SUPPORTING INFORMATION

A novel diterpene and six new sesquiterpenes from the sea hare *Aplysia dactylomela*

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1. Experimental section

Figure S1. HRESIMS spectrum of compound **1**

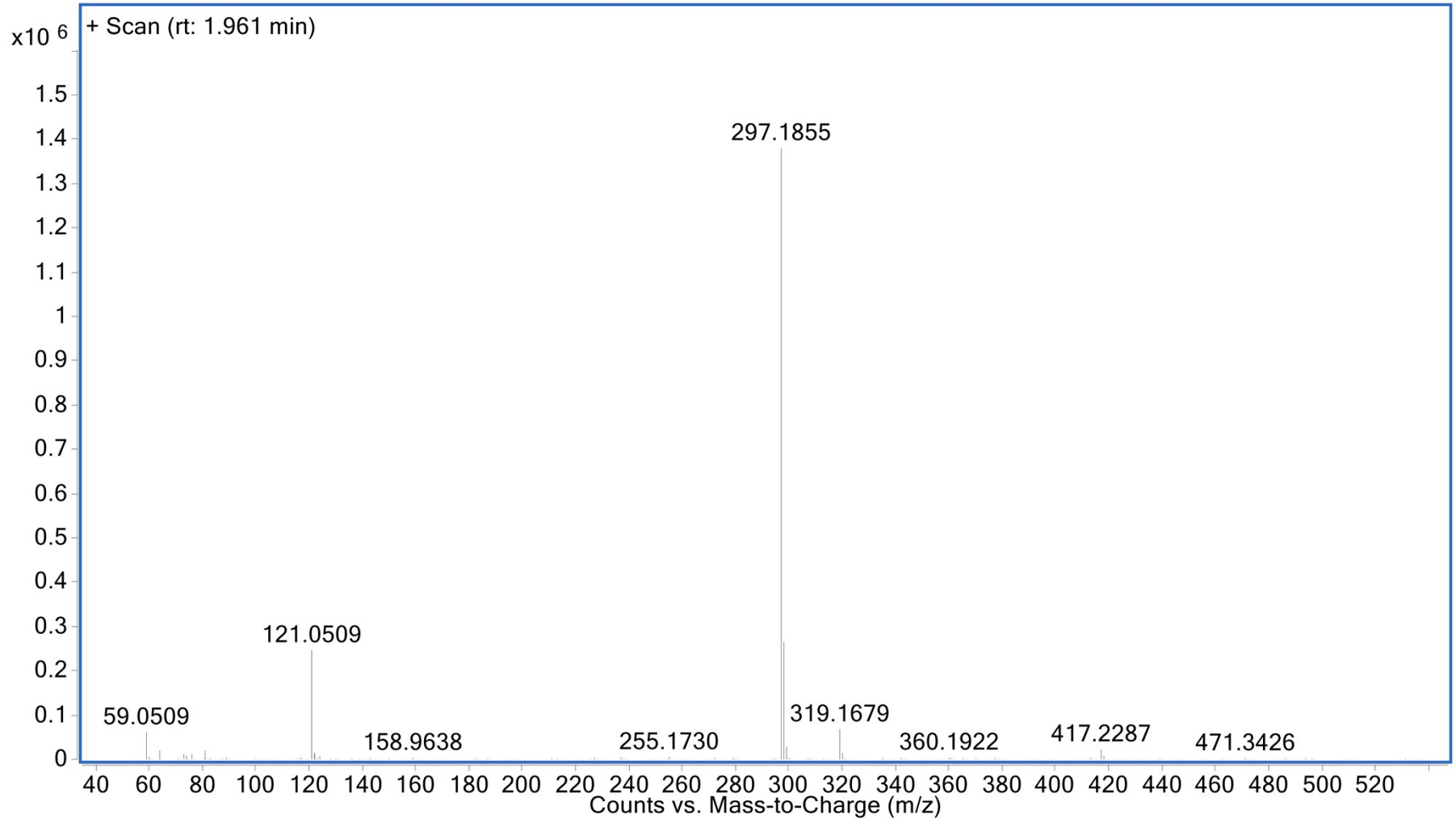


Figure S2a. ^{1}H NMR spectrum (600 MHz, $CDCl_3$) of compound **1**

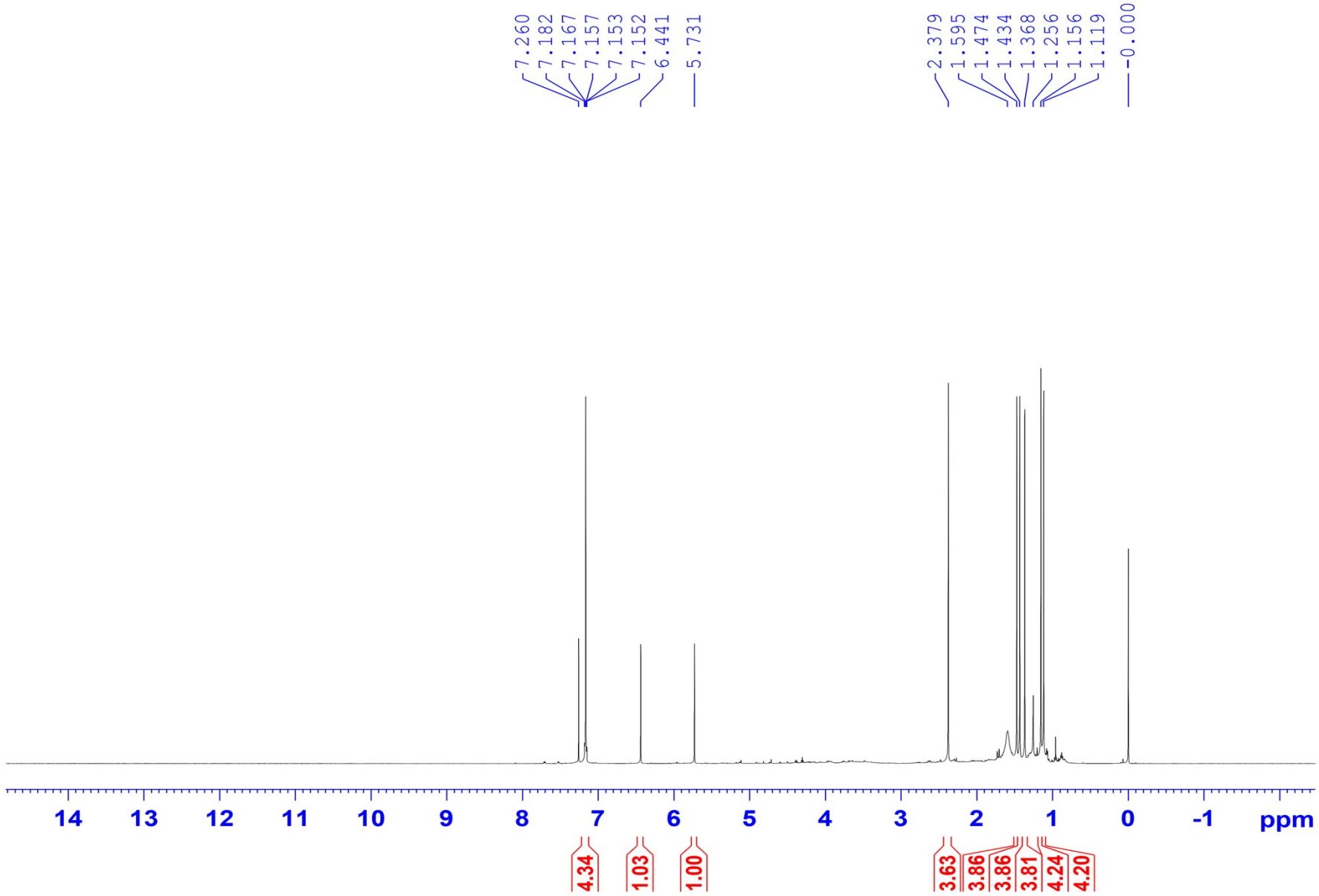


Figure S2b. Expanded ^{1}H NMR spectrum (600 MHz, $CDCl_3$) of compound **1**

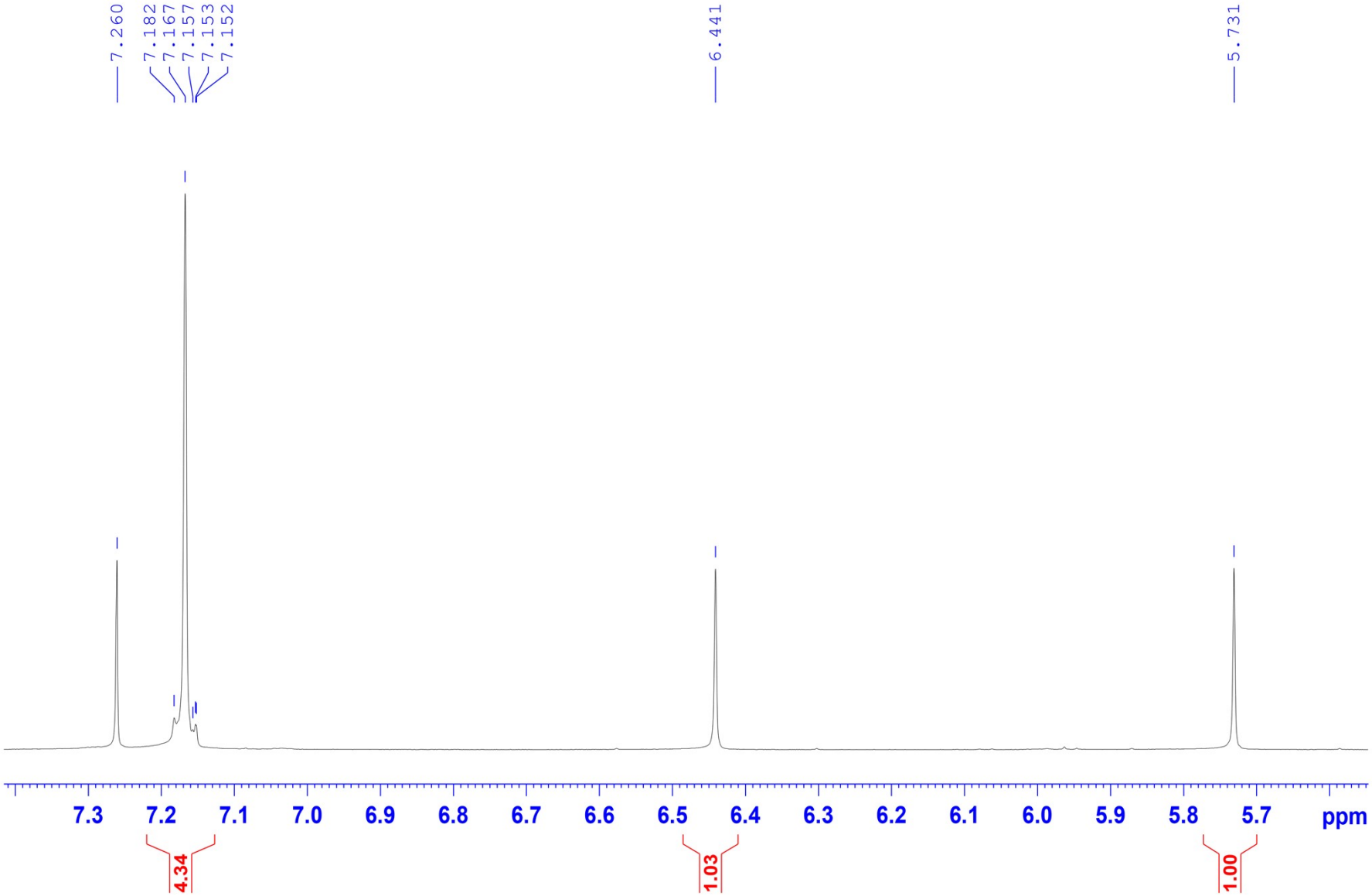


Figure S3. ^{13}C NMR spectrum (150 MHz, $CDCl_3$) of compound **1**

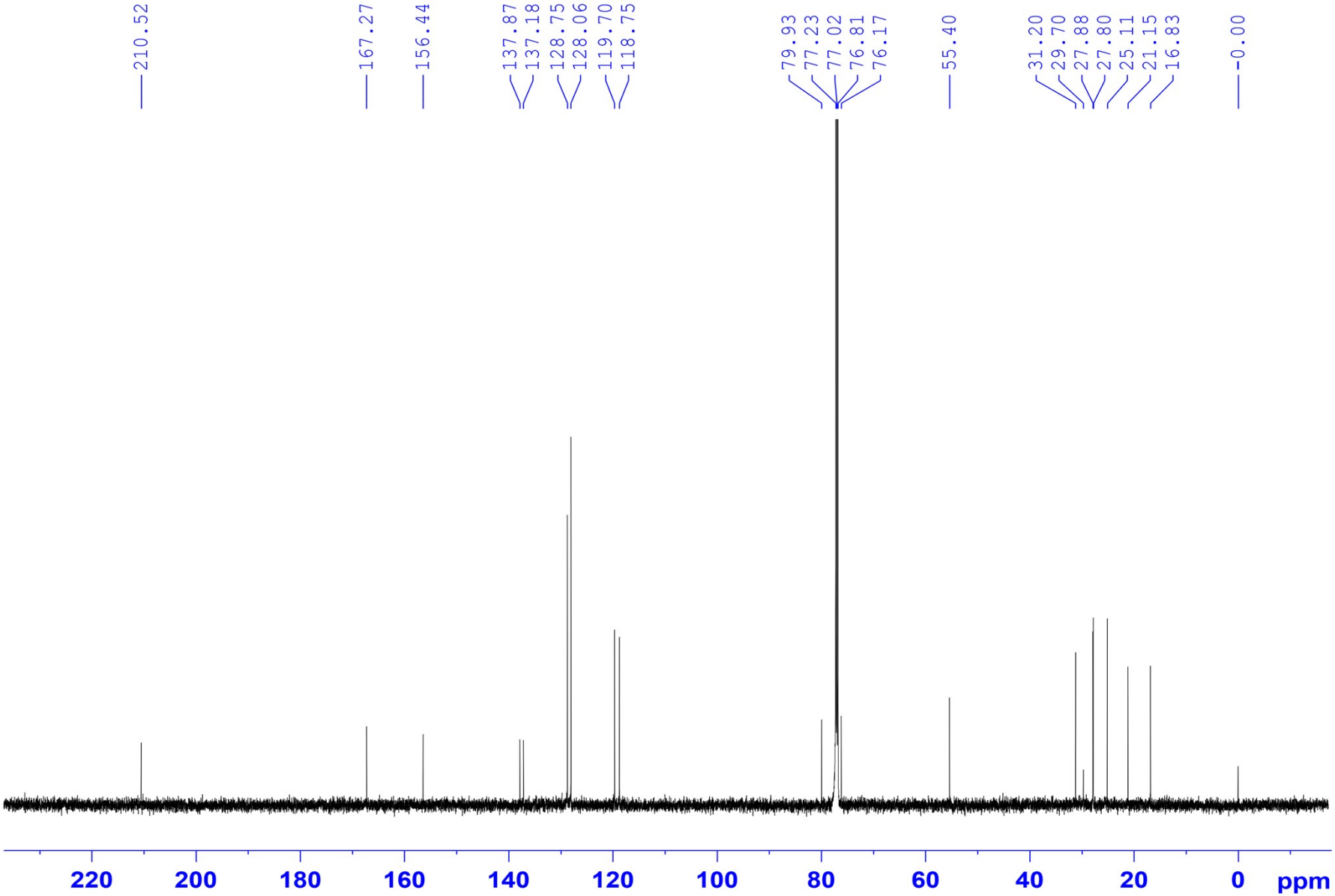


Figure S4a. HSQC spectrum (in $CDCl_3$) of compound **1**

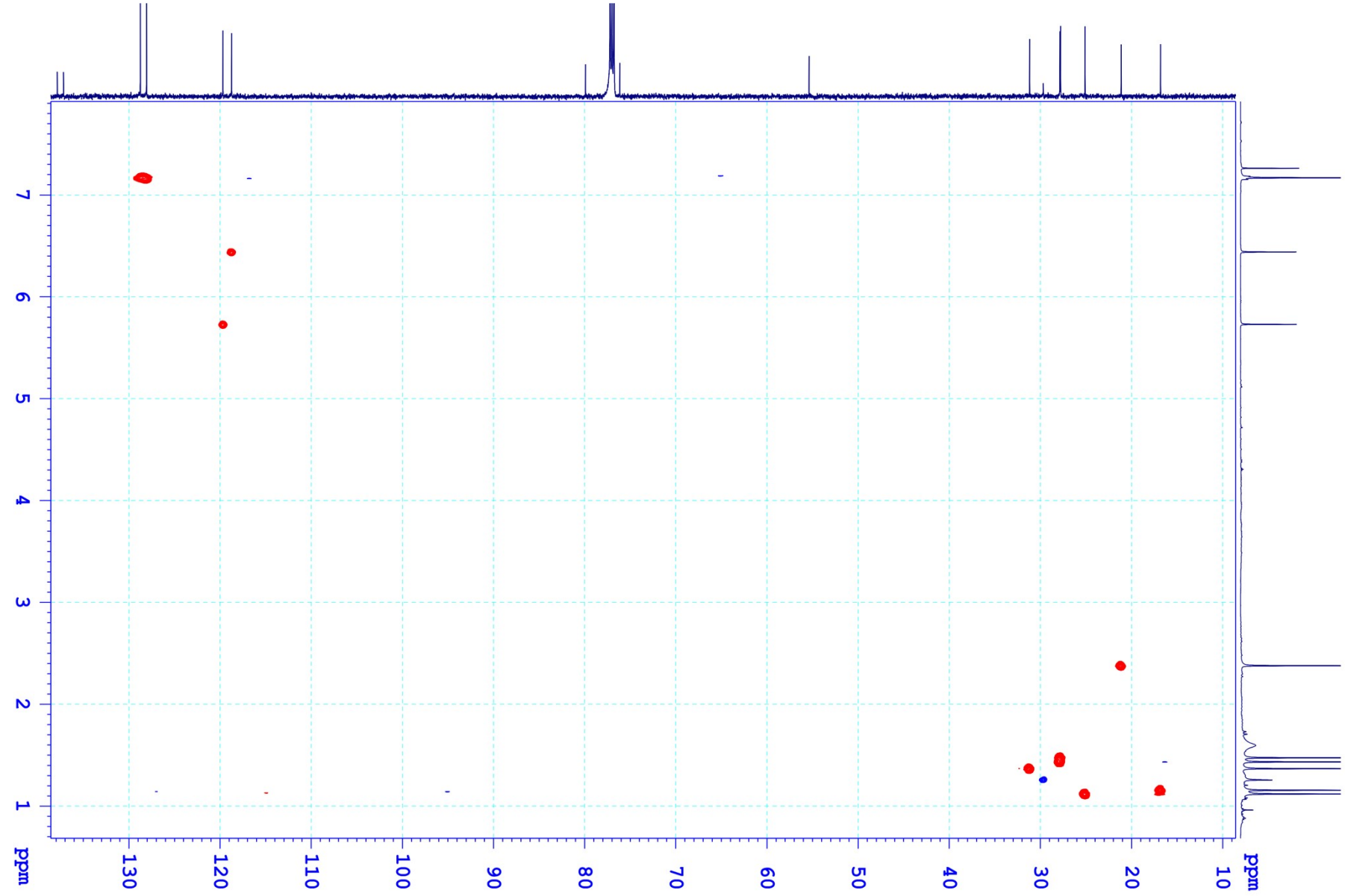


Figure S4b. Expanded HSQC spectrum (in $CDCl_3$) of compound **1**

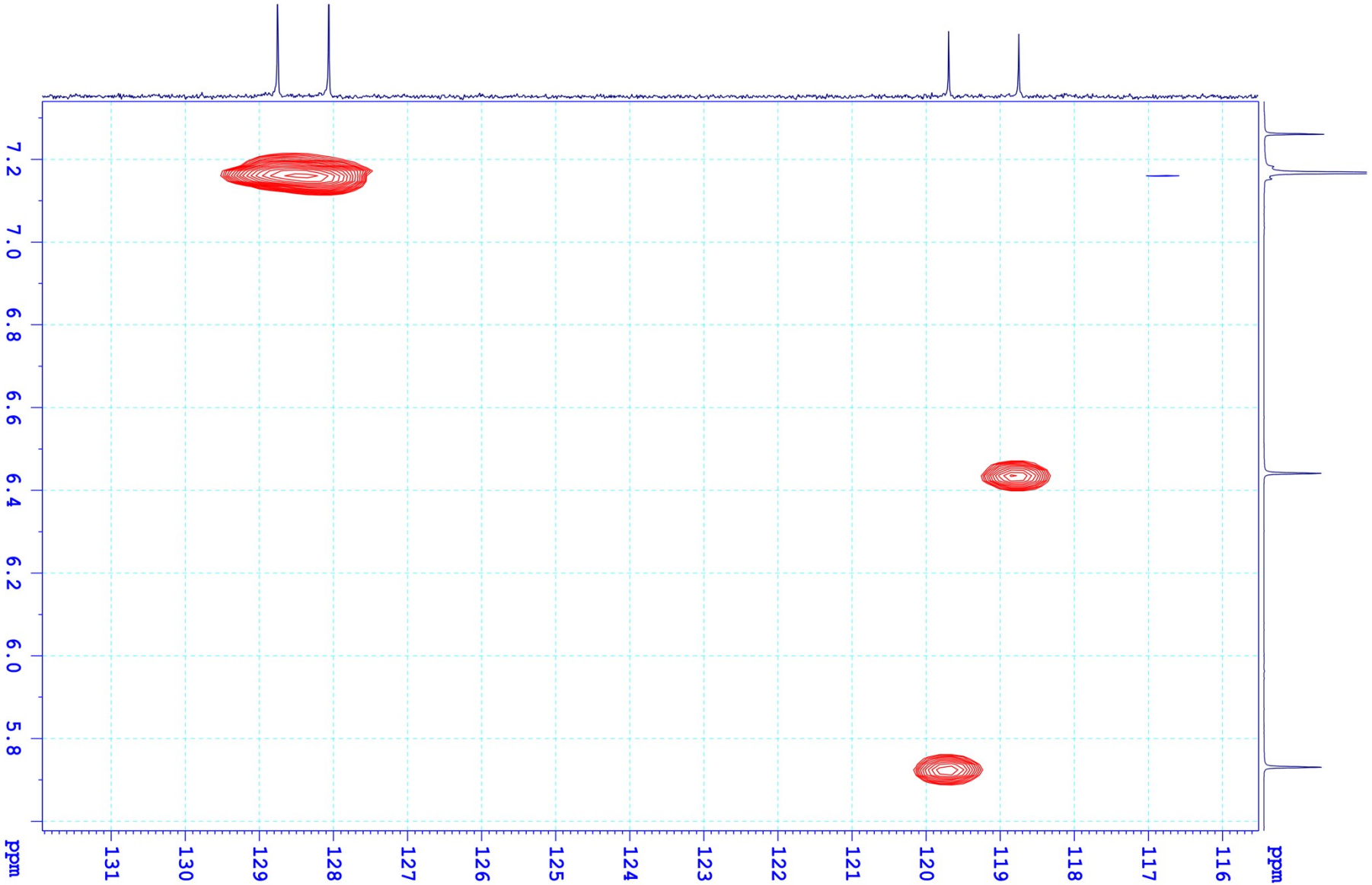


Figure S5. HMBC spectrum (in $CDCl_3$) of compound **1**

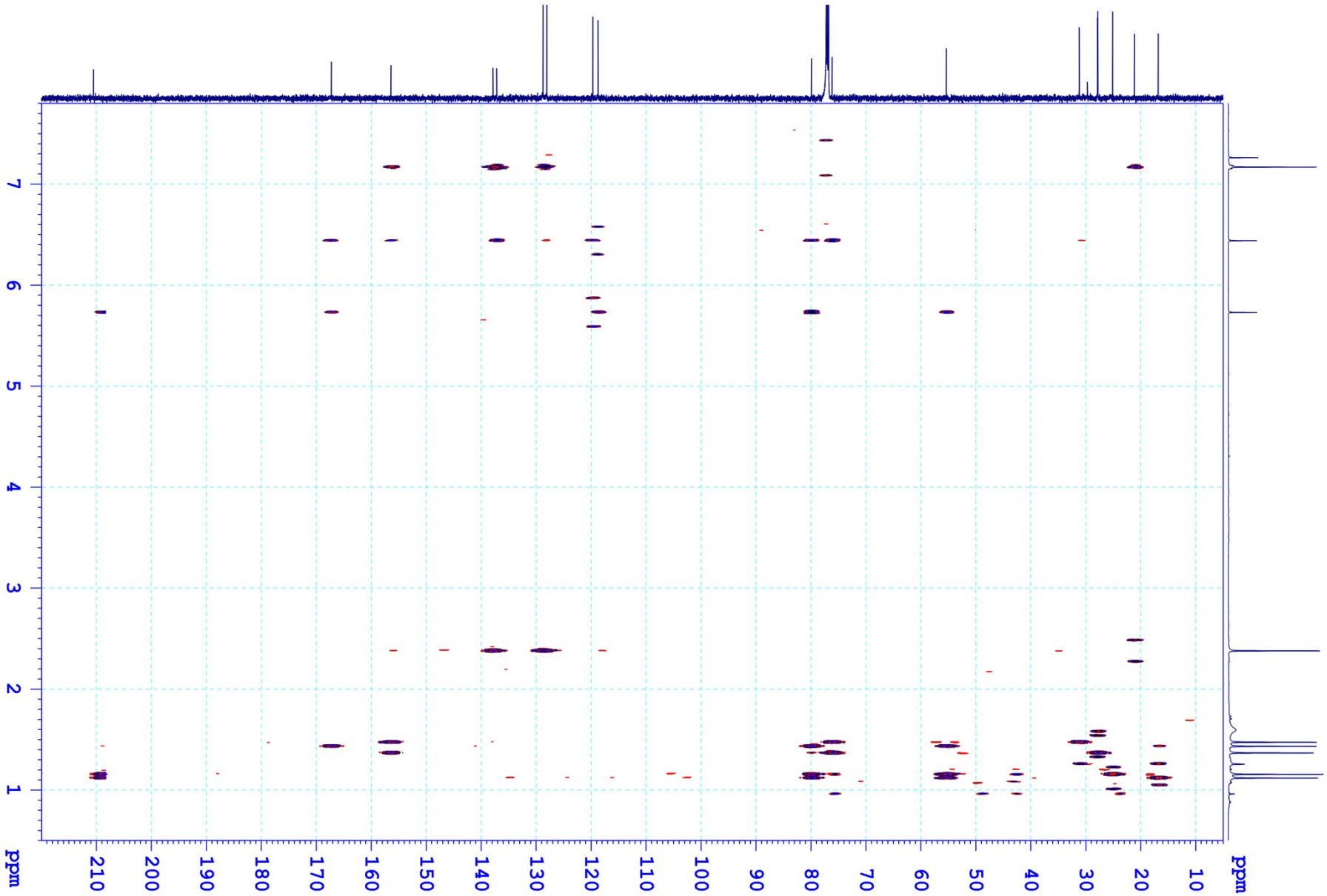


Figure S6. NOESY spectrum (in $CDCl_3$) of compound **1**

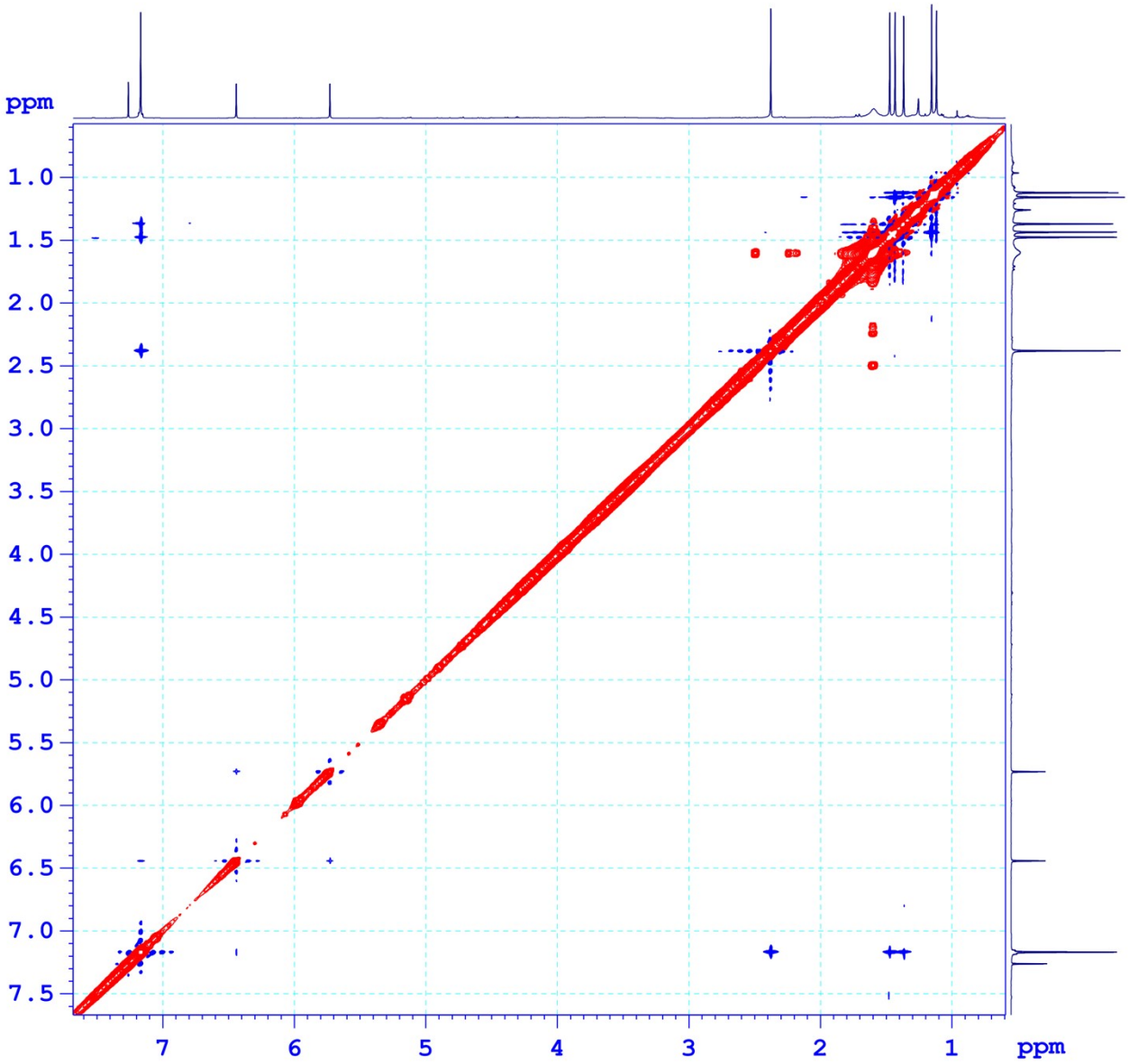


Figure S7. ECD spectrum (in MeOH) of compound **1**

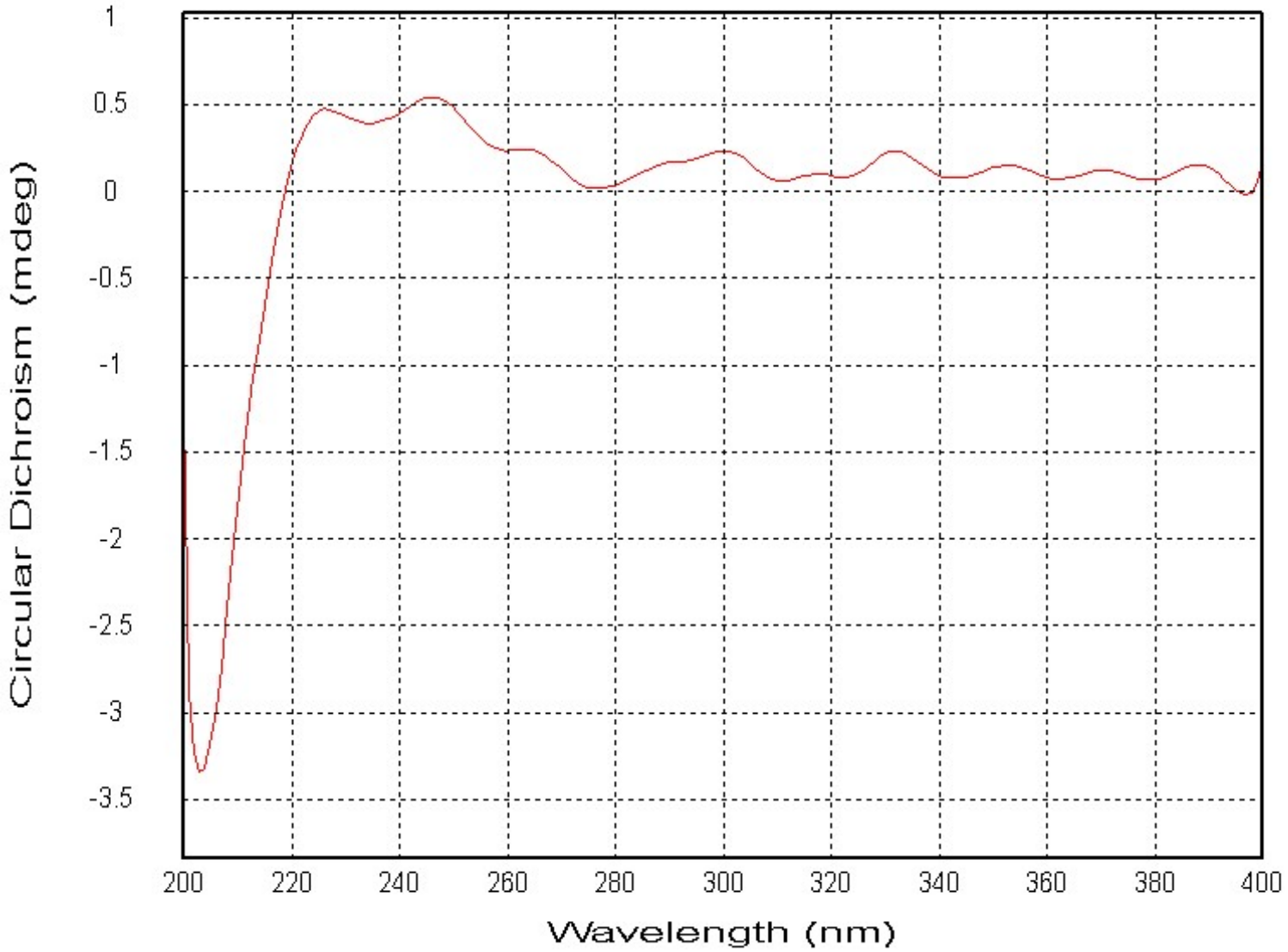


Figure S8. IR spectrum of compound **1**

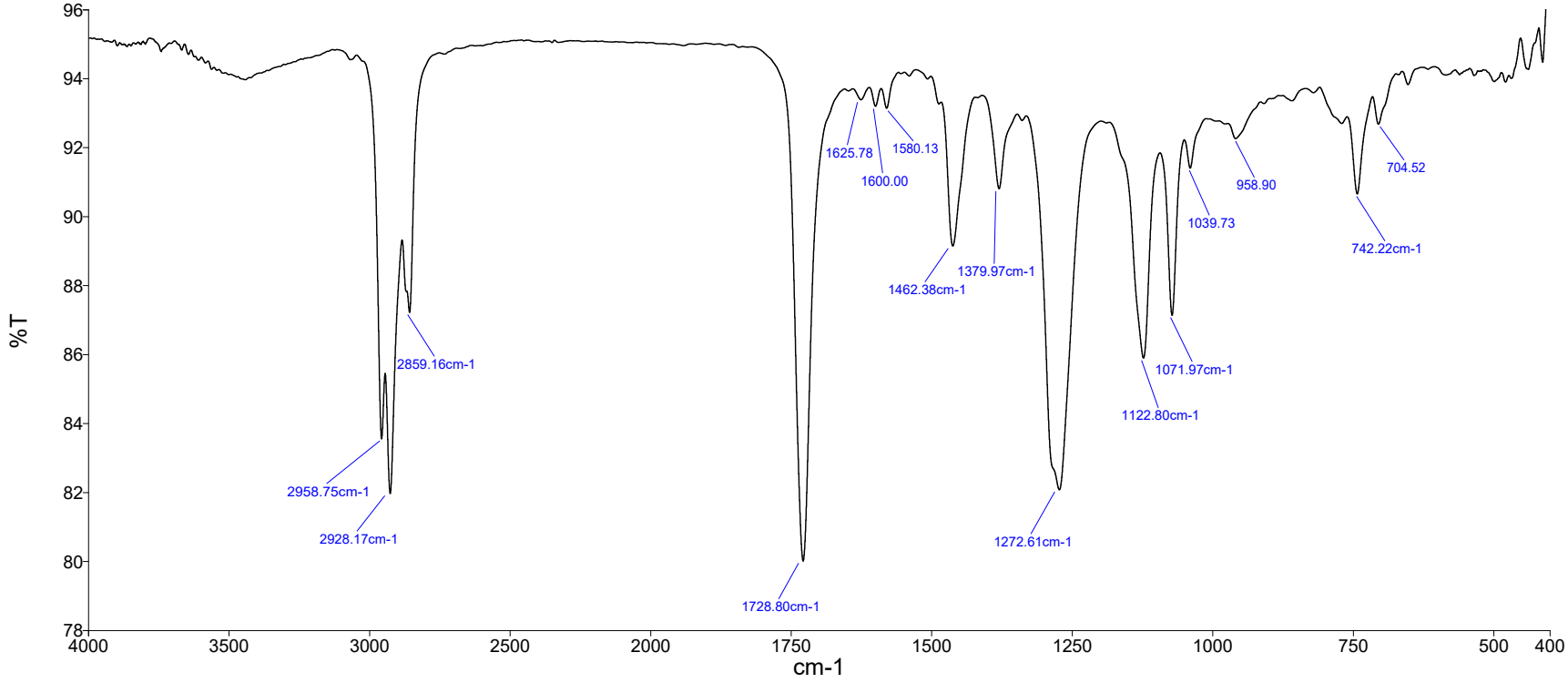


Figure S9a. ^{1}H NMR spectrum (600 MHz, DMSO-d_6) of compound **1**

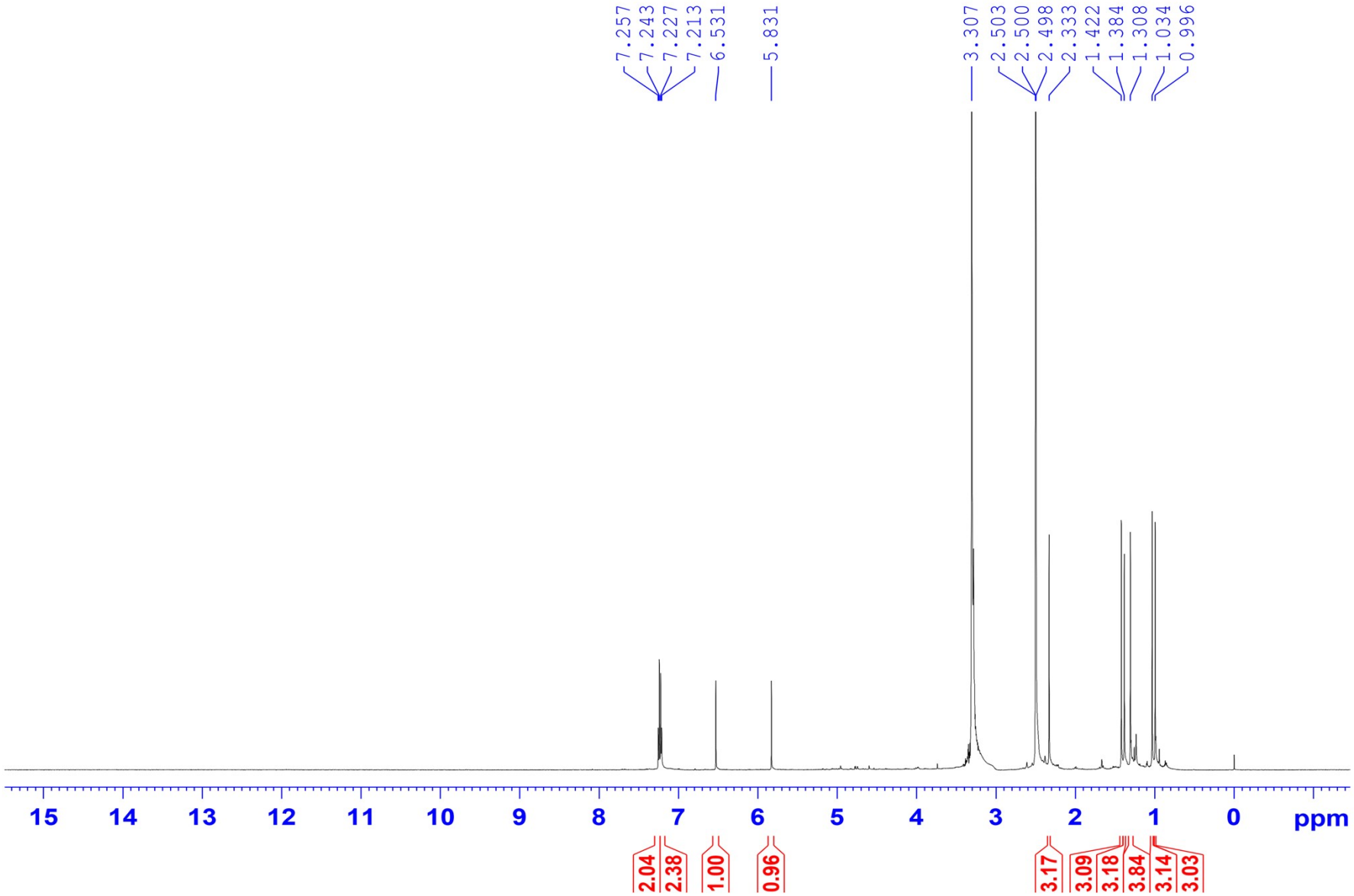


Figure S9b. Expanded ^{1}H NMR spectrum (600 MHz, DMSO-d_6) of compound **1**

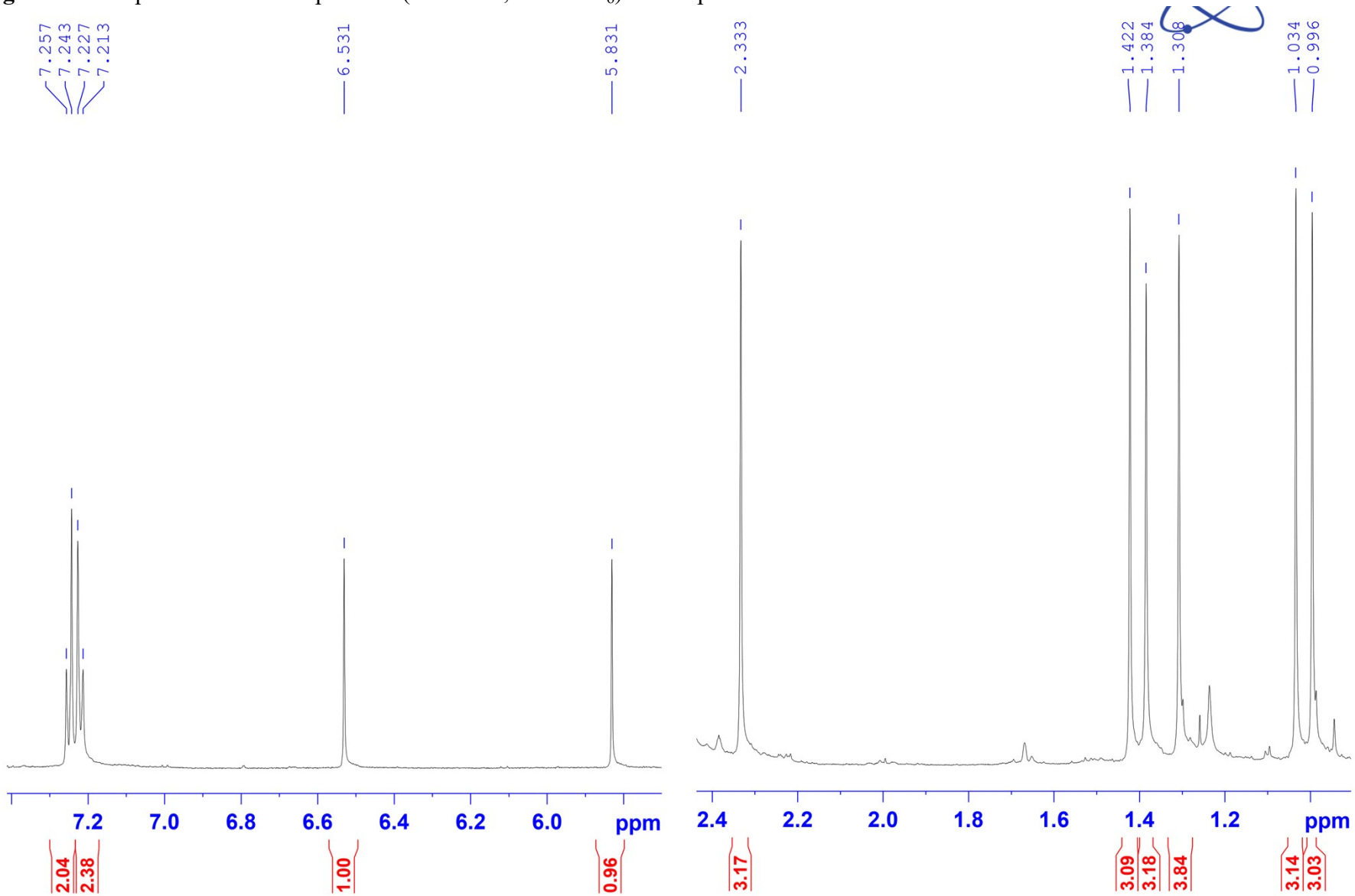


