Antiproliferative prenylated xanthones and benzophenones from the roots of *Cudrania tricuspidata* on HSC-T6 cells

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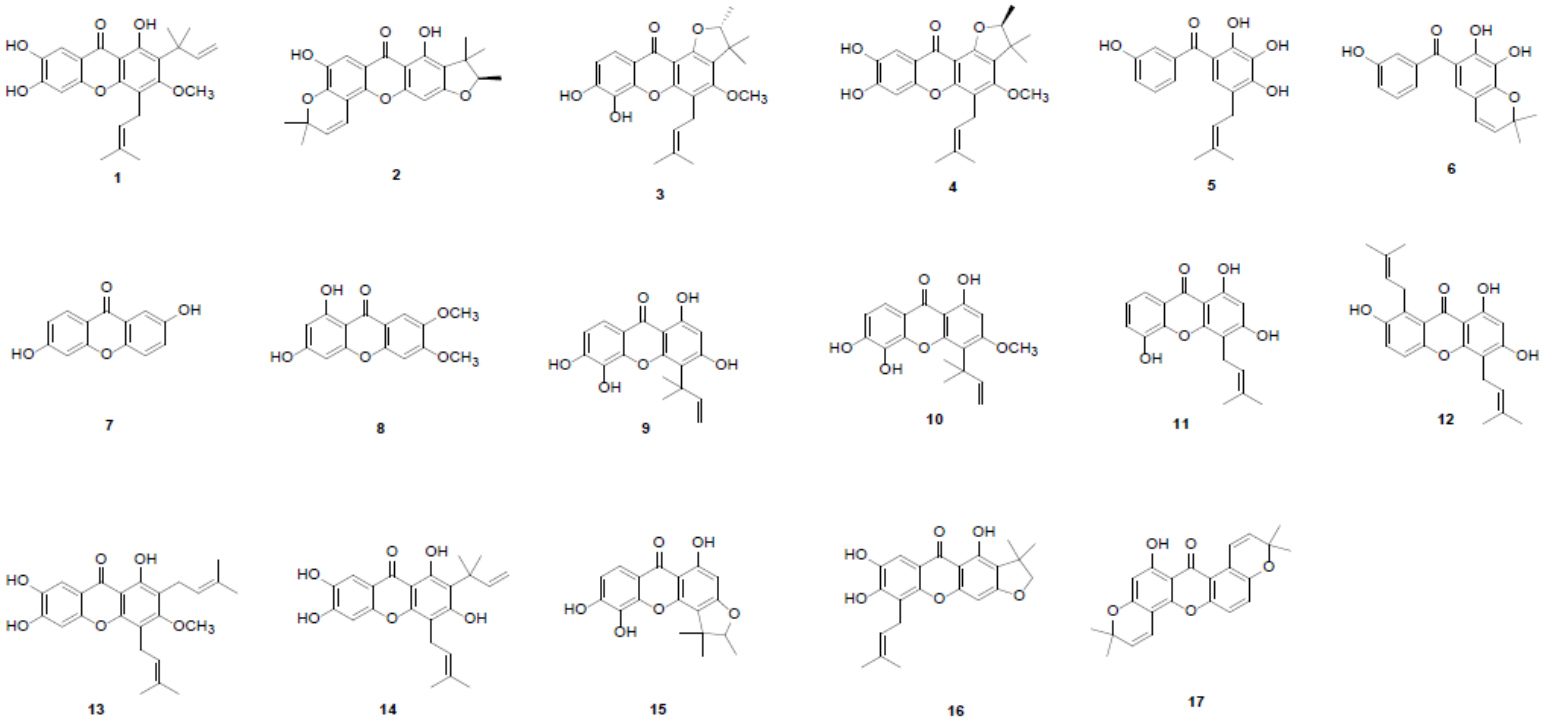
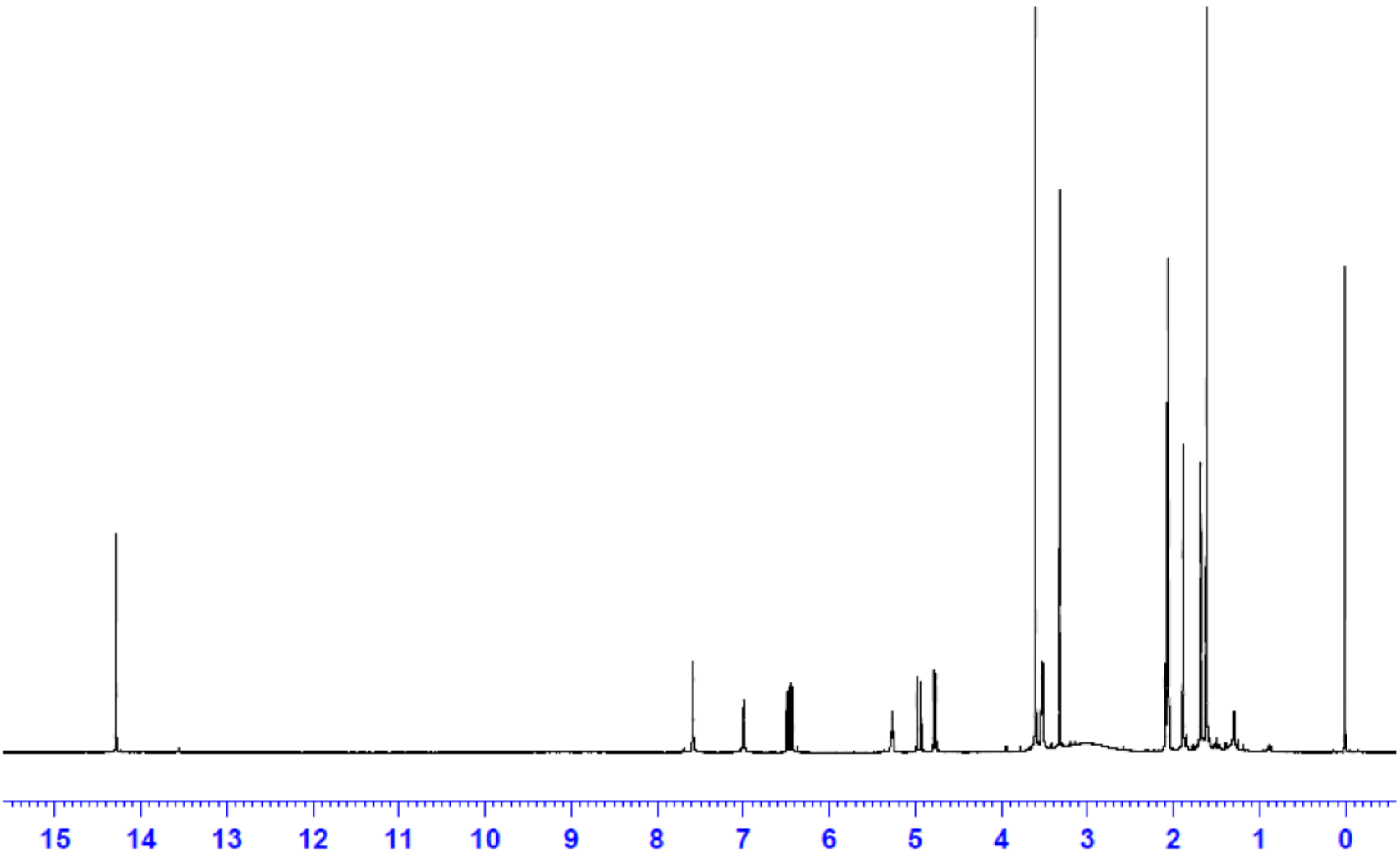
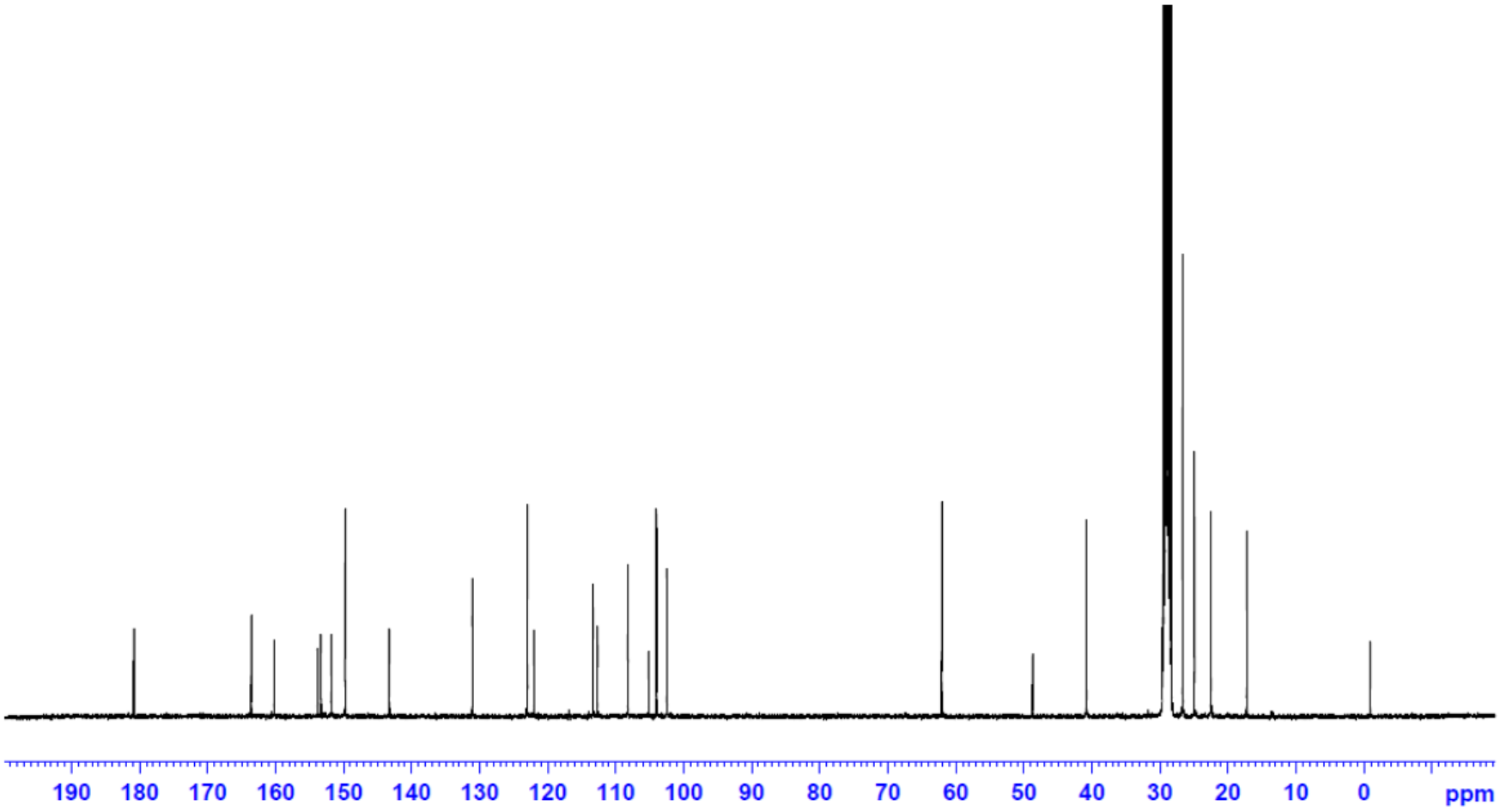


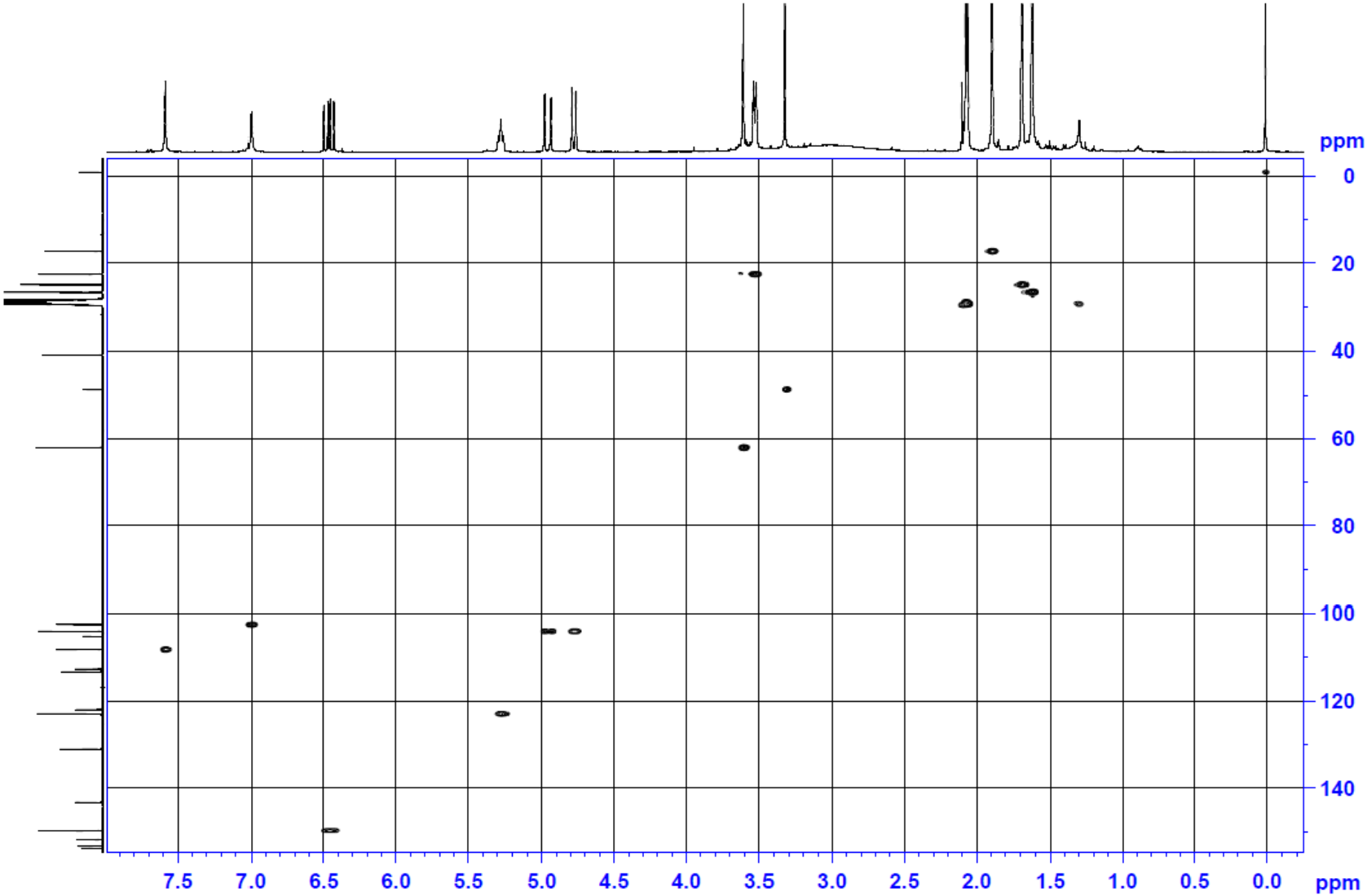
S1. Chemical constituents isolated from *C. tricuspidata* roots.



