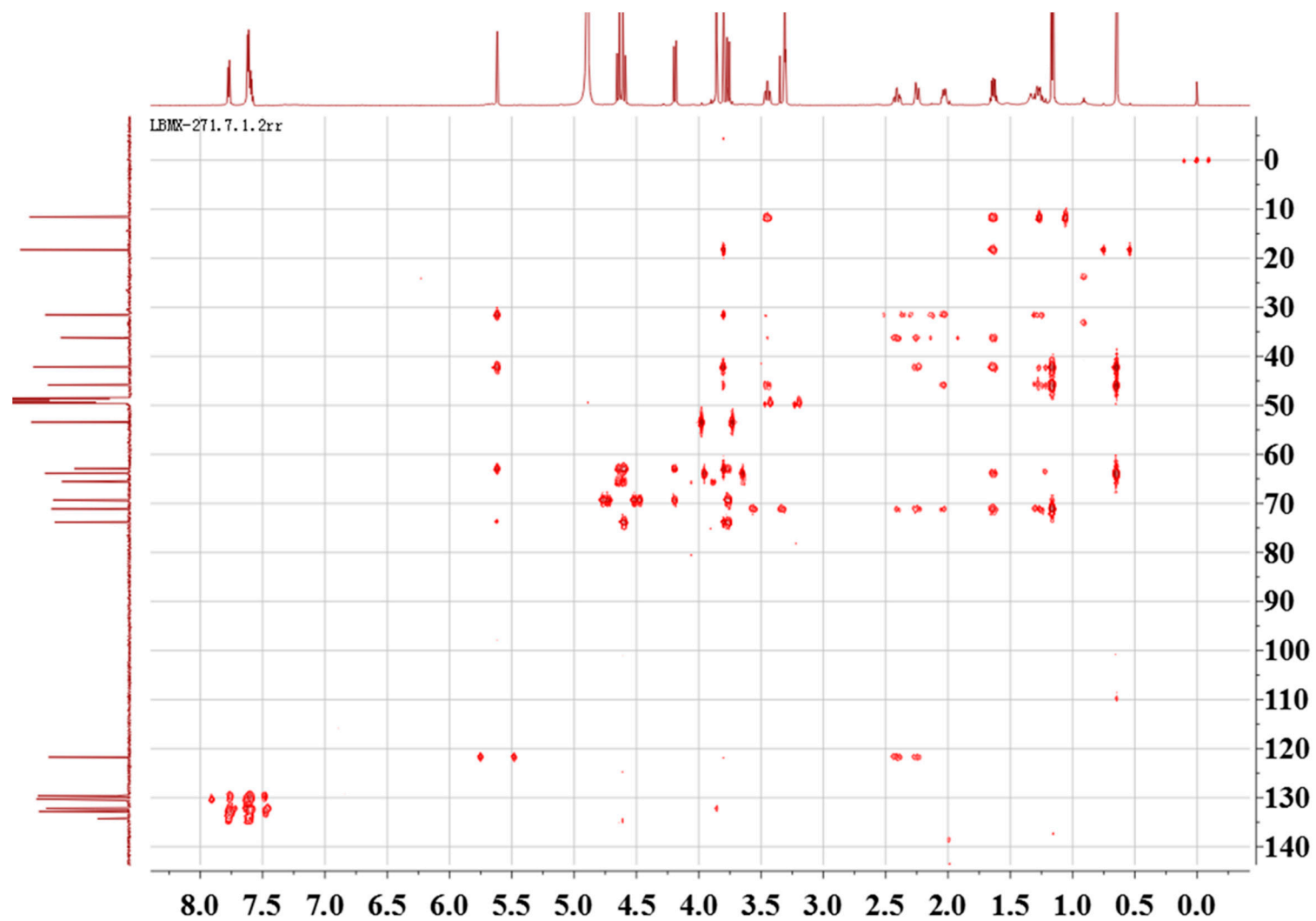


Figure S9 COSY spectrum of **1** in CD₃OD

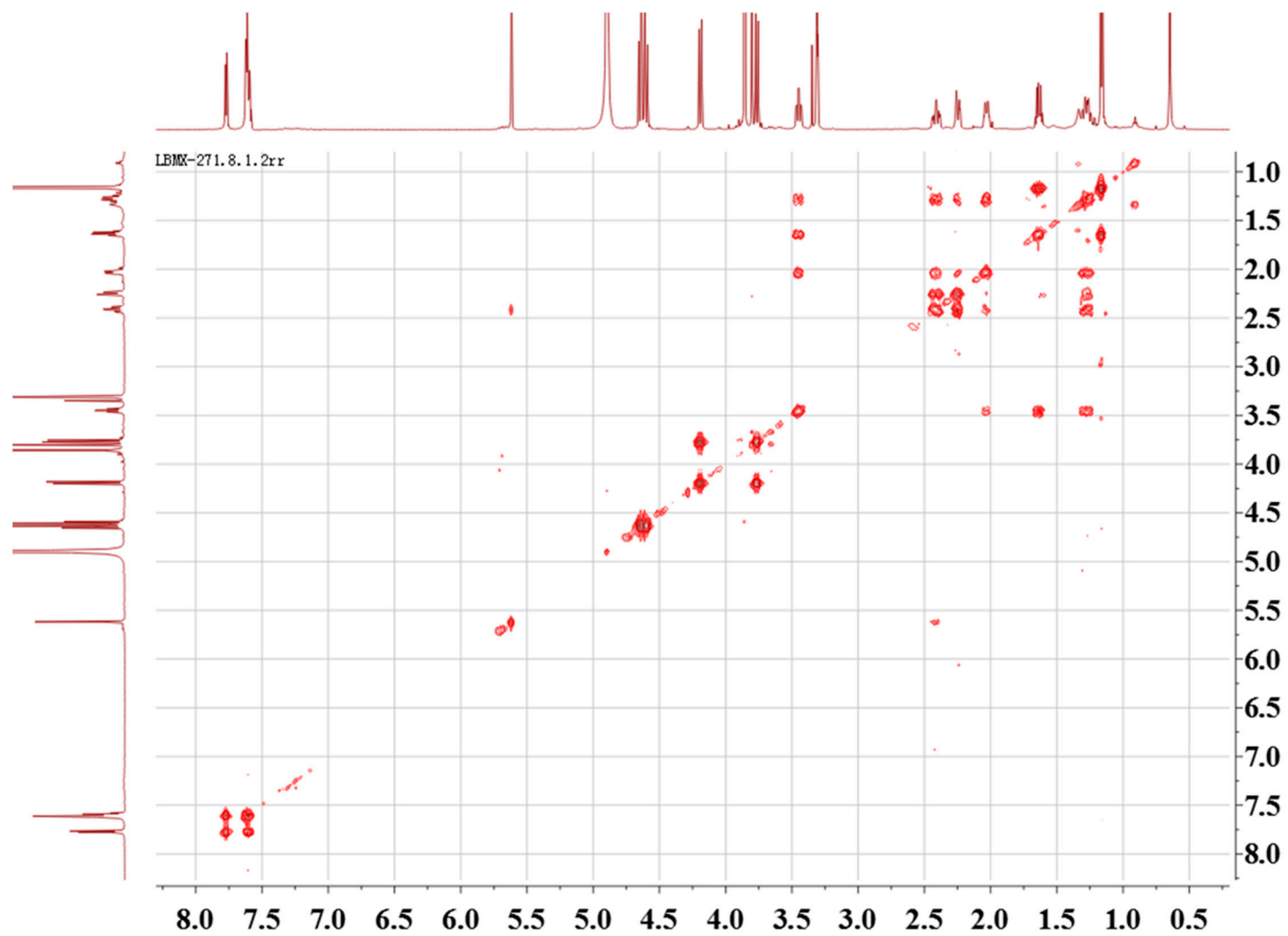


Figure S10 ROESY spectrum of **1** in CD₃OD

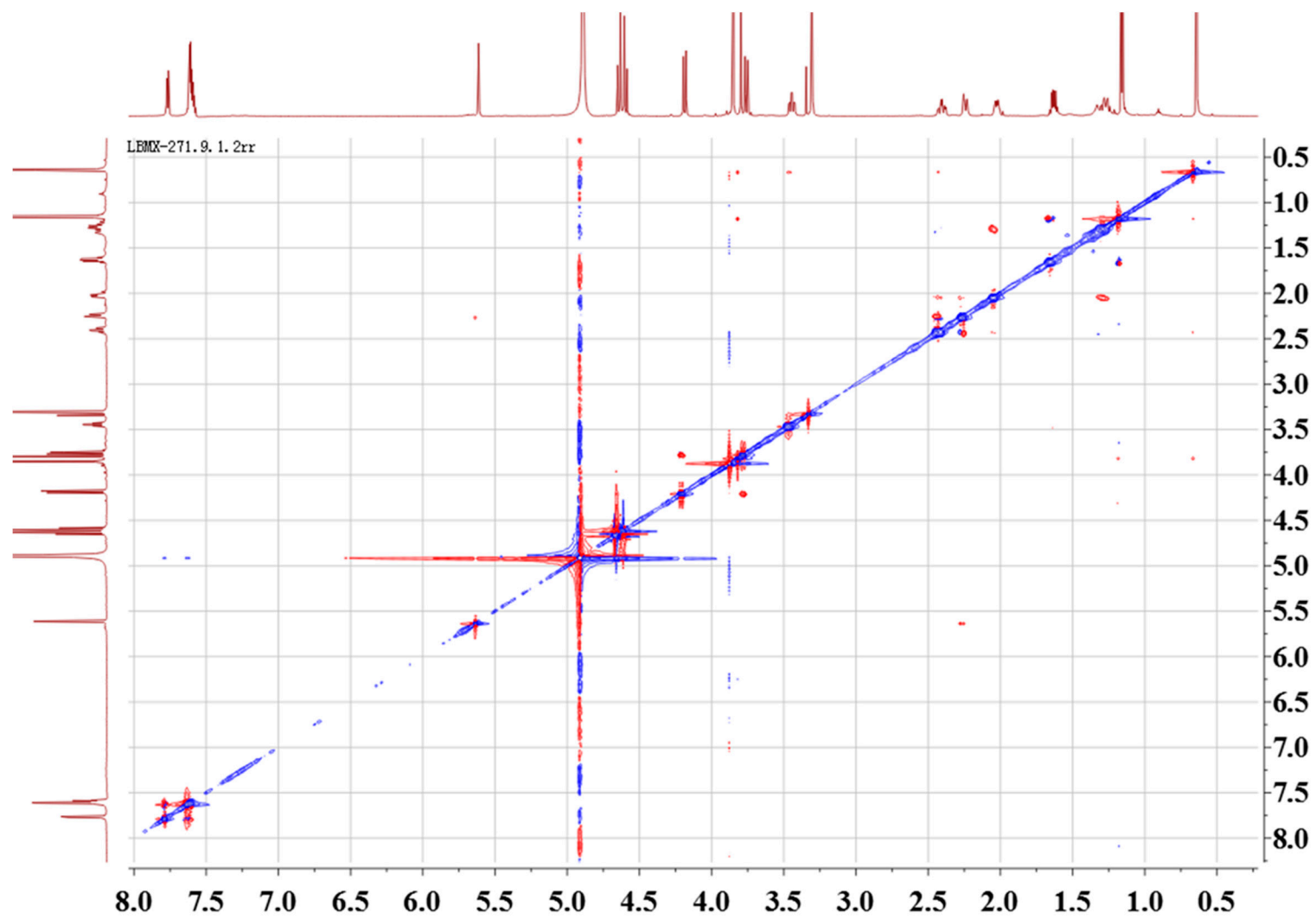


Figure S11 HRMS spectrum of **1**

LBMX-271 #11 RT: 0.14 AV: 1 NL: 7.18E8

T: FTMS + p ESI Full lock ms [150.0000-1100.0000]