Figure S10. ^{13}C NMR spectrum (150 MHz, DMSO-d_6) of compound **1**

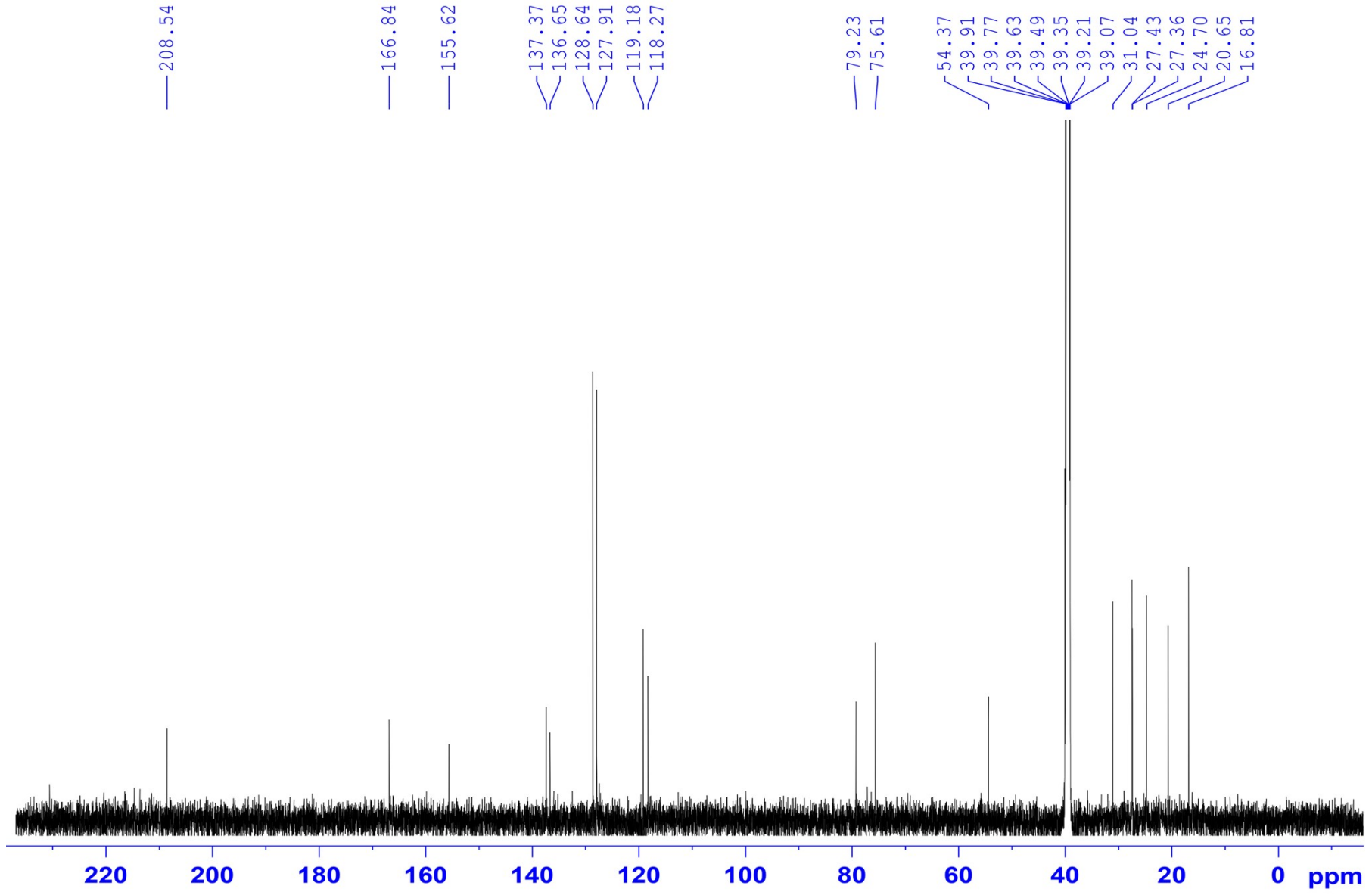


Figure S11a. HSQC spectrum (in DMSO-d_6) of compound **1**

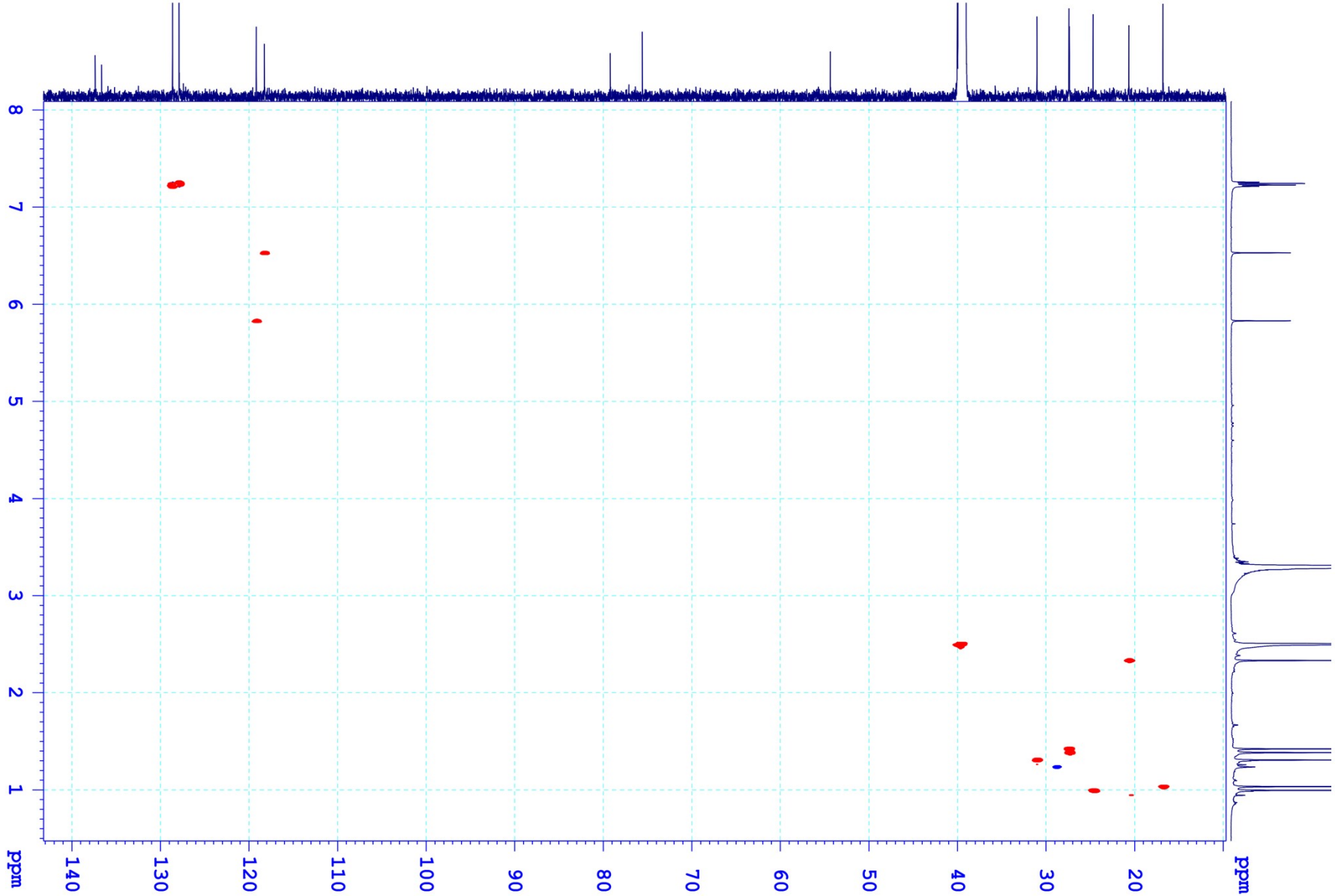


Figure S11b. Expanded HSQC spectrum (in DMSO-d_6) of compound **1**

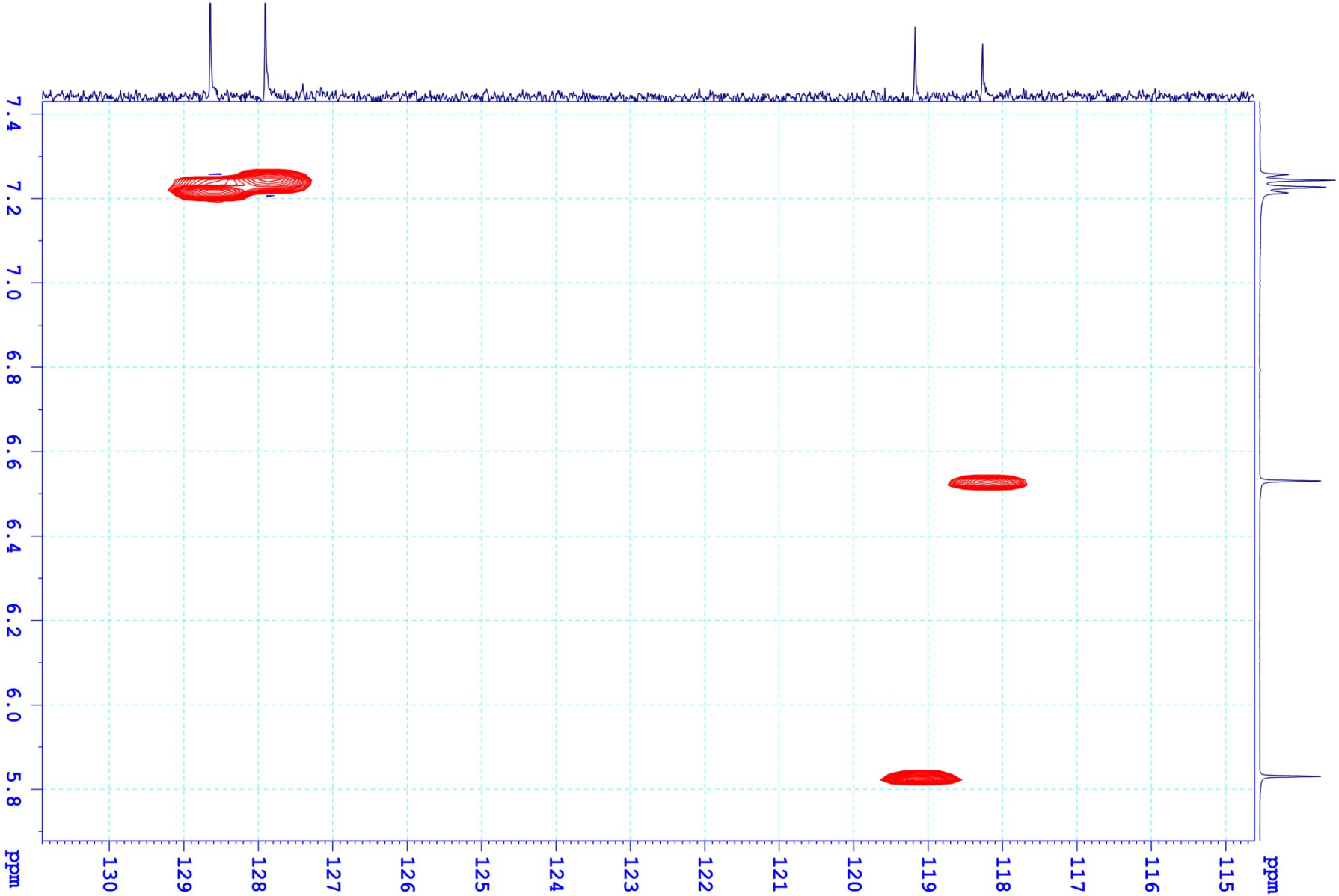


Figure S12a. HMBC spectrum (in DMSO-d_6) of compound **1**

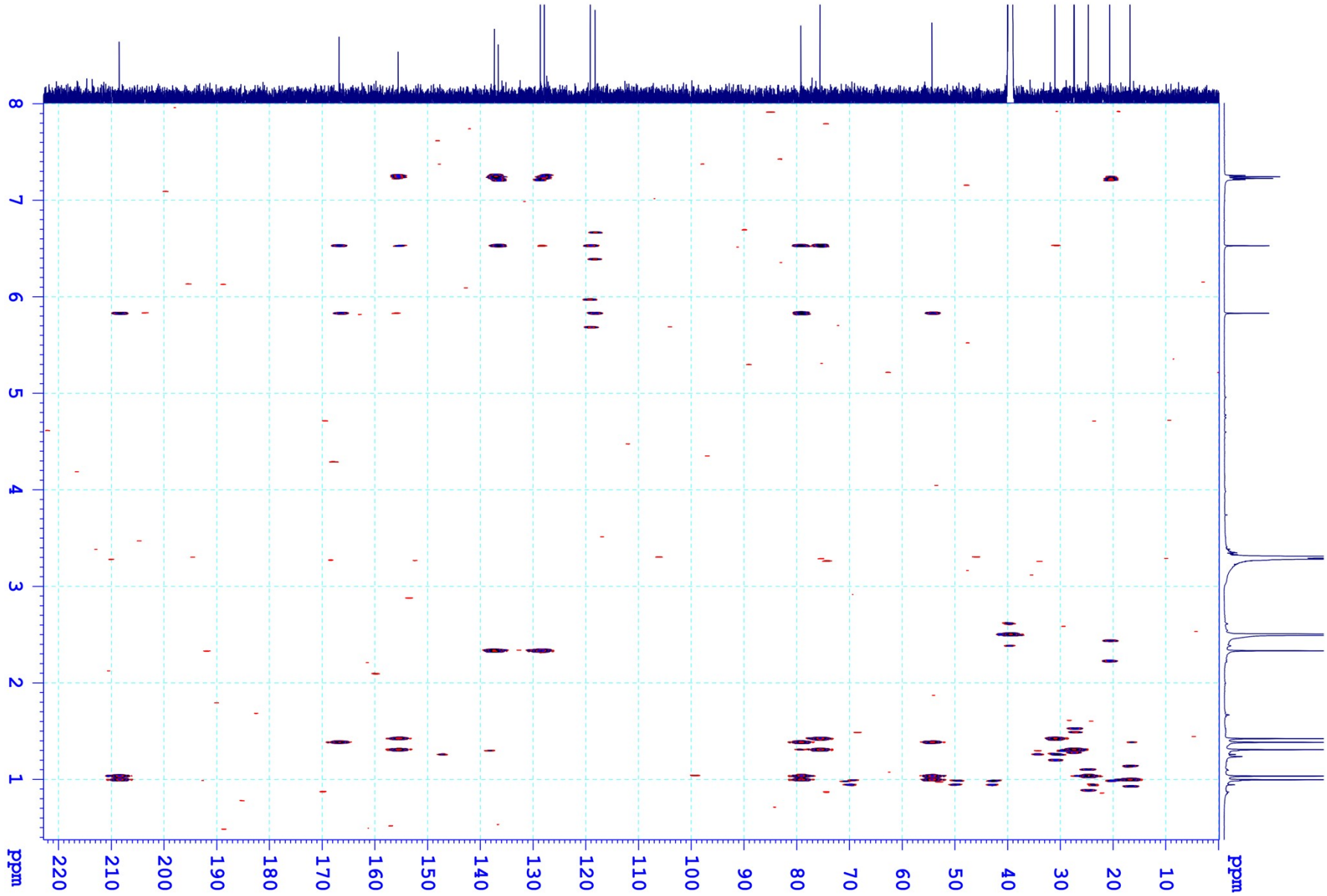


Figure S12b. Expanded HMBC spectrum (in DMSO-d_6) of compound **1**

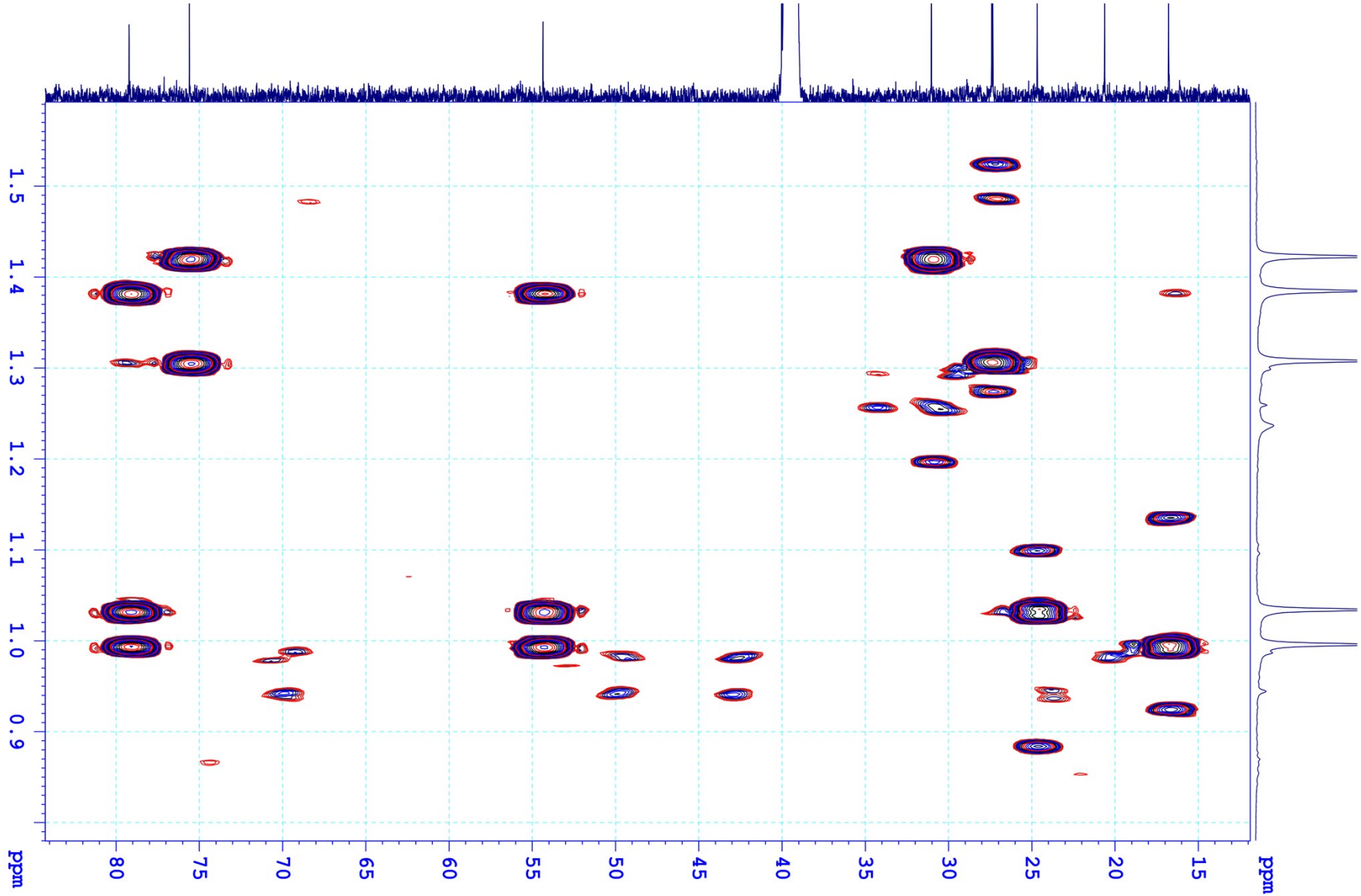


Figure S13. NOESY spectrum (in DMSO-d_6) of compound **1**

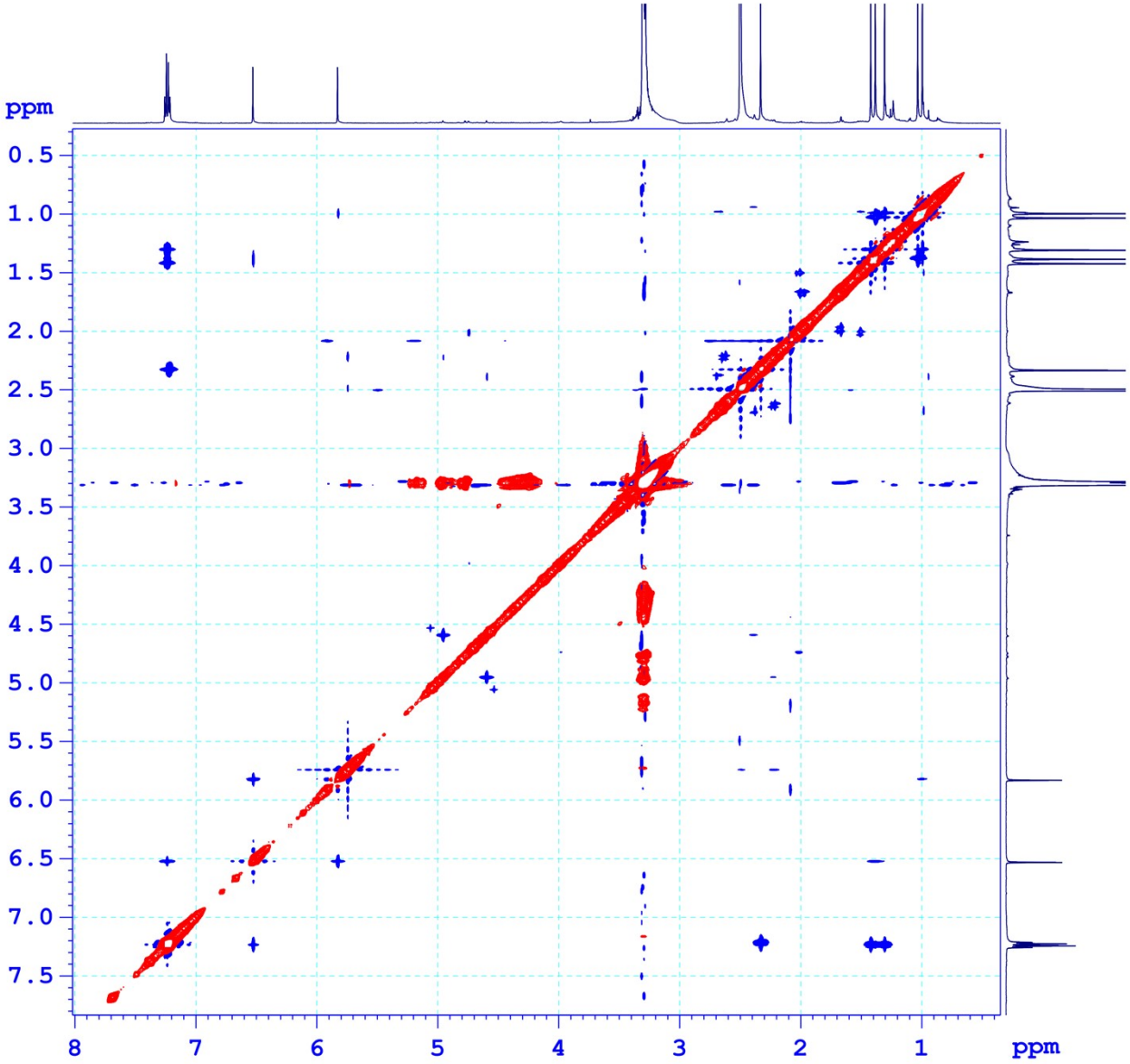


Figure S14. HRESIMS spectrum of compound **2**

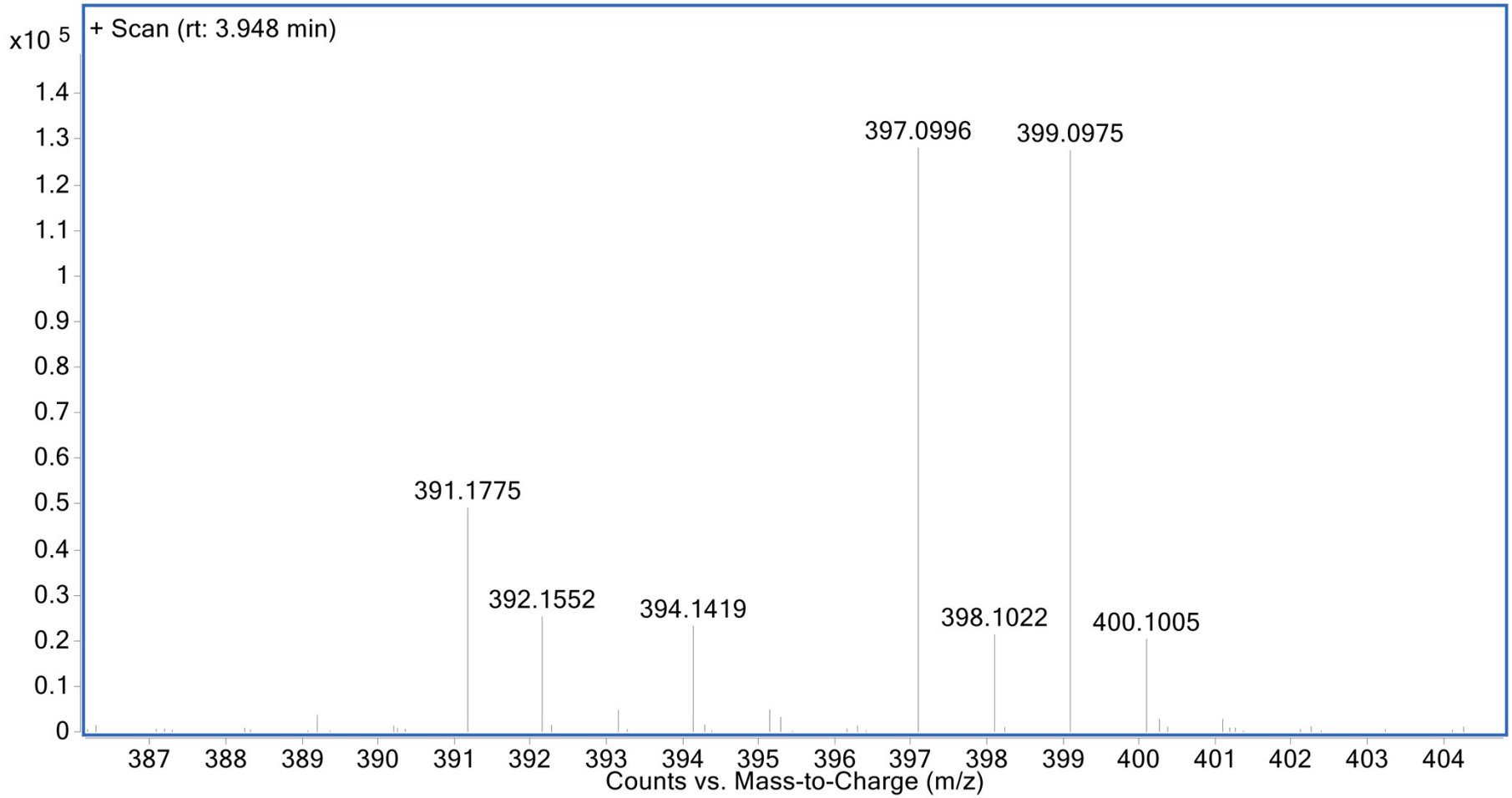


Figure S15. ^{1}H NMR spectrum (600 MHz, $CDCl_3$) of compound **2**

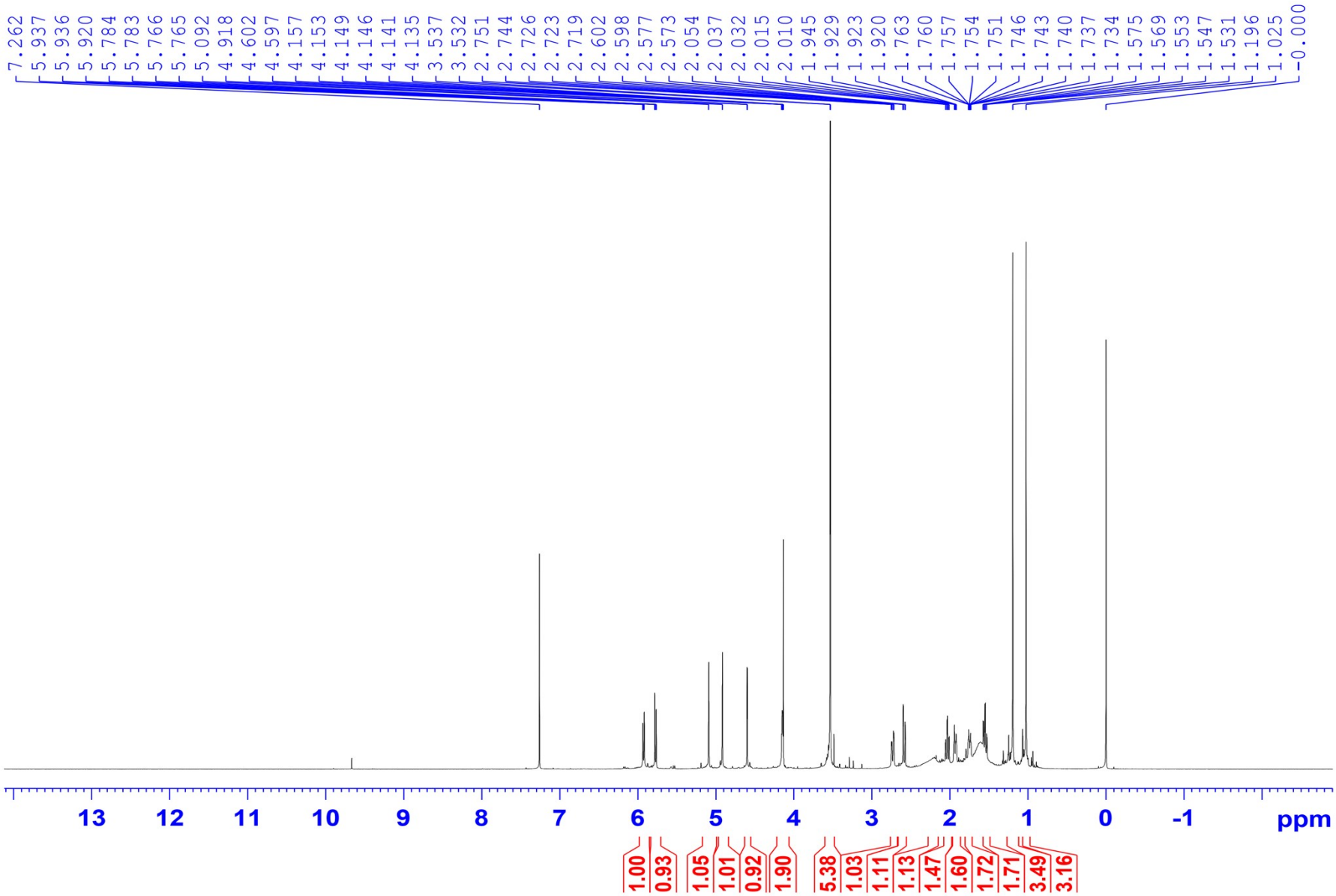


Figure S16. ^{13}C NMR spectrum (150 MHz, $CDCl_3$) of compound **2**

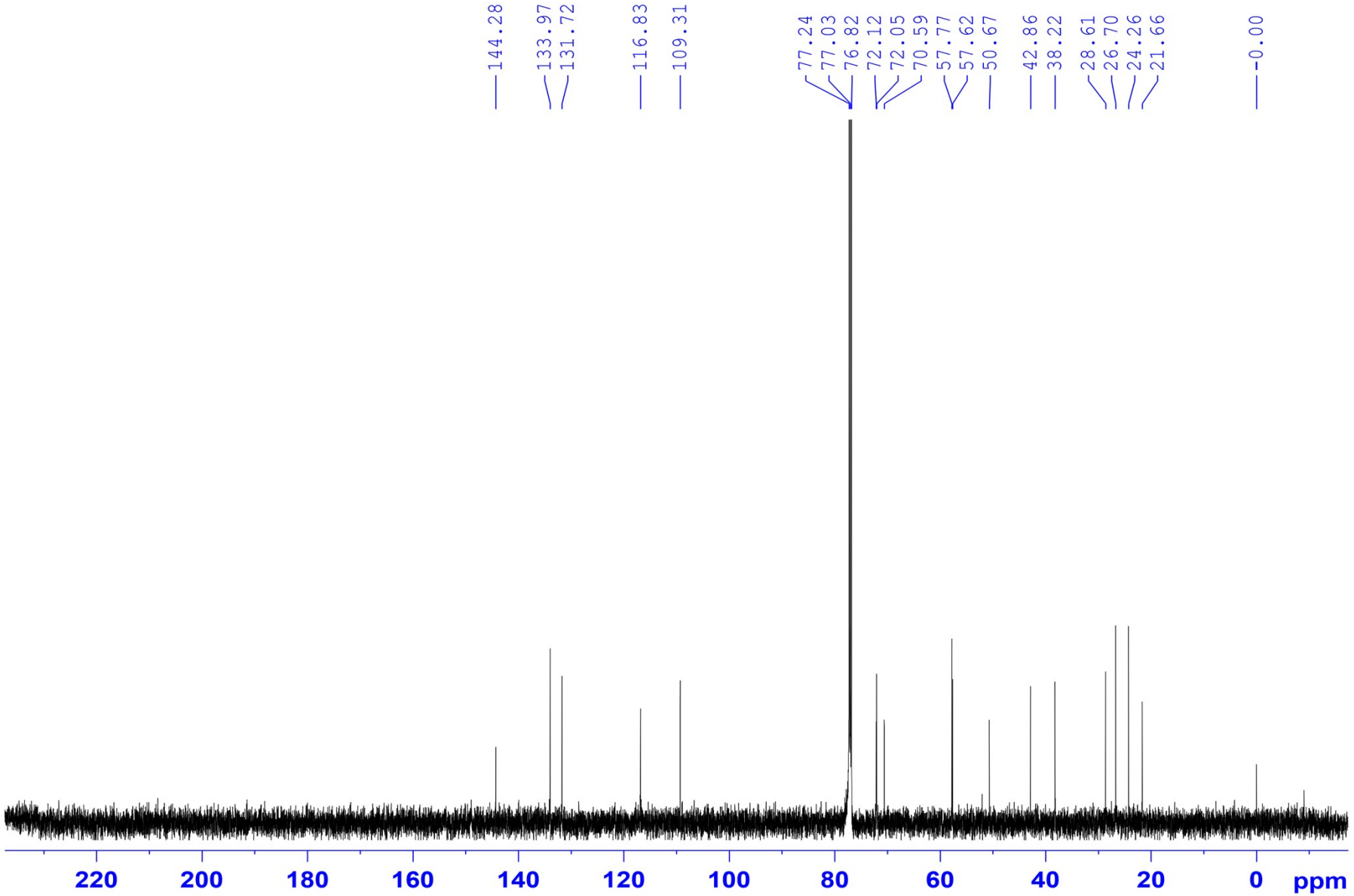


Figure S17. HSQC spectrum (in $CDCl_3$) of compound **2**

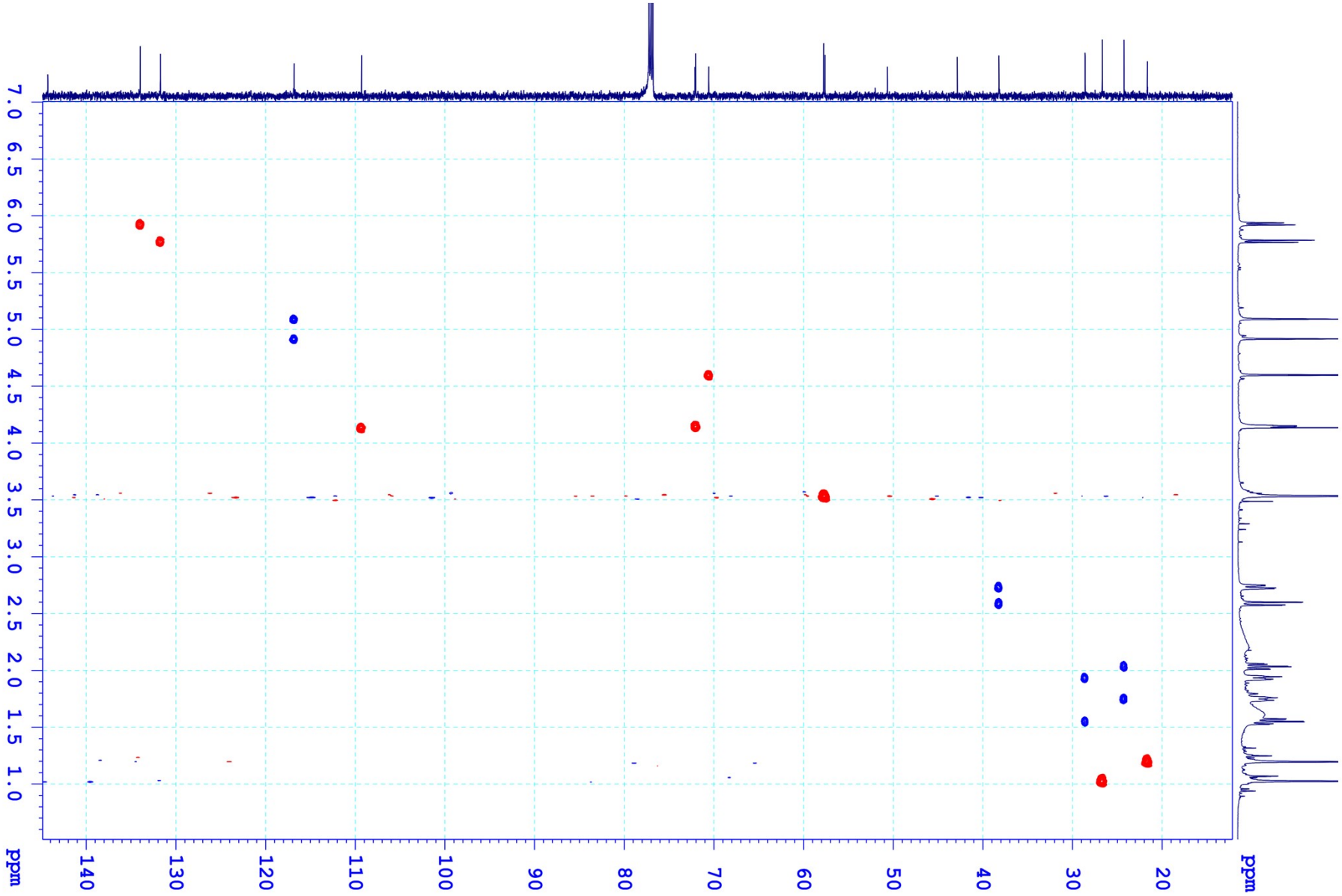


Figure S18. HMBC spectrum (in $CDCl_3$) of compound **2**

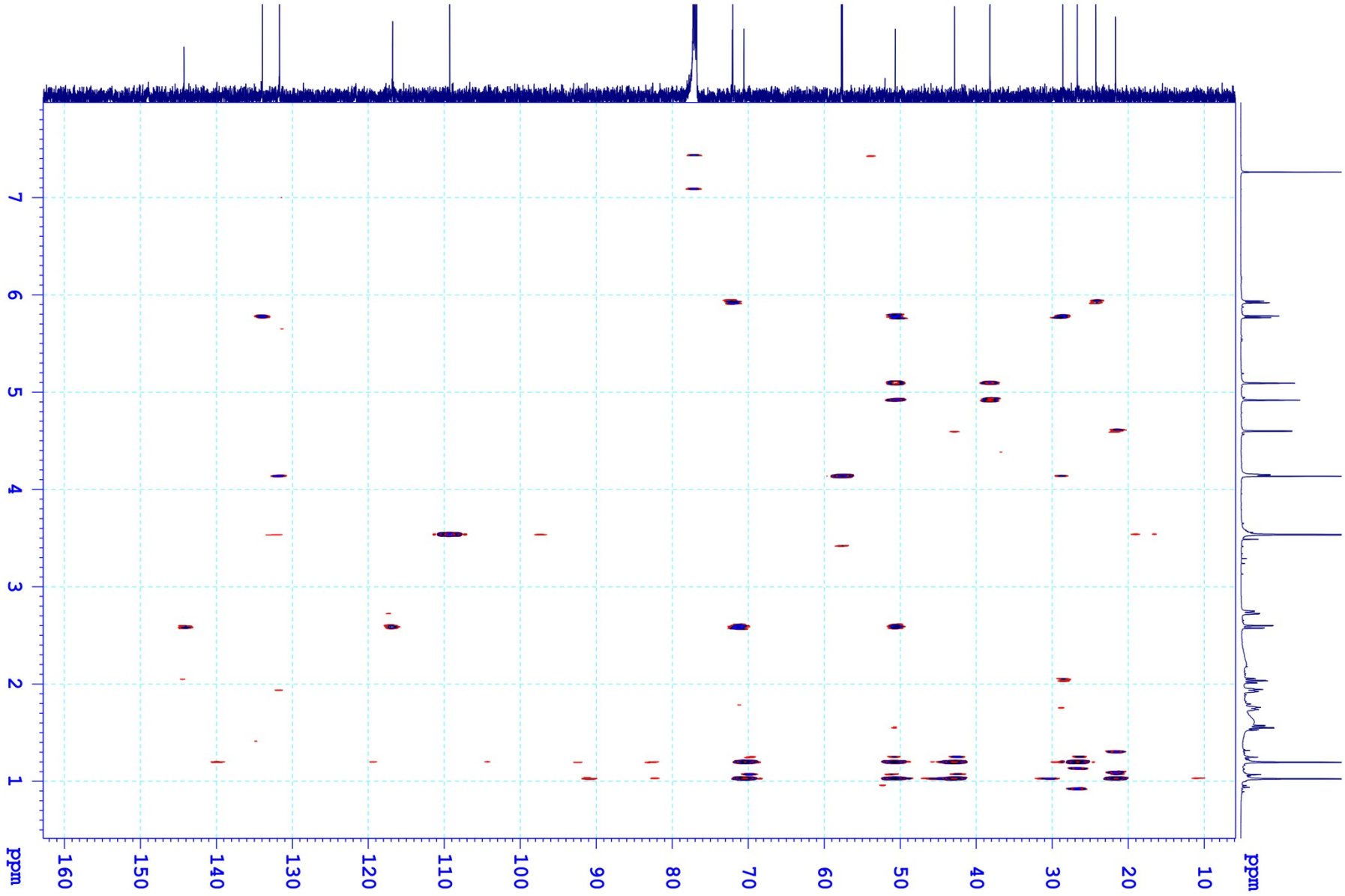


Figure S19. COSY spectrum (in $CDCl_3$) of compound **2**

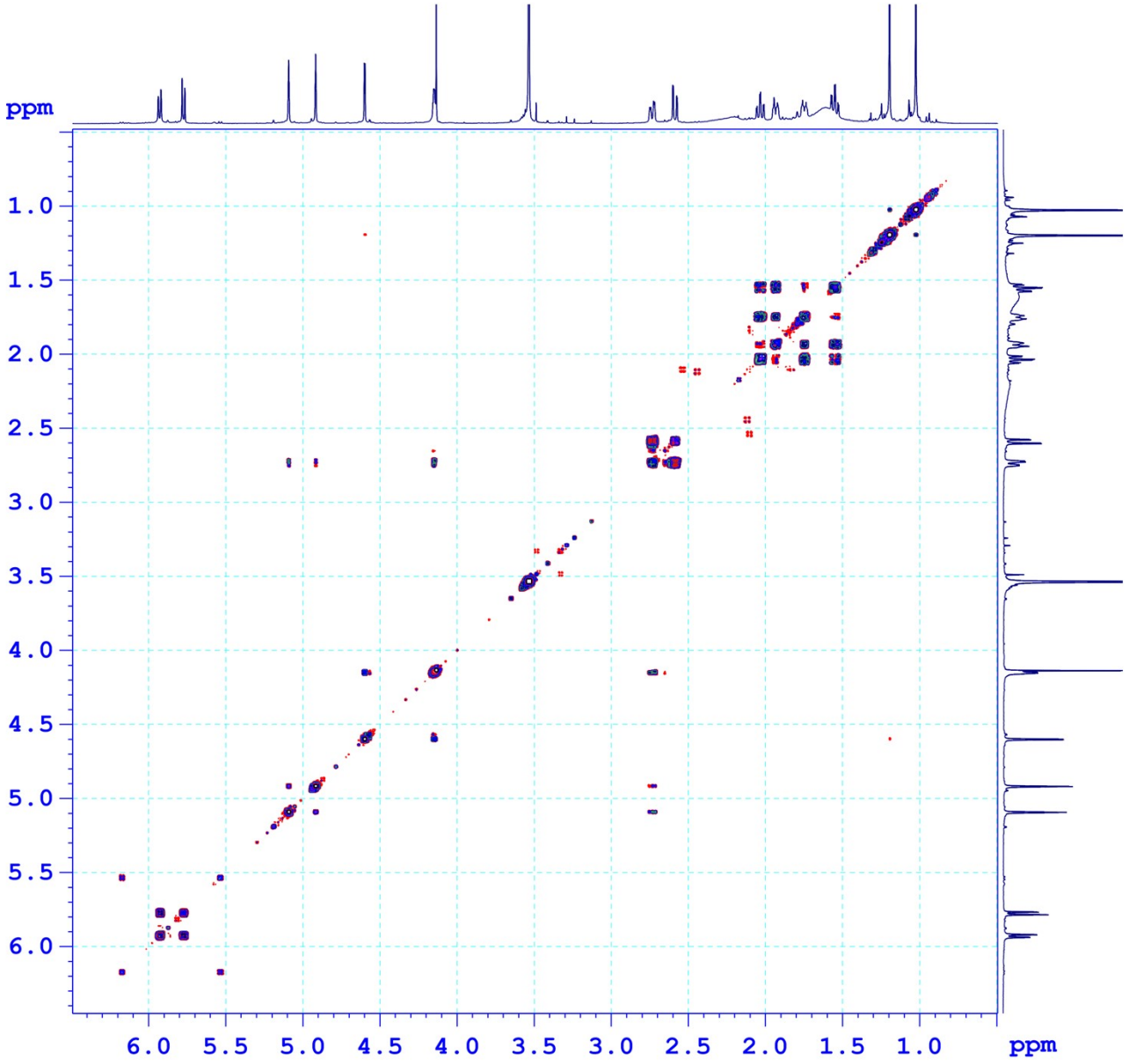


Figure S20. NOESY spectrum (in $CDCl_3$) of compound **2**

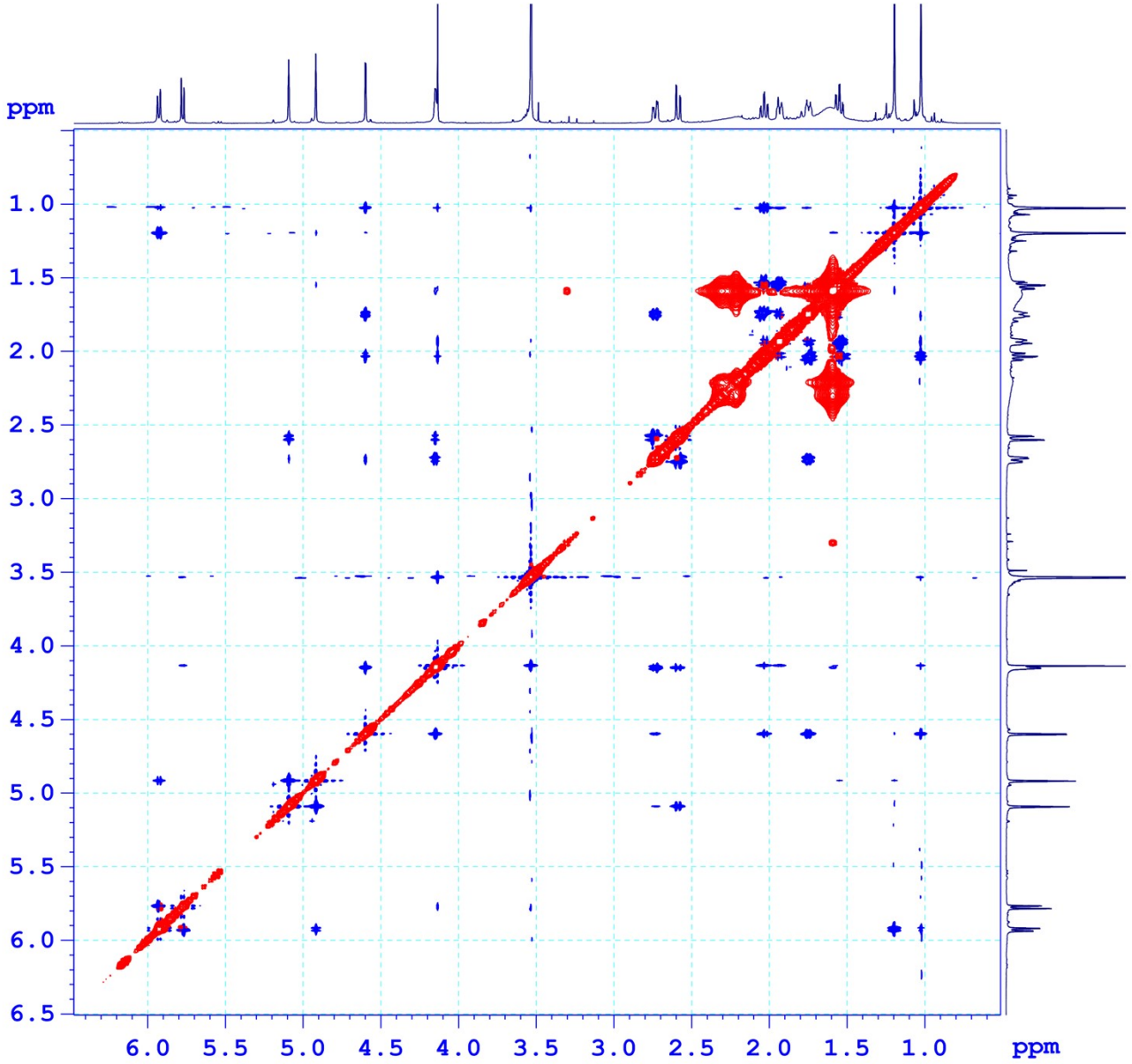


Figure S21. ECD spectra recorded in ACN (left) and in MeOH (right) of compound **2**