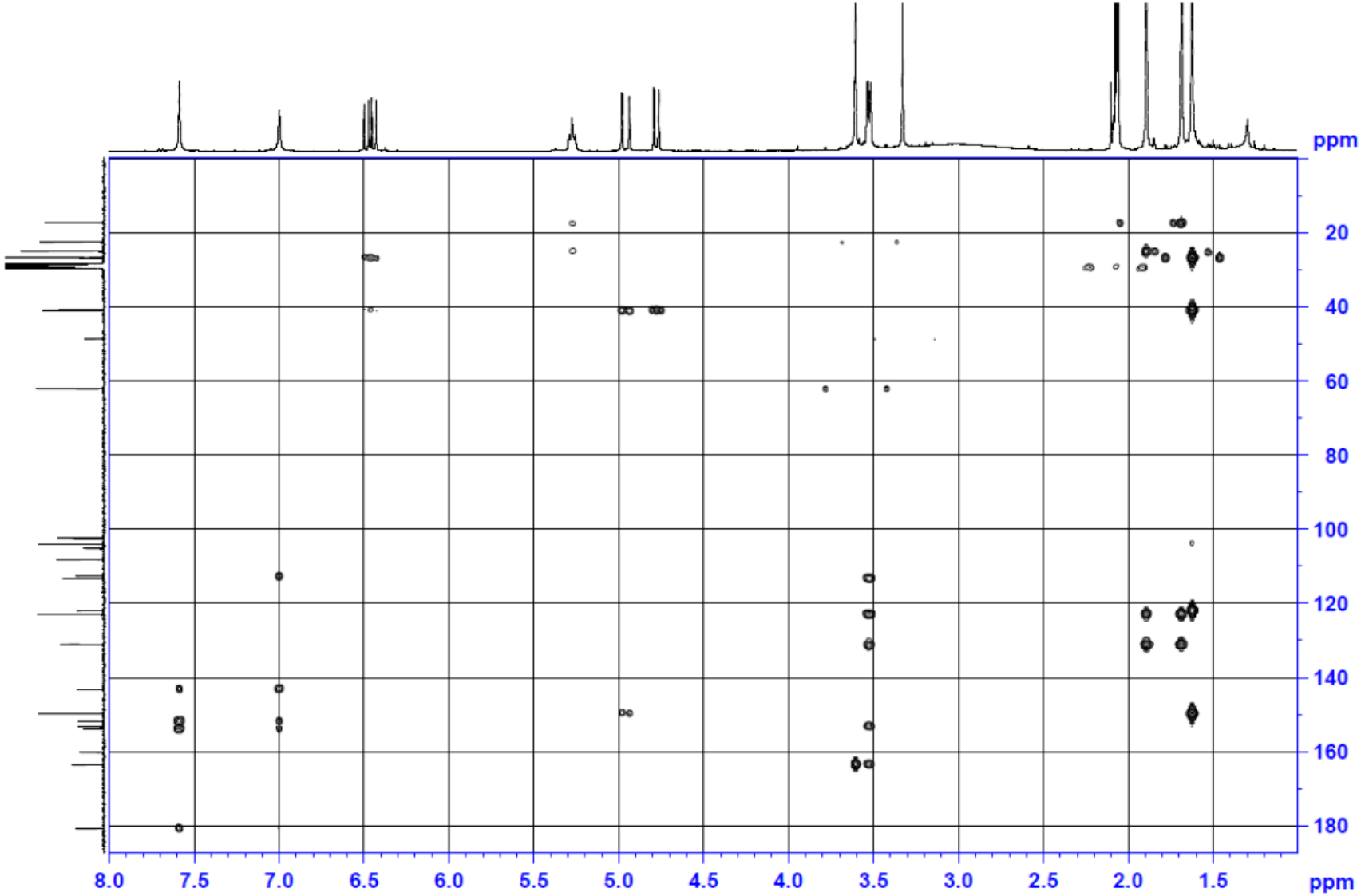
S2. ^{1}H-NMR spectrum of compound **1** (Acetone-d_6, 400 MHz)



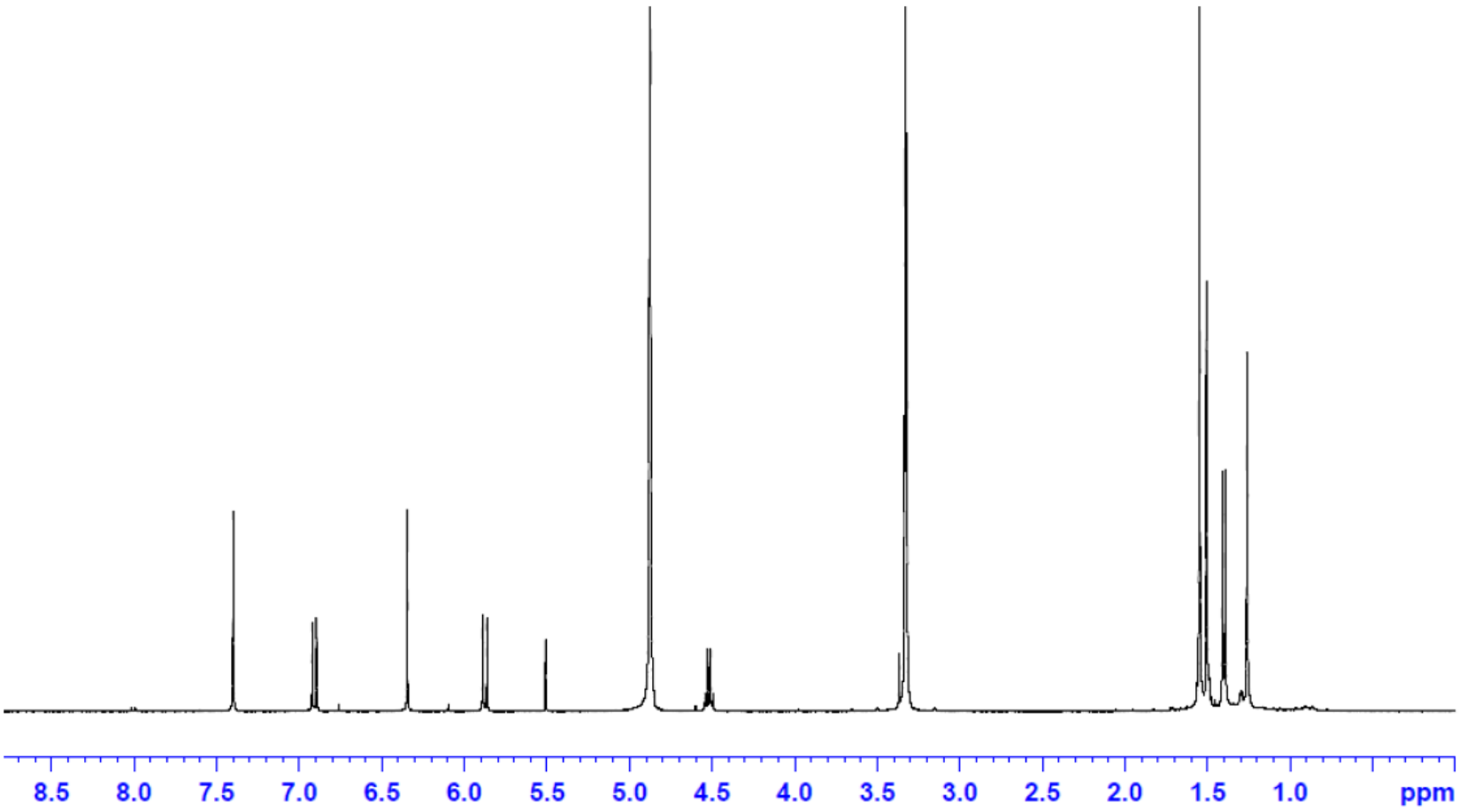
S3. ^{13}C-NMR spectrum of compound **1** (Acetone-d_6, 100 MHz)



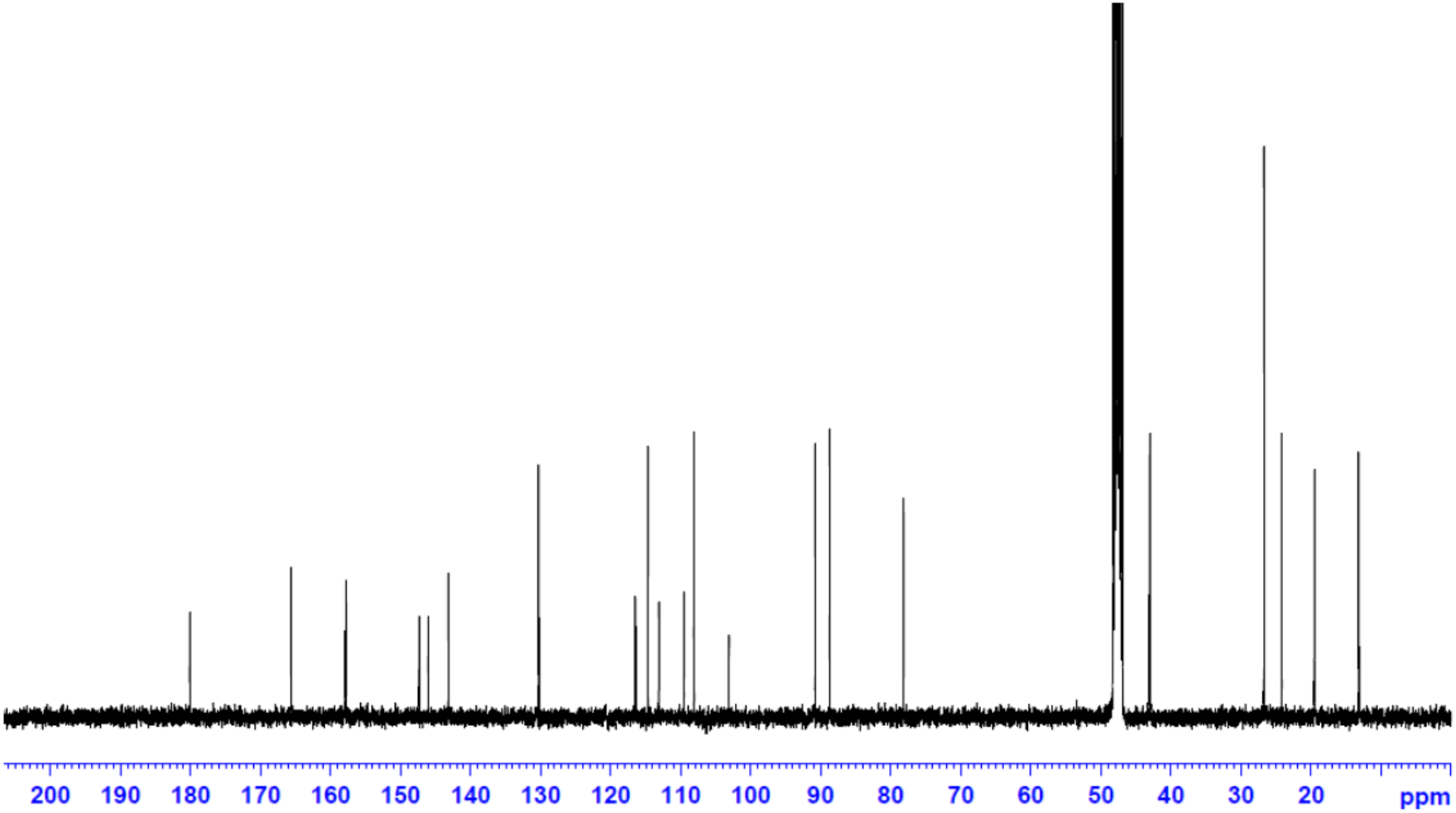
S4. HSQC spectrum of compound **1** (Acetone-d_6, 100 MHz)



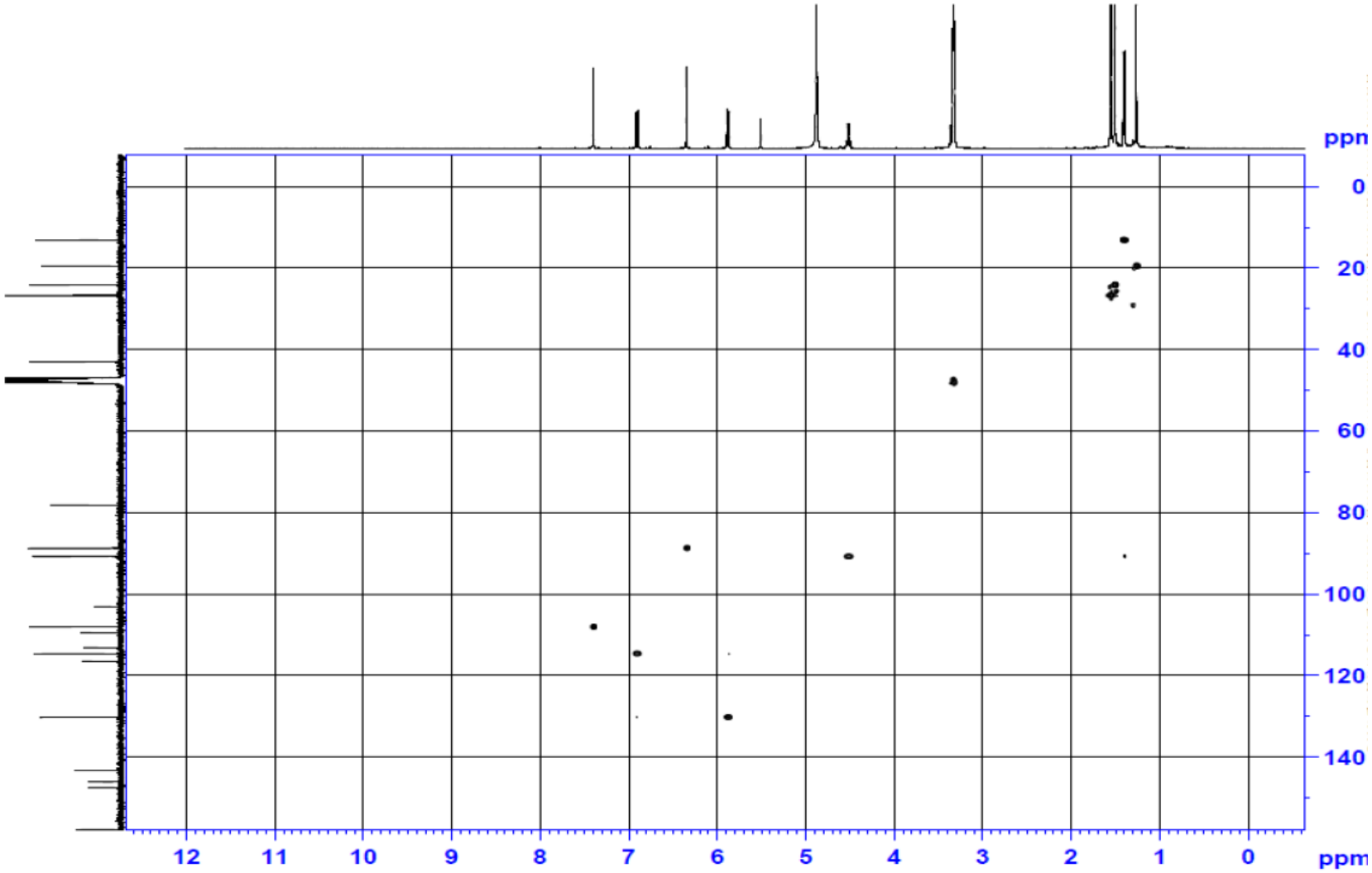
S5. HMBC spectrum of compound **1** (Acetone-d_6, 100 MHz)