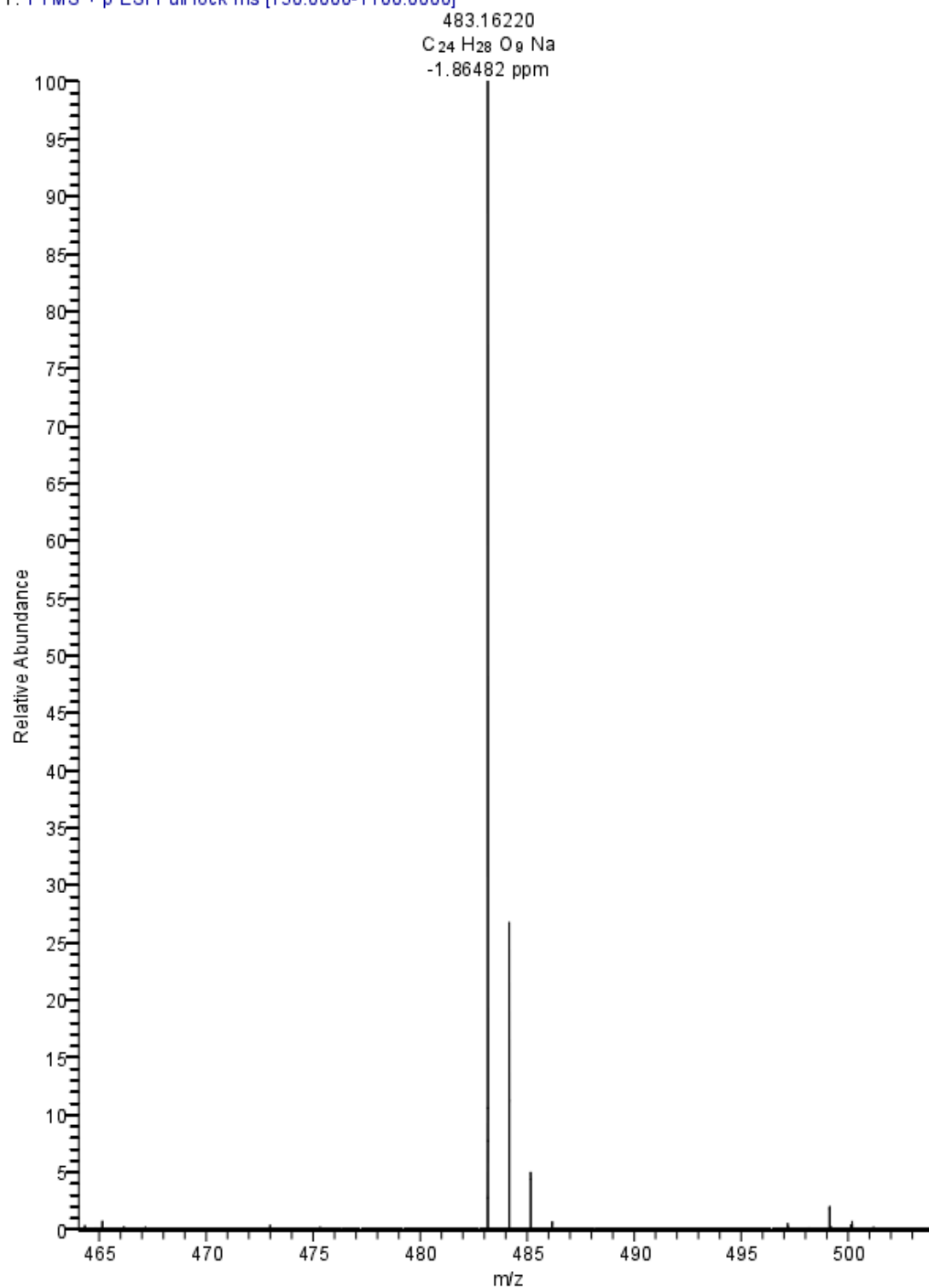


Figure S12 ^1H NMR spectrum of **2** in CD_3OD

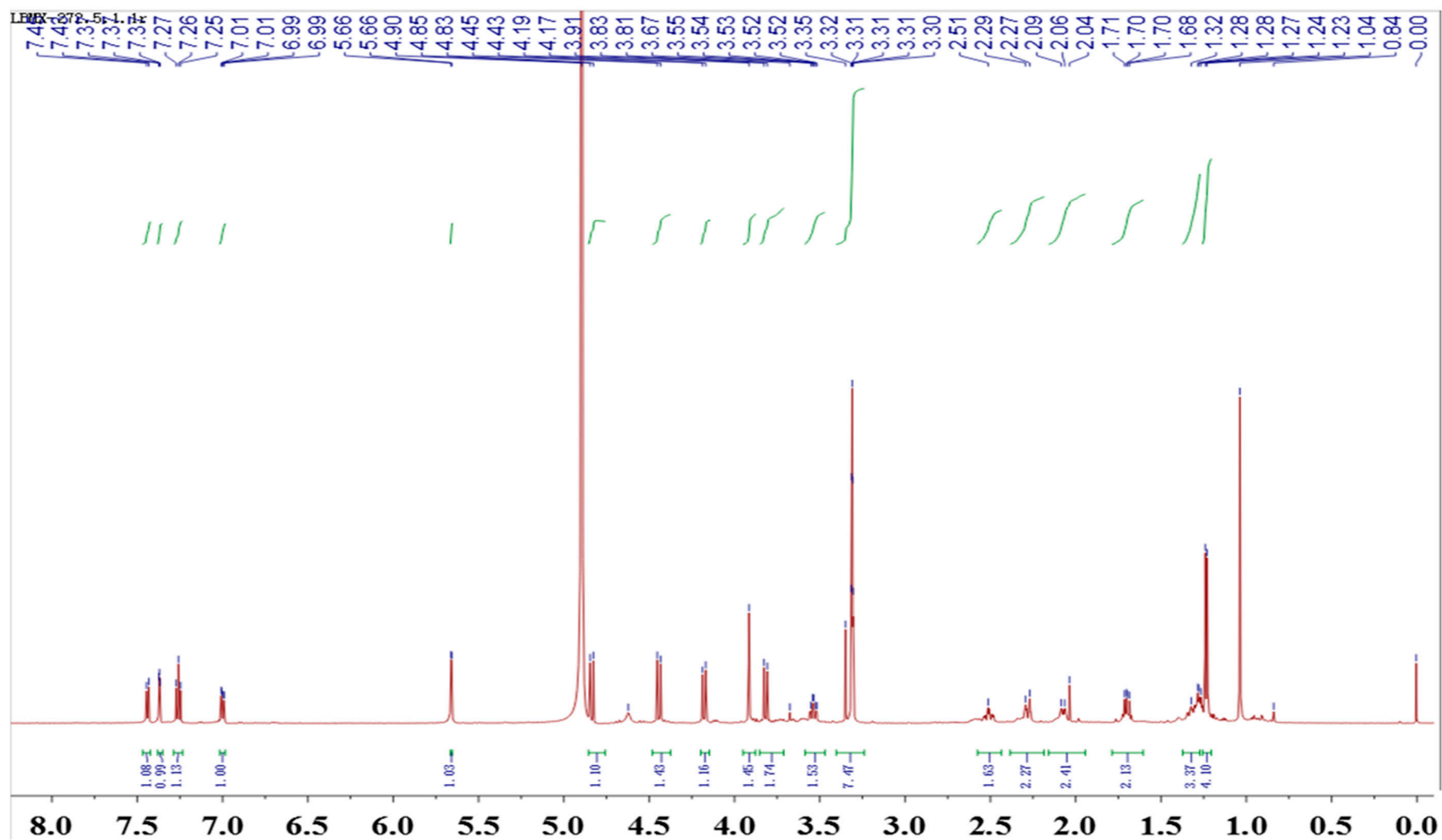


Figure S13 ^{13}C NMR spectrum of **2** in CD_3OD

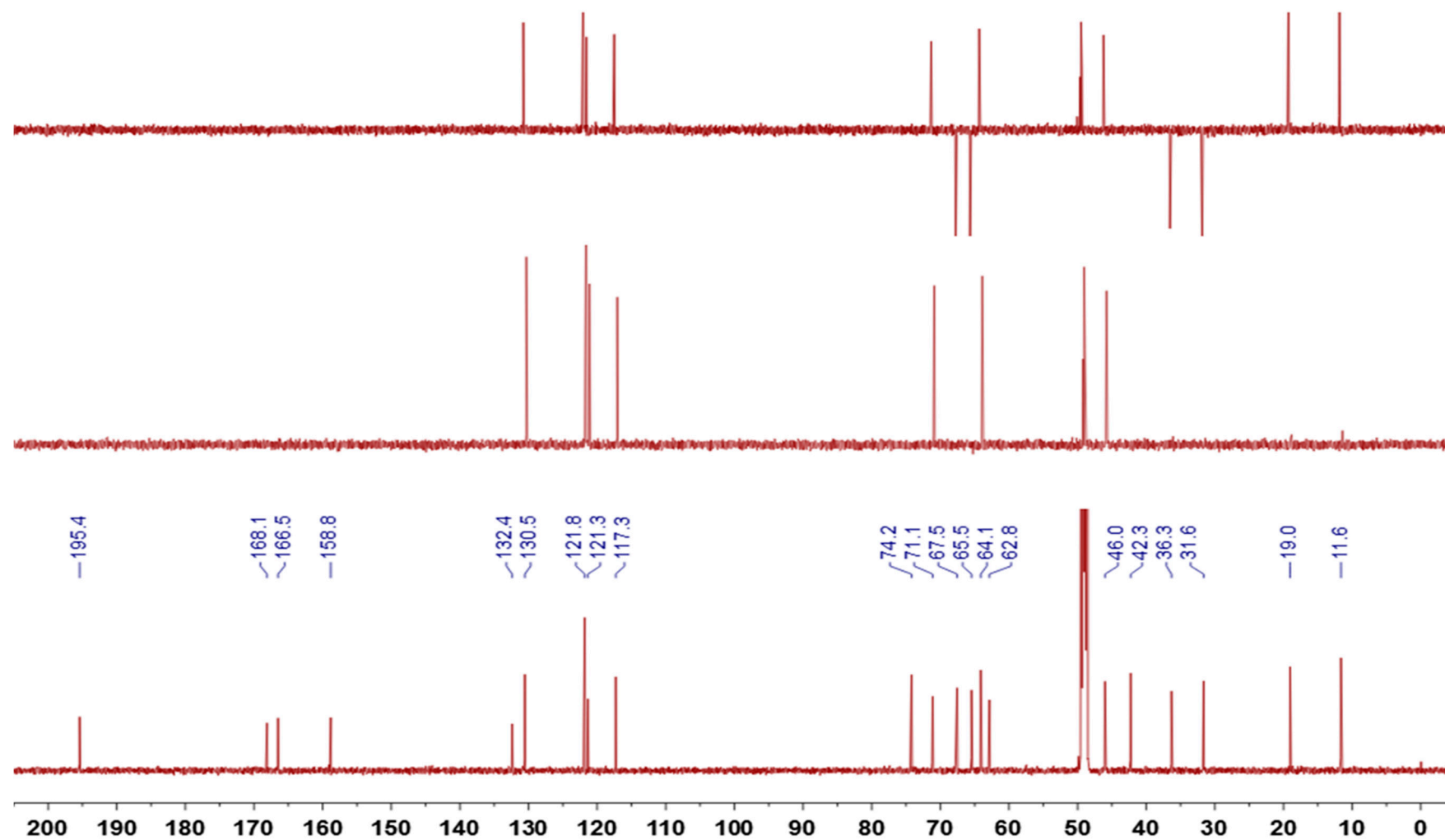


Figure S14 HSQC spectrum of **2** in CD₃OD

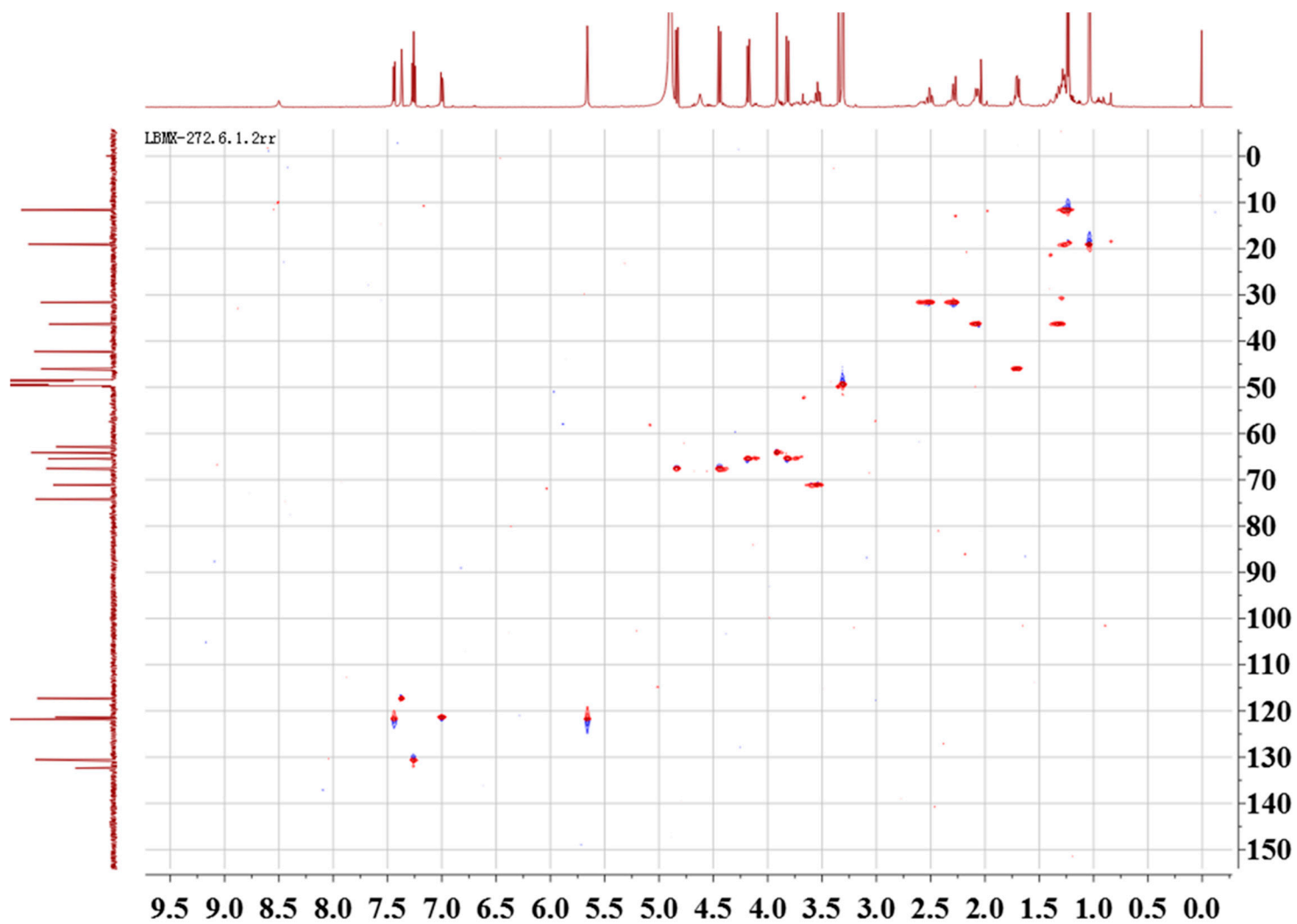


Figure S15 HMBC spectrum of **2** in CD₃OD