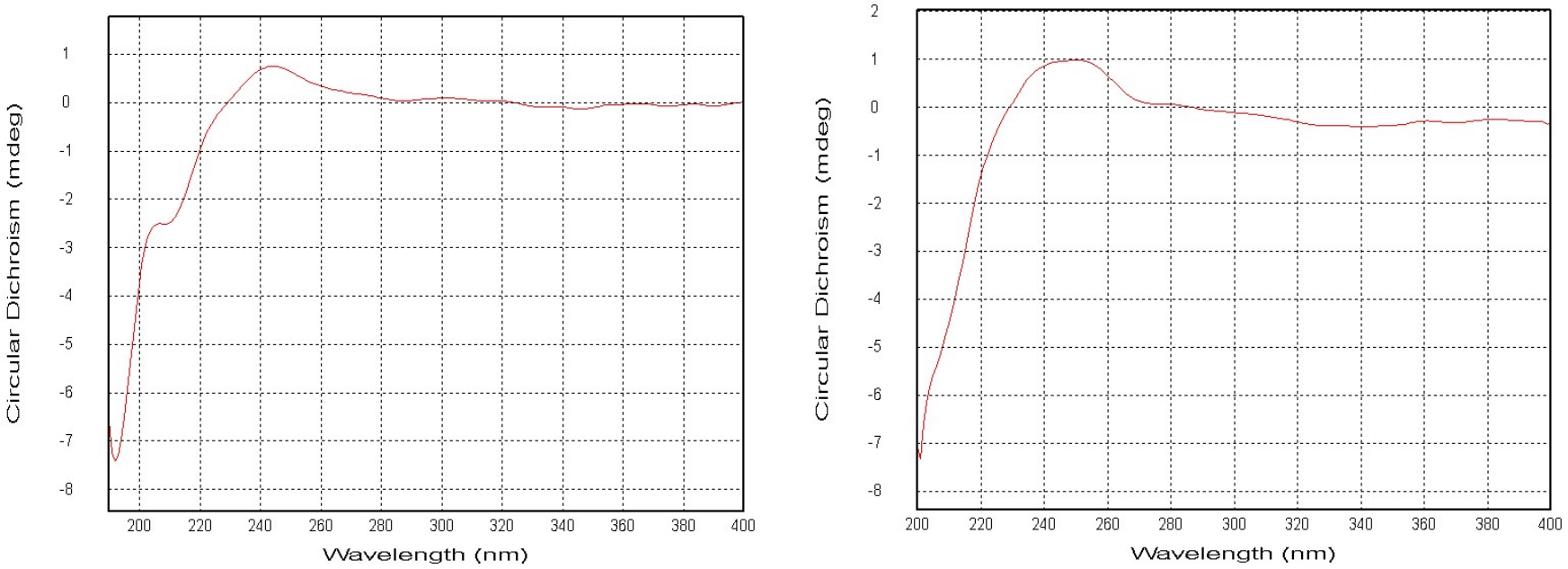


Figure S22. IR spectrum of compound **2**

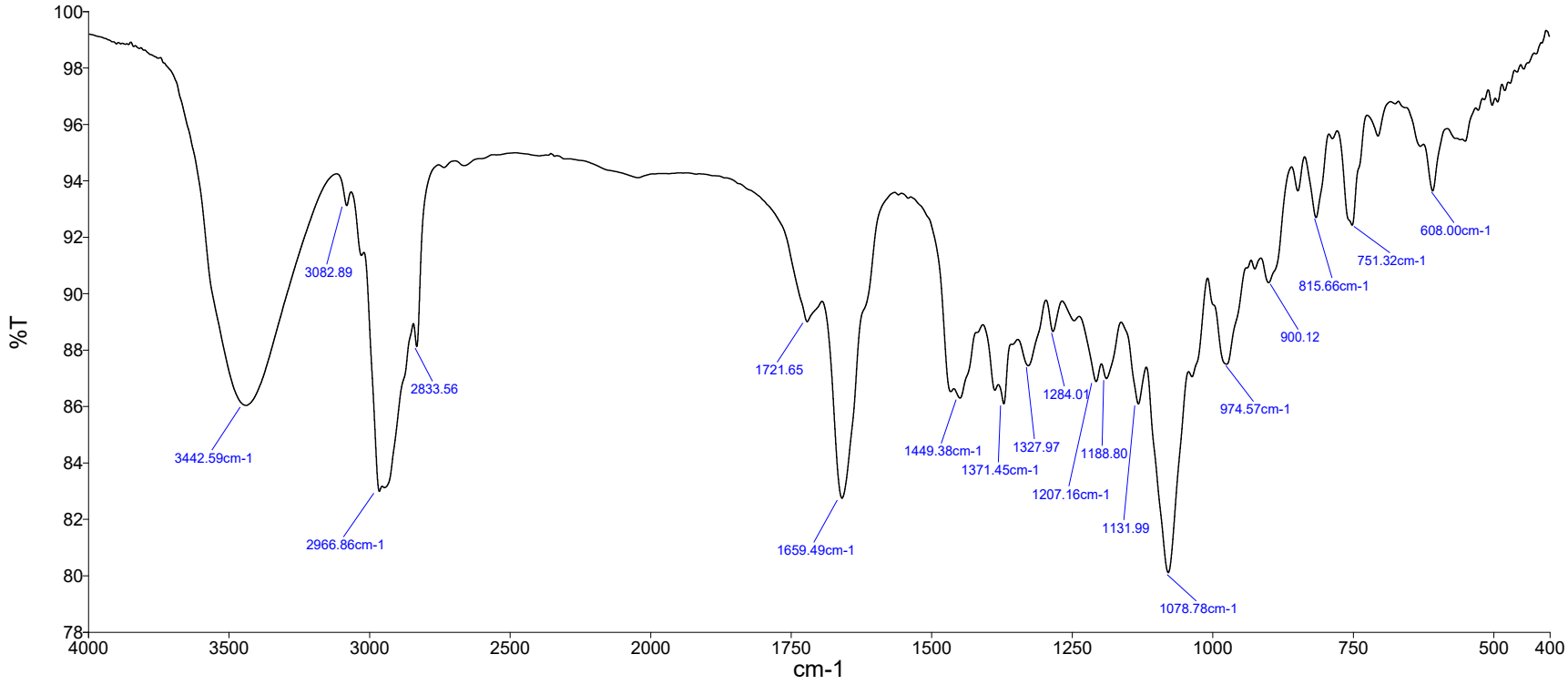


Figure S23. HRESIMS spectrum of compound **3**

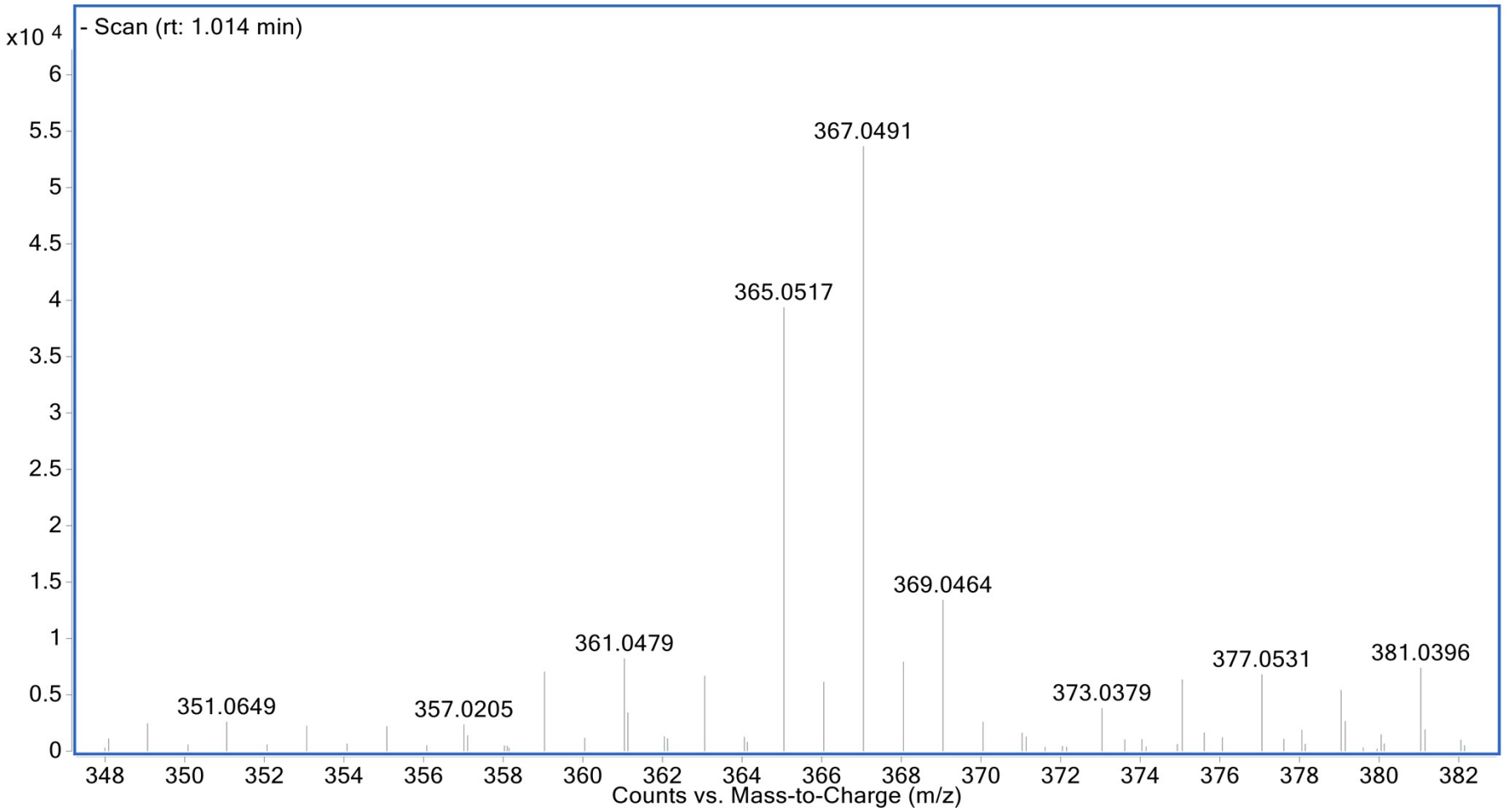


Figure S24. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of compound **3**

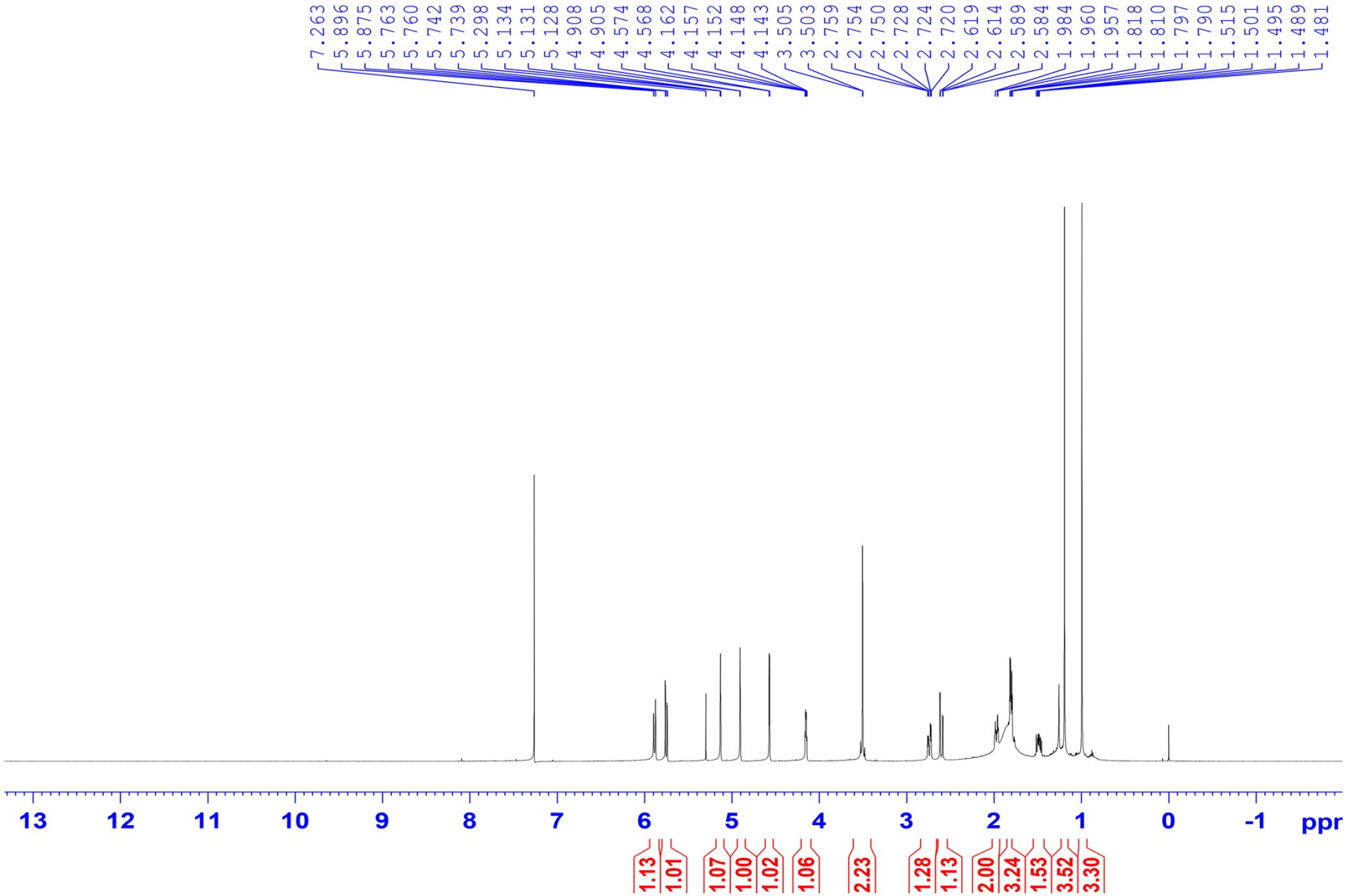


Figure S25. ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of compound **3**

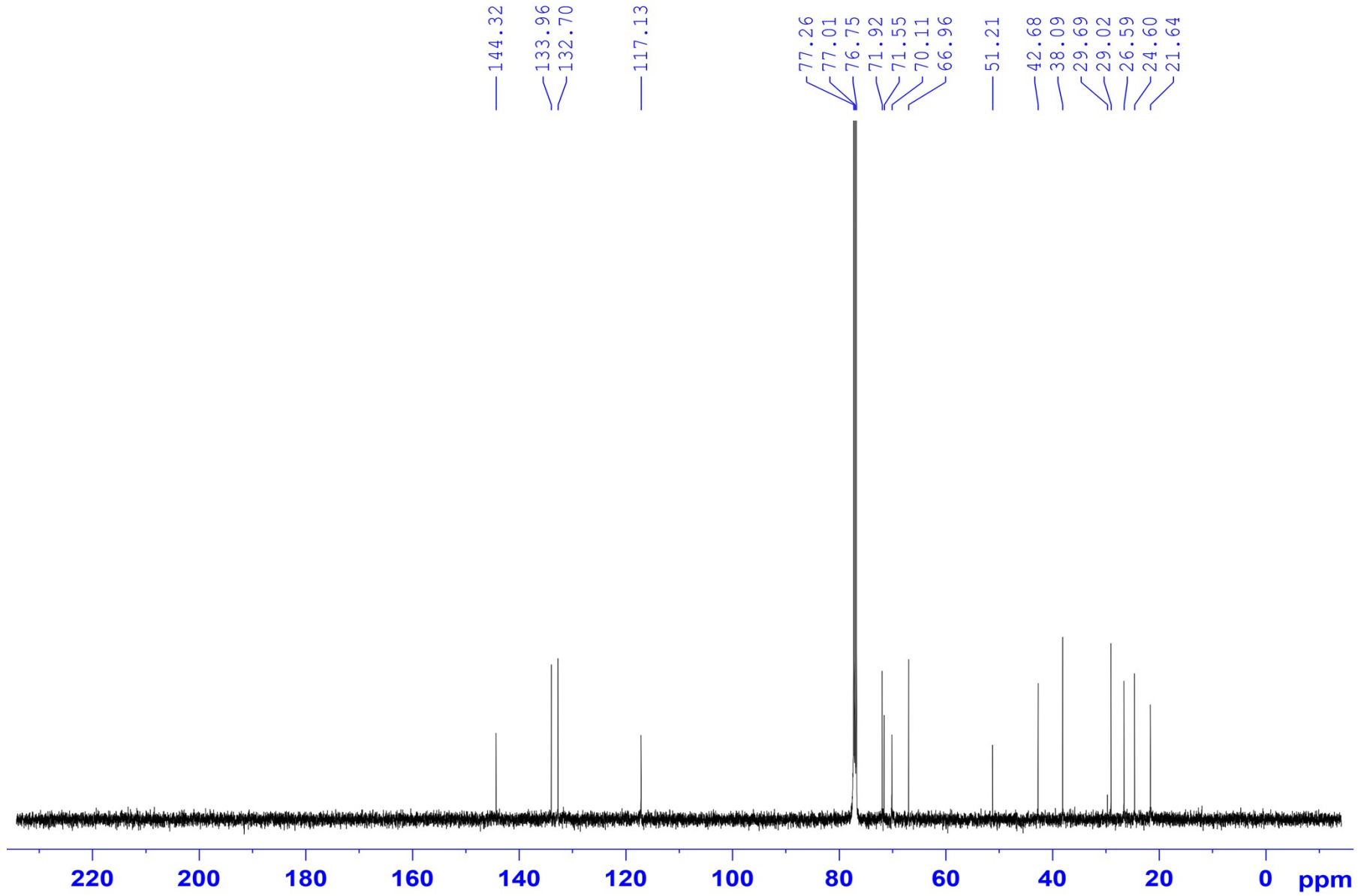


Figure S26. HSQC spectrum (in $CDCl_3$) of compound **3**

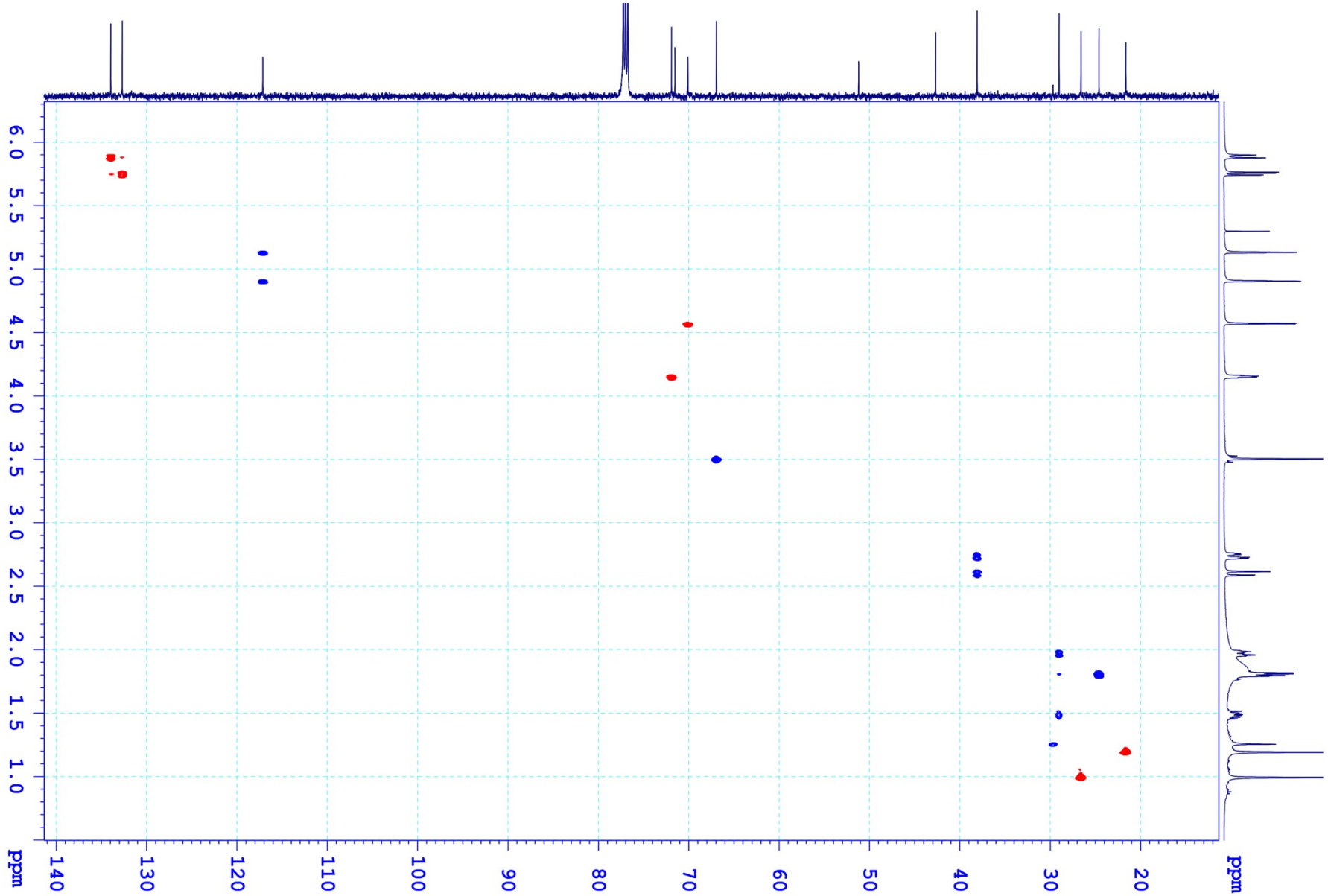


Figure S27. HMBC spectrum (in $CDCl_3$) of compound **3**

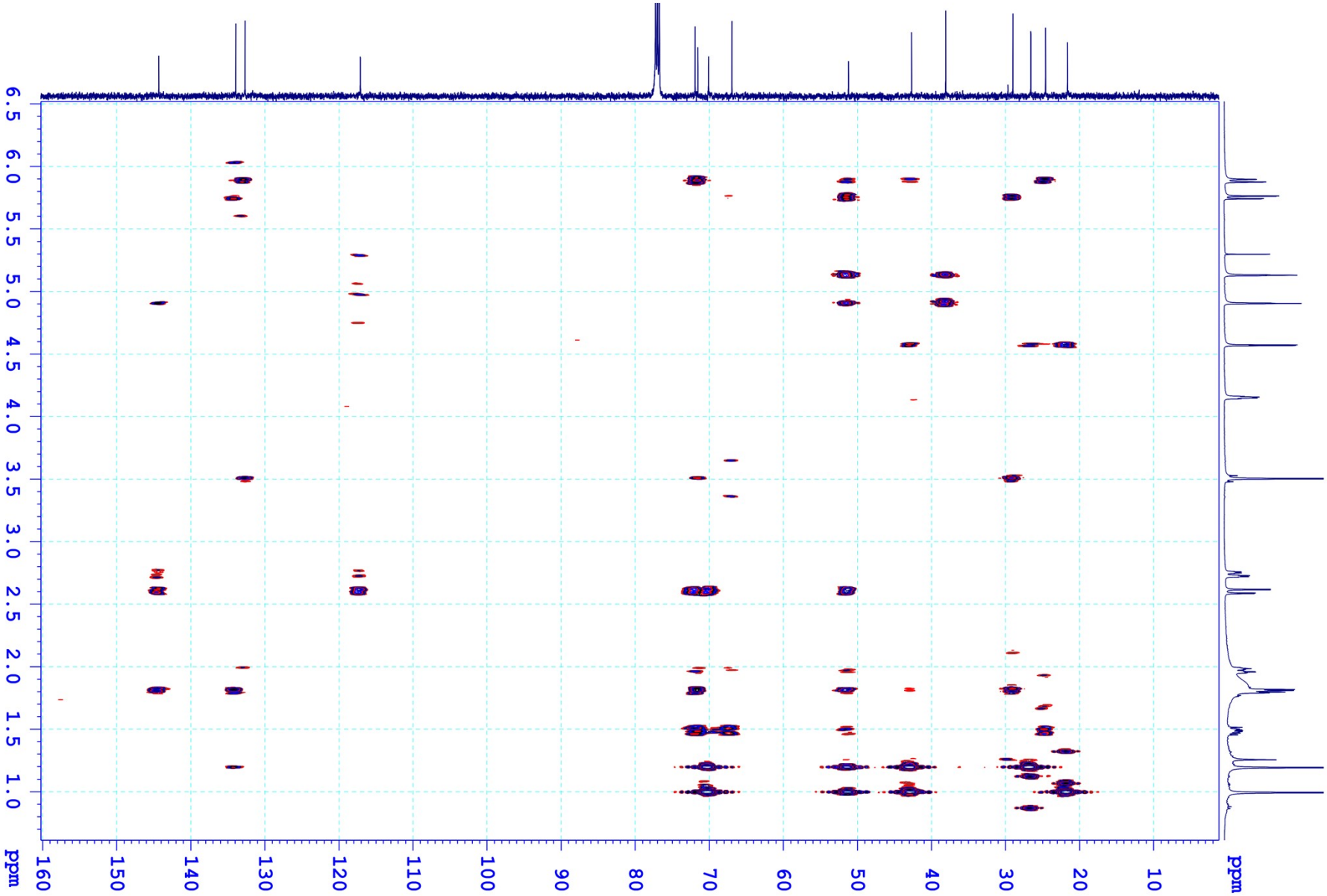


Figure S28. COSY spectrum (in $CDCl_3$) of compound **3**

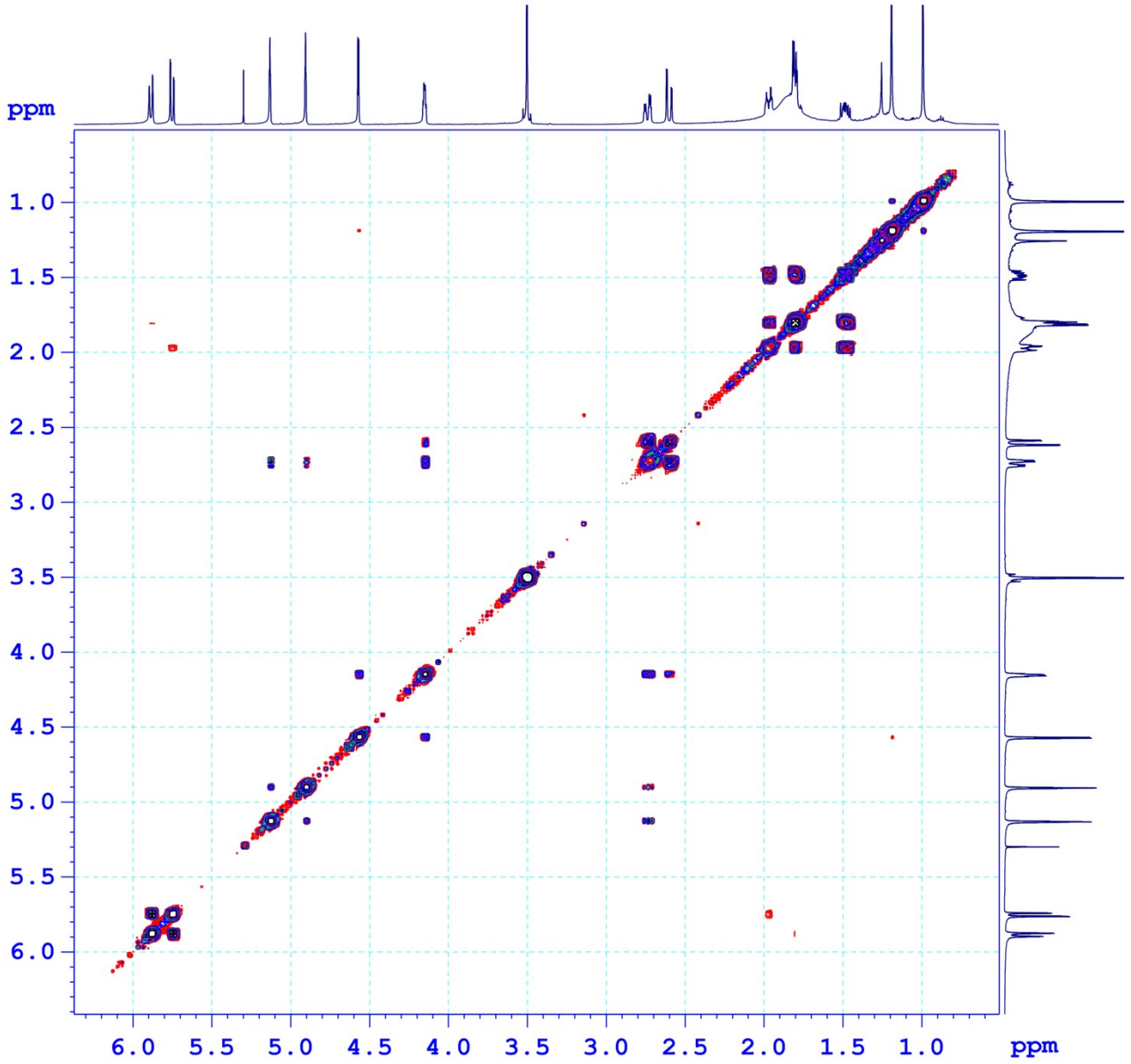


Figure S29. NOESY spectrum (in $CDCl_3$) of compound **3**

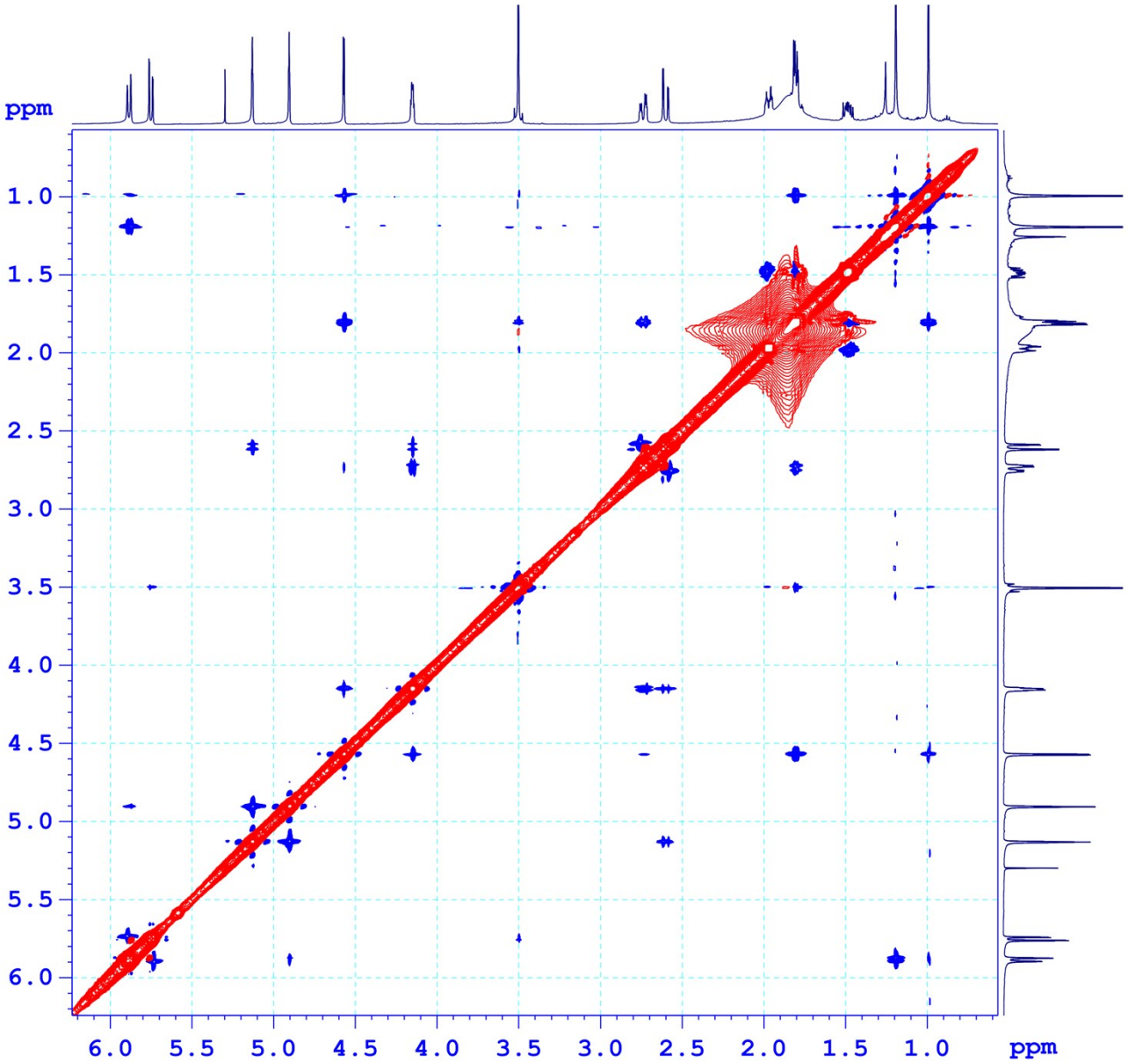


Figure S30. ECD spectrum (in ACN) of compound **3**

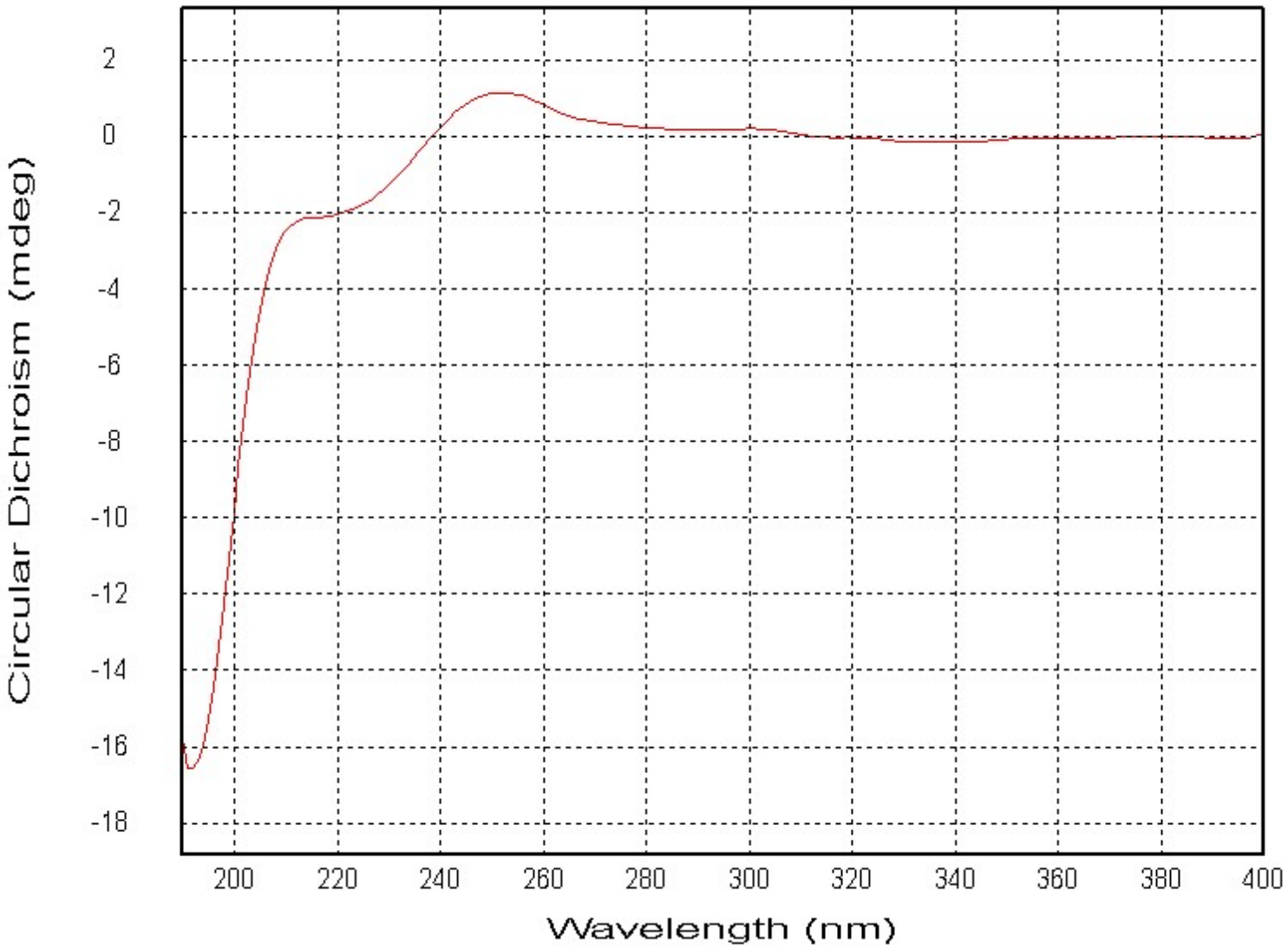


Figure S31. IR spectrum of compound **3**

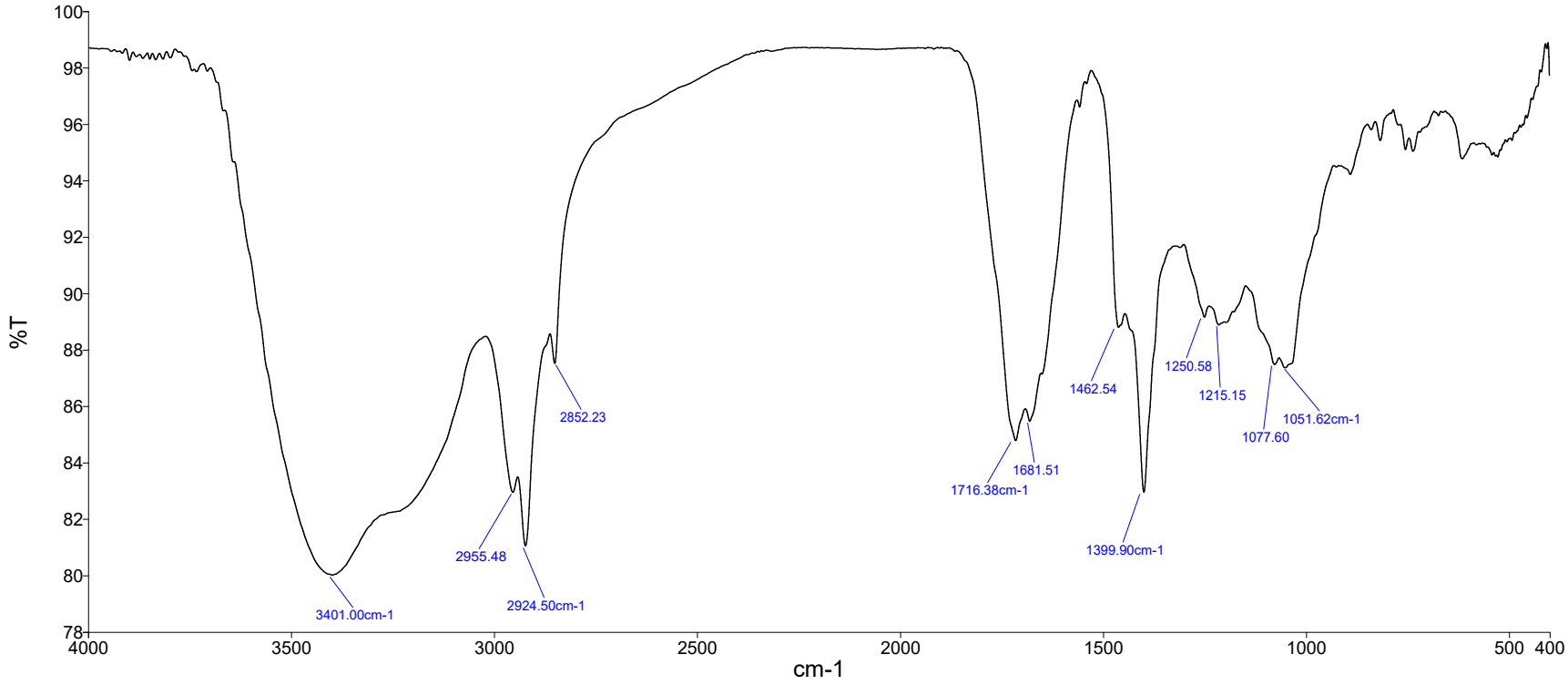


Figure S32. HRESIMS spectrum of compound **4**

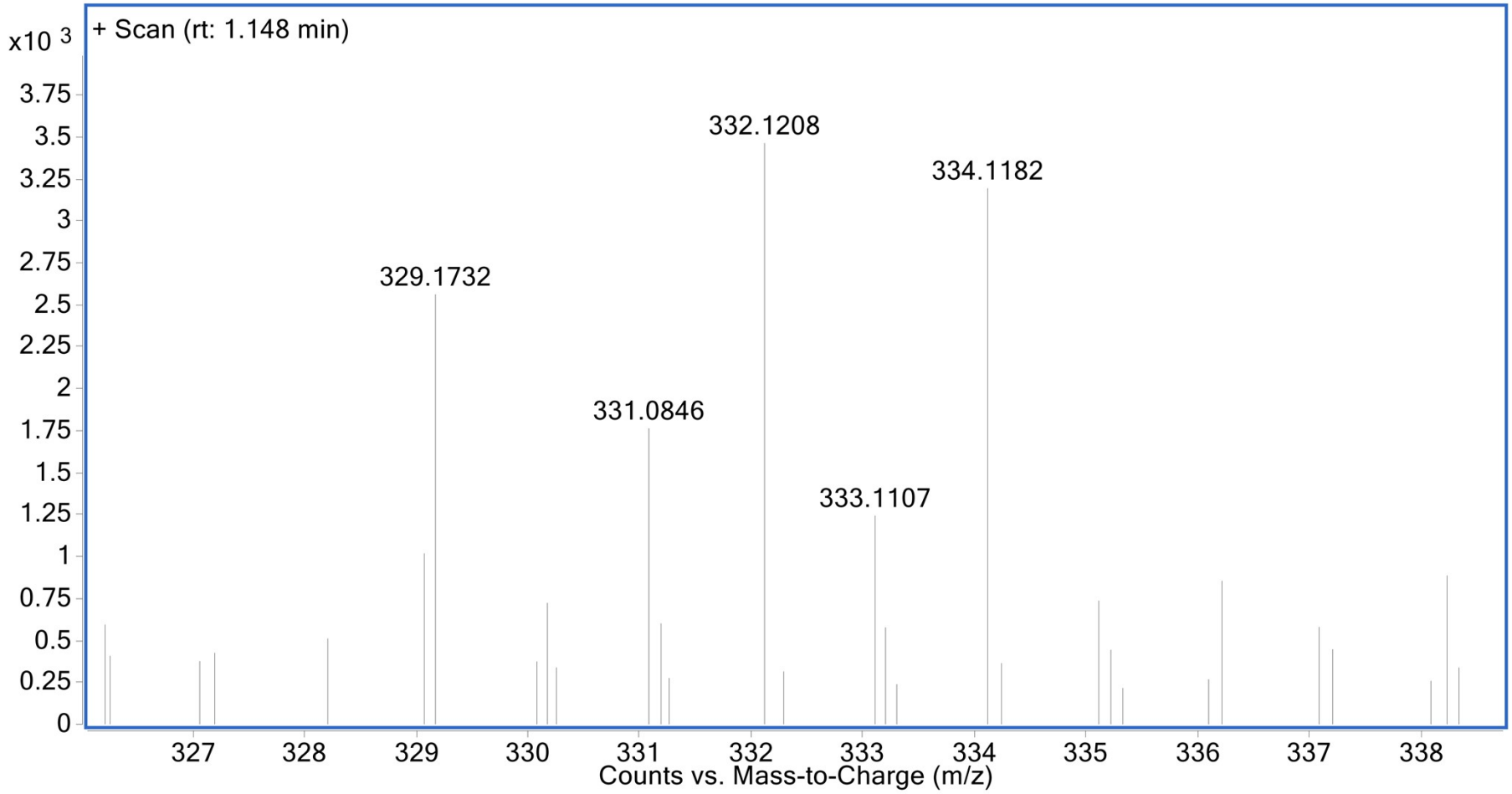


Figure S33. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of compound **4**

