

SUPPLEMENTARY MATERIALS FOR:

**Dentifragilones A–B and Other Benzoic Acid Derivatives From the European
Basidiomycete *Dentipellis fragilis***

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Display Report

Analysis Info

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Method 27278.m
Sample Name Dent F4F1
Comment

Acquisition Date 24.03.2021 16:04:52

Operator esu
Instrument amaZon speed

Acquisition Parameter

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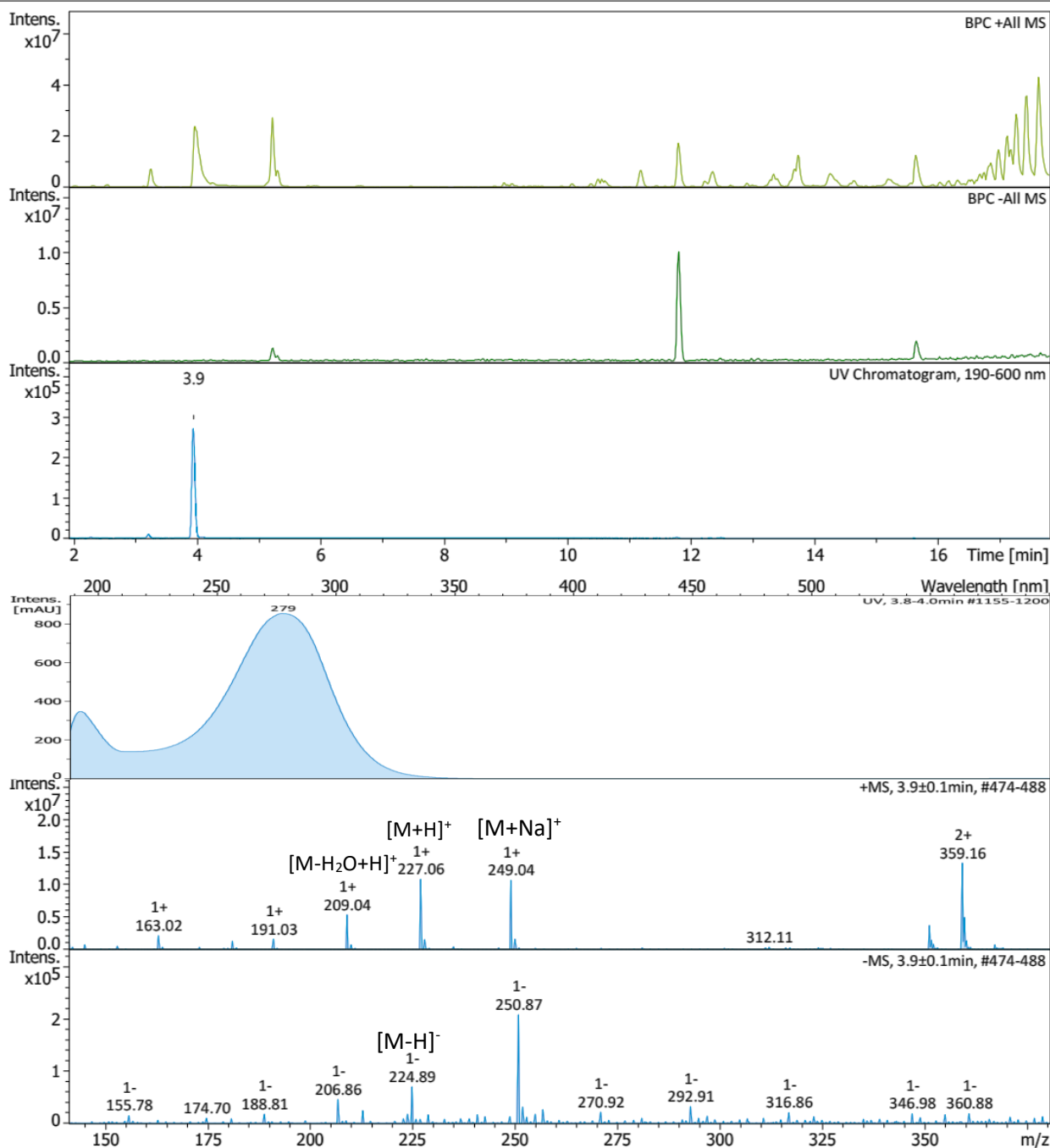


Figure S1. LR-ESI-MS of 1.

Display Report

Analysis Info

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Comment Screening01
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Acquisition Date 07.06.2021 16:39:26

Operator ate06

Instrument maXis

Acquisition Parameter

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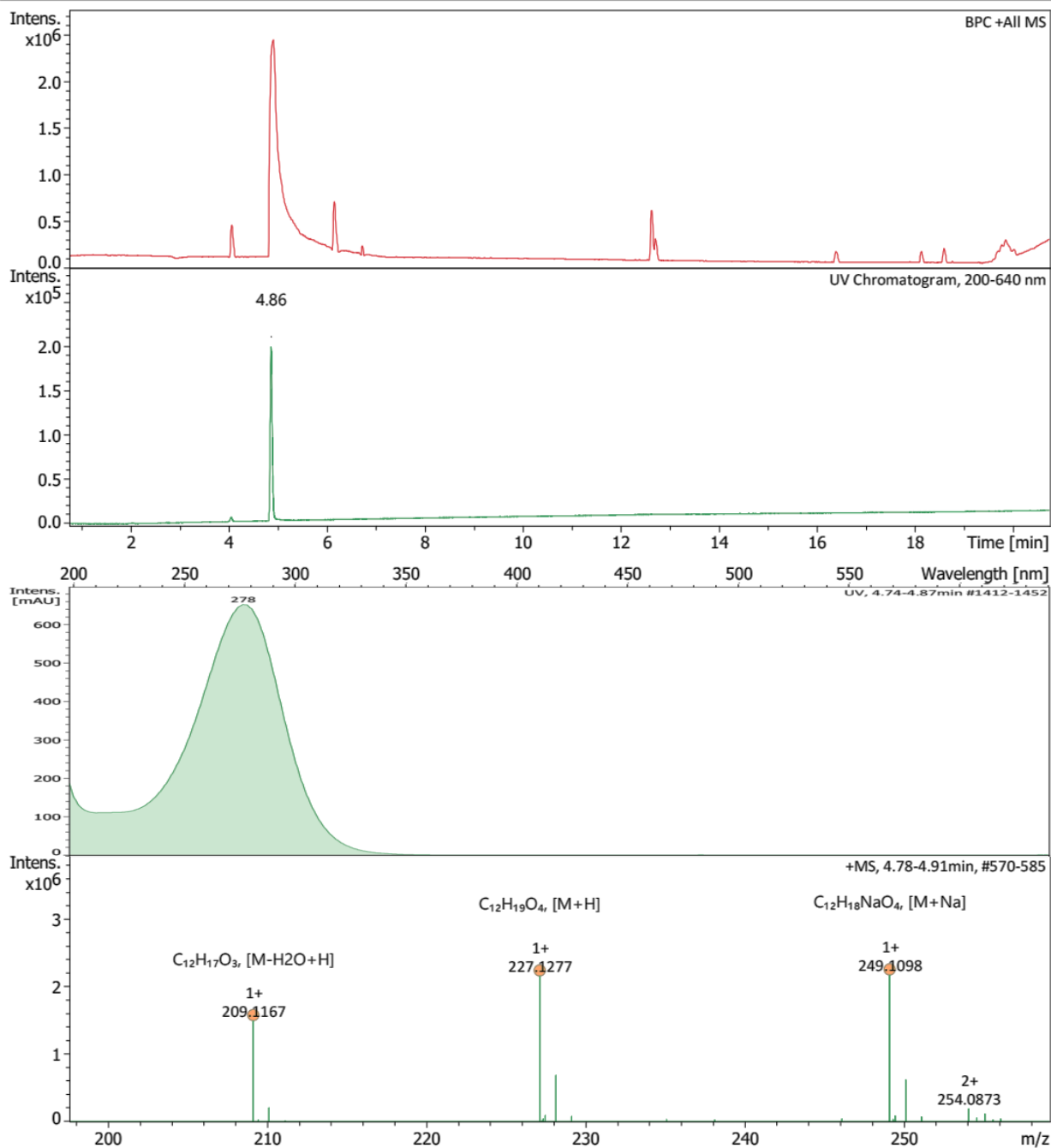


Figure S2. HR-ESI-MS of 1.

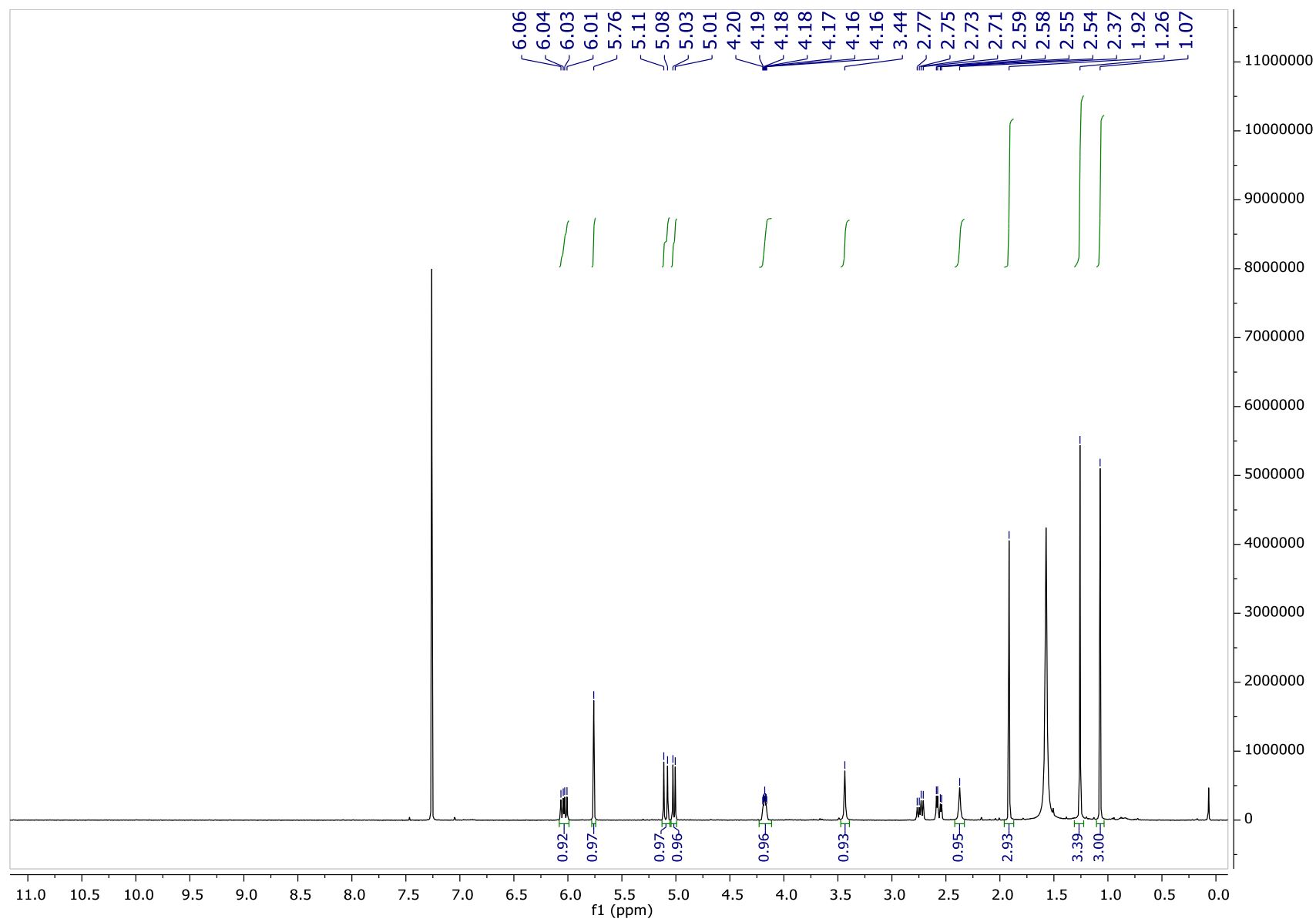


Figure S3. ^1H NMR spectrum of **1** in chloroform-*d* at 500 MHz.