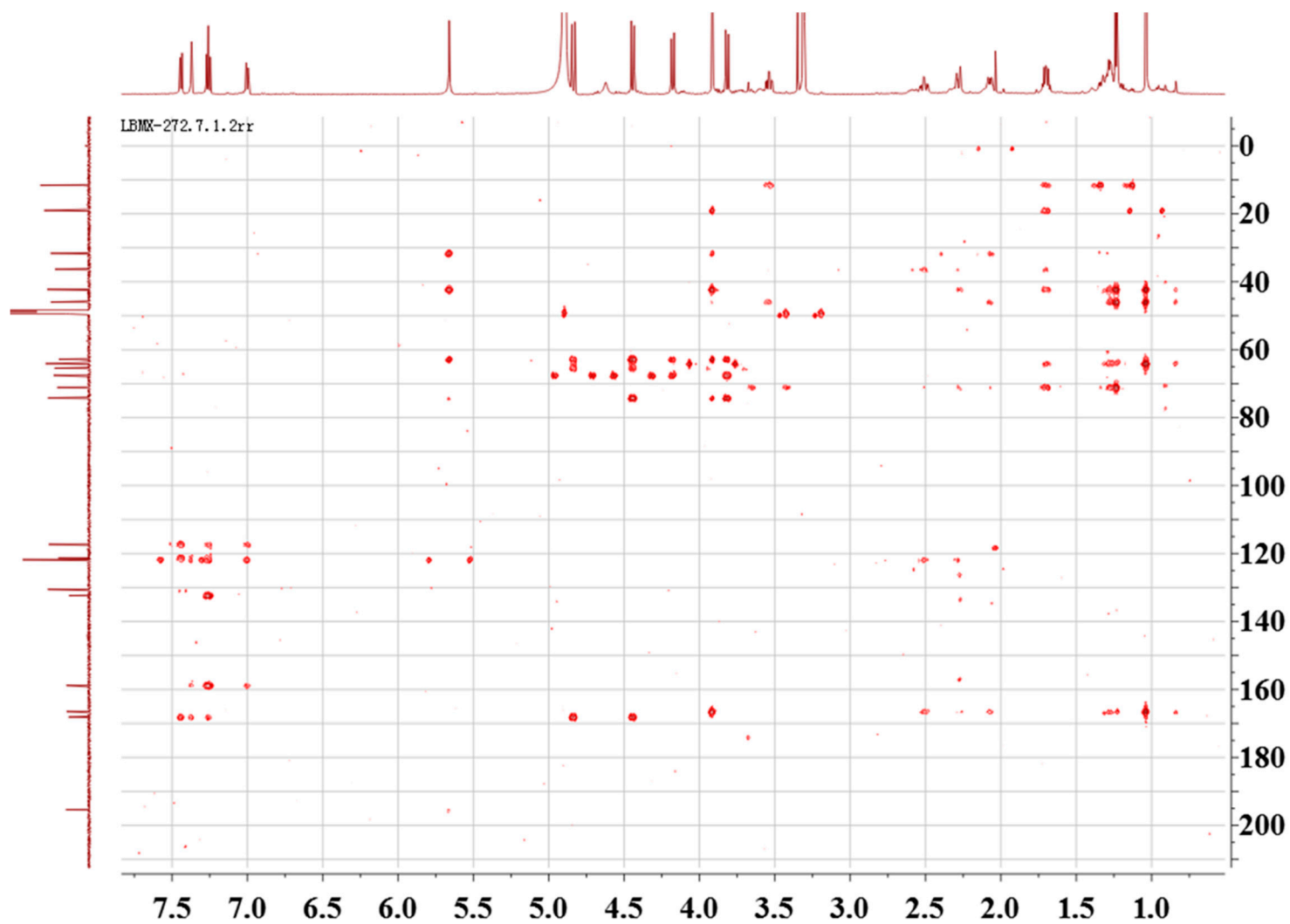


Figure S16 COSY spectrum of **2** in CD₃OD

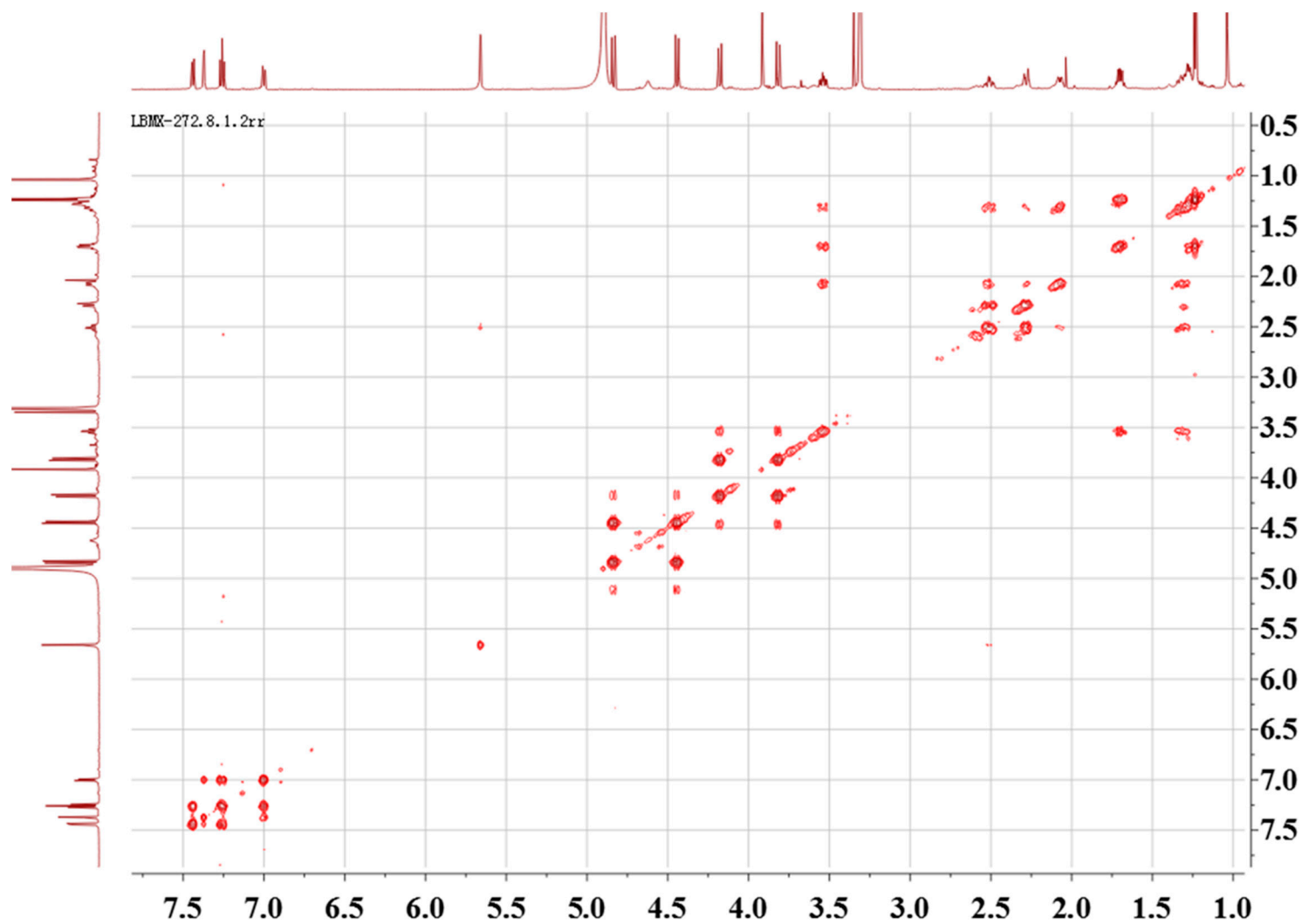


Figure S17 Roesy spectrum of **2** in CD₃OD

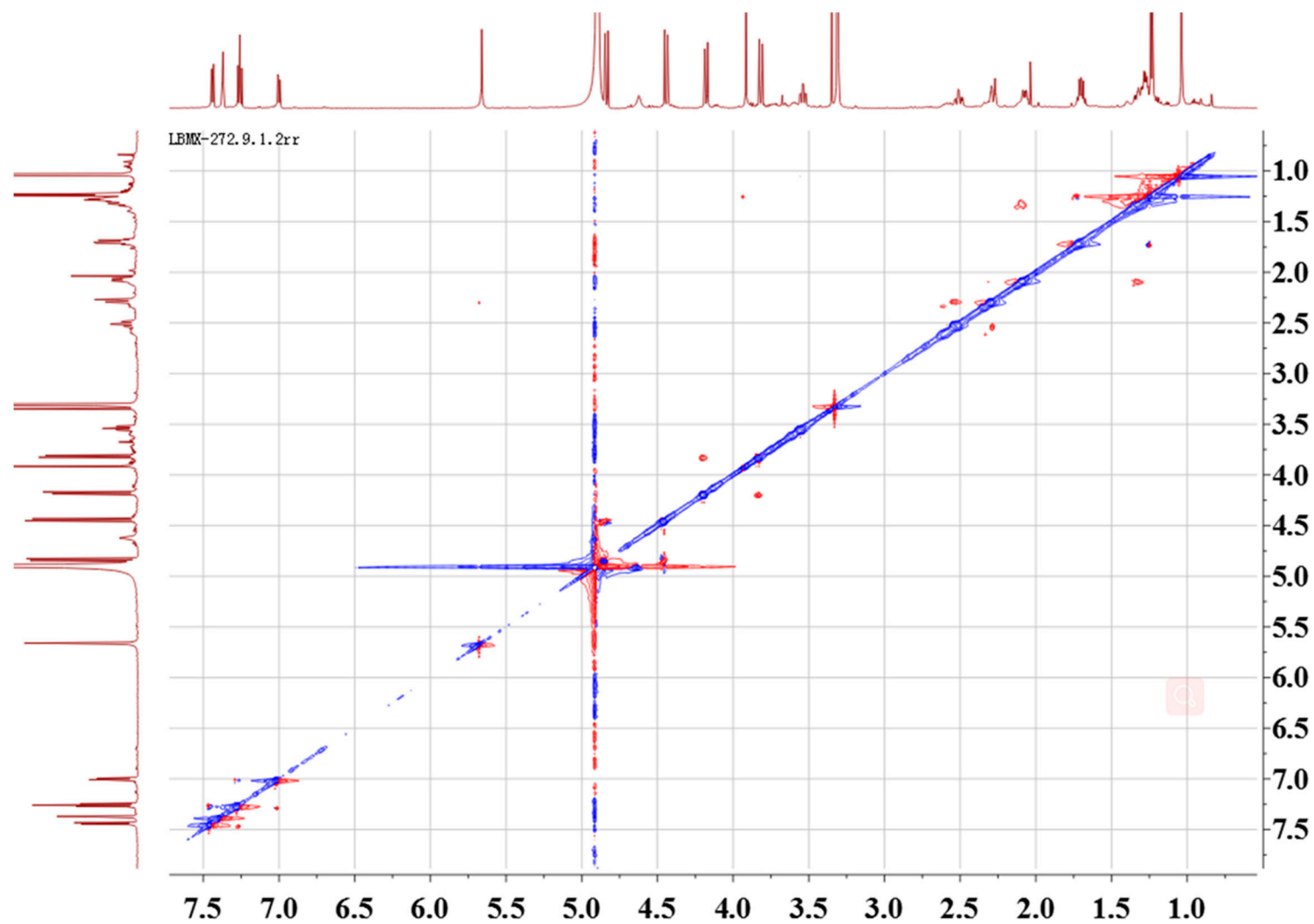


Figure S18 HRMS spectrum of **2**

LBMX-272 #13 RT: 0.17 AV: 1 NL: 1.47E8

T: FTMS + p ESI Full lock ms [150.0000-1100.0000]