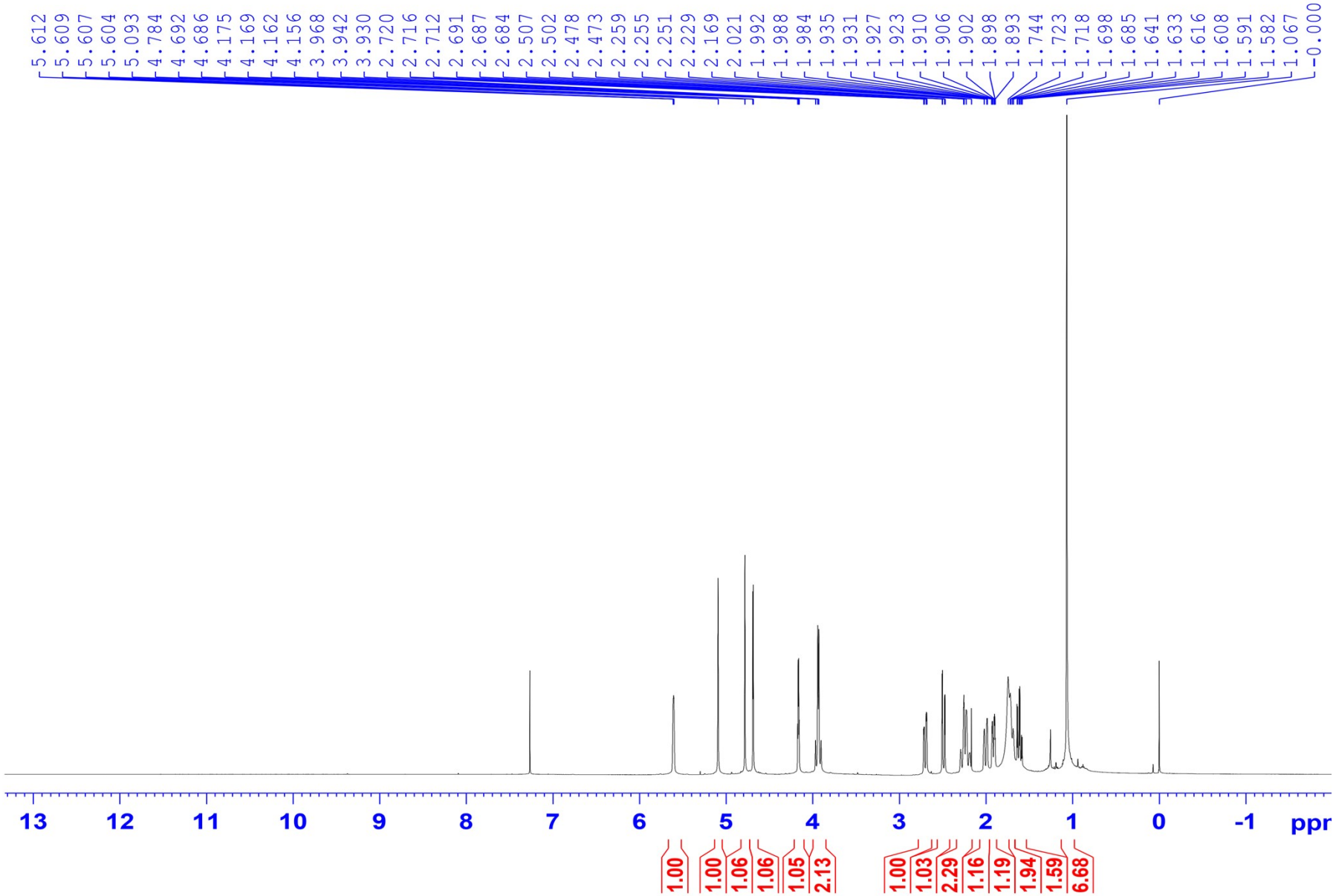


Figure S34. ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of compound **4**

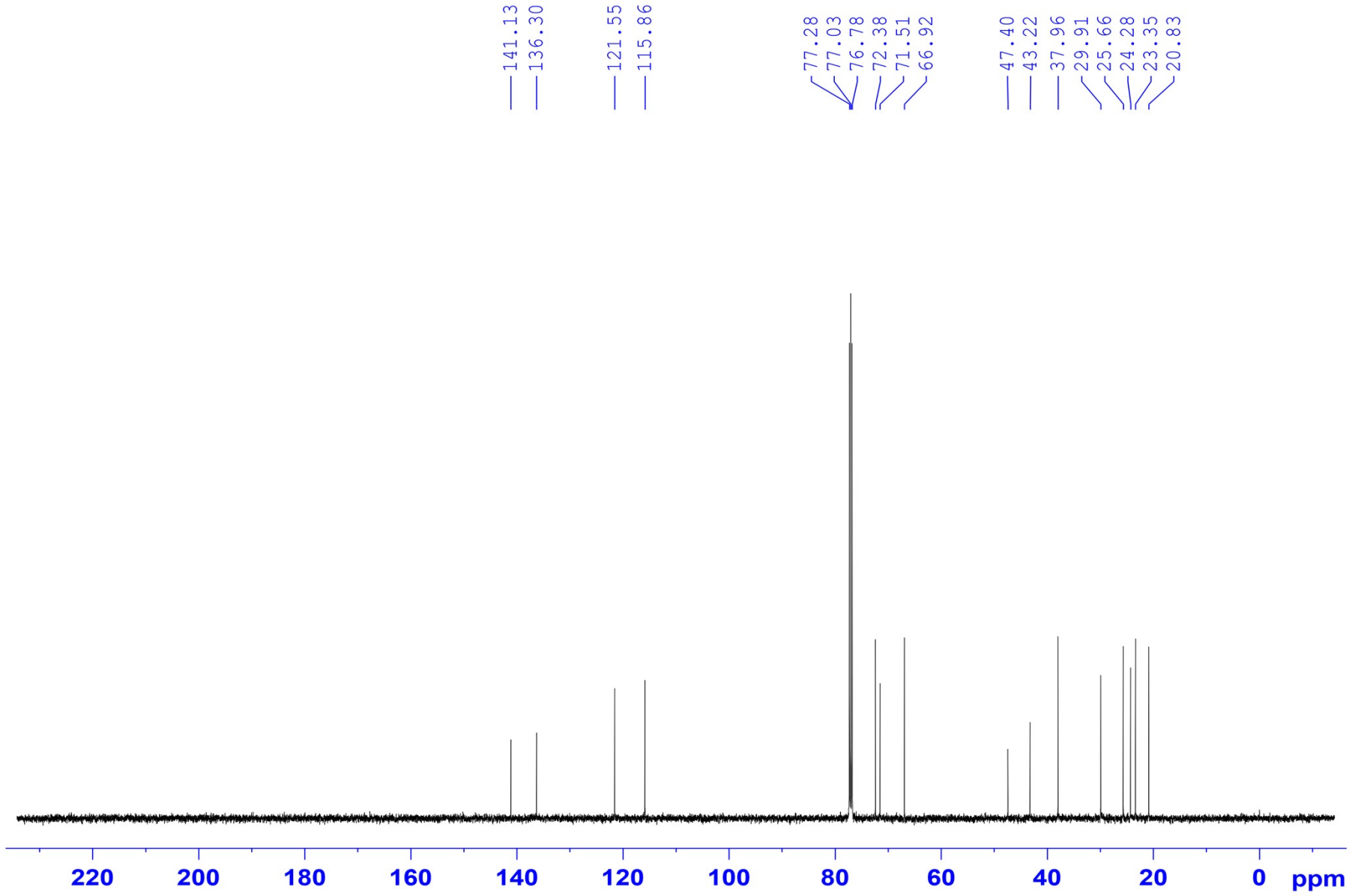


Figure S35. HSQC spectrum (in $CDCl_3$) of compound **4**

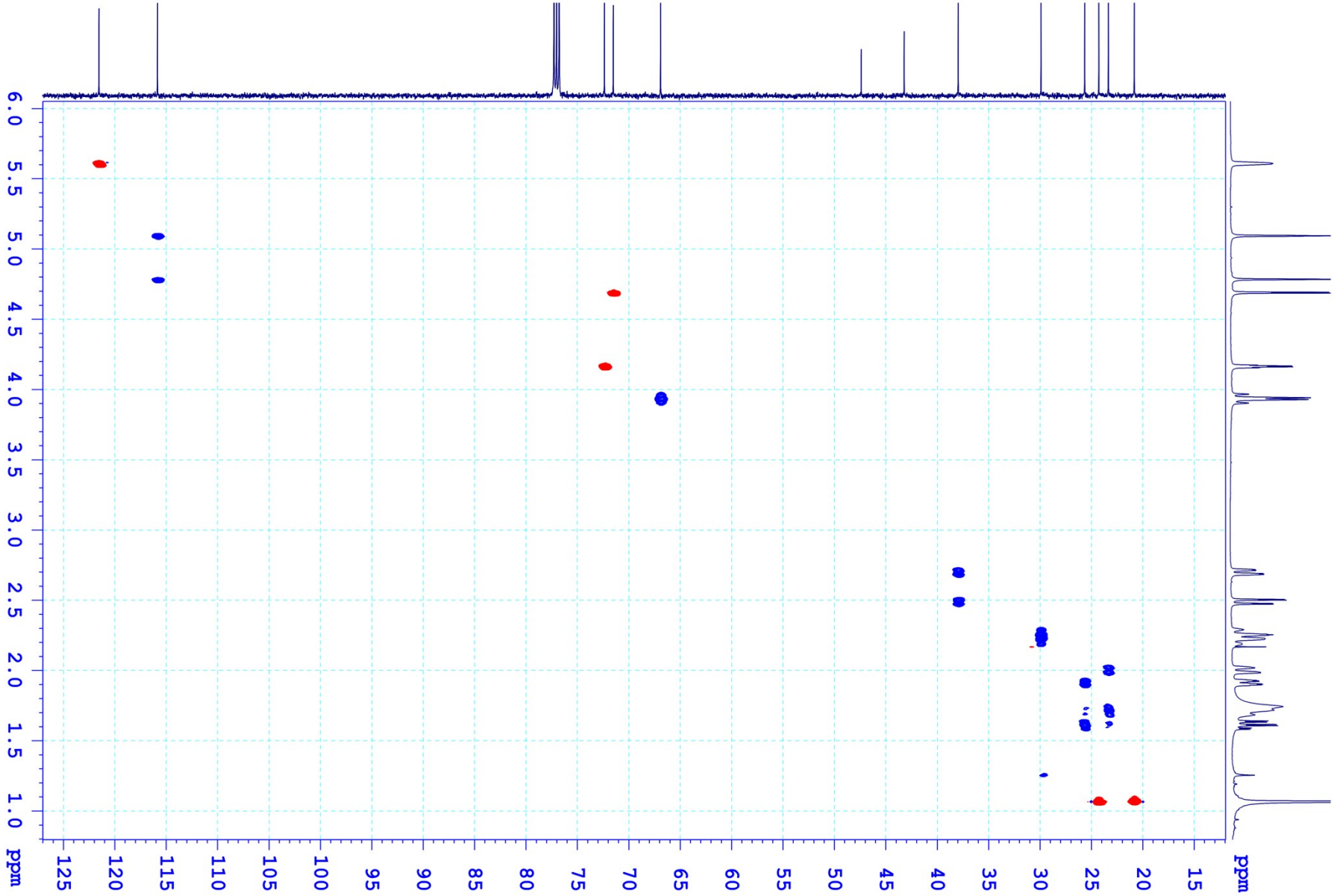


Figure S36. HMBC spectrum (in $CDCl_3$) of compound **4**

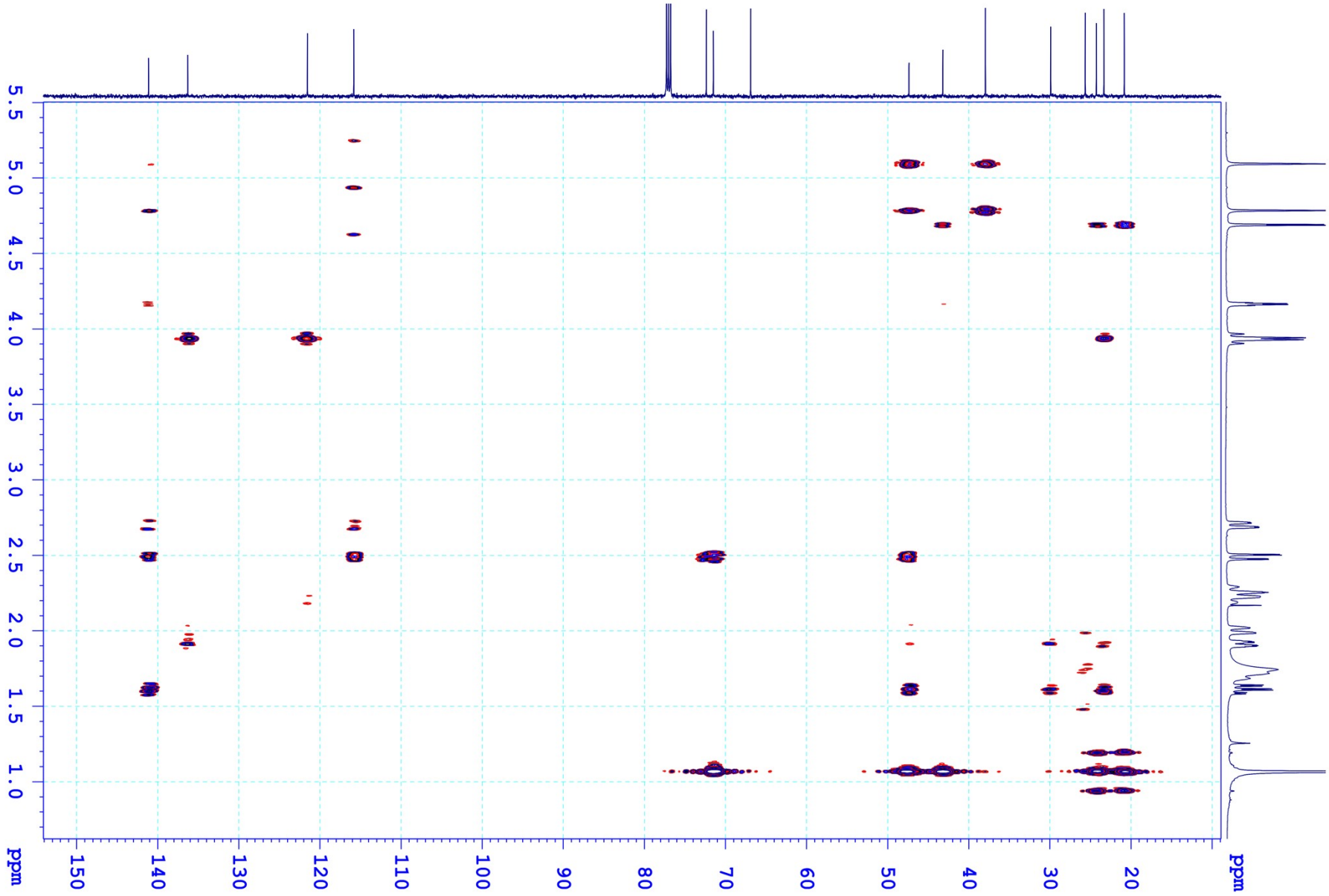


Figure S37. COSY spectrum (in $CDCl_3$) of compound **4**

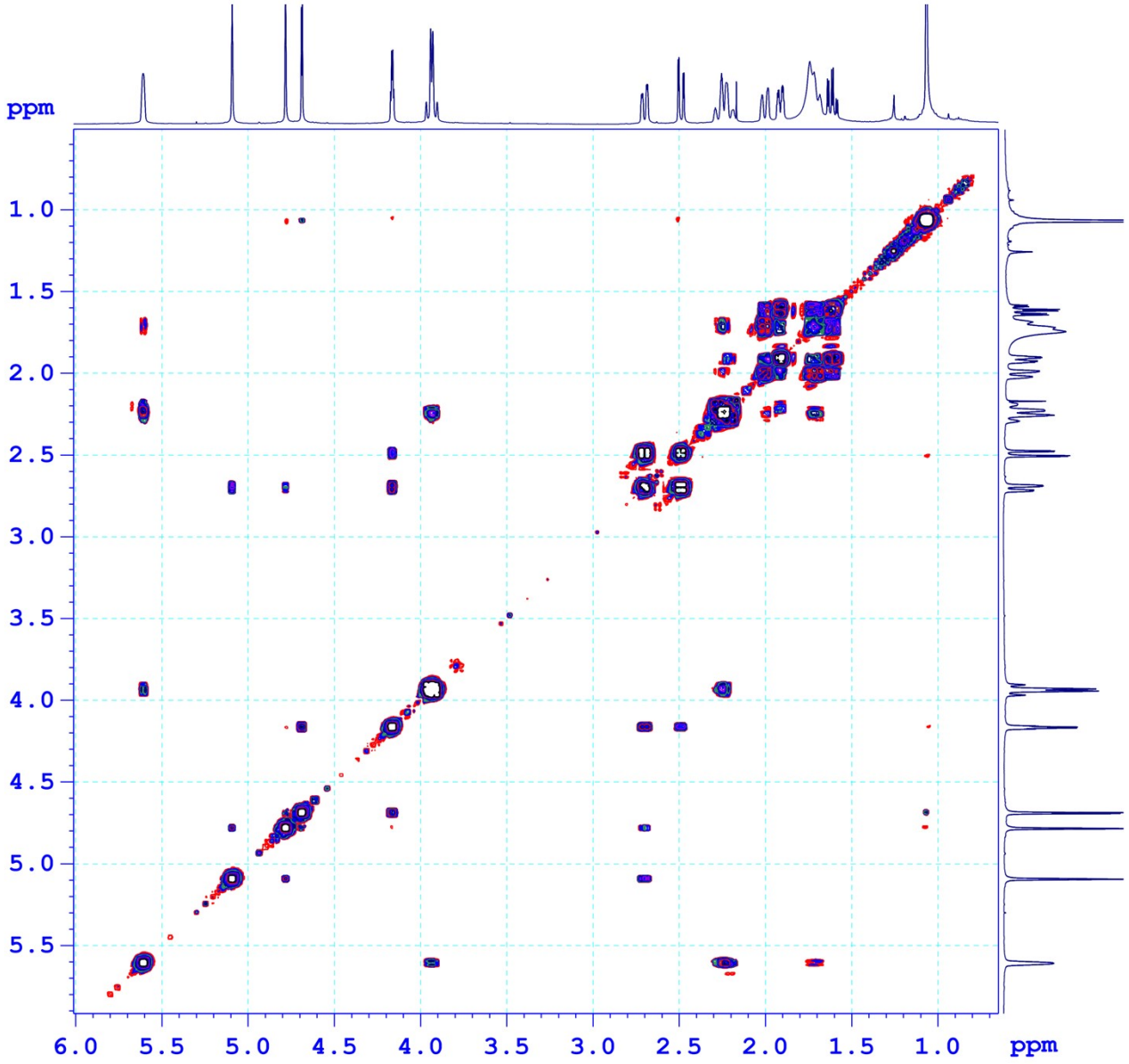


Figure S38. NOESY spectrum (in $CDCl_3$) of compound **4**

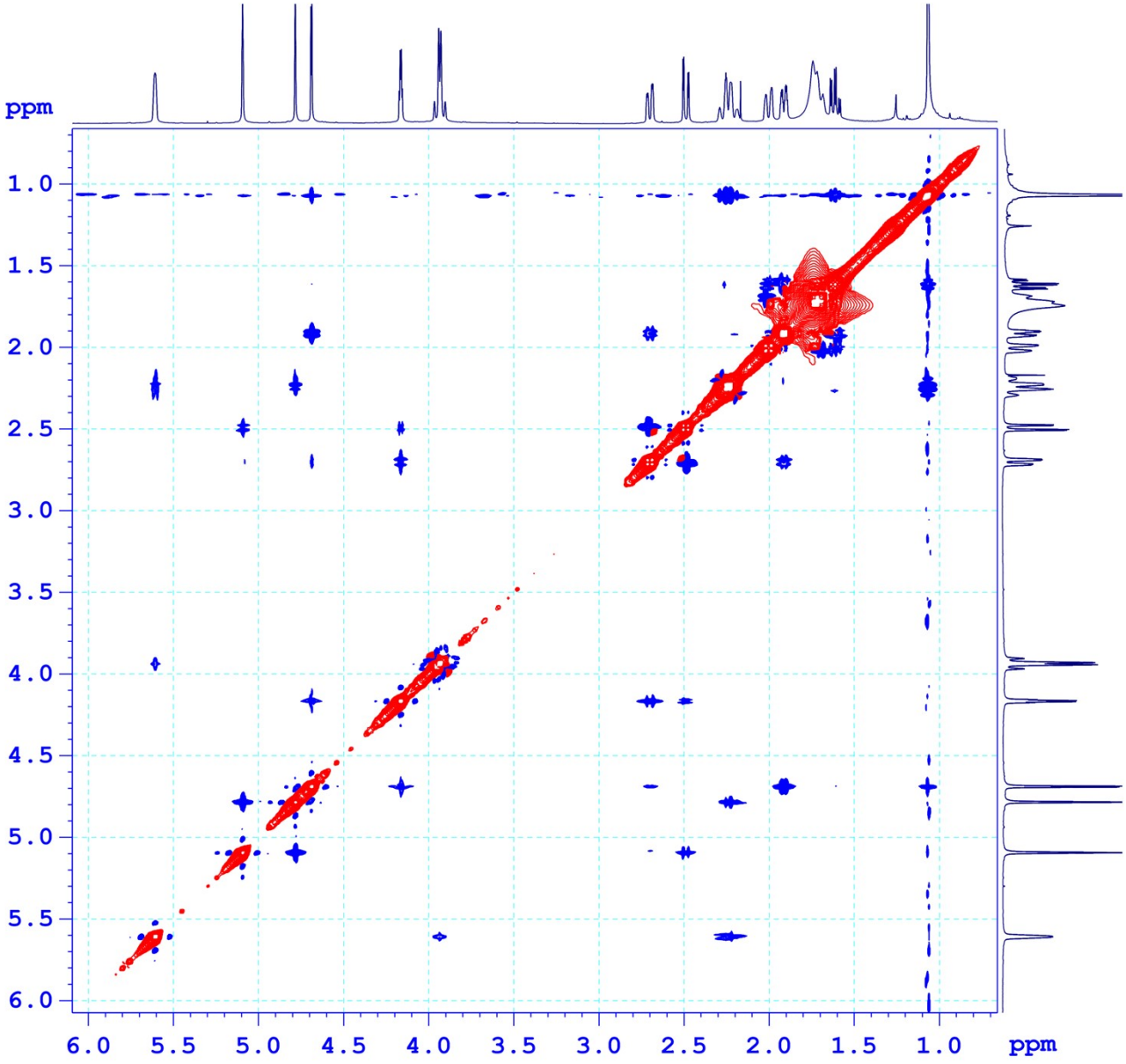


Figure S39. ECD spectrum (in ACN) of compound **4**

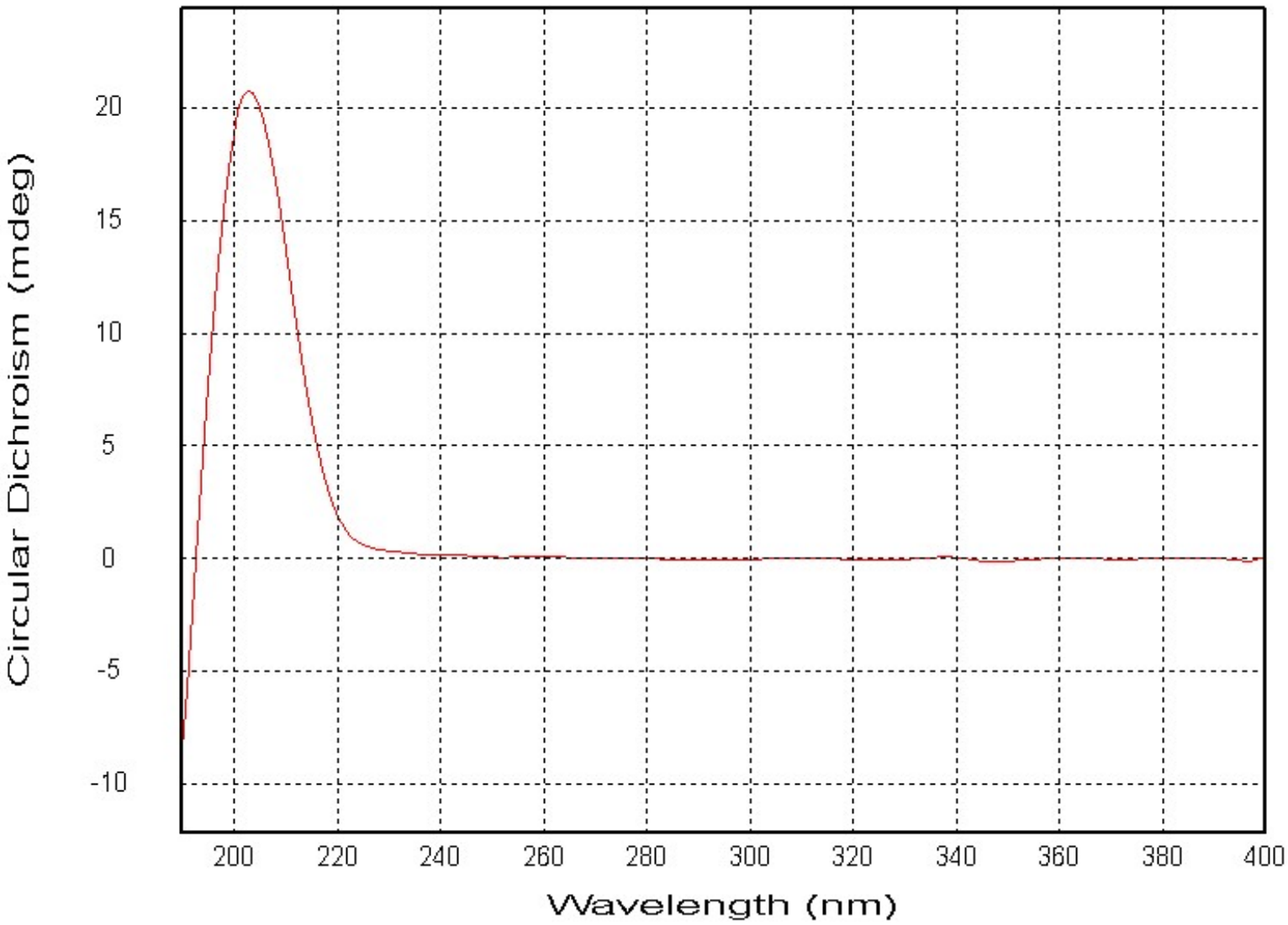


Figure S40. IR spectrum of compound **4**

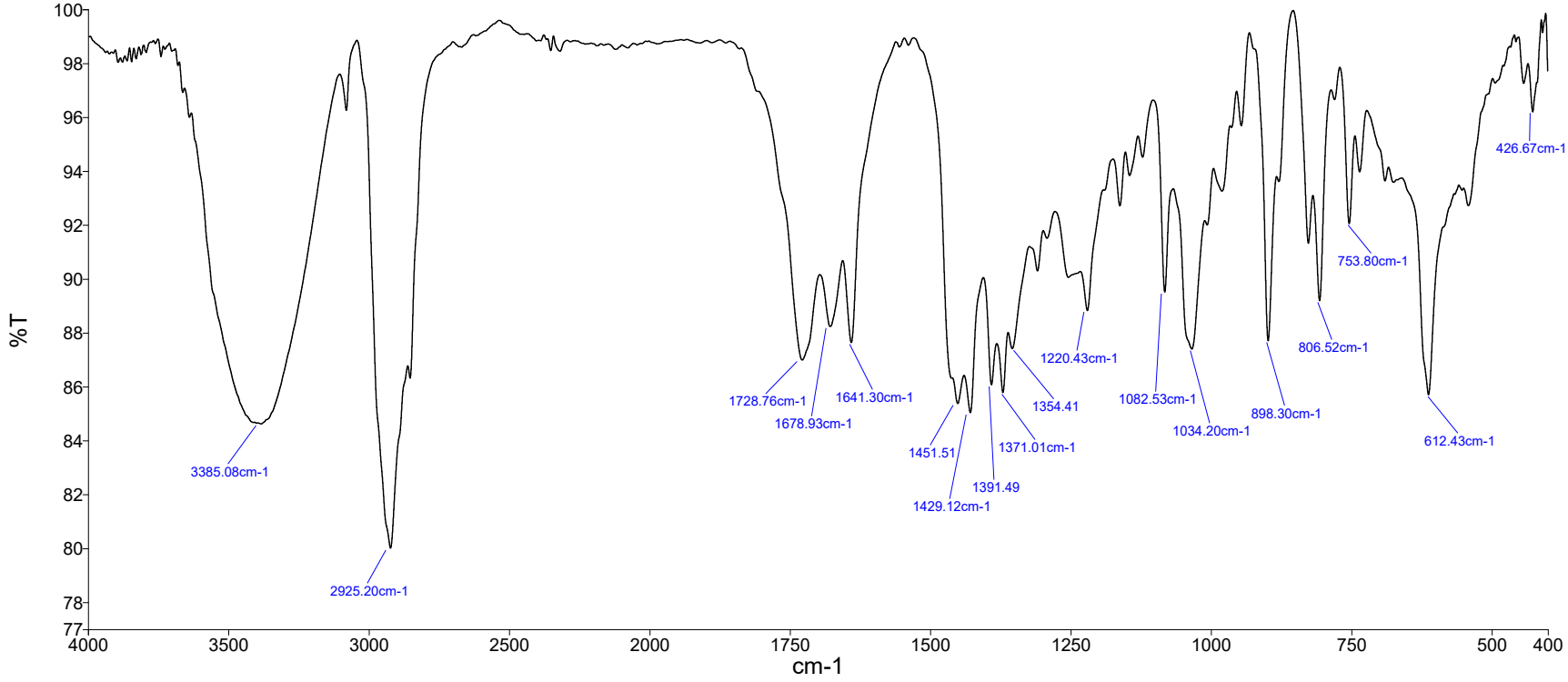


Figure S41. HRESIMS spectrum of compound **5**

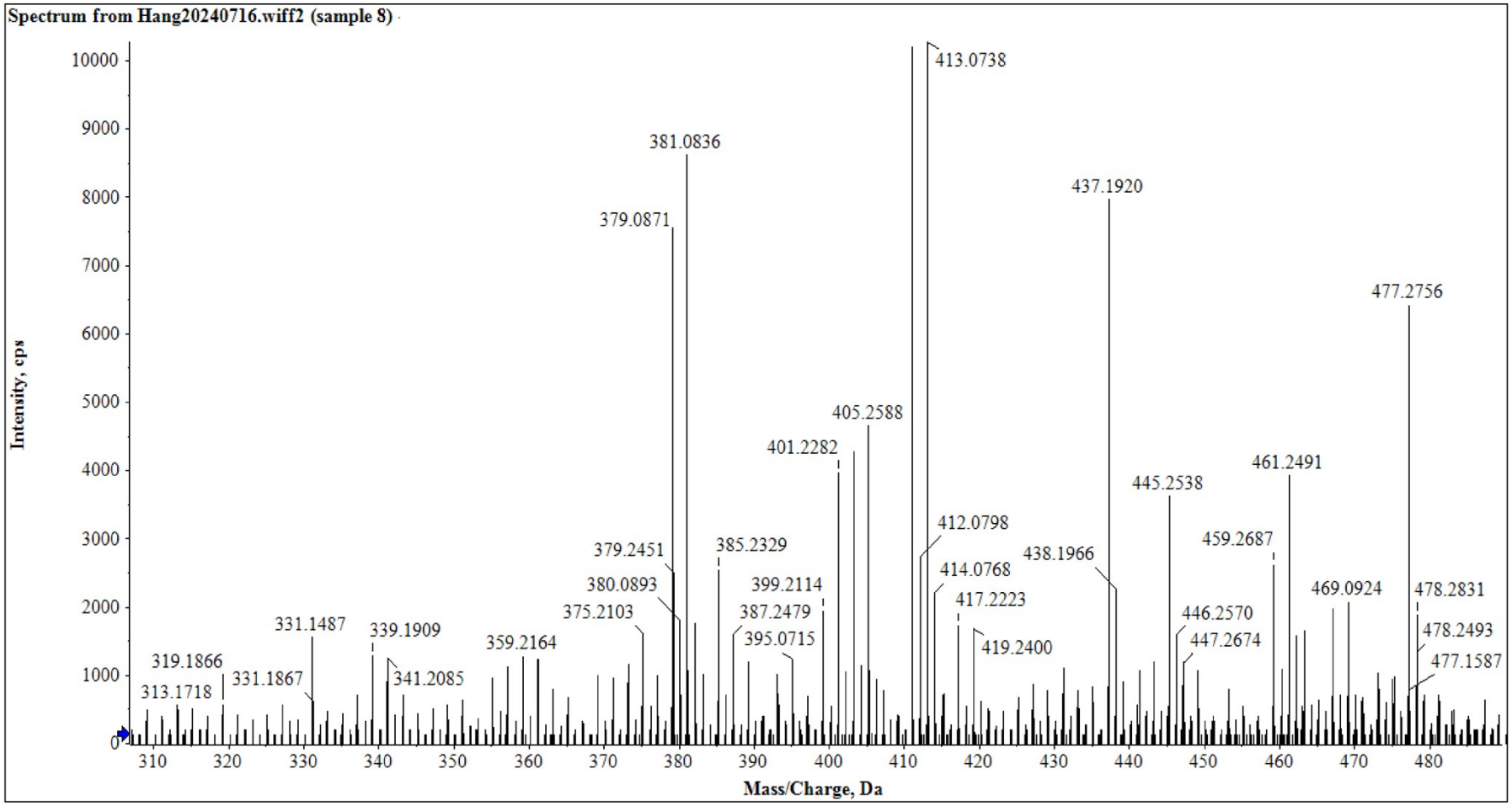


Figure S42. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of compound **5**

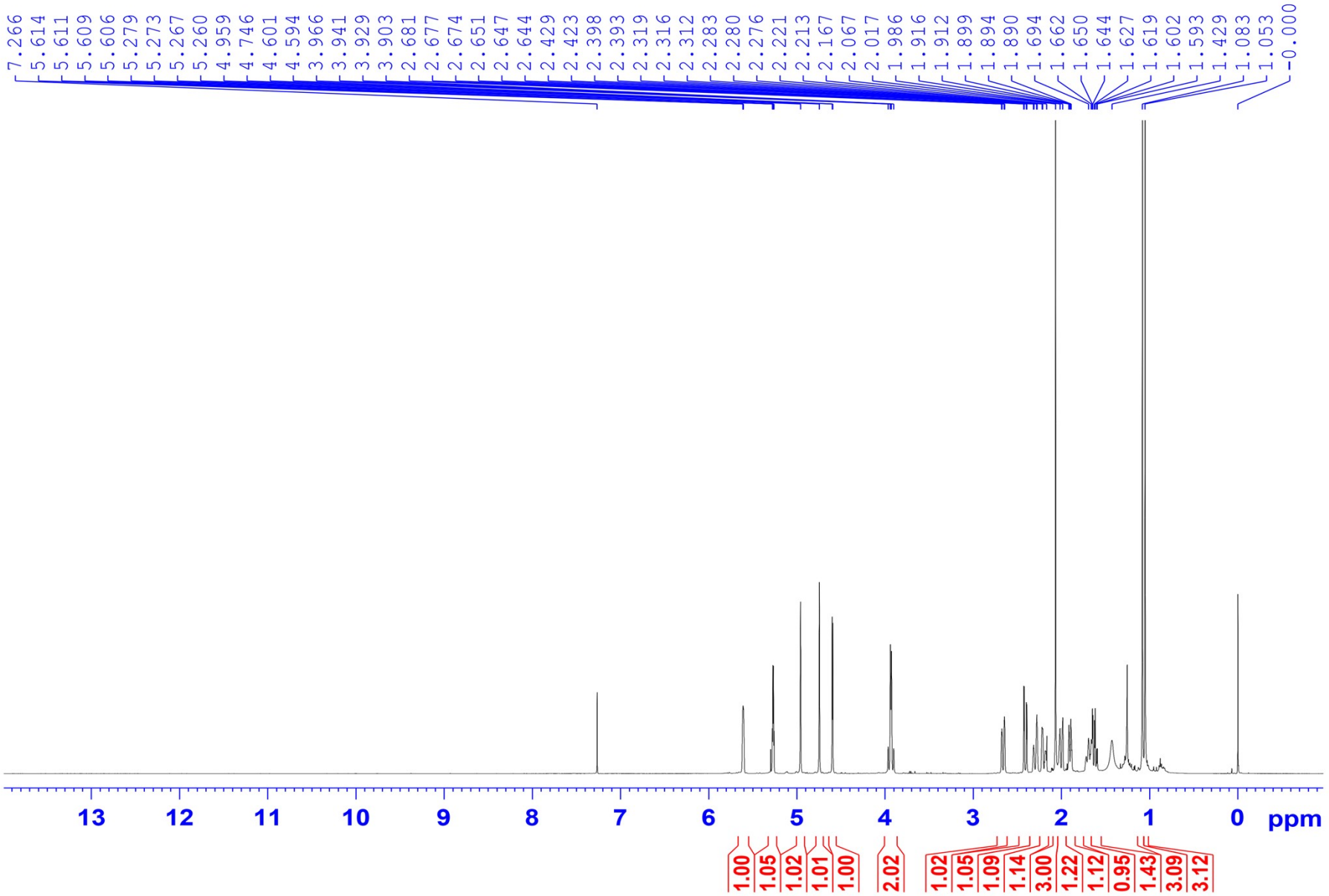


Figure S43. ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of compound **5**