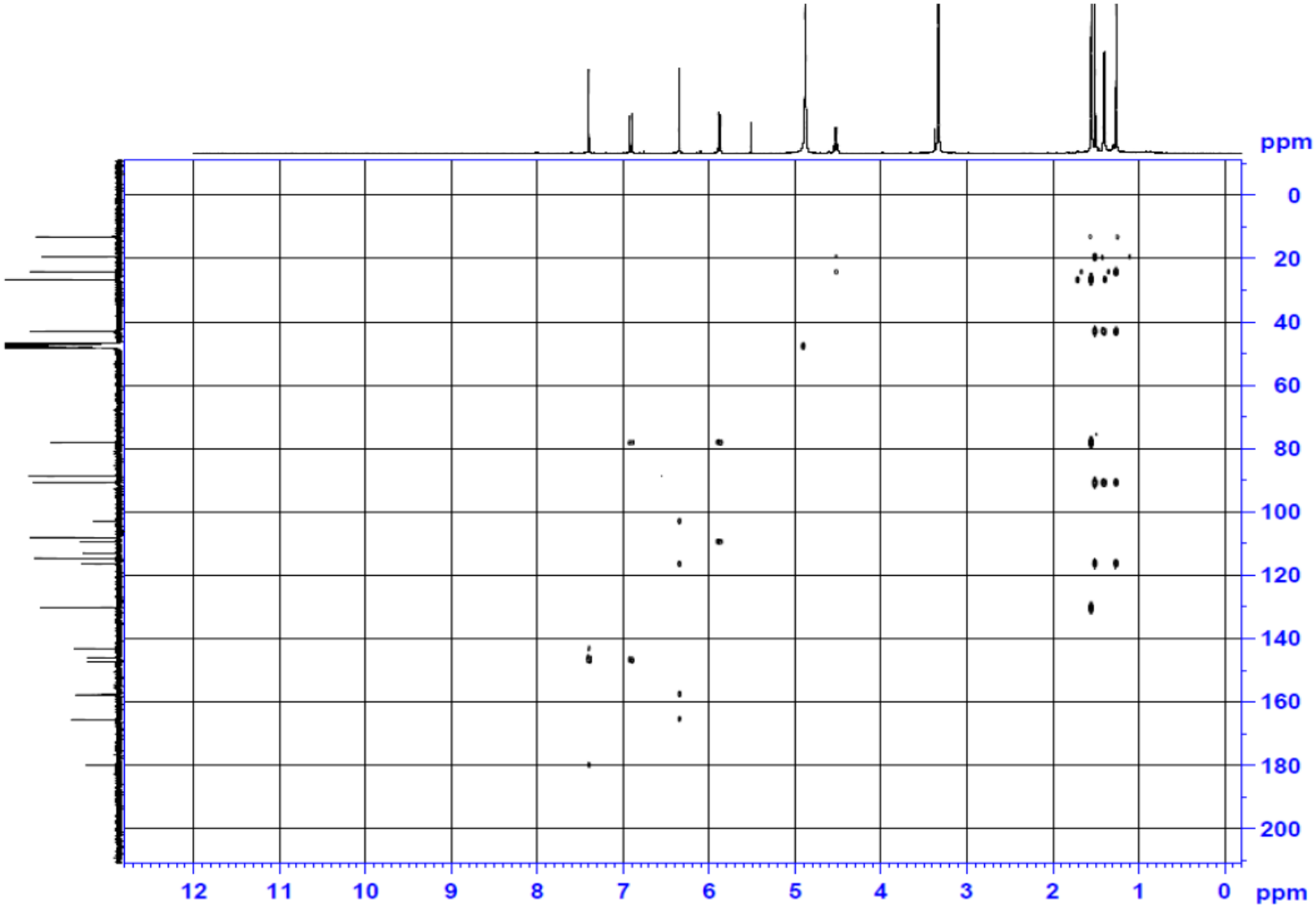
S6. ^{1}H-NMR spectrum of compound **2** (CD_3OD, 400 MHz)



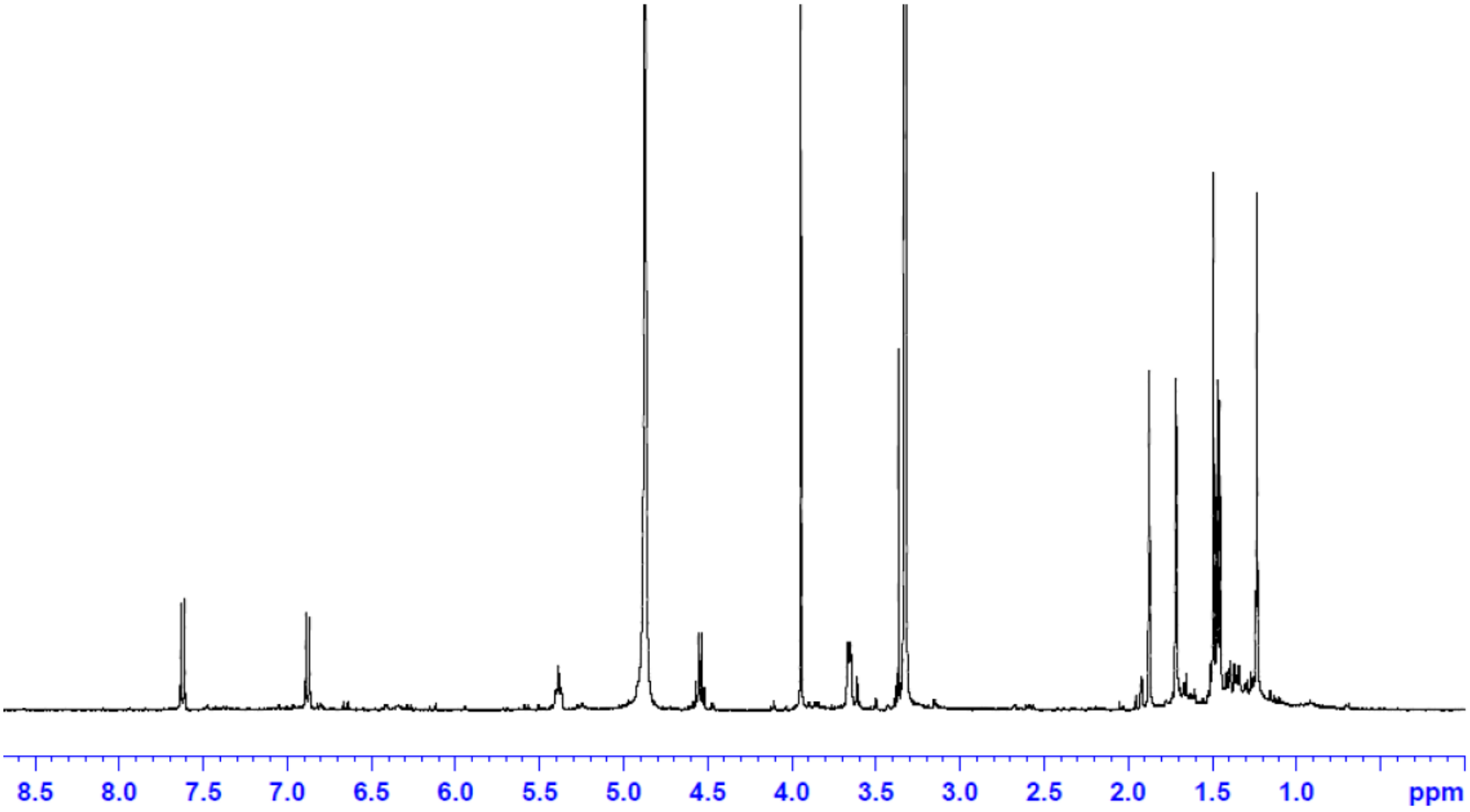
S7. ^{13}C-NMR spectrum of compound **2** (CD_3OD, 100 MHz)



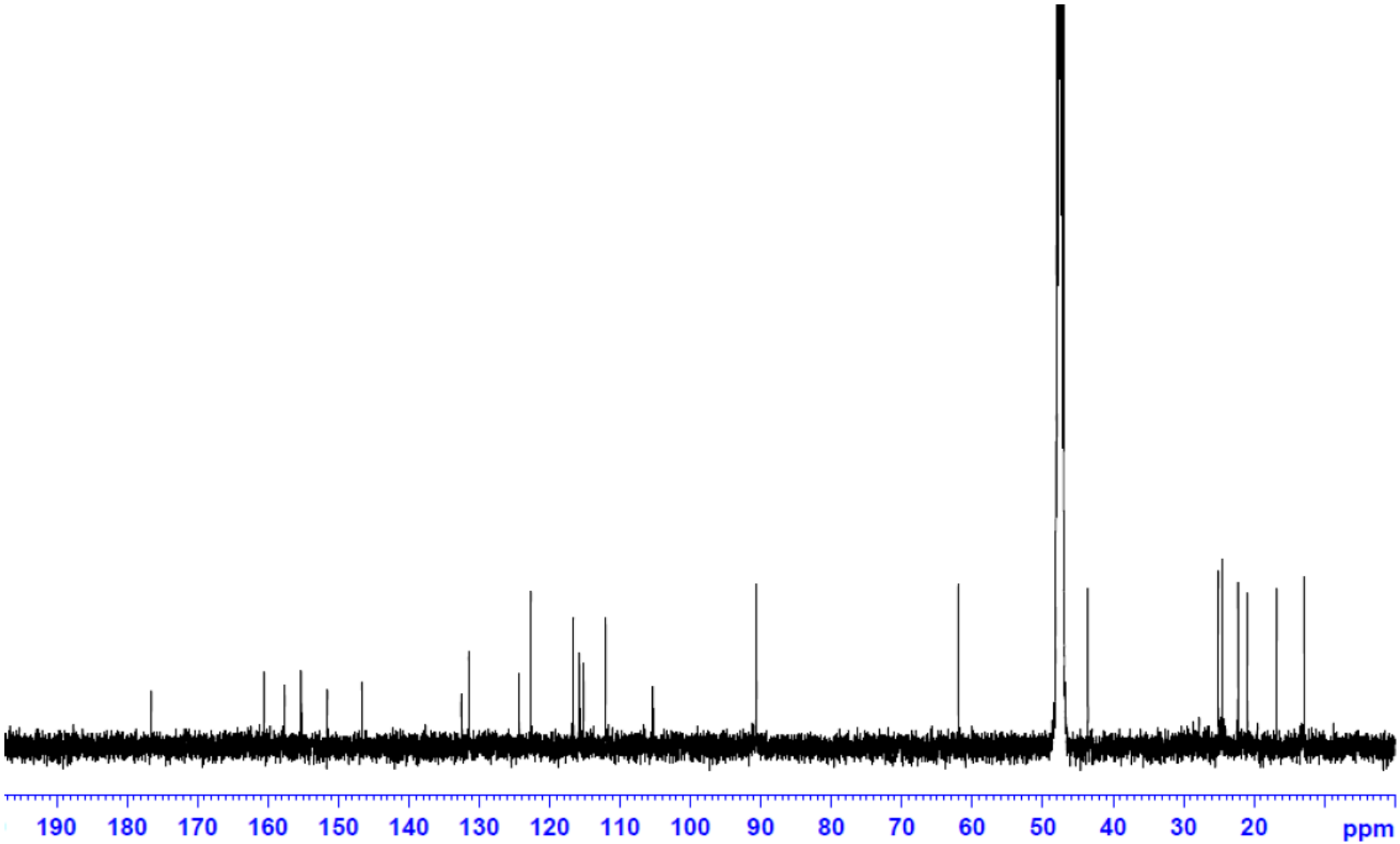
S8. HSQC spectrum of compound **2** (CD_3OD, 100 MHz)