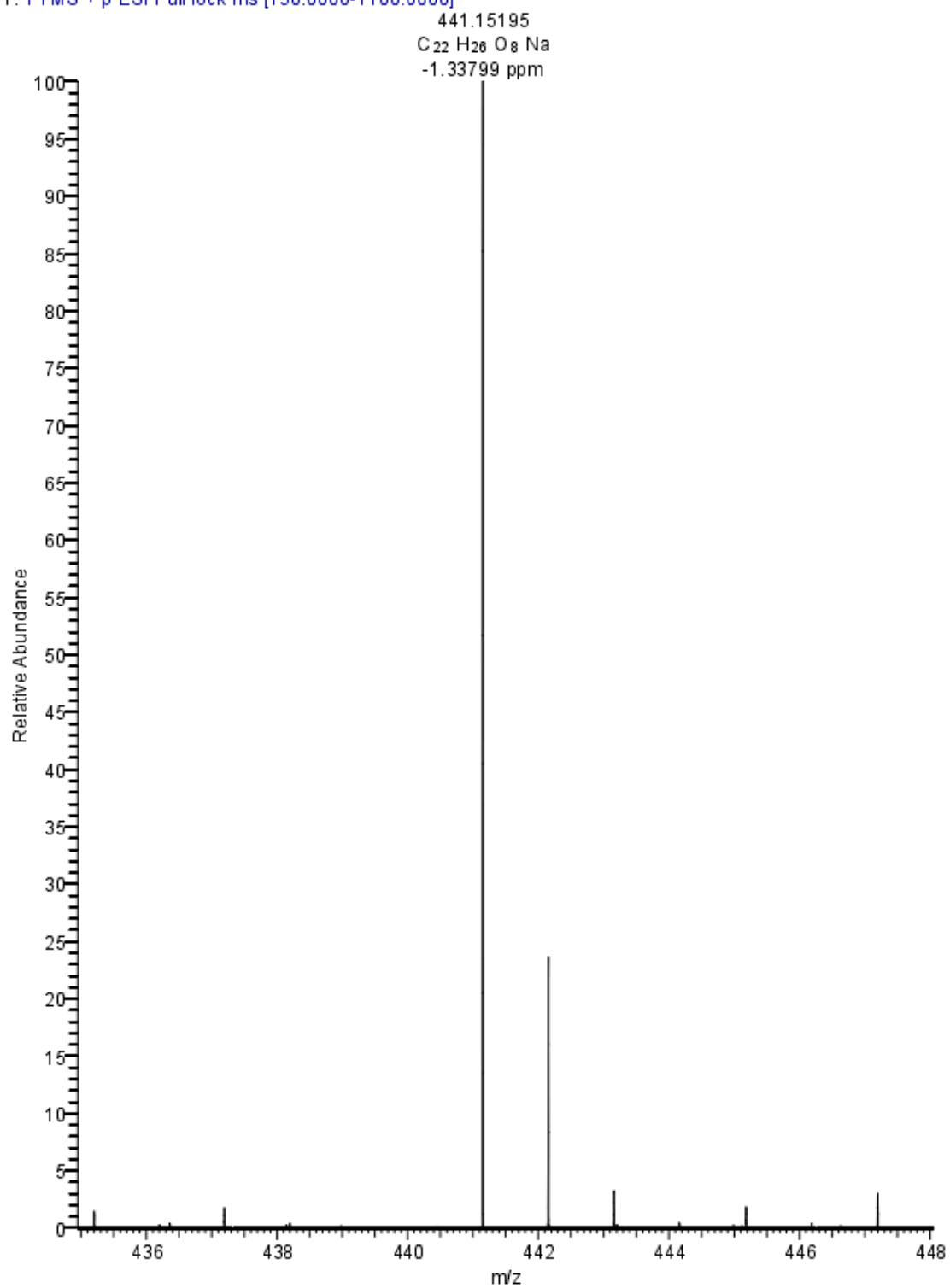


Figure S19 ^1H NMR spectrum of **3** in CD_3OD

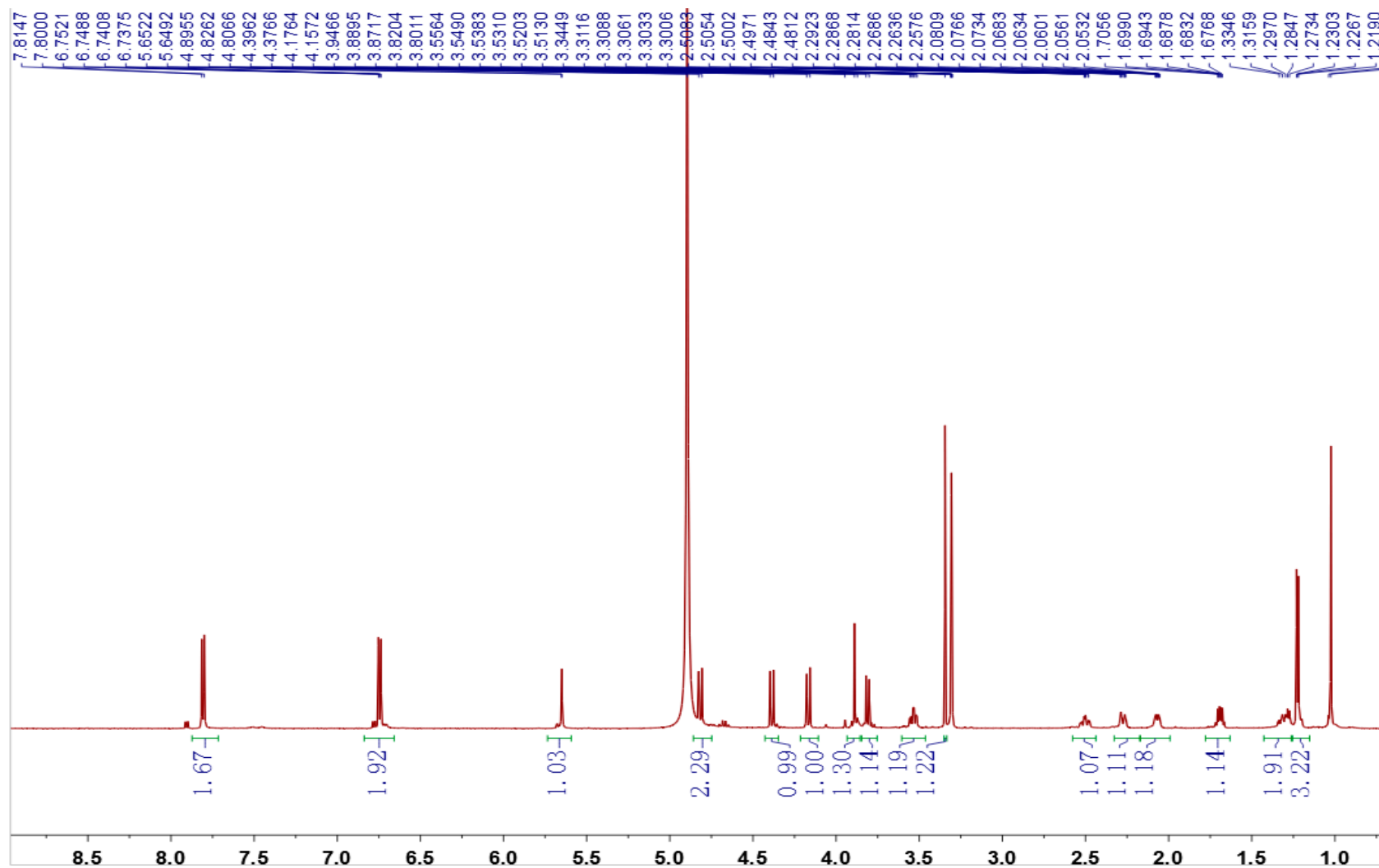


Figure S20 ^{13}C NMR spectrum of **3** in CD_3OD

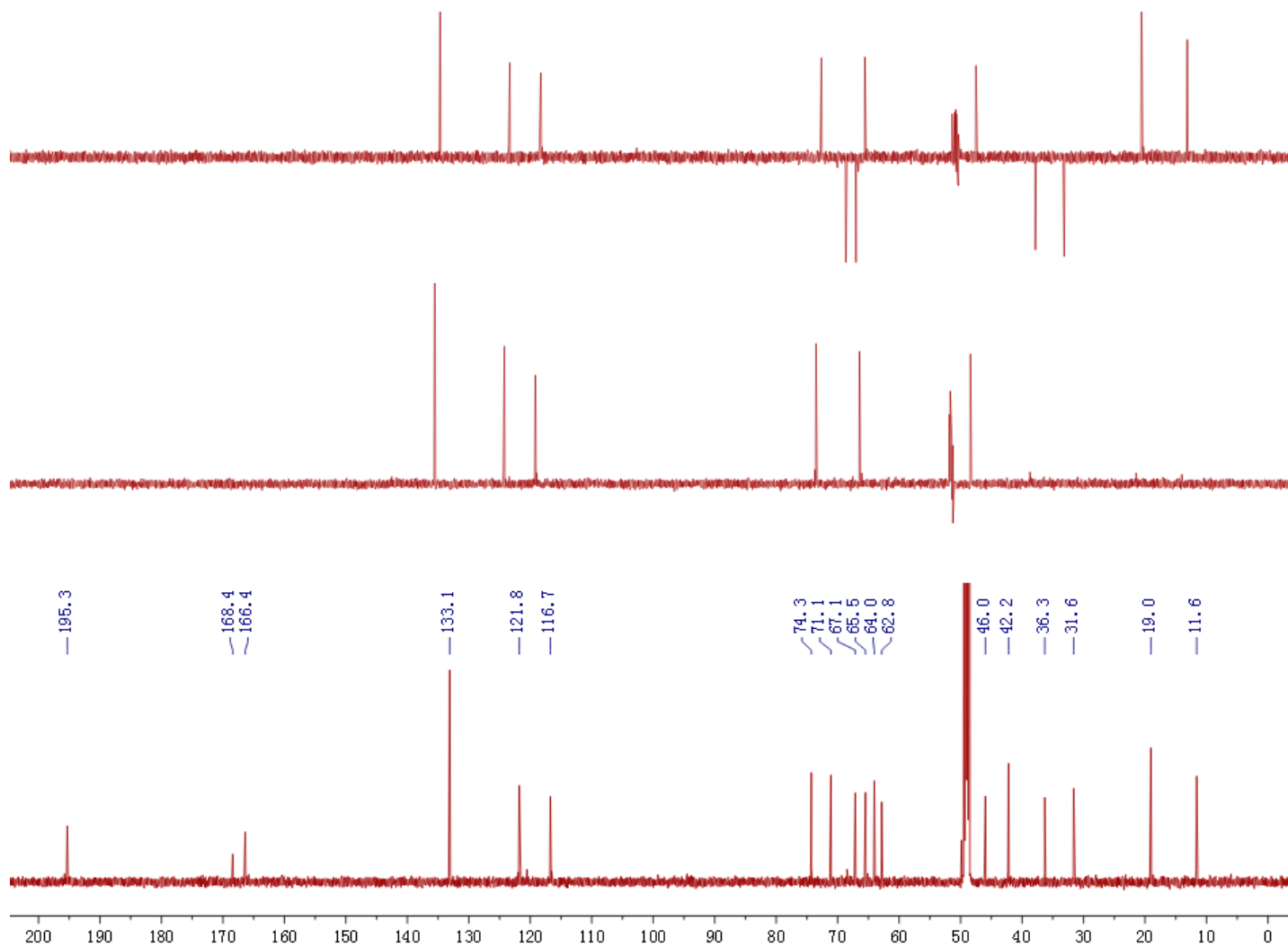


Figure S21 HSQC spectrum of **3** in CD₃OD