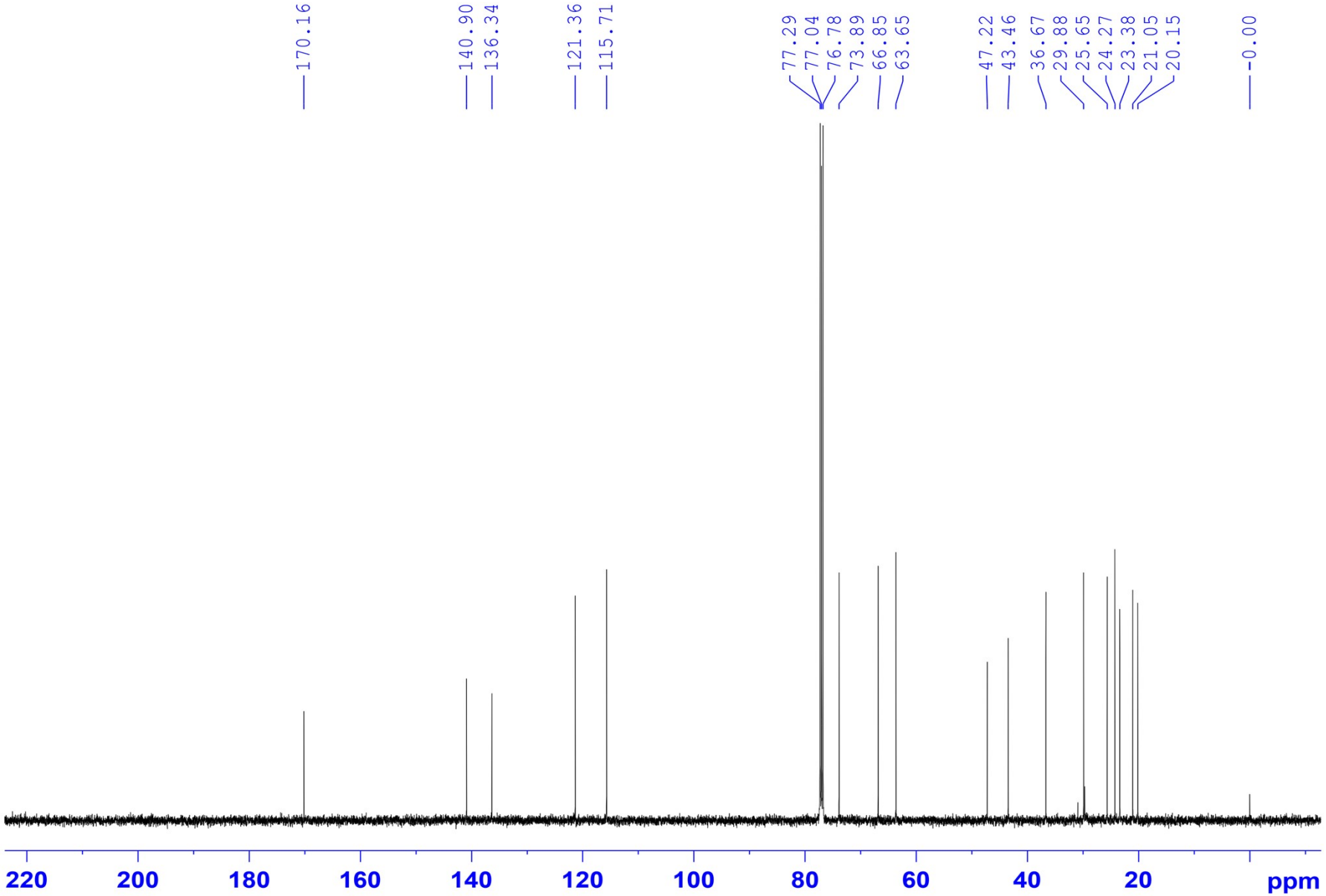


Figure S44. HSQC spectrum (in $CDCl_3$) of compound **5**

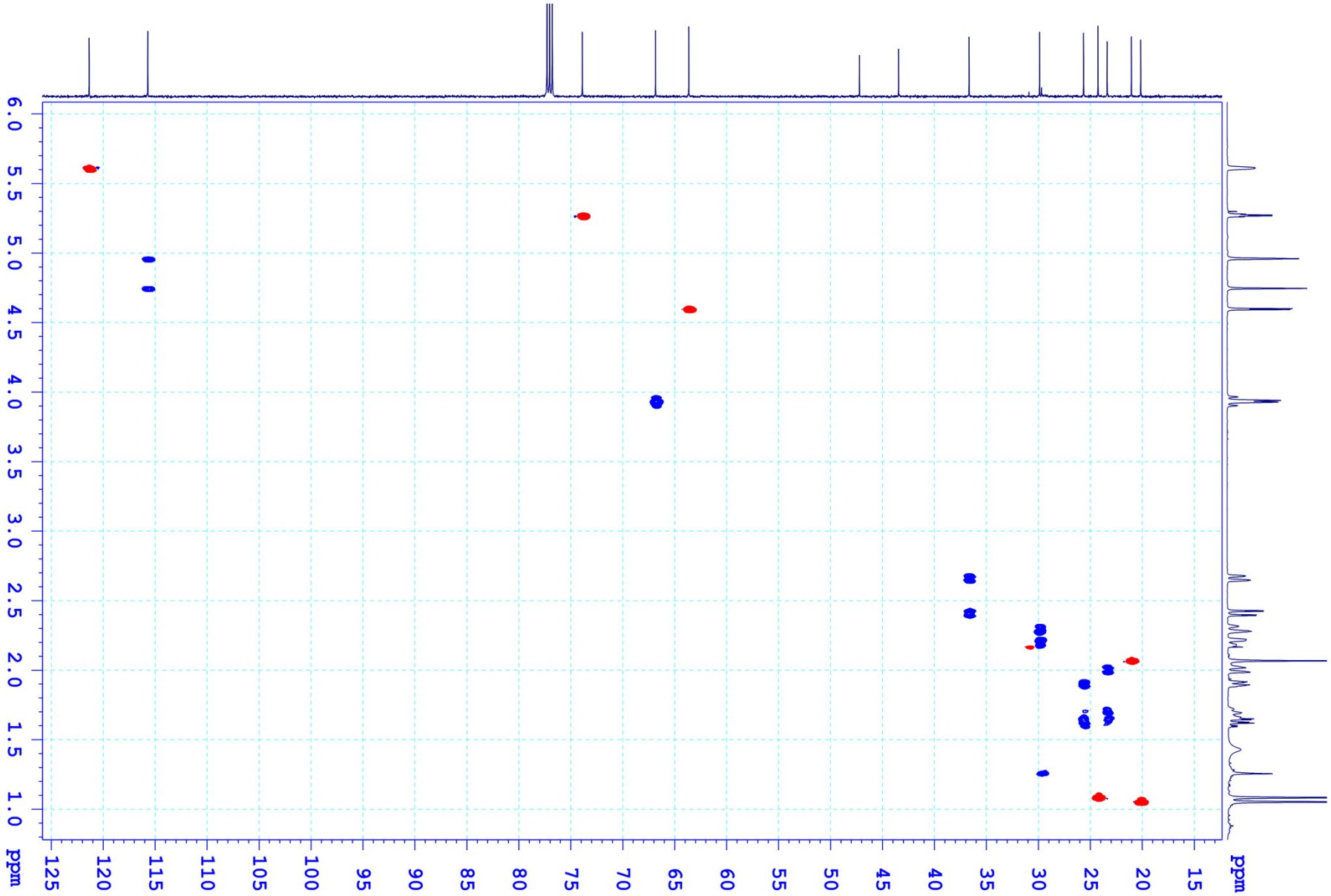


Figure S45. HMBC spectrum (in $CDCl_3$) of compound **5**

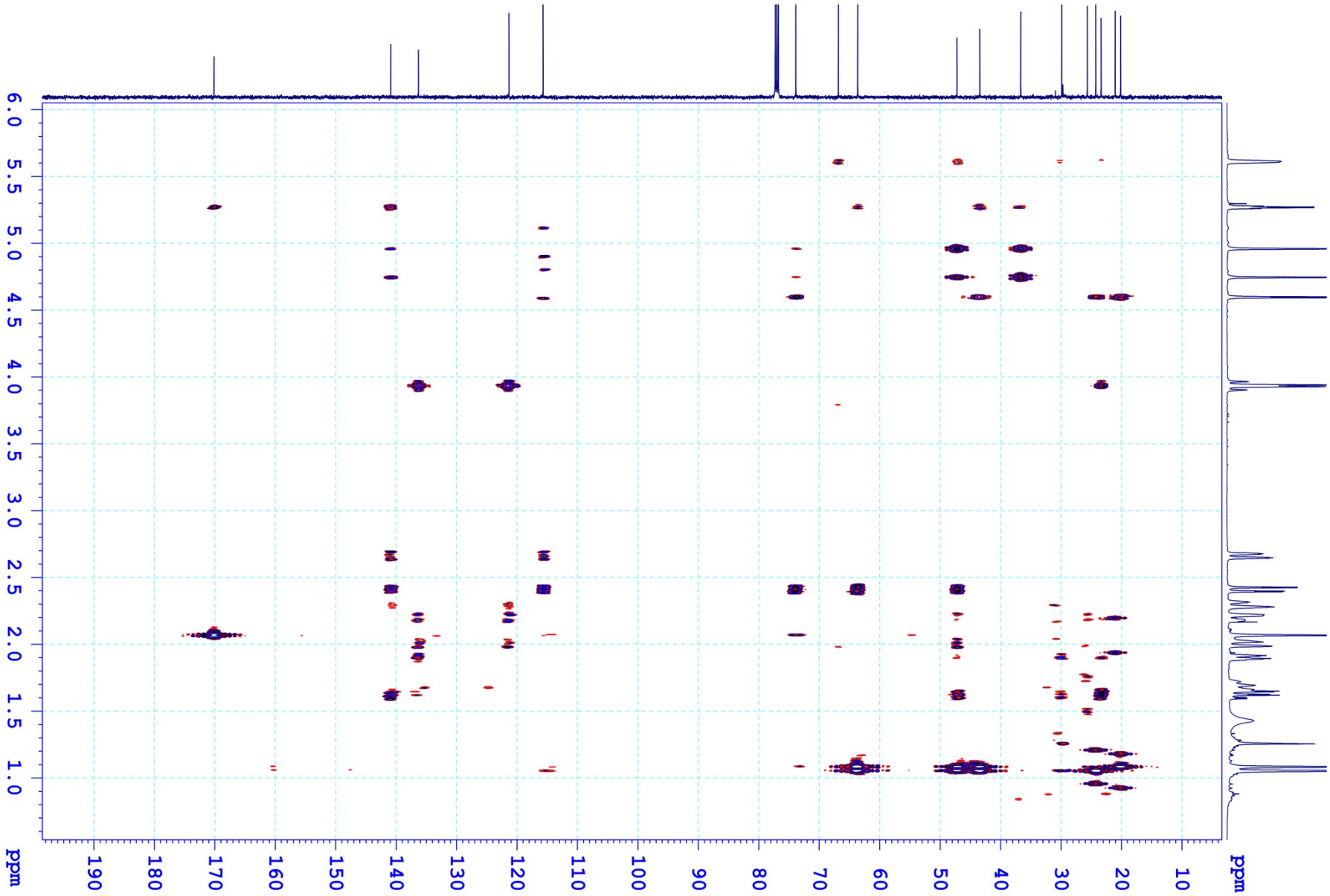


Figure S46. COSY spectrum (in $CDCl_3$) of compound **5**

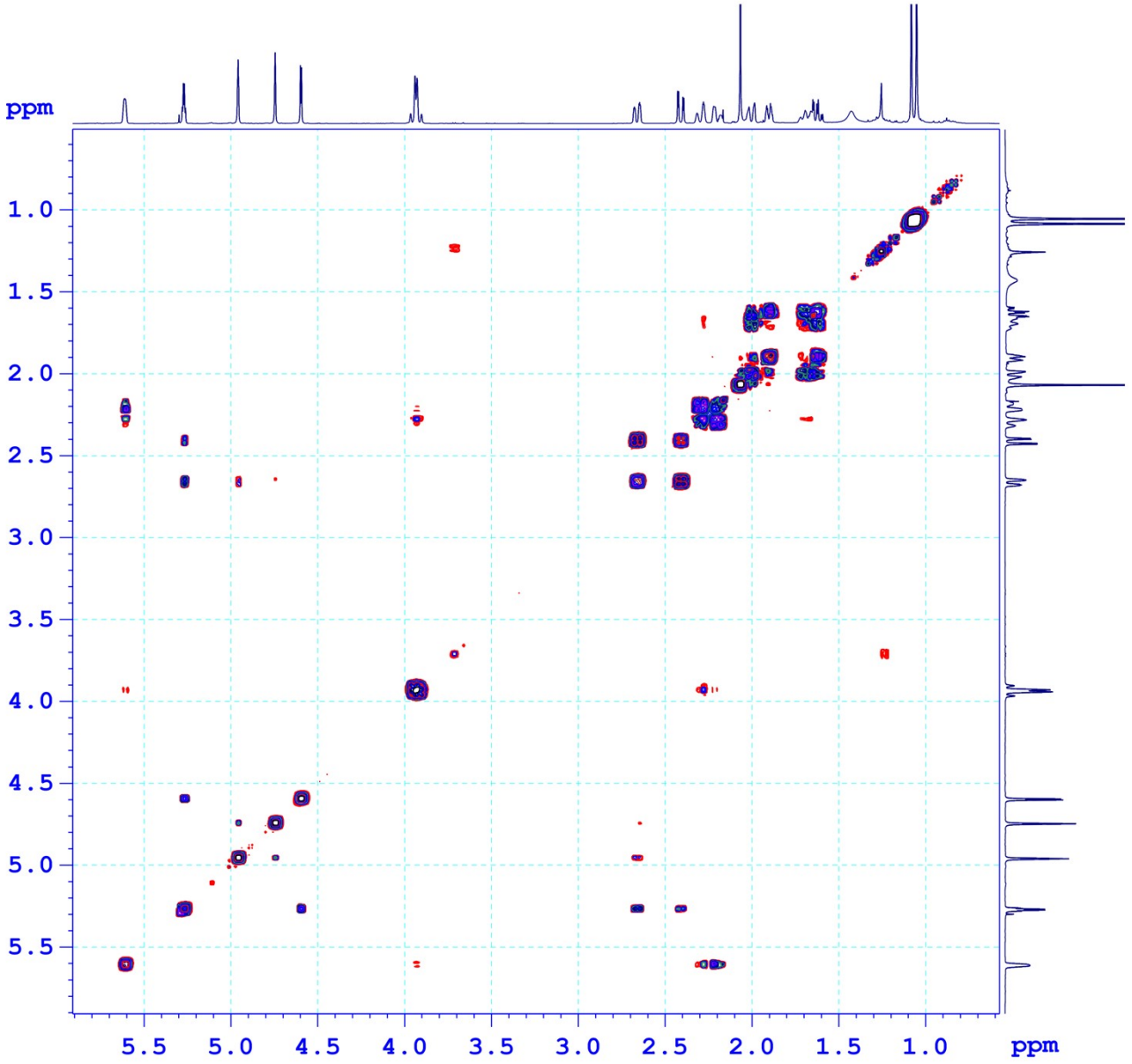


Figure S47. NOESY spectrum (in $CDCl_3$) of compound **5**

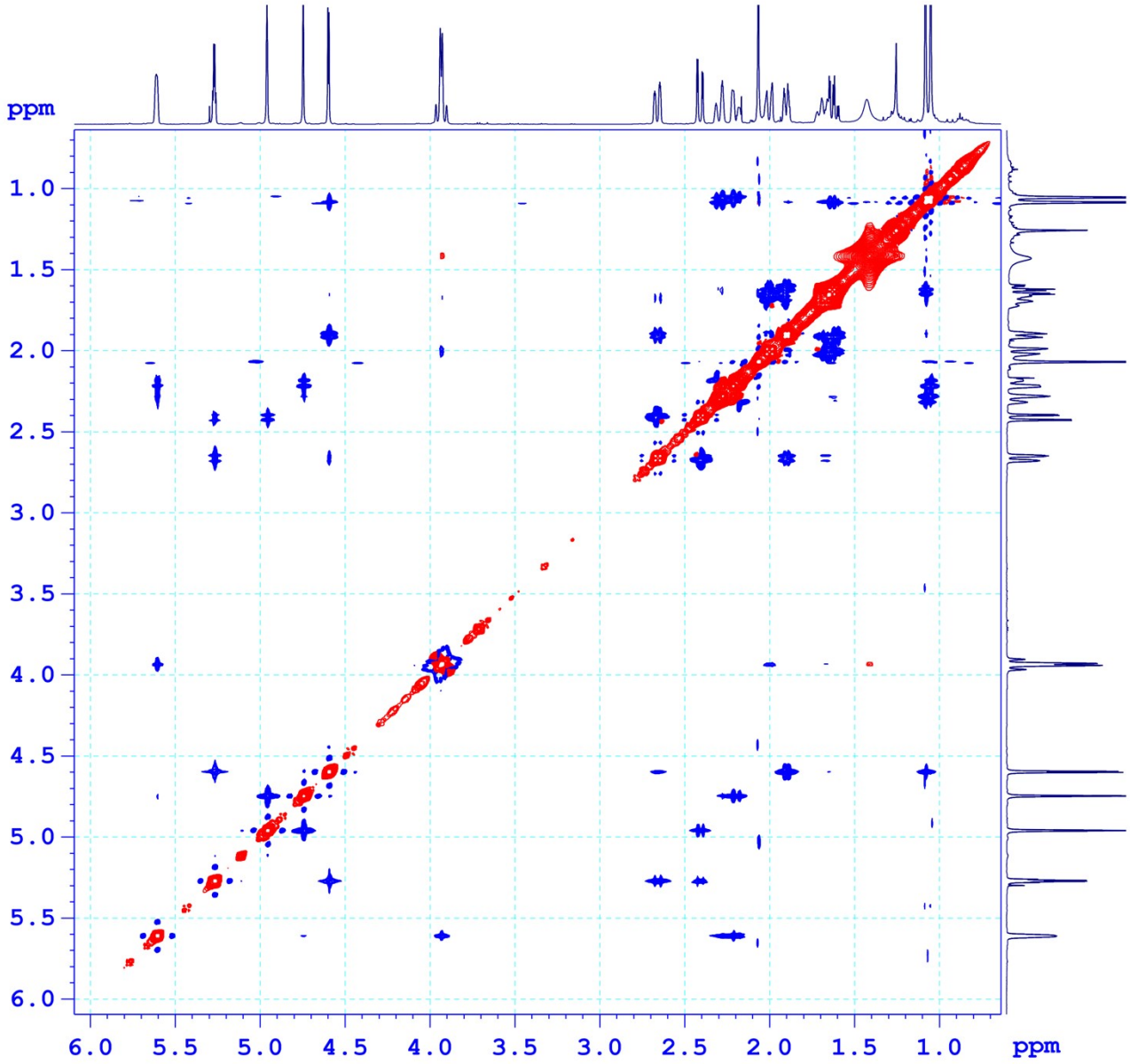


Figure S48. ECD spectrum (in ACN) of compound **5**

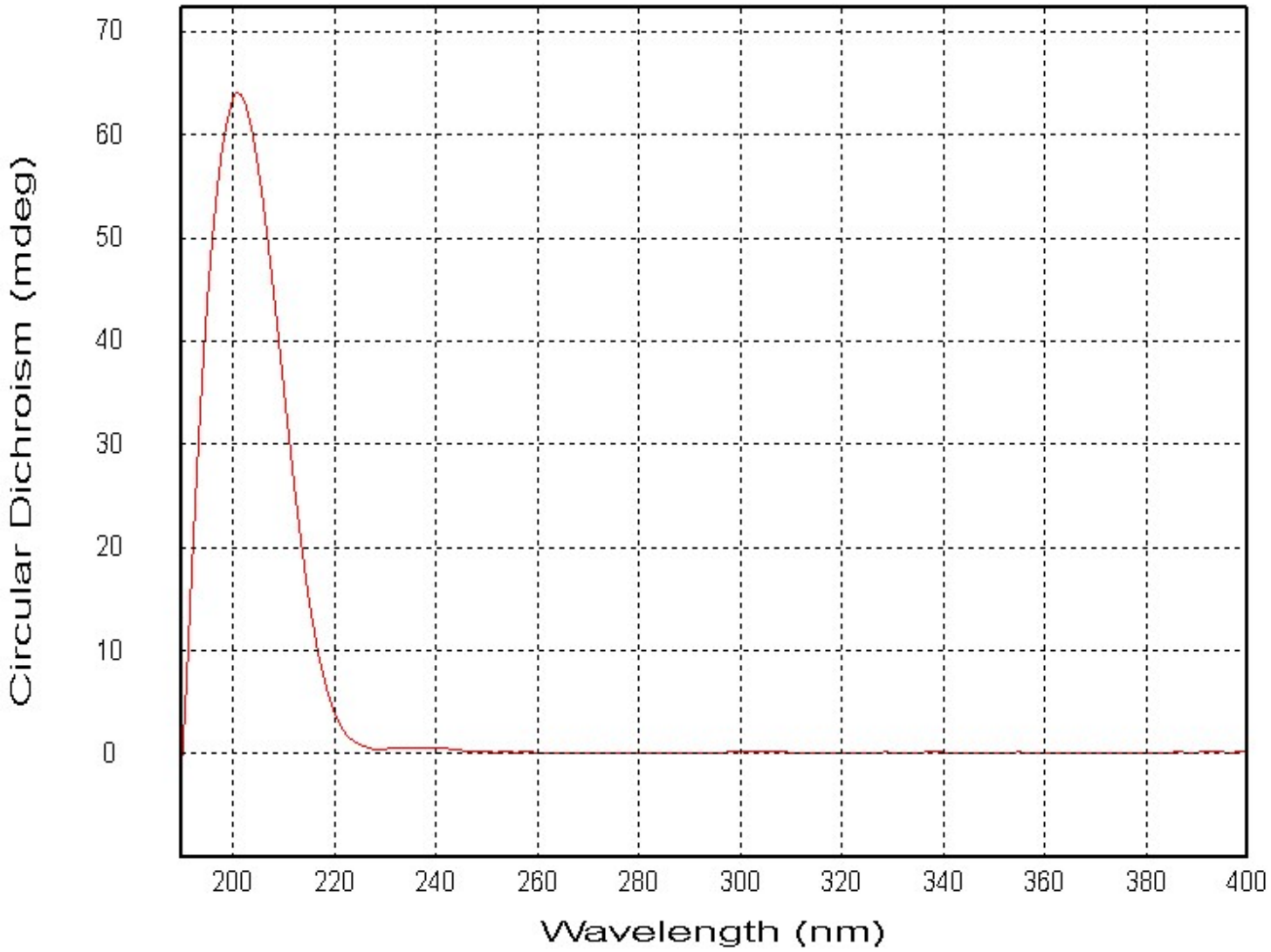


Figure S49. IR spectrum of compound **5**

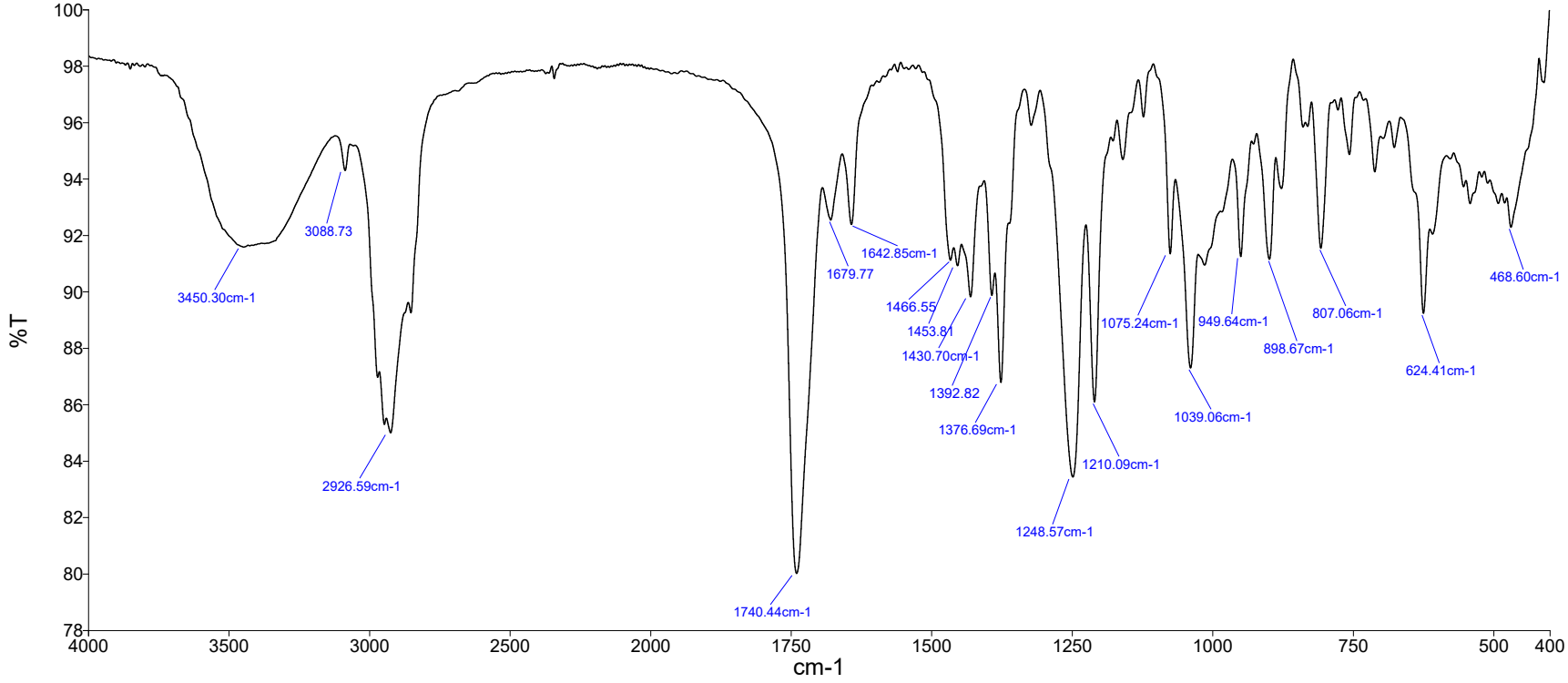


Figure S50. HRESIMS spectrum of compound **6**

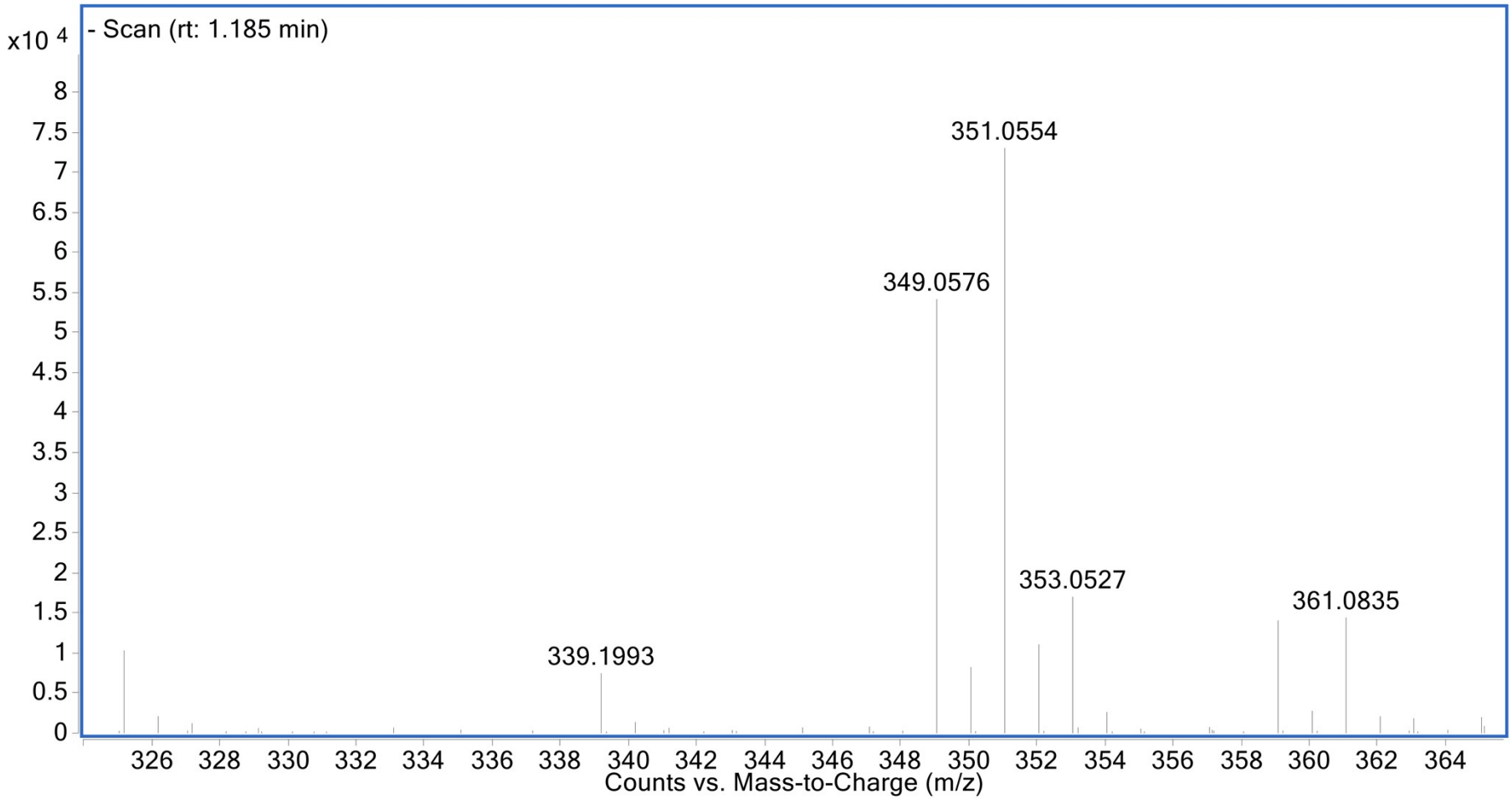


Figure S51. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of compound **6**

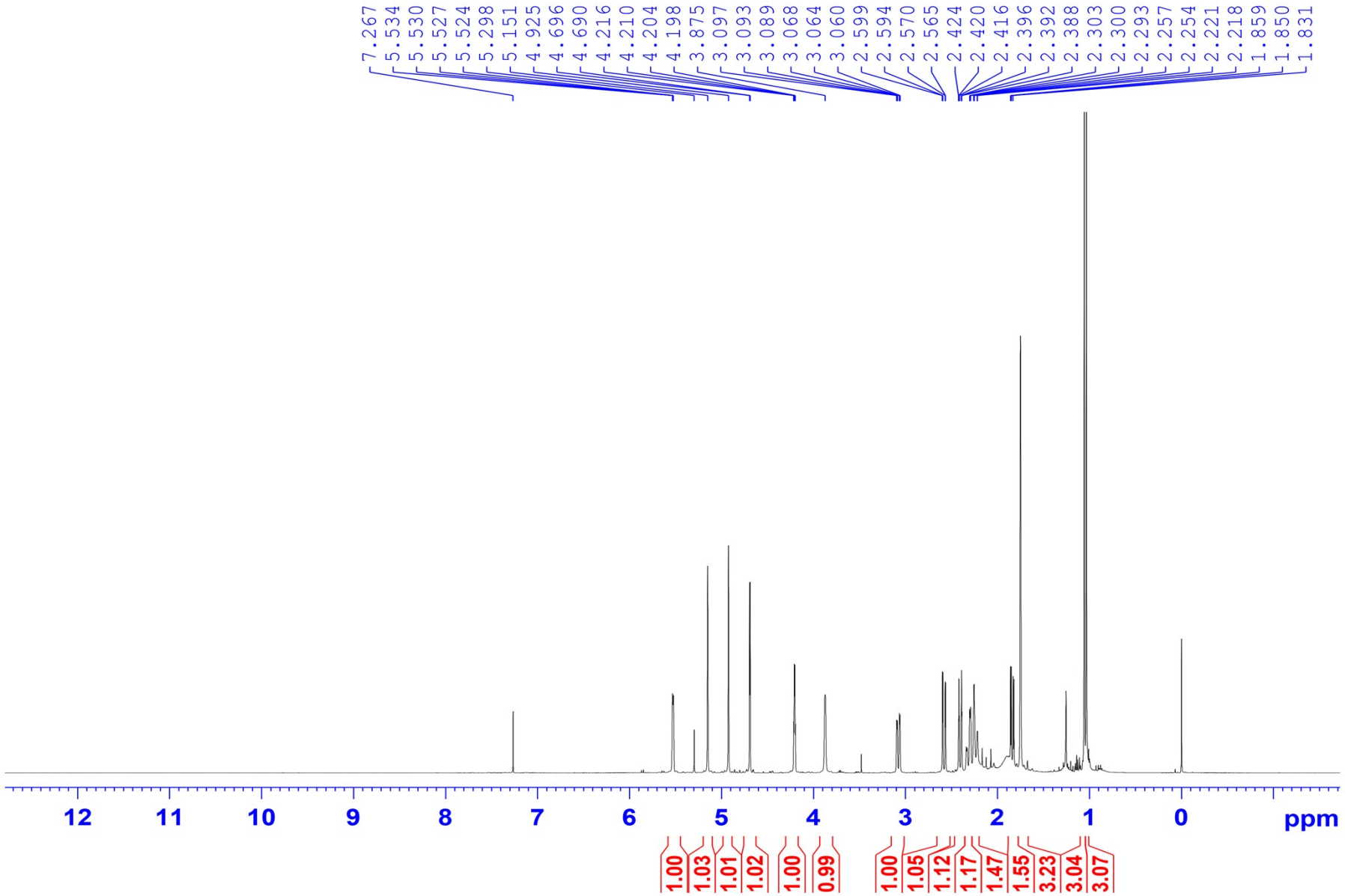


Figure S52. ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of compound **6**