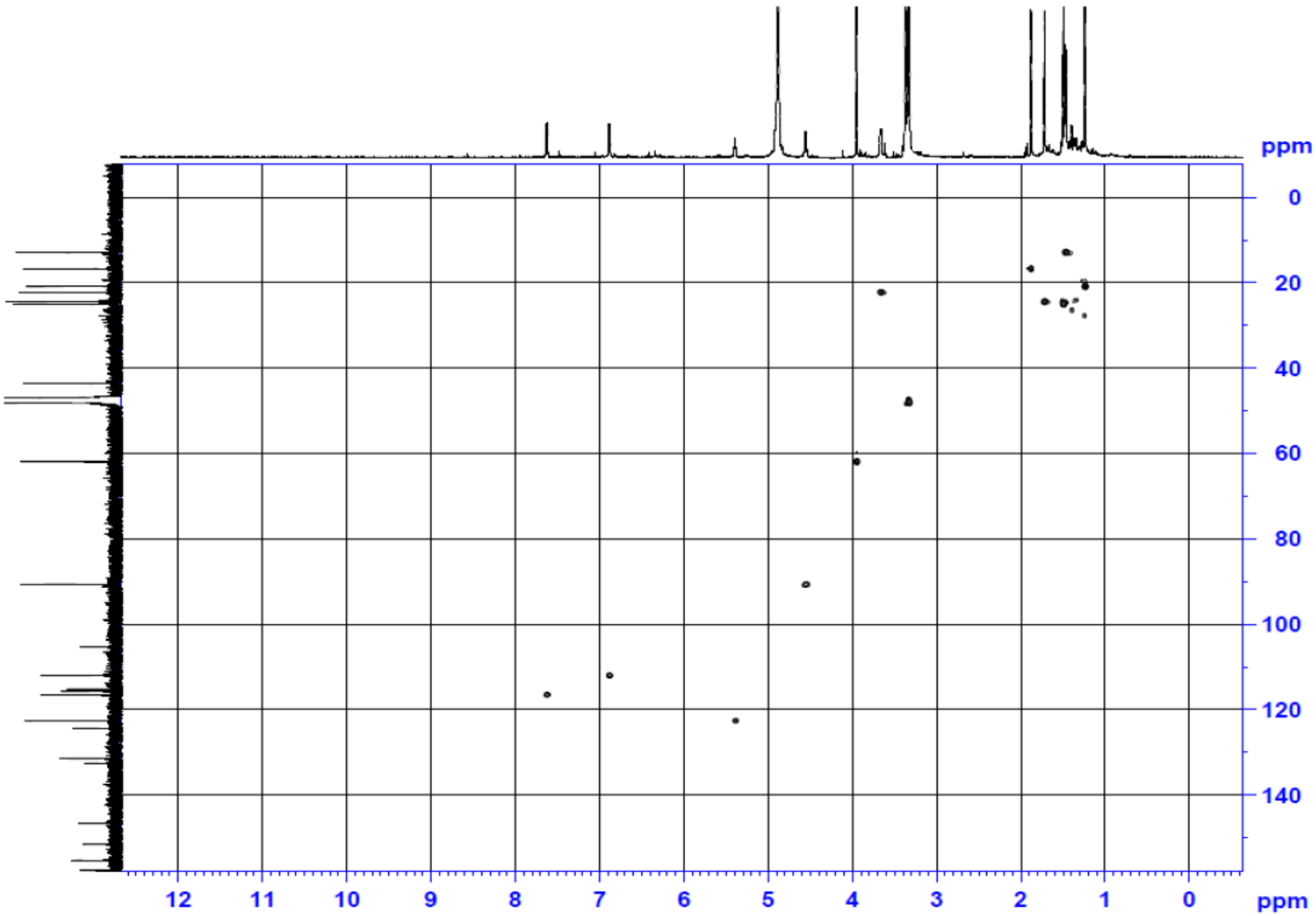
S9. HMBC spectrum of compound **2** (CD_3OD, 100 MHz)



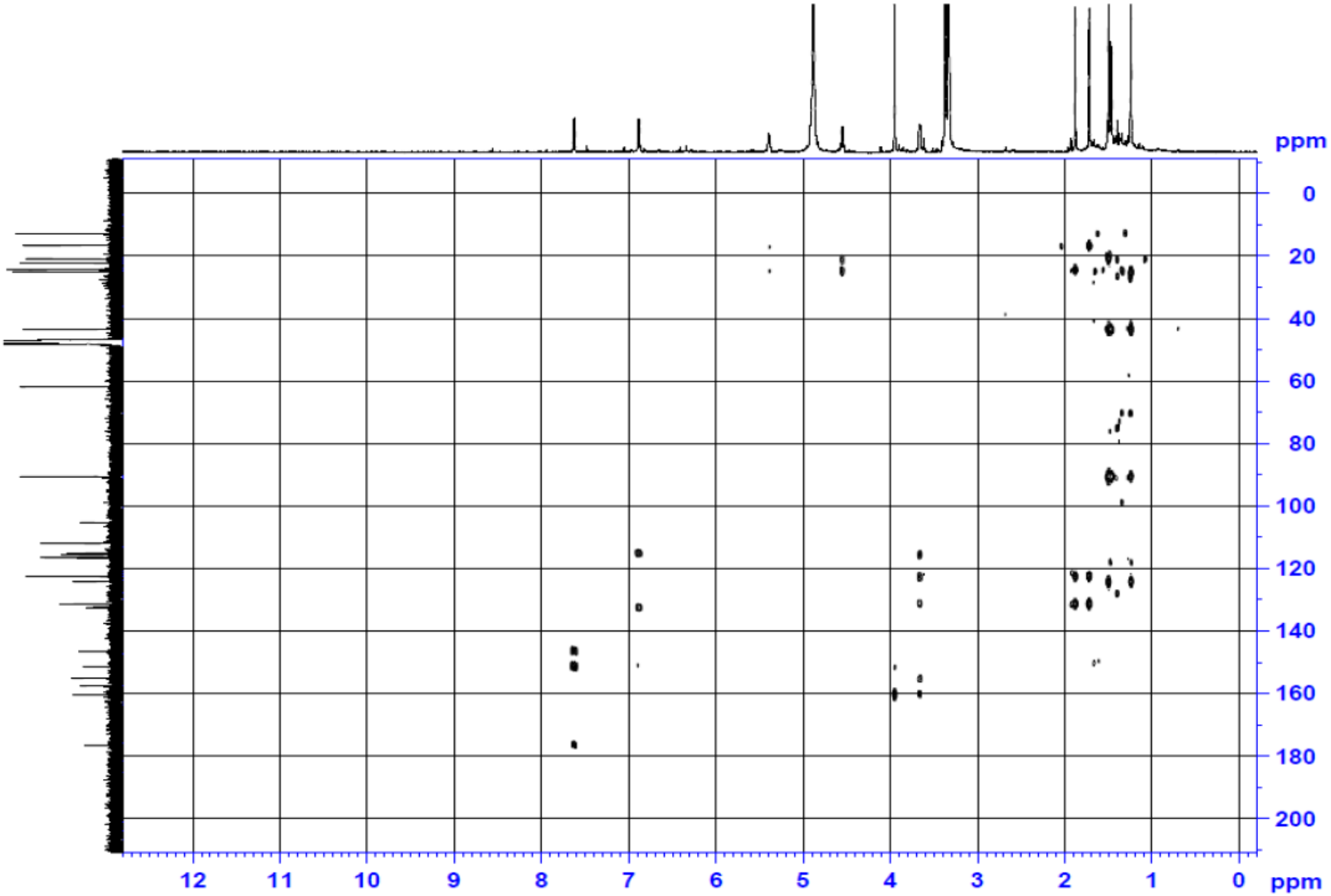
S10. ^{1}H-NMR spectrum of compound **3** (CD_3OD, 400 MHz)



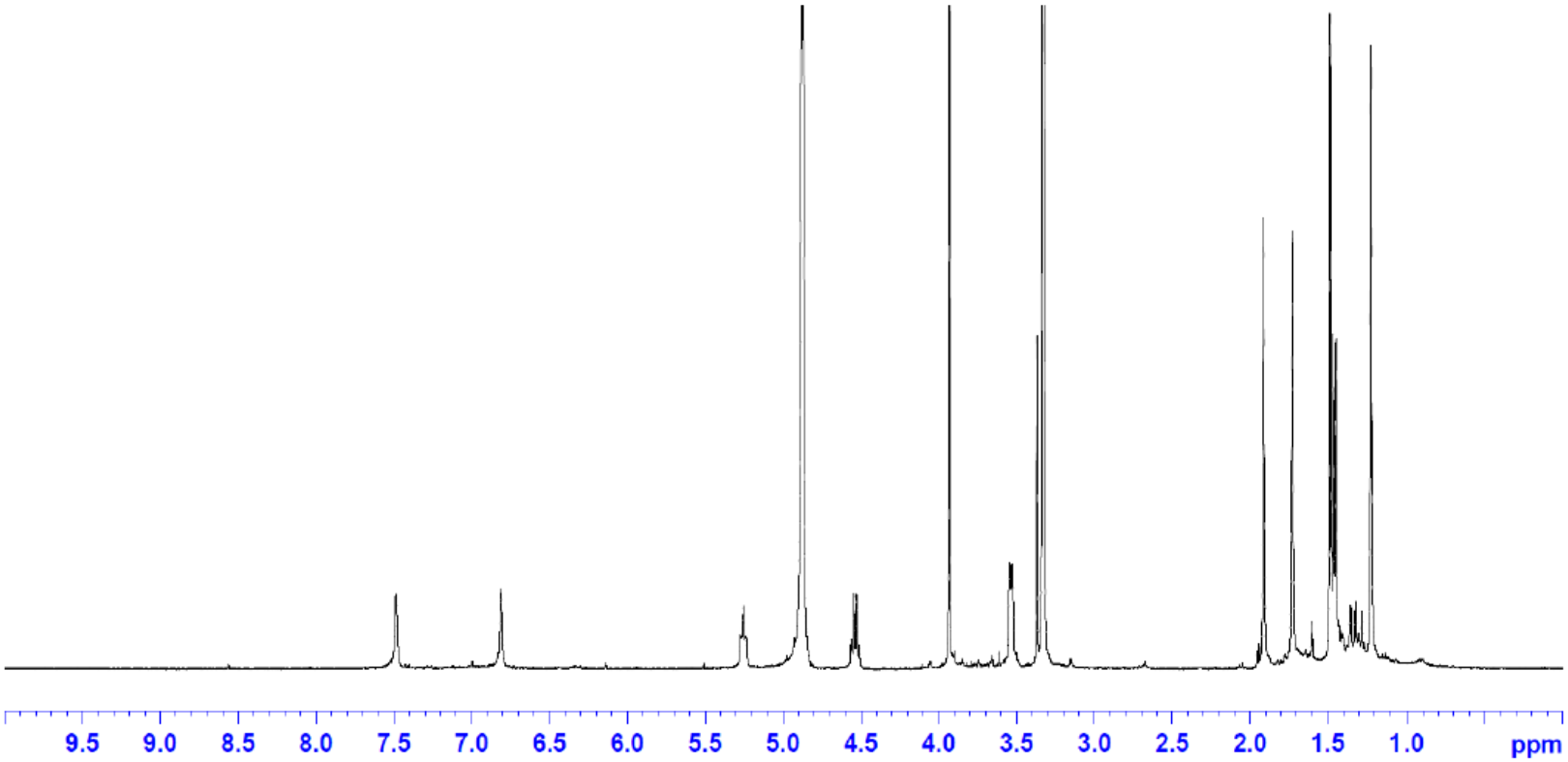
S11. ^{13}C-NMR spectrum of compound **3** (CD_3OD, 125 MHz)



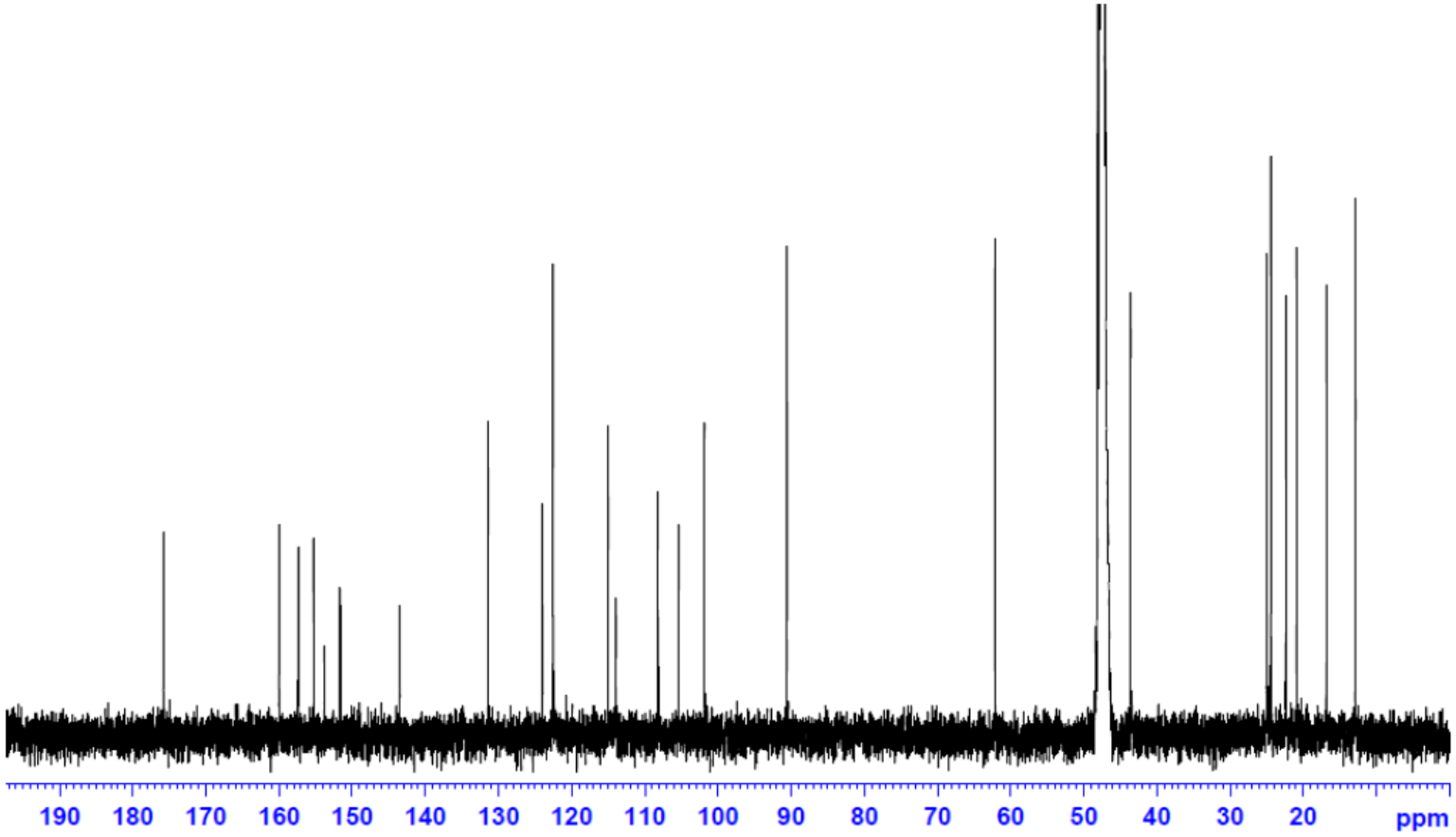
S12. HSQC spectrum of compound **3** (CD_3OD, 100 MHz)