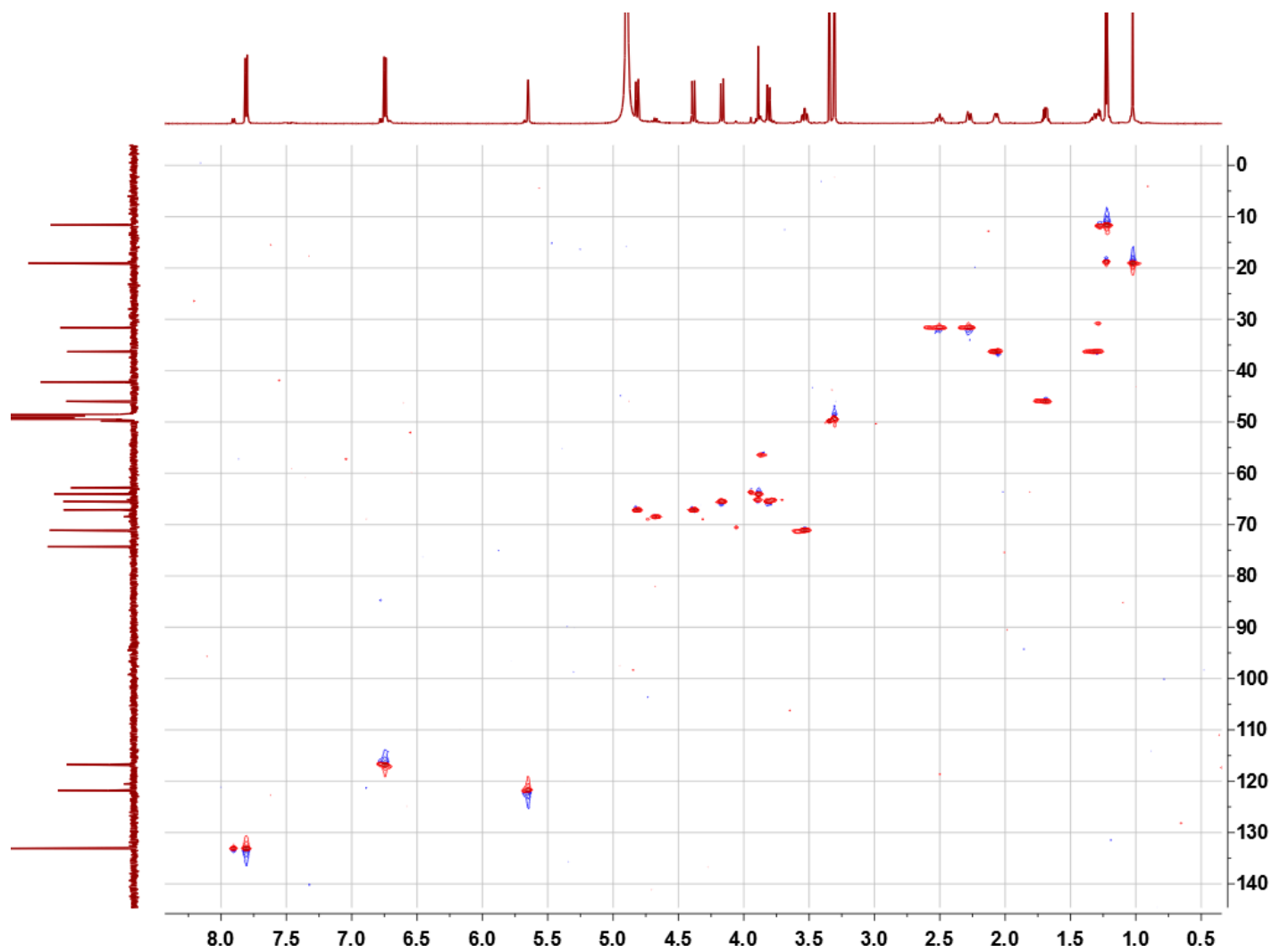


Figure S22 HMBC spectrum of **3** in CD₃OD

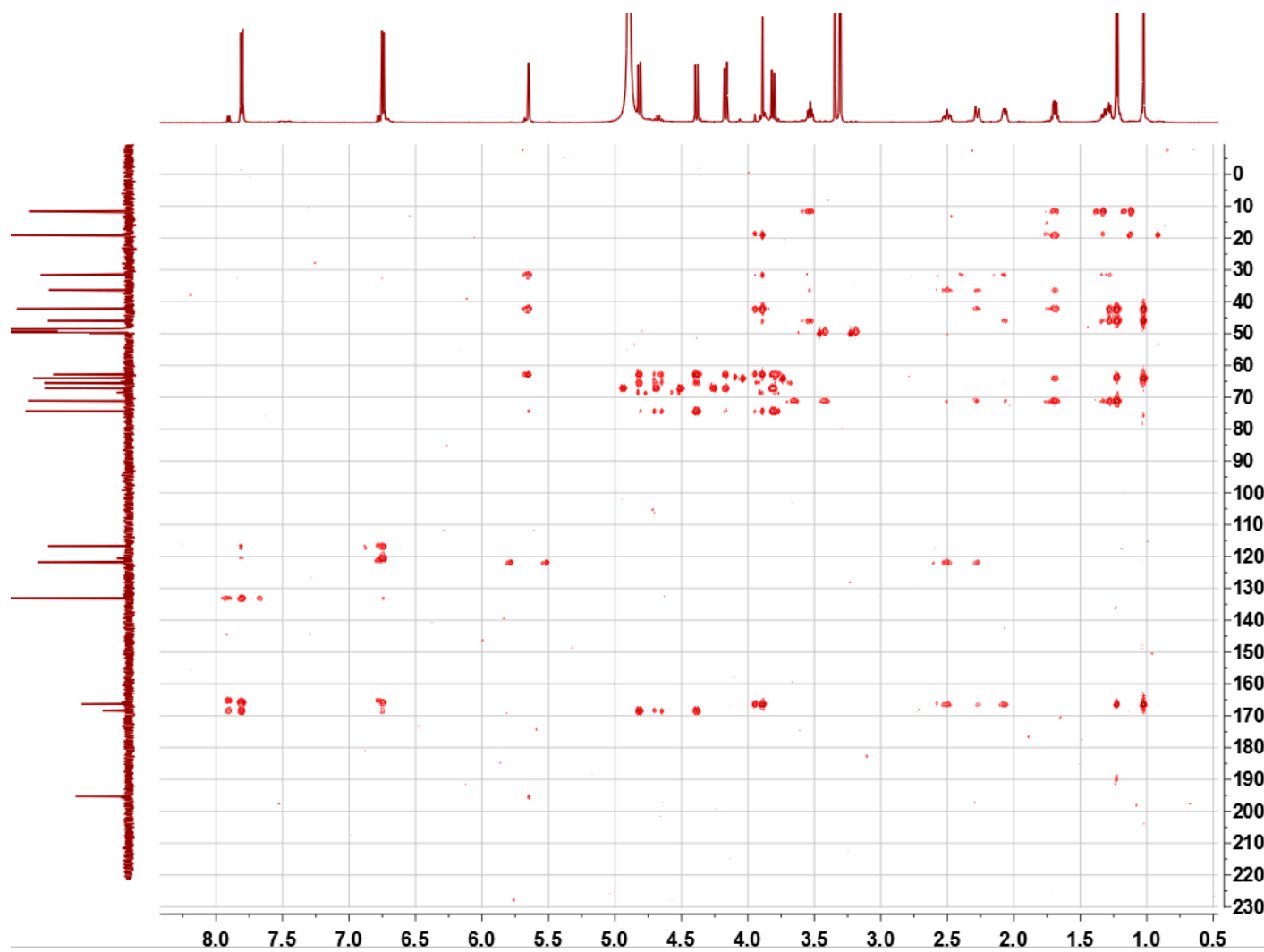


Figure S23 COSY spectrum of **3** in CD₃OD

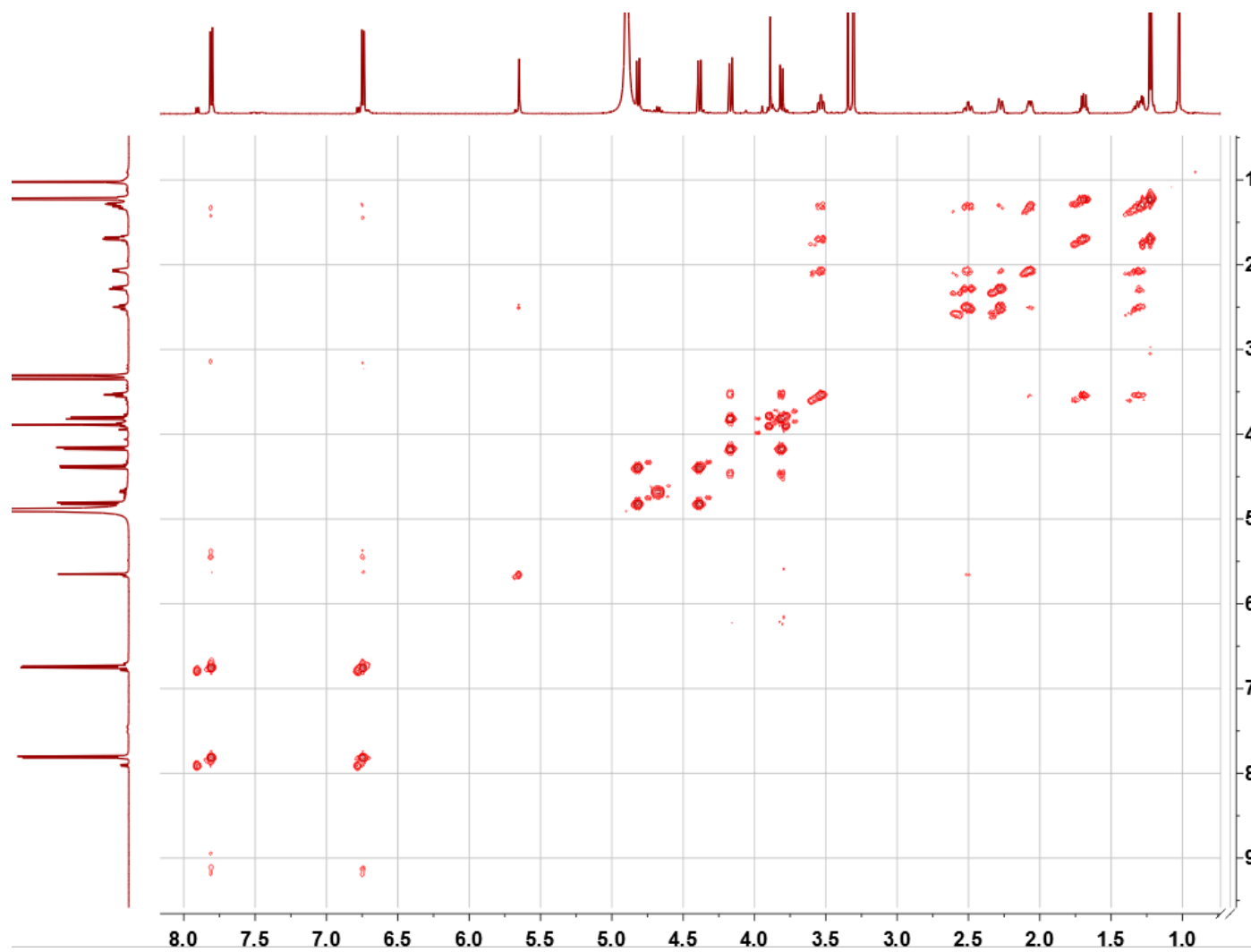


Figure S24 Roesy spectrum of **3** in CD₃OD

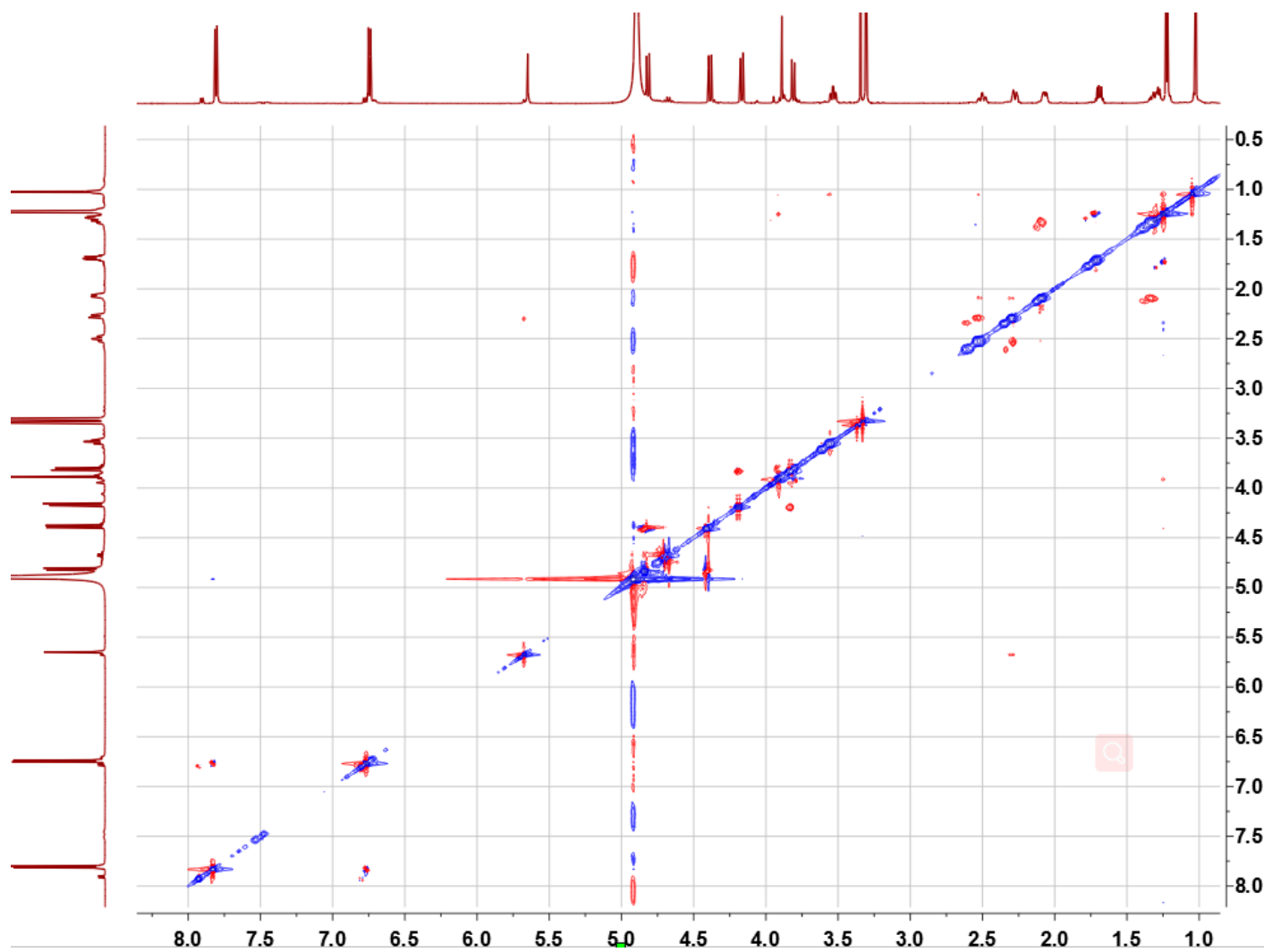


