

Supplementary Material

Penicacids H-J, three new mycophenolic acid derivatives from the marine-derived fungus *Rhizopus oryzae*

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ABSTRACT

Chemical investigation of secondary metabolites in crude methanol extract of the mycelial cells in solid rice medium of a marine-derived fungus *Rhizopus oryzae* is found to have enriched the metabolic profile of this genus by affording three mycophenolic acid derivatives recognized as new fungal metabolites trivially named as penicacids H-J (**1-3**) along with two known naphtho- γ -pyrone dimers, asperpyrone A (**4**) and dianhydroaurasperone C (**5**). The structure elucidation of isolated compounds was unambiguously determined based on extensive 1D and 2D NMR spectroscopic analyses in addition to comparing coupling constant and optical rotation values with related congeners in literature. All isolated compounds were assessed for their antibacterial activity against four different bacterial microorganisms and they revealed moderate to weak activities with minimum inhibitory concentration (MIC) values ranging from 62.5 to 250 $\mu\text{g/mL}$.

Keywords: *Rhizopus oryzae*; marine-derived; penicacid; antibacterial activity.

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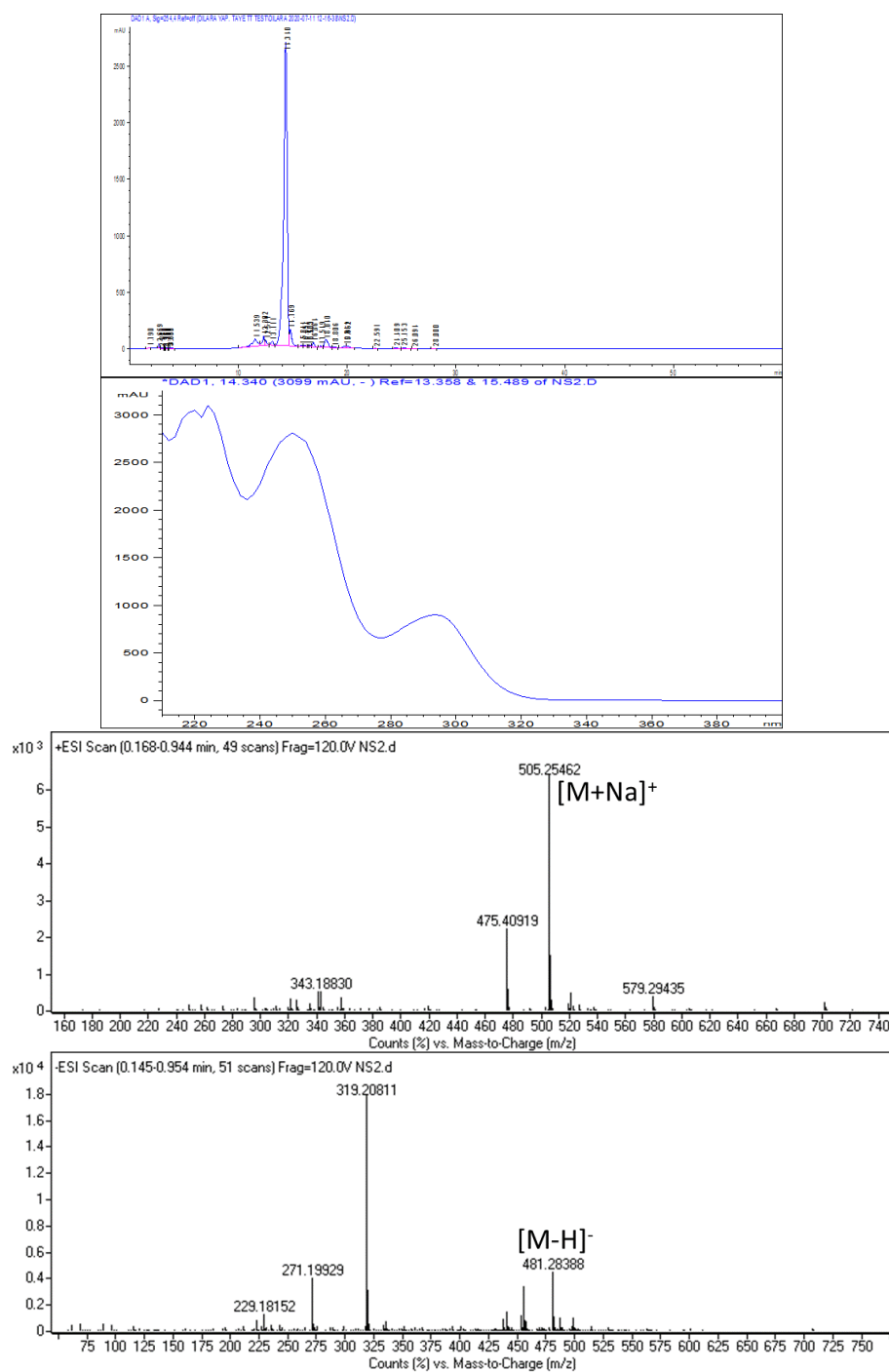


Figure S1. HPLC chromatogram and HRESIMS of **1**.

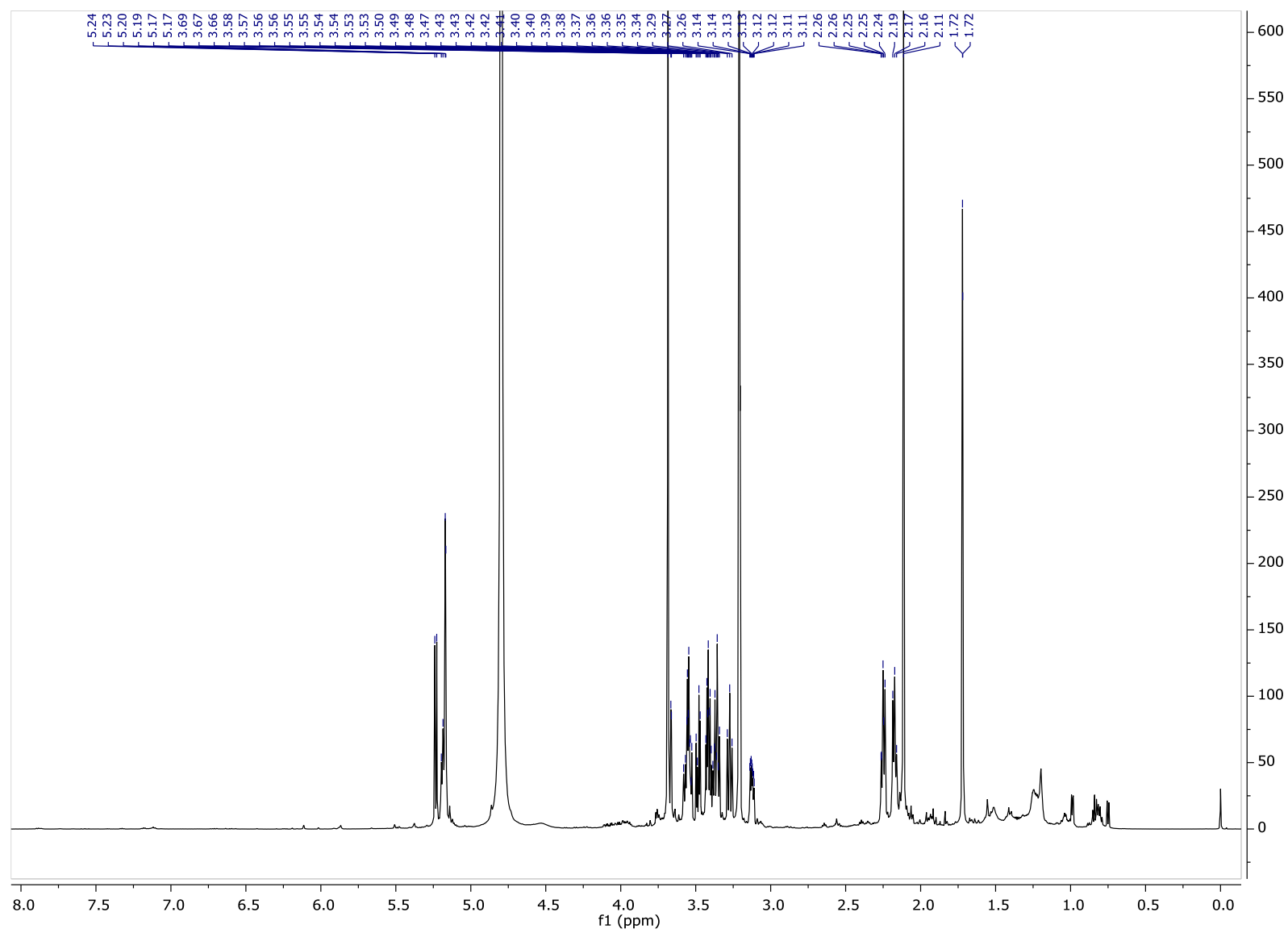


Figure S2. ^1H -NMR spectrum of **1** in $\text{methanol-}d_4$ at 600 MHz.

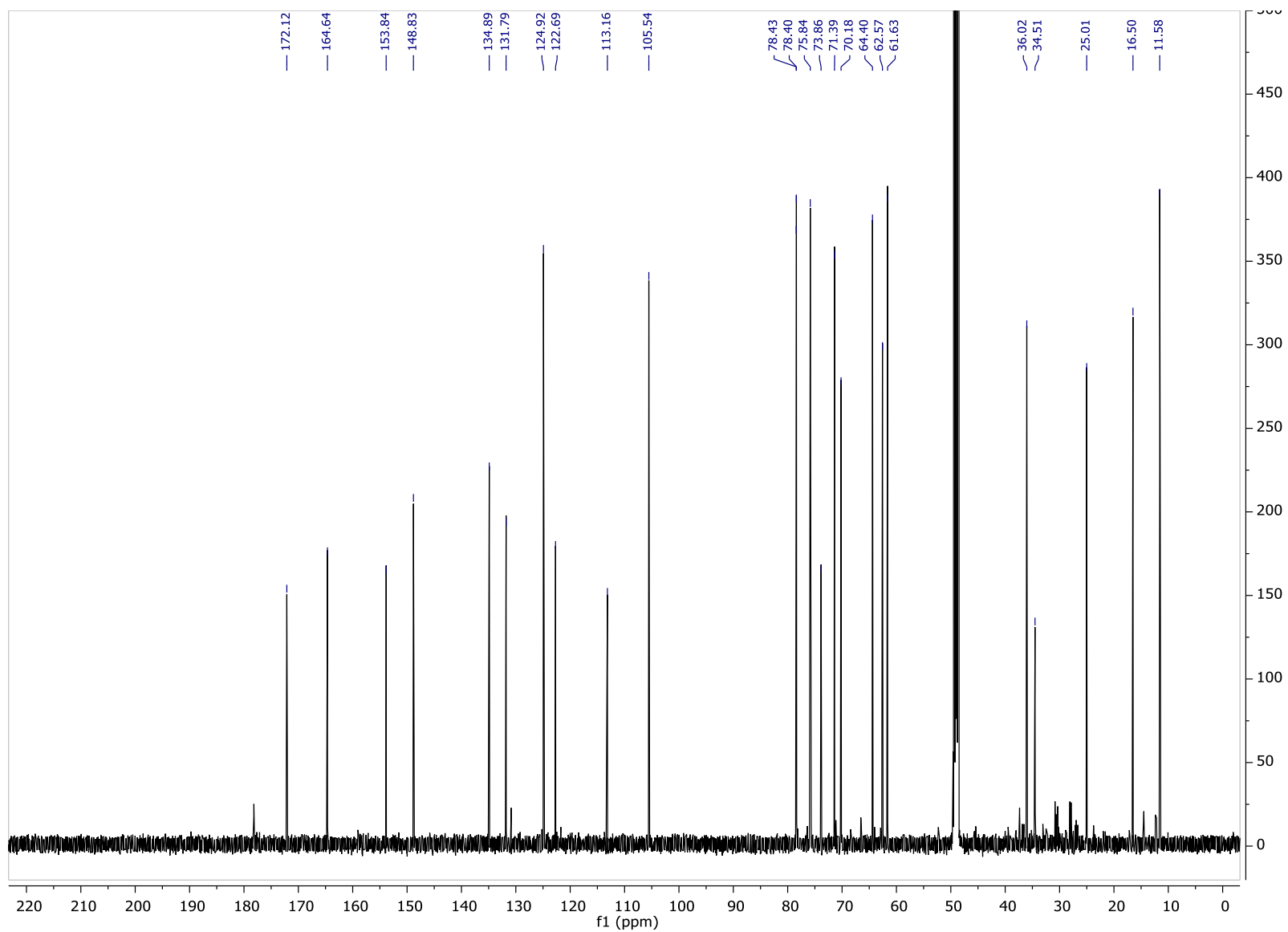


Figure S3. ^{13}C -NMR spectrum of **1** in methanol- d_4 at 150 MHz.