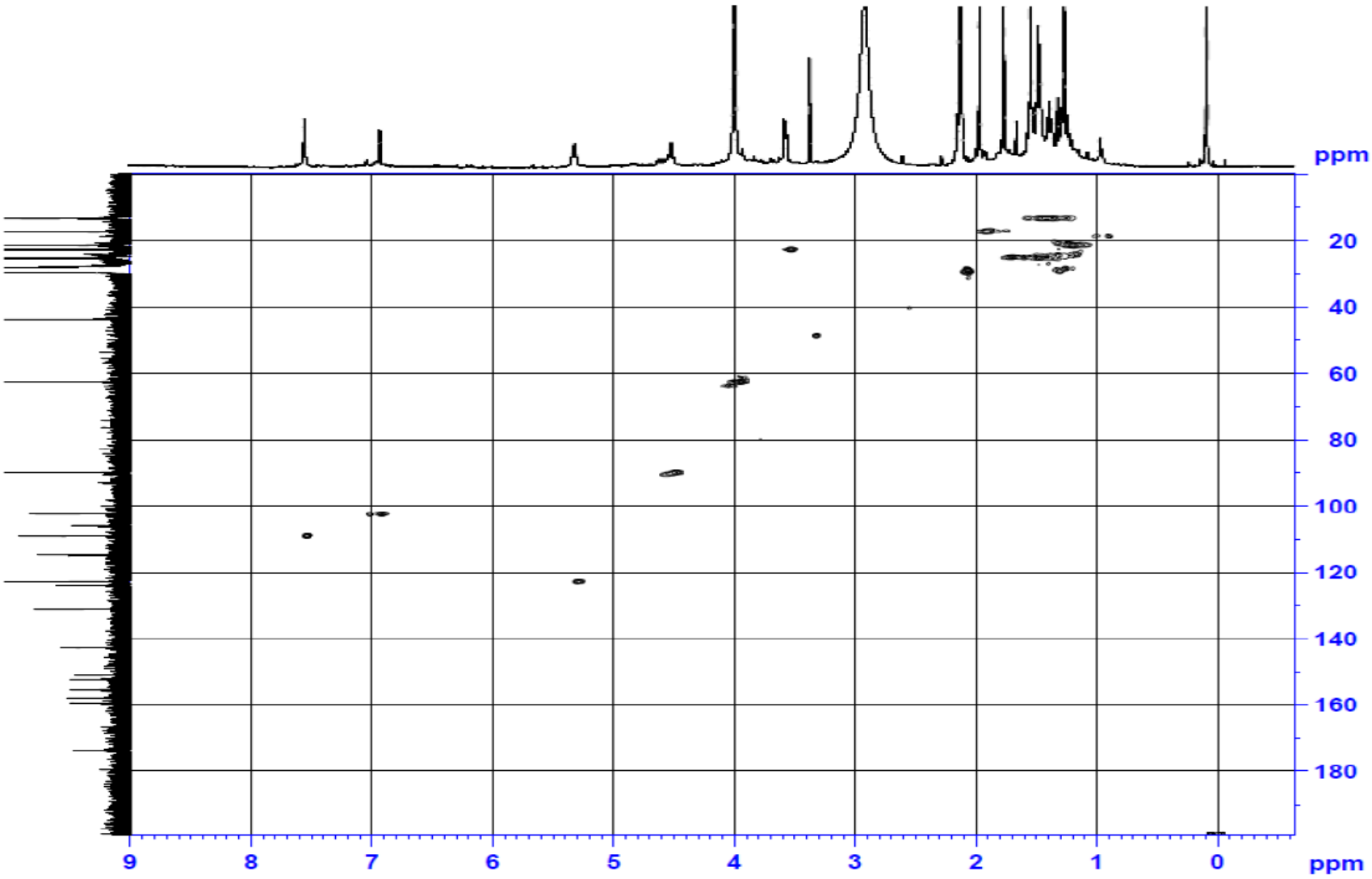
S13. HMBC spectrum of compound **3** (CD_3OD, 100 MHz)



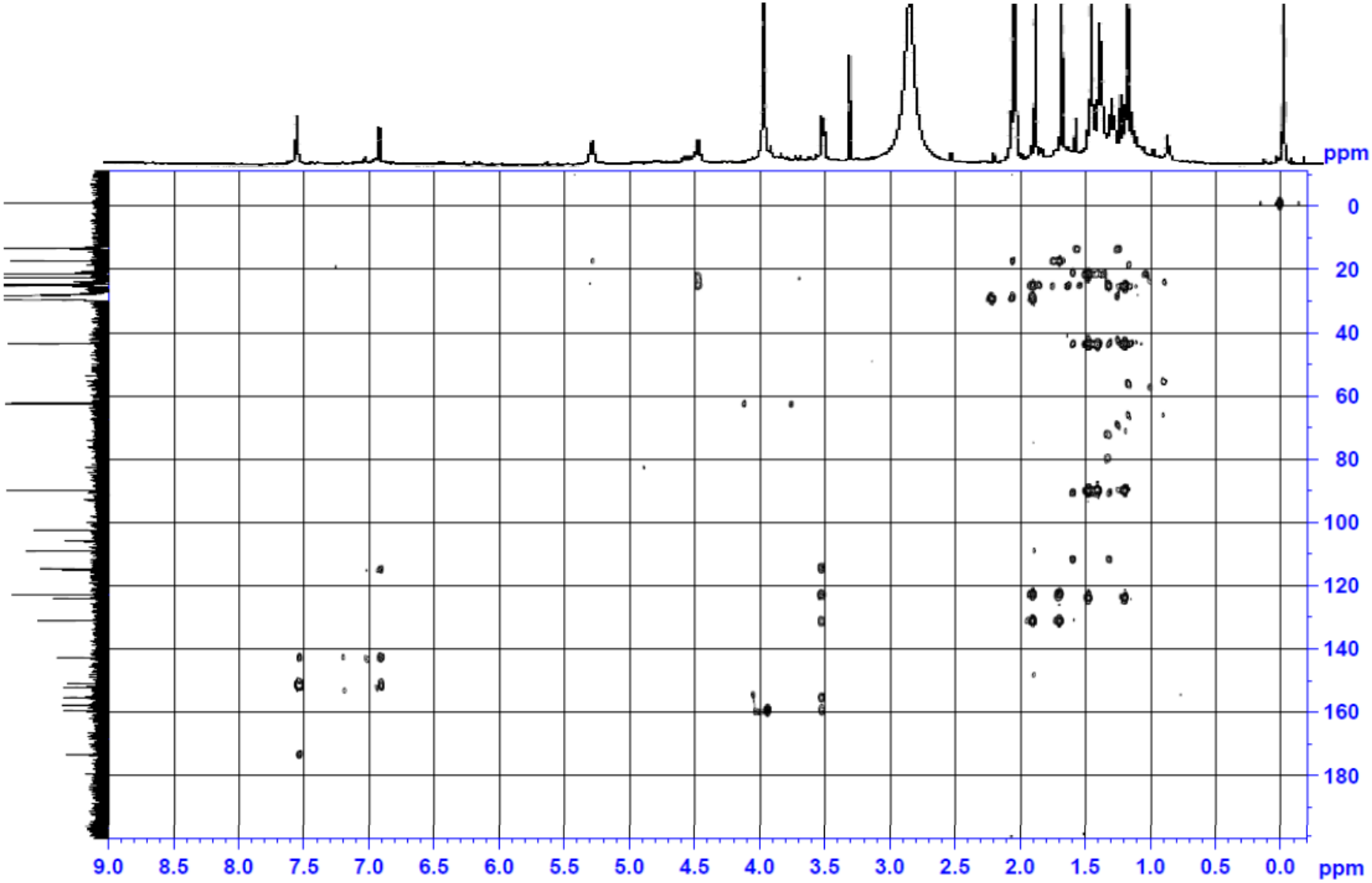
S14. ^{1}H-NMR spectrum of compound **4** (CD_3OD, 400 MHz)



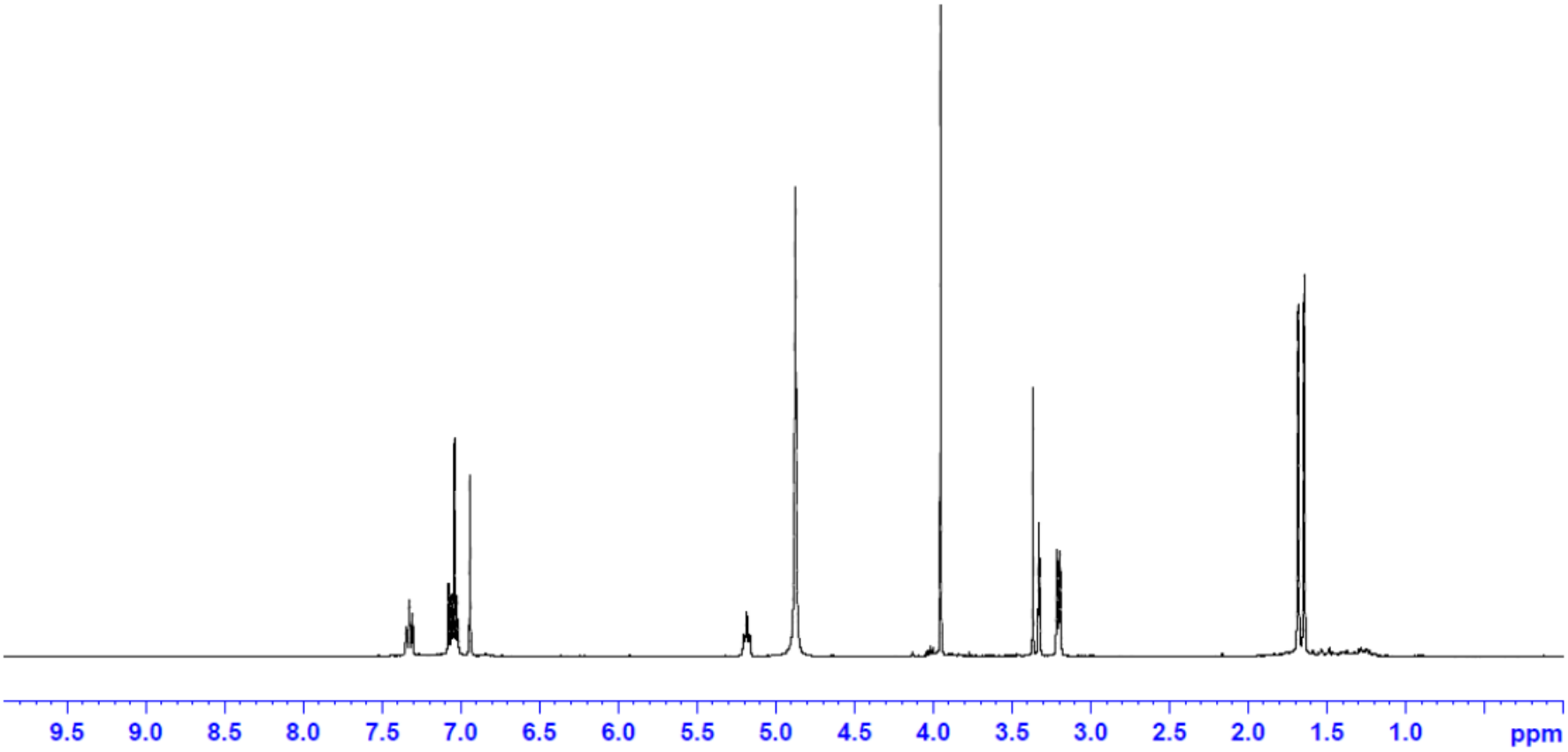
S15. ^{13}C-NMR spectrum of compound **4** (CD_3OD, 100 MHz)



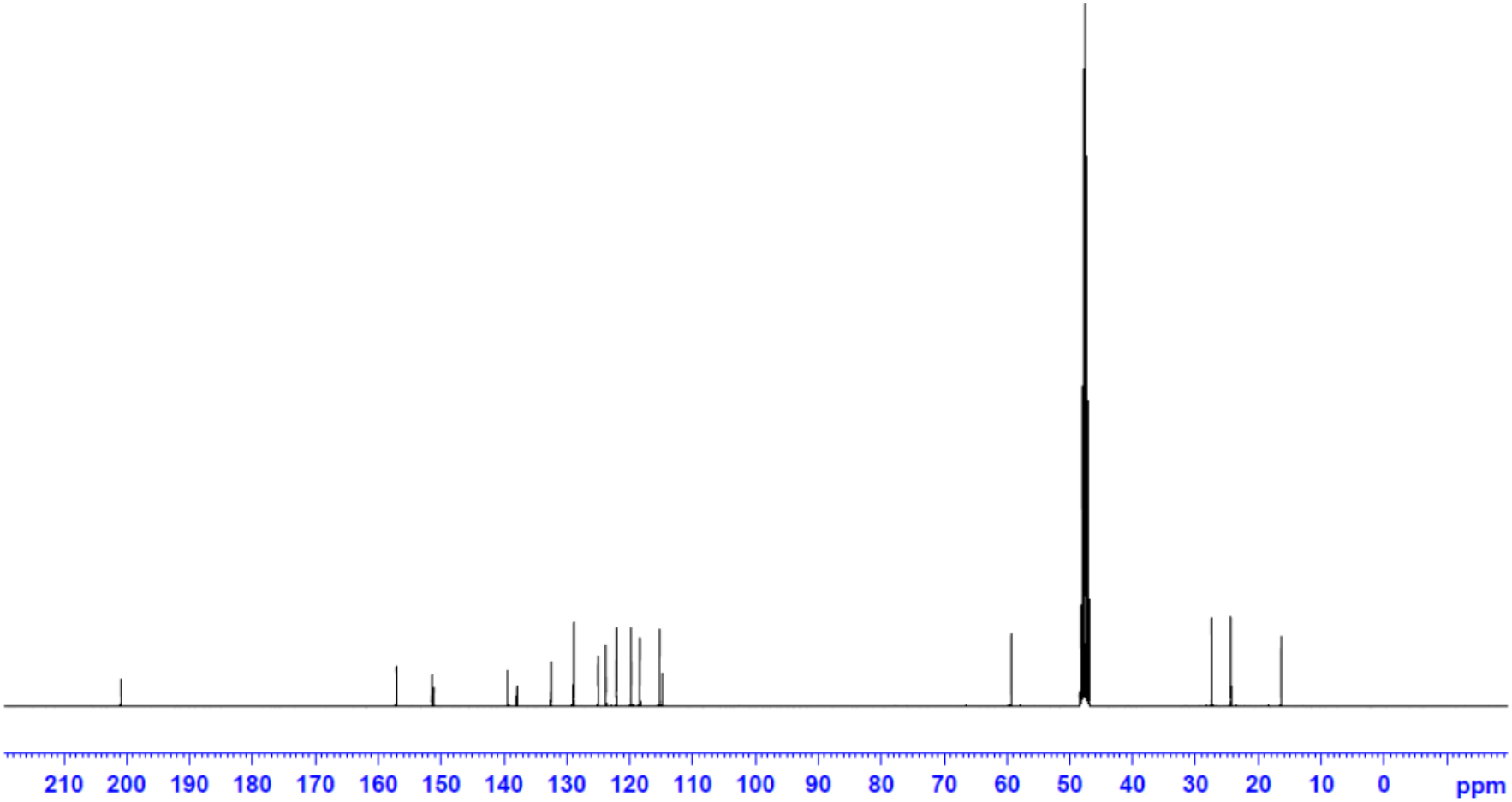
S16. HSQC spectrum of compound **4** (Acetone-d_6, 100 MHz)