Figure S25 HRMS spectrum of **3**

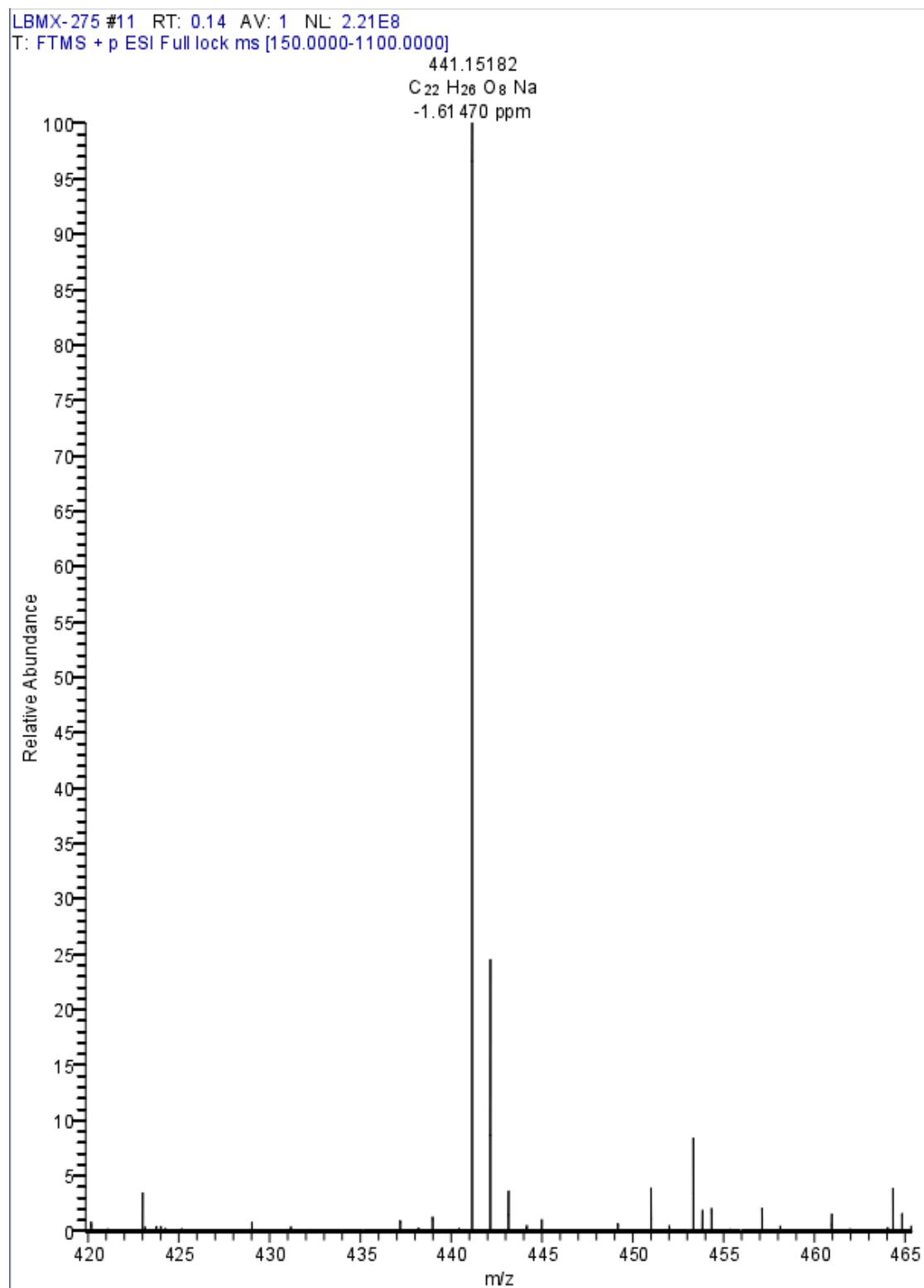


Figure S26 ^1H NMR spectrum of **4** in CD_3OD

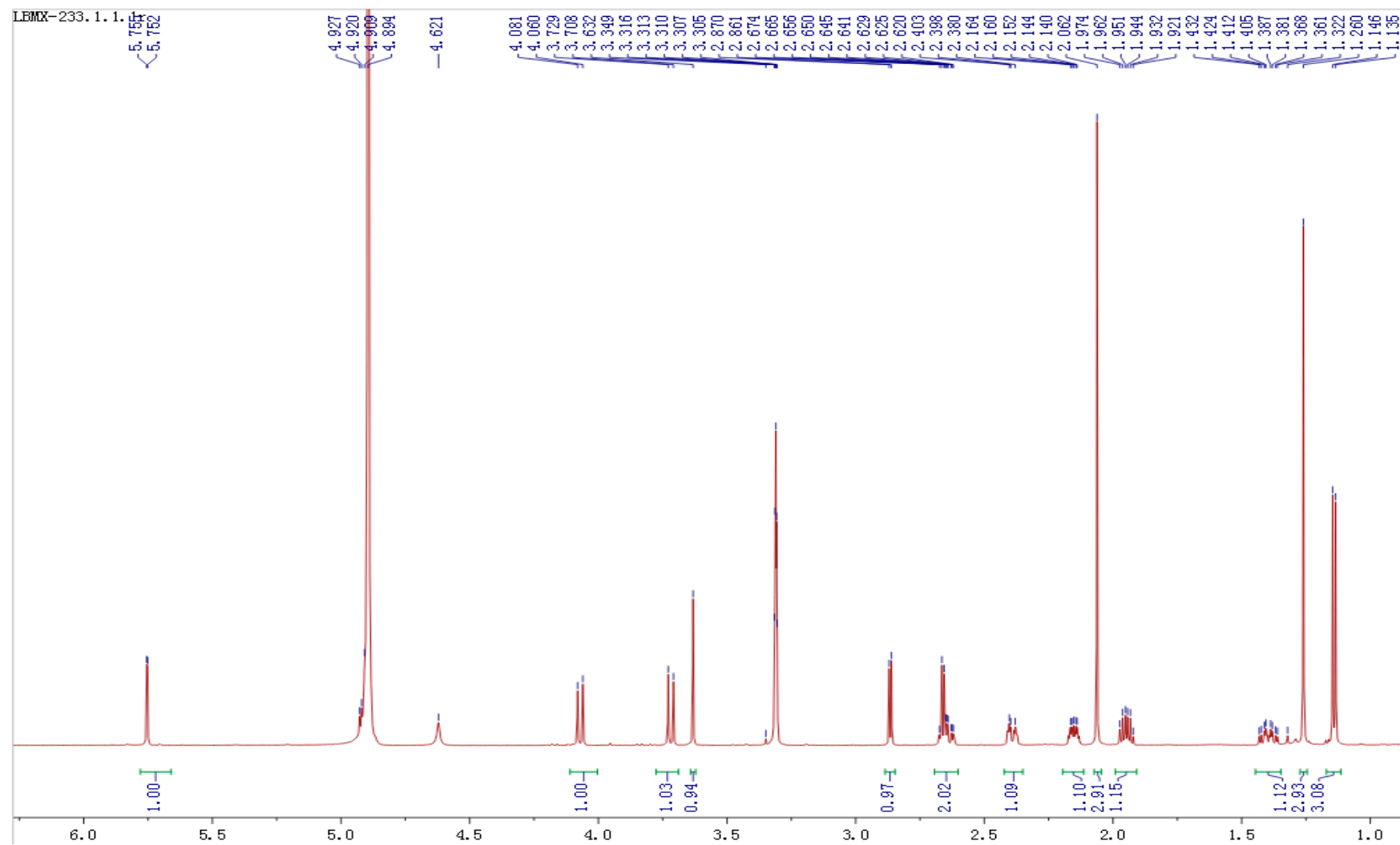


Figure S27 ^{13}C NMR spectrum of **4** in CD_3OD

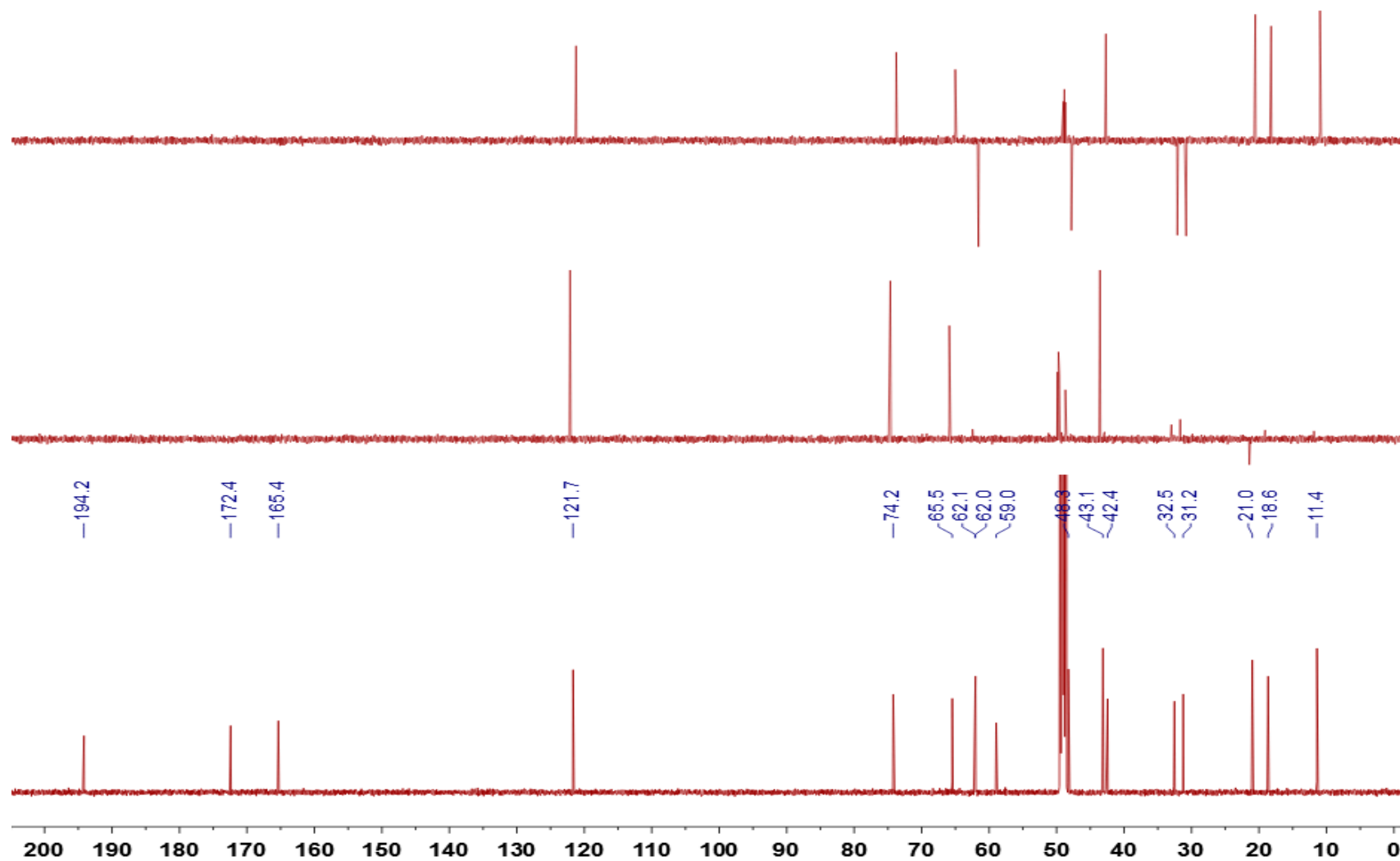