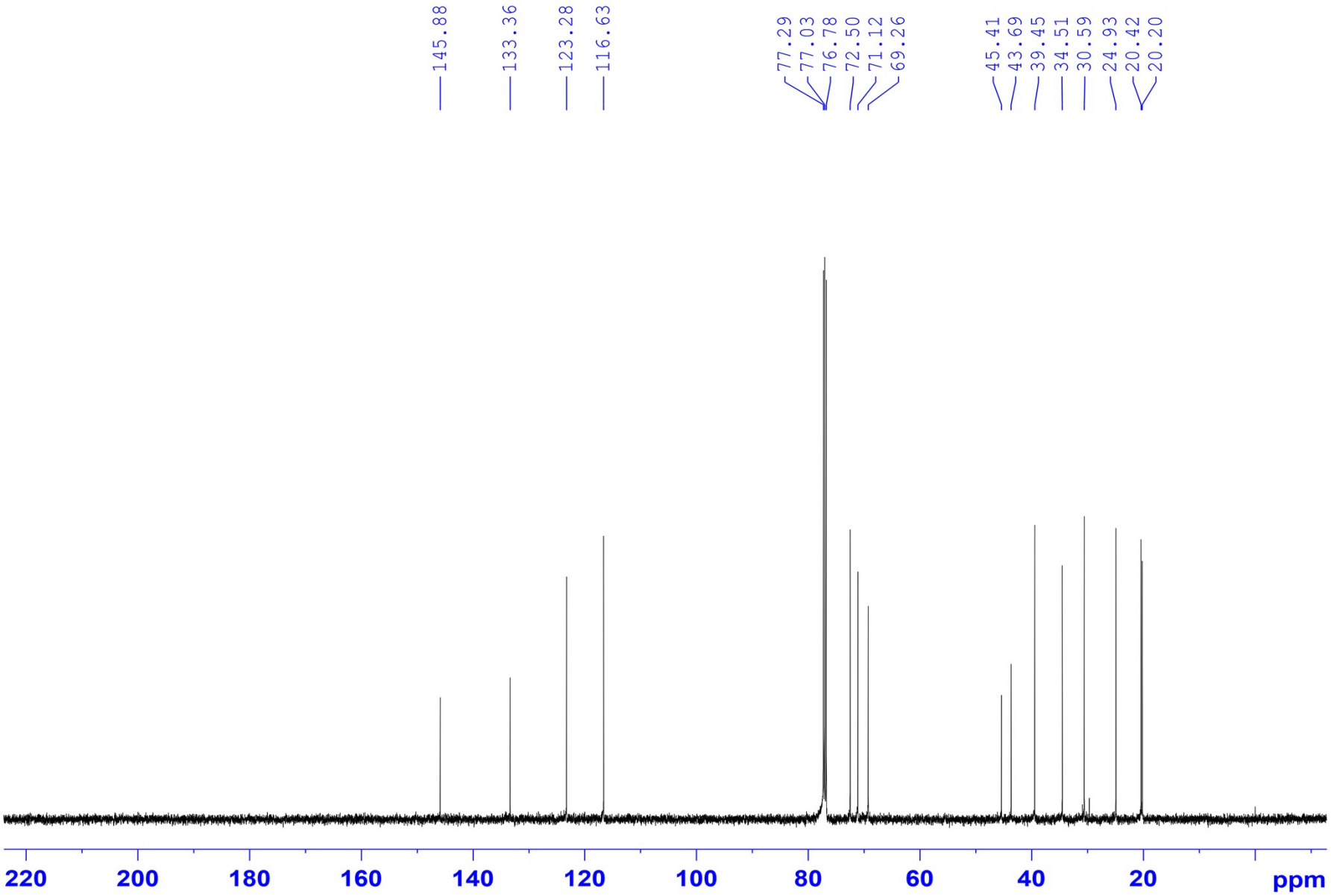


Figure S53. HSQC spectrum (in $CDCl_3$) of compound **6**

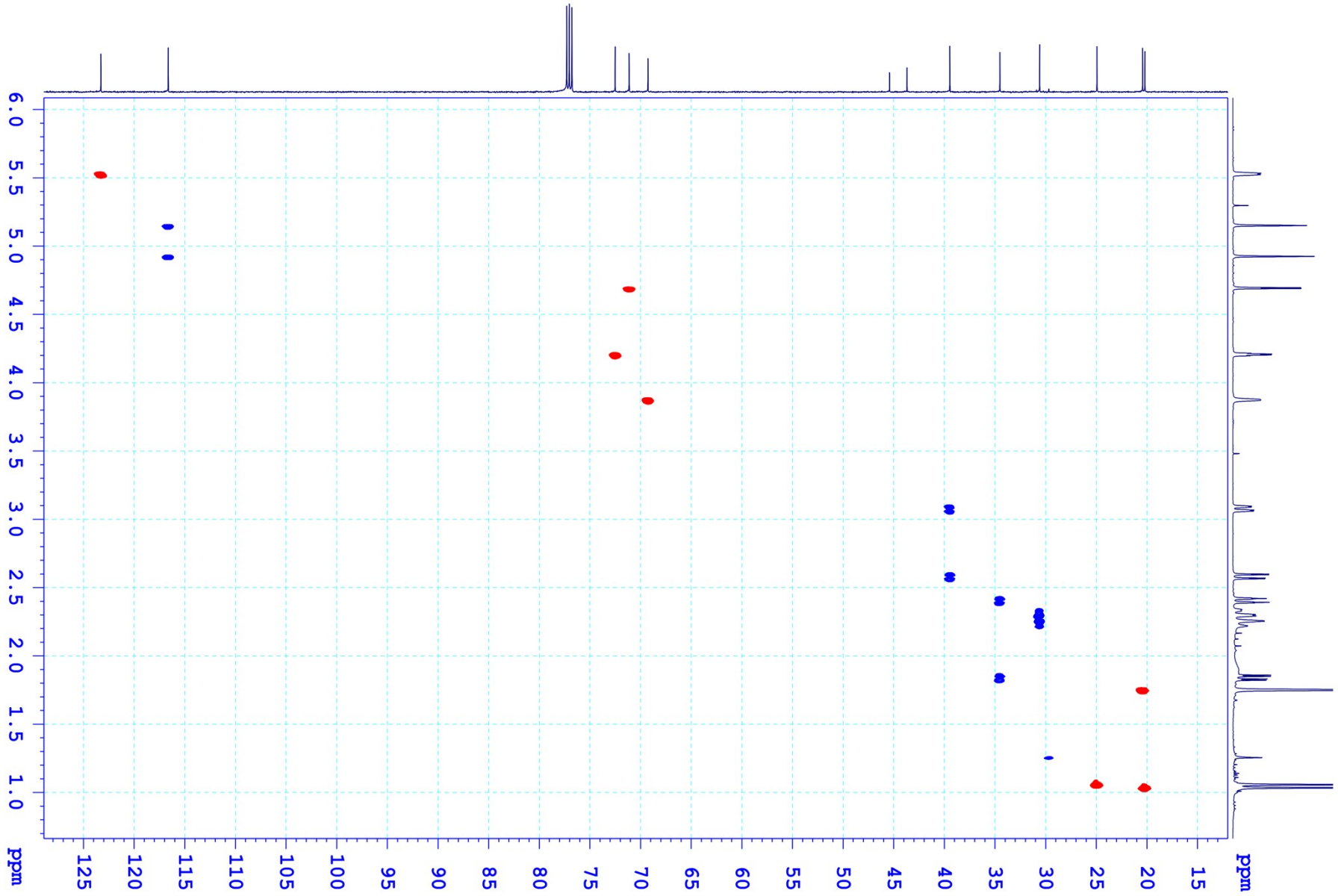


Figure S54. HMBC spectrum (in $CDCl_3$) of compound **6**

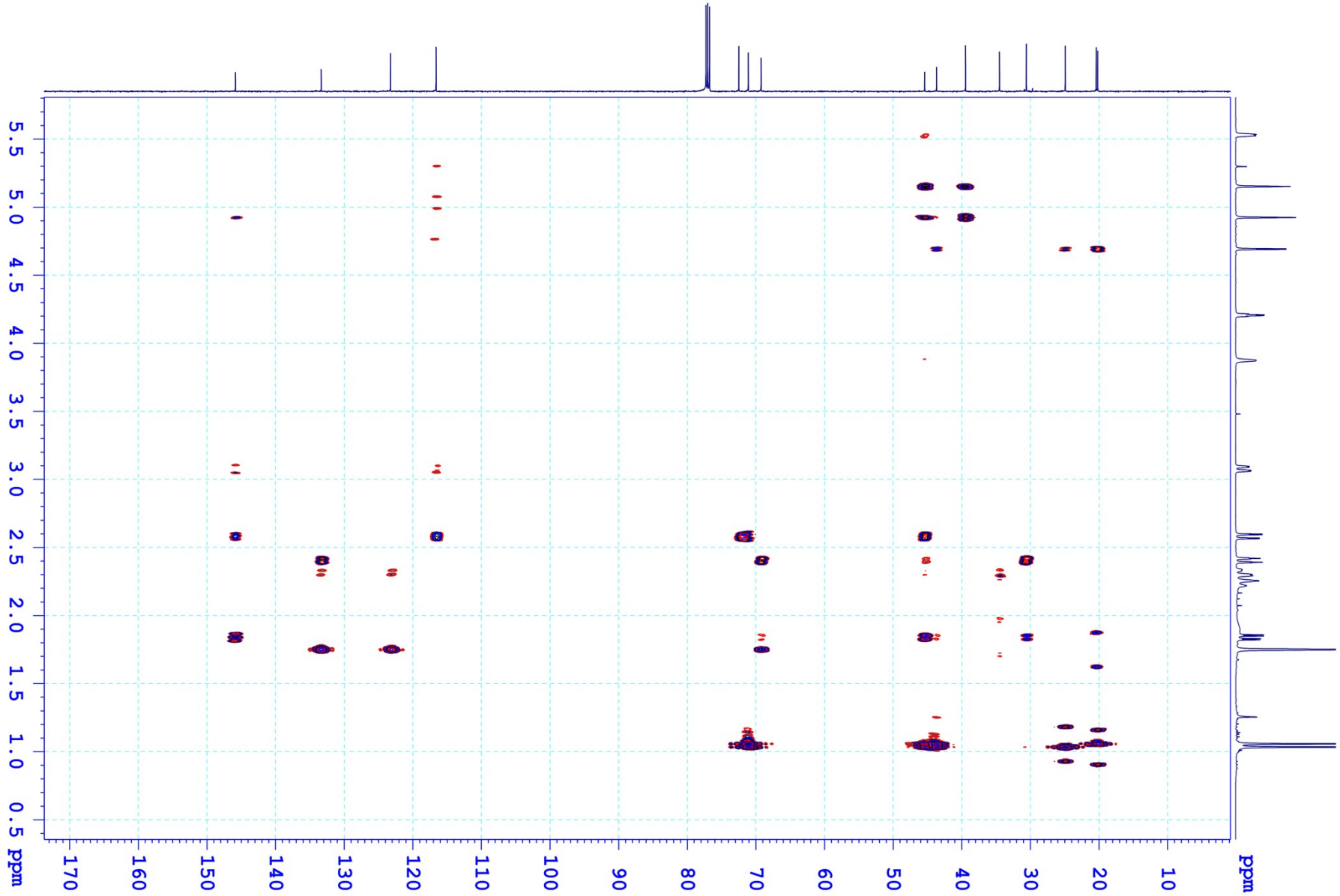


Figure S55. COSY spectrum (in $CDCl_3$) of compound **6**

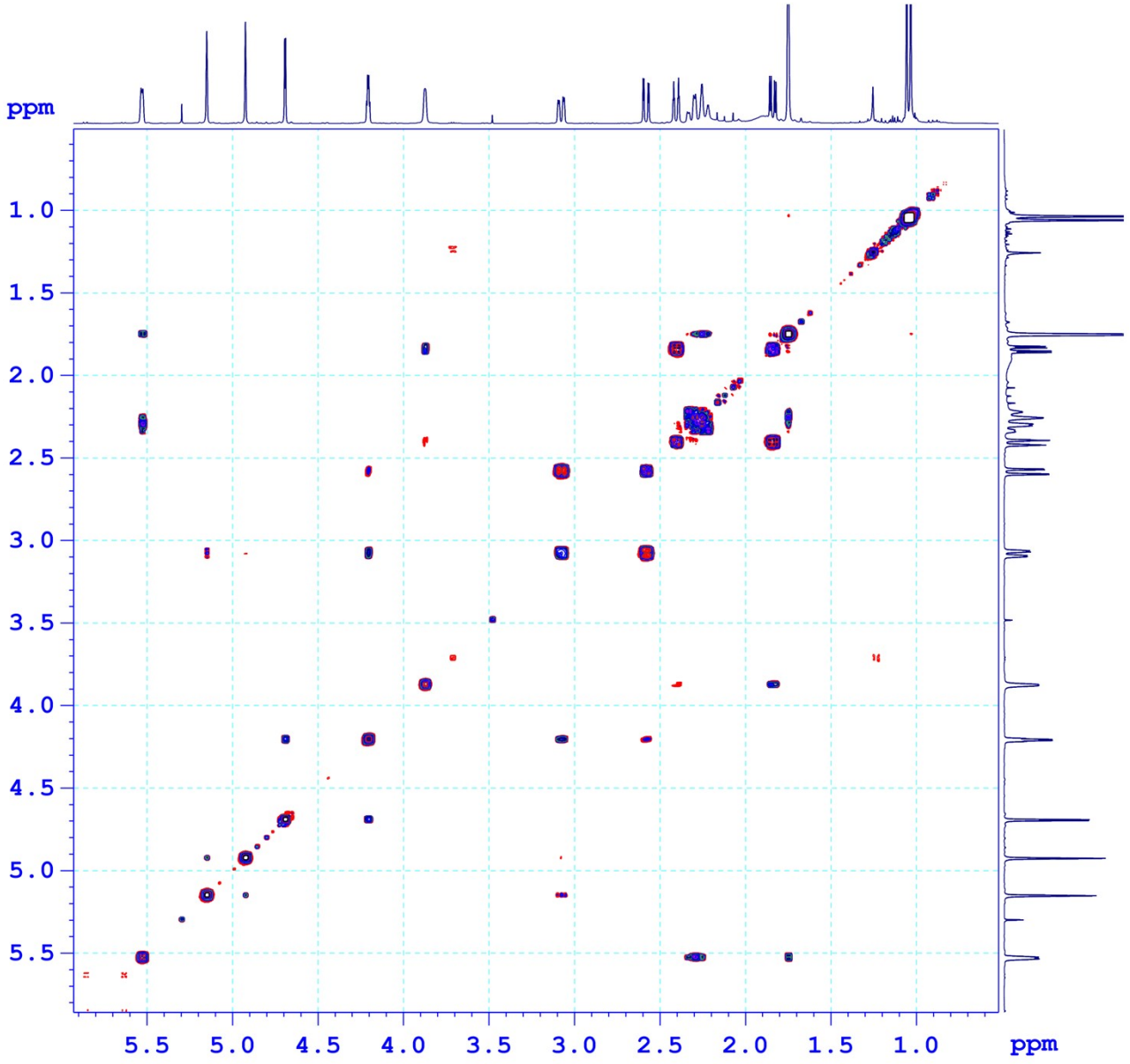


Figure S56. NOESY spectrum (in $CDCl_3$) of compound **6**

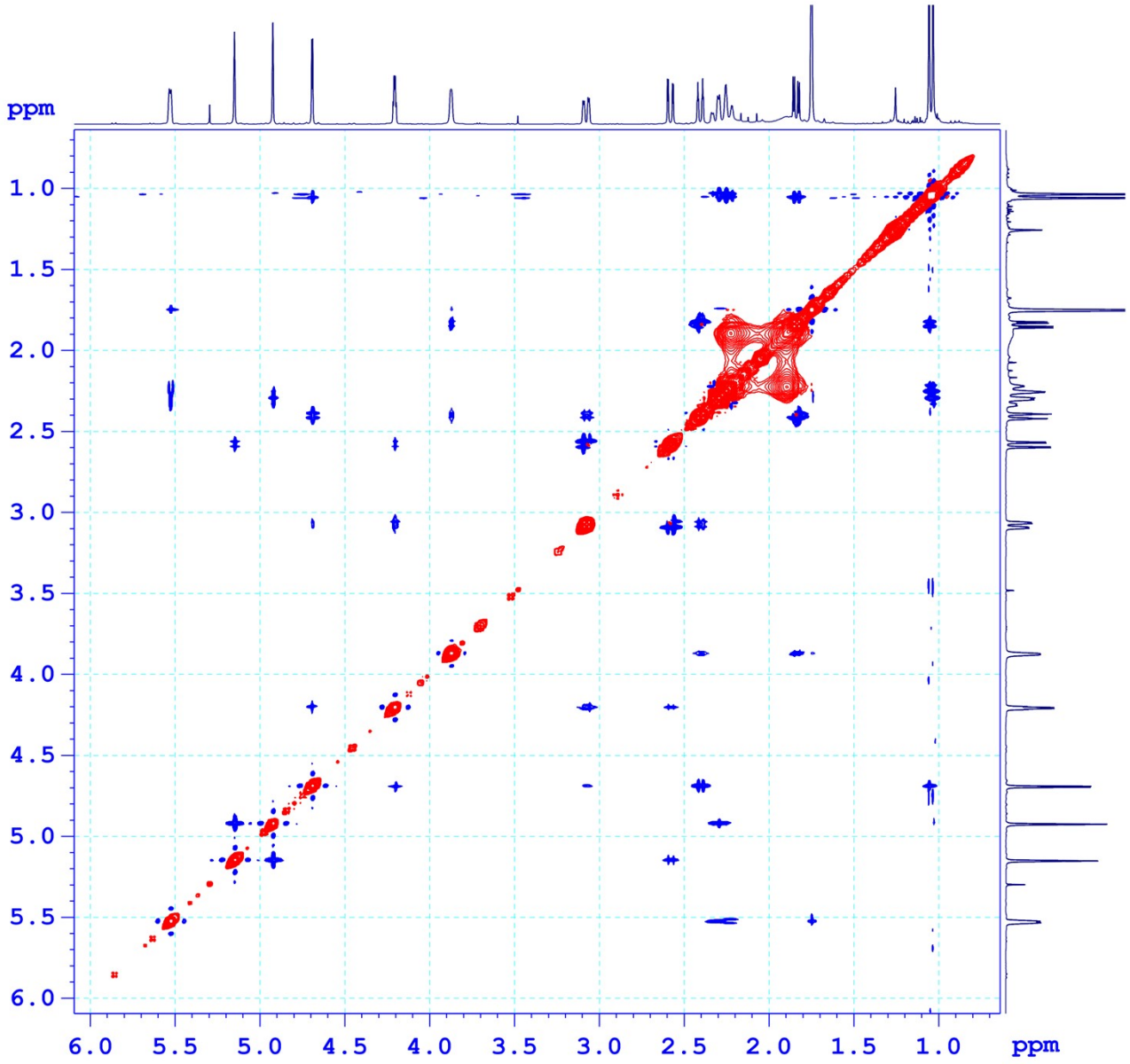


Figure S57. ECD spectrum (in ACN) of compound **6**

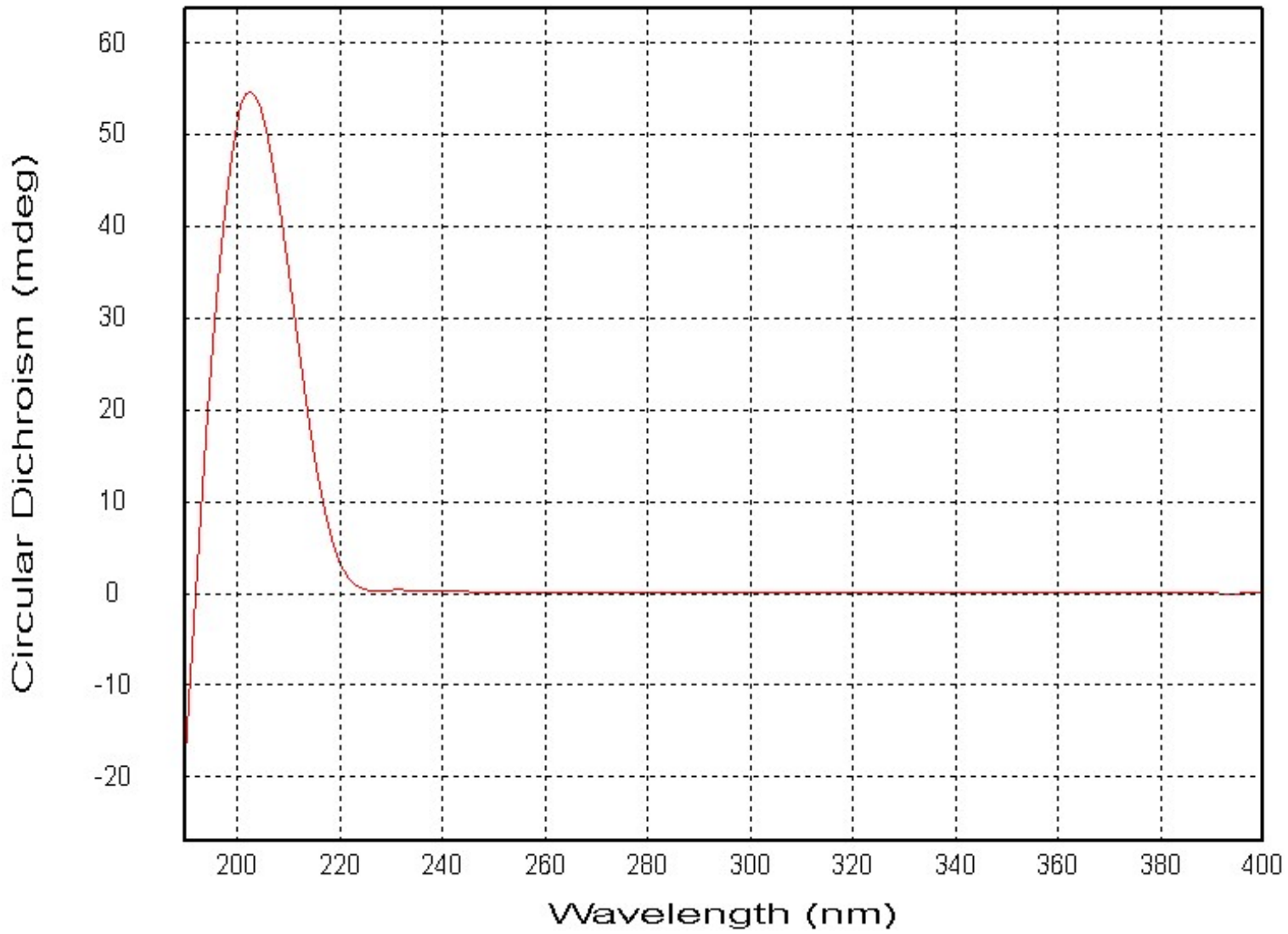


Figure S58. IR spectrum of compound **6**

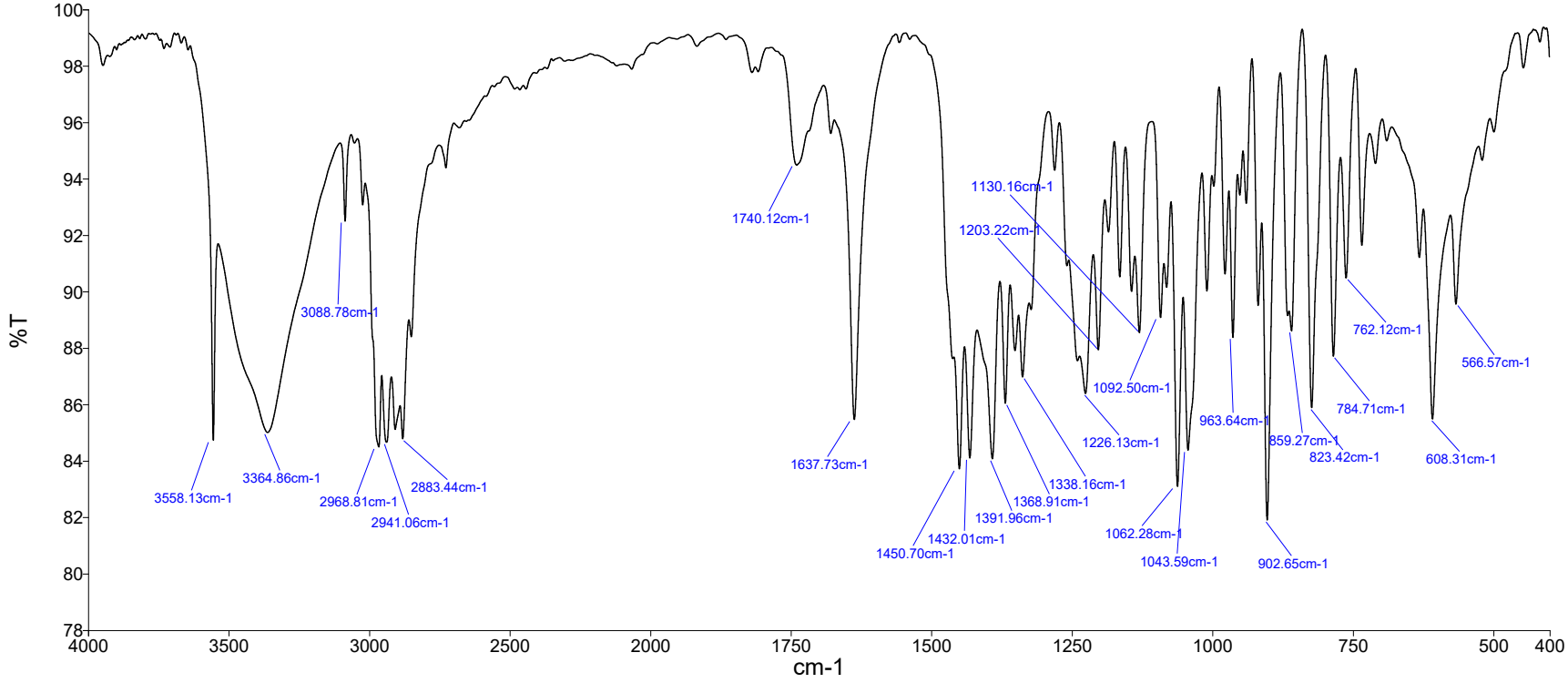


Figure S59. HRESIMS spectrum of compound **7**

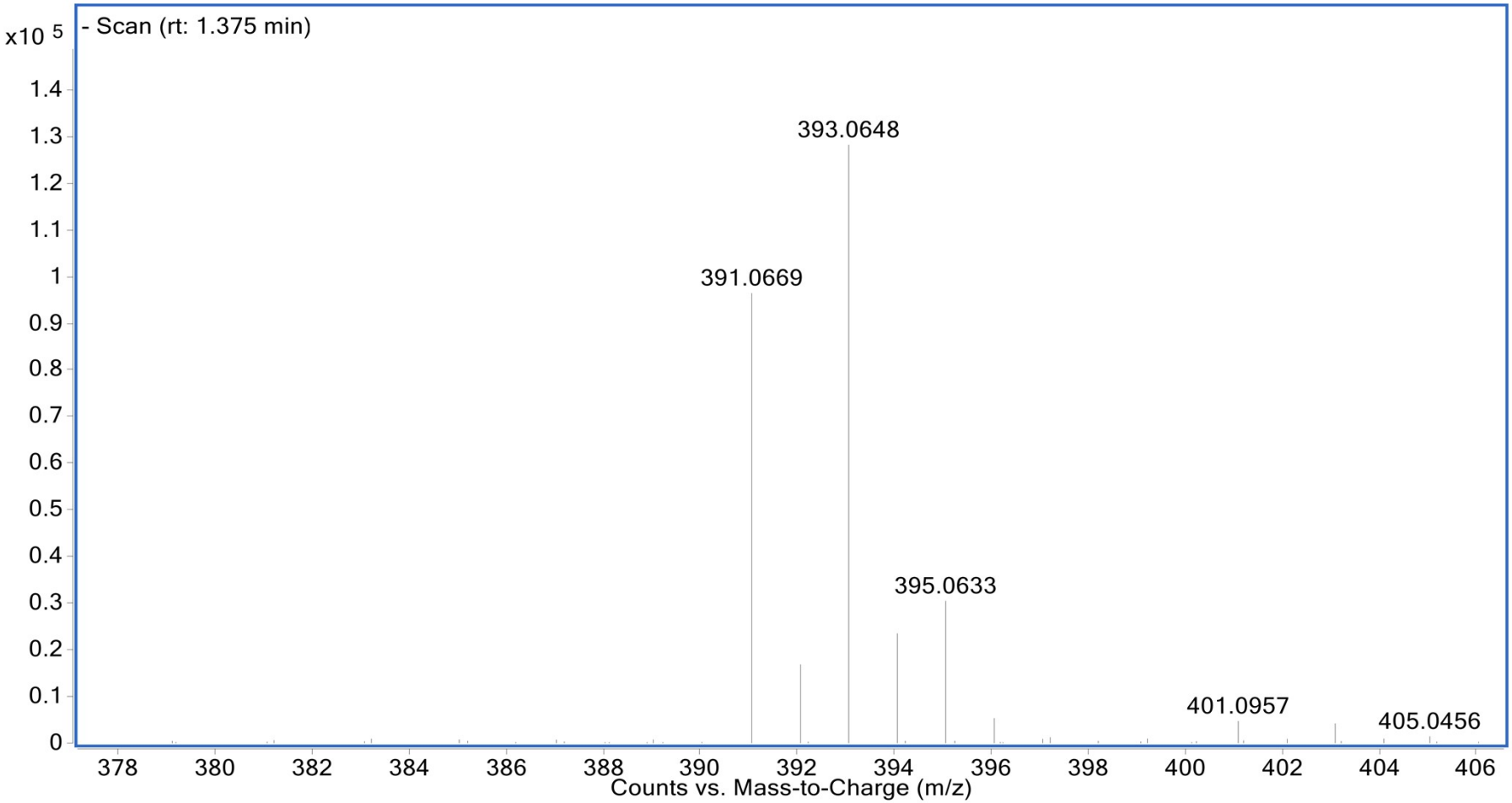


Figure S60. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of compound **7**

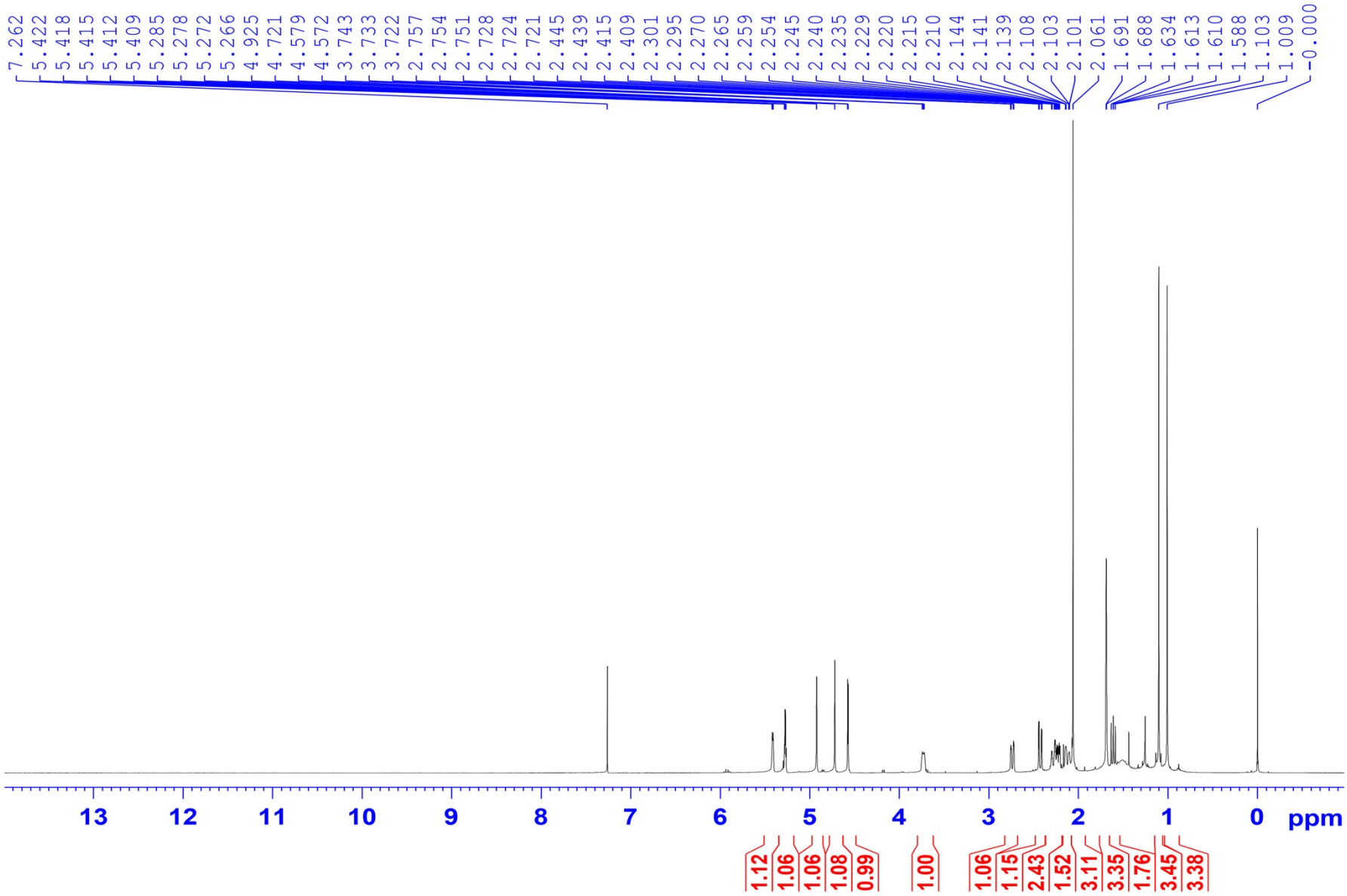


Figure S61. ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of compound **7**

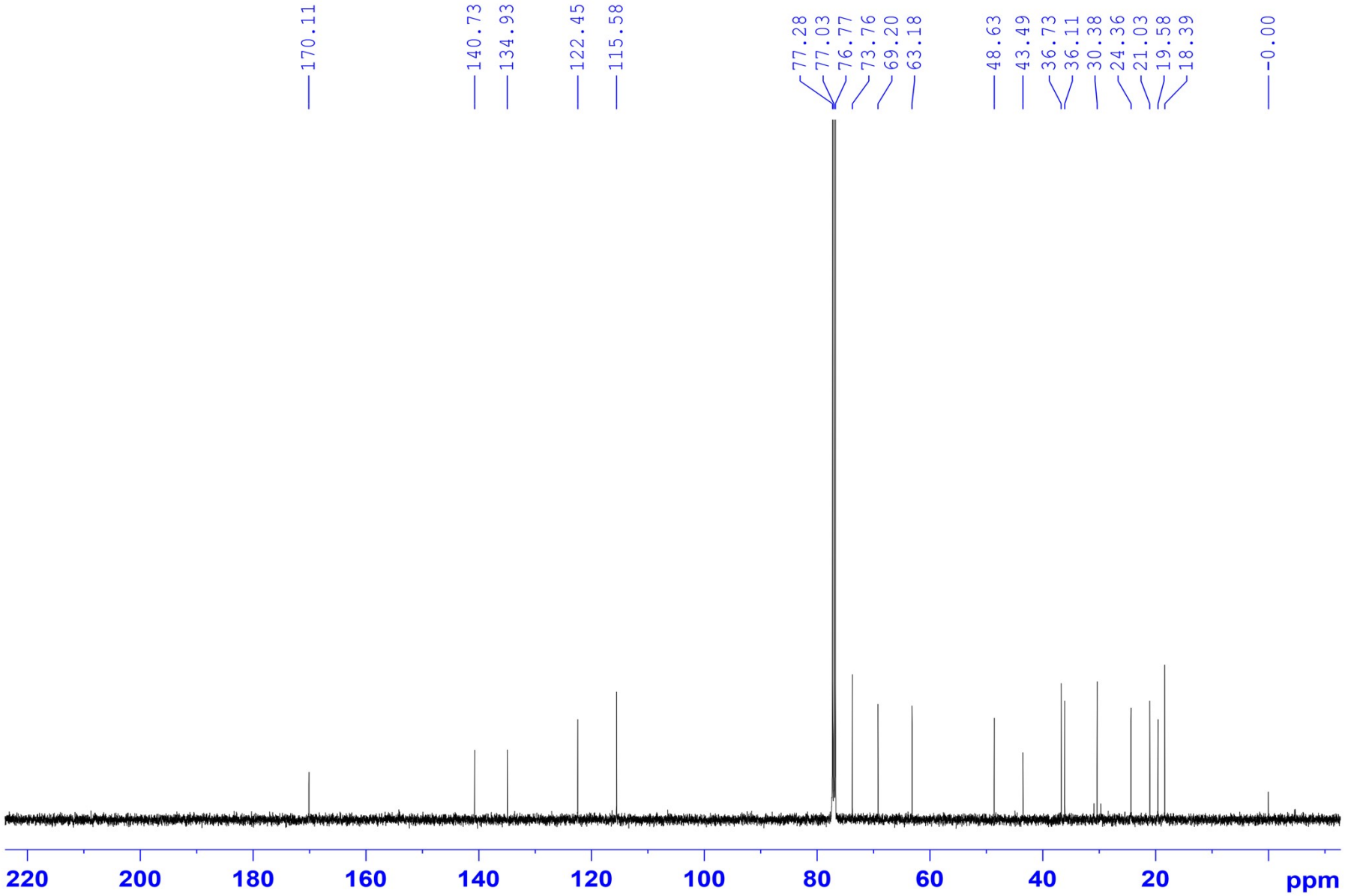


Figure S62. HSQC spectrum (in $CDCl_3$) of compound **7**

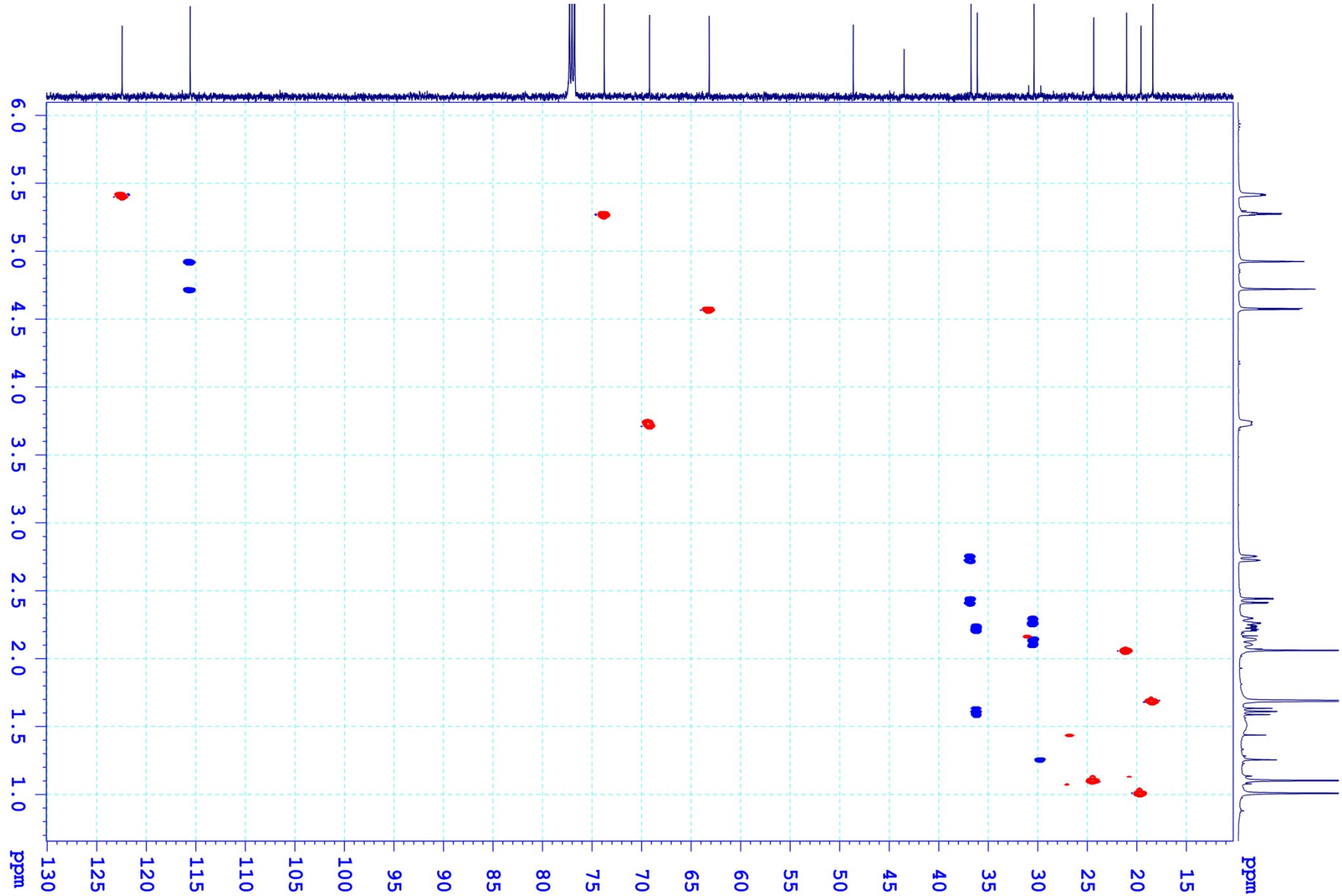


Figure S63. HMBC spectrum (in $CDCl_3$) of compound **7**

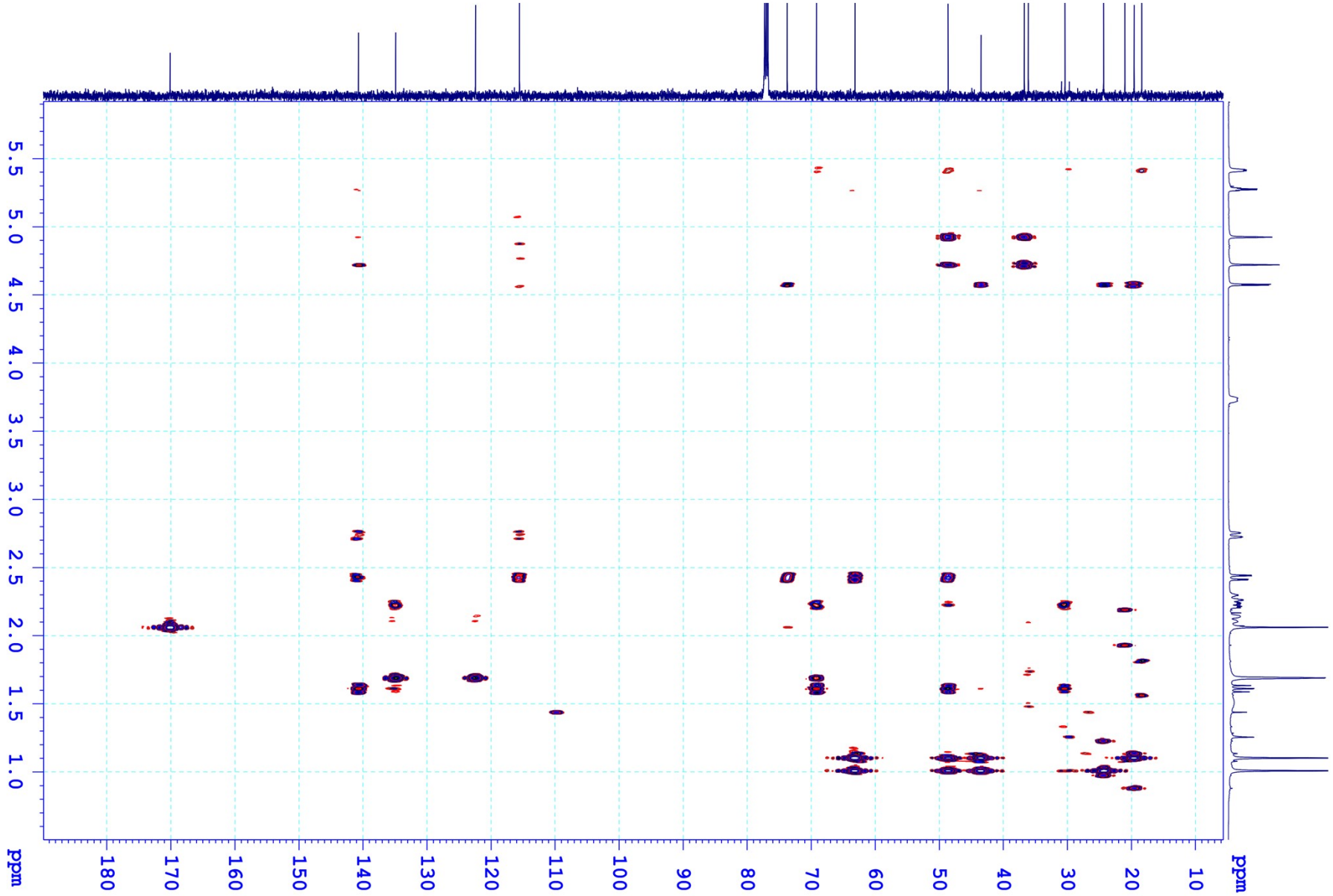


Figure S64. COSY spectrum (in $CDCl_3$) of compound **7**

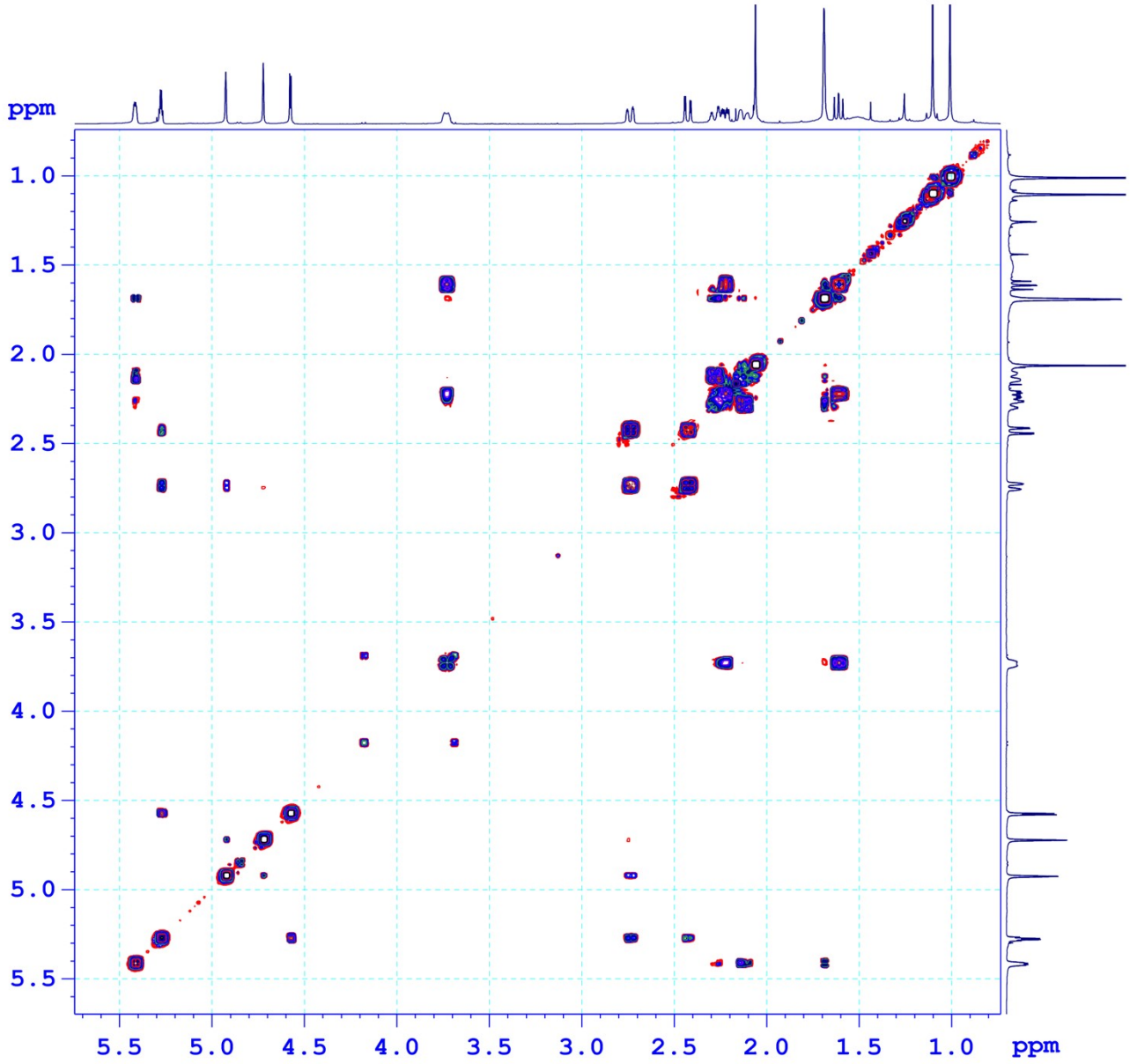


Figure S65. NOESY spectrum (in $CDCl_3$) of compound **7**

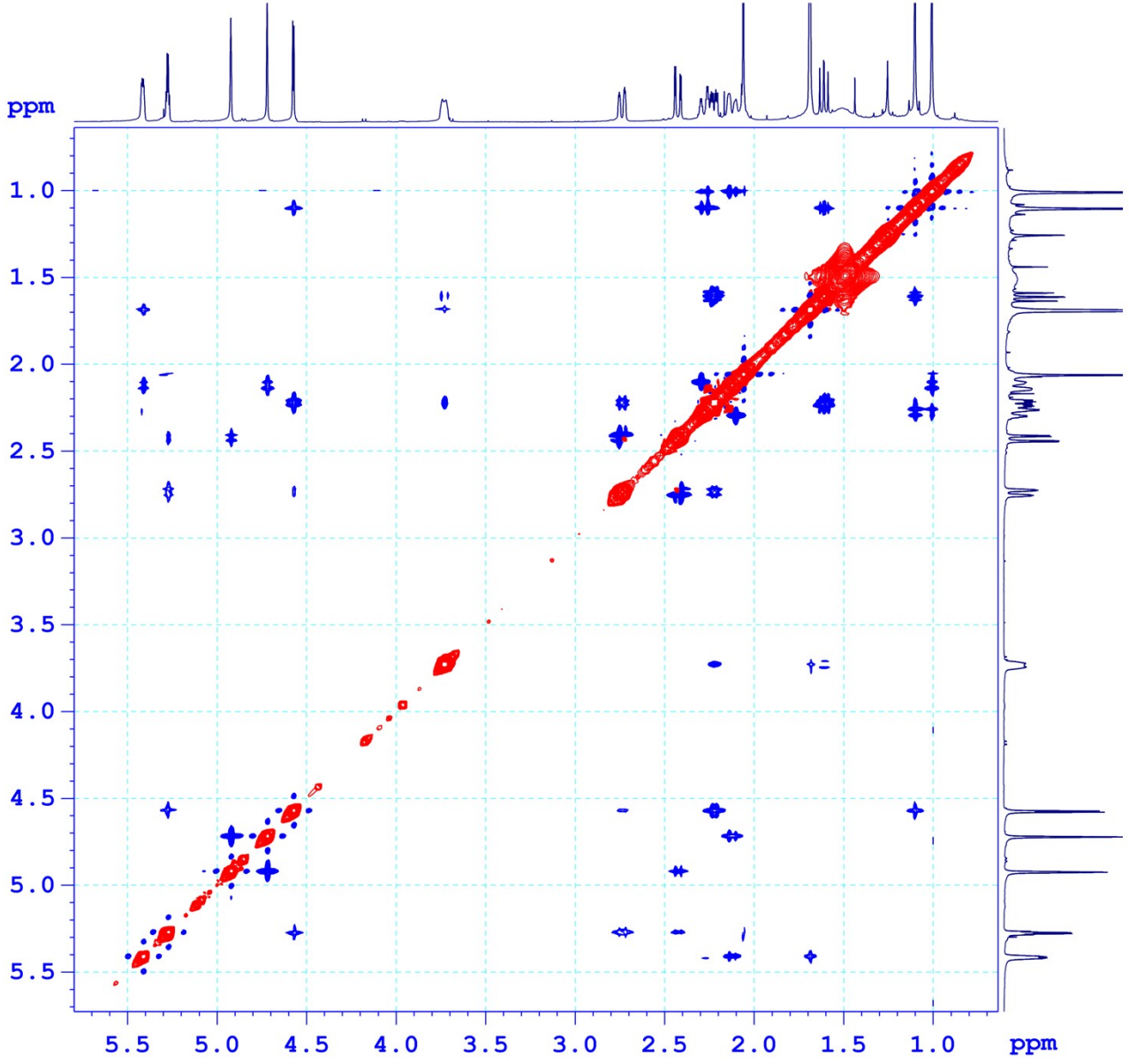


Figure S66. ECD spectrum (in ACN) of compound **7**

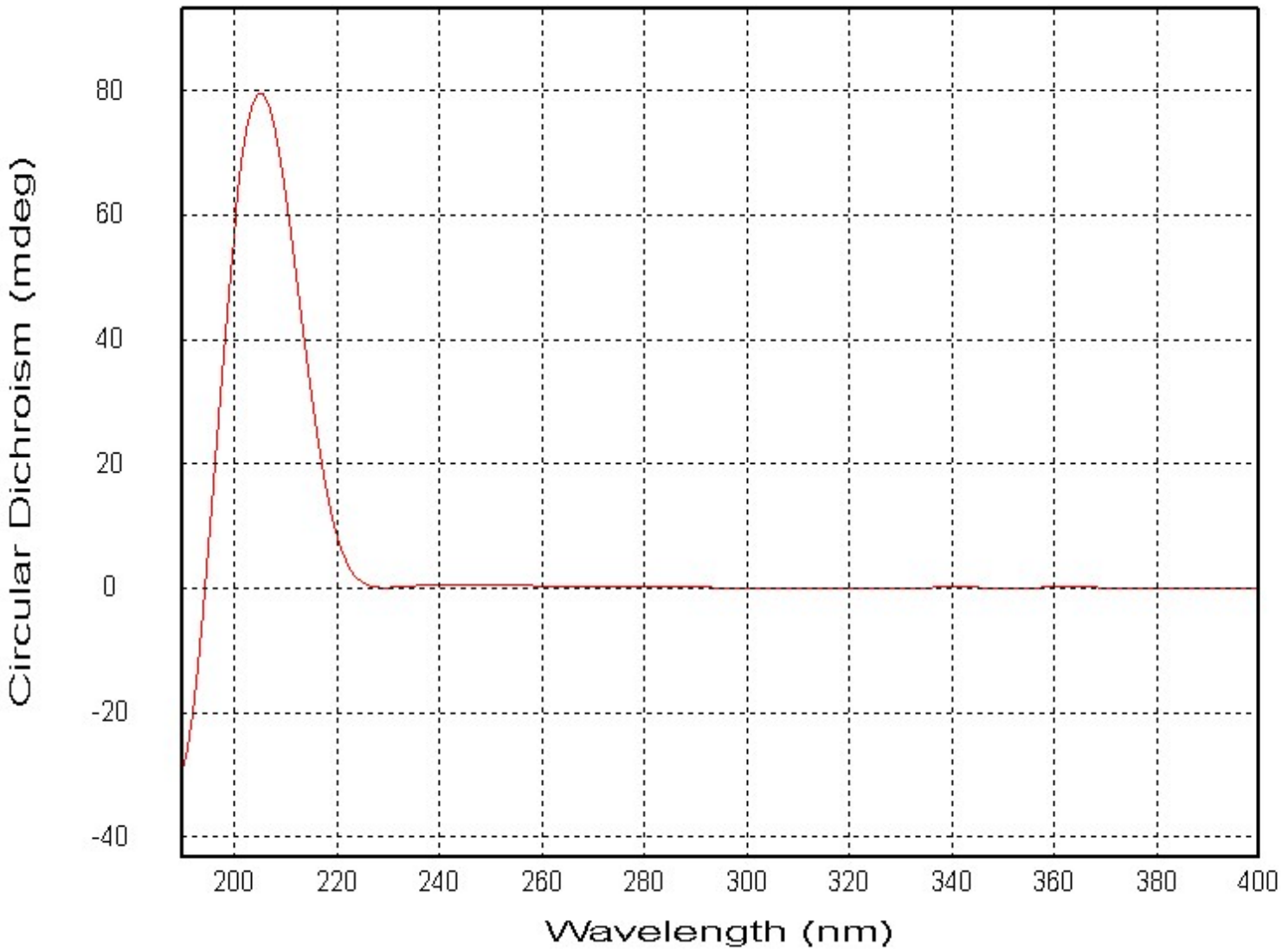
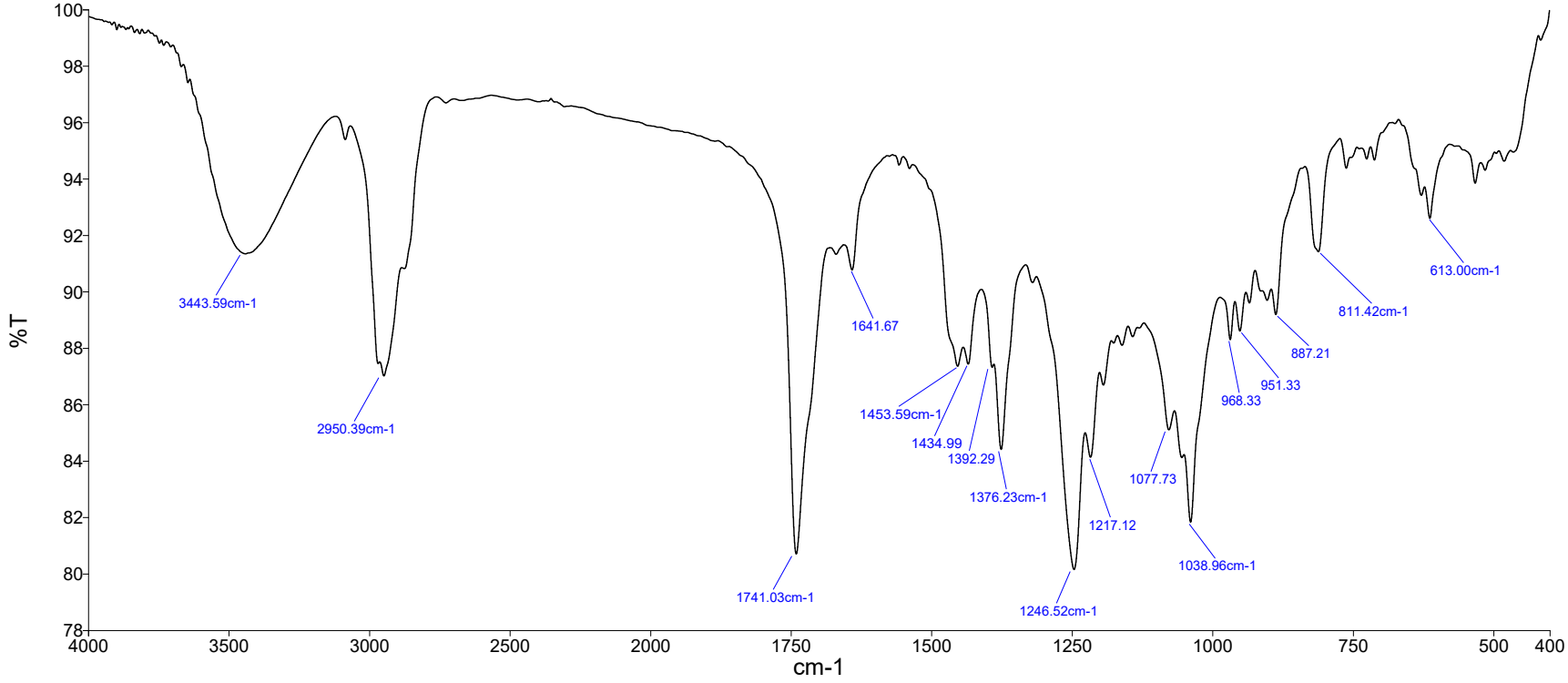


Figure S67. IR spectrum of compound **7**



2. Computational methods

All DFT calculations were performed with Gaussian 16 program package using the default pruned (99 × 590) integration grid.[1] Conformational analysis were carried out by Spartan□14 software using the Molecular Mechanics force field (MMFF) for compounds **2**–**7**, and using a PM3 semiempirical method for compound **1**. Conformers within a 5 kcal/mol energy window were further optimized at the B3LYP/6-31G(d,p)/IEFPCM-ACN level for compound **2**, at the ωB97X-D/6-311+G(d,p)/IEFPCM-ACN level for compound **3**, and at the B3LYP/6-31G(d)/IEFPCM-ACN level for compounds **4**, **6**, and **7**. The Gibbs free energy of all optimized conformer of compound **2** were calculated at M062X/6-31G(d,p)/IEFPCM-ACN level. Geometry optimizations of compounds **1** were calculated at the B3LYP/6-31G(d) level (for NMR calculation) and at the B3LYP/6-311+G(2d,p)/IEFPCM-MeOH level (for ECD calculation). To confirm that each optimized conformer corresponded to a true energy minimum, frequency calculations were performed at the same theoretical level.