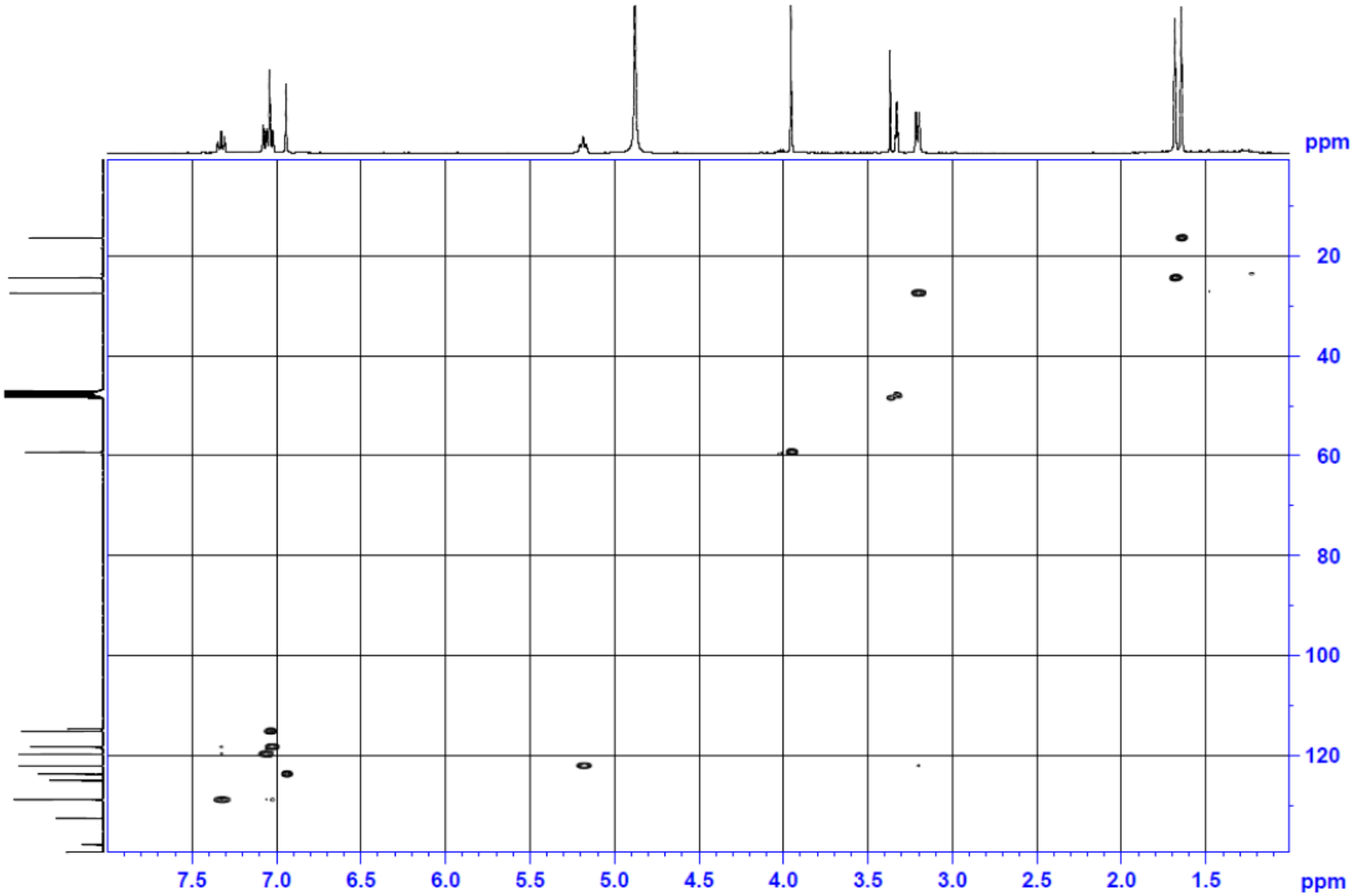
S17. HMBC spectrum of compound **4** (Acetone-d_6, 100 MHz)



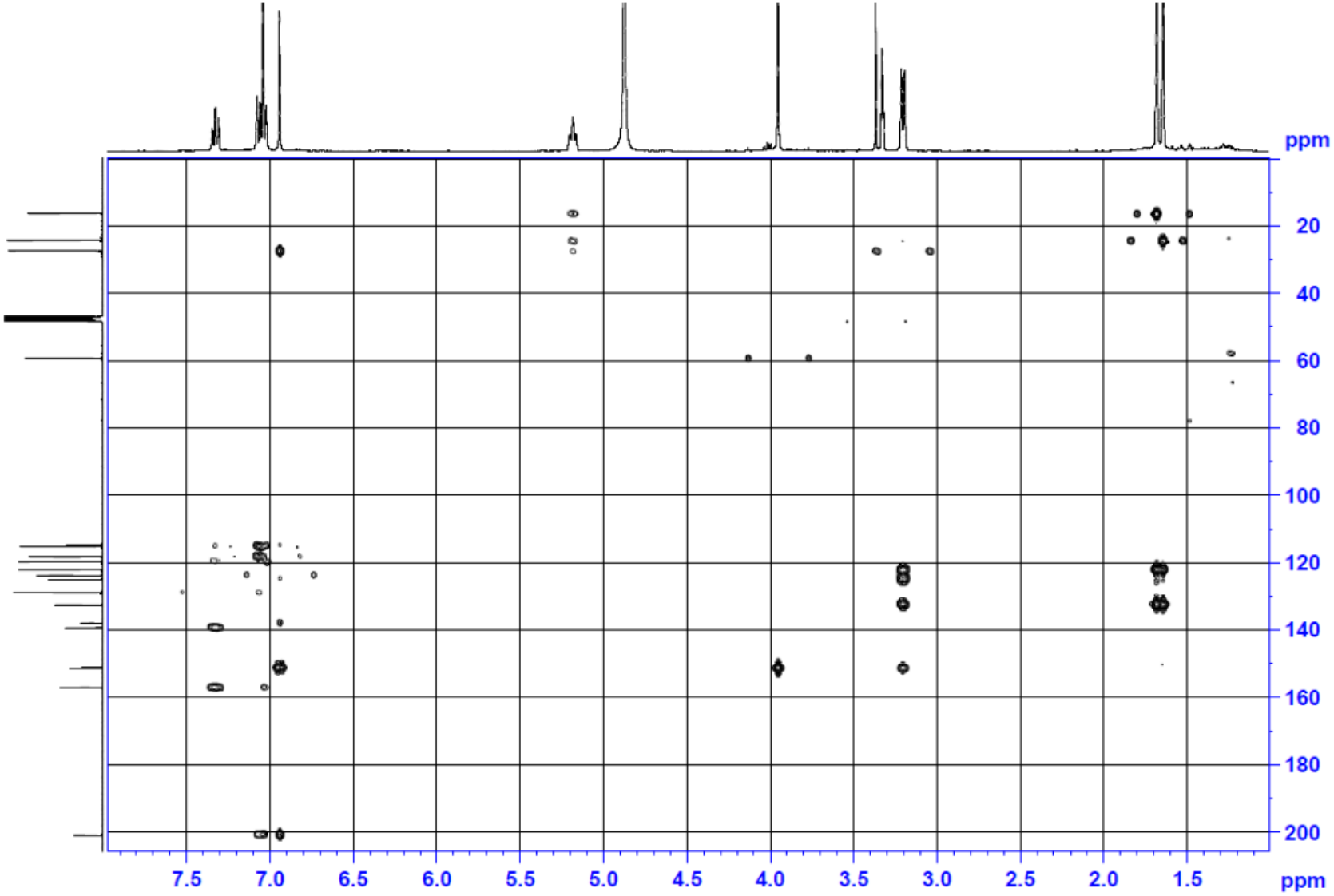
S18. ^{1}H-NMR spectrum of compound **5** (CD_3OD, 400 MHz)



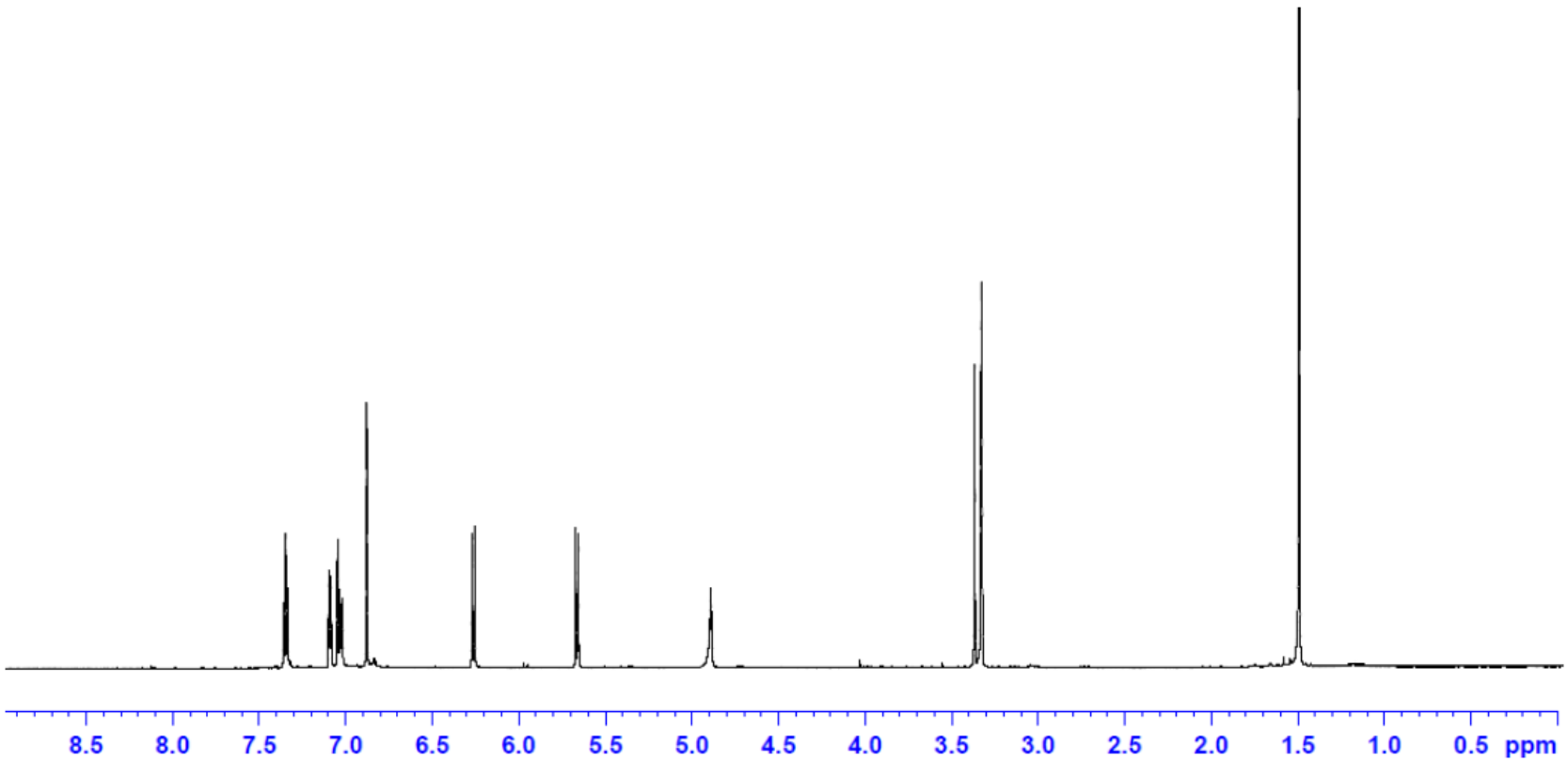
S19. ^{13}C-NMR spectrum of compound **5** (CD_3OD, 100 MHz)



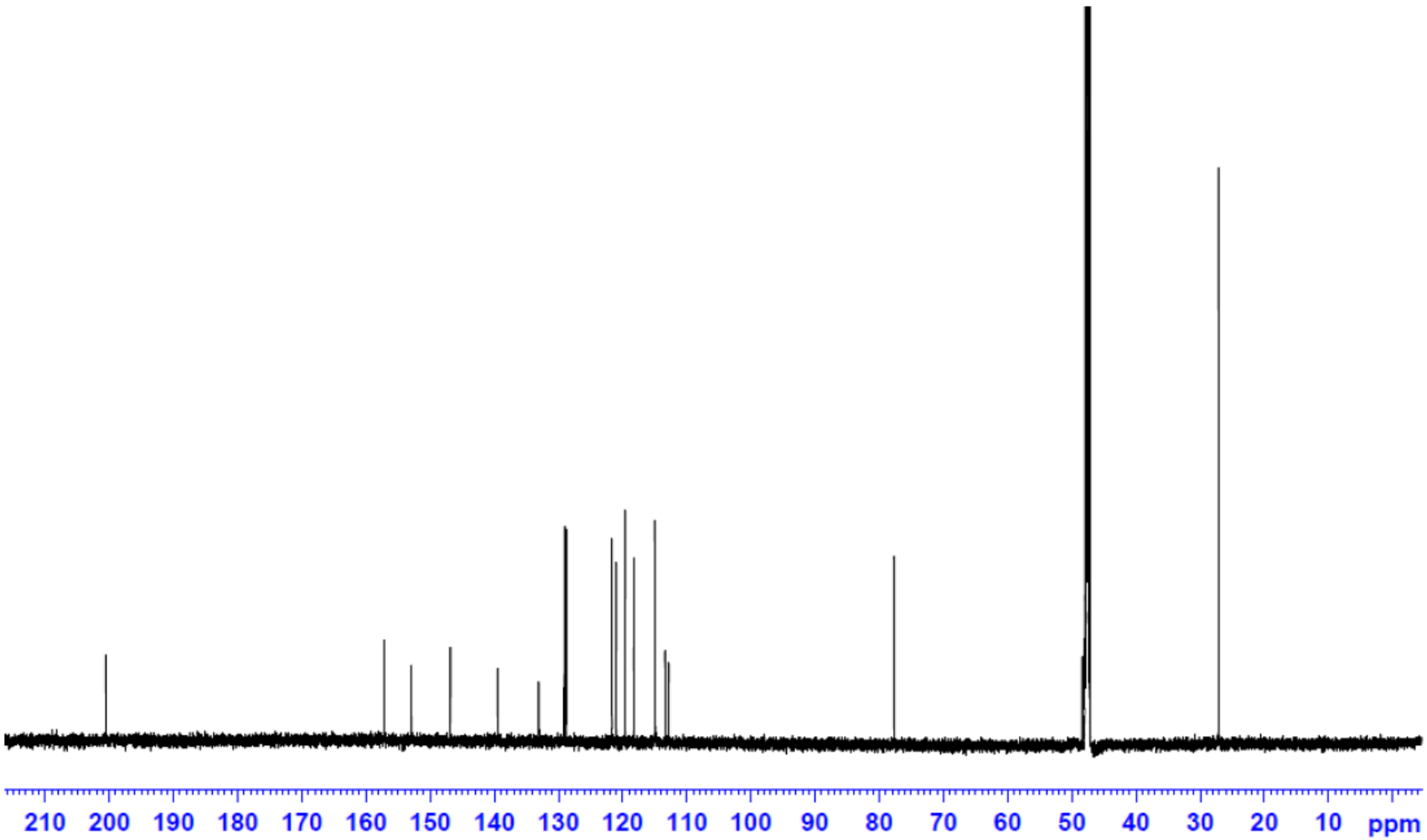
S20. HSQC spectrum of compound **5** (CD_3OD, 100 MHz)