Figure S28 HSQC spectrum of **4** in CD₃OD

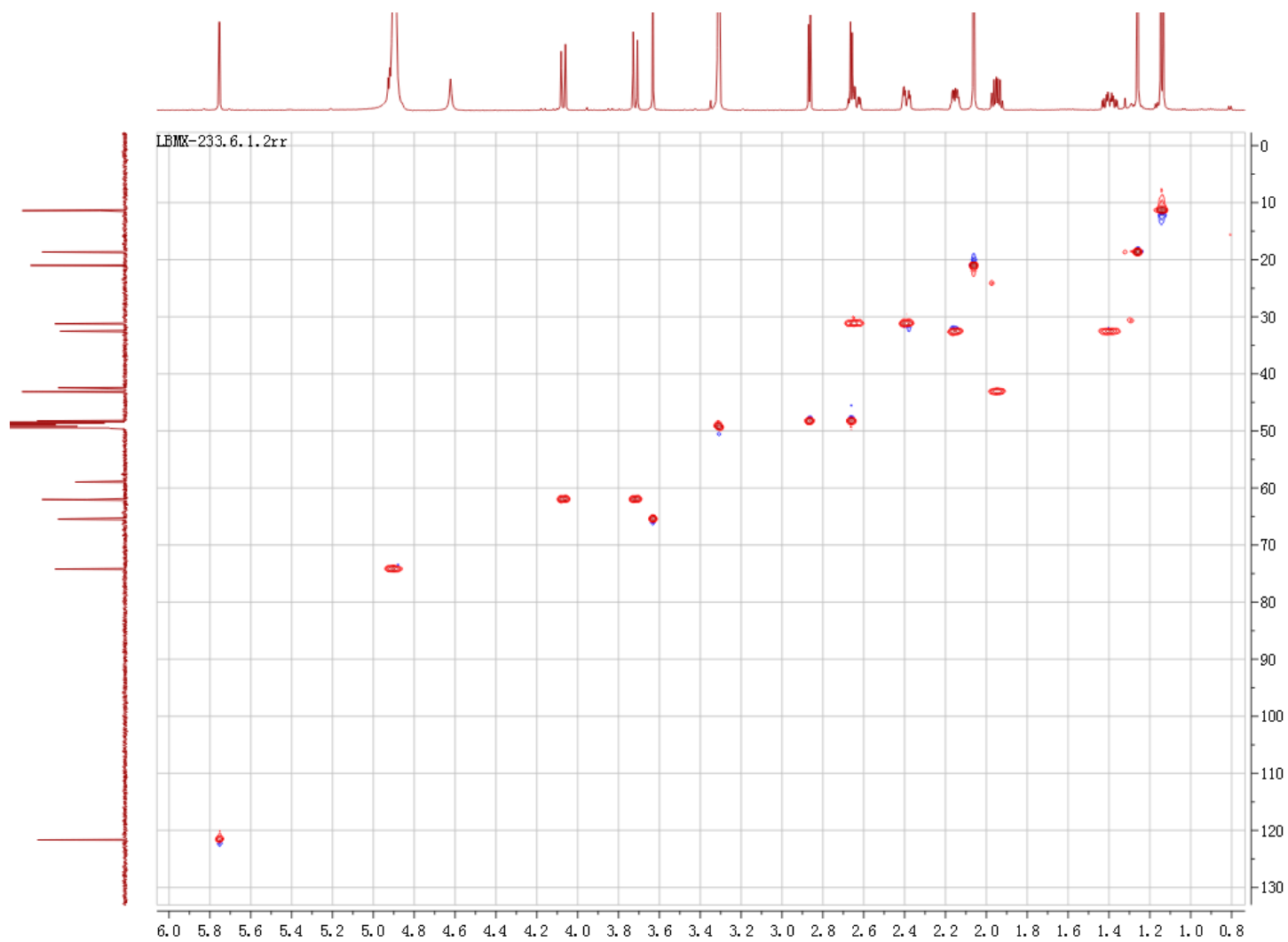


Figure S29 HMBC spectrum of **4** in CD₃OD

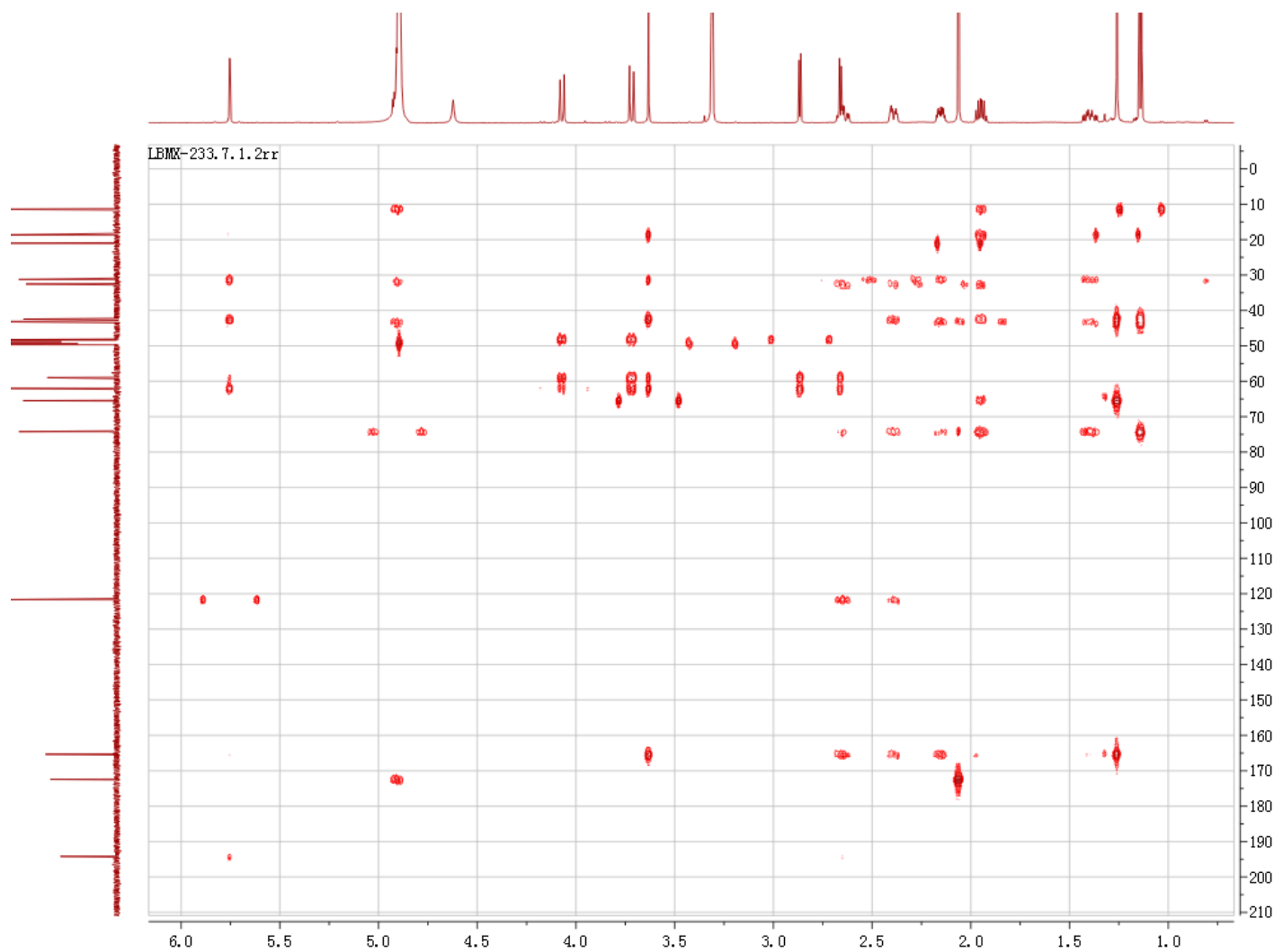


Figure S30 COSY spectrum of **4** in CD₃OD

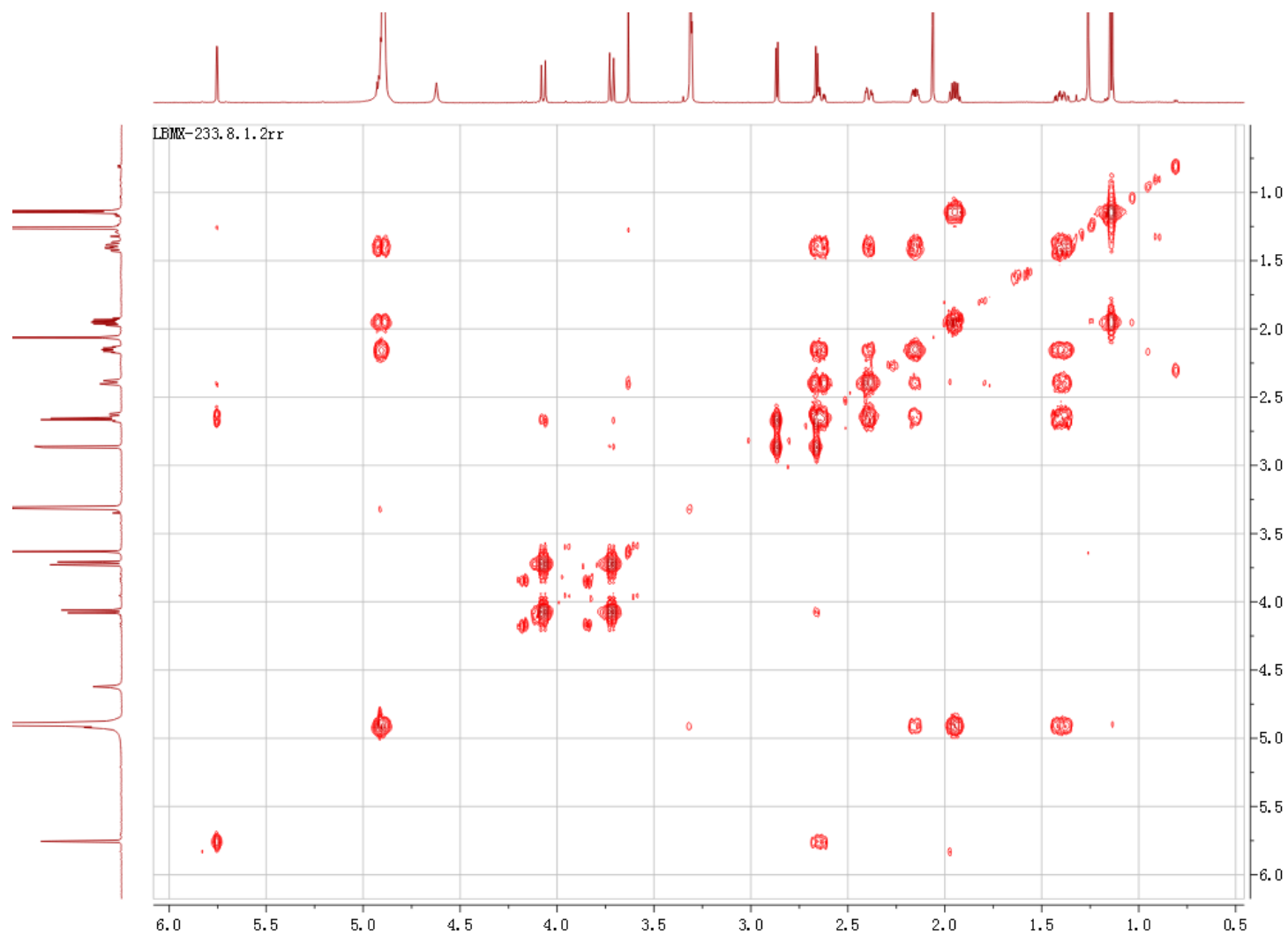


Figure S31 Roesy spectrum of 4 in CD₃OD