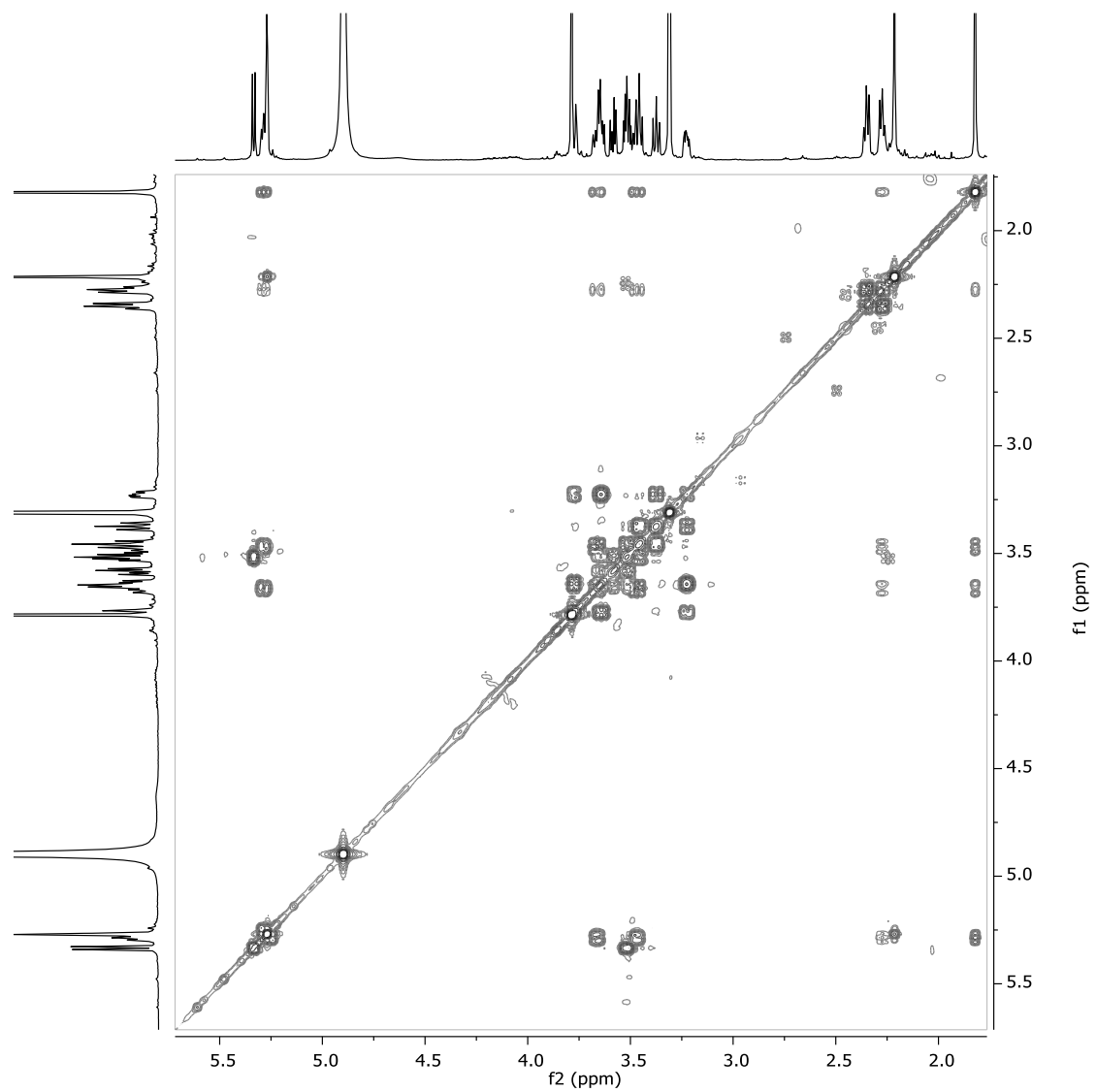


Figure S4. ^1H - ^1H COSY spectrum of **1** in methanol- d_4 at 600 MHz.

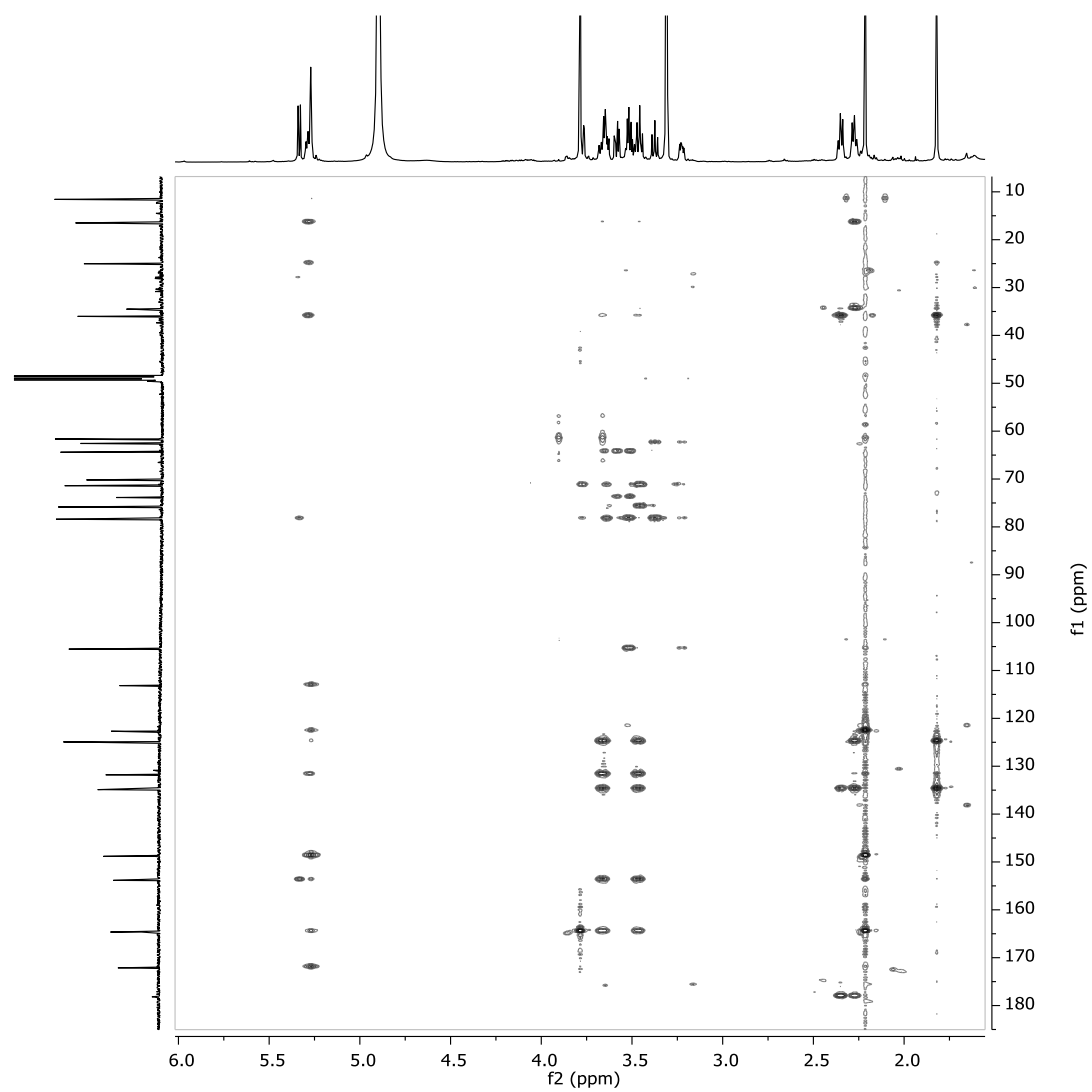


Figure S5. gHMBC spectrum of **1** in methanol- d_4 at 600 MHz.

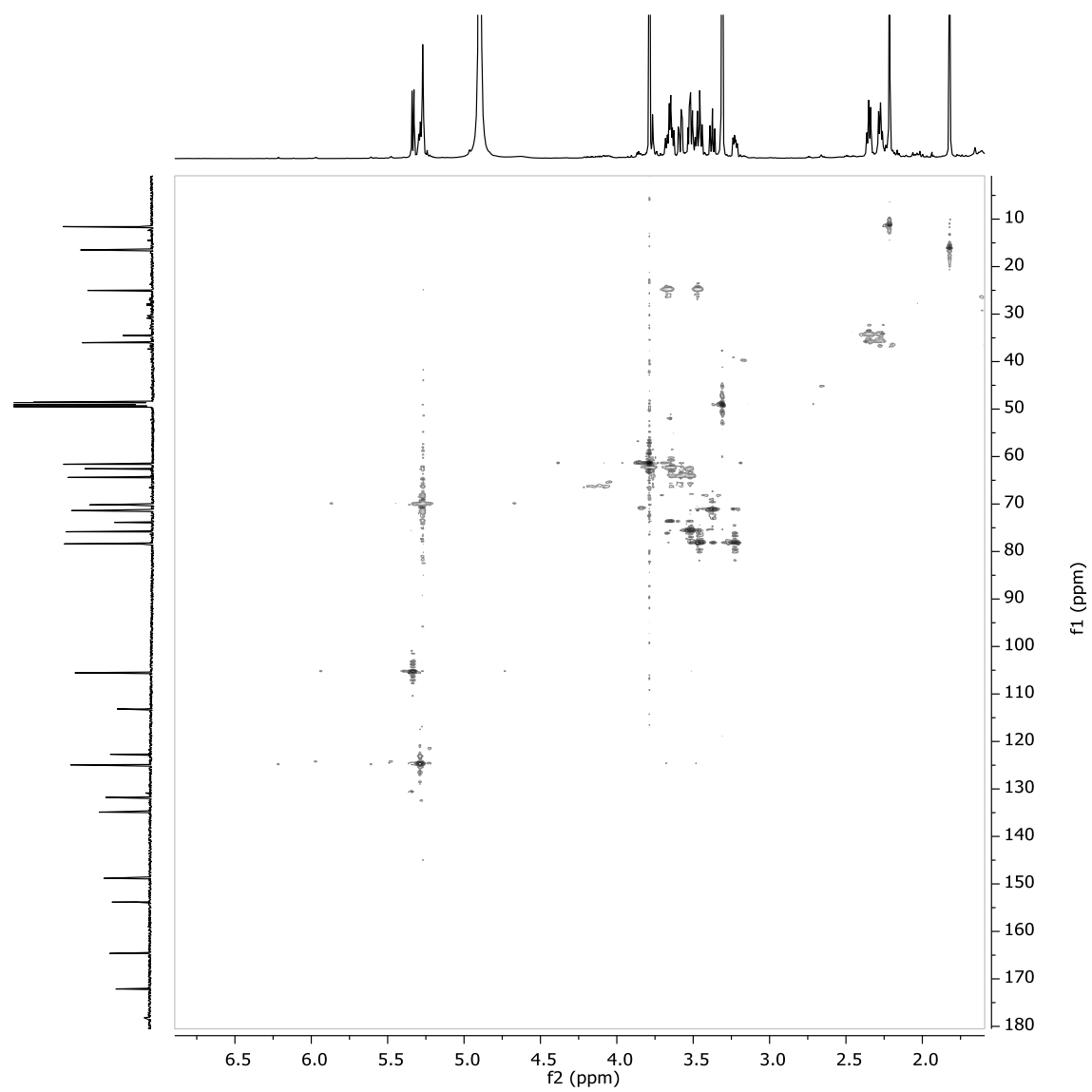


Figure S6. gHMQC spectrum of **1** in methanol- d_4 at 600 MHz.

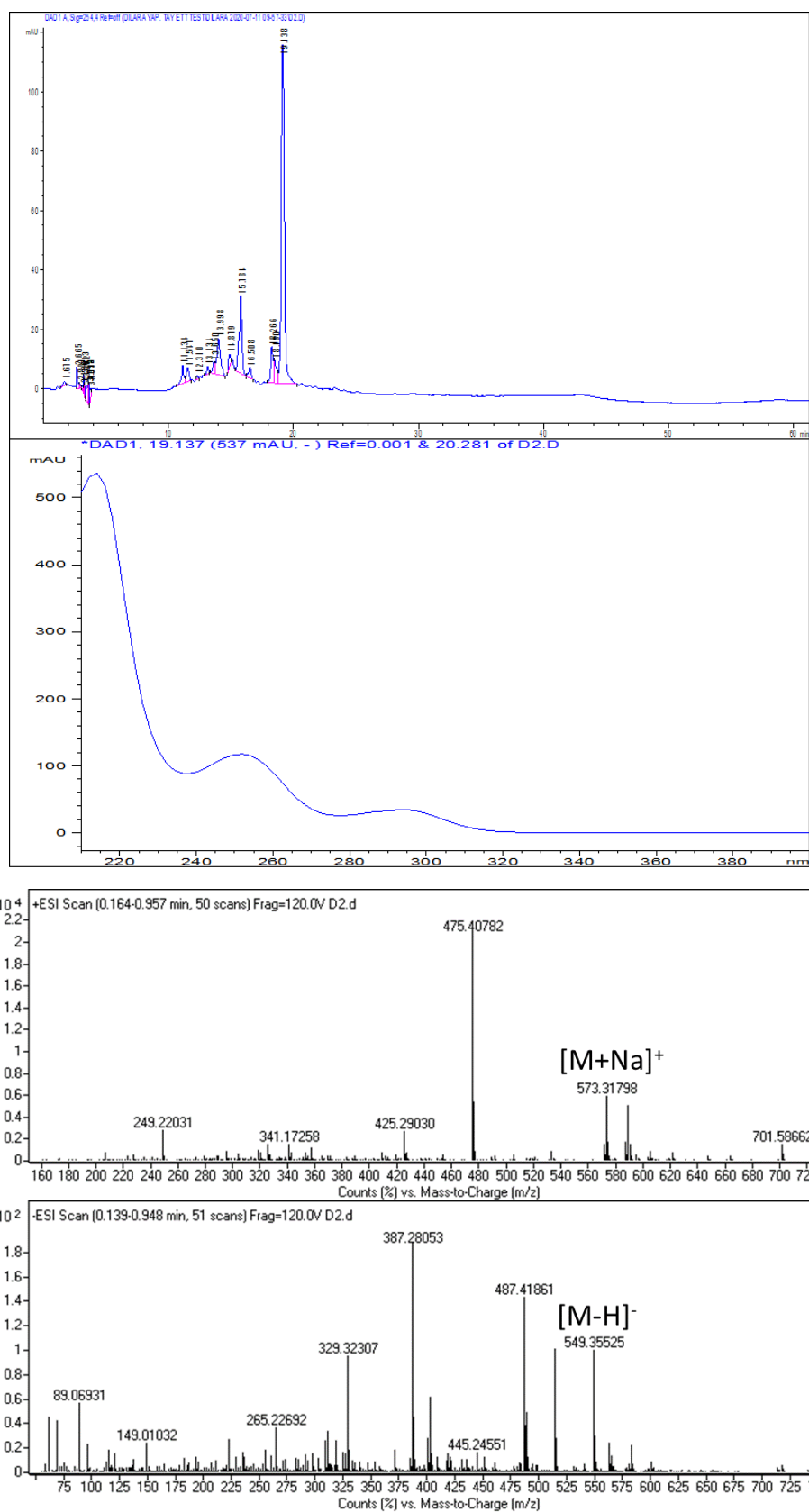


Figure S7. HPLC chromatogram and HRESIMS spectrum of **2**.

