

Chemistry & Biodiversity

Supporting Information

p*-Terphenyl and Orsellinic Acid Derivatives from the European Polyporales *Terana coerulea* and *Sparassis brevipes

Winnie Chemutai Sum, Sherif S. Ebada,* Harald Kellner, and Marc Stadler*

Supporting Information for:

p-Terphenyl and Orsellinic Acid Derivatives from European Polyporales

Terana coerulea and *Sparassis brevipes*

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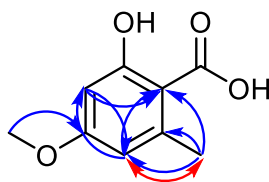
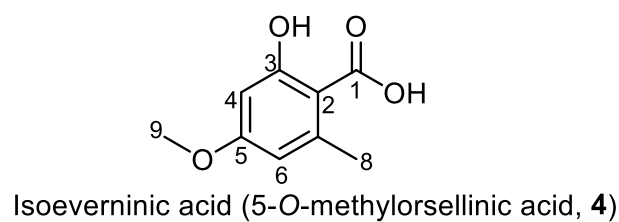


Figure S1. Key ^1H - ^1H COSY, HMBC and ROESY correlations of **4**.

Table S1. ^1H and ^{13}C NMR data of compound (**4**) and isoevernic acid (5-*O*-methylorsellinic acid).^[1,2]

pos.	4		Isoevernic acid ^[1,2]	
	$\delta_{\text{C}},^{a,b}$ type	δ_{H}^a (multi, J [Hz])	$\delta_{\text{C}},^c$ type	δ_{H}^c (multi, J [Hz])
1	173.6, CO		174.1, CO	
2	105.9, C		105.5, C	
3	166.3, C		167.2, C	
4	101.8, CH	6.15 d (2.5)	99.4, CH	6.33 d (2.5)
5	164.0, C		165.1, C	
6	112.6, CH	6.20 dd (2.5, 1.0)	111.4, CH	6.35 d (2.5)
7	144.7, C		144.5, C	
8	24.4, CH ₃	2.44 s	24.3, CH ₃	2.57 s
9	52.26, CH ₃	3.87 s	55.7, CH ₃	3.80 s

[1] Y. Nishitoba, H. Nishimura, T. Nishiyama, J. Mizutani, *Phytochemistry* **1987**, 26, 3181-3185.

[2] J. Guo, Z.-L. Li, A.-L. Wang, X.-Q. Liu, J. Wang, X. Guo, Y.-K. Jing, H.-M. Hua, *Planta Med.* **2011**, 77, 2042-2046..

^a Measured in methanol-*d*₄ at 125 MHz for ^{13}C and 500 MHz for ^1H .

^b Assignment confirmed by HMBC and HSQC spectra.

^c Measured in chloroform-*d* at 75 MHz for ^{13}C and 300 MHz for ^1H .

Generic Display Report

Analysis Info

Analysis Name S:\DATA\AmaZon\wsu20_Winnier Sum Chemutal\IHI CRUDEV\IHI769\769 HPLC FRACTIONS\IHI769
Method R3F4F2F4_BB4_01_47253.d Operator tti
Sample Name IHI769 R3F4F2F4 Instrument amaZon speed
Comment

Acquisition Date 18.05.2023 16:57:46

Operator tti
Instrument amaZon speed

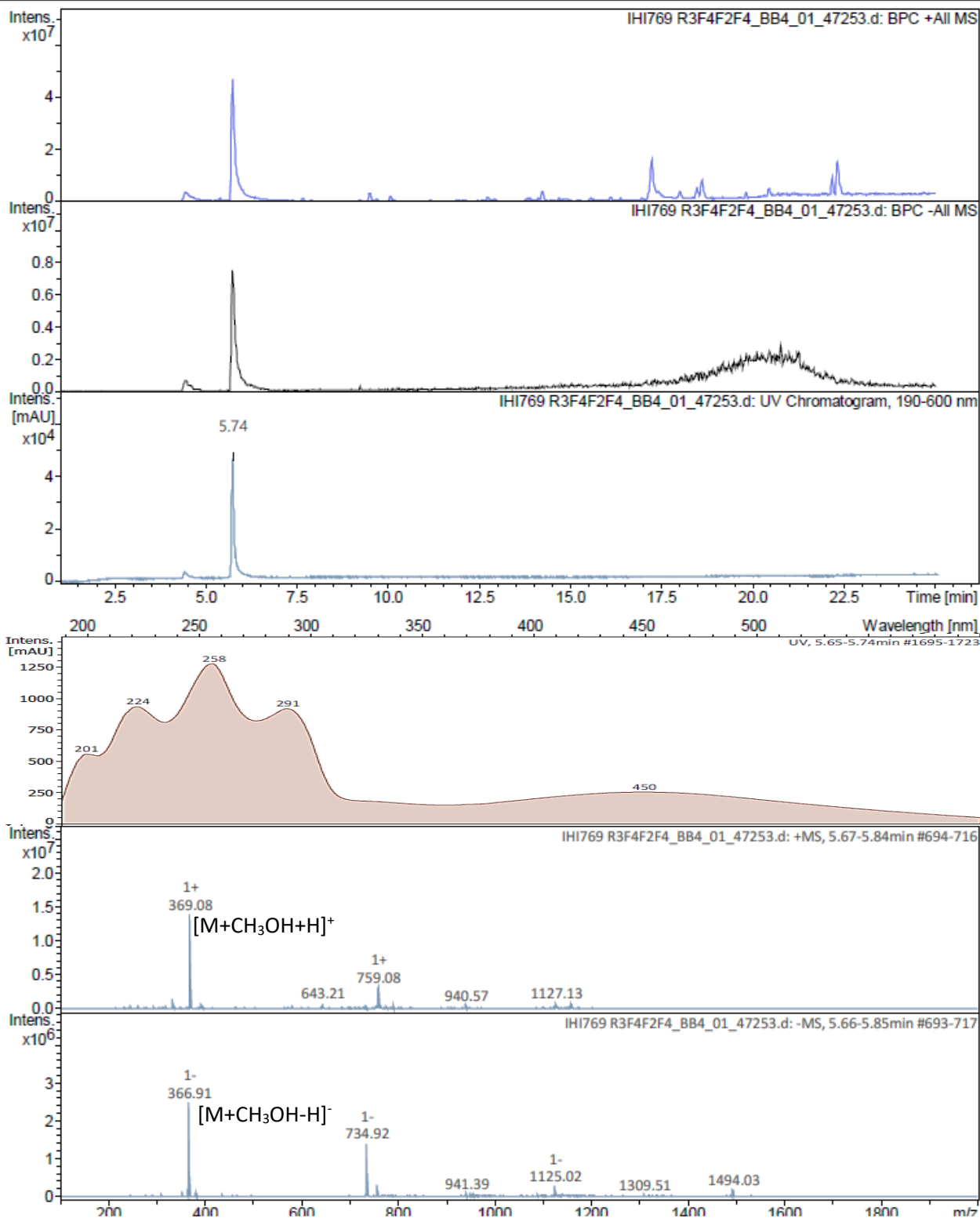


Figure S2. LR-ESI-MS of 1.

Generic Display Report

Analysis Info

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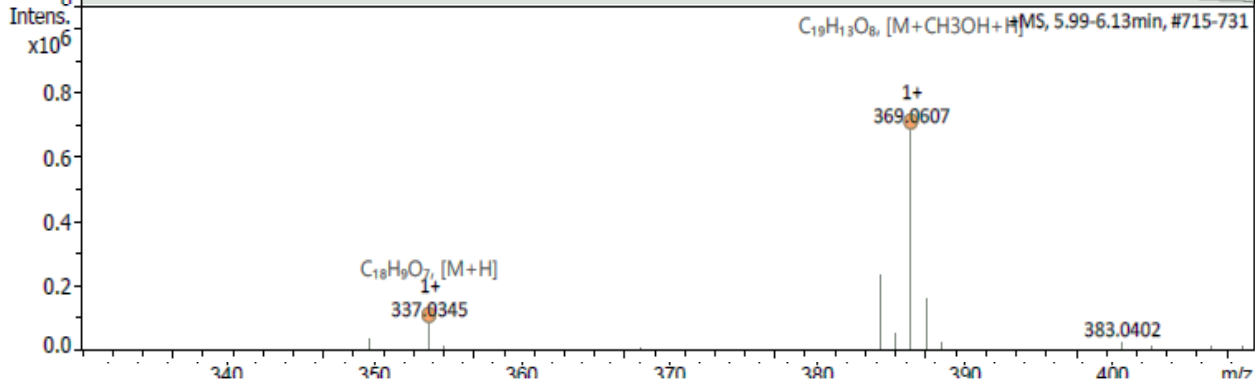
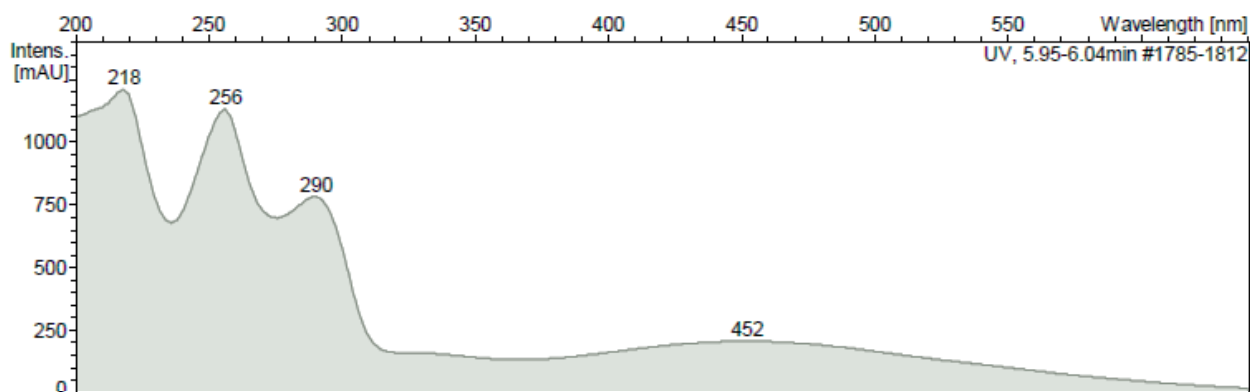
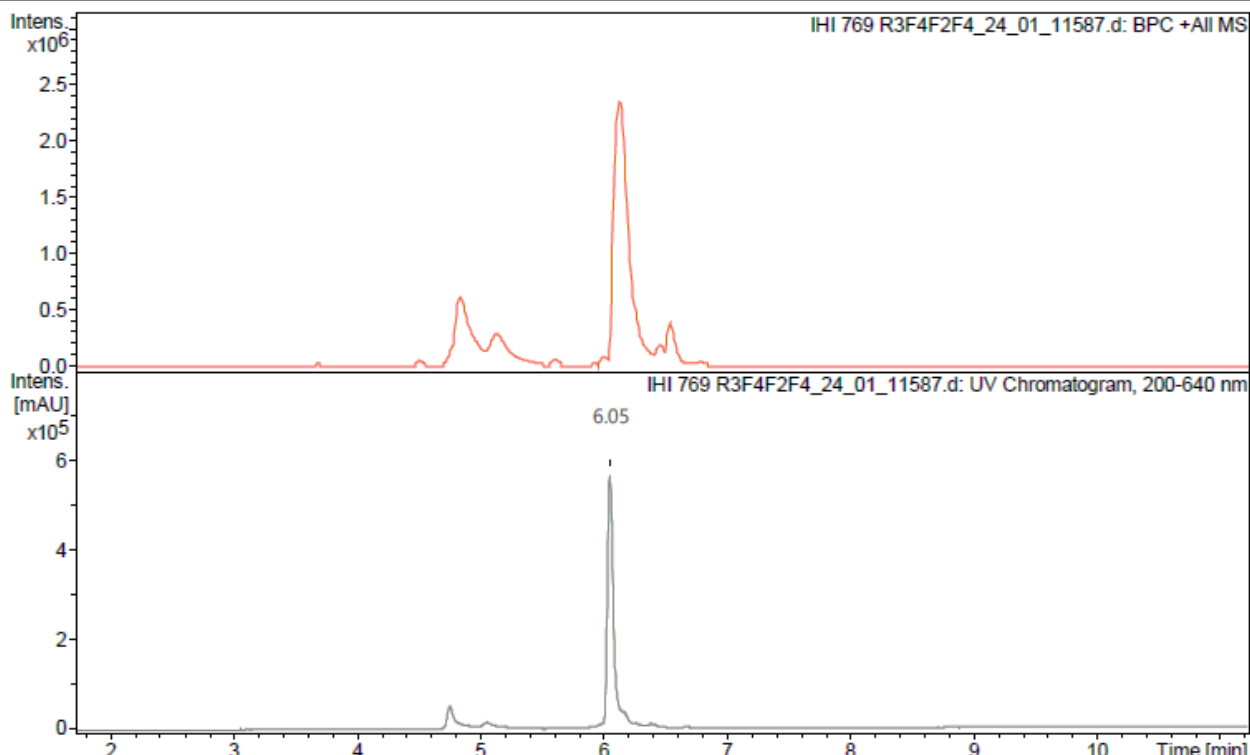


Figure S3. HR-ESI-MS of 1.

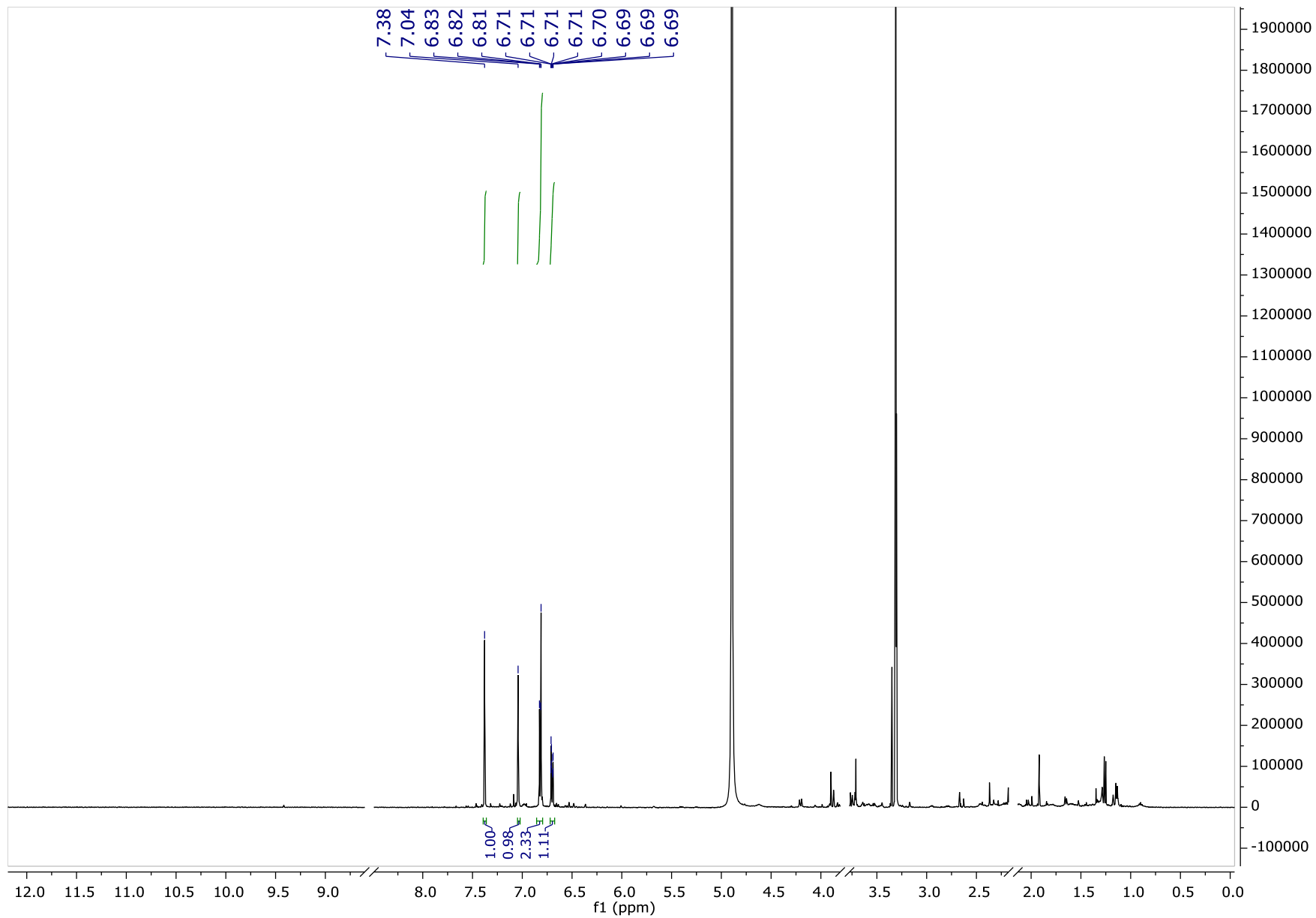


Figure S4. ¹H NMR spectrum of **1** in methanol-*d*₄ at 500 MHz.

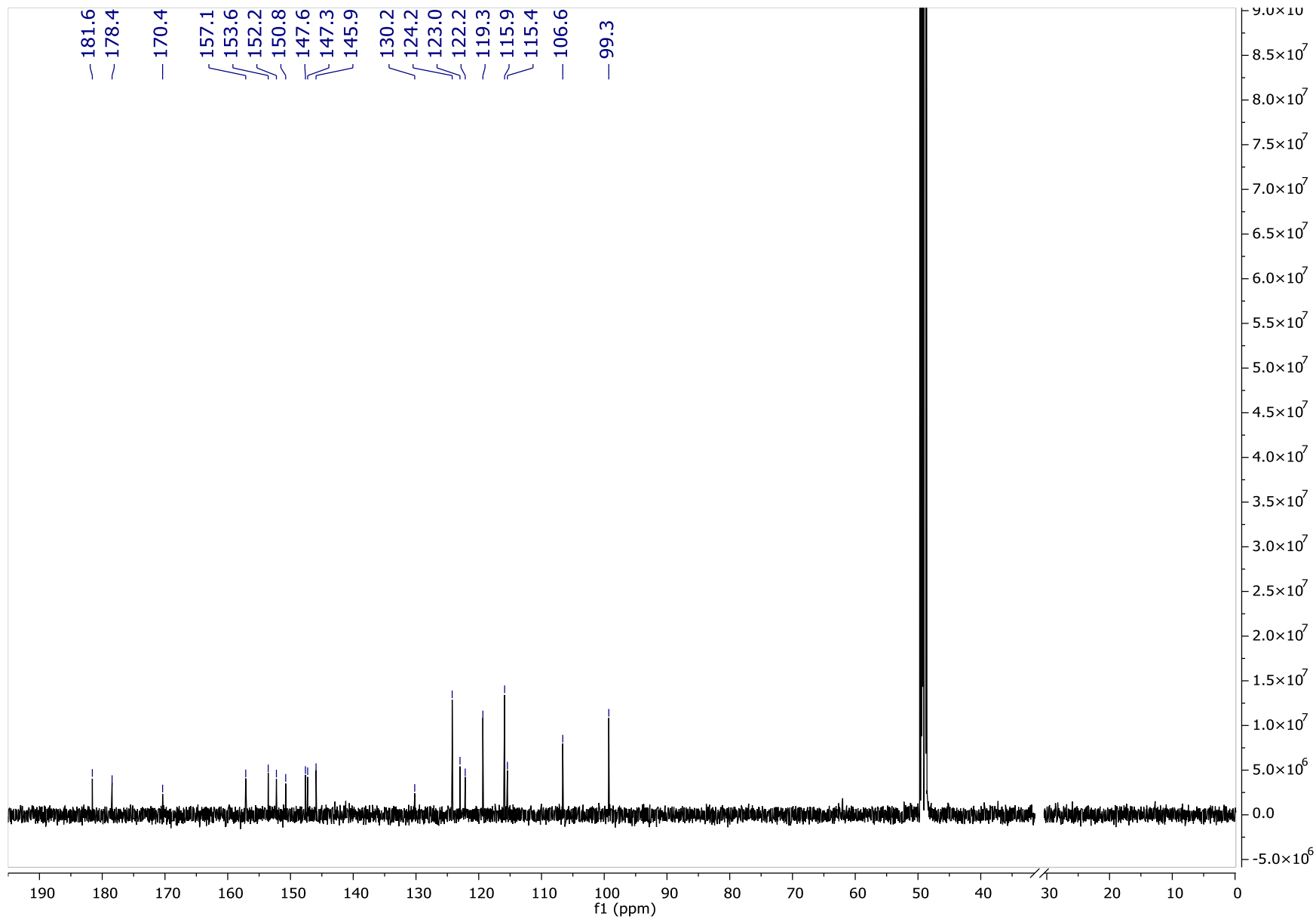


Figure S5. ^{13}C NMR spectrum of **1** in methanol- d_4 at 125 MHz.

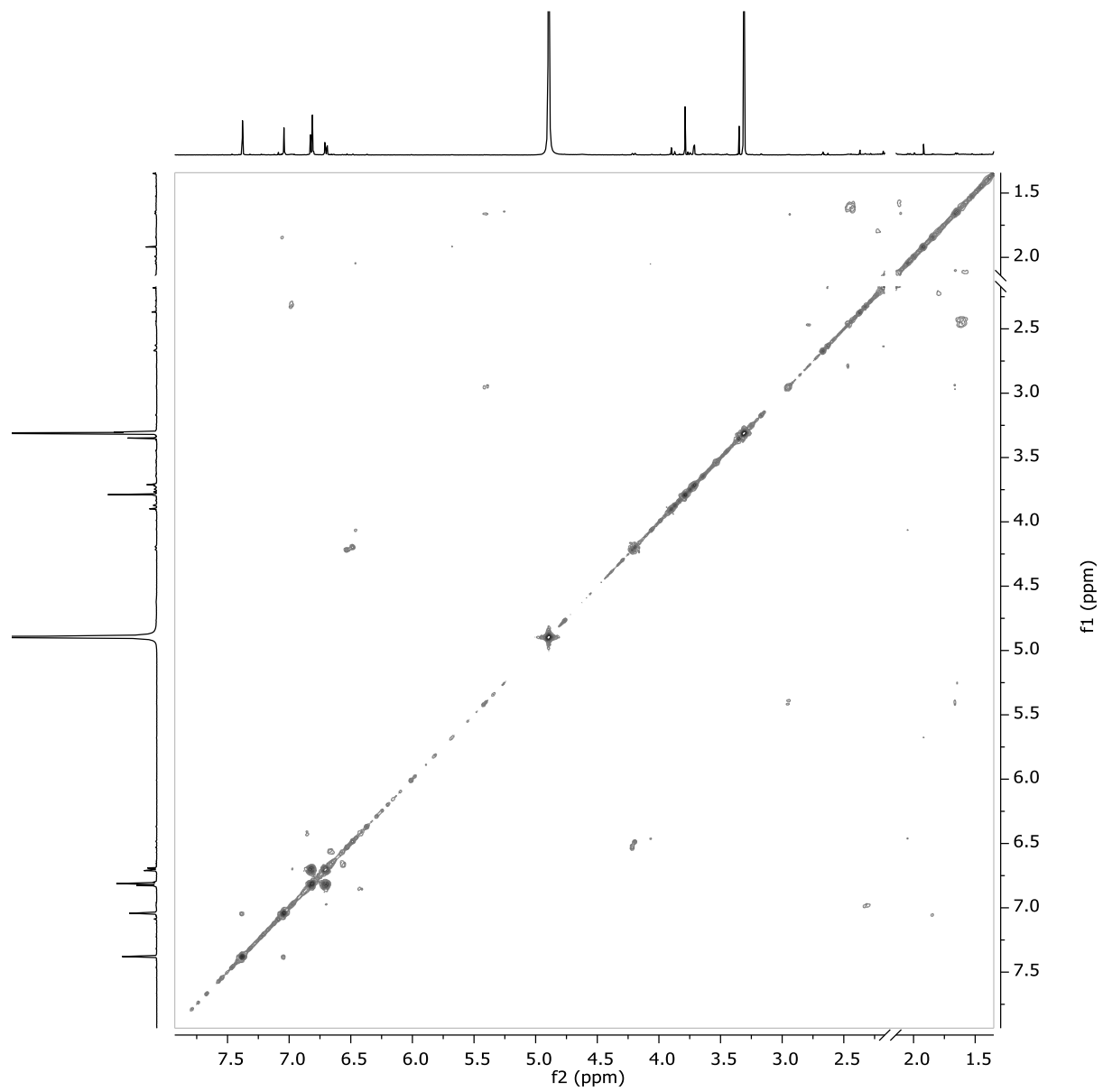


Figure S6. ^1H - ^1H NMR spectrum of **1** in CD_3OD at 500 MHz.

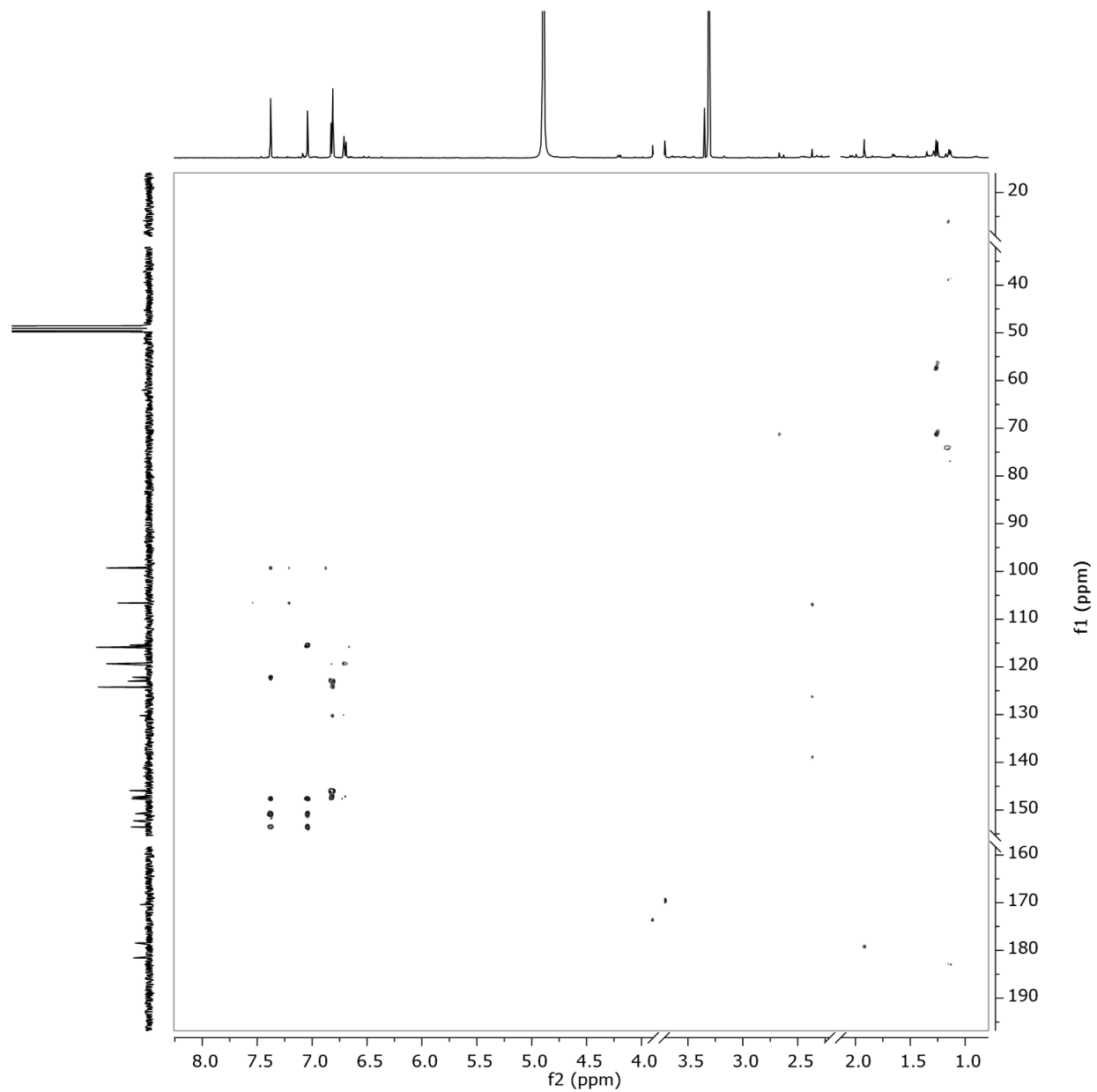


Figure S7. HMBC spectrum of **1** in methanol-*d*₄ at 500 MHz.

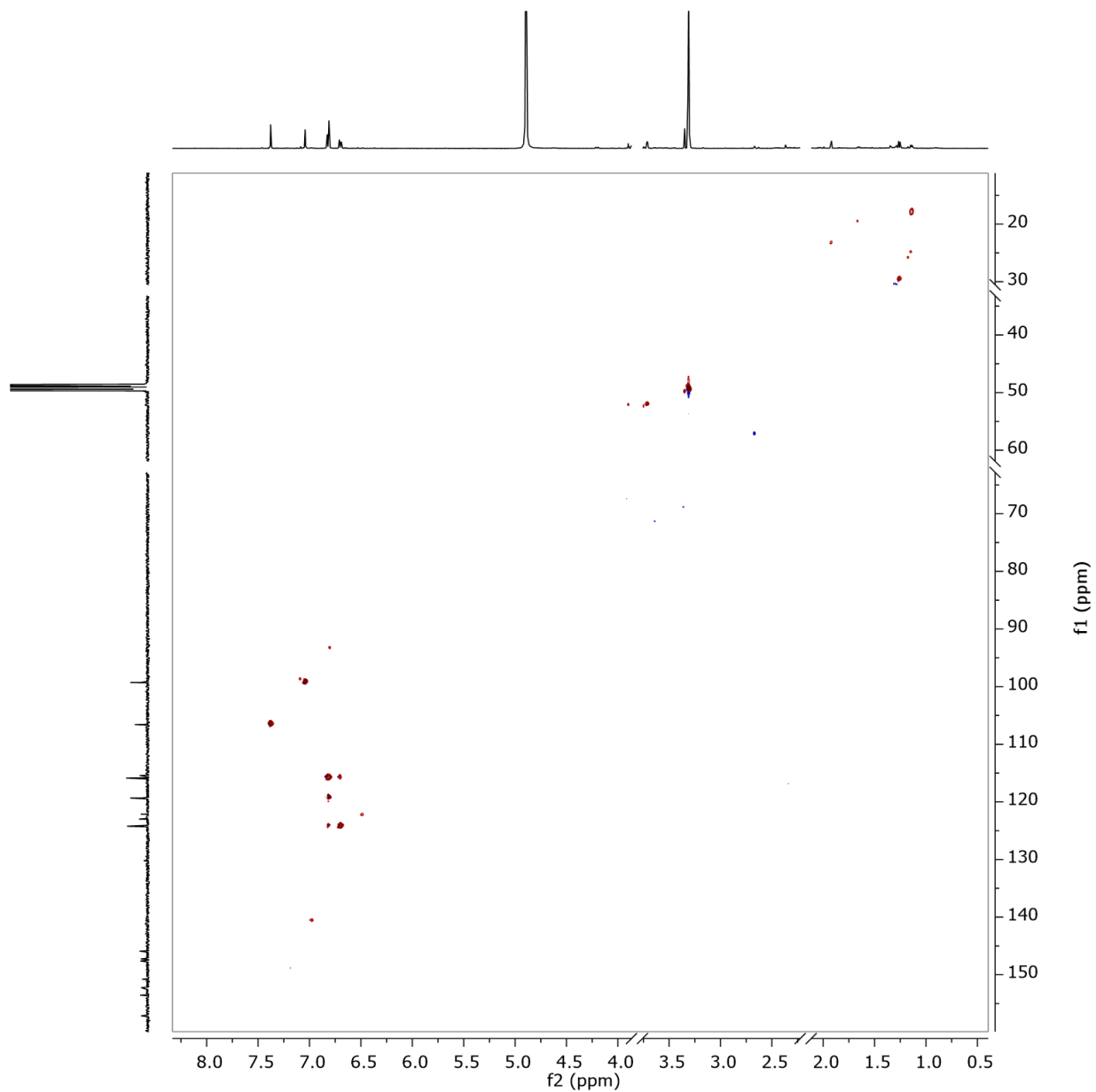


Figure S8. HSQC spectrum of **1** in methanol-*d*₄ at 500 MHz.

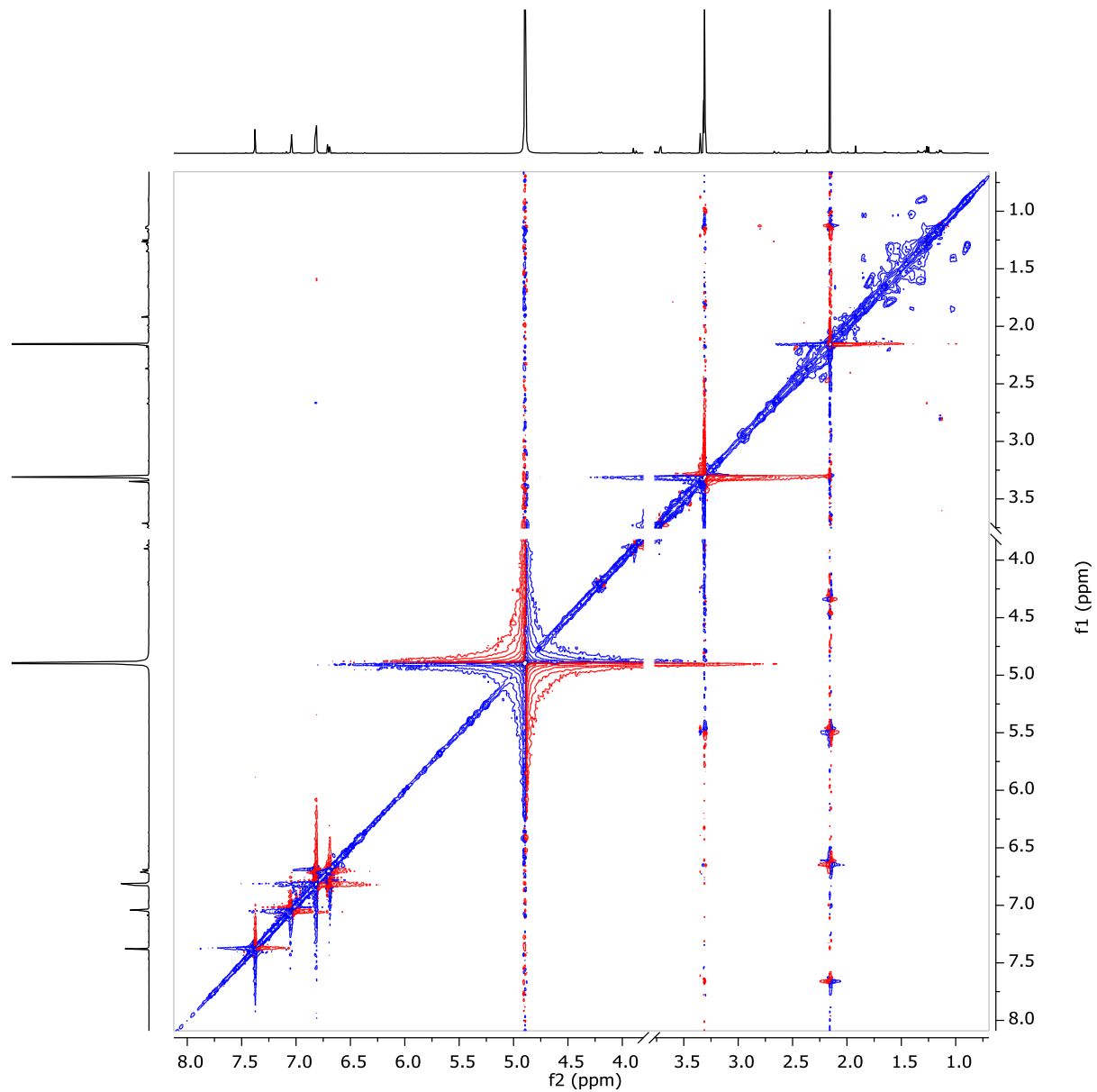


Figure S9. ROESY spectrum of **1** in methanol-*d*₄ at 500 MHz.

Display Report

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Sample Name IHI 752B R2F1
Comment

Acquisition Date 22.05.2023 16:58:12

Operator tti
Instrument amaZon speed

Acquisition Parameter

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SPS Target Mass	1000 m/z	Averages	6 Spectra		

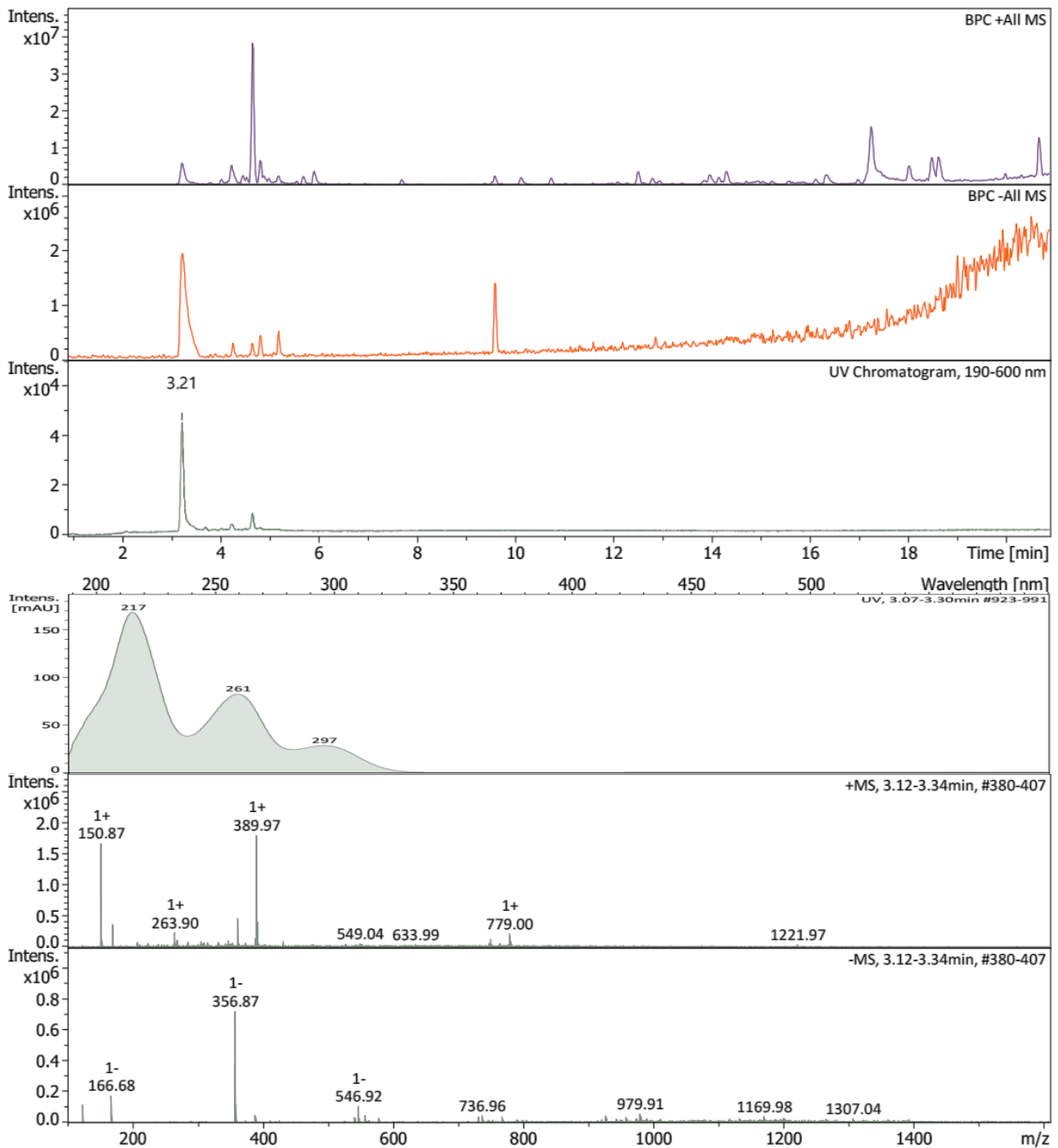


Figure S10. LR-ESI-MS of 2.

Display Report

Analysis Info

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Comment Screening01
Waters Acquity UPLC BEH C_18 1,7um 2.1x50mm

Acquisition Date 23.05.2023 18:58:34

Operator ate06
Instrument maXis

Acquisition Parameter

Ion Polarity Positive

SPS Target Mass

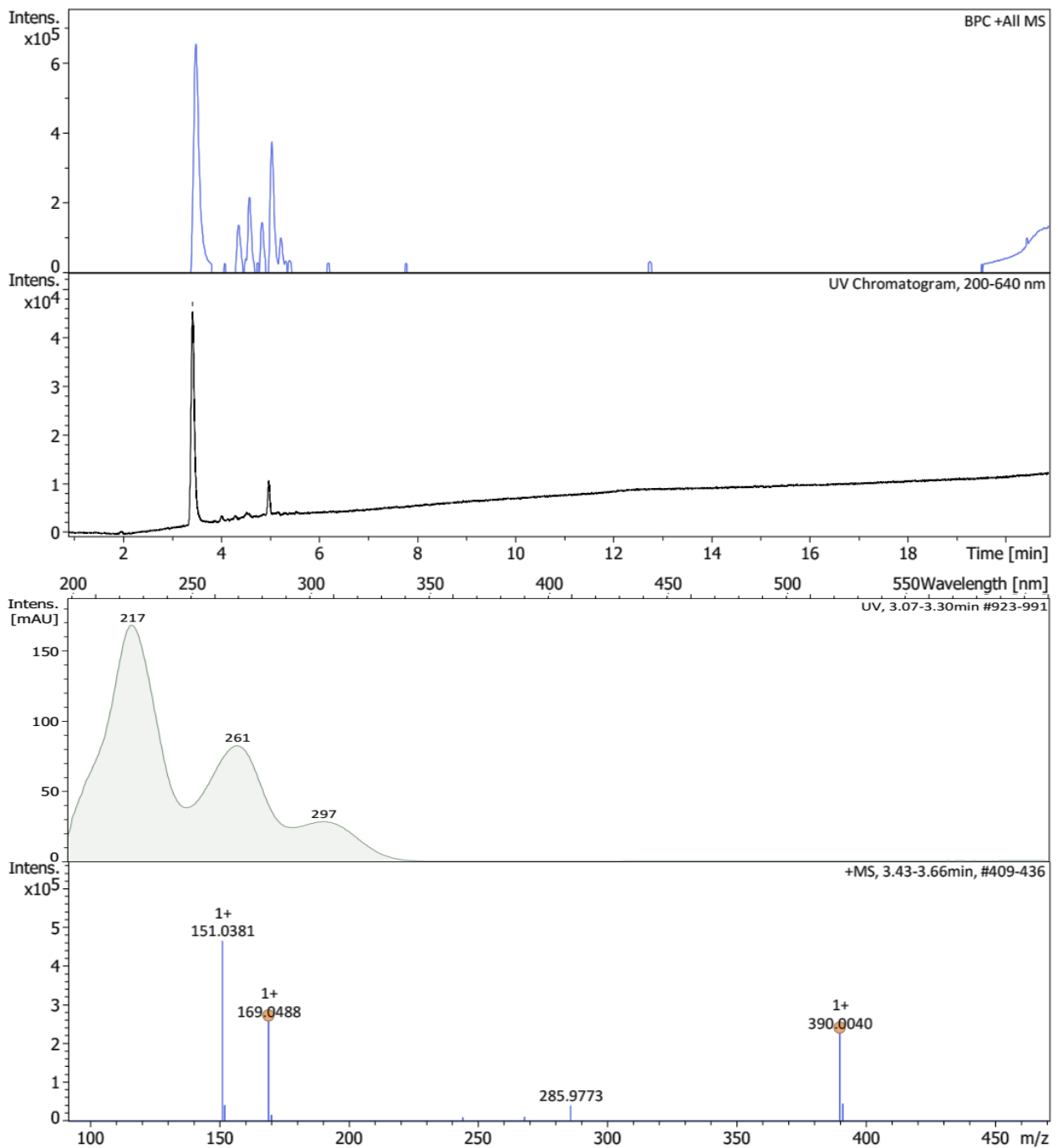


Figure S11. HR-ESI-MS of 2.

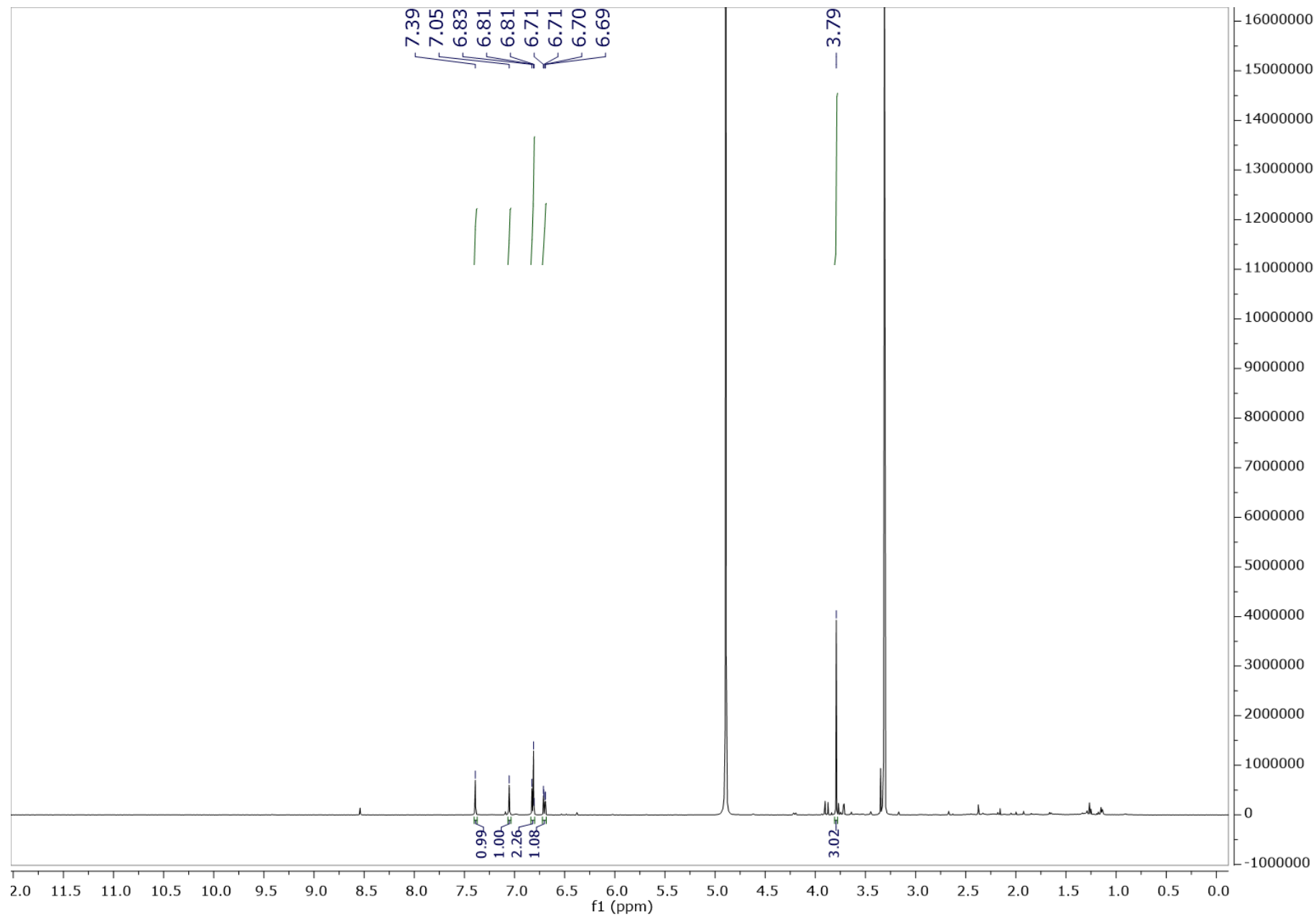


Figure S12. ^1H NMR spectrum of **2** in methanol- d_4 at 500 MHz.

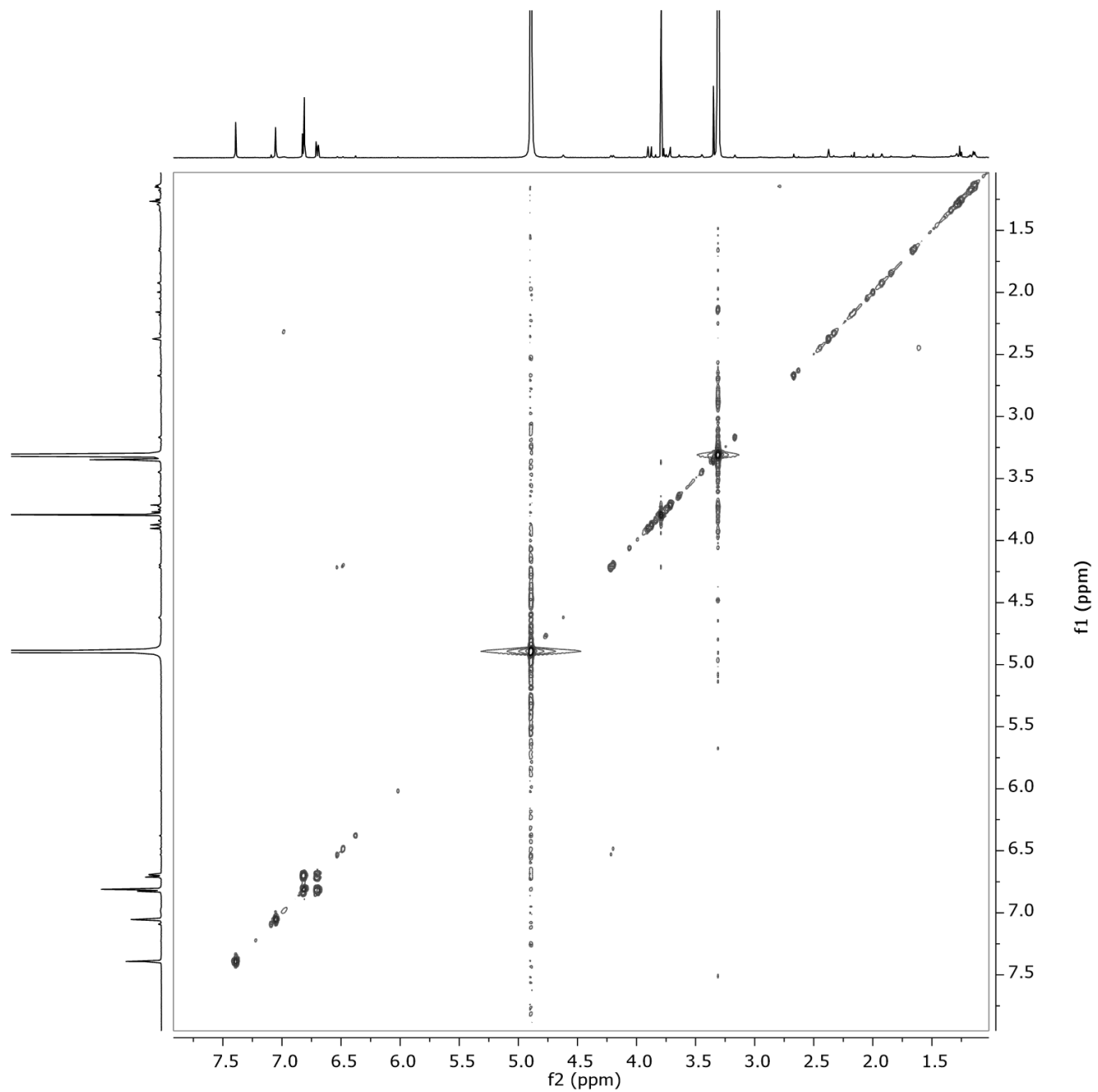


Figure S13. ^1H - ^1H COSY spectrum of **2** in methanol- d_4 at 500 MHz.

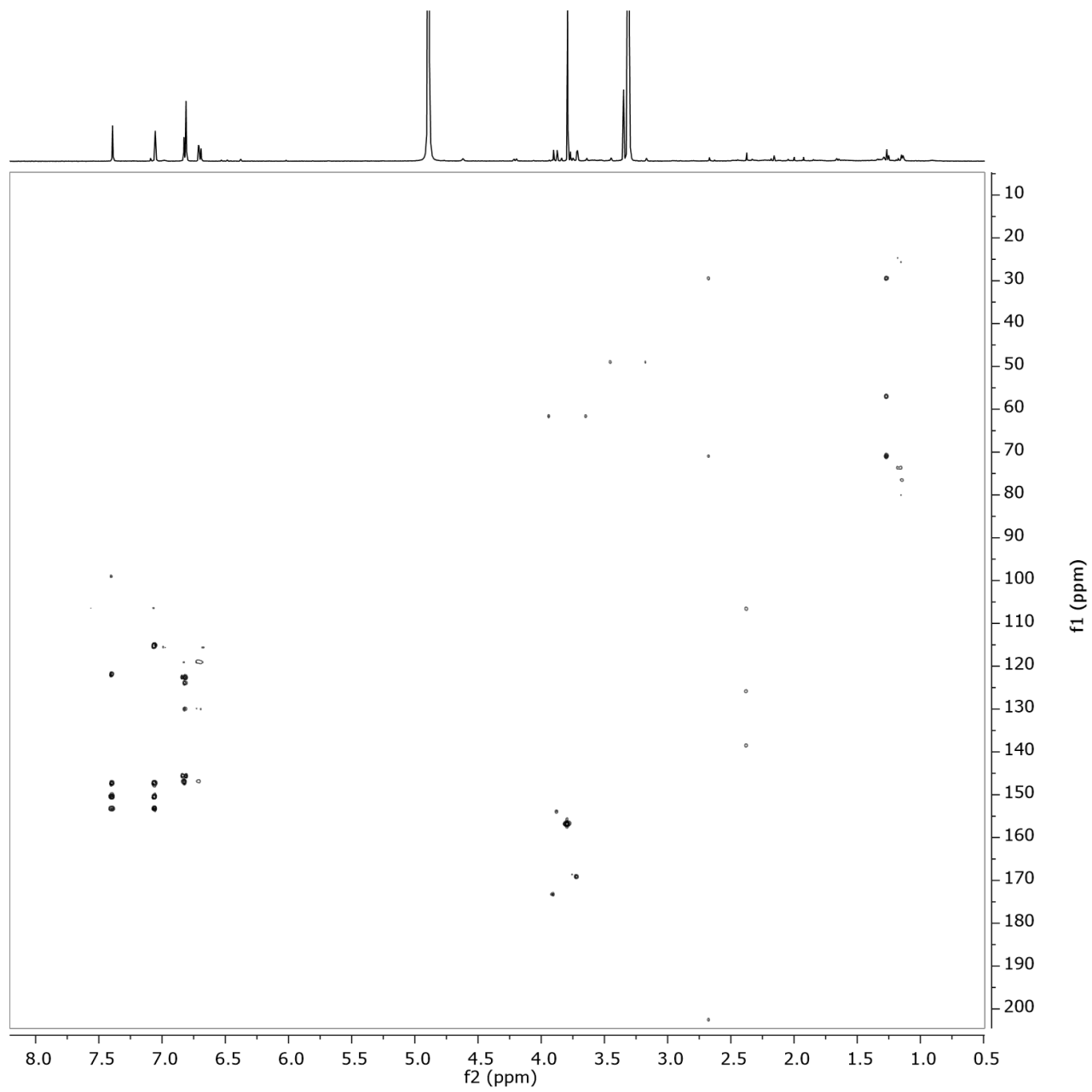


Figure S14. HMBC spectrum of **2** in methanol- d_4 at 500 MHz.

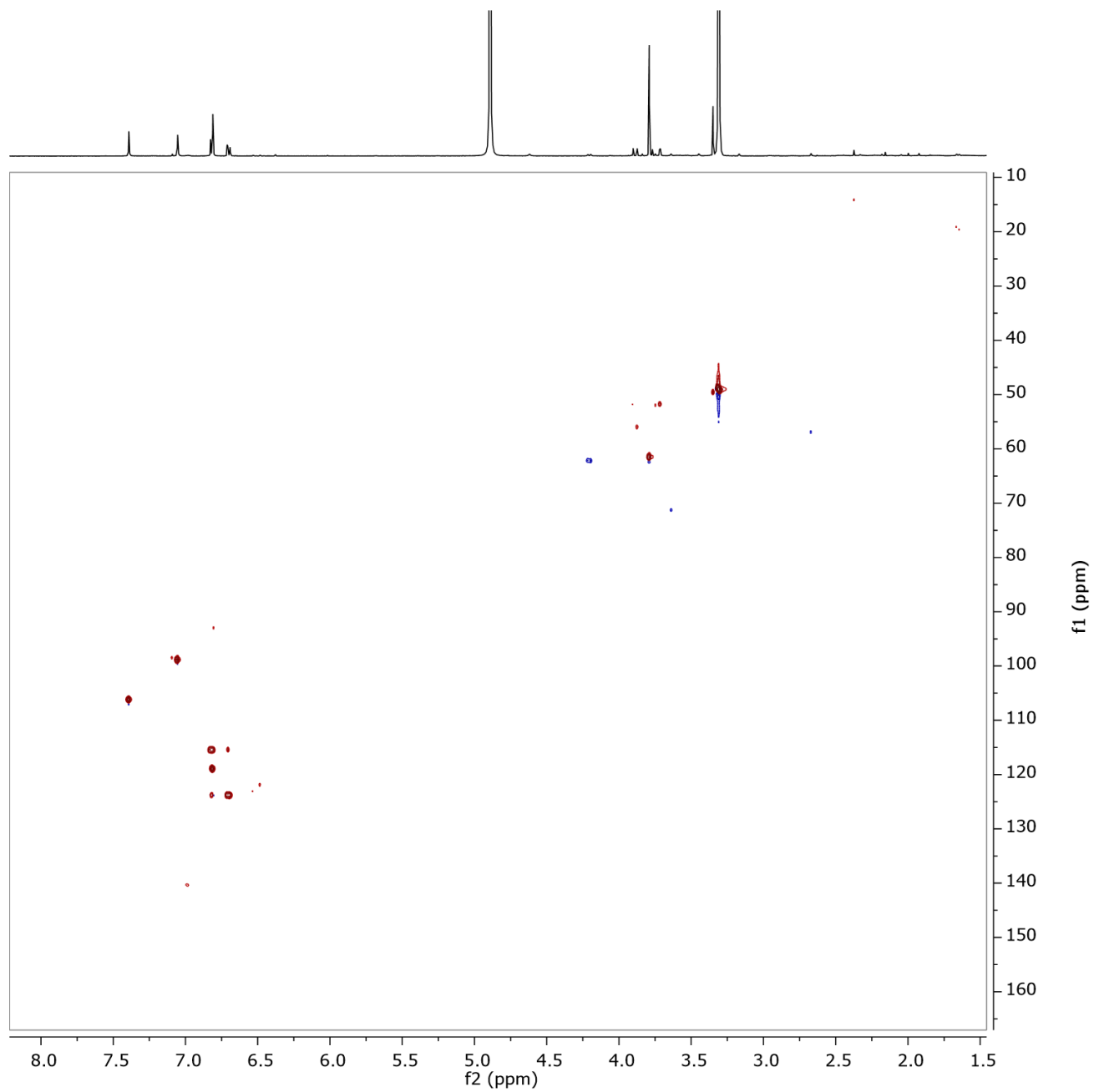


Figure S15. HSQC spectrum of **2** in methanol-*d*₄ at 500 MHz.

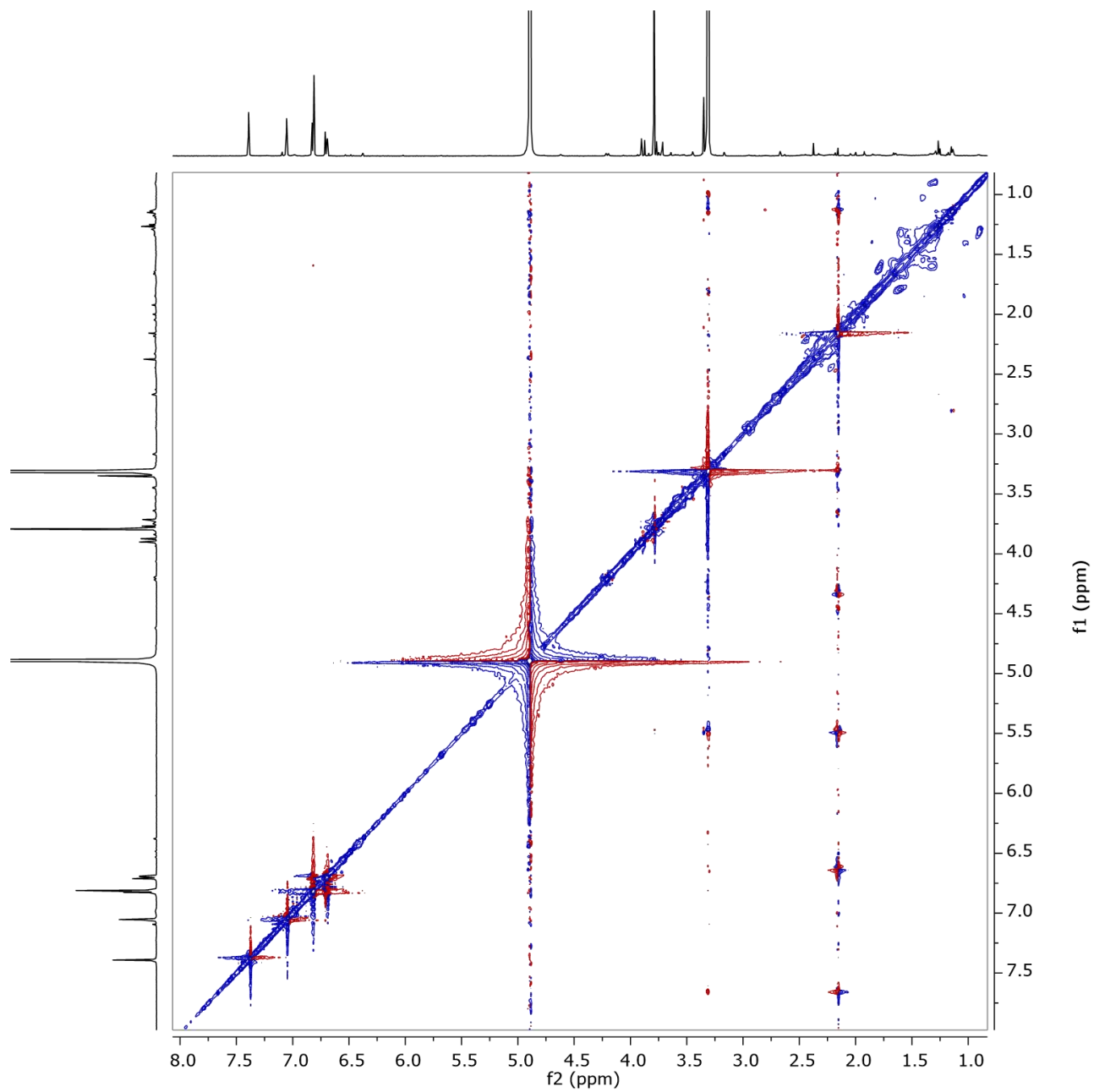


Figure S16. ROESY spectrum of **2** in methanol- d_4 at 500 MHz

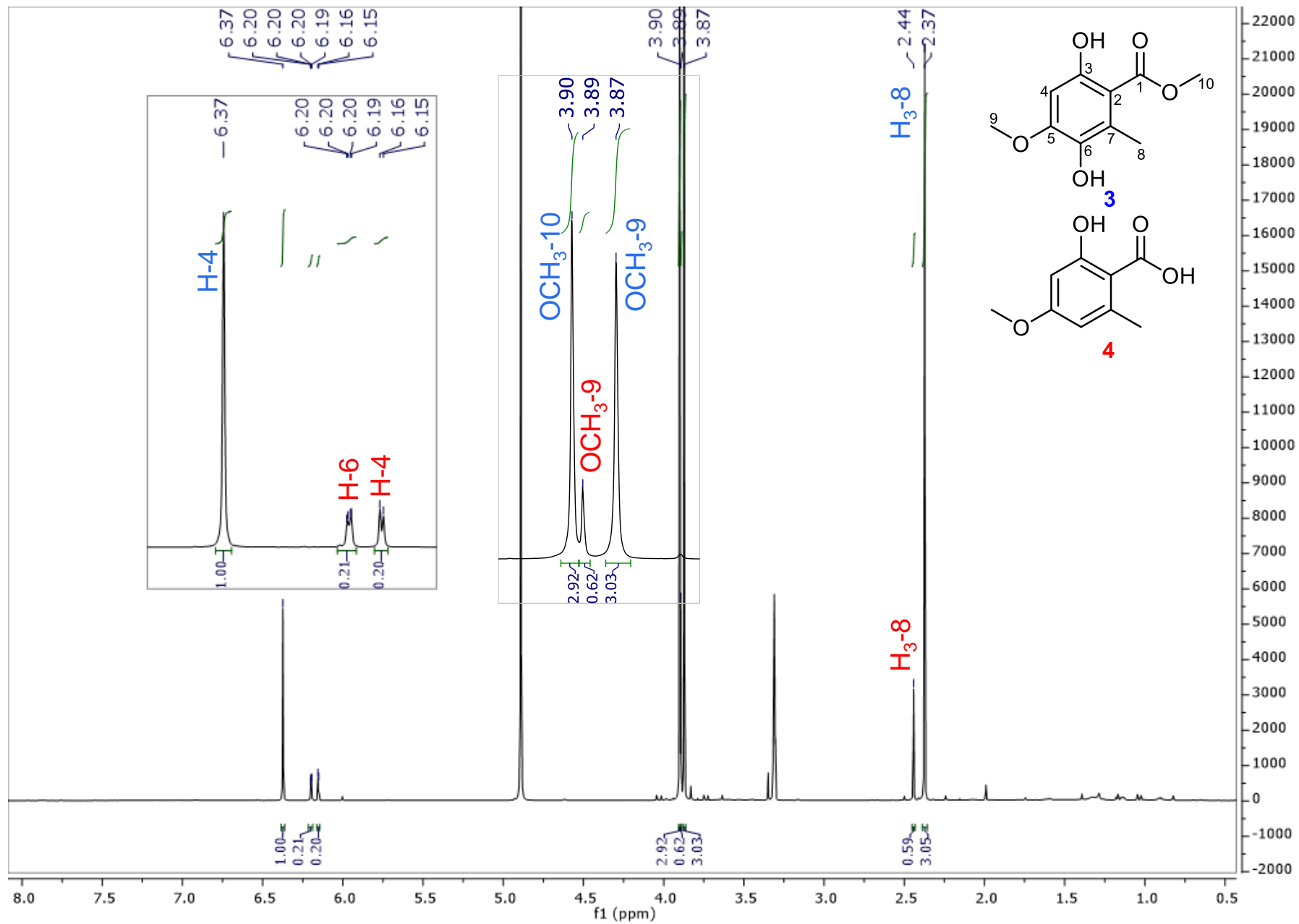


Figure S17. ^1H NMR spectrum of **3** and **4** in methanol- d_4 at 500 MHz.

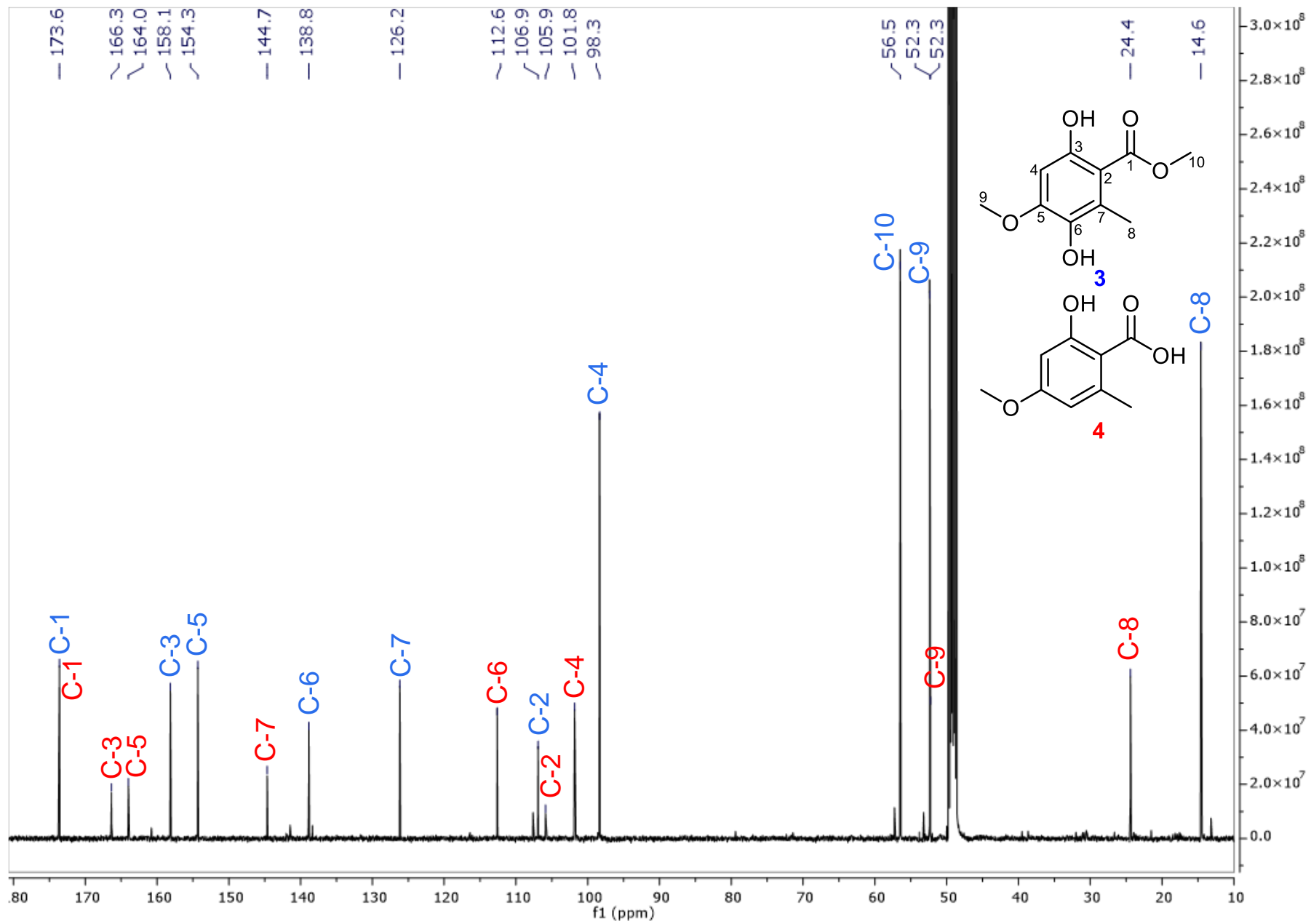


Figure S18. ^{13}C NMR spectrum of **3** and **4** in methanol- d_4 at 125 MHz.

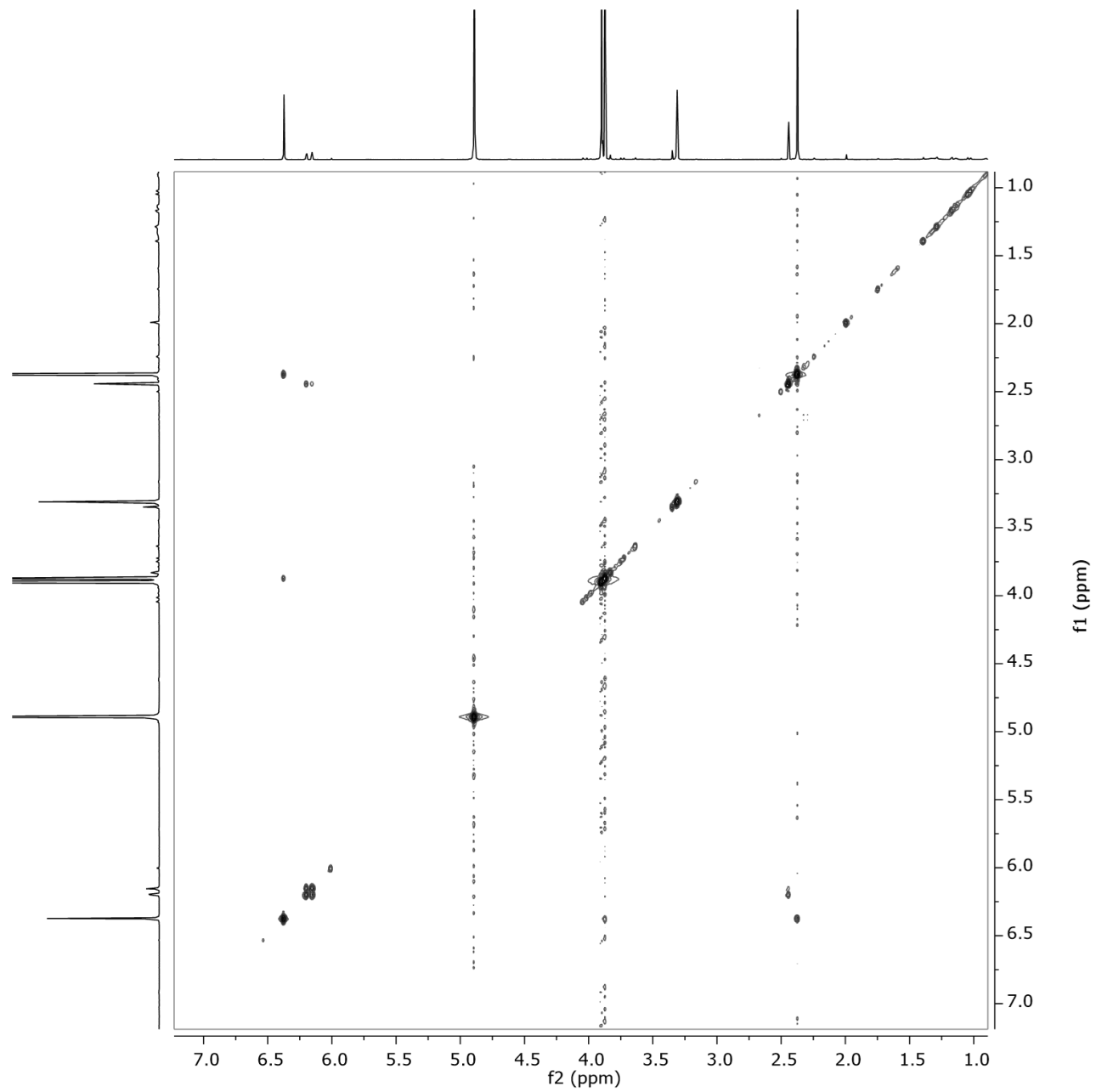


Figure S19. ^1H - ^1H COSY spectrum of **3** and **4** in methanol- d_4 at 500 MHz.

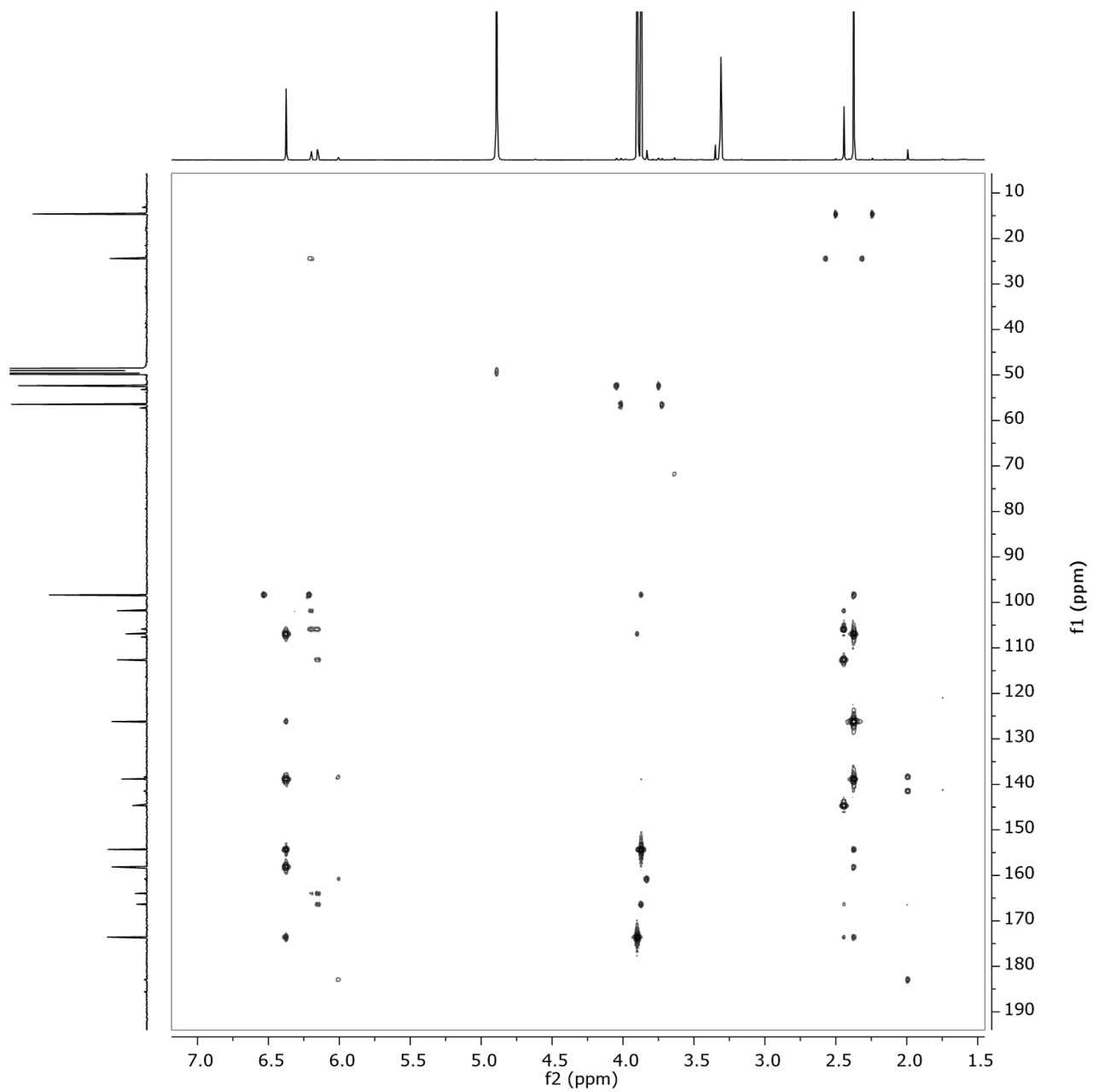


Figure S20. HMBC spectrum of **3** and **4** in methanol-*d*₄ at 500 MHz.

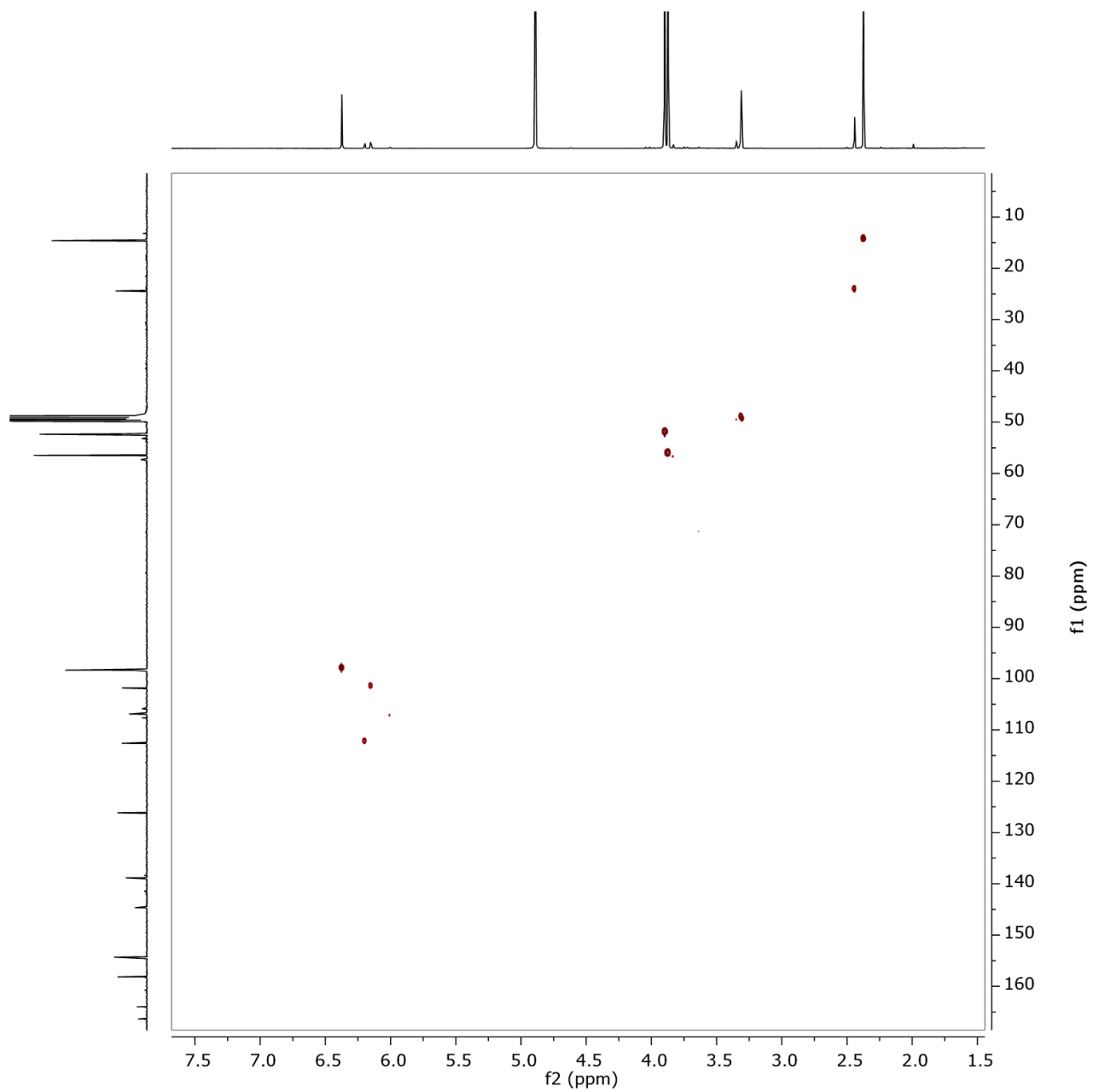


Figure S21. HSQC spectrum of **3** and **4** in methanol-*d*₄ at 500 MHz.

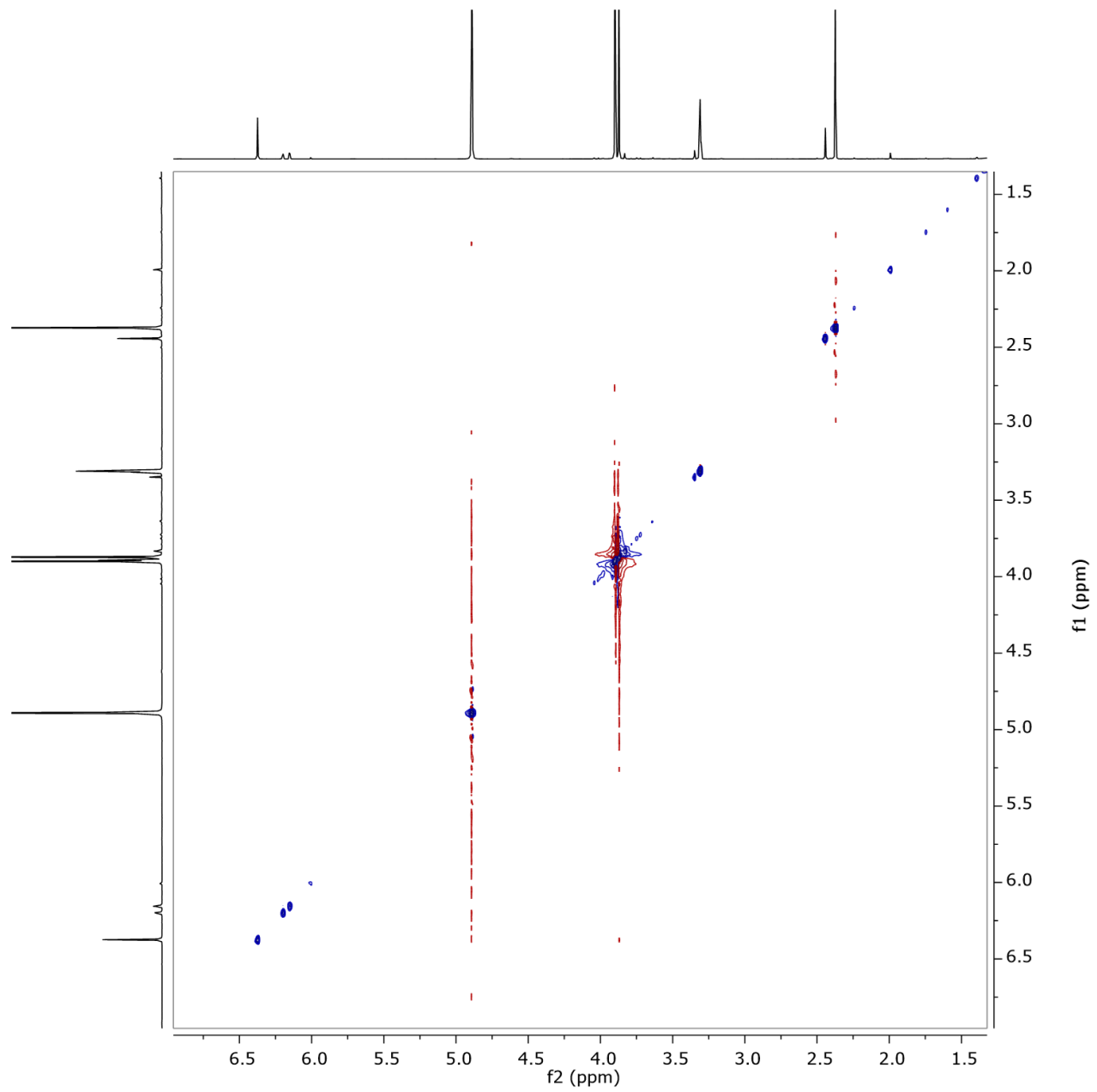


Figure S22. ROESY spectrum of **3** and **4** in methanol-*d*₄ at 500 MHz.