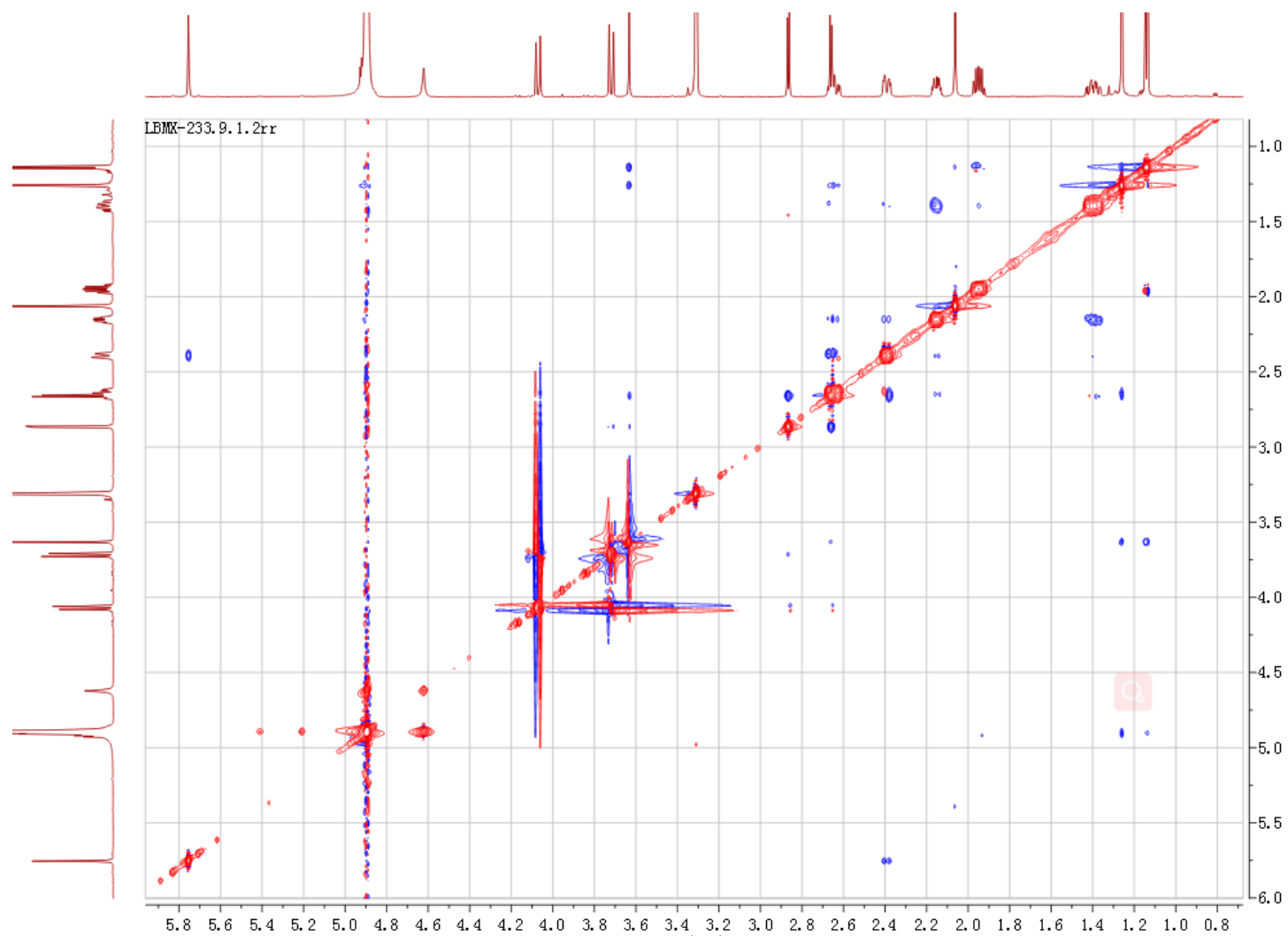


Figure S32 HRMS spectrum of **4**

LBMX-233 #13 RT: 0.17 AV: 1 SB: 8 1.32-1.53 NL: 1.58E8
T: FTMS + p ESI Full ms [150.0000-1100.0000]

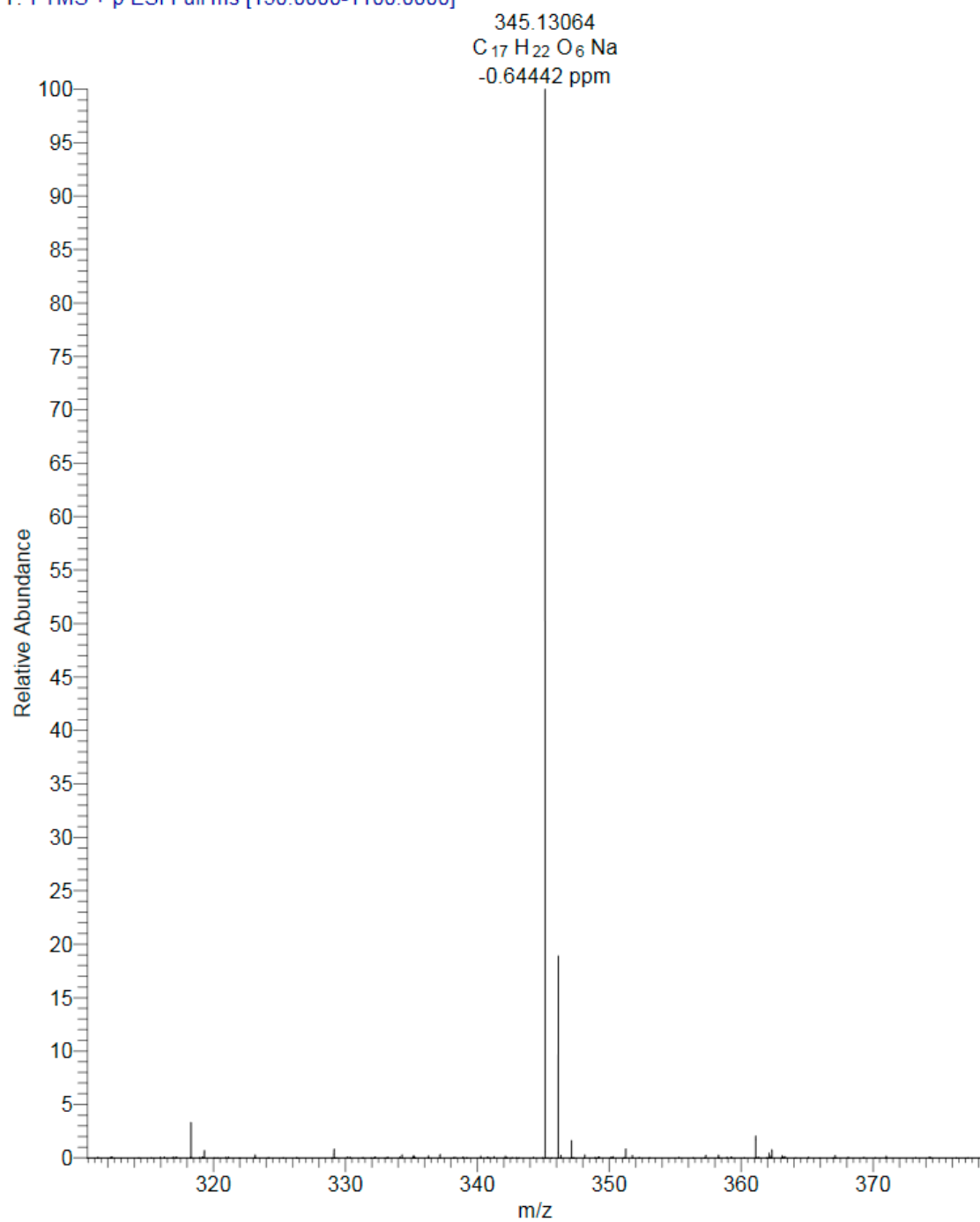


Figure S33 CD spectrum of **1-4** in MeOH