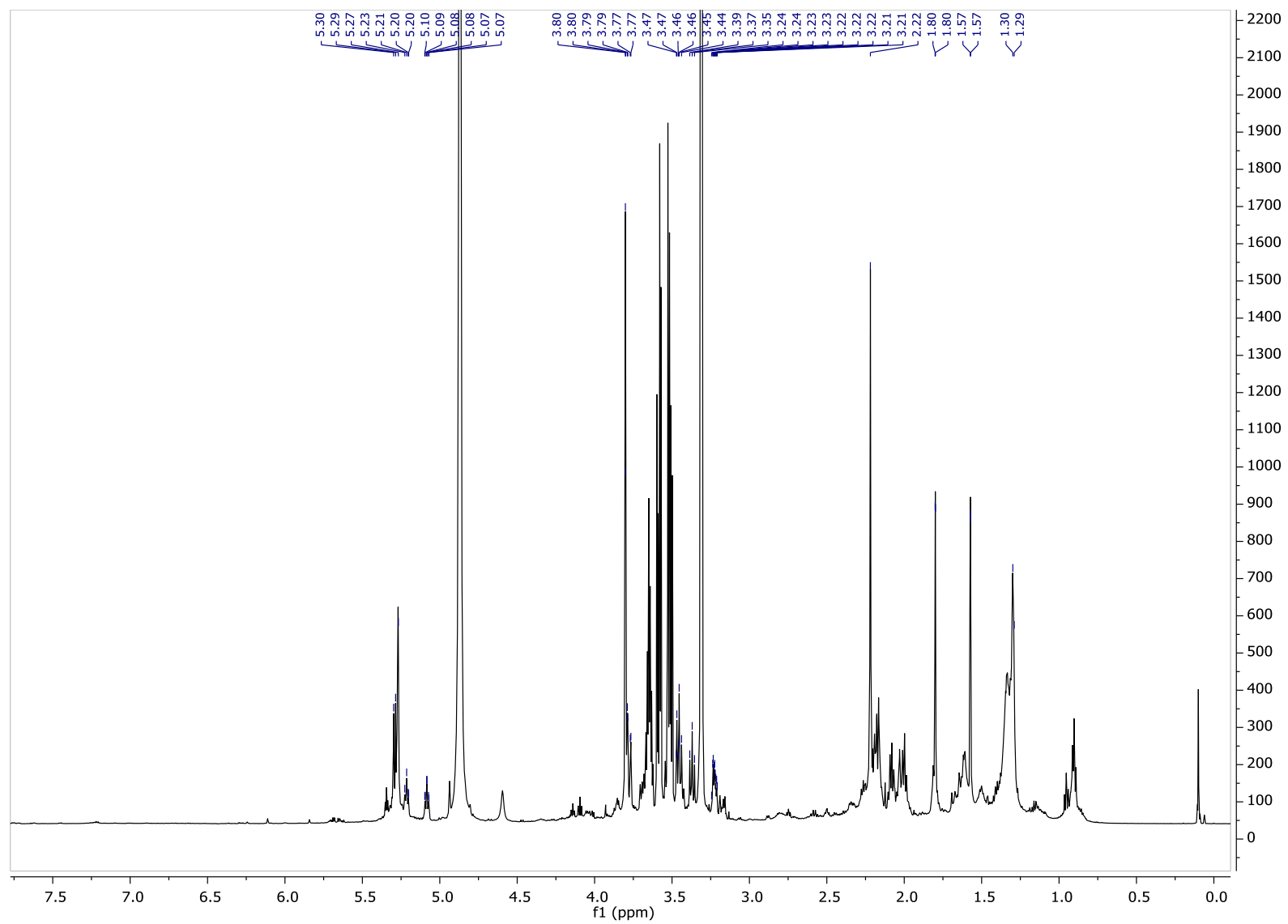


Figure S8. ^1H -NMR spectrum of **2** in methanol- d_4 at 600 MHz.

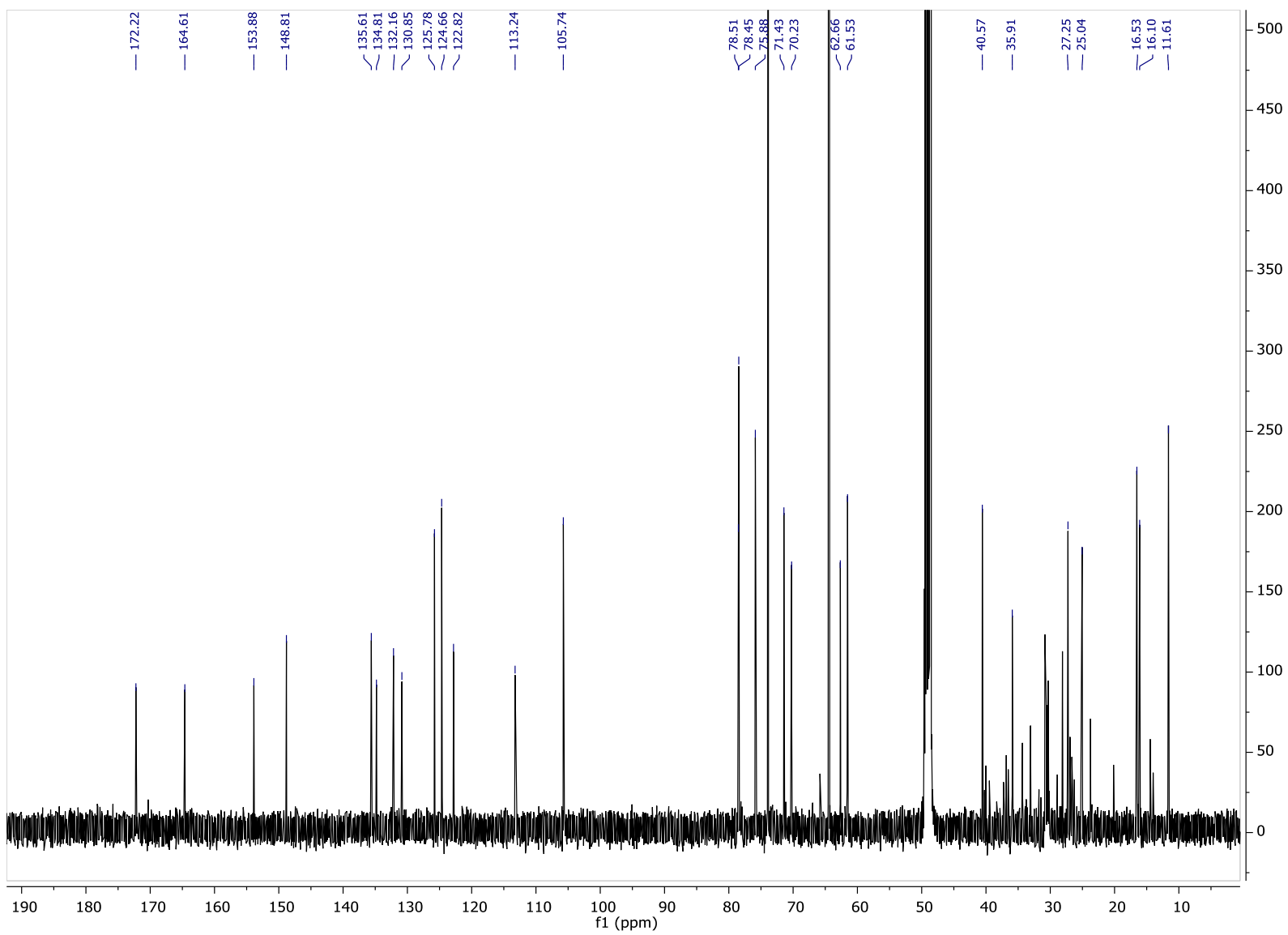


Figure S9. ^{13}C -NMR spectrum of **2** in methanol- d_4 at 150 MHz.

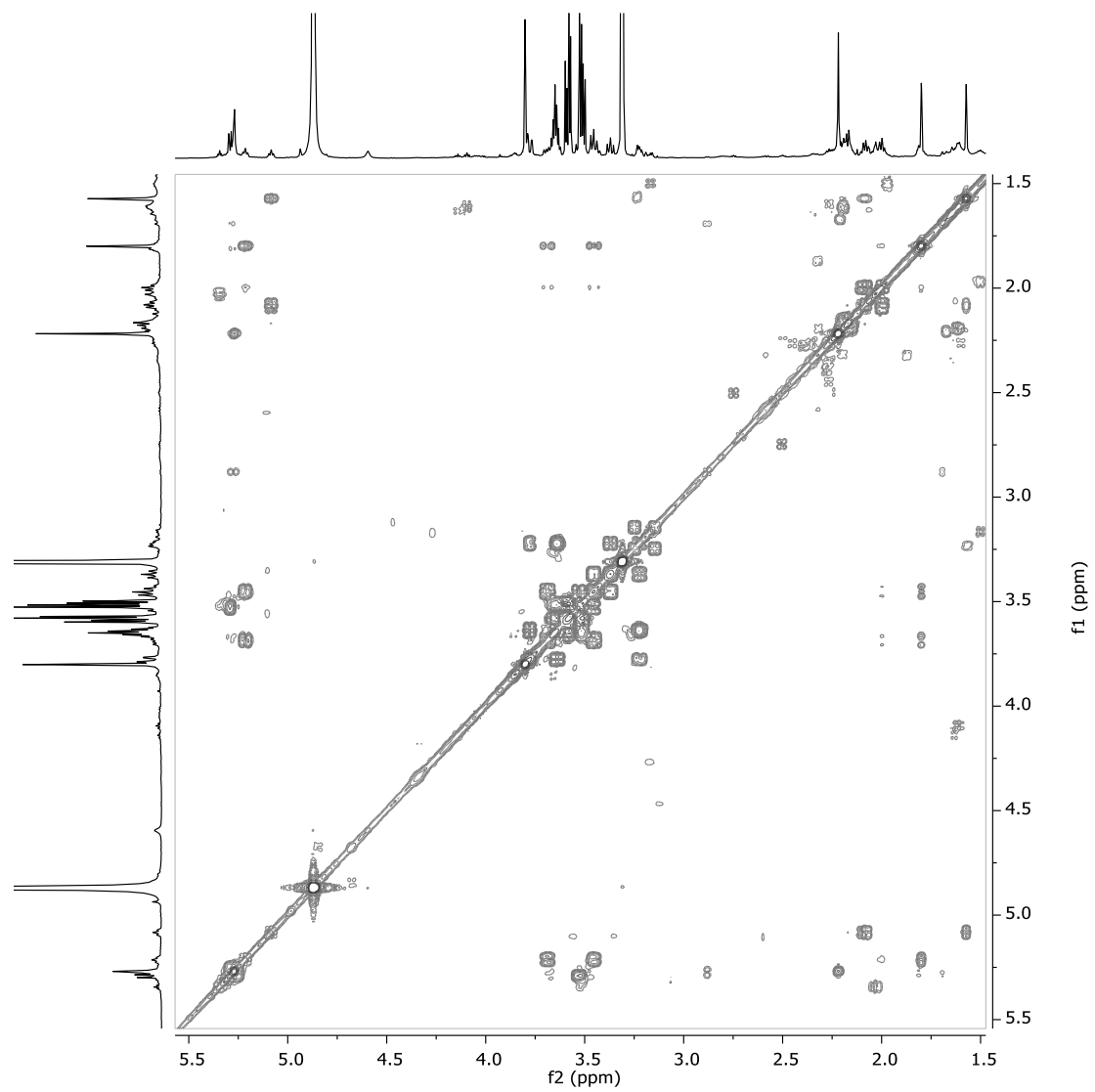


Figure S10. ^1H - ^1H COSY spectrum of **2** in methanol- d_4 at 600 MHz.

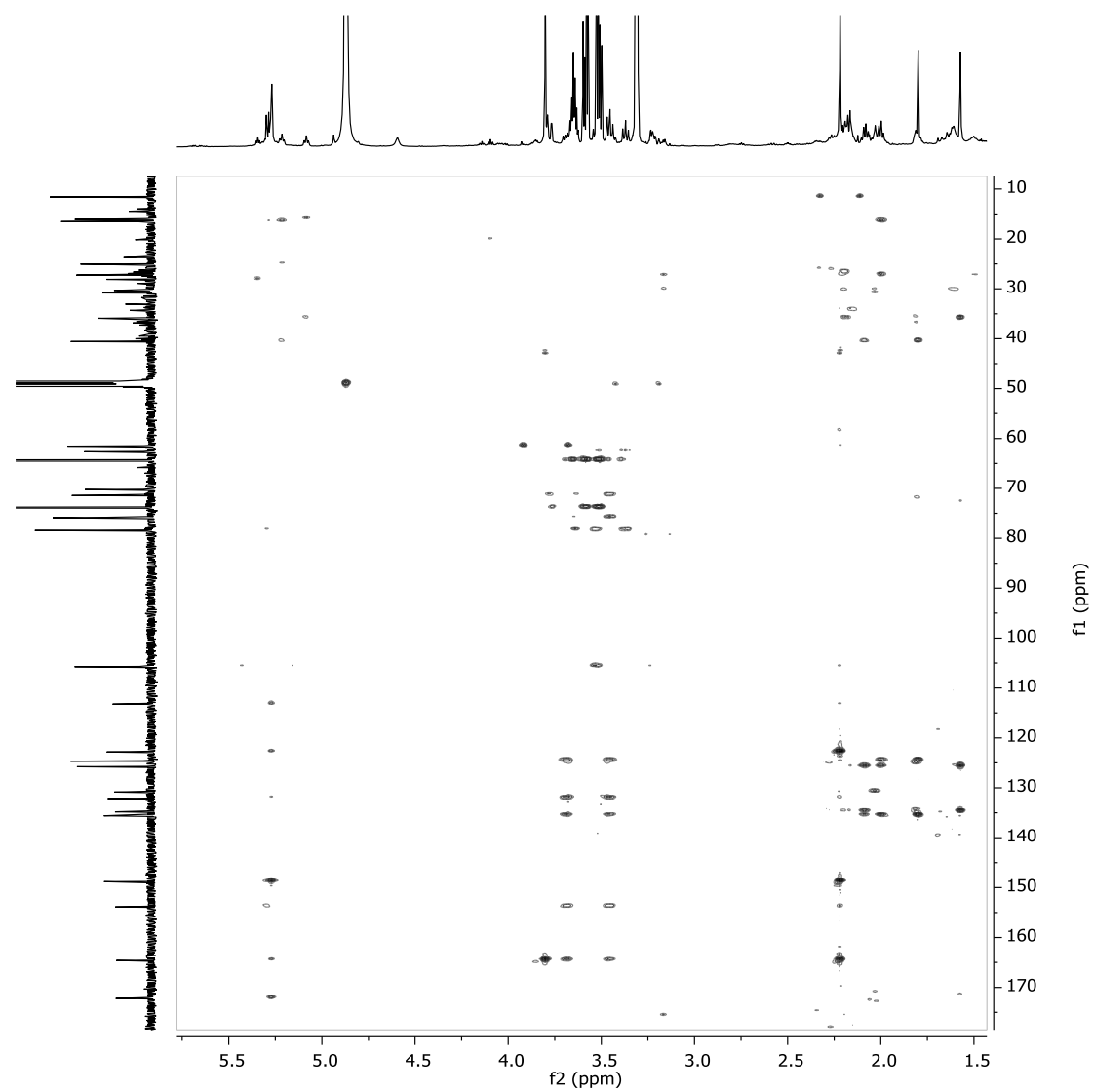


Figure S11. gHMBC spectrum of **2** in methanol- d_4 at 600 MHz.