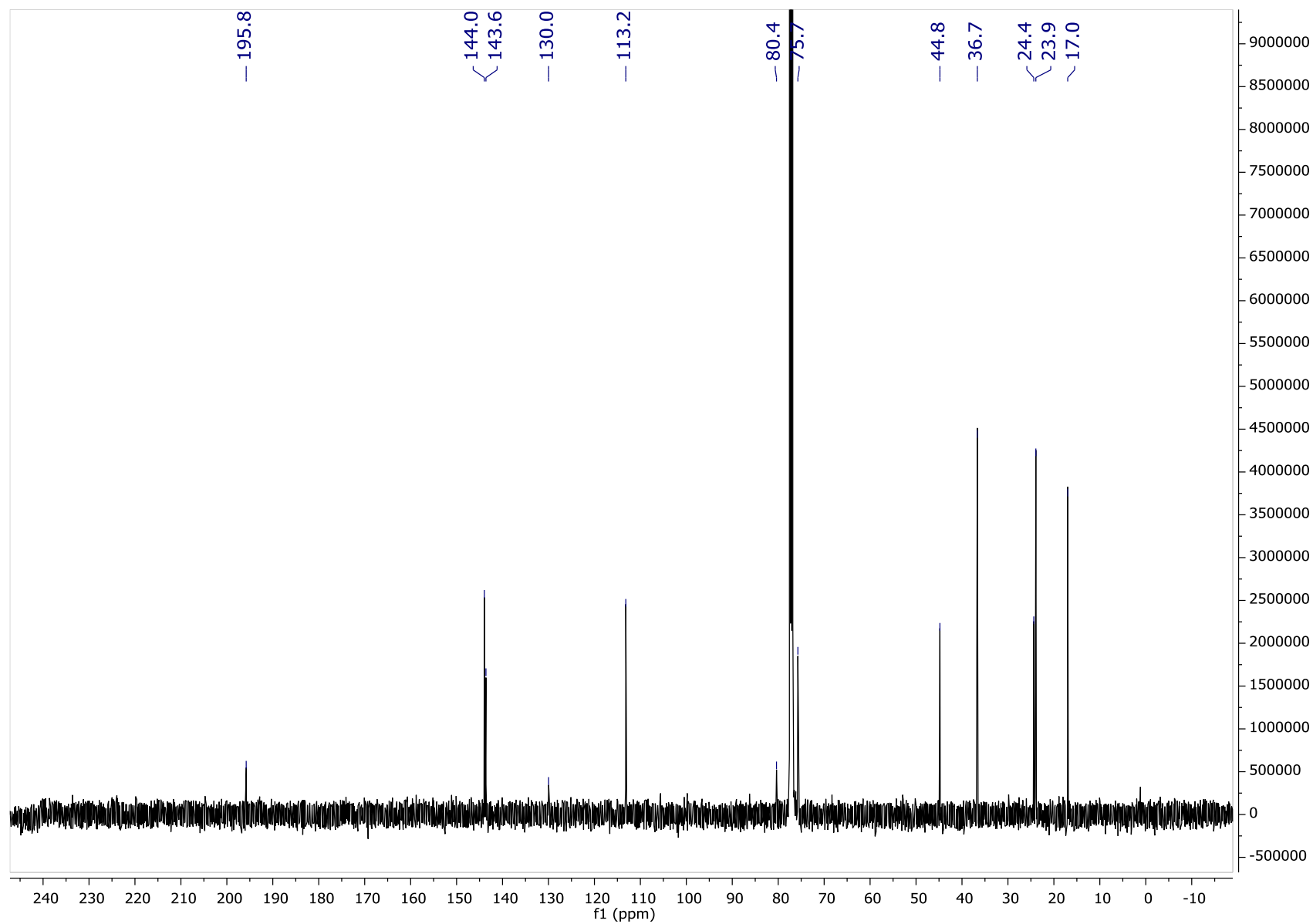


Figure S4. ^{13}C NMR spectrum of **1** in chloroform-*d* at 125 MHz.

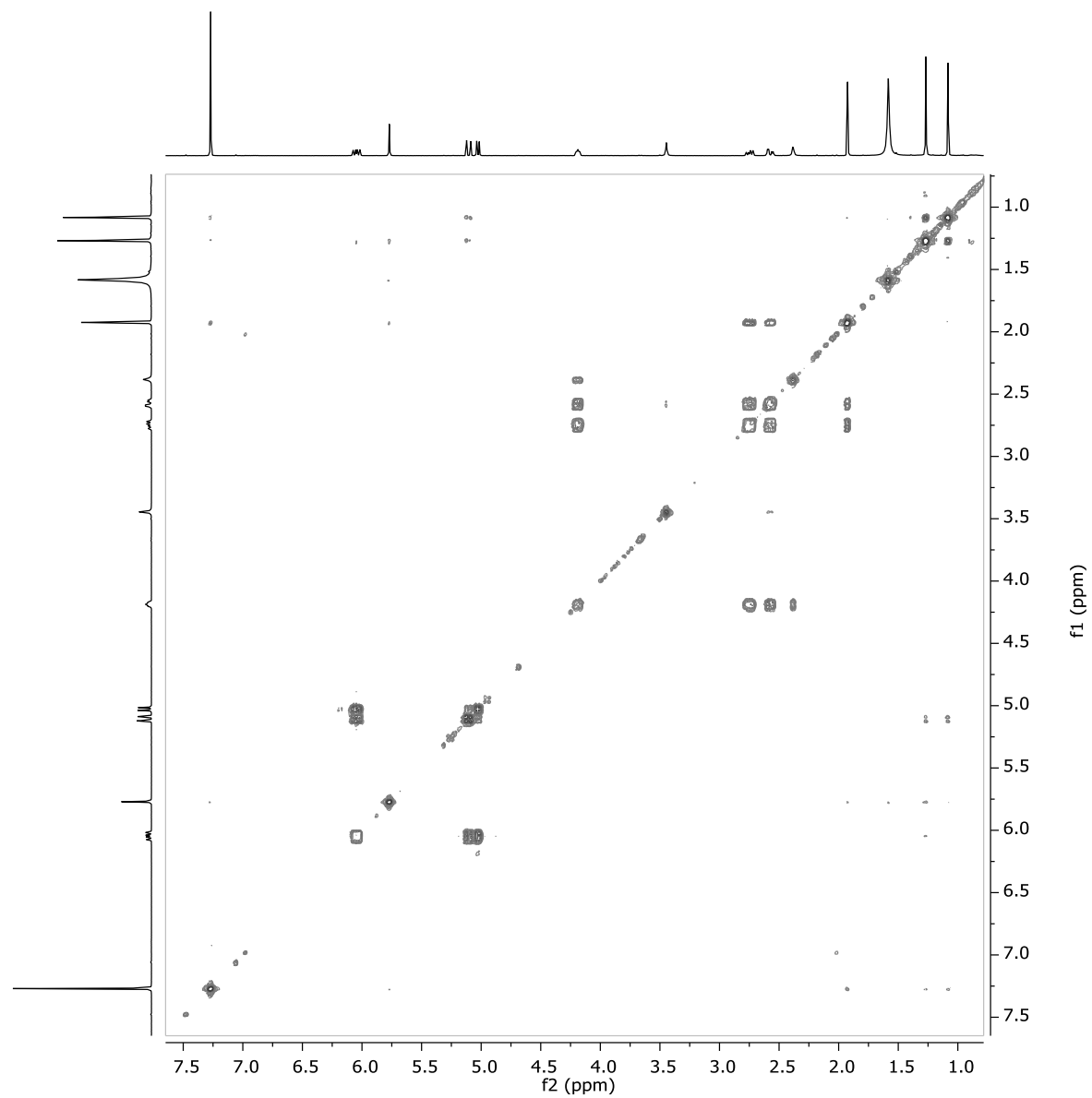


Figure S5. ^1H - ^1H COSY spectrum of **1** in chloroform-*d* at 500 MHz.

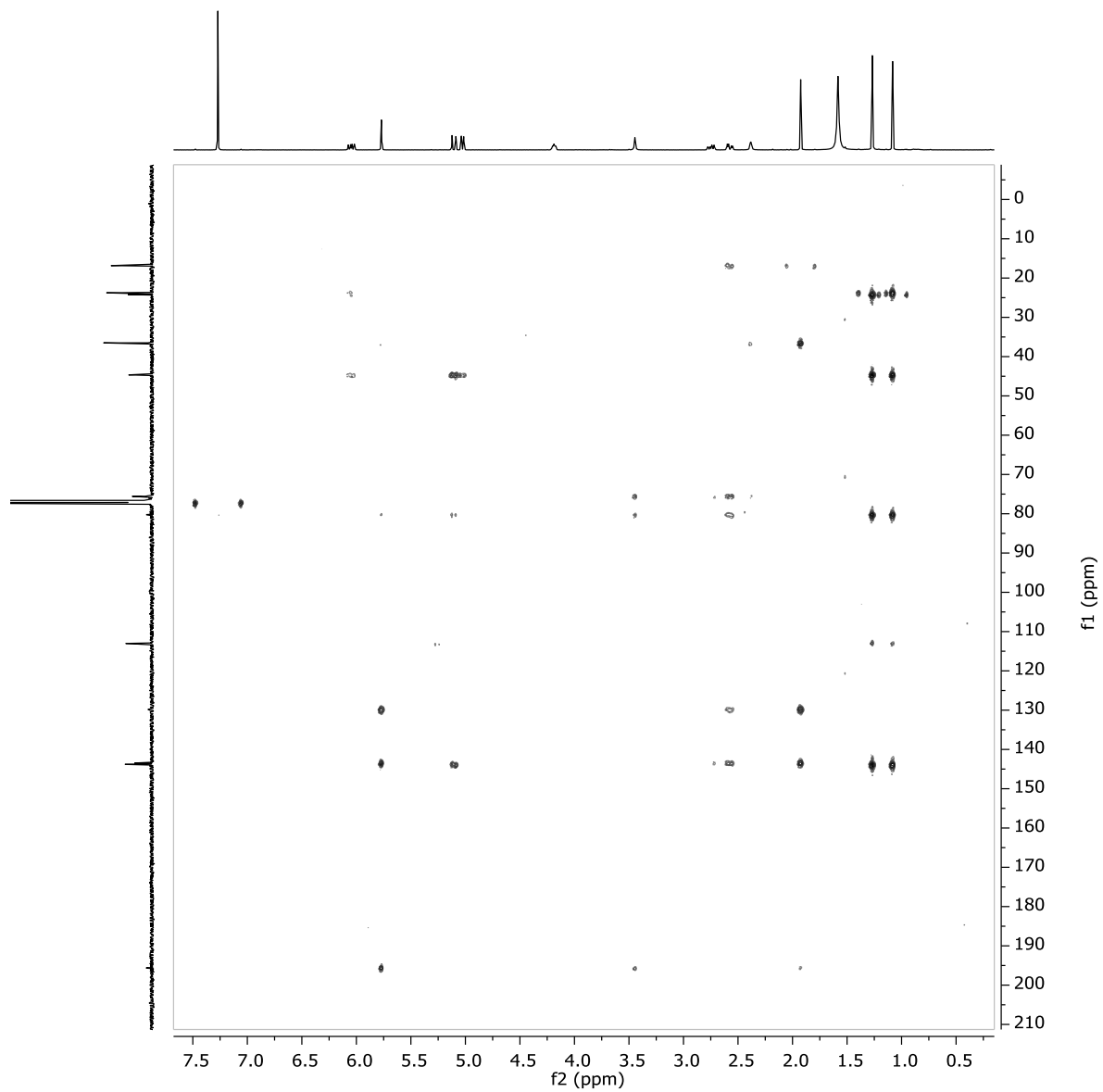


Figure S6. HMBC spectrum of **1** in chloroform-*d* at 500 MHz.

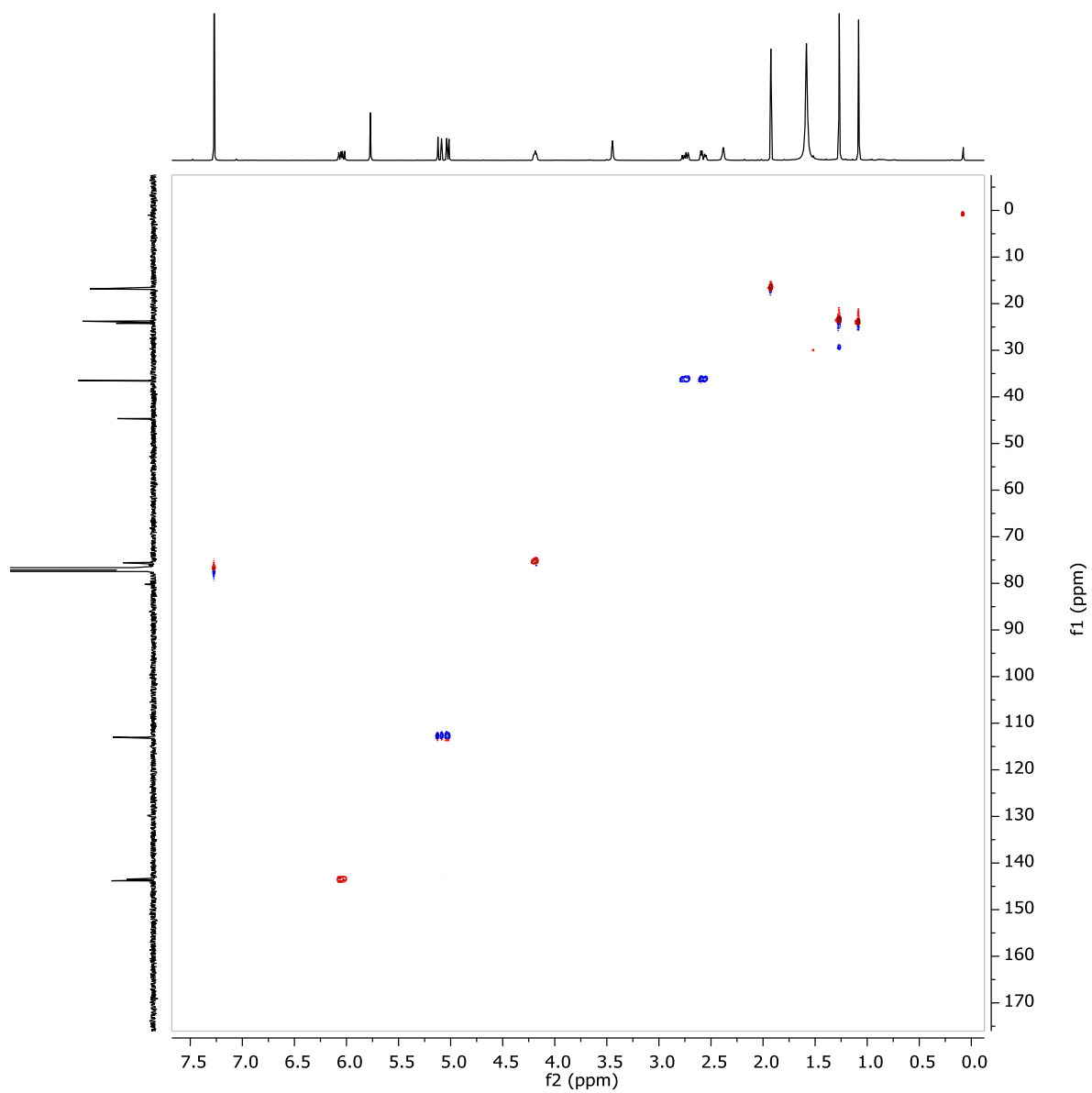


Figure S7. HSQC spectrum of **1** in methanol- d_4 at 500 MHz.

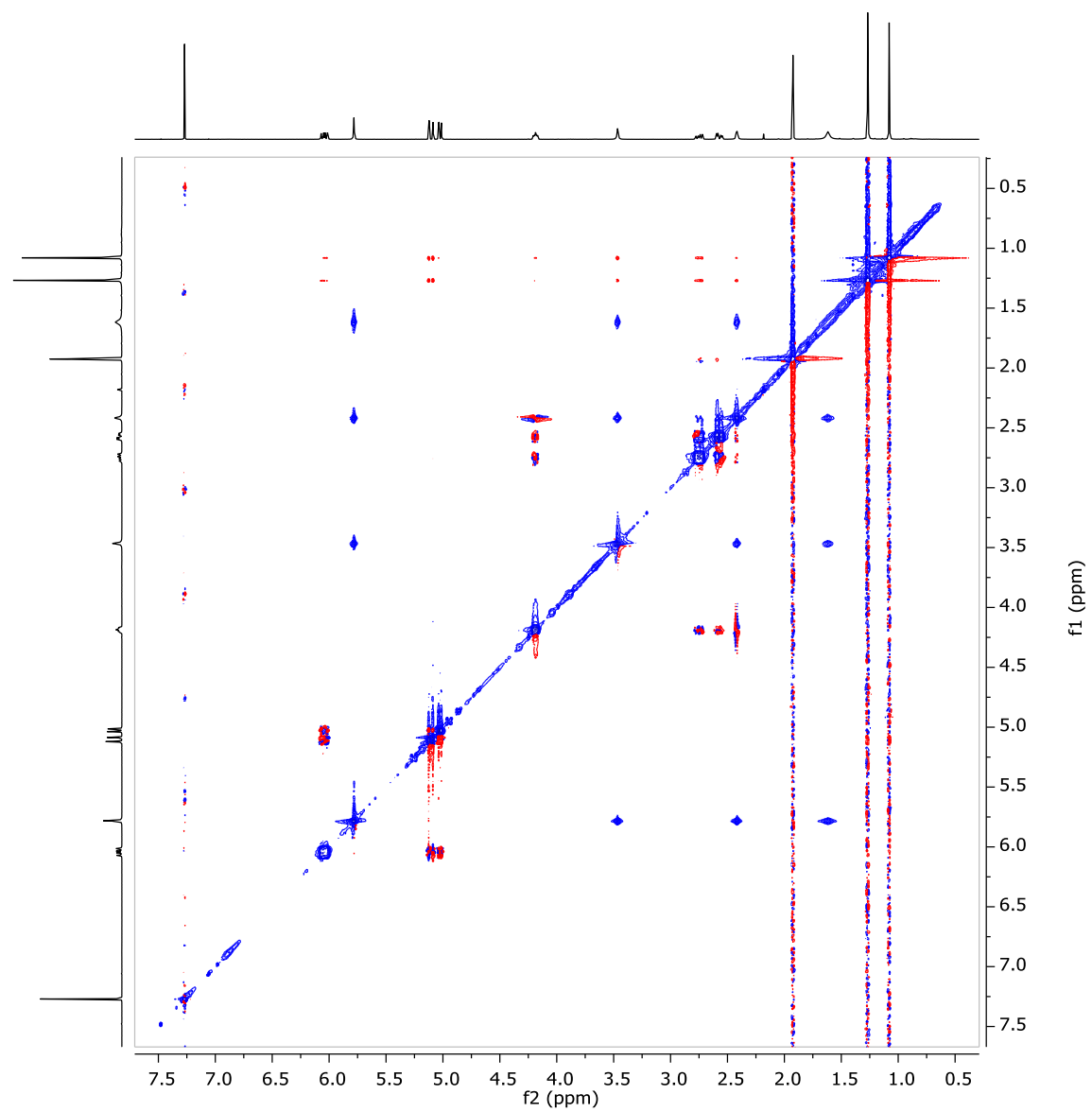


Figure S8. ROESY spectrum of **1** in methanol-*d*₄ at 500 MHz.

Display Report

Analysis Info

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Method 29109.m
Sample Name Dent 7B
Comment

Acquisition Date 28.05.2021 22:23:48

Operator esu
Instrument amaZon speed

Acquisition Parameter

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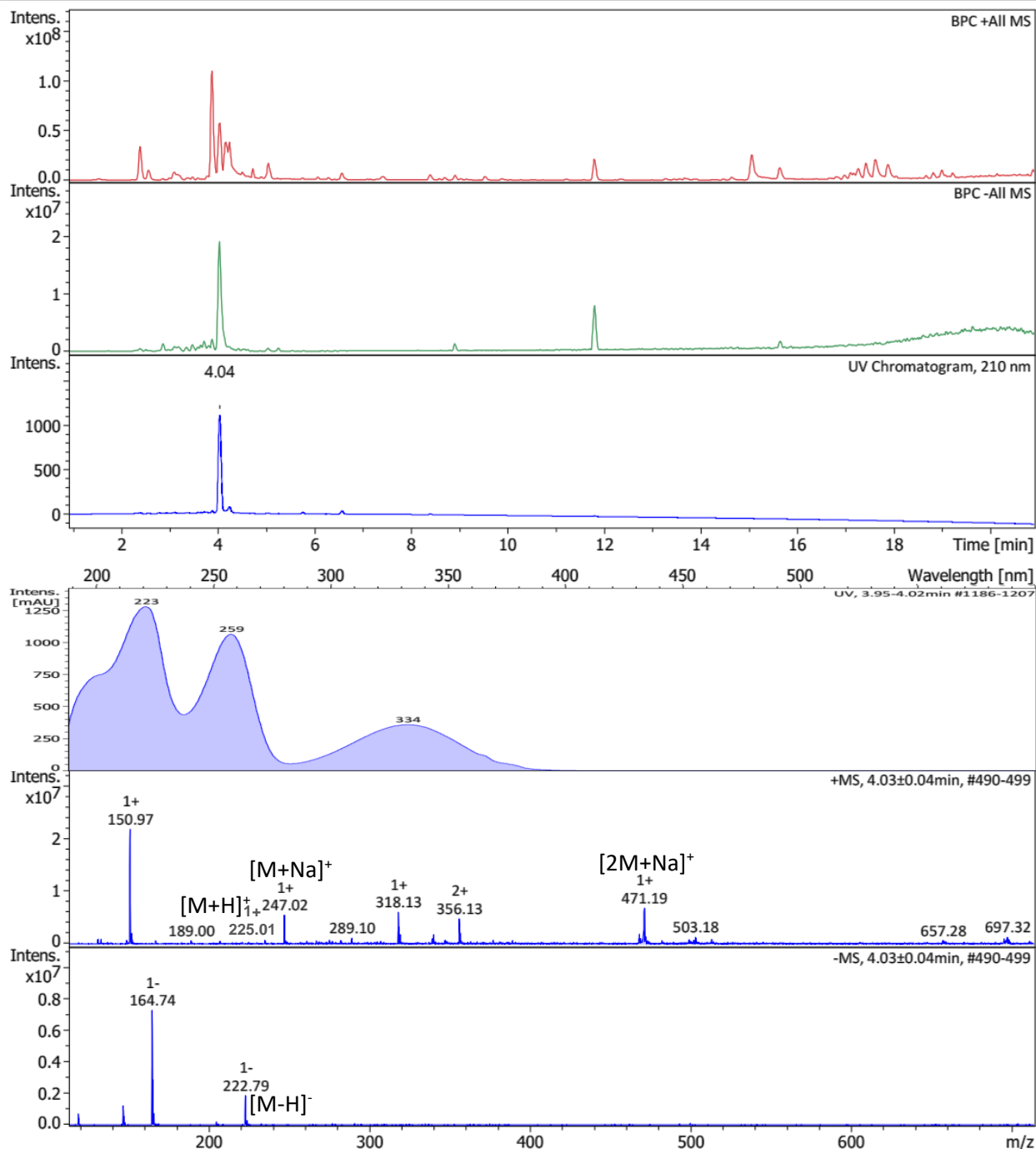


Figure S9. LR-ESI-MS of **2**.

Display Report

Analysis Info

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Sample Name Dent Rice F19
Comment Screening01
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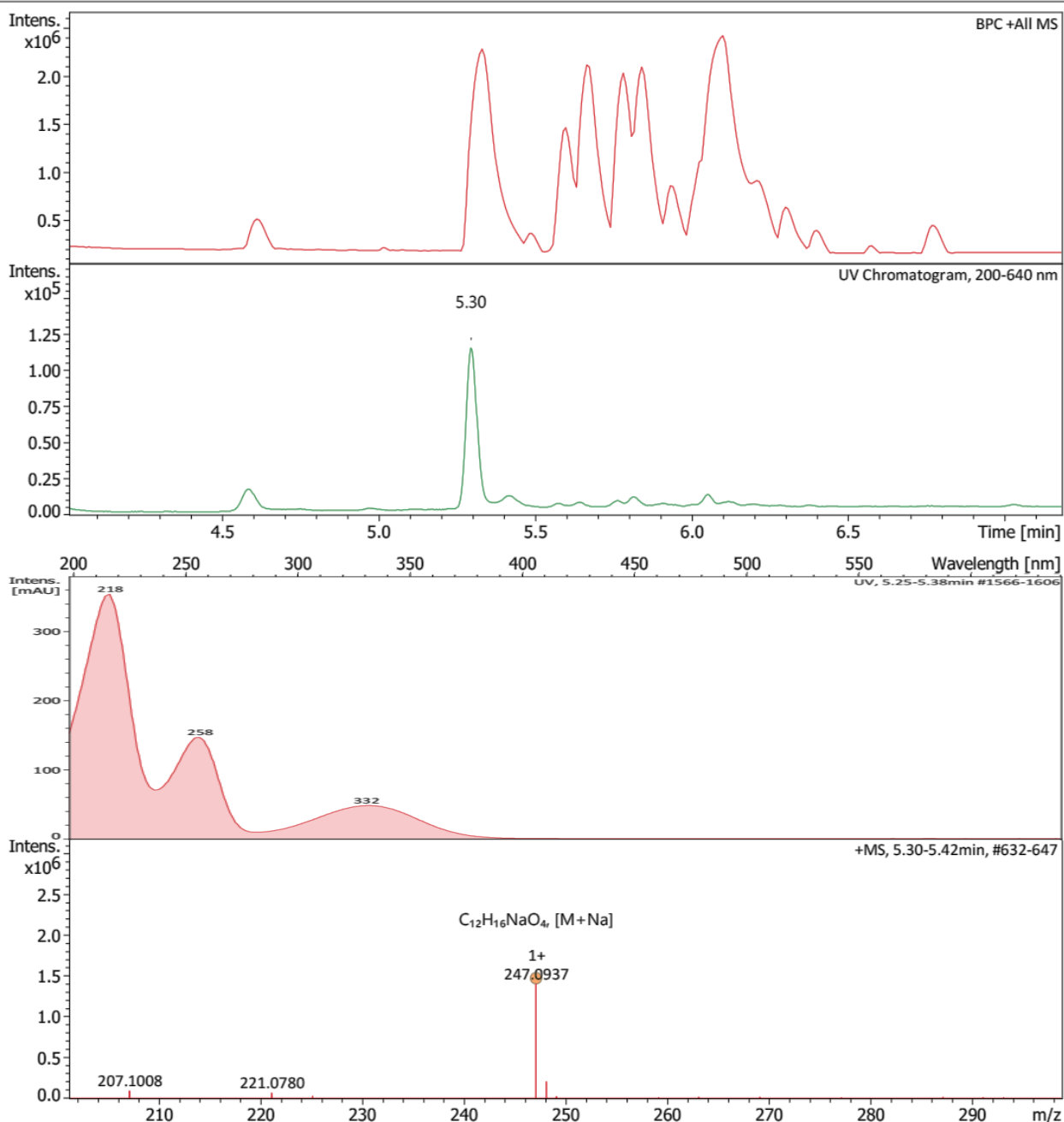
Acquisition Date 23.02.2022 11:36:13

Operator ate06

Instrument maxIs 255552.00037

Acquisition Parameter

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Scan End	2500 m/z	Set Charging Voltage	0 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Dent Rice F19_P1-B-1_01_9608.d

Bruker Compass DataAnalysis 6.1

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by: sel22

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Figure S10. HR-ESI-MS of **2**.

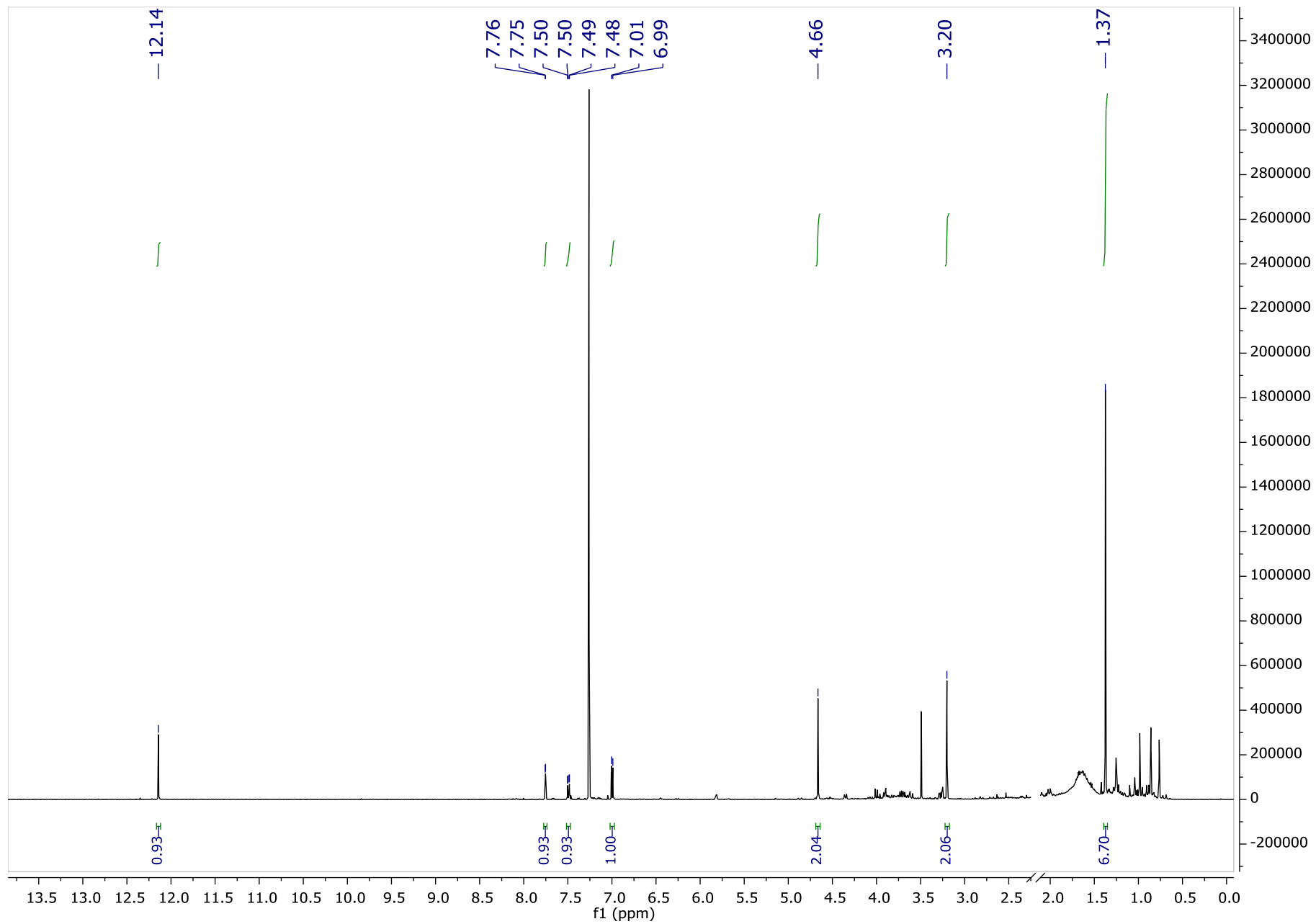


Figure S11. ^1H NMR spectrum of **2** in chloroform-*d* at 500 MHz.

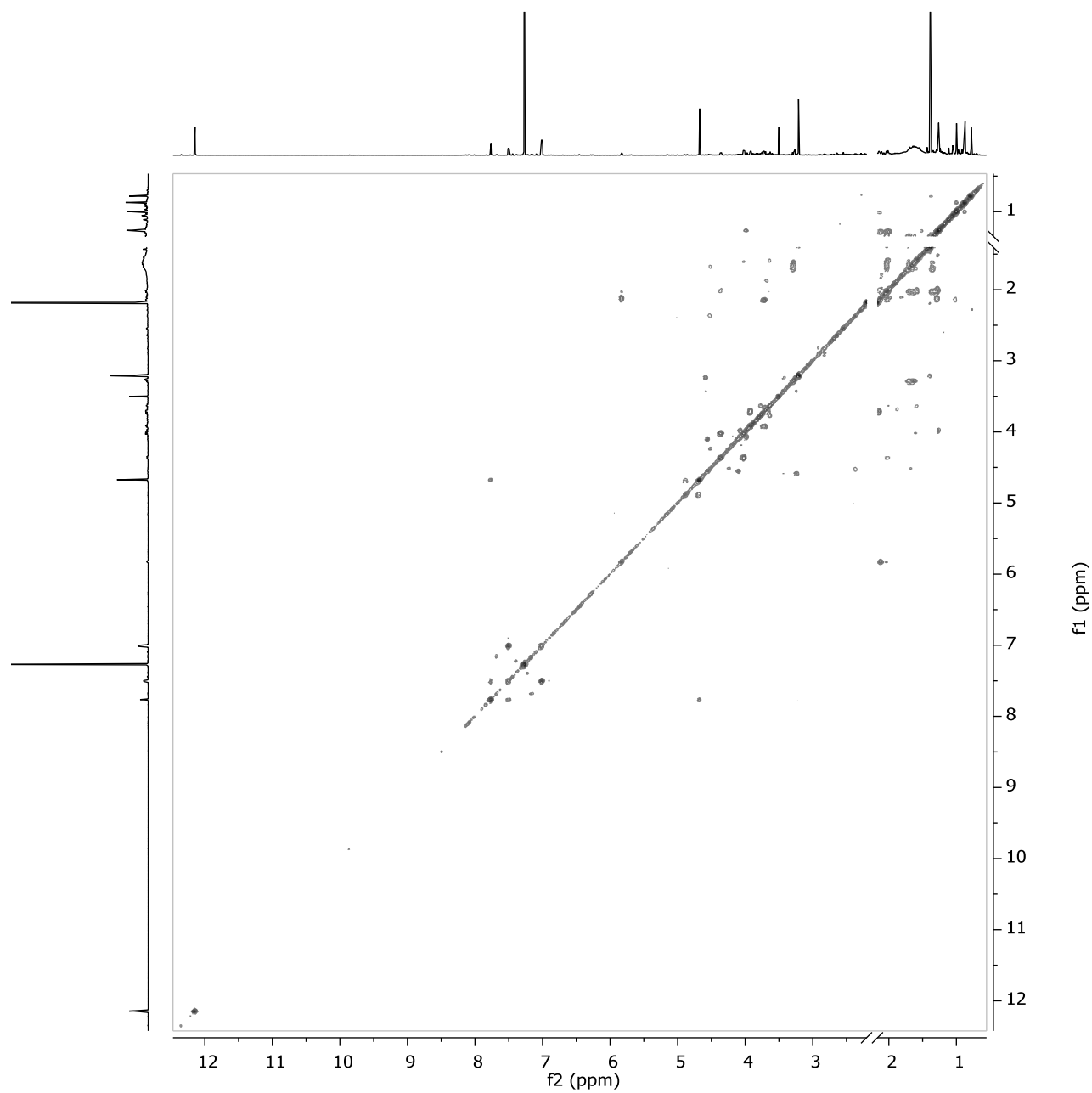


Figure S12. ^1H - ^1H COSY spectrum of **2** in chloroform-*d* at 500 MHz.

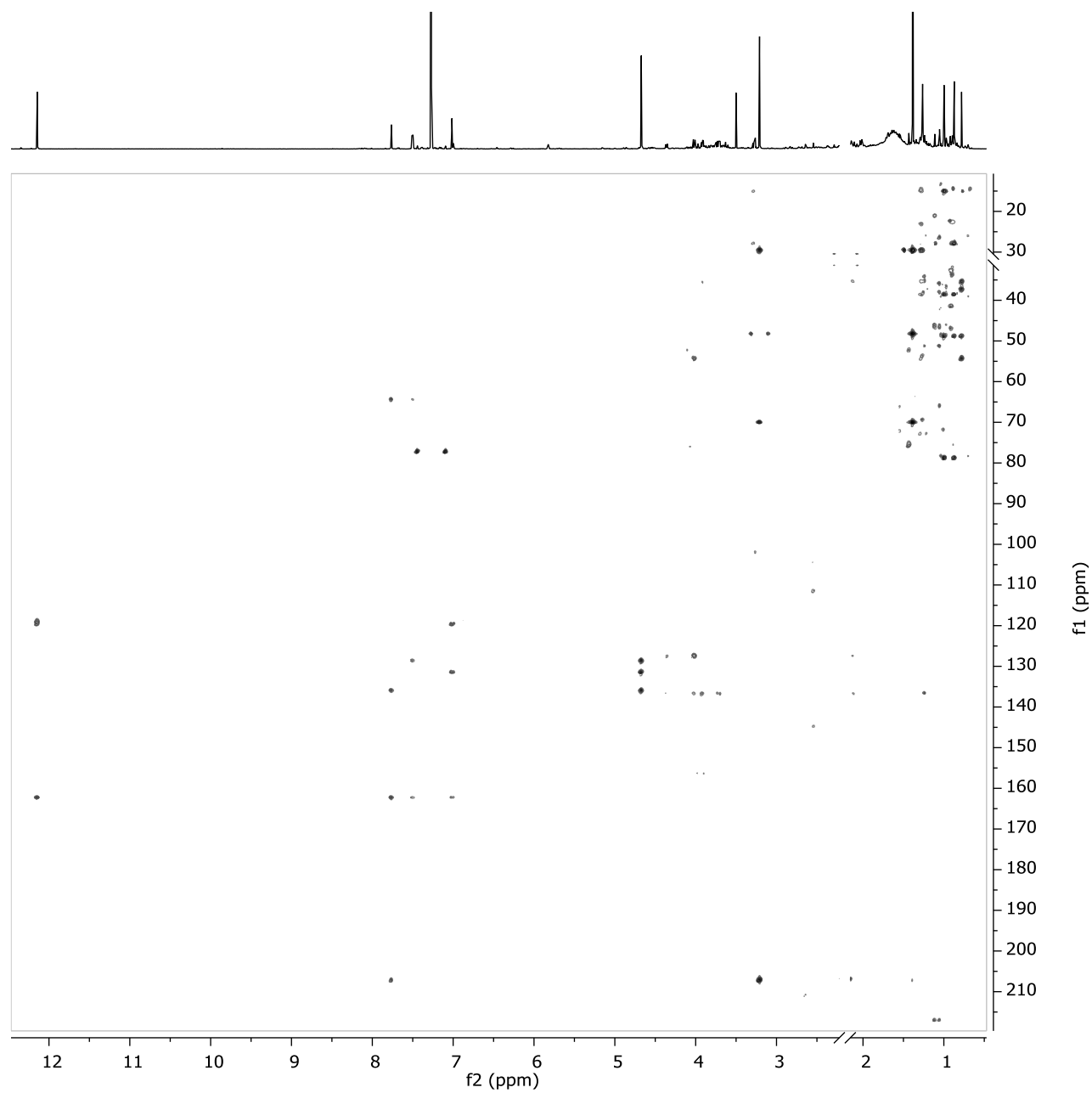


Figure S13. HMBC spectrum of **2** in chloroform-*d* at 500 MHz.

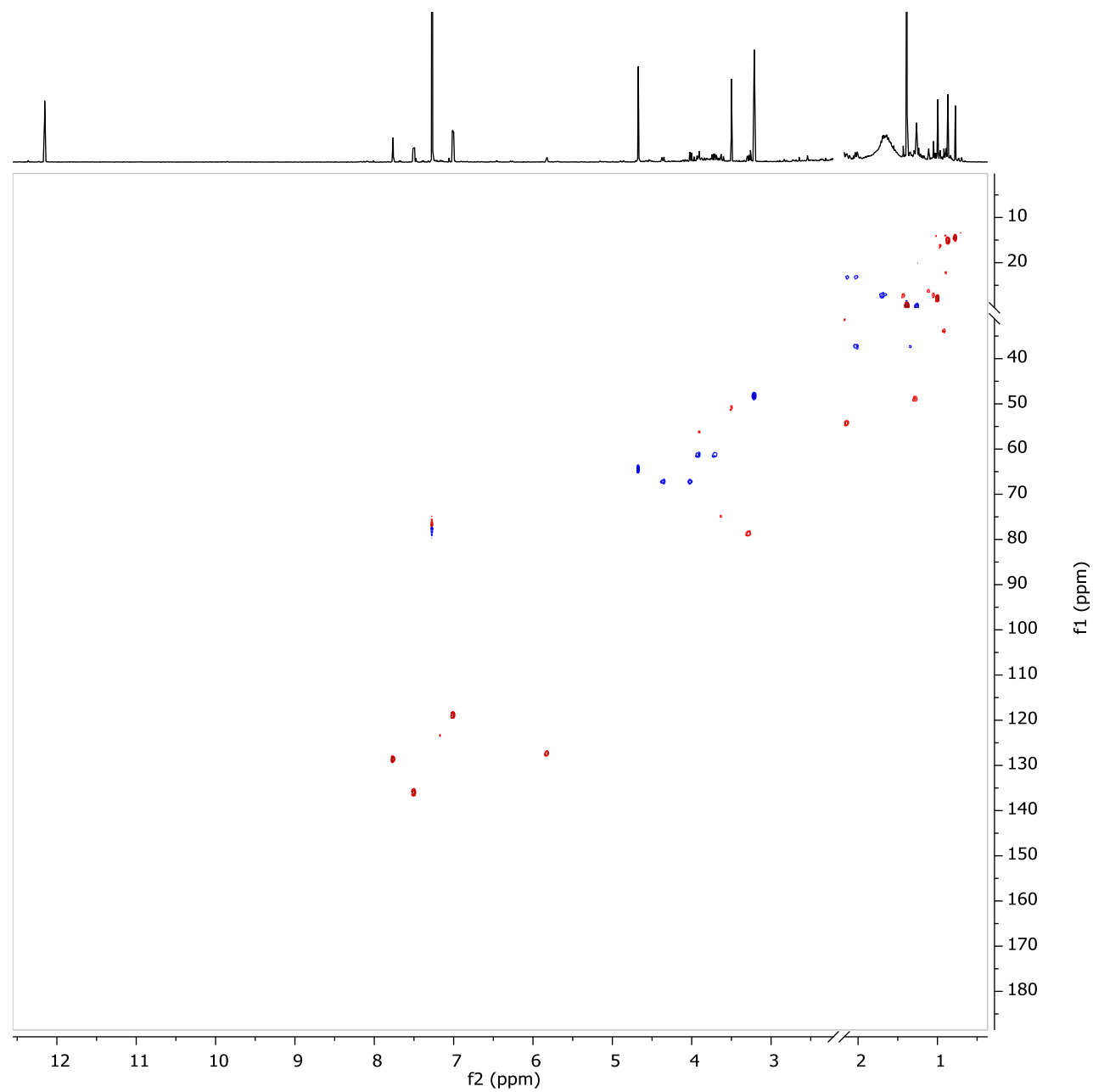


Figure S14. HSQC spectrum of **2** in methanol- d_4 at 500 MHz.

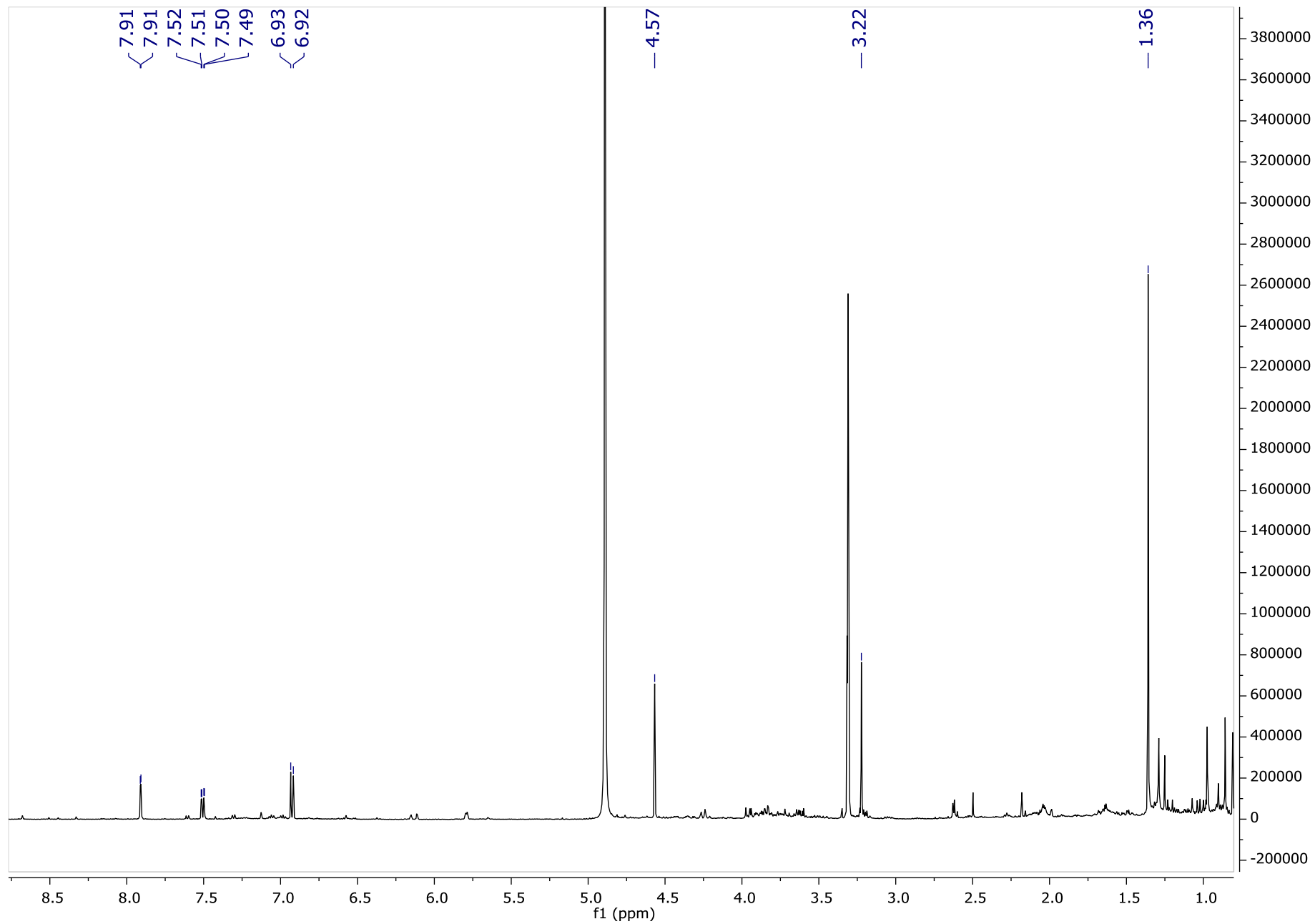


Figure S15. ¹H NMR spectrum of **2** in methanol-*d*₄ at 500 MHz.

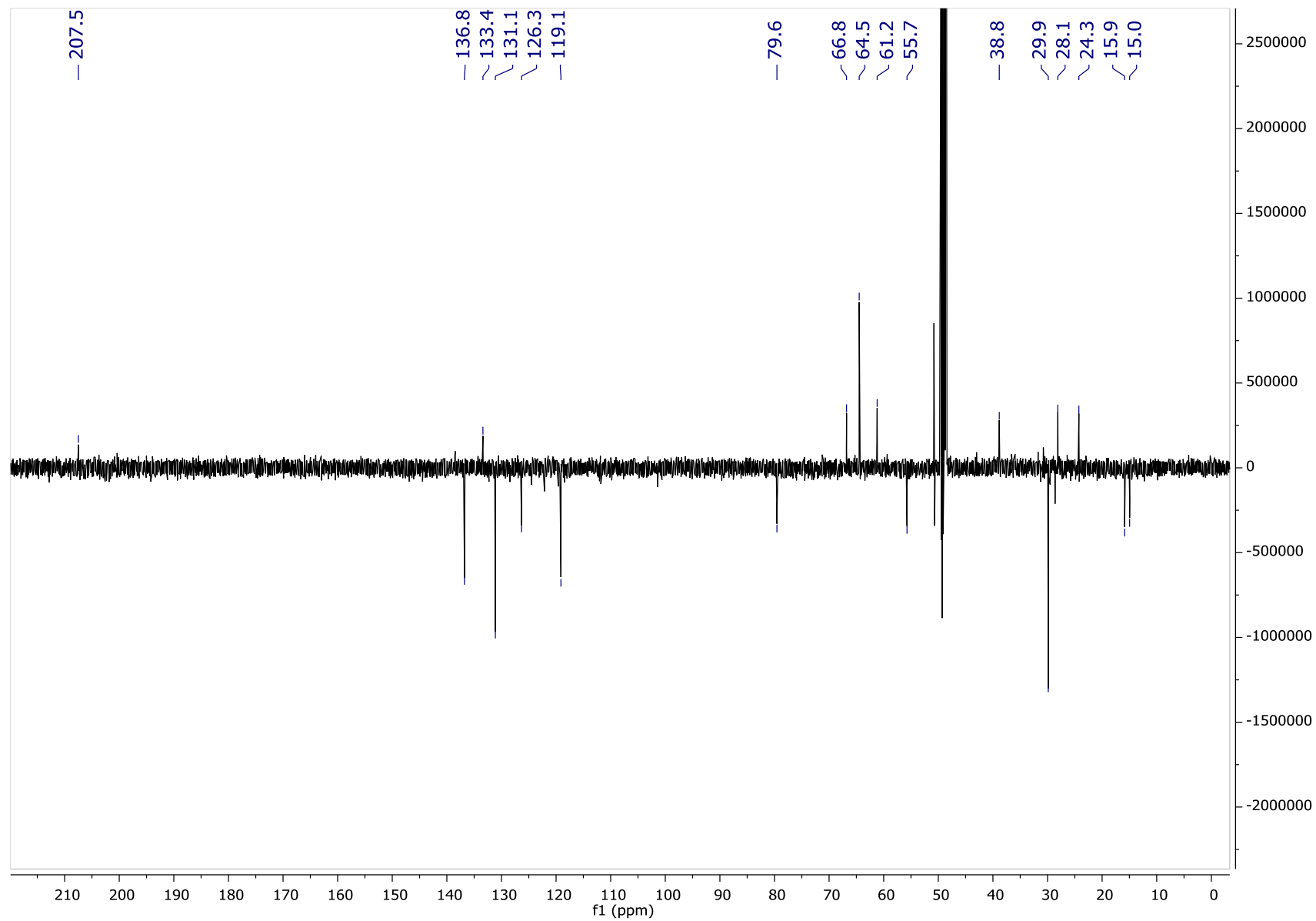


Figure S16. DEPTQ spectrum of **2** in methanol- d_4 at 125 MHz.

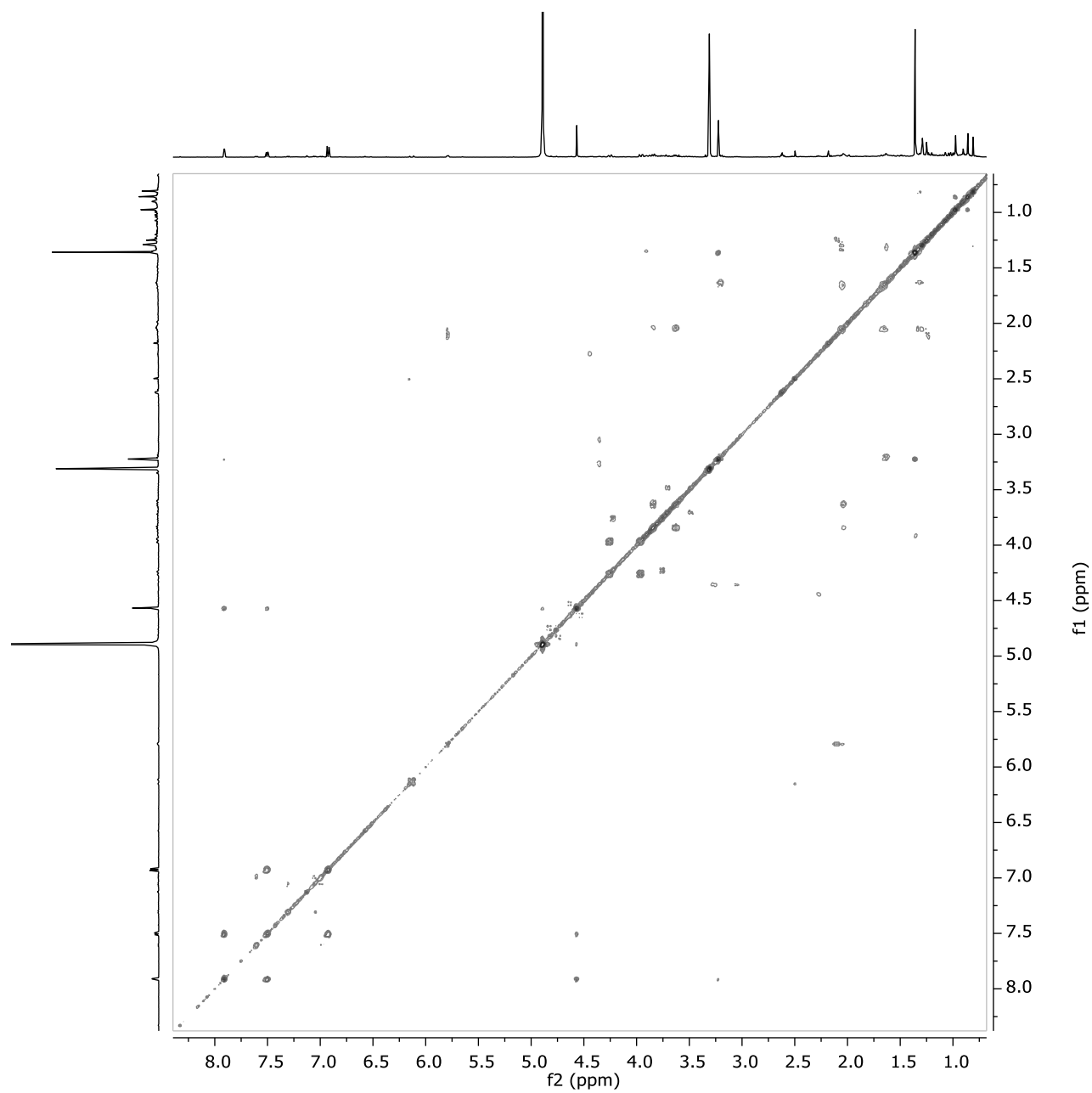


Figure S17. ^1H - ^1H COSY spectrum of **2** in methanol- d_4 at 500 MHz.

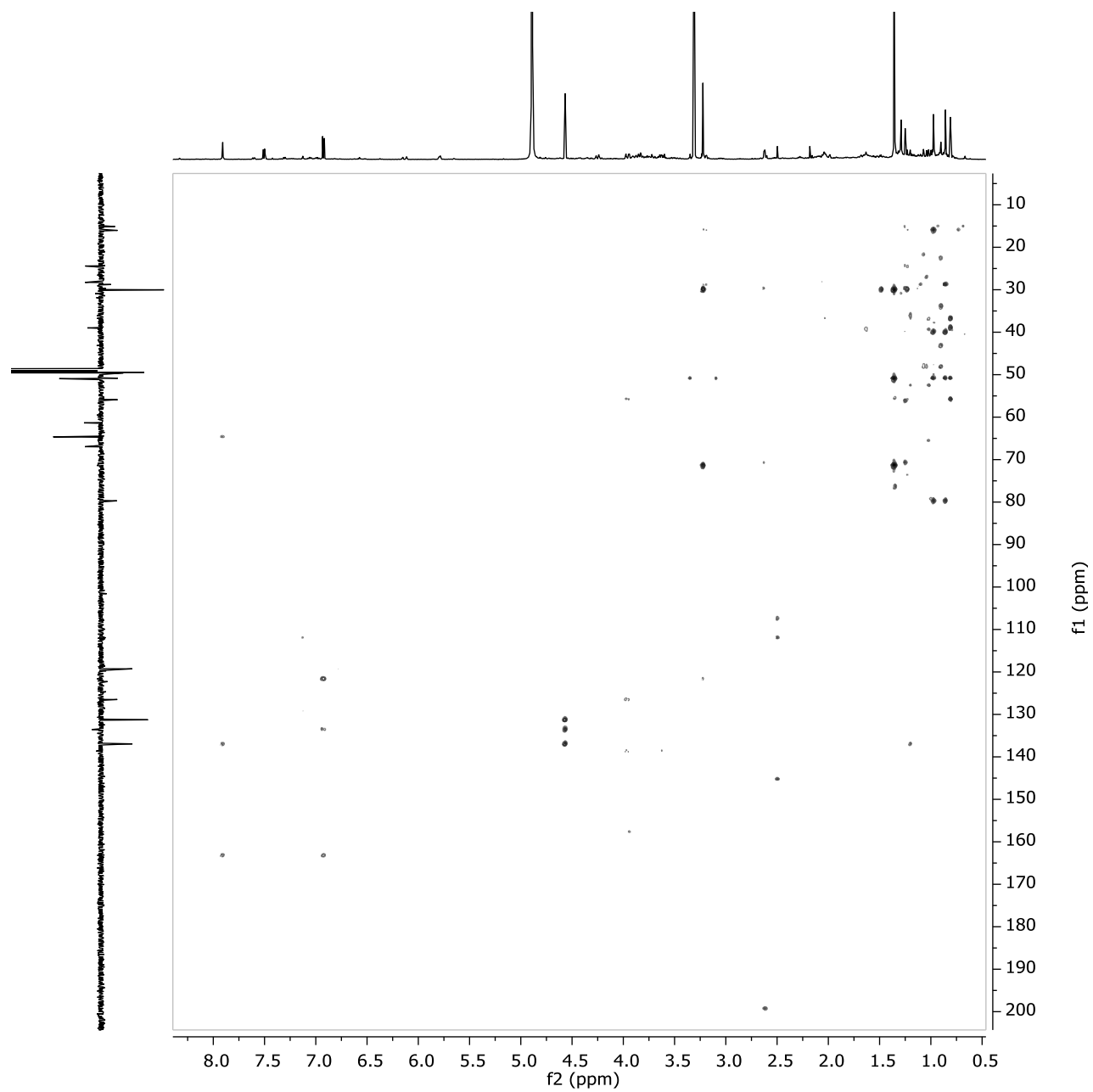


Figure S18. HMBC spectrum of **2** in methanol- d_4 at 500 MHz.

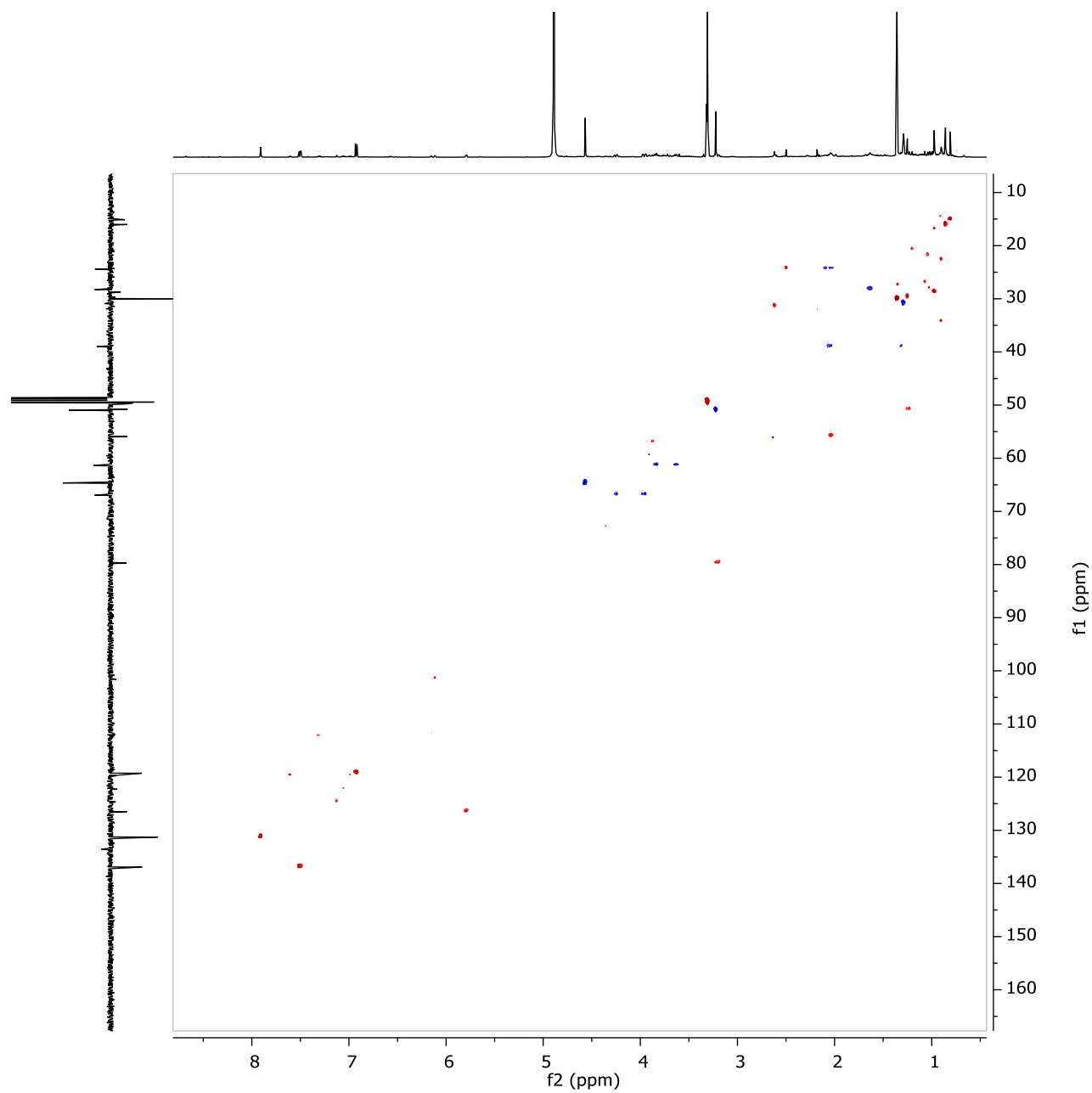


Figure S19. HSQC spectrum of **2** in methanol-*d*₄ at 500 MHz.

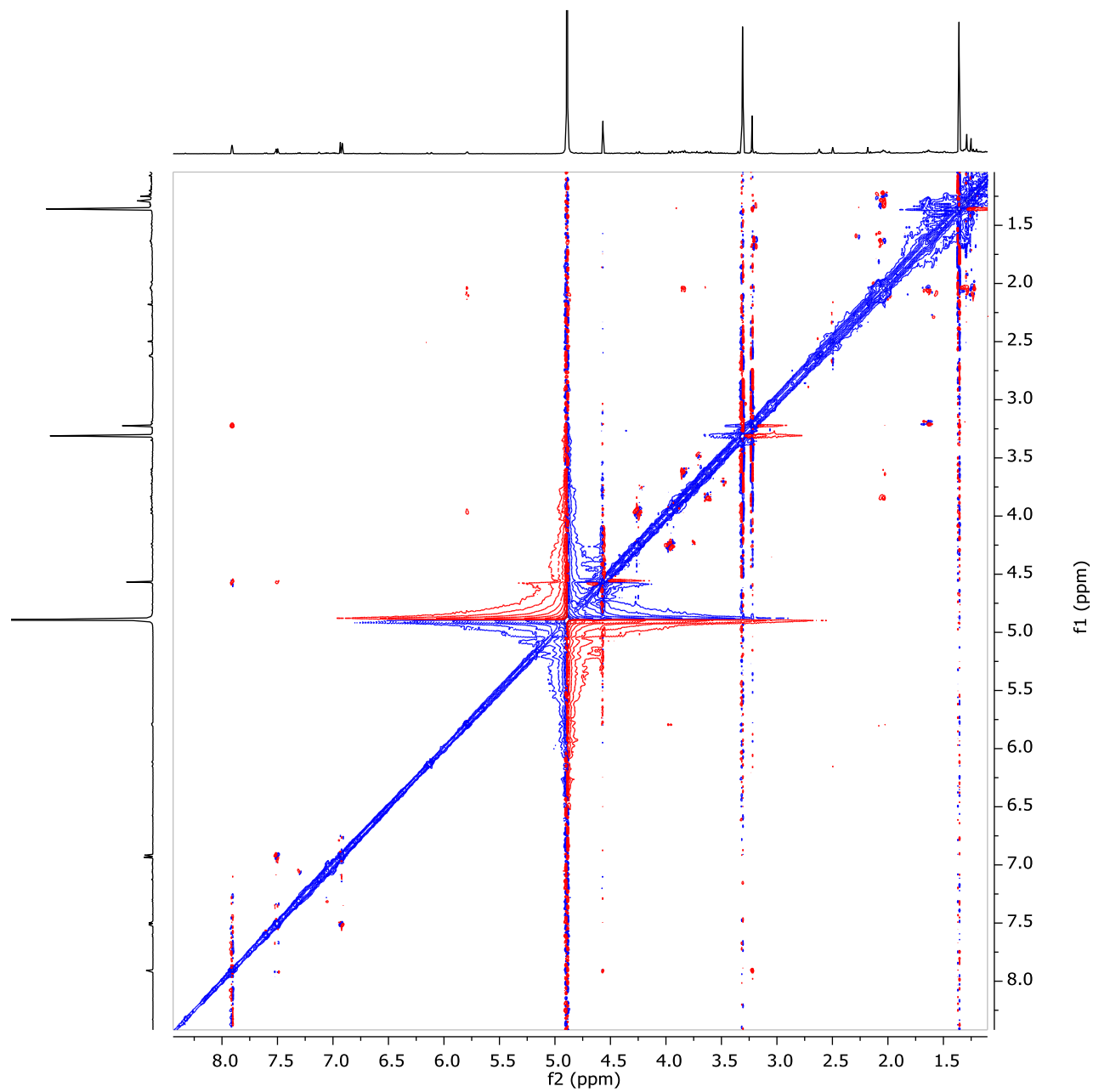


Figure S20. ROESY spectrum of **2** in methanol-*d*₄ at 500 MHz.

Display Report

Analysis Info

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Method 29108.m
Sample Name Dent 6B
Comment

Acquisition Date 28.05.2021 21:47:42

Operator esu
Instrument amaZon speed

Acquisition Parameter

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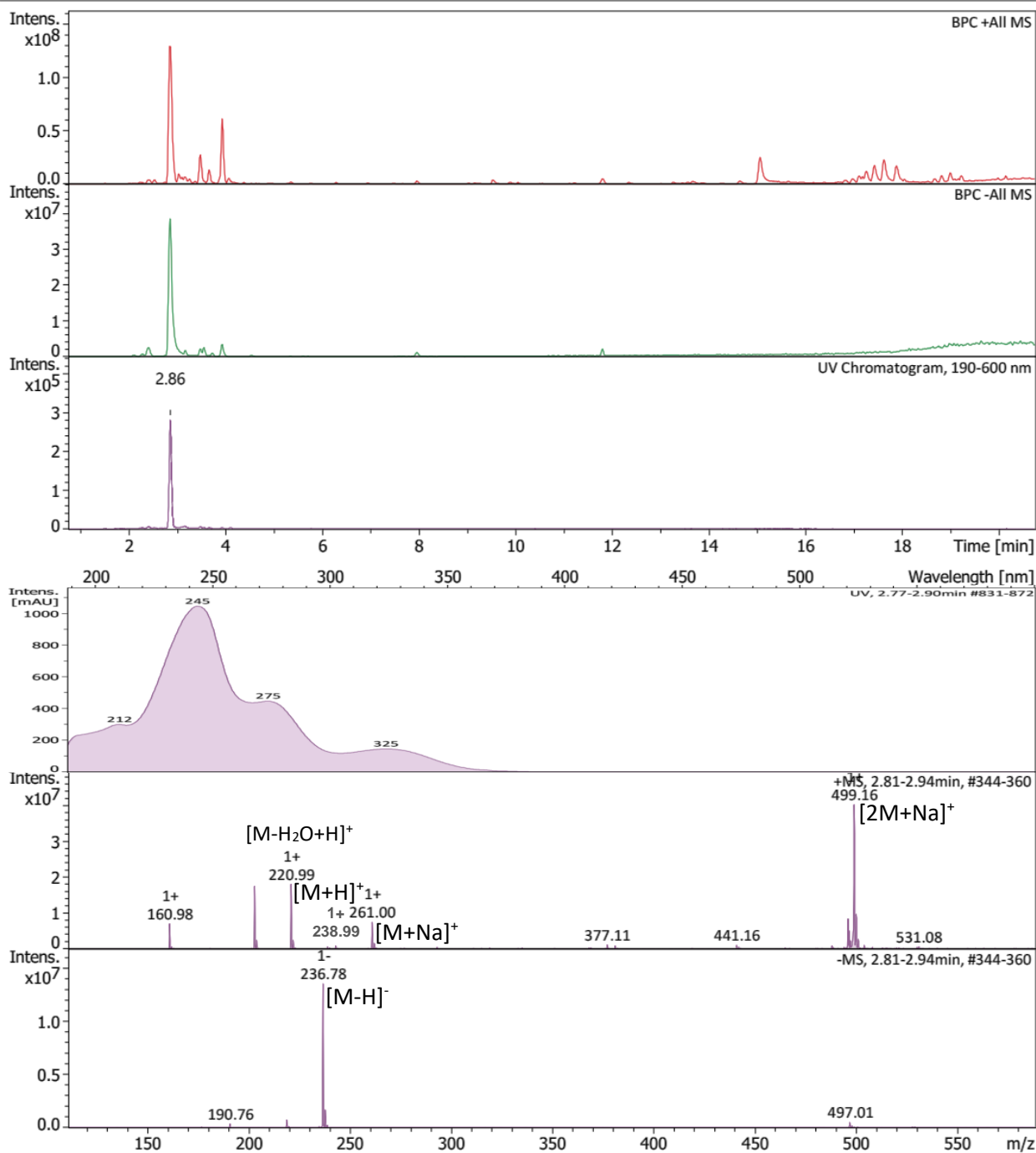


Figure S21. LR-ESI-MS of **3**.

Display Report

Analysis Info

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Comment Screening01
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Acquisition Date 02.06.2021 18:51:46

Acquisition Parameter

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SPS Target Mass

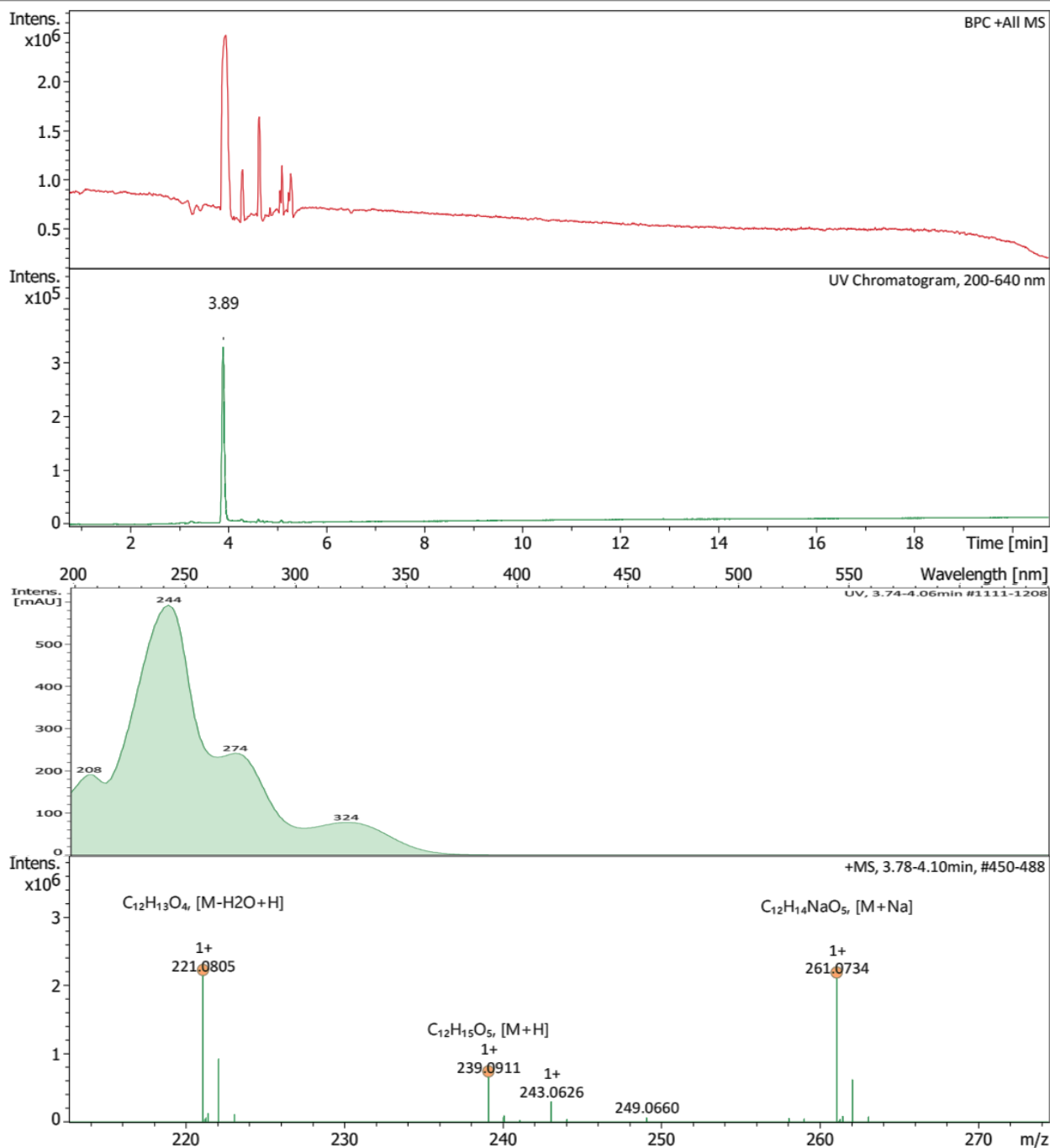


Figure S22. HR-ESI-MS of **3**.

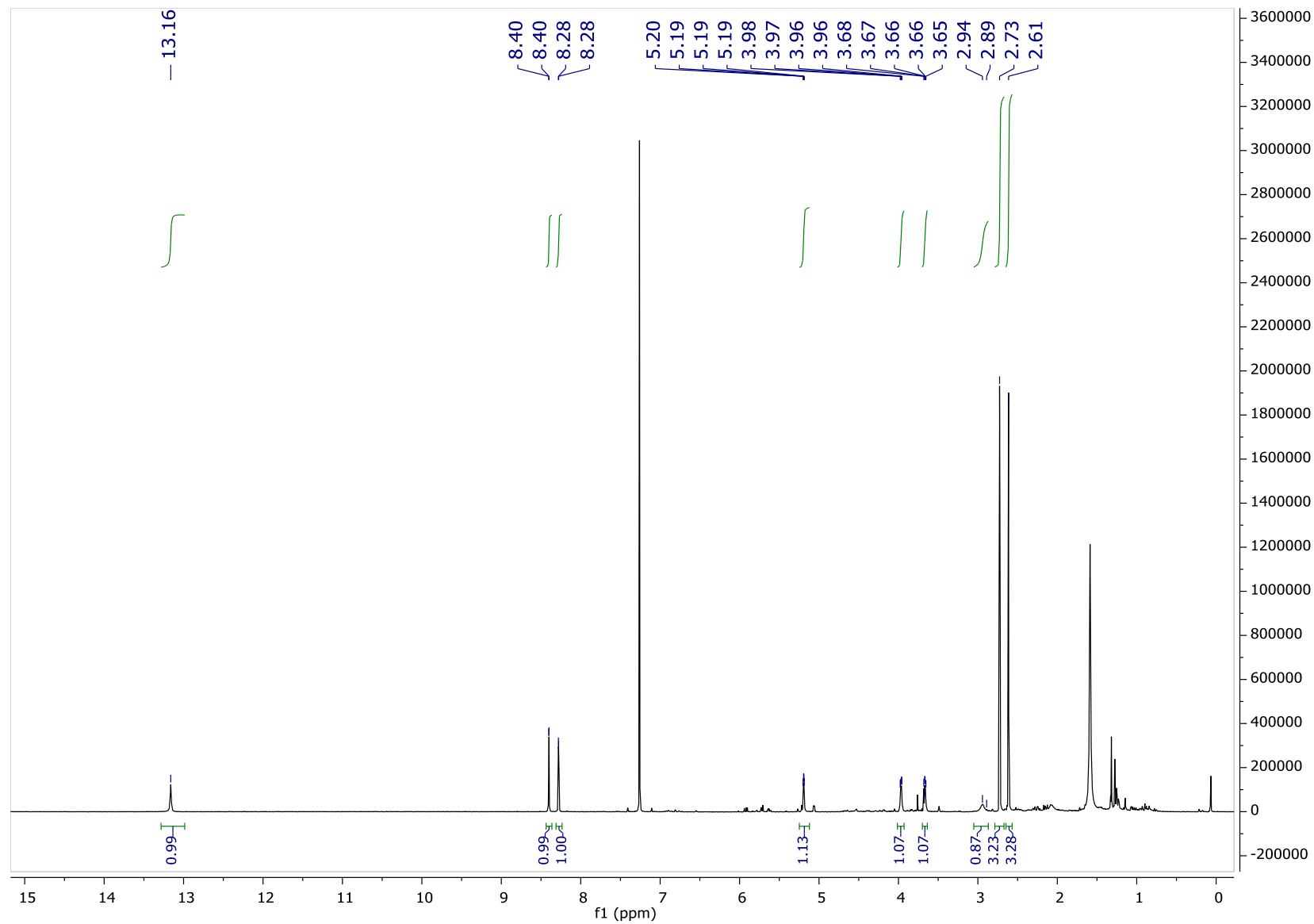


Figure S23. ^1H NMR spectrum of **3** in chloroform-*d* at 700 MHz.