The stable conformers of **1** were further subjected to NMR calculations at the mPW1PW91/6–31+G(d,p)/IEFPCM-$CHCl_3$ level by gauge independent atomic orbitals (GIAO) method.[2, 3] The shielding values were averaged according to the Boltzmann distribution theory. The NMR data of methanol and benzen were calculated at the same level and used as multi-standard references.[4] In particular, unscaled chemical shifts (δ_u) of sp^2 carbons were computed using benzene as a reference, while methanol was used for calculating δ_u of sp^3 carbons and all protons. The scaled chemical shifts (δ_{calc}) were corrected using the formula $\delta_{calc} = (\delta_u - b)/m$, where m and b are the slope and intercept, respectively, resulting from a linear regression plot of the δ_u against experimental chemical shifts (δ_{exp}). The comparison of the experimental and calculated NMR chemical shifts was carried out using the corrected mean absolute error (CMAE), root mean square deviation (RMSD), and linear correlation coefficient (R^2).

$$CMAE = \frac{1}{n}\sum_{i=1}^{n}\left|\delta_{exp} - \delta_{calc}\right|$$

$$RMSD = \sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(\delta_{exp} - \delta_{calc}\right)^2}$$

The time-dependent density functional theory (TD-DFT) calculations of the 48 lowest excited states were computed at the B3LYP/cc-PVDZ/IEFPCM-MeOH level for compound **1**, at the B3LYP/6311+G(d,p)/IEFPCM-ACN level for compound **2**, at the B3LYP/631+G(d,p)/IEFPCM-

ACN level for compound **3**, and at the CAM-B3LYP/LanL2DZ/IEFPCM-ACN level for compounds **4**, **6** and **7**. The ECD spectra of individual conformers were simulated using SpecDis 1.71 software.[5] The final ECD spectrum of each compound was obtained by Boltzmann-weighted averaging of the conformer spectra based on their relative free energies at 298 K.

References

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3. N. Grimblat, M. M. Zanardi and A. M. Sarotti, *J. Org. Chem.*, 2015, **80**, 12526-12534.
4. A. M. Sarotti and S. C. Pellegrinet, *J. Org. Chem.*, 2009, **74**, 7254-7260.
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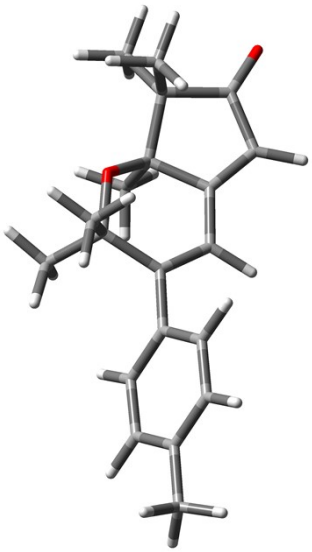
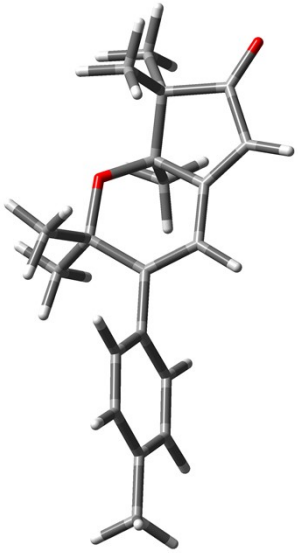
3. Calculated NMR data of compound 1

Figure S61. Optimized conformers of **1** calculated at B3LYP/6-31G(d) level



1a



1b

Table S1. Electronic energies and Boltzmann populations of **1a** and **1b** calculated at IEFPCM-$CHCl_3$/MPW1PW91/6-31+G(d,p)

Conformer	Electronic energy (Hartree)	Imaginary frequencies	Boltz. Pop.
1a	-926.8706144	0	0.57350022
1b	-926.8703348	0	0.42649978

Table S2. ^{13}C NMR data calculated for **1** at IEFPCM-$CHCl_3$/MPW1PW91/6-31+G(d,p) level

C	Shielding value			δ_{exp}	δ_{calc}	$\lvert\Delta\delta\rvert$
	1a	1b	Average			
1	69.0649	70.9673	69.88	128.06	127.79	0.27
2	69.4523	70.8813	70.06	128.75	127.60	1.15
3	58.8475	58.5819	58.73	137.87	138.81	0.94
4	70.9694	69.8332	70.48	128.75	127.18	1.57
5	71.1911	69.1323	70.31	128.06	127.35	0.71
6	59.8577	59.5977	59.75	137.18	137.81	0.63
7	36.1041	36.2367	36.16	156.44	161.16	4.72
8	76.7747	77.5188	77.09	118.75	120.64	1.89
9	28.974	29.3847	29.15	167.27	168.10	0.83
10	78.0337	78.206	78.11	119.70	119.64	0.06
11	-9.1524	-9.0617	-9.11	210.52	205.97	4.55
12	136.6637	136.5614	136.62	55.40	57.52	2.12
13	113.6752	113.354	113.54	79.93	80.37	0.44
14	116.7898	116.1868	116.53	76.17	77.41	1.24
15	163.8757	165.7654	164.68	31.20	29.75	1.45
16	168.3535	167.6093	168.04	27.80	26.43	1.37
17	173.4628	173.7704	173.59	21.15	20.93	0.22
18	169.9808	169.8277	169.92	25.11	24.57	0.54
19	178.0139	178.185	178.09	16.83	16.48	0.35
20	167.2295	167.0025	167.13	27.88	27.32	0.56
CMAE (ppm)						**1.28**
RMSD (ppm)						**1.79**

Table S3. ^{1}H NMR data calculated for **1** at IEFPCM-$CHCl_3$/MPW1PW91/6-31+G(d,p) level

H	Shielding value			δ_{exp}	δ_{calc}	$\lvert\Delta\delta\rvert$
	1a	1b	Average			
1	24.0946	23.9429	24.0299	7.16	7.1591	0.0009
2	23.9578	23.9808	23.9676	7.17	7.2172	0.0472
4	23.9684	23.9289	23.9516	7.17	7.2322	0.0622
5	23.9618	24.1003	24.0209	7.16	7.1675	0.0075
8	24.7846	24.8609	24.8171	6.44	6.4238	0.0162
10	25.6902	25.7459	25.7140	5.73	5.5862	0.1438
15	30.5405	29.7513	30.1984	1.37	1.3979	0.0279
16	29.6852	29.9858	30.1004	1.47	1.4894	0.0194
17	29.358	28.935	29.1358	2.38	2.3903	0.0103
18	30.7096	30.723	30.5108	1.12	1.1061	0.0139
19	30.6718	30.6675	30.5044	1.16	1.1121	0.0479
20	30.6149	30.6299	30.1145	1.43	1.4763	0.0463
CMAE (ppm)						**0.0370**
RMSD (ppm)						**0.0524**

Table S4. Cartesian coordinates of the optimized conformers of **1** calculated at B3LYP/6-31G(d) level

Atomic Number	Coordinates (Angstroms)			Atomic Number	Coordinates (Angstroms)		
	X	Y	Z		X	Y	Z
Conformer **1a**				Conformer **1b**			
6	-2.874035	-1.049063	0.811579	6	3.047129	0.265283	-1.176111
6	-4.258361	-1.213548	0.804318	6	4.430339	0.097814	-1.143624
6	-5.06869	-0.500376	-0.086962	6	5.067947	-0.496426	-0.04677
6	-4.439542	0.377315	-0.979505	6	4.265624	-0.937551	1.0122
6	-3.056936	0.551486	-0.973152	6	2.880684	-0.780797	0.982106
6	-2.24543	-0.1566	-0.071755	6	2.243985	-0.165604	-0.107774
6	-6.571065	-0.656507	-0.075264	6	6.570898	-0.640711	-0.002632
6	-0.756452	-0.038825	-0.065914	6	0.753873	-0.049358	-0.112634
6	-0.011947	-1.126308	-0.374319	6	0.008266	-1.172891	-0.225231
6	-0.107585	1.258937	0.434926	6	0.107202	1.333107	0.042246
6	1.427422	-1.062089	-0.367063	6	-1.430191	-1.114711	-0.152183
8	1.335637	1.198576	0.486302	8	-1.337642	1.295922	0.056421

6	-0.513357	1.467789	1.908698	6	0.414054	2.229419	-1.173974
6	-0.515478	2.505761	-0.379367	6	0.613806	2.03314	1.322827
6	2.361159	-2.039175	-0.360253	6	-2.376813	-1.995295	-0.545818
6	3.696299	-1.443528	-0.172039	6	-3.709375	-1.379518	-0.411071
6	3.49785	0.056973	0.178101	6	-3.501701	0.126228	-0.090042
6	2.056149	0.320035	-0.381748	6	-2.03955	0.124211	0.479268
6	4.628378	0.921208	-0.390317	6	-4.601847	0.662462	0.831958
6	2.069514	0.865316	-1.824235	6	-2.003255	-0.010936	2.015216
6	3.518183	0.15373	1.721584	6	-3.568078	0.875882	-1.441135
8	4.773688	-2.013469	-0.210536	8	-4.792719	-1.912887	-0.581238
1	-2.267998	-1.614297	1.514243	1	2.5874	0.702916	-2.056202
1	-4.715116	-1.910741	1.503302	1	5.024635	0.427581	-1.992985
1	-5.040193	0.928443	-1.699814	1	4.728877	-1.415872	1.872362
1	-2.604555	1.21938	-1.699124	1	2.280374	-1.136985	1.814819
1	-6.868661	-1.645512	0.288599	1	6.989059	-0.791295	-1.003672
1	-6.996272	-0.521076	-1.07551	1	6.874426	-1.486927	0.622548
1	-7.042796	0.087203	0.580949	1	7.044072	0.258398	0.41443
1	-0.503235	-2.064246	-0.624423	1	0.495568	-2.129264	-0.402044
1	-1.593986	1.602125	2.00987	1	1.472879	2.493322	-1.227952
1	-0.007136	2.359096	2.29304	1	-0.168069	3.150867	-1.073951
1	-0.203741	0.609185	2.511813	1	0.11503	1.735432	-2.103504
1	-1.576394	2.73606	-0.25084	1	1.691245	2.214916	1.266111
1	-0.311535	2.387882	-1.447034	1	0.416526	1.439285	2.21878
1	0.068322	3.355703	-0.013272	1	0.099886	2.993719	1.427255
1	2.191907	-3.10931	-0.42323	1	-2.219843	-2.987656	-0.956115
1	5.582389	0.571681	0.015646	1	-5.572725	0.521873	0.347445
1	4.497014	1.972642	-0.110181	1	-4.463353	1.732122	1.026616
1	4.700467	0.860772	-1.4799	1	-4.642165	0.139523	1.791588
1	2.719135	0.26357	-2.46706	1	-2.64812	-0.827534	2.353871
1	2.426421	1.899525	-1.831718	1	-2.338084	0.920134	2.482145
1	1.065315	0.839329	-2.256321	1	-0.989041	-0.228763	2.360828
1	3.372513	1.189543	2.040003	1	-3.419339	1.948376	-1.288935
1	4.486101	-0.200446	2.091606	1	-4.551215	0.713196	-1.895266
1	2.730985	-0.452561	2.179348	1	-2.803115	0.525861	-2.140568

4. Calculated ECD data

Figure S62. Optimized conformers of **1**-(13*R*) calculated at B3LYP/6-311+G(2d,p)/IEFPCM-MeOH level

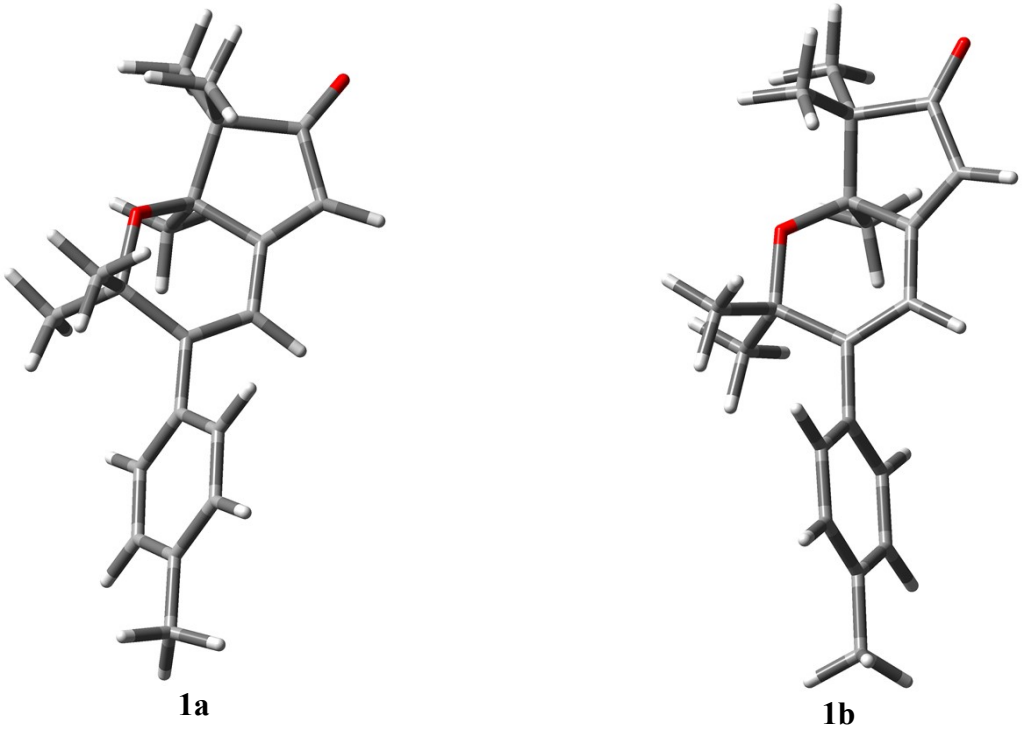


Table S5. Energies and Boltzmann populations of **1a** and **1b** calculated at B3LYP/6-311+G(2d,p)/IEFPCM-MeOH level

Conformer	Gibbs free energy (Hartree)	Imaginary frequencies	Boltz. Pop.
1a	-926.953910	0	0.383555547
1b	-926.954358	0	0.616444453

Table S6. Cartesian coordinates of the optimized conformers of **1** calculated at B3LYP/6-311+G(2d,p)/IEFPCM-MeOH level

Atomic Number	Coordinates (Angstroms)			Atomic Number	Coordinates (Angstroms)		
	X	Y	Z		X	Y	Z
Conformer **1a**				Conformer **1b**			
6	-2.868278	-1.016984	0.84133	6	2.894625	-0.59629	1.079573
6	-4.248872	-1.182915	0.833	6	4.276989	-0.74805	1.104994
6	-5.053577	-0.504902	-0.084196	6	5.053202	-0.496546	-0.027541
6	-4.422388	0.339917	-1.000323	6	4.392765	-0.095919	-1.191517
6	-3.043667	0.517316	-0.991697	6	3.01247	0.067366	-1.22066

6	-2.240109	-0.157147	-0.066099	6	2.238401	-0.176213	-0.081627
6	-6.552498	-0.663798	-0.075796	6	6.553672	-0.636565	0.006754
6	-0.753654	-0.036269	-0.061232	6	0.750096	-0.060338	-0.086291
6	-0.011143	-1.115807	-0.377176	6	0.005677	-1.182133	-0.124369
6	-0.113679	1.264411	0.429046	6	0.115351	1.329581	-0.03356
6	1.421705	-1.047953	-0.373436	6	-1.426821	-1.113347	-0.060169
8	1.33377	1.1906	0.505853	8	-1.33501	1.294991	-0.053247
6	-0.540212	1.502092	1.888263	6	0.460777	2.137837	-1.294781
6	-0.507477	2.493429	-0.411912	6	0.59832	2.107712	1.206127
6	2.348261	-2.028443	-0.374952	6	-2.366466	-2.02266	-0.391185
6	3.672037	-1.44764	-0.173934	6	-3.687394	-1.405426	-0.322552
6	3.496671	0.046723	0.183731	6	-3.501265	0.115132	-0.110682
6	2.054027	0.325279	-0.373259	6	-2.039605	0.165225	0.46432
6	4.621841	0.91527	-0.382925	6	-4.597171	0.718125	0.770758
6	2.079389	0.881487	-1.808211	6	-2.017629	0.151468	2.003453
6	3.526996	0.133025	1.725862	6	-3.574165	0.762072	-1.511643
8	4.745174	-2.033806	-0.209981	8	-4.76706	-1.961119	-0.470735
1	-2.269523	-1.558098	1.564353	1	2.31769	-0.806162	1.972485
1	-4.705286	-1.855132	1.55151	1	4.756964	-1.074514	2.021206
1	-5.016668	0.863763	-1.741193	1	4.96482	0.085156	-2.095127
1	-2.59262	1.16368	-1.733228	1	2.535527	0.360695	-2.147051
1	-6.846695	-1.638797	0.316161	1	7.030263	0.324779	0.222694
1	-6.969083	-0.556355	-1.078871	1	6.94257	-0.982974	-0.952527
1	-7.021975	0.09754	0.555065	1	6.86952	-1.338935	0.779708
1	-0.496257	-2.054205	-0.623167	1	0.485742	-2.148774	-0.23138
1	-1.616556	1.656015	1.963305	1	1.524306	2.365618	-1.346144
1	-0.033421	2.39348	2.262094	1	-0.089726	3.079522	-1.258503
1	-0.259602	0.653162	2.512863	1	0.164968	1.597825	-2.194956
1	-1.565465	2.724717	-0.293349	1	1.672184	2.288818	1.148461
1	-0.299817	2.358169	-1.472177	1	0.393107	1.57586	2.133639
1	0.068569	3.347689	-0.053389	1	0.086229	3.070588	1.236629
1	2.167479	-3.092745	-0.451882	1	-2.198201	-3.041068	-0.716548
1	5.57123	0.619677	0.066153	1	-5.563383	0.610054	0.275692
1	4.451771	1.967701	-0.144944	1	-4.419106	1.784096	0.929487
1	4.725577	0.820412	-1.463755	1	-4.670668	0.234024	1.744486
1	2.730763	0.283862	-2.446658	1	-2.664263	-0.633988	2.395977

1	2.439307	1.91096	-1.805618	1	-2.357108	1.112398	2.391807
1	1.083071	0.862483	-2.247926	1	-1.011185	-0.037324	2.374465
1	3.406717	1.167739	2.047045	1	-3.449393	1.842195	-1.434221
1	4.489359	-0.233889	2.088141	1	-4.551225	0.55584	-1.953079
1	2.735332	-0.458724	2.185991	1	-2.804054	0.379114	-2.181754

Figure S63. The most stable conformers of (3*R*,6*R*,9*S*,10*R*)-**2** calculated at B3LYP/6-31G(d,p)/IEFPCM-ACN level

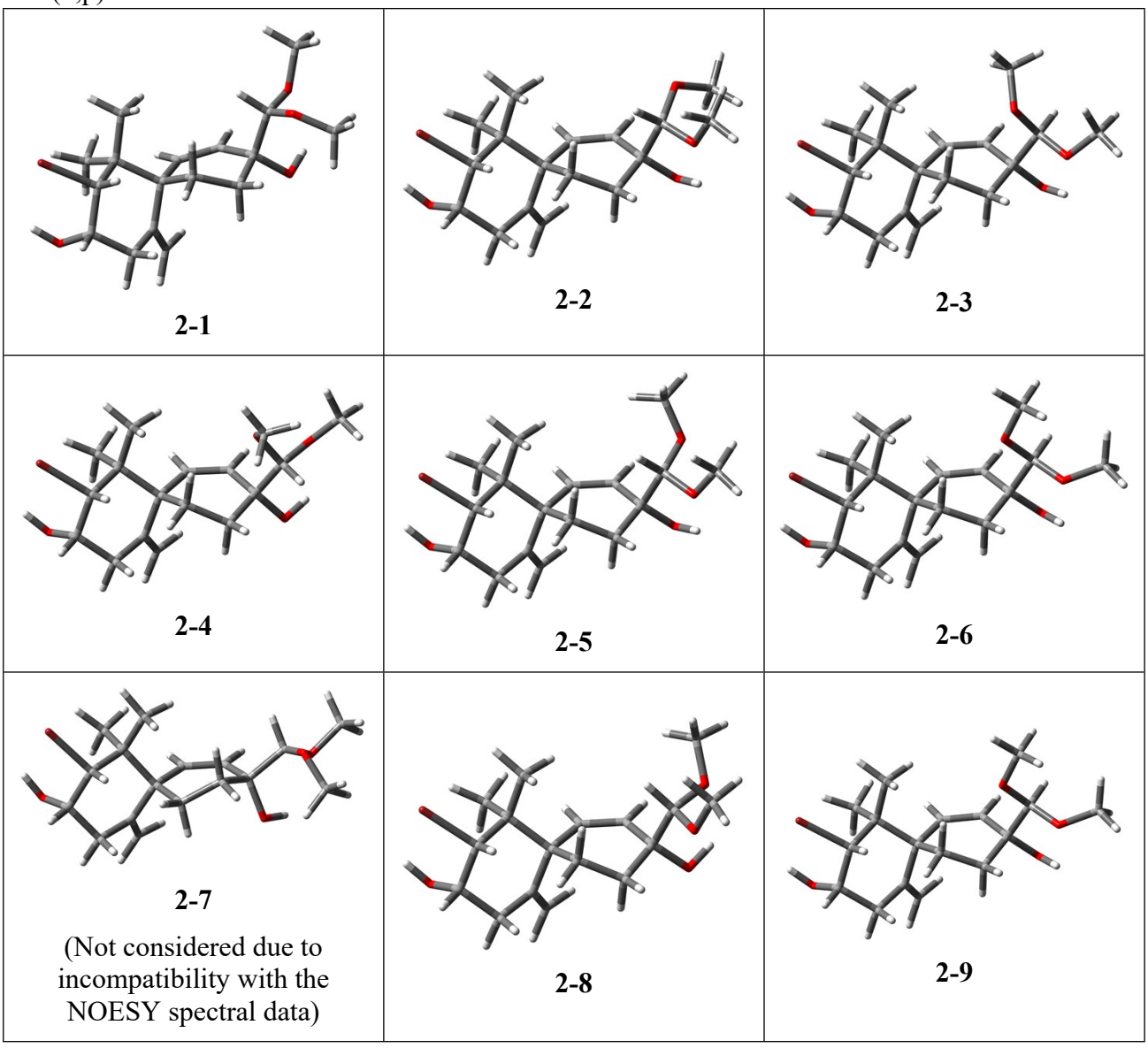


Table S7. Gibbs free energies and Boltzmann populations of the most stable conformers of (3*R*,6*R*,9*S*,10*R*)-**2** calculated at M062X/6-31G(d,p)/IEFPCM-ACN level

Conformer	Gibbs free energy (Hartree)	Imaginary frequencies	Boltz. Pop.
2-1	-3535.948589	0	0.318621577
2-2	-3535.948077	0	0.185255687
2-3	-3535.947996	0	0.17002553
2-4	-3535.947718	0	0.126661032
2-5	-3535.946462	0	0.033490618
2-6	-3535.946367	0	0.030284904
2-7	-3535.946364	0	0.030188831
2-8	-3535.946185	0	0.024975375
2-9	-3535.947290	0	0.080496445

Table S8. Cartesian coordinates of the most stable conformers of (3*R*,6*R*,9*S*,10*R*)-**2** calculated at B3LYP/6-31G(d,p)/IEFPCM-ACN level

Atomic Number	Coordinates (Angstroms)			Atomic Number	Coordinates (Angstroms)		
	X	Y	Z		X	Y	Z
Conformer **2-1**				Conformer **2-2**			
6	-2.455499	-0.245136	-0.566861	6	-1.450935	-0.295886	0.648055
6	-3.039889	1.14921	-0.831577	6	-0.848176	2.040003	-0.201885
6	-1.894532	2.161907	-0.971637	6	-3.062194	1.020927	-0.965011
6	-0.841493	2.042528	0.109711	6	-1.923816	2.006121	-1.267008
6	-0.246346	0.634344	0.307213	6	-2.467782	-0.321543	-0.517435
6	-1.461108	-0.38869	0.609478	6	-0.24545	0.673123	0.177851
6	0.547979	0.229302	-0.974223	6	0.745997	0.820518	1.320138
6	1.893016	0.95843	-1.080366	6	2.077421	0.783754	1.208968
6	2.830058	0.602518	0.076261	6	2.830643	0.612621	-0.086643
6	2.053651	0.583367	1.379651	6	1.866715	0.78767	-1.275867
6	0.721295	0.616476	1.479045	6	0.520168	0.089725	-1.050421
8	-3.90144	1.612013	0.198778	8	3.841116	1.634482	-0.119812
6	-2.125832	-0.058954	1.966262	6	3.525333	-0.780787	-0.14451
6	-0.952206	-1.844275	0.681875	6	-0.449401	3.203788	0.322486
35	-4.033413	-1.50464	-0.374342	35	-4.035637	-1.543995	-0.119449
6	3.527352	-0.775871	-0.124801	6	-2.091072	0.223944	1.956269
6	-0.452469	3.120156	0.799461	6	-0.936046	-1.726139	0.917753

8	3.83181	1.631093	0.143645	8	-3.907259	1.622849	0.005293
8	4.521152	-0.837932	0.875775	8	4.126246	-1.212408	1.058522
8	4.040867	-1.025099	-1.415865	8	4.444675	-0.705453	-1.211975
6	5.135737	-0.213125	-1.857751	6	5.276127	-0.489913	1.512903
6	5.098602	-2.130748	1.058556	6	4.975227	-1.964341	-1.627075
1	-2.00544	-0.61783	-1.487131	1	-3.627874	0.839872	-1.89013
1	-3.588961	1.102311	-1.782836	1	-1.487377	1.724506	-2.232905
1	-2.329845	3.1652	-0.974791	1	-2.363558	2.99855	-1.399831
1	-1.438701	2.014929	-1.958262	1	-2.032391	-0.819205	-1.384073
1	-0.031508	0.426233	-1.879192	1	0.328795	1.004747	2.305132
1	0.729478	-0.848493	-0.961444	1	2.689359	0.908502	2.098385
1	2.372201	0.722706	-2.033767	1	2.338904	0.415814	-2.190806
1	1.734944	2.041289	-1.046454	1	1.713011	1.86412	-1.401374
1	2.658209	0.57109	2.284162	1	0.691703	-0.97789	-0.891532
1	0.287169	0.669379	2.472738	1	-0.075542	0.165112	-1.963293
1	-4.577003	0.927209	0.327644	1	2.772527	-1.554221	-0.345234
1	-3.078079	-0.589211	2.042603	1	4.46852	1.35569	-0.806017
1	-1.49936	-0.401273	2.793561	1	-0.908433	4.139256	0.014226
1	-2.322054	1.006566	2.085715	1	0.344707	3.267055	1.05797
1	-0.089952	-1.911936	1.351319	1	-3.040014	-0.290646	2.124941
1	-1.738057	-2.493697	1.075063	1	-1.448629	0.003317	2.812265
1	-0.66062	-2.242529	-0.29373	1	-2.288647	1.295453	1.926169
1	2.793466	-1.579572	0.020628	1	-0.670072	-2.262394	0.002801
1	0.326211	3.076481	1.552651	1	-0.055592	-1.69707	1.565951
1	-0.903971	4.091345	0.615672	1	-1.709039	-2.310581	1.422435
1	4.53226	1.281916	0.717559	1	-4.578243	0.962562	0.241205
1	4.827774	0.816852	-2.056001	1	5.671986	-1.060587	2.355633
1	5.946722	-0.203056	-1.122927	1	6.041182	-0.425273	0.732773
1	5.494645	-0.6741	-2.780445	1	5.024682	0.522587	1.840112
1	5.830637	-2.03805	1.862401	1	4.174145	-2.628854	-1.975474
1	4.332599	-2.861667	1.348077	1	5.518583	-2.456417	-0.814146
1	5.597698	-2.478913	0.148686	1	5.659838	-1.76143	-2.452119
Conformer **2-3**				Conformer **2-4**			
6	-2.334864	-0.22956	-0.593201	6	-2.389406	-0.279684	-0.483412
6	-2.895011	1.152509	-0.956377	6	-3.002932	1.066035	-0.892314
6	-1.734985	2.146099	-1.112354	6	-1.877058	2.061079	-1.208139

6	-0.725073	2.079406	0.013474	6	-0.77955	2.08628	-0.165651
6	-0.146515	0.679424	0.300711	6	-0.156111	0.718995	0.176123
6	-1.379992	-0.314454	0.621517	6	-1.341921	-0.269648	0.654938
6	0.683323	0.19717	-0.92921	6	0.588709	0.158343	-1.075085
6	2.009015	0.957153	-1.063111	6	1.892818	0.912626	-1.357321
6	2.930985	0.783242	0.159463	6	2.901578	0.814835	-0.205855
6	2.124632	0.750677	1.433045	6	2.190753	0.85958	1.129757
6	0.789979	0.718808	1.497597	6	0.864702	0.850814	1.294223
8	-3.786305	1.680643	0.015836	8	-3.824435	1.647467	0.110303
6	-2.086716	0.095321	1.934531	6	-1.95182	0.215908	1.990379
6	-0.887939	-1.767266	0.789431	6	-0.808656	-1.701393	0.876204
35	-3.932608	-1.461357	-0.38195	35	-3.940147	-1.519289	-0.066604
6	3.847687	-0.467406	0.060869	6	3.822832	-0.425444	-0.327502
6	-0.36322	3.189391	0.665643	6	-0.382288	3.244329	0.372509
8	3.821008	1.908728	0.283623	8	3.762204	1.963754	-0.324576
8	4.684931	-0.242129	-1.048805	8	3.102052	-1.627152	-0.179455
8	3.129495	-1.668388	-0.124193	8	4.787411	-0.280391	0.695154
6	3.152502	-2.570992	0.980188	6	5.87339	-1.200615	0.630222
6	5.77394	-1.156969	-1.156862	6	3.2975	-2.597897	-1.209502
1	-1.859727	-0.659257	-1.475059	1	-1.975049	-0.759948	-1.369788
1	-3.411855	1.056699	-1.921963	1	-3.592599	0.897297	-1.804771
1	-2.159907	3.150957	-1.188663	1	-2.324716	3.0527	-1.31946
1	-1.243561	1.93869	-2.070537	1	-1.460012	1.792471	-2.186334
1	0.117676	0.307101	-1.858188	1	-0.042063	0.199976	-1.966649
1	0.908328	-0.8636	-0.817012	1	0.828172	-0.89123	-0.90221
1	2.534425	0.641696	-1.969583	1	2.346544	0.551151	-2.287097
1	1.816289	2.030821	-1.155451	1	1.683748	1.977765	-1.500907
1	2.705301	0.801381	2.352937	1	2.836783	0.955473	1.999655
1	0.331676	0.764683	2.480553	1	0.477414	0.978292	2.300407
1	-4.472747	1.009898	0.160357	1	-4.48387	0.978675	0.354653
1	-3.043702	-0.426529	2.01008	1	-2.891687	-0.310463	2.173163
1	-1.490563	-0.200634	2.801284	1	-1.285278	-0.017038	2.824372
1	-2.281313	1.166511	1.985323	1	-2.158736	1.286138	1.988276
1	-0.061206	-1.808045	1.504047	1	0.095269	-1.679343	1.490941
1	-1.697739	-2.392481	1.173353	1	-1.55926	-2.302875	1.394656
1	-0.549633	-2.211553	-0.150278	1	-0.570723	-2.213186	-0.060171

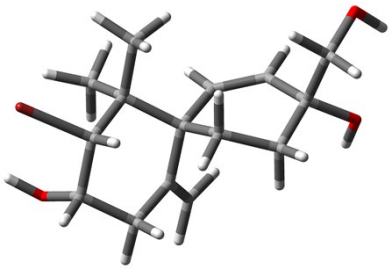
1	4.456758	-0.53453	0.978096	1	4.321633	-0.40305	-1.310561
1	0.384556	3.183999	1.450612	1	0.426685	3.301236	1.092141
1	-0.805625	4.150027	0.415829	1	-0.856545	4.18074	0.091059
1	4.49277	1.774737	-0.404405	1	4.521046	1.77792	0.251555
1	2.64581	-3.480347	0.651262	1	6.57893	-0.914664	1.412231
1	4.180306	-2.820897	1.27315	1	5.535442	-2.226801	0.810654
1	2.623448	-2.163399	1.849415	1	6.377101	-1.152826	-0.344838
1	6.352337	-0.858683	-2.032761	1	4.352617	-2.875837	-1.315472
1	6.415882	-1.113809	-0.266729	1	2.726793	-3.481034	-0.916177
1	5.413784	-2.182097	-1.291219	1	2.924402	-2.240743	-2.177056
Conformer **2-5**				Conformer **2-6**			
6	-1.39098	-0.365686	0.575875	6	-2.377306	-0.262361	-0.560147
6	-0.845947	2.082699	0.0753	6	-2.939957	1.095618	-1.001445
6	-3.030241	1.131498	-0.840561	6	-1.781699	2.080738	-1.214511
6	-1.914725	2.174968	-0.993243	6	-0.768052	2.079464	-0.089679
6	-2.40443	-0.246754	-0.587255	6	-0.191228	0.699132	0.281801
6	-0.208827	0.690952	0.260183	6	-1.423917	-0.276316	0.657878
6	0.774134	0.699777	1.419975	6	0.637821	0.1421	-0.916937
6	2.106154	0.727119	1.310141	6	1.982799	0.862068	-1.076391
6	2.864623	0.778483	0.006915	6	2.888173	0.737593	0.163335
6	1.898207	1.087285	-1.150984	6	2.072553	0.80898	1.427369
6	0.58017	0.31176	-1.03223	6	0.73777	0.807595	1.480106
8	3.840597	1.821974	0.142406	8	-3.832557	1.676548	-0.061119
6	3.630589	-0.553113	-0.234465	6	-2.132382	0.20664	1.944824
6	-0.481179	3.169008	0.764664	6	-0.927896	-1.716549	0.908687
35	-3.94442	-1.549466	-0.378285	35	-3.97157	-1.485225	-0.280943
6	-2.047218	-0.057916	1.941998	6	3.780278	-0.534483	0.151697
6	-0.842883	-1.807385	0.637376	6	-0.399284	3.226214	0.491215
8	-3.890032	1.568481	0.202455	8	3.806265	1.844173	0.222524
8	4.371658	-0.936907	0.907587	8	4.694456	-0.419335	-0.933999
8	4.512739	-0.287787	-1.299242	8	2.97099	-1.665803	0.015243
6	3.946572	-2.144967	1.533589	6	3.665315	-2.906196	0.117986
6	5.269018	-1.413345	-1.741132	6	6.077456	-0.548845	-0.594651
1	-3.590551	1.071664	-1.784502	1	-1.899527	-0.739768	-1.41566
1	-1.467047	2.04162	-1.985532	1	-3.456443	0.944028	-1.960107
1	-2.376944	3.166124	-0.989255	1	-2.208361	3.079126	-1.34601

1	-1.956282	-0.604403	-1.51438	1	-1.292631	1.8207	-2.161088
1	0.350105	0.723523	2.418972	1	0.081838	0.22496	-1.854443
1	2.723258	0.743826	2.204622	1	0.835404	-0.917254	-0.756834
1	2.383922	0.868334	-2.106978	1	2.509781	0.48534	-1.958997
1	1.701357	2.163643	-1.122331	1	1.815853	1.93331	-1.230364
1	0.795408	-0.75992	-1.018919	1	2.647077	0.906179	2.34739
1	-0.018074	0.486721	-1.929662	1	0.271837	0.927077	2.453138
1	2.934485	-1.36074	-0.510051	1	-4.51805	1.014012	0.120701
1	4.50903	1.635908	-0.536869	1	-3.091463	-0.306995	2.045643
1	-0.963592	4.126786	0.589269	1	-1.53938	-0.044264	2.827753
1	0.30687	3.146838	1.50892	1	-2.323192	1.279821	1.937254
1	-2.98361	-0.614175	2.028414	1	-0.078118	-1.711148	1.596932
1	-1.401693	-0.385731	2.760524	1	-1.725924	-2.312747	1.357825
1	-2.27097	1.001459	2.06749	1	-0.618843	-2.223449	-0.009204
1	-0.548966	-2.193663	-0.342309	1	4.350882	-0.580085	1.094027
1	0.026104	-1.855886	1.299693	1	0.351719	3.265225	1.27222
1	-1.608044	-2.478926	1.034162	1	-0.838714	4.171678	0.184713
1	-4.545552	0.865718	0.338092	1	4.39338	1.721784	-0.540526
1	2.94582	-2.045406	1.971333	1	4.356117	-3.0493	-0.720126
1	3.94504	-2.987548	0.829977	1	4.22574	-2.969957	1.060887
1	4.661821	-2.351748	2.332422	1	2.910126	-3.693766	0.097216
1	5.883634	-1.071605	-2.575454	1	6.300267	-1.530194	-0.160387
1	4.606986	-2.218734	-2.086302	1	6.63815	-0.436825	-1.524745
1	5.914283	-1.794745	-0.943892	1	6.391554	0.23239	0.107775
Conformer **2-7**				Conformer **2-8**			
6	-2.551351	-0.279727	-0.523202	6	-2.399346	-0.305866	-0.534821
6	-3.222267	1.067032	-0.815946	6	-3.058432	1.033767	-0.890795
6	-2.135905	2.09865	-1.142992	6	-1.968431	2.085202	-1.143116
6	-1.02183	2.125825	-0.121359	6	-0.881619	2.101807	-0.088894
6	-0.314299	0.775528	0.110495	6	-0.214725	0.743074	0.20307
6	-1.433137	-0.311673	0.54892	6	-1.370718	-0.307566	0.620528
6	0.426124	0.414664	-1.225617	6	0.56656	0.273343	-1.064825
6	1.704182	-0.423514	-1.079449	6	1.882436	1.037531	-1.253288
6	2.716726	0.233199	-0.143409	6	2.854672	0.78534	-0.098358
6	2.019795	0.692033	1.123356	6	2.108385	0.865317	1.220193
6	0.706307	0.915543	1.223043	6	0.777658	0.867663	1.347255

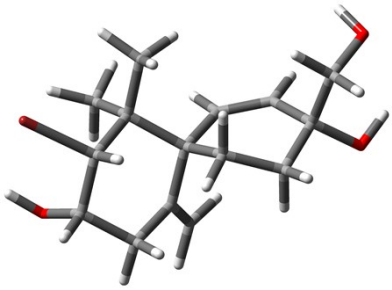
8	-3.990543	1.571298	0.267101	8	-3.915751	1.535797	0.124598
6	-1.978682	0.02672	1.955194	6	-2.016695	0.099499	1.965236
6	-0.83651	-1.731907	0.602793	6	-0.790179	-1.727396	0.793949
35	-4.044559	-1.584702	-0.093805	35	-3.907211	-1.619896	-0.19961
6	3.851562	-0.754745	0.23306	6	3.58667	-0.581085	-0.200445
6	-0.665984	3.27342	0.46498	6	-0.525188	3.249219	0.498449
8	3.277202	1.371323	-0.827549	8	3.847926	1.818544	-0.143905
8	4.832738	0.018414	0.888411	8	4.62408	-0.589824	0.77994
8	4.380138	-1.51303	-0.833777	8	4.145761	-0.69406	-1.476242
6	5.123483	-0.807574	-1.834917	6	4.765287	-1.95265	-1.72663
6	5.821894	-0.744021	1.580022	6	4.503353	-1.570342	1.810258
1	-2.185683	-0.695642	-1.461909	1	-1.953351	-0.728454	-1.435404
1	-3.863664	0.933148	-1.698766	1	-3.628281	0.885445	-1.819164
1	-2.608925	3.081205	-1.226711	1	-2.452767	3.063462	-1.210013
1	-1.730027	1.853881	-2.132694	1	-1.53294	1.883238	-2.129242
1	0.711406	1.357905	-1.70242	1	-0.039719	0.385054	-1.966678
1	-0.24683	-0.087601	-1.925537	1	0.785485	-0.794313	-0.98005
1	1.482182	-1.423607	-0.700431	1	2.354897	0.760888	-2.198182
1	2.159625	-0.55354	-2.065233	1	1.687481	2.11487	-1.281071
1	2.658657	0.875172	1.984631	1	2.728997	0.973902	2.107791
1	0.324075	1.272908	2.174785	1	0.361551	1.006946	2.340295
1	-4.618076	0.873087	0.513265	1	-4.553437	0.83245	0.326073
1	-2.862915	-0.581307	2.160611	1	-2.93862	-0.468288	2.111783
1	-1.234162	-0.209628	2.719309	1	-1.352579	-0.143092	2.798467
1	-2.262057	1.075629	2.046659	1	-2.263831	1.160413	2.004081
1	0.052716	-1.749484	1.237911	1	0.092376	-1.700474	1.439315
1	-1.566835	-2.427049	1.024396	1	-1.532623	-2.37773	1.262676
1	-0.56409	-2.106098	-0.388044	1	-0.506854	-2.190526	-0.155111
1	3.446113	-1.515303	0.916122	1	2.896936	-1.416748	-0.0039
1	0.154327	3.343062	1.170436	1	0.275184	3.303992	1.22786
1	-1.187615	4.198067	0.233237	1	-1.027098	4.180587	0.25043
1	4.022702	1.667446	-0.282156	1	4.562649	1.514707	0.43939
1	4.482954	-0.16757	-2.447122	1	5.625072	-2.113224	-1.067329
1	5.909968	-0.191627	-1.387798	1	4.053384	-2.779477	-1.594147
1	5.582686	-1.575887	-2.460702	1	5.105185	-1.93676	-2.763678
1	6.508066	-0.029602	2.037653	1	4.464272	-2.584636	1.394826

1	5.362414	-1.358984	2.364636	1	5.392876	-1.476576	2.43634
1	6.375629	-1.39474	0.895738	1	3.613885	-1.404105	2.42928
Conformer **2-9**							
6	-2.431059	-0.248597	-0.495961	1	-1.440421	1.823427	-2.169057
6	-3.001387	1.123215	-0.880841	1	-0.082208	0.181524	-1.985451
6	-1.845328	2.087231	-1.184569	1	0.759207	-0.959097	-0.950232
6	-0.744108	2.058763	-0.145986	1	2.326728	0.431234	-2.303663
6	-0.164023	0.665764	0.166741	1	1.699993	1.880226	-1.531584
6	-1.378882	-0.290711	0.637417	1	2.849374	0.765676	1.977621
6	0.552449	0.100434	-1.099116	1	0.487389	0.853994	2.293203
6	1.882296	0.810273	-1.376424	1	-4.480299	1.063811	0.370226
6	2.894147	0.682959	-0.221769	1	-2.922723	-0.305623	2.16192
6	2.192137	0.714787	1.113361	1	-1.305399	-0.076115	2.810807
6	0.865992	0.742842	1.281808	1	-2.138416	1.268967	2.000239
8	-3.800164	1.714658	0.134148	1	0.017607	-1.756615	1.443803
6	-1.966859	0.19265	1.983523	1	-1.65596	-2.327585	1.346951
6	-0.889696	-1.741707	0.833522	1	-0.671804	-2.246027	-0.111626
35	-4.019619	-1.442602	-0.090696	1	4.390813	-0.454056	-1.298752
6	3.806417	-0.562302	-0.367139	1	0.497237	3.211807	1.137026
6	-0.311167	3.193319	0.414534	1	-0.757017	4.149065	0.152488
8	3.8437	1.768627	-0.285748	1	3.360753	2.579404	-0.071408
8	2.991868	-1.697025	-0.423828	1	6.613457	-0.555744	1.3707
8	4.694972	-0.694037	0.726871	1	6.459558	-0.706886	-0.397295
6	6.028573	-0.245141	0.501734	1	6.074684	0.843146	0.400412
6	3.691185	-2.890964	-0.768099	1	4.451886	-3.135671	-0.020003
1	-2.036652	-0.728502	-1.391535	1	2.949365	-3.690364	-0.807756
1	-3.599085	0.988701	-1.793751	1	4.173297	-2.796649	-1.751051
1	-2.261842	3.094344	-1.275841	-	-	-	-

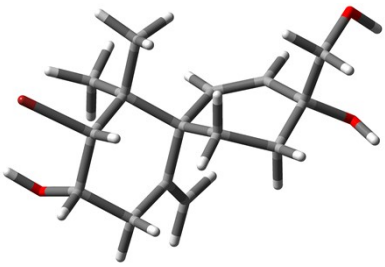
Figure S64. The most stable conformers of (3*R*,6*R*,9*S*,10*R*)-**3** calculated at ωB97X-D/6-311+G(d,p)/IEFPCM-ACN level



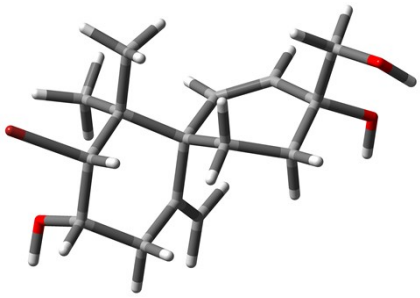
3-1



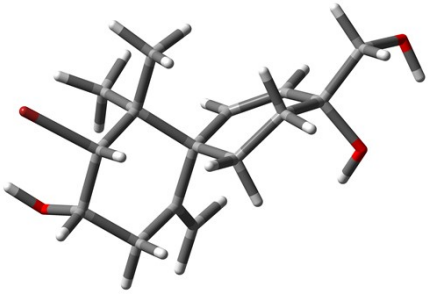
3-2



3-3

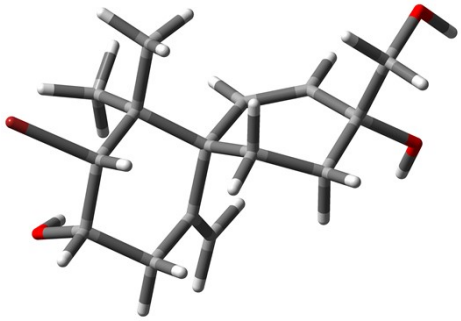


3-4

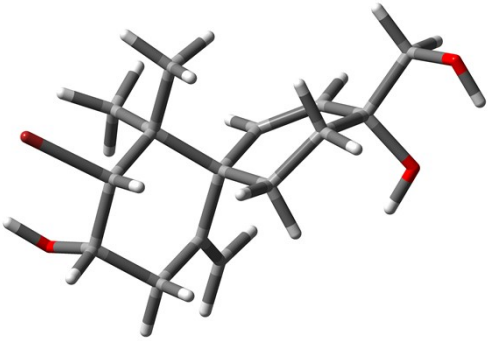


3-5

(Not considered due to incompatibility with the NOESY spectral data)



3-6



3-7

(Not considered due to incompatibility with the NOESY spectral data)

Table S9. Gibbs free energies and Boltzmann populations of the most stable conformers of (3*R*,6*R*,9*S*,10*R*)-**3** calculated at ωB97X-D/6-311+G(d,p)/IEFPCM-ACN level

Conformer	Gibbs free energy	Imaginary	Boltz. Pop.