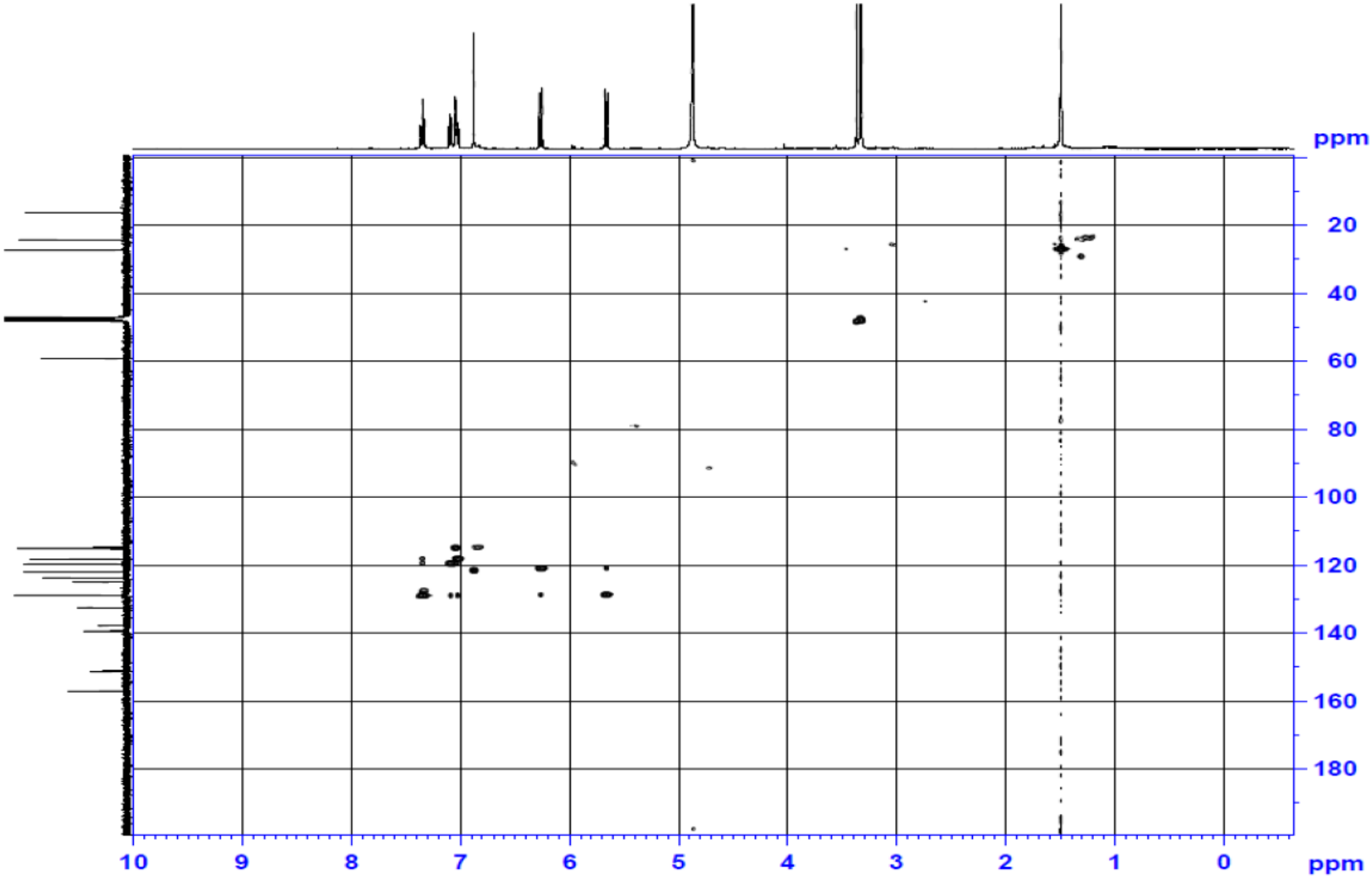
S21. HMBC spectrum of compound **5** (CD_3OD, 100 MHz)



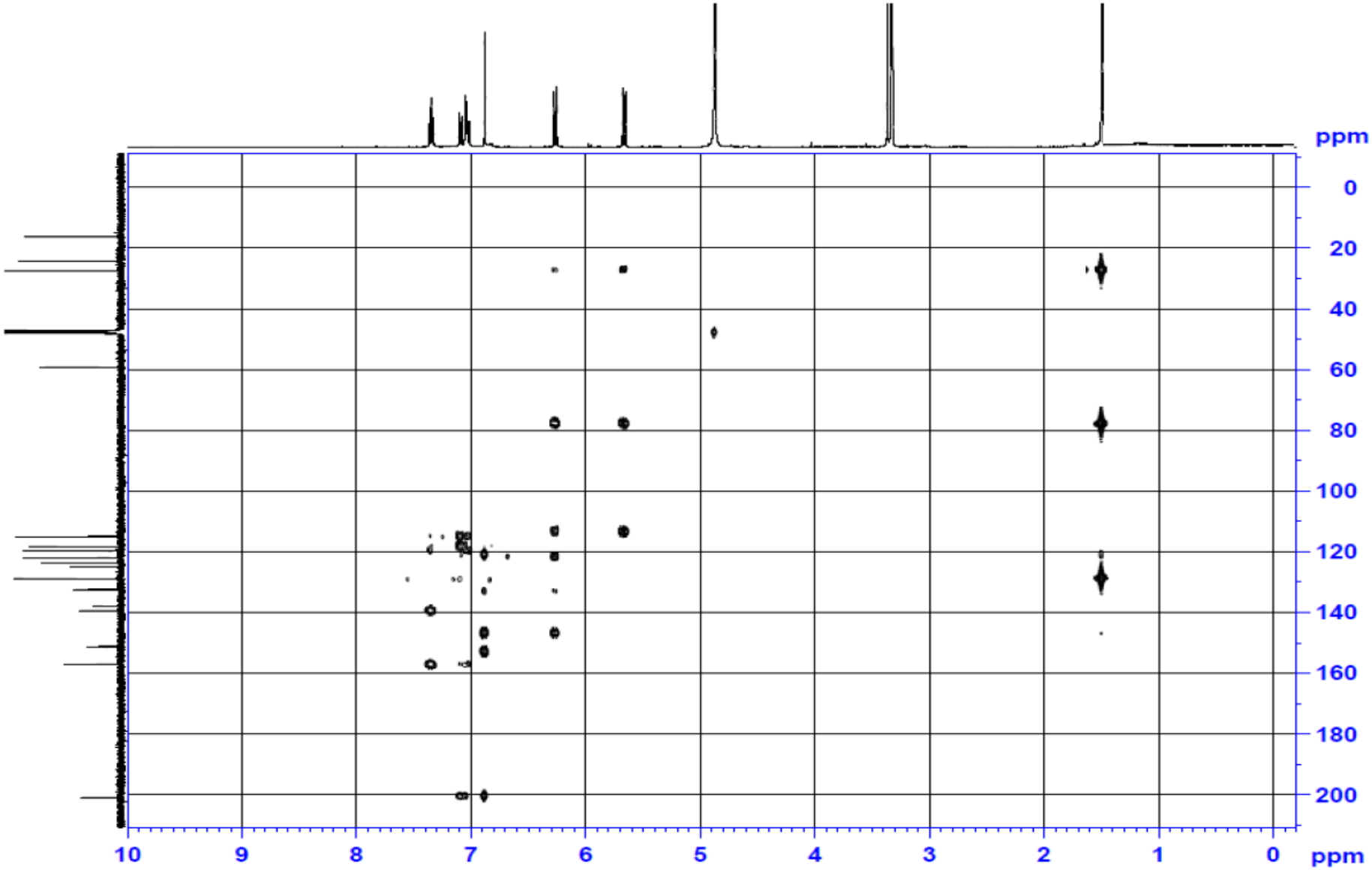
S22. ^{1}H-NMR spectrum of compound **6** (CD_3OD, 700 MHz)



S23. ^{13}C-NMR spectrum of compound **6** (CD_3OD, 175 MHz)



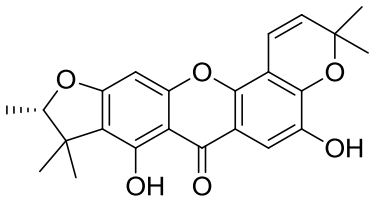
S24. HSQC spectrum of compound **6** (CD_3OD, 175 MHz)



S25. HMBC spectrum of compound **6** (CD_3OD, 175 MHz)

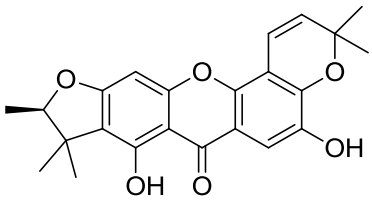
Optical Rotations

Compound **2** (14*S*)



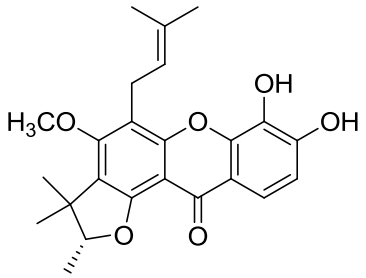
Frequency:	0.7722602145762712E-01	
Frequency / eV:	2.101427864516412	
Frequency / nm:	590.0000000000000	
Frequency / cm^(-1):	16949.15253984299	
1/3*trace:	313.0550069999875	(dipole polarizability)
1/3*trace:	-0.8072258753087465	(rotatory dispersion)
specific rotation [alpha] in deg*[dm(g/cc)]^(-1)	-78.95854378028110	

Compound **2**_enantiomer (14*R*)



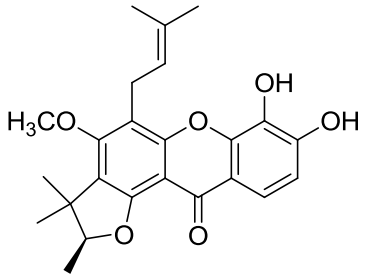
Frequency:	0.7722602145762712E-01	
Frequency / eV:	2.101427864516412	
Frequency / nm:	590.0000000000000	
Frequency / cm^(-1):	16949.15253984299	
1/3*trace:	314.9800375626319	(dipole polarizability)
1/3*trace:	0.9525011236660188	(rotatory dispersion)
specific rotation [alpha] in deg*[dm(g/cc)]^(-1)	93.16859626803318	

Compound **3** (14*R*)



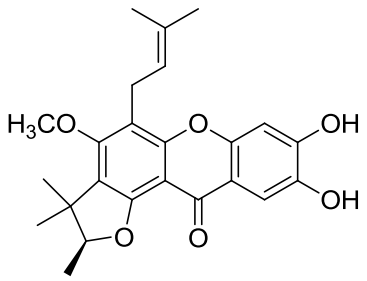
Frequency:		0.7722602145762712E-01
Frequency / eV:		2.101427864516412
Frequency / nm:		590.0000000000000
Frequency / cm^(-1):		16949.15253984299
1/3*trace:	310.3356209521055	(dipole polarizability)
1/3*trace:	-2.207448579294767	(rotatory dispersion)
specific rotation [alpha] in deg*[dm(g/cc)]^(-1)		-207.4817420928886

Compound **3**_enantiomer (14*S*)



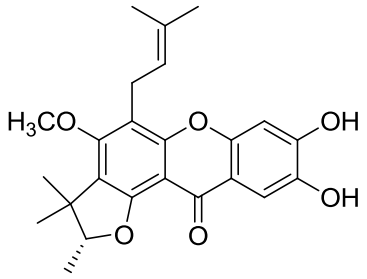
Frequency:		0.7722602145762712E-01
Frequency / eV:		2.101427864516412
Frequency / nm:		590.0000000000000
Frequency / cm^(-1):		16949.15253984299
1/3*trace:	312.0317236550798	(dipole polarizability)
1/3*trace:	1.581090651628422	(rotatory dispersion)
specific rotation [alpha] in deg*[dm(g/cc)]^(-1)		148.6093247578386

Compound **4** (14*S*)



Frequency:		0.7722602145762712E-01
Frequency / eV:		2.101427864516412
Frequency / nm:		590.0000000000000
Frequency / cm^(-1):		16949.15253984299
1/3*trace:	315.3679800552995	(dipole polarizability)
1/3*trace:	1.023197870090321	(rotatory dispersion)
specific rotation [alpha] in deg*[dm(g/cc)]^(-1)		96.17205971787421

Compound **4**_enantiomer (14*R*)



Frequency:		0.7722602145762712E-01
Frequency / eV:		2.101427864516412
Frequency / nm:		590.0000000000000
Frequency / cm^(-1):		16949.15253984299
1/3*trace:	314.3718018572110	(dipole polarizability)
1/3*trace:	-0.9810681426525202	(rotatory dispersion)
specific rotation [alpha] in deg*[dm(g/cc)]^(-1)		-92.21221697241549

Calculated ECDs and CD spectra

Computational analysis. The ground-state geometries were optimized with density functional theory (DFT) calculations, using Turbomole 6.5 at the basis set def-SV(P) for all atoms and functional B3LYP/DFT level, the ground states were further confirmed by the harmonic frequency calculation. The calculated ECD data corresponding to the optimized structures were obtained with TDDFT at the functional B3LYP/DFT level at the basis set def2-TZVPP for all atoms. The CD spectra were simulated by overlapping for each transition, where σ is the width of the band at 1/e height. ΔEi and Ri are the excitation energies and rotatory strengths for transition i, respectively. In the current work a value of σ was 0.10 eV.

$$\Delta\epsilon(E) = \frac{1}{2.297 \times 10^{-39}} \frac{1}{\sqrt{2\pi\sigma}} \sum_{i}^{A} \Delta E_i R_i e^{[-(E-\Delta E_i)^2/(2\sigma)^2]}$$

Compound **2**

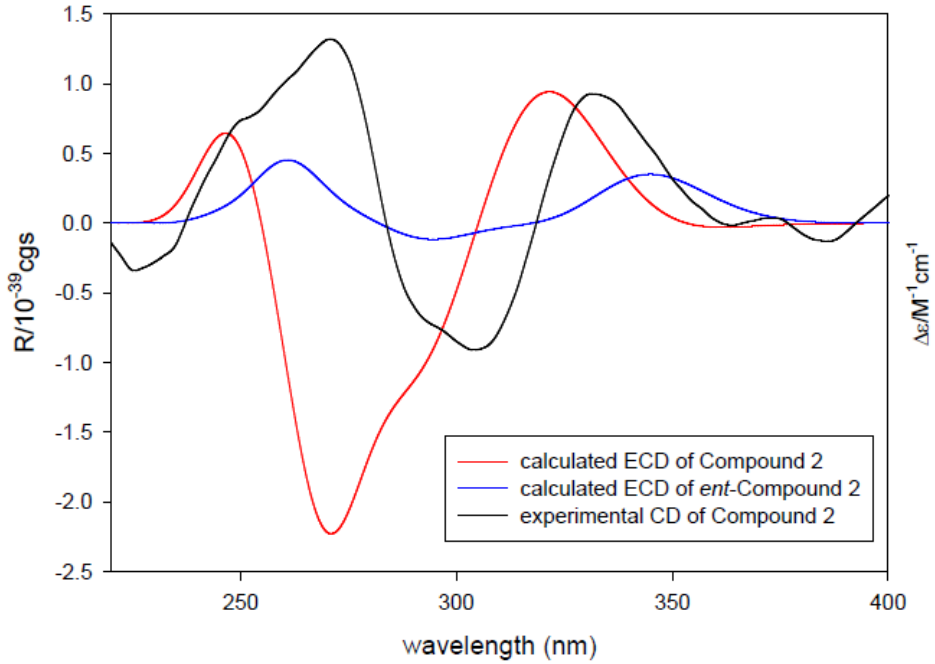
total energy = -1339.23308144284
kinetic energy = 1327.18577061588
potential energy .= -2666.41885205872

Parameters of Level DFT
DFT settings (Functional B3-LYP / Gridsize M3)
Geometry optimization options (Energy 10^{-6} Hartree, Gradient norm $|dE / dxyz| = 10^{-3}$ Hartree/Bohr)

Energy minimized coordinates of Compound 2 at the basis set def-SV(P) for all atoms (Å).