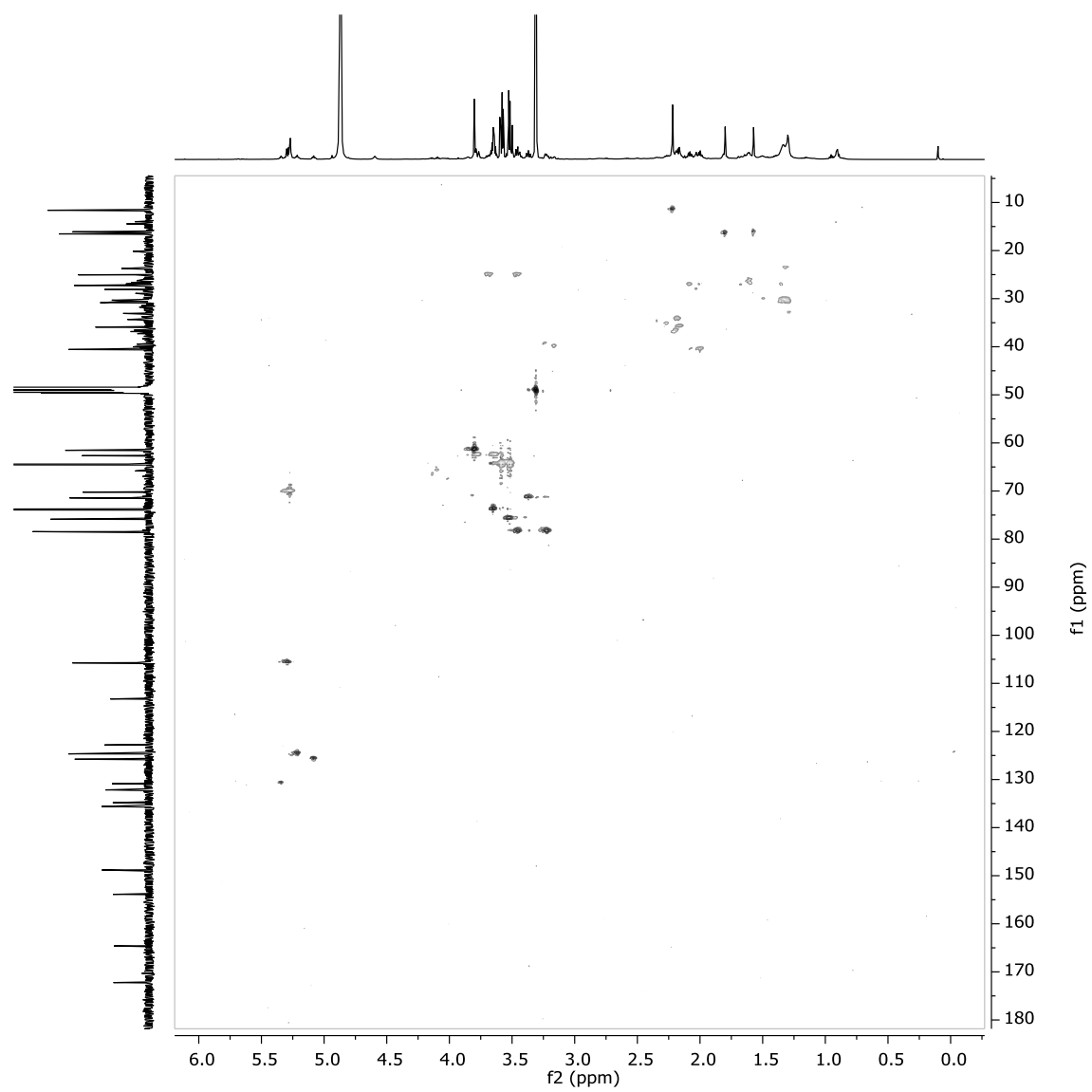


Figure S12. gHMQC spectrum of **2** in methanol- d_4 at 600 MHz.

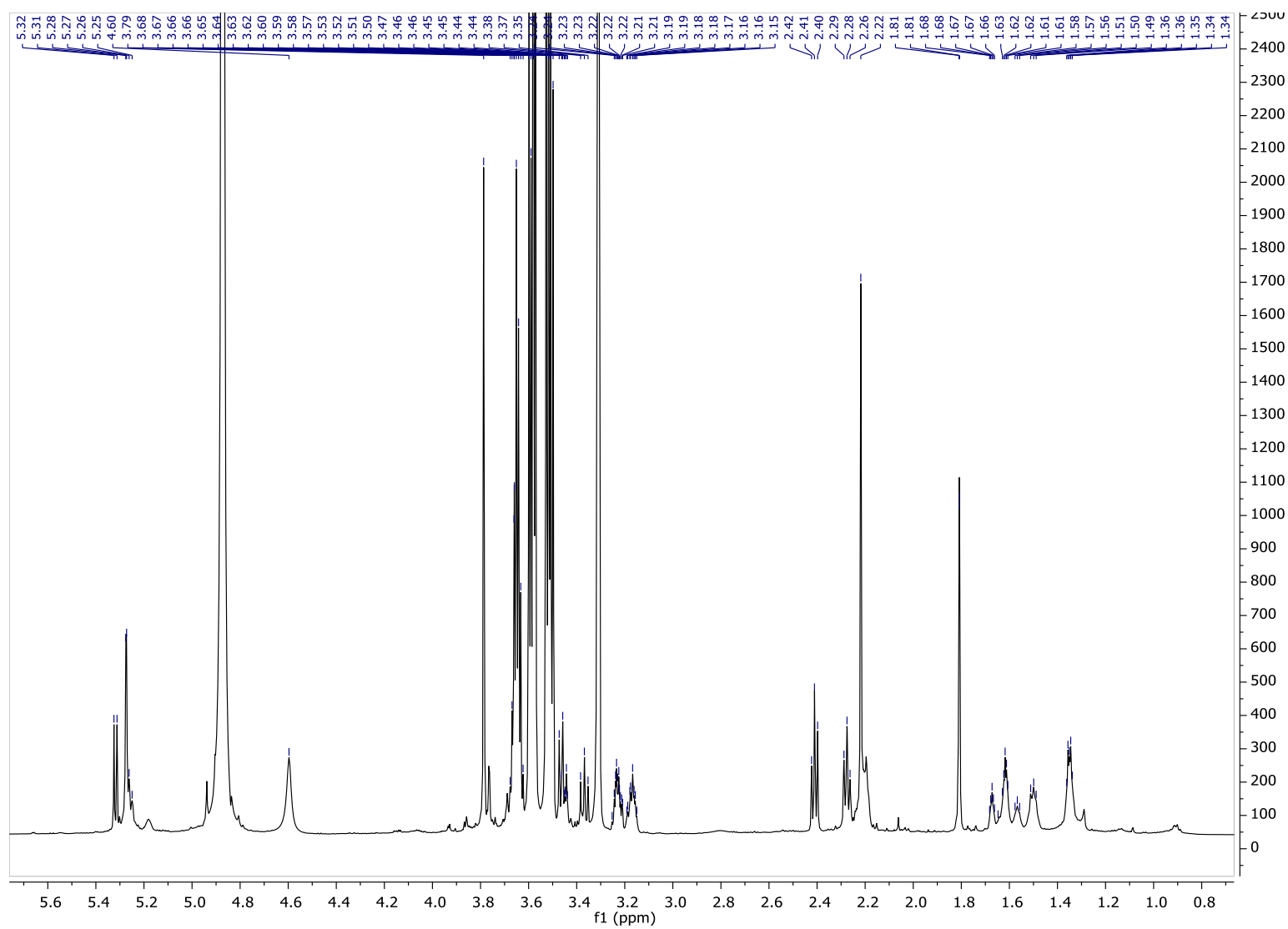


Figure S13. ^1H -NMR spectrum of **3** in methanol- d_4 at 400 MHz.

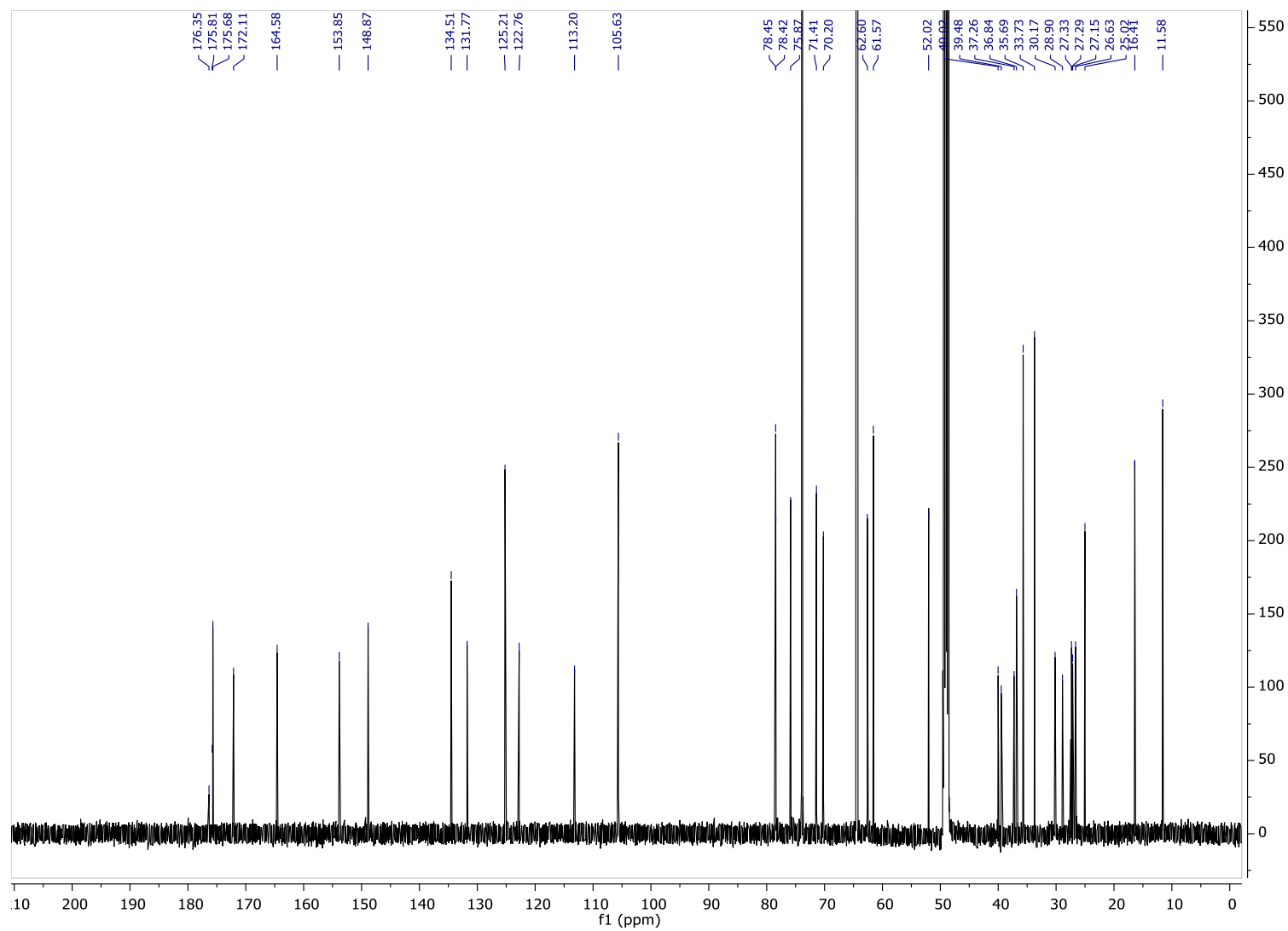


Figure S14. ^{13}C -NMR spectrum of **3** in methanol- d_4 at 100 MHz.

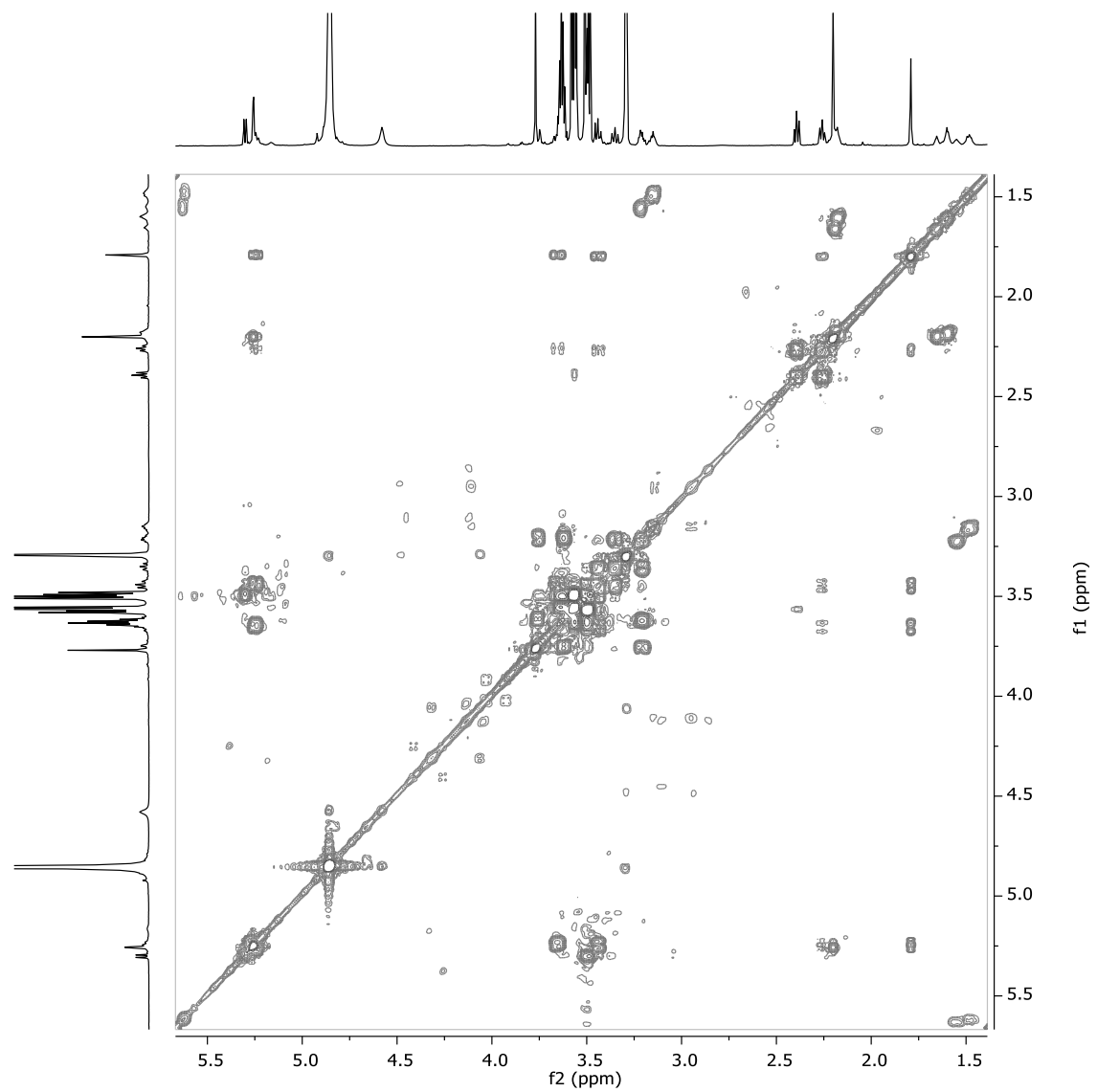


Figure S15. ^1H - ^1H COSY spectrum of **3** in methanol- d_4 at 400 MHz.

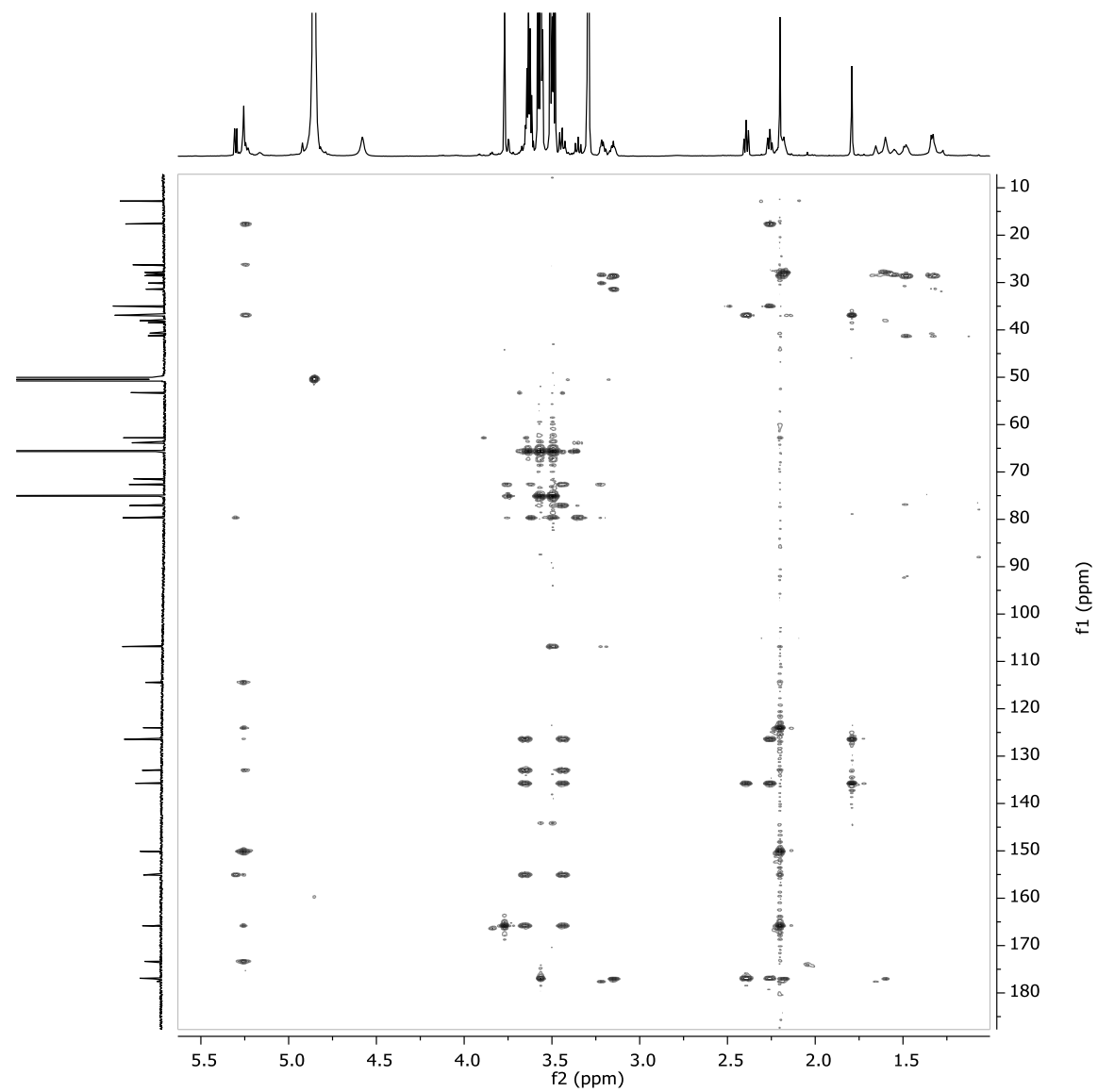


Figure S16. gHMBC spectrum of **3** in methanol- d_4 at 400 MHz.

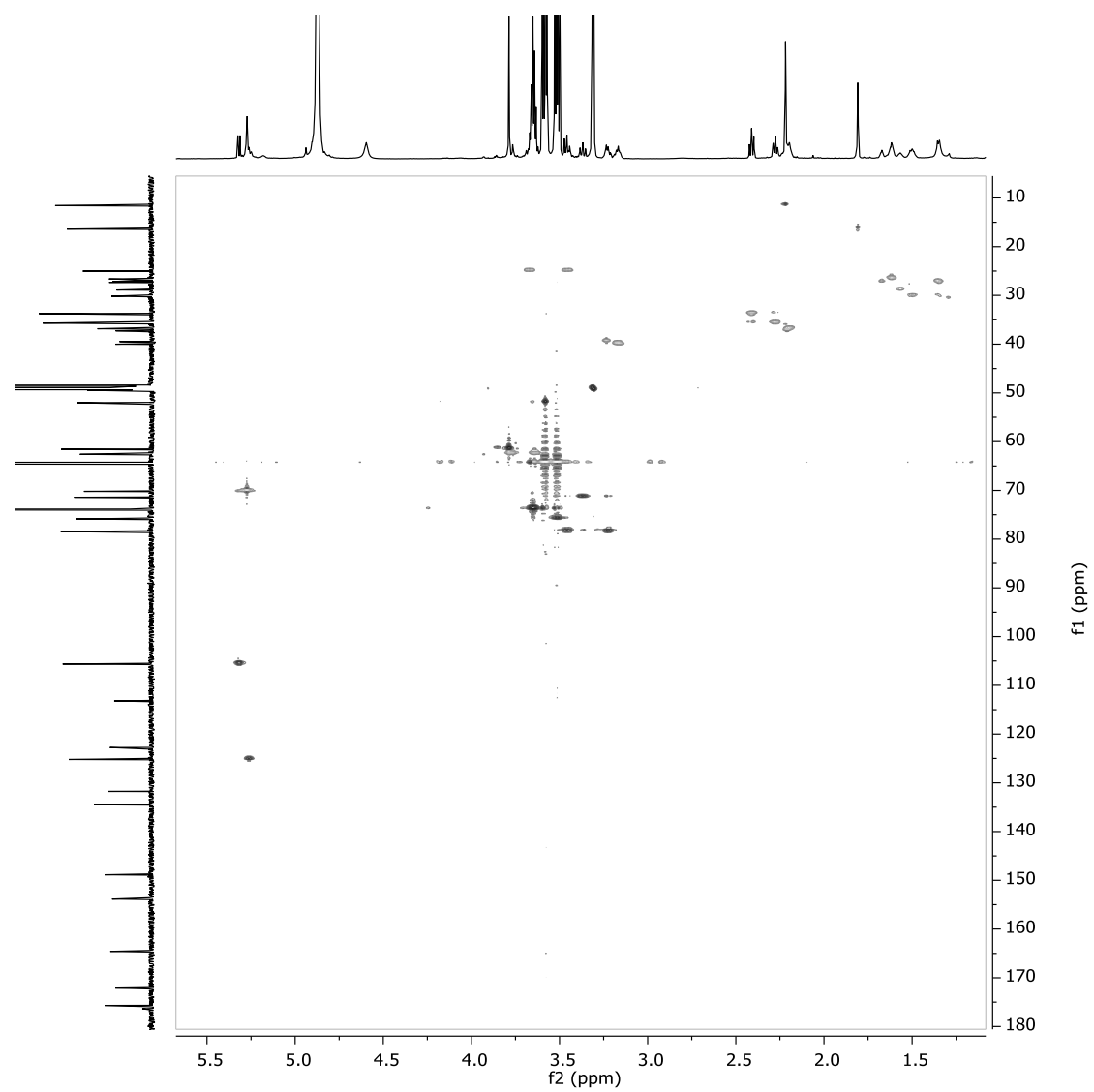
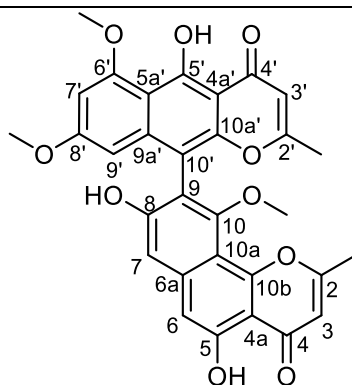


Figure S17. gHMQC spectrum of **3** in methanol- d_4 at 400 MHz.

Table S1. ^1H and ^{13}C NMR data of asperpyrone A (**4**) in methanol- d_4 at 400 and 100 MHz.



Asperpyrone A (**4**)

Chemical Formula: $\text{C}_{31}\text{H}_{24}\text{O}_{10}$

Exact Mass: 556.13695

Molecular Weight: 556.52300

#	δ_{H} (multi, $J[\text{Hz}]$)	δ_{C} , type
2		170.8, C
3	6.42, s (1H)	112.3, CH
4		184.5, CO
4a		111.0, C
5		155.5, C
6	6.92, s (1H)	107.0, CH
6a		140.1, C
7	7.04, s (1H)	107.6, CH
8		158.4, C
9		118.4, C
10		159.6, C
10a		109.6, C
10b		154.7, C
2-Me	2.53, s (3H)	20.5, CH_3
10-OMe	3.48, s (3H)	62.0, CH_3
2'		171.4, C
3'	6.11, s (1H)	108.9, CH
4'		186.2, C
4a'		103.3, C
5'		162.0, C
5a'		110.8, C
6'		162.3, C
7'	6.53, d (2.2, 1H)	98.3, CH
8'		163.4, C
9'	6.32, d (2.2, 1H)	97.6, CH
9a'		140.0, C
10'		108.2, C
10a'		150.2, C
2'-Me	2.18, s (3H)	20.6, CH_3
6'-OMe	3.99, s (3H)	56.5, CH_3
8'-OMe	3.62, s (3H)	55.7, CH_3

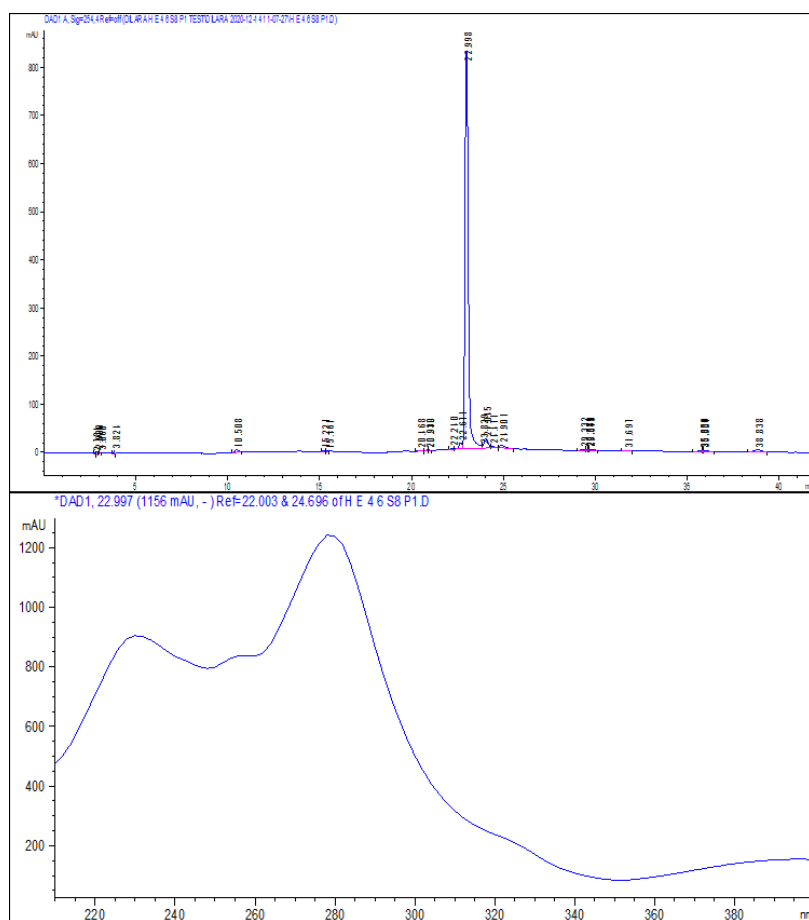


Figure S18. HPLC chromatogram of **4**.

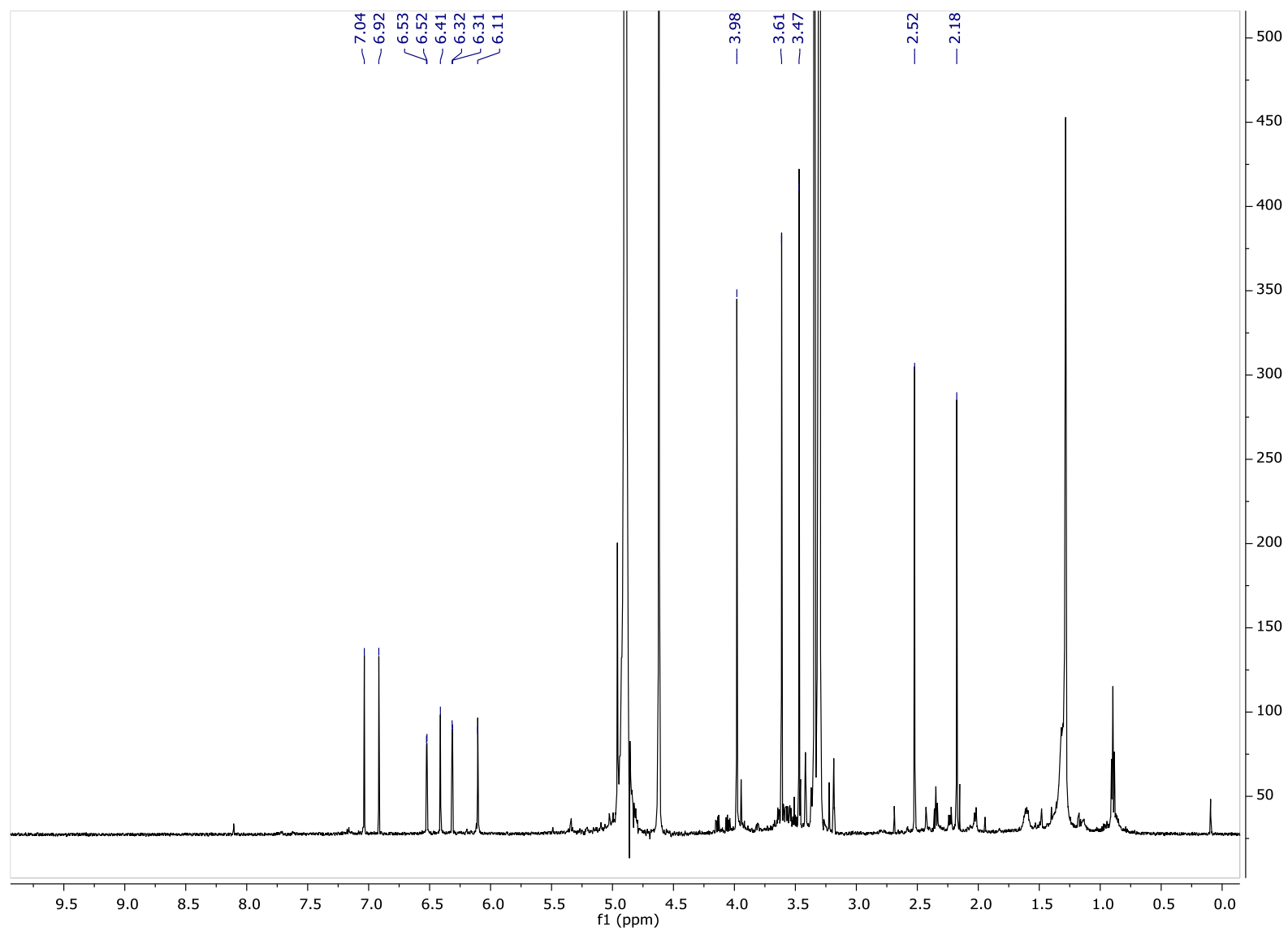


Figure S19. ^1H -NMR spectrum of **4** in methanol- d_4 at 400 MHz.

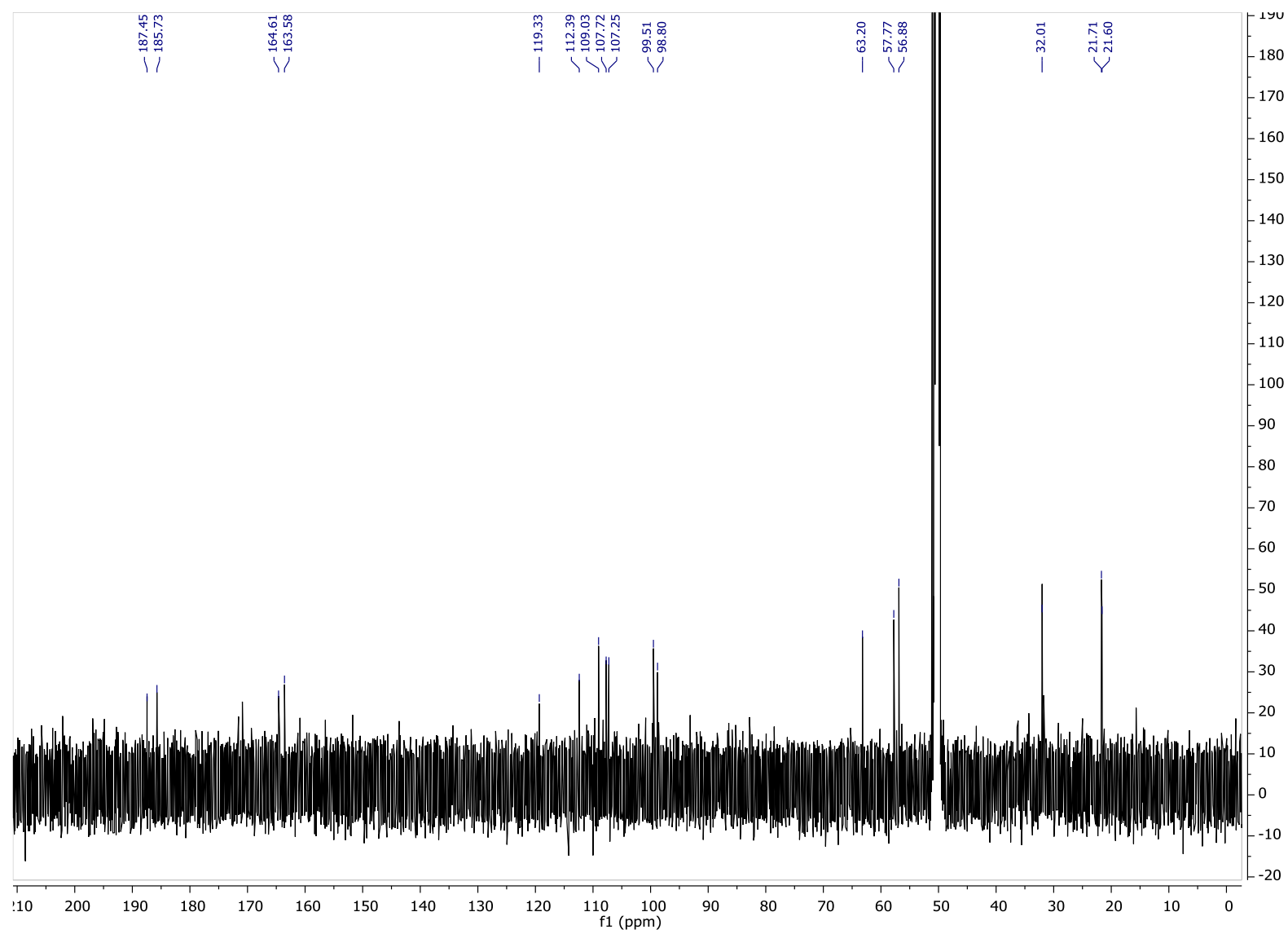


Figure S20. ¹³C-NMR spectrum of **4** in methanol-*d*₄ at 400 MHz.

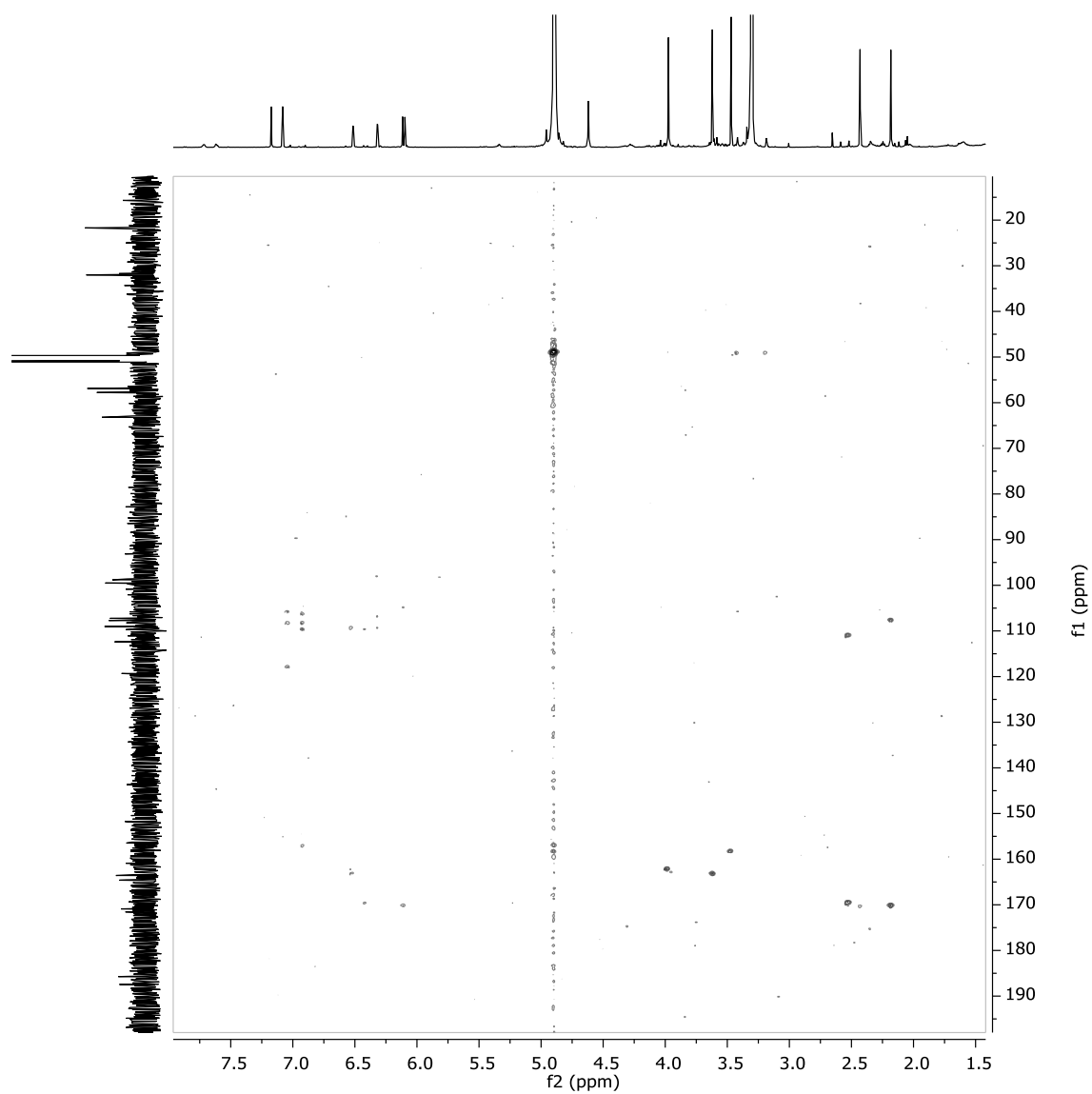


Figure S21. gHMBC spectrum of **4** in methanol- d_4 at 400 MHz.

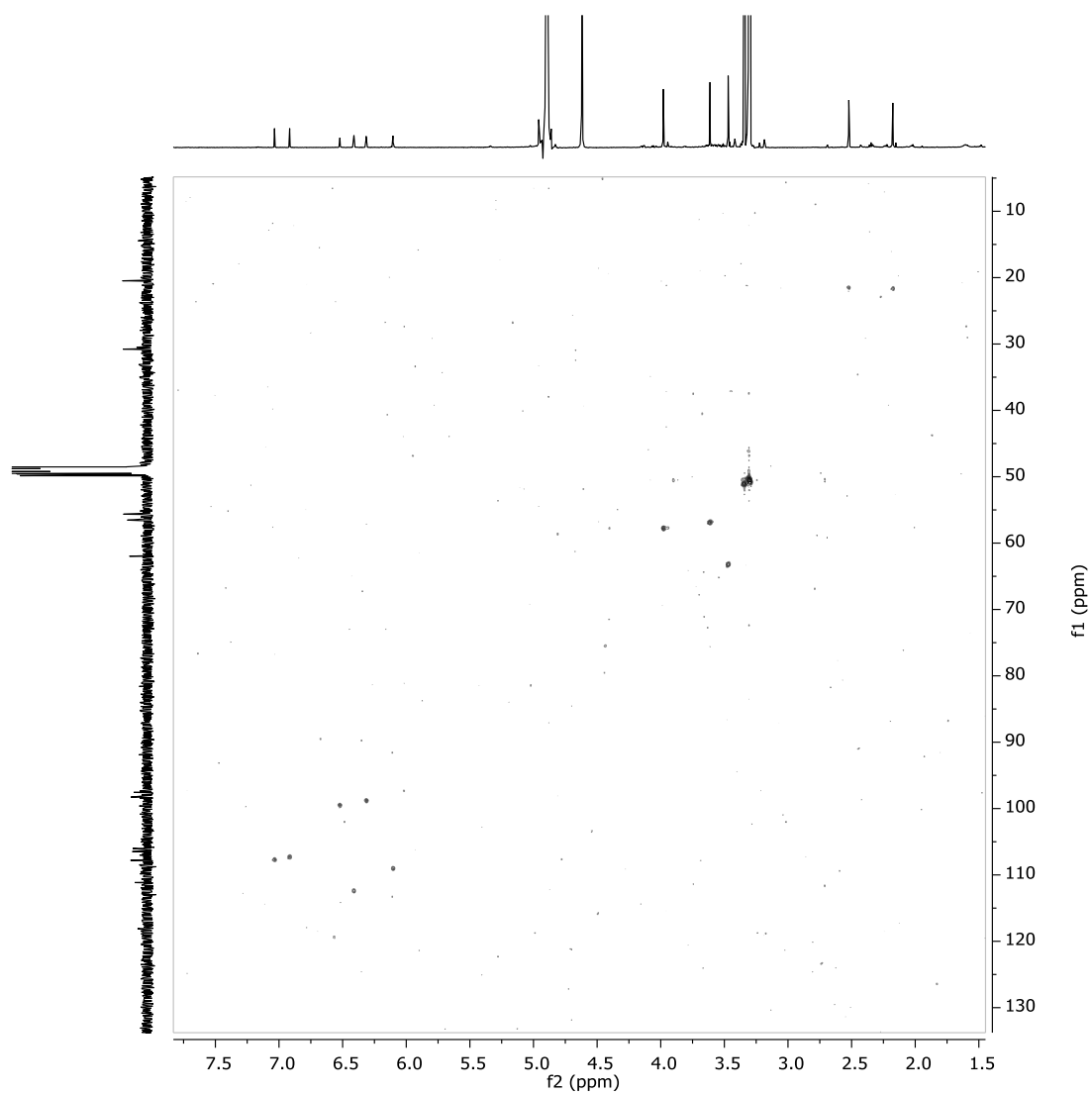
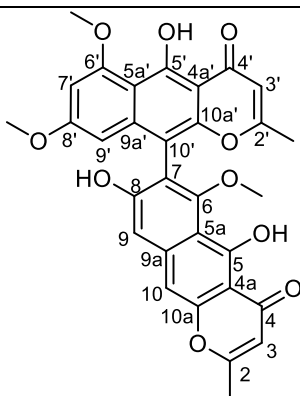


Figure S22. gHMQC spectrum of **4** in methanol- d_4 at 400 MHz.

Table S2. ^1H and ^{13}C NMR data of dianhydroaurasperone C (**5**) in methanol- d_4 at 400 and 100 MHz.



Dianhydroaurasperone C (**5**)
 Chemical Formula: $\text{C}_{31}\text{H}_{24}\text{O}_{10}$
 Exact Mass: 556.13695
 Molecular Weight: 556.52300

#	δ_{H} (multi, J [Hz])	δ_{C} , type
2		171.1, C
3	6.10, s (1H)	107.5, CH
4		186.1, C
4a		106.2, C
5		163.3, C
5a		112.8, C
6		160.9, C
7		119.9, C
8		162.6, C
9	7.09, s (1H)	106.3, CH
9a		140.2, C
10	7.18, s (1H)	101.7, CH
10a		155.7, C
2-Me	2.44, s (3H)	20.4, CH_3
2-OMe	3.47, s (3H)	62.3, CH_3
2'		171.6, C
3'	6.12, s (1H)	107.6, CH
4'		186.2, C
4a'		106.2, C
5'		163.4, C
6'		110.5, C
6a'		163.5, C
7'	6.52, d (1H, 2.3)	98.1, CH
8'		164.5, C
9'	6.32, d (1H, 2.3)	97.3, CH
9a'		140.3, C
10'		108.2, C
10a'		152.3, C
2'-Me	2.19, s (3H)	20.2, CH_3
6'-OMe	3.95, s (3H)	56.3, CH_3
8'-OMe	3.63, s (3H)	55.4, CH_3

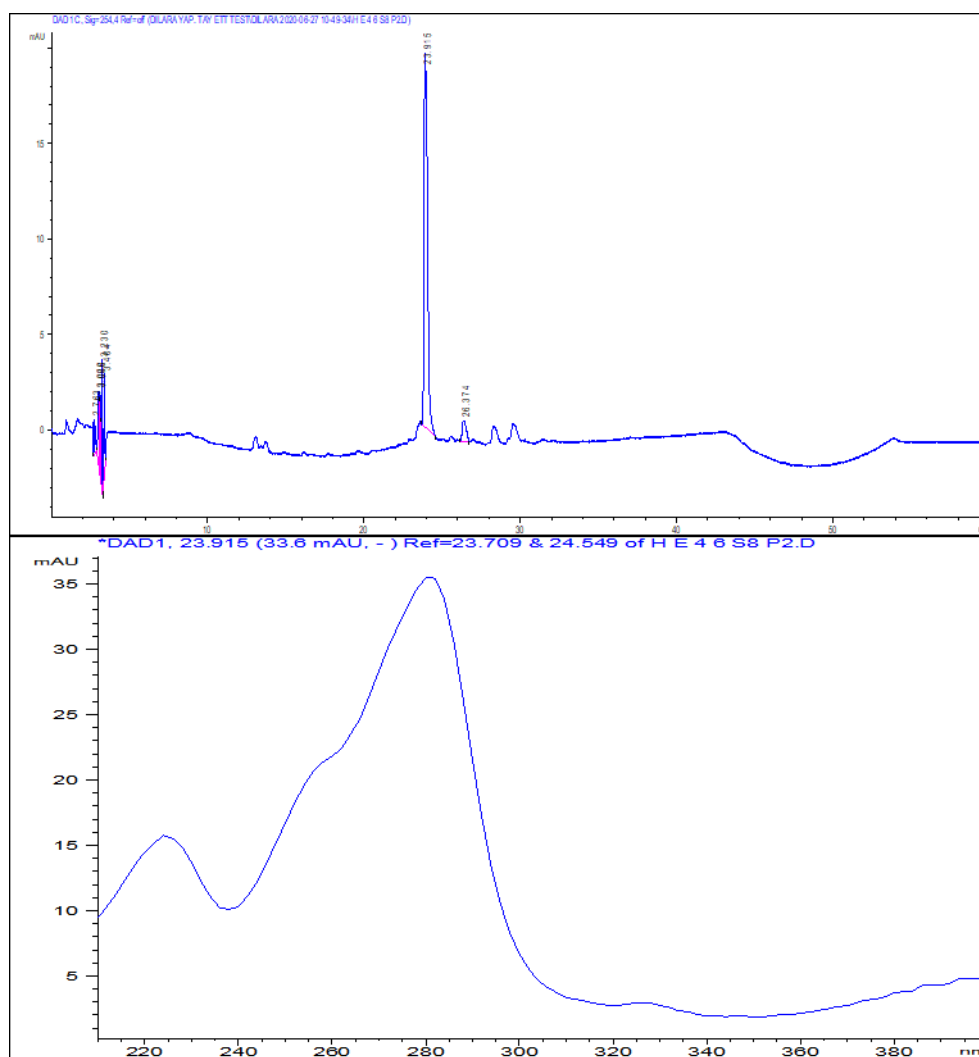


Figure S23. HPLC chromatogram of **5**.

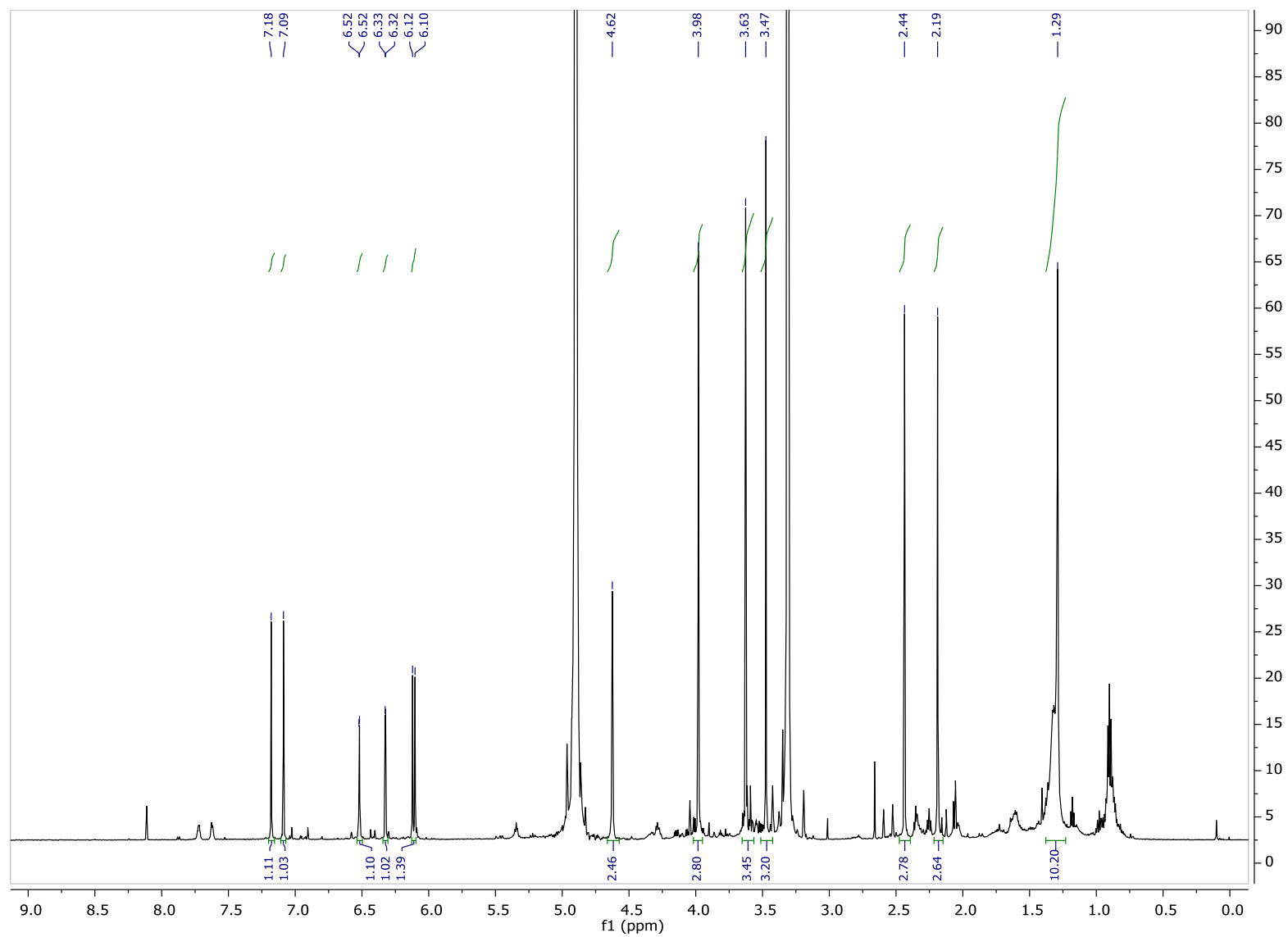


Figure S24. ^1H -NMR spectrum of **5** in $\text{methanol-}d_4$ at 400 MHz.

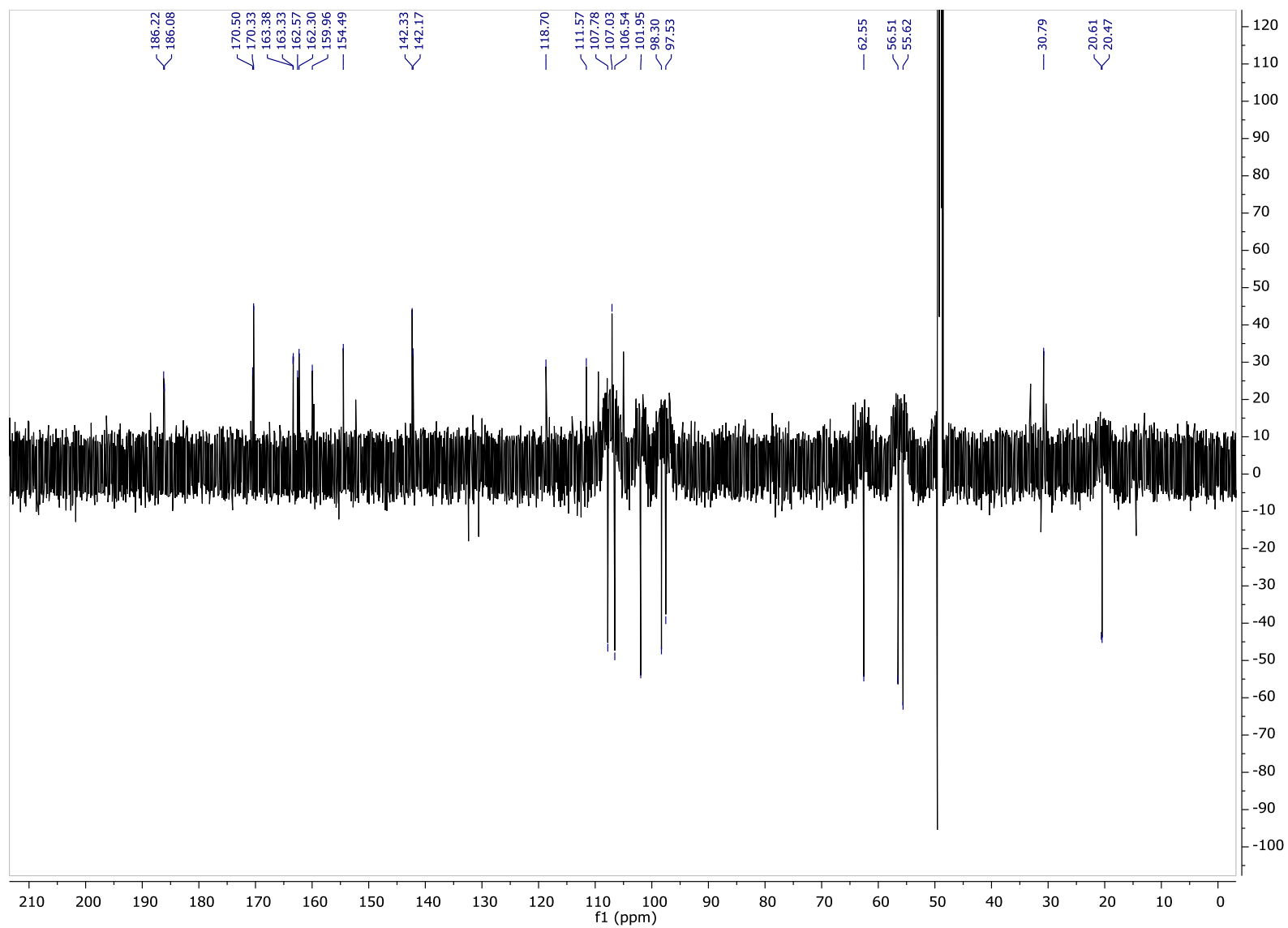


Figure S25. APT-NMR spectrum of **5** in methanol- d_4 at 400 MHz.

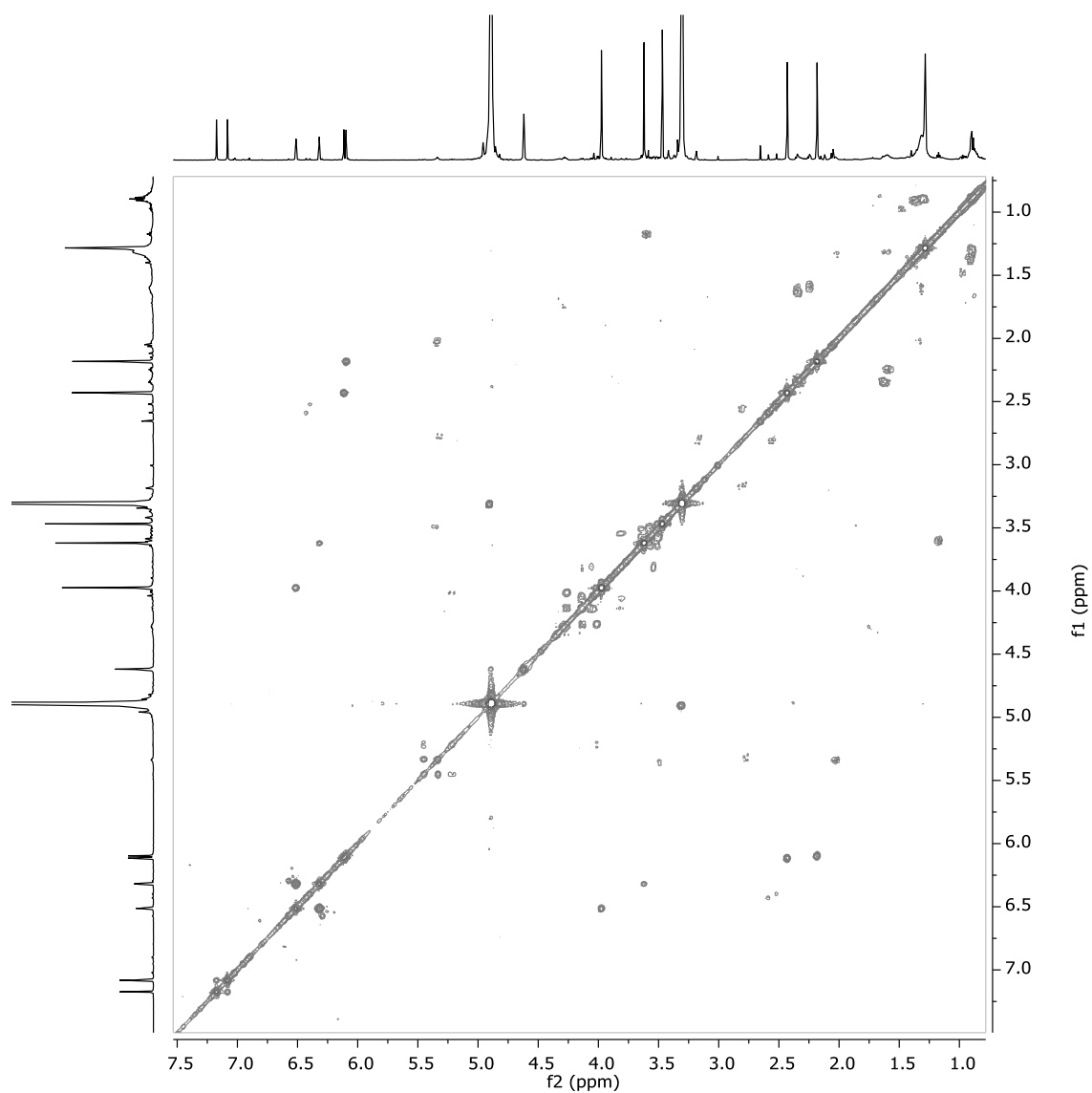


Figure S26. ^1H – ^1H COSY spectrum of **5** in methanol- d_4 at 400 MHz.

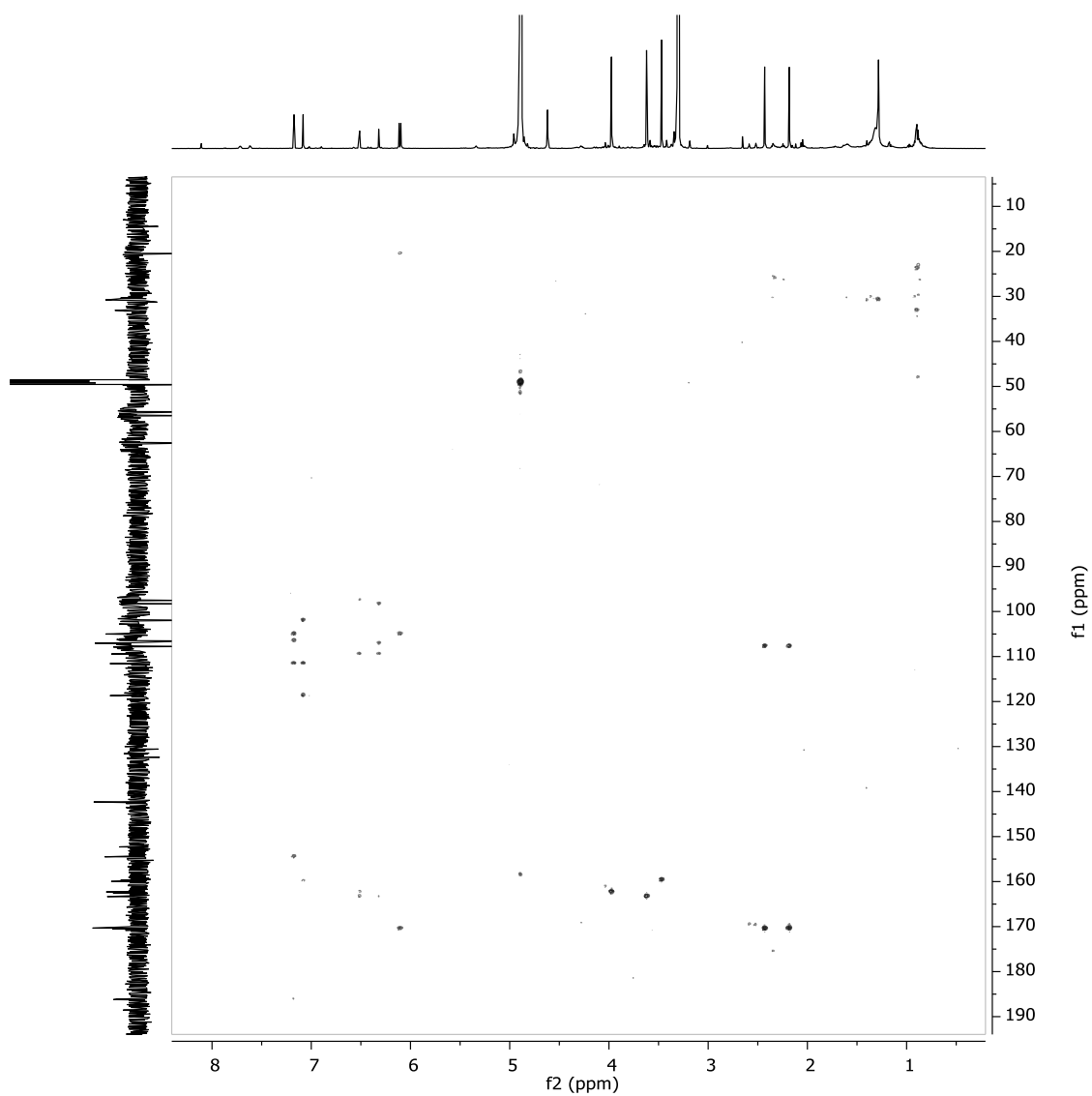


Figure S27. gHMBC spectrum of **5** in methanol- d_4 at 400 MHz.

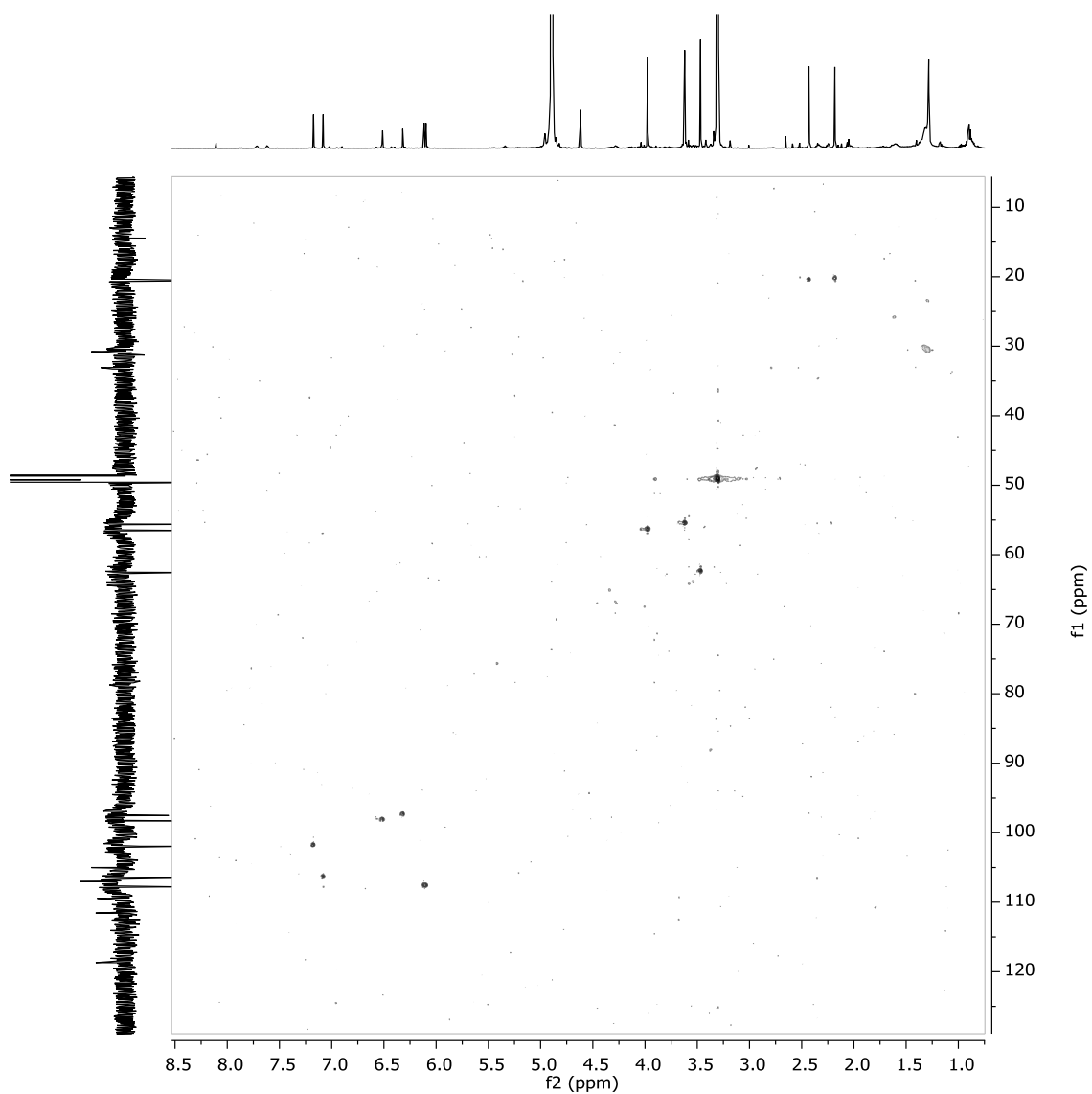


Figure S28. gHMQC spectrum of **5** in methanol- d_4 at 400 MHz.

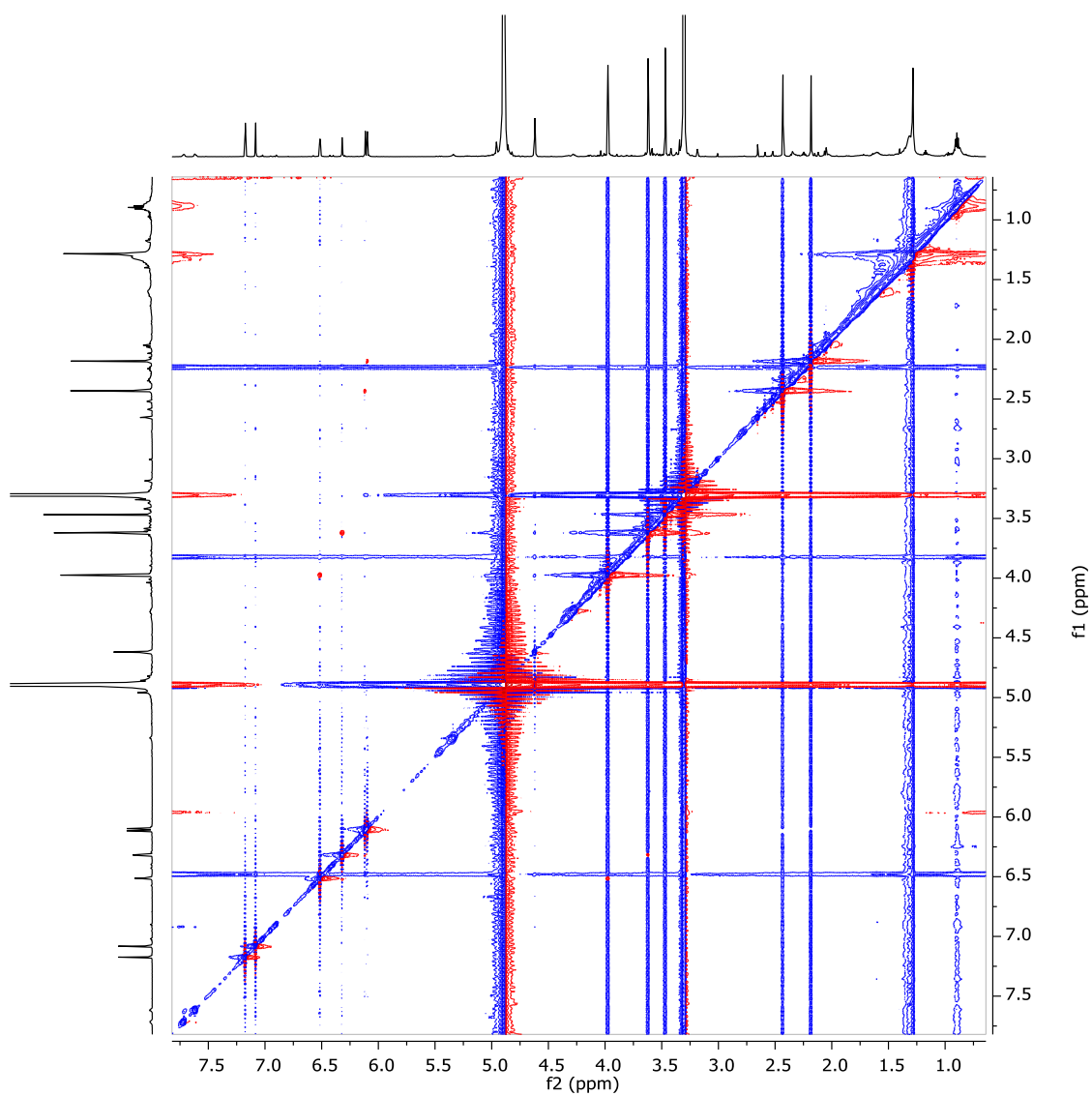


Figure S29. NOESY spectrum of **5** in methanol- d_4 at 400 MHz.