	(Hartree)	frequencies	
3-1	-3384.945402	0	0.40108247
3-2	-3384.944734	0	0.197685598
3-3	-3384.944401	0	0.138933084
3-4	-3384.943925	0	0.083919114
3-5	-3384.943786	0	0.072431142
3-6	-3384.943686	0	0.065152116
3-7	-3384.943244	0	0.040796476

Table S10. Cartesian coordinates of the most stable conformers of (3*R*,6*R*,9*S*,10*R*)-**3** calculated at ωB97X-D/6-311+G(d,p)/IEFPCM-ACN level

Atomic Number	Coordinates (Angstroms)			Atomic Number	Coordinates (Angstroms)		
	X	Y	Z		X	Y	Z
Conformer **3-1**				Conformer **3-2**			
6	-1.862158	-0.120542	-0.512752	6	-0.790041	-0.428402	0.565211
6	-2.245262	1.352113	-0.685998	6	0.094335	1.905082	0.071944
6	-0.982746	2.178689	-0.915524	6	-2.264342	1.344875	-0.676176
6	0.118779	1.873533	0.067665	6	-1.018424	2.19671	-0.903116
6	0.501702	0.394262	0.185627	6	-1.853175	-0.121256	-0.51301
6	-0.806214	-0.441216	0.568987	6	0.502412	0.431677	0.183384
6	1.110768	-0.083306	-1.159	6	1.546834	0.256885	1.265802
6	2.521946	0.45809	-1.367855	6	2.840922	0.041479	1.054101
6	3.487497	-0.060157	-0.302809	6	3.486986	-0.037961	-0.309293
6	2.838491	-0.01428	1.056788	6	2.532378	0.50258	-1.365845
6	1.544043	0.202459	1.267514	6	1.115367	-0.027521	-1.166204
8	-2.923313	1.905534	0.426218	6	0.685338	2.892021	0.741077
6	-1.289607	-0.065084	1.98129	8	-2.950968	1.877878	0.440805
6	-0.500296	-1.948204	0.56507	6	-1.276159	-0.067027	1.980362
35	-3.543166	-1.162735	-0.280839	35	-3.51441	-1.195896	-0.284647
6	3.983871	-1.469555	-0.642303	6	-0.458532	-1.930013	0.555238
6	0.71895	2.852378	0.740491	6	3.92249	-1.475108	-0.632988
8	4.691309	0.722828	-0.28393	8	4.93363	-1.924734	0.259571
8	4.899656	-1.963051	0.315872	8	4.654154	0.787582	-0.325866
1	-1.511091	-0.48668	-1.477029	1	-2.902747	1.416122	-1.564559
1	-2.880409	1.429876	-1.576154	1	-0.670341	2.018533	-1.925483
1	-1.253362	3.235245	-0.872296	1	-1.308681	3.247581	-0.849649

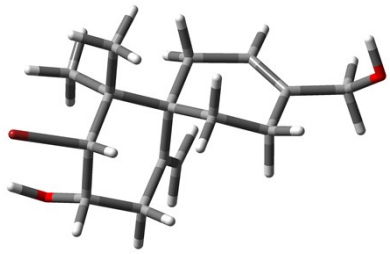
1	-0.633126	1.984588	-1.934481	1	-1.496514	-0.474712	-1.480061
1	0.490263	0.211114	-2.006006	1	1.208913	0.355533	2.291372
1	1.141782	-1.174174	-1.170321	1	3.509258	-0.050845	1.907588
1	2.889585	0.190838	-2.362794	1	2.897084	0.24194	-2.363674
1	2.506913	1.551547	-1.313803	1	2.537138	1.594173	-1.292465
1	3.505728	-0.146193	1.903843	1	1.133732	-1.118036	-1.199795
1	1.204019	0.275232	2.294439	1	0.500302	0.288836	-2.009101
1	-3.7007	1.368042	0.604462	1	1.512283	2.716447	1.418806
1	-2.312202	-0.415585	2.132438	1	0.355644	3.918643	0.616578
1	-0.671596	-0.556007	2.735381	1	-3.715888	1.322463	0.618244
1	-1.272582	1.01068	2.153228	1	-2.291275	-0.437818	2.133743
1	0.435801	-2.143803	1.094379	1	-0.645386	-0.548518	2.730023
1	-1.294363	-2.492467	1.079532	1	-1.27912	1.008167	2.15643
1	-0.418359	-2.361225	-0.442685	1	-0.372396	-2.338965	-0.453794
1	3.145239	-2.166798	-0.6698	1	0.482038	-2.11098	1.081794
1	4.445028	-1.438869	-1.638493	1	-1.241895	-2.489226	1.070091
1	1.536235	2.664754	1.426759	1	4.37004	-1.486758	-1.629623
1	0.405659	3.88365	0.612337	1	3.063068	-2.152183	-0.624634
1	4.492541	1.58569	0.088101	1	4.524605	-2.202709	1.081944
1	5.579983	-1.291304	0.419901	1	5.341615	0.308728	0.149868
Conformer **3-3**				Conformer **3-4**			
6	-0.787436	-0.424136	0.566178	6	-0.847788	-0.336983	0.676496
6	0.094993	1.909452	0.068448	6	0.139383	1.862889	-0.138442
6	-2.263578	1.345008	-0.678723	6	-2.18683	1.239117	-0.922637
6	-1.019034	2.198716	-0.906065	6	-0.890731	1.997951	-1.229511
6	-1.850149	-0.120281	-0.513329	6	-1.837583	-0.184677	-0.503657
6	0.504315	0.436537	0.18326	6	0.493531	0.423217	0.251317
6	1.548303	0.264869	1.267384	6	1.455771	0.418061	1.421121
6	2.842648	0.045737	1.065174	6	2.759498	0.170938	1.33945
6	3.480781	-0.059831	-0.292671	6	3.494547	-0.122169	0.058498
6	2.53792	0.496096	-1.35597	6	2.61961	0.222417	-1.145837
6	1.115908	-0.02444	-1.166389	6	1.189433	-0.269989	-0.950126
6	0.686423	2.898207	0.734538	6	0.698943	2.940777	0.406201
8	-2.951836	1.878456	0.436998	8	-2.939424	1.878182	0.093164
35	-3.509798	-1.197213	-0.28486	35	-3.518456	-1.206001	-0.239998
6	-1.274989	-0.06033	1.980226	6	-1.410438	0.250354	1.983175

6	-0.454064	-1.925357	0.5599	6	-0.560147	-1.827791	0.921522
6	3.891714	-1.508271	-0.605107	6	3.960301	-1.583216	0.055141
8	4.813435	-2.011374	0.341601	8	4.779867	-1.881485	-1.05809
8	4.688323	0.716396	-0.216071	8	4.722822	0.619833	0.019878
1	-2.901486	1.413987	-1.567648	1	-2.7838	1.183438	-1.840003
1	-0.671467	2.021223	-1.928716	1	-0.49033	1.61688	-2.175015
1	-1.310994	3.249103	-0.852592	1	-1.130671	3.050536	-1.400266
1	-1.492116	-0.474471	-1.479633	1	-1.41732	-0.680847	-1.377694
1	1.207029	0.364641	2.291553	1	1.047514	0.670363	2.393301
1	3.510822	-0.05797	1.914756	1	3.371169	0.193907	2.238081
1	2.90268	0.235279	-2.35512	1	3.05414	-0.212196	-2.048757
1	2.547815	1.587573	-1.277654	1	2.614843	1.310461	-1.275184
1	1.126987	-1.114657	-1.205046	1	1.207256	-1.348103	-0.781985
1	0.506893	0.300681	-2.010213	1	0.632844	-0.118262	-1.875497
1	1.513917	2.724197	1.411979	1	1.461021	2.871303	1.173299
1	0.355992	3.924382	0.608283	1	0.408097	3.936083	0.085324
1	-3.715472	1.321541	0.615262	1	-3.211525	2.737191	-0.235658
1	-2.290115	-0.431248	2.13315	1	-2.451781	-0.050081	2.107983
1	-0.644791	-0.54031	2.731285	1	-0.856992	-0.137391	2.840762
1	-1.278579	1.015157	2.154506	1	-1.372512	1.33911	1.99794
1	-0.367642	-2.337044	-0.448013	1	-0.430721	-2.392704	-0.004215
1	0.486624	-2.103882	1.087034	1	0.344671	-1.941946	1.524218
1	-1.236788	-2.484186	1.076113	1	-1.38646	-2.282597	1.470538
1	4.322541	-1.536634	-1.616541	1	3.098494	-2.251042	0.012155
1	3.02296	-2.16845	-0.585152	1	4.496239	-1.77805	0.993066
1	5.49966	-1.343717	0.439135	1	5.451655	-1.1938	-1.096344
1	5.026565	0.837592	-1.107975	1	4.518993	1.550173	-0.101998
Conformer **3-5**				Conformer **3-6**			
6	-1.884747	-0.136151	-0.507788	6	-0.821655	-0.465325	0.554058
6	-2.363953	1.30786	-0.666063	6	0.121033	1.836137	0.041386
6	-1.162517	2.188503	-0.990453	6	-2.238753	1.366854	-0.678494
6	-0.028449	1.995113	-0.019216	6	-0.949145	2.138055	-0.976421
6	0.484774	0.554539	0.089975	6	-1.891547	-0.117055	-0.510182
6	-0.74015	-0.392688	0.502768	6	0.49677	0.355296	0.172545
6	1.111546	0.194219	-1.293124	6	1.53254	0.163308	1.261762
6	2.271132	-0.7985	-1.253187	6	2.831255	-0.030809	1.054951

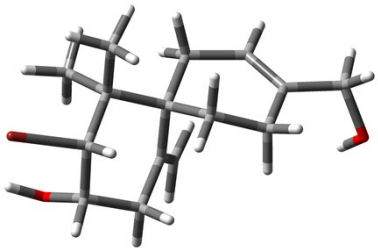
6	3.382822	-0.346034	-0.315758	6	3.48943	-0.051089	-0.301129
6	2.808111	0.098087	1.0013	6	2.514774	0.432669	-1.374933
6	1.545076	0.479733	1.164812	6	1.115848	-0.138135	-1.160246
8	-2.99177	1.838436	0.485199	6	0.66236	2.811645	0.768686
6	-1.169812	-0.093861	1.94987	8	-2.941128	1.931542	0.412437
6	-0.327203	-1.869085	0.427218	6	-1.280286	-0.109889	1.982926
35	-3.485396	-1.27152	-0.167916	35	-3.572499	-1.140869	-0.273198
6	4.408142	-1.466539	-0.132179	6	-0.537762	-1.97625	0.524466
6	0.496445	3.031099	0.630617	6	4.035476	-1.442704	-0.638155
8	4.142525	0.733634	-0.897769	8	4.955886	-1.909732	0.32845
8	5.523919	-1.047318	0.627424	8	4.66559	0.772266	-0.272281
1	-1.582154	-0.486301	-1.493689	1	-2.914399	1.459169	-1.530544
1	-3.061062	1.338885	-1.511662	1	-0.60748	1.87083	-1.980664
1	-1.487235	3.230494	-1.004752	1	-1.17816	3.205391	-0.991347
1	-0.828541	1.940988	-2.003898	1	-1.548181	-0.47867	-1.479447
1	1.483171	1.122911	-1.738308	1	1.186382	0.213167	2.288156
1	0.354173	-0.177963	-1.984811	1	3.495711	-0.164604	1.903785
1	1.932736	-1.787347	-0.937381	1	2.890338	0.160422	-2.365489
1	2.684365	-0.905833	-2.259954	1	2.475909	1.526137	-1.33634
1	3.492169	0.126184	1.844559	1	1.174321	-1.227633	-1.143593
1	1.240817	0.803149	2.154324	1	0.490006	0.118739	-2.015287
1	-3.724953	1.262424	0.72122	1	1.437806	2.623564	1.501796
1	-2.13385	-0.560383	2.159825	1	0.345775	3.841081	0.634318
1	-0.448332	-0.518275	2.650658	1	-2.320112	2.129428	1.117977
1	-1.263015	0.975192	2.14011	1	-2.340185	-0.332758	2.110985
1	0.603481	-2.030136	0.975752	1	-0.733678	-0.707551	2.71455
1	-1.094295	-2.497726	0.883156	1	-1.113539	0.93969	2.236622
1	-0.189782	-2.207188	-0.602759	1	-0.47149	-2.372599	-0.490906
1	3.949804	-2.304296	0.397012	1	0.400552	-2.1923	1.042283
1	4.723661	-1.814687	-1.124999	1	-1.334614	-2.517389	1.037454
1	1.331984	2.932153	1.313209	1	4.506221	-1.393439	-1.629029
1	0.099599	4.030234	0.481868	1	3.219974	-2.166418	-0.677524
1	3.713826	1.564495	-0.681315	1	5.616739	-1.219707	0.437958
1	5.807599	-0.209542	0.247284	1	4.434755	1.627026	0.100041
Conformer **3-7**							
6	-1.82715	-0.206875	-0.526886	1	-1.510152	3.111498	-1.317186

6	-2.343715	1.19624	-0.848952	1	-0.74507	1.75944	-2.142665
6	-1.153465	2.088968	-1.181007	1	1.56679	1.071589	-1.657597
6	-0.080301	2.032726	-0.126388	1	0.512544	-0.294576	-1.848836
6	0.473601	0.630112	0.151419	1	2.062625	-1.733448	-0.556087
6	-0.742724	-0.324809	0.5717	1	2.876917	-0.954429	-1.901363
6	1.206732	0.17127	-1.147563	1	3.361059	0.495364	2.135185
6	2.393724	-0.767333	-0.939777	1	1.078013	1.108317	2.224671
6	3.424522	-0.195112	0.0291	1	-3.789393	1.224753	0.450442
6	2.741192	0.349697	1.253425	1	-2.235303	-0.396906	2.147163
6	1.458961	0.698013	1.295758	1	-0.587396	-0.243486	2.735863
8	-3.062267	1.805119	0.206618	1	-1.416959	1.164092	2.038845
6	-1.275774	0.086566	1.955444	1	0.621386	-1.85785	1.277944
6	-0.275602	-1.784277	0.659198	1	-1.049416	-2.399404	1.122155
35	-3.407171	-1.368897	-0.180784	1	-0.058362	-2.208126	-0.324309
6	4.464027	-1.240301	0.430824	1	5.145576	-0.790917	1.164948
6	0.366188	3.145189	0.451734	1	3.967373	-2.092848	0.898401
8	4.205532	0.844556	-0.592493	1	1.158446	3.144319	1.19073
8	5.18617	-1.73592	-0.680095	1	-0.053191	4.109453	0.183071
1	-1.449792	-0.632944	-1.455468	1	3.631575	1.587809	-0.791942
1	-2.985327	1.122267	-1.734812	1	5.532239	-0.973072	-1.152116

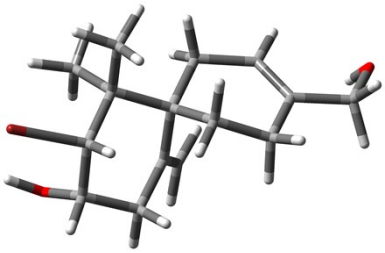
Figure S65. The most stable conformers of (6*R*,9*S*,10*R*)-**4** calculated at B3LYP/6-31G(d)/IEFPCM-ACN level



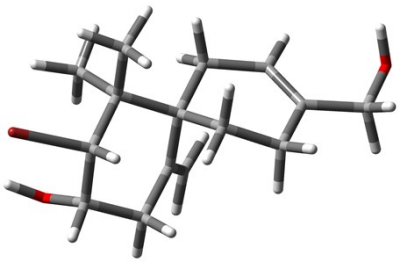
4-1



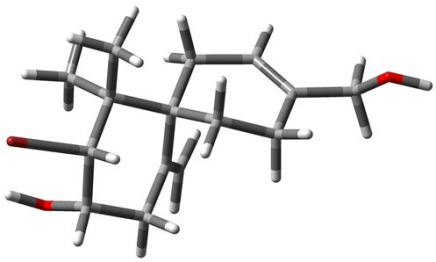
4-2



4-3



4-4



4-5

Table S11. Gibbs free energies and Boltzmann populations of the most stable conformers of (6*R*,9*S*,10*R*)-**4** calculated at B3LYP/6-31G(d)/IEFPCM-ACN level

Conformer	Gibbs free energy (Hartree)	Imaginary frequencies	Boltz. Pop.
4-1	-3307.246762	0	0.322937983
4-2	-3307.246558	0	0.260187033
4-3	-3307.246361	0	0.211189317
4-4	-3307.246034	0	0.149369662
4-5	-3307.245113	0	0.056316005

Table S12. Cartesian coordinates of the most stable conformers of (6*R*,9*S*,10*R*)-**4** calculated at B3LYP/6-31G(d)/IEFPCM-ACN level

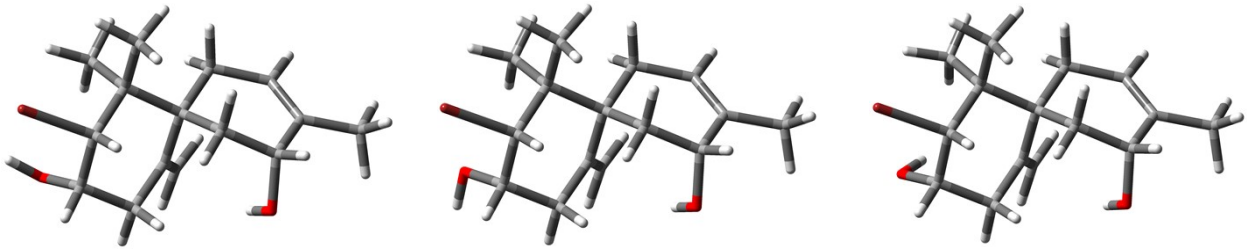
Atomic Number	Coordinates (Angstroms)			Atomic Number	Coordinates (Angstroms)		
	X	Y	Z		X	Y	Z
Conformer **4-1**				Conformer **4-2**			
6	-1.298355	-0.210777	1.958633	6	-1.299041	-0.577883	1.882665
6	-0.803196	-2.172767	0.484149	6	-1.015961	-2.256263	0.046357
6	1.23426	2.395905	0.904888	6	1.4711	1.922961	1.285663
8	-2.376306	2.132384	0.272794	8	-2.152005	2.141311	0.705393
35	-3.618161	-0.716227	-0.375301	35	-3.676086	-0.393798	-0.442473
6	1.353028	-0.634679	-0.957046	6	1.271204	-0.683609	-1.131951
6	1.614789	-0.416382	1.512151	6	1.57591	-0.976761	1.32387
6	-0.331035	1.962387	-0.950069	6	-0.140761	2.013337	-0.578121
6	0.584312	1.494182	0.160441	6	0.730562	1.251203	0.396755
6	0.693608	-0.031492	0.32297	6	0.687592	-0.280151	0.258268
6	-0.787291	-0.628747	0.562003	6	-0.84405	-0.765507	0.418417
6	-1.694746	-0.09	-0.576567	6	-1.700902	0.069328	-0.570889
6	-1.759232	1.425399	-0.794648	6	-1.614627	1.597336	-0.49265
6	3.09214	-0.299242	1.225012	6	3.055375	-0.938906	1.026324
6	3.626979	-0.130706	0.009125	6	3.593959	-0.603878	-0.152982
6	2.752791	-0.064476	-1.219356	6	2.719325	-0.213292	-1.320625
6	5.116058	-0.000103	-0.187157	6	5.085843	-0.572347	-0.3605
8	5.658815	-1.02029	-1.038772	8	5.556086	0.722654	-0.76459
1	-0.75107	-0.745396	2.7406	1	-0.803166	-1.305454	2.531943
1	-2.355817	-0.470322	2.061475	1	-2.376693	-0.746667	1.962535
1	-1.195119	0.862483	2.127159	1	-1.085045	0.426728	2.251327

1	-0.580208	-2.541762	-0.521863	1	-0.839317	-2.443447	-1.017442
1	-0.085657	-2.620996	1.176866	1	-0.341699	-2.897743	0.620378
1	-1.795148	-2.544053	0.756464	1	-2.038028	-2.575039	0.269354
1	1.102385	3.460262	0.724139	1	1.444795	3.009786	1.318197
1	1.923991	2.130684	1.698172	1	2.134692	1.442246	1.995593
1	-3.245042	1.715554	0.415864	1	-3.058158	1.792955	0.785742
1	1.446415	-1.717053	-0.817409	1	1.255401	-1.776291	-1.206193
1	0.729693	-0.489625	-1.845016	1	0.657443	-0.308383	-1.956981
1	1.371341	0.188164	2.3927	1	1.398621	-0.538544	2.312001
1	1.413751	-1.451486	1.81671	1	1.278864	-2.028595	1.424124
1	0.046716	1.634824	-1.927204	1	0.195607	1.847355	-1.609621
1	-0.377968	3.055565	-0.978859	1	-0.078462	3.090458	-0.393897
1	-1.42485	-0.562122	-1.521511	1	-1.486541	-0.234895	-1.595623
1	-2.312899	1.604857	-1.727724	1	-2.152928	2.006398	-1.360011
1	3.749158	-0.363876	2.093347	1	3.710692	-1.222445	1.850851
1	2.687663	0.978378	-1.565855	1	2.758999	0.875803	-1.461727
1	3.230247	-0.623767	-2.033328	1	3.123373	-0.645967	-2.246522
1	5.626684	0.009243	0.787143	1	5.376199	-1.239595	-1.181741
1	5.355709	0.941746	-0.696685	1	5.605229	-0.913485	0.547397
1	5.450927	-1.871133	-0.619003	1	5.297314	1.342641	-0.063152
Conformer **4-3**				Conformer **4-4**			
6	-1.179886	-0.480706	1.904291	6	-1.178826	-0.515546	1.895594
6	-0.901174	-2.235317	0.139803	6	-0.855805	-2.231018	0.100669
6	1.400847	2.138962	1.014802	6	1.350235	2.174284	1.064719
8	-2.255855	2.118939	0.648321	8	-2.303973	2.084082	0.683013
35	-3.691682	-0.55498	-0.279065	35	-3.679765	-0.602332	-0.299522
6	1.220763	-0.60345	-1.246065	6	1.236778	-0.529116	-1.245577
6	1.677058	-0.744271	1.199829	6	1.686329	-0.70473	1.198735
6	-0.319396	2.036823	-0.748475	6	-0.361013	2.067927	-0.707268
6	0.650644	1.378929	0.209025	6	0.618965	1.413465	0.24244
6	0.69178	-0.157891	0.152889	6	0.692535	-0.12079	0.158688
6	-0.79756	-0.719669	0.426811	6	-0.785512	-0.718989	0.415669
6	-1.757738	0.011401	-0.549552	6	-1.75704	0.009646	-0.551174
6	-1.758359	1.543721	-0.552361	6	-1.790029	1.541395	-0.52593
6	3.134282	-0.649116	0.815176	6	3.142854	-0.566554	0.823759
6	3.582946	-0.338685	-0.405492	6	3.591437	-0.234481	-0.391259

6	2.626231	-0.06225	-1.539929	6	2.632363	0.045966	-1.523356
6	5.054184	-0.23051	-0.737396	6	5.063776	-0.100641	-0.712936
8	5.932485	-0.313585	0.378989	8	5.948339	-0.472693	0.337884
1	-0.603045	-1.140669	2.558772	1	-0.590138	-1.174468	2.540521
1	-2.238459	-0.709576	2.056896	1	-2.232672	-0.77046	2.039368
1	-1.009797	0.553626	2.207926	1	-1.032923	0.516553	2.218609
1	-0.774783	-2.467674	-0.922262	1	-0.719103	-2.441488	-0.964699
1	-0.157902	-2.806226	0.702935	1	-0.103545	-2.796233	0.657594
1	-1.888013	-2.599424	0.439092	1	-1.836279	-2.621017	0.387975
1	1.311654	3.222761	0.993596	1	1.238729	3.256214	1.062192
1	2.1335	1.73518	1.70437	1	2.088368	1.773675	1.75026
1	-3.132814	1.723747	0.802329	1	-3.172988	1.667791	0.826035
1	1.266279	-1.697492	-1.264498	1	1.304831	-1.621451	-1.284312
1	0.543333	-0.307412	-2.053156	1	0.557005	-0.231743	-2.050233
1	1.529041	-0.258752	2.170694	1	1.523348	-0.24114	2.177781
1	1.442283	-1.80207	1.374915	1	1.474972	-1.770722	1.352896
1	-0.034216	1.834905	-1.789083	1	-0.06787	1.890319	-1.750117
1	-0.310644	3.124152	-0.622979	1	-0.375468	3.152801	-0.562721
1	-1.585587	-0.334178	-1.569194	1	-1.573707	-0.313387	-1.576279
1	-2.369989	1.875468	-1.403979	1	-2.405359	1.875829	-1.373827
1	3.852258	-0.86559	1.604582	1	3.860753	-0.756482	1.619957
1	2.591188	1.020143	-1.73571	1	2.573422	1.131427	-1.695437
1	3.000949	-0.519156	-2.467089	1	3.018068	-0.382834	-2.458997
1	5.227062	0.700361	-1.304937	1	5.300355	0.947898	-0.940019
1	5.347241	-1.051992	-1.404937	1	5.286875	-0.669853	-1.631358
1	5.708566	0.423511	0.970378	1	5.797899	-1.415638	0.514294
Conformer **4-5**							
6	-1.30947	-0.214301	1.957715	1	-0.598028	-2.545602	-0.524371
6	-0.822341	-2.176927	0.481458	1	-0.110416	-2.63123	1.175978
6	1.243588	2.377047	0.91898	1	-1.817812	-2.541989	0.74939
8	-2.36589	2.138902	0.272281	1	1.119271	3.442687	0.740277
35	-3.624304	-0.700029	-0.38597	1	1.928497	2.105352	1.714265
6	1.349118	-0.65063	-0.949266	1	-3.237789	1.727395	0.411463
6	1.604355	-0.43956	1.520222	1	1.434383	-1.733842	-0.811247
6	-0.31719	1.957818	-0.943082	1	0.730084	-0.499664	-1.839304
6	0.590846	1.481193	0.169848	1	1.361931	0.164349	2.401541

6	0.689507	-0.045509	0.329363	1	1.395204	-1.474055	1.82124
6	-0.79629	-0.633209	0.562153	1	0.062123	1.629727	-1.919407
6	-1.695796	-0.086299	-0.578732	1	-0.356928	3.051353	-0.96978
6	-1.749486	1.429934	-0.794158	1	-1.42551	-0.55844	-1.52354
6	3.083466	-0.331445	1.238266	1	-2.298358	1.614779	-1.729035
6	3.62338	-0.163574	0.025251	1	3.736568	-0.401197	2.108816
6	2.753765	-0.090356	-1.206286	1	2.697065	0.953527	-1.551734
6	5.108046	-0.008012	-0.163631	1	3.228577	-0.651874	-2.019699
8	5.589656	-1.058728	-1.014917	1	5.616477	-0.030298	0.811877
1	-0.768643	-0.75417	2.740553	1	5.319487	0.970953	-0.624306
1	-2.369093	-0.466671	2.056347	1	6.47976	-0.806369	-1.306566
1	-1.199326	0.857886	2.12868				

Figure S66. The most stable conformers of (4*R*,6*S*,9*S*,10*R*)-**6** calculated at B3LYP/6-31G(d)/IEFPCM-ACN level



6-1 **6-2** **6-3**

Table S13. Gibbs free energies and Boltzmann populations of the most stable conformers of (4*R*,6*S*,9*S*,10*R*)-**6** calculated at B3LYP/6-31G(d)/IEFPCM-ACN level

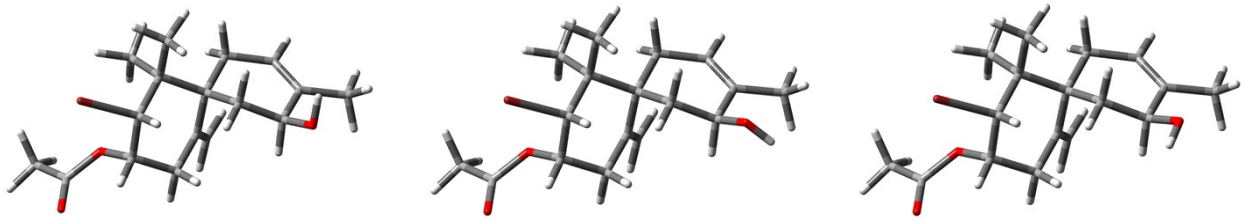
Conformer	Gibbs free energy (Hartree)	Imaginary frequencies	Boltz. Pop.
4-1	-3307.251552	0	0.946586675
4-2	-3307.247967	0	0.021241001
4-3	-3307.248359	0	0.032172325

Table S14. Cartesian coordinates of the most stable conformers of (4*R*,6*S*,9*S*,10*R*)-**6** calculated at B3LYP/6-31G(d)/IEFPCM-ACN level

Atomic Number	Coordinates (Angstroms)			Atomic Number	Coordinates (Angstroms)		
	X	Y	Z		X	Y	Z
Conformer **6-1**				Conformer **6-2**			
6	-1.566669	0.091146	-0.531743	6	-1.586854	0.096073	-0.507847
6	-1.508943	1.604344	-0.29612	6	-1.520685	1.60606	-0.303231
6	-0.043474	2.052904	-0.312831	6	-0.045678	2.039909	-0.389097
6	0.830644	1.204114	0.585932	6	0.834969	1.22739	0.534639
6	0.820634	-0.307498	0.284952	6	0.814664	-0.294771	0.294639
6	-0.708251	-0.825063	0.38157	6	-0.715656	-0.803137	0.415183
8	-2.072333	2.013418	0.942868	8	-2.102059	1.952332	0.948178
6	-0.860033	-2.275587	-0.132046	6	-0.870434	-2.263698	-0.069365
6	-1.177419	-0.785093	1.852764	6	-1.173022	-0.737032	1.888832
6	1.416115	-0.57378	-1.130976	6	1.406674	-0.618827	-1.110869
6	2.880237	-0.133731	-1.291558	6	2.871941	-0.190828	-1.291755
6	3.750454	-0.58561	-0.136473	6	3.742856	-0.599346	-0.120936
6	3.192648	-1.005826	1.005812	6	3.185873	-0.972514	1.037945
6	1.710287	-1.098552	1.278932	6	1.703666	-1.050069	1.316521
6	1.54146	1.789604	1.559725	6	1.548957	1.847919	1.484351
6	5.24016	-0.500826	-0.343817	6	5.232456	-0.527757	-0.334194
35	-3.53287	-0.414896	-0.479647	35	-3.533346	-0.443769	-0.485361
8	3.020112	1.283709	-1.520281	8	3.016852	1.215516	-1.578199
1	-1.331646	-0.103195	-1.578566	1	-1.329247	-0.102693	-1.548264
1	-2.041246	2.091819	-1.125609	1	-2.080588	2.083761	-1.1194
1	0.320991	2.00748	-1.346014	1	0.291046	1.936826	-1.428244
1	-0.005779	3.103349	-0.007437	1	0.022809	3.106936	-0.146631
1	-2.974505	1.647194	0.972472	1	-2.051807	2.918167	1.030999
1	-1.877911	-2.626136	0.05947	1	-1.878181	-2.620366	0.159019
1	-0.178103	-2.961017	0.378236	1	-0.165527	-2.933303	0.430952
1	-0.683176	-2.358809	-1.208962	1	-0.725794	-2.364049	-1.149758
1	-0.979956	0.180803	2.320631	1	-0.945847	0.227582	2.345448
1	-2.253666	-0.97255	1.904368	1	-2.254213	-0.889567	1.946855
1	-0.679046	-1.567418	2.432734	1	-0.693066	-1.528036	2.473064
1	1.382077	-1.652457	-1.318817	1	1.369017	-1.703934	-1.255316
1	0.833231	-0.099303	-1.926045	1	0.823361	-0.174786	-1.923103
1	3.258956	-0.581792	-2.2192	1	3.247366	-0.677541	-2.201136

1	3.838974	-1.330798	1.822017	1	3.832855	-1.266992	1.865172
1	1.43145	-2.160045	1.255958	1	1.421209	-2.110808	1.333999
1	1.514994	-0.777512	2.307182	1	1.510444	-0.690024	2.332173
1	2.20336	1.246991	2.225328	1	2.208076	1.328964	2.171256
1	1.482078	2.864032	1.717264	1	1.496494	2.928322	1.598003
1	5.792029	-0.7854	0.557764	1	5.785206	-0.77608	0.577529
1	5.563719	-1.156206	-1.164671	1	5.552625	-1.217925	-1.127437
1	5.534641	0.518552	-0.622961	1	5.529437	0.478135	-0.656273
1	2.809627	1.713483	-0.67292	1	2.804738	1.680321	-0.749988
Conformer **6-3**							
6	-1.592086	0.100256	-0.520048	1	0.05582	3.095709	-0.198613
6	-1.504025	1.614696	-0.293628	1	-1.372527	1.967304	1.621261
6	-0.027587	2.027435	-0.423801	1	-1.889443	-2.62714	0.077029
6	0.824744	1.208528	0.523372	1	-0.178444	-2.954077	0.348873
6	0.810733	-0.312883	0.275146	1	-0.729973	-2.343499	-1.220387
6	-0.720675	-0.822173	0.380603	1	-0.857534	0.094596	2.394599
8	-2.059295	2.054144	0.93939	1	-2.266873	-0.863176	1.915587
6	-0.87883	-2.27023	-0.138638	1	-0.766535	-1.664307	2.393006
6	-1.177446	-0.802816	1.858419	1	1.390073	-1.713275	-1.270989
6	1.416376	-0.628046	-1.125483	1	0.835595	-0.189331	-1.942304
6	2.879739	-0.186265	-1.28986	1	3.269341	-0.66906	-2.195206
6	3.741834	-0.585626	-0.109496	1	3.817057	-1.260428	1.874964
6	3.176286	-0.972218	1.040966	1	1.421211	-2.139271	1.288467
6	1.691765	-1.075149	1.298017	1	1.479636	-0.739999	2.318328
6	1.476188	1.821506	1.523821	1	2.09564	1.296521	2.242381
6	5.232855	-0.490655	-0.303208	1	1.4223	2.901592	1.639262
35	-3.543159	-0.4103	-0.469646	1	5.777096	-0.73731	0.613992
8	3.014644	1.221548	-1.575154	1	5.57278	-1.170842	-1.096754
1	-1.35189	-0.092058	-1.566856	1	5.519664	0.521425	-0.614711
1	-2.094766	2.107092	-1.071773	1	2.820398	1.686826	-0.743495
1	0.299907	1.889507	-1.460022				

Figure S67. The most stable conformers of (4*S*,6*S*,9*S*,10*R*)-**7** calculated at B3LYP/6-31G(d)/IEFPCM-ACN level



7-1 **7-2** **7-3**

Table S15. Gibbs free energies and Boltzmann populations of the most stable conformers of (4*S*,6*S*,9*S*,10*R*)-**7** calculated at B3LYP/6-31G(d)/IEFPCM-ACN level

Conformer	Gibbs free energy (Hartree)	Imaginary frequencies	Boltz. Pop.
7-1	-3459.887391	0	0.605617987
7-2	-3459.886040	0	0.144804463
7-3	-3459.886554	0	0.24957755

Table S16. Cartesian coordinates of the most stable conformers of (4*S*,6*S*,9*S*,10*R*)-**7** calculated at B3LYP/6-31G(d)/IEFPCM-ACN level

Atomic Number	Coordinates (Angstroms)			Atomic Number	Coordinates (Angstroms)		
	X	Y	Z		X	Y	Z
Conformer **7-1**				Conformer **7-2**			
6	-1.018551	-0.755256	-0.493589	6	-1.015864	-0.753286	-0.494812
6	-1.341206	0.677813	-0.906001	6	-1.340622	0.680437	-0.903208
6	-0.038153	1.46033	-1.108519	6	-0.038933	1.466367	-1.101092
6	0.900935	1.314958	0.069341	6	0.899359	1.318679	0.077101
6	1.290304	-0.131259	0.423886	6	1.290966	-0.128223	0.427788
6	-0.058982	-0.969739	0.711628	6	-0.057405	-0.969766	0.711021
8	-2.127239	1.325886	0.118899	8	-2.129906	1.323531	0.122422
6	0.221357	-2.48646	0.817209	6	0.225623	-2.486305	0.812116
6	-0.685869	-0.500623	2.043127	6	-0.687194	-0.50586	2.042937
6	2.101331	-0.746916	-0.753932	6	2.100389	-0.74152	-0.751259
6	3.380075	0.036239	-1.078193	6	3.373607	0.041627	-1.071946
6	4.209948	0.303054	0.16291	6	4.208644	0.29112	0.171335
6	3.656159	0.196158	1.377852	6	3.655433	0.190402	1.386247

6	2.223571	-0.187205	1.662162	6	2.220719	-0.184923	1.668567
6	1.323778	2.407635	0.714788	6	1.319962	2.410202	0.726018
6	5.638521	0.735238	-0.047021	6	5.646964	0.688717	-0.038091
35	-2.770751	-1.723374	-0.262847	35	-2.766766	-1.725129	-0.269551
8	4.129098	-0.63968	-2.100903	8	4.080129	-0.74067	-2.052049
6	-3.316405	1.871694	-0.235278	6	-3.318846	1.869193	-0.232499
8	-3.739458	1.904888	-1.372824	8	-3.738826	1.907062	-1.371065
6	-4.026634	2.4195	0.976347	6	-4.033476	2.409997	0.979683
1	-0.611302	-1.256997	-1.371986	1	-0.606642	-1.25161	-1.374192
1	-1.929457	0.672433	-1.824004	1	-1.927322	0.676863	-1.822217
1	0.428737	1.08594	-2.02906	1	0.43001	1.096217	-2.02229
1	-0.282949	2.511893	-1.286178	1	-0.285753	2.518054	-1.275293
1	-0.688028	-3.007469	1.128639	1	-0.683166	-3.010033	1.120768
1	0.993487	-2.704243	1.559946	1	0.9974	-2.704829	1.554974
1	0.535987	-2.919794	-0.137496	1	0.542642	-2.91575	-0.143478
1	-0.75055	0.587286	2.107289	1	-0.75422	0.581731	2.11017
1	-1.696094	-0.906486	2.14271	1	-1.69671	-0.914099	2.139854
1	-0.09583	-0.863956	2.889643	1	-0.097617	-0.87039	2.889239
1	1.512643	-0.837525	-1.671886	1	1.509891	-0.82741	-1.668377
1	2.403068	-1.76345	-0.474236	1	2.411116	-1.756403	-0.481697
1	3.121548	0.997593	-1.54274	1	3.109547	1.013577	-1.519757
1	4.268115	0.402579	2.256657	1	4.270941	0.383763	2.26563
1	1.833888	0.450935	2.46257	1	1.830277	0.455131	2.467095
1	2.219093	-1.201461	2.081482	1	2.212229	-1.198714	2.088886
1	2.009915	2.377496	1.553475	1	2.006045	2.378779	1.564708
1	0.997512	3.396329	0.400591	1	0.9923	3.399288	0.414459
1	5.685645	1.650383	-0.653977	1	5.724821	1.596947	-0.653621
1	6.214944	-0.022947	-0.589573	1	6.205141	-0.097125	-0.562262
1	6.137197	0.933225	0.907008	1	6.149198	0.884987	0.914158
1	4.402789	-1.497554	-1.734688	1	4.728002	-0.160026	-2.480494
1	-4.919277	2.963049	0.665376	1	-3.371323	3.065318	1.553024
1	-4.312645	1.592628	1.635356	1	-4.924855	2.955577	0.668624
1	-3.362419	3.078506	1.543068	1	-4.322261	1.579134	1.632458
Conformer **7-3**							
6	-1.017099	-0.755186	-0.492158	1	0.426417	1.087645	-2.029252
6	-1.34234	0.677057	-0.905436	1	-0.287266	2.512752	-1.286957

6	-0.040634	1.461723	-1.108643	1	-0.682324	-3.006174	1.130798
6	0.899062	1.318644	0.06905	1	0.998441	-2.698796	1.562829
6	1.290588	-0.126702	0.425549	1	0.542804	-2.915916	-0.134559
6	-0.057341	-0.9672	0.713302	1	-0.752208	0.589444	2.107743
8	-2.129371	1.32433	0.119165	1	-1.695223	-0.905928	2.143747
6	0.226091	-2.483236	0.8197	1	-0.095234	-0.860166	2.891133
6	-0.685656	-0.498397	2.044237	1	1.509836	-0.835353	-1.664008
6	2.105498	-0.744719	-0.748356	1	2.416807	-1.757719	-0.474487
6	3.384916	0.038347	-1.07035	1	3.124421	1.014054	-1.514404
6	4.216232	0.289322	0.167918	1	4.267959	0.406806	2.258955
6	3.656227	0.198046	1.380783	1	1.832174	0.464434	2.461782
6	2.221916	-0.178422	1.665251	1	2.214365	-1.190655	2.08931
6	1.319463	2.41276	0.713815	1	2.005795	2.384734	1.552421
6	5.651648	0.698115	-0.038178	1	0.99155	3.400565	0.398522
35	-2.767651	-1.726419	-0.26152	1	5.719286	1.594606	-0.670299
8	4.189745	-0.693443	-2.009565	1	6.219207	-0.086339	-0.551111
6	-3.319318	1.868309	-0.235161	1	6.141667	0.916028	0.91619
8	-3.742429	1.900556	-1.372732	1	3.698249	-0.717759	-2.846236
6	-4.030369	2.415306	0.976331	1	-4.315407	1.588098	1.635347
1	-0.608882	-1.256829	-1.370199	1	-3.367056	3.075164	1.543112
1	-1.930766	0.670144	-1.823324	1	-4.923685	2.957694	0.665261