Atom	X	Y	Z
C	-3.2904	1.097	0.0935
C	-3.4031	0.3909	1.3015
C	-2.2499	0.0114	1.9876
C	-0.9635	0.3849	1.4831
C	-2.0734	1.4754	-0.4522
C	-0.9252	1.1073	0.2631
O	0.2448	1.5064	-0.303
C	1.4425	1.2378	0.29
C	1.5207	0.5396	1.4959
C	0.2997	0.0516	2.1828
C	2.7898	0.3058	2.0621
C	2.5996	1.7045	-0.3675

C	3.8521	1.4465	0.2134
C	3.9512	0.7507	1.4472
C	2.578	2.4995	-1.592
C	3.7256	2.7822	-2.2303
C	5.0532	2.2274	-1.7543
O	4.9948	1.8995	-0.3374
C	5.4102	0.9421	-2.5205
H	4.6285	0.1764	-2.3746
H	6.3727	0.5377	-2.1593
H	5.4929	1.1456	-3.6034
C	6.1688	3.2698	-1.8668
H	5.905	4.1777	-1.2978
H	6.3319	3.5484	-2.923
H	7.1102	2.8632	-1.4588
C	-4.878	0.0434	1.5149
C	-5.5137	1.0619	0.5023
O	-4.4889	1.3493	-0.4773
C	-6.7873	0.6625	-0.2192
H	-5.6895	2.0079	1.0522
H	-7.1111	1.4822	-0.8836
H	-7.5986	0.4694	0.5046
H	-6.6397	-0.2391	-0.8362
C	-5.1323	-1.431	1.1282
H	-4.8336	-1.631	0.0851
H	-6.1963	-1.7056	1.2458
H	-4.5371	-2.1023	1.773
C	-5.4253	0.3228	2.9285
H	-5.118	1.3182	3.2933
H	-5.0949	-0.4304	3.6699
H	-6.5307	0.2811	2.9307
O	0.3735	-0.5647	3.237
O	-2.3064	-0.7097	3.1285
H	-3.235	-0.8395	3.3805
O	5.1996	0.559	1.9521
H	5.1274	0.0868	2.7987
H	-1.9958	2.0321	-1.386
H	2.8208	-0.2458	3.0071
H	1.6162	2.8678	-1.9572
H	3.7349	3.391	-3.1409



S26. Experimental CD spectra of Compound **2** (black), calculated ECD spectra of 1 (red), and *ent*-1 (blue)

Compound **3**

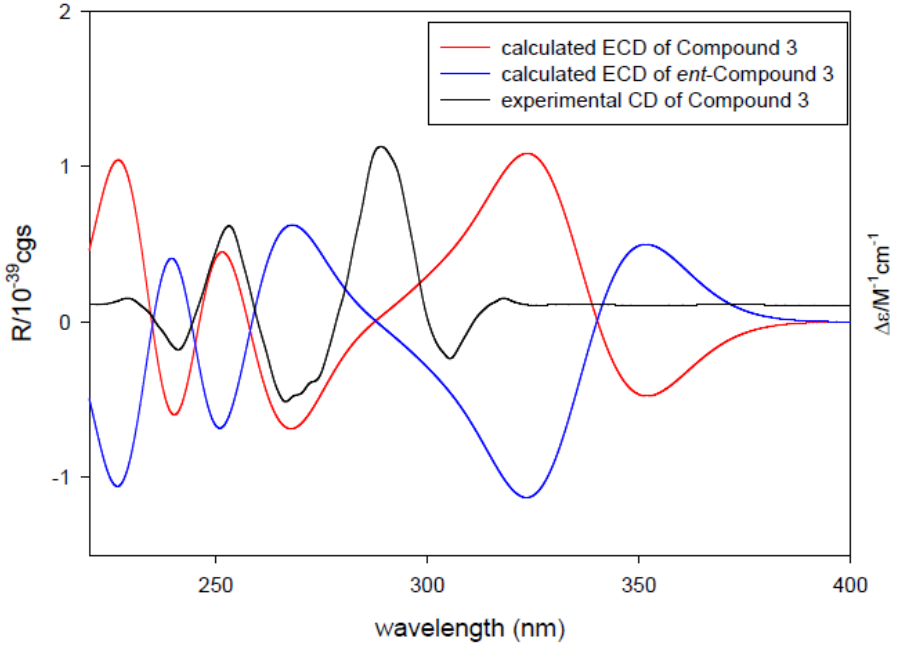
total energy = -1379.65975149120
kinetic energy = 1367.07877719219
potential energy .= -2746.73852868339

Parameters of Level DFT
DFT settings (Functional B3-LYP / Gridsize M3)
Geometry optimization options (Energy 10^{-6} Hartree, Gradient norm $\left| dE / dxyz \right| = 10^{-3}$ Hartree/Bohr)

Energy minimized coordinates of Compound 3 at the basis set def-SV(P) for all atoms (Å).

Atom	X	Y	Z
C	-8.3784	4.1787	0.181
C	-8.3514	2.7902	0.4454
C	-7.0936	2.1613	0.4848
C	-5.8677	2.8257	0.2347
C	-7.1998	4.8725	-0.1168
C	-5.9766	4.1923	-0.0943
C	-4.5701	2.1064	0.2911
O	-7.1153	0.8227	0.7747
C	-5.9554	0.1035	0.8368
C	-4.6906	0.6668	0.6136
C	-3.559	-0.1644	0.7074
C	-6.1011	-1.2535	1.1455
C	-4.9611	-2.0656	1.2366
C	-3.6871	-1.5135	1.0144
C	-6.925	6.3414	-0.4466
C	-5.4686	6.1882	-1.01
O	-4.9353	4.9793	-0.4186
C	-7.8552	6.933	-1.5185
H	-7.8672	6.3055	-2.427
H	-7.5195	7.9474	-1.806
H	-8.8905	7.0037	-1.1476
C	-6.9686	7.2084	0.8309
H	-6.2949	6.8163	1.6127
H	-7.9909	7.2322	1.2435
H	-6.676	8.2517	0.6141
C	-4.4756	7.3143	-0.7936
H	-5.5527	5.9836	-2.0955
H	-3.5091	7.0482	-1.2551
H	-4.2997	7.5022	0.2783
H	-4.8379	8.2452	-1.2646
O	-9.5814	4.8447	0.1469
C	-10.1437	5.2219	1.3953
H	-10.3534	4.3466	2.0394
H	-11.0918	5.7365	1.1699

H	-9.4785	5.9104	1.9491
O	-3.49	2.6412	0.0944
O	-5.0931	-3.3778	1.5374
H	-6.0423	-3.5725	1.6532
O	-7.3125	-1.8436	1.3785
H	-8.0224	-1.1898	1.2526
C	-9.6266	1.9713	0.5688
C	-9.9641	1.2446	-0.7166
H	-10.4623	2.6503	0.8018
H	-9.5422	1.2711	1.415
C	-10.31	-0.0436	-0.8942
H	-9.9285	1.8863	-1.6076
C	-10.4276	-1.0674	0.2099
H	-10.2214	-0.6579	1.2133
H	-9.7467	-1.9227	0.0287
H	-11.4493	-1.4943	0.2413
C	-10.6221	-0.5793	-2.2725
H	-10.5219	0.1973	-3.0498
H	-11.6531	-0.9831	-2.3208
H	-9.9456	-1.4167	-2.5363
H	-2.8179	-2.1714	1.0919
H	-2.5816	0.291	0.5313



S27. Experimental CD spectra of Compound **3** (black), calculated ECD spectra of 1 (red), and *ent*-1 (blue)

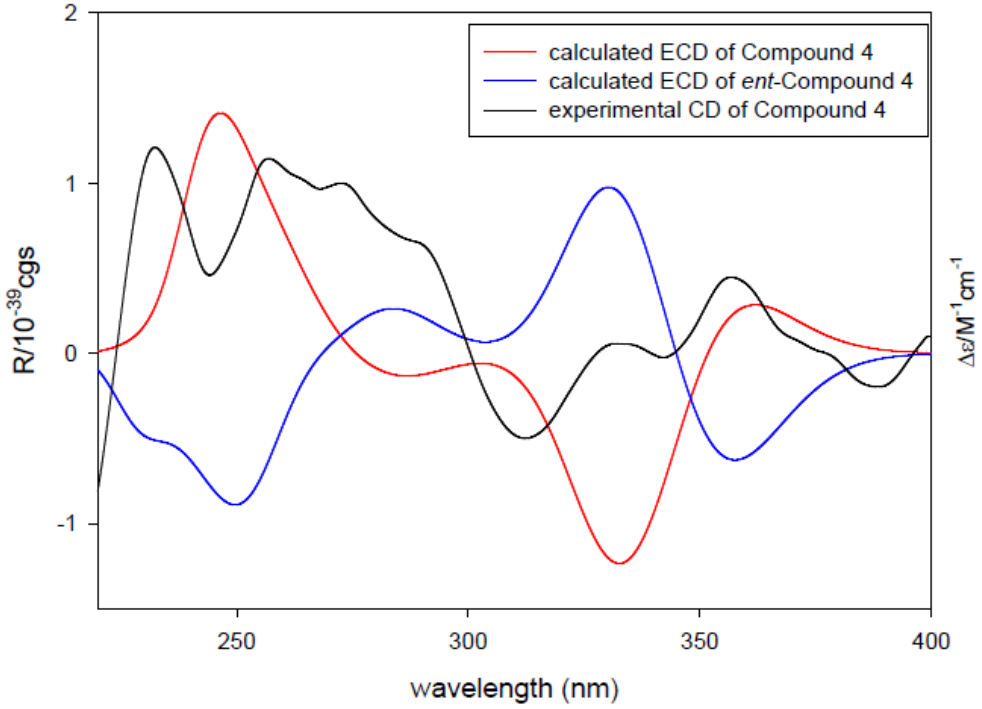
Compound **4**
total energy = -1379.65188980715
kinetic energy = 1367.10638886374
potential energy .= -2746.75827867089

Parameters of Level DFT
DFT settings (Functional B3-LYP / Gridsize M3)
Geometry optimization options (Energy 10^{-6} Hartree, Gradient norm $\left| dE / dxyz \right| = 10^{-3}$ Hartree/Bohr)

Energy minimized coordinates of Compound 4 at the basis set def-SV(P) for all atoms (Å).

Atom	X	Y	Z
C	-4.8252	3.5258	0.4445
C	-6.0767	2.922	0.1904
C	-6.1949	1.5312	0.0957
C	-5.078	0.7231	0.315
C	-3.7254	2.6683	0.6558
C	-3.8048	1.2523	0.6126
C	-2.6121	0.4093	0.8472
O	-2.533	3.2908	0.8966
C	-1.393	2.5772	1.1077
C	-1.3745	1.1805	1.0962
C	-0.1496	0.5202	1.325
C	-0.2187	3.3096	1.3425
C	0.9847	2.6454	1.5669
C	1.0224	1.2208	1.558
C	-4.6243	5.0343	0.3801
C	-4.7391	5.572	-1.0303
H	-3.6492	5.2806	0.8179
H	-5.373	5.5402	1.0154
C	-3.804	6.2172	-1.7525
C	-2.4069	6.5368	-1.276
H	-2.2427	7.6326	-1.2492
H	-1.6559	6.127	-1.9796
H	-2.182	6.1338	-0.2763
C	-4.1047	6.6863	-3.1579
H	-3.9709	7.7829	-3.2506
H	-5.1359	6.4403	-3.4635
H	-3.4108	6.2248	-3.8887
C	-7.4145	0.6339	-0.0971
C	-6.674	-0.7249	-0.3585
O	-5.3584	-0.5907	0.2319
C	-8.265	0.6192	1.1916
H	-7.6697	0.31	2.0685
H	-9.1263	-0.0673	1.0987
H	-8.6625	1.6294	1.392
C	-8.2937	1.0019	-1.3044

H	-7.6925	1.0784	-2.2279
H	-8.792	1.9722	-1.1474
H	-9.0726	0.2323	-1.4647
C	-7.3059	-2.0083	0.1465
H	-6.5087	-0.8086	-1.4505
H	-6.665	-2.8667	-0.1186
H	-8.296	-2.1609	-0.3191
H	-7.4258	-1.9992	1.2425
O	-2.622	-0.8137	0.8385
O	2.2301	0.6395	1.7832
H	2.1276	-0.3267	1.7536
O	2.1537	3.2855	1.7998
H	2.0092	4.2467	1.7844
H	-0.2616	4.4029	1.3457
H	-0.1624	-0.5745	1.3108
H	-5.7129	5.3916	-1.5056
O	-7.2045	3.6667	-0.0421
C	-7.727	4.507	0.9759
H	-7.5386	5.5726	0.7474
H	-7.2964	4.2644	1.964
H	-8.8196	4.3483	1.0151



S28. Experimental CD spectra of Compound **4** (black), calculated ECD spectra of 1 (red), and *ent*-1 (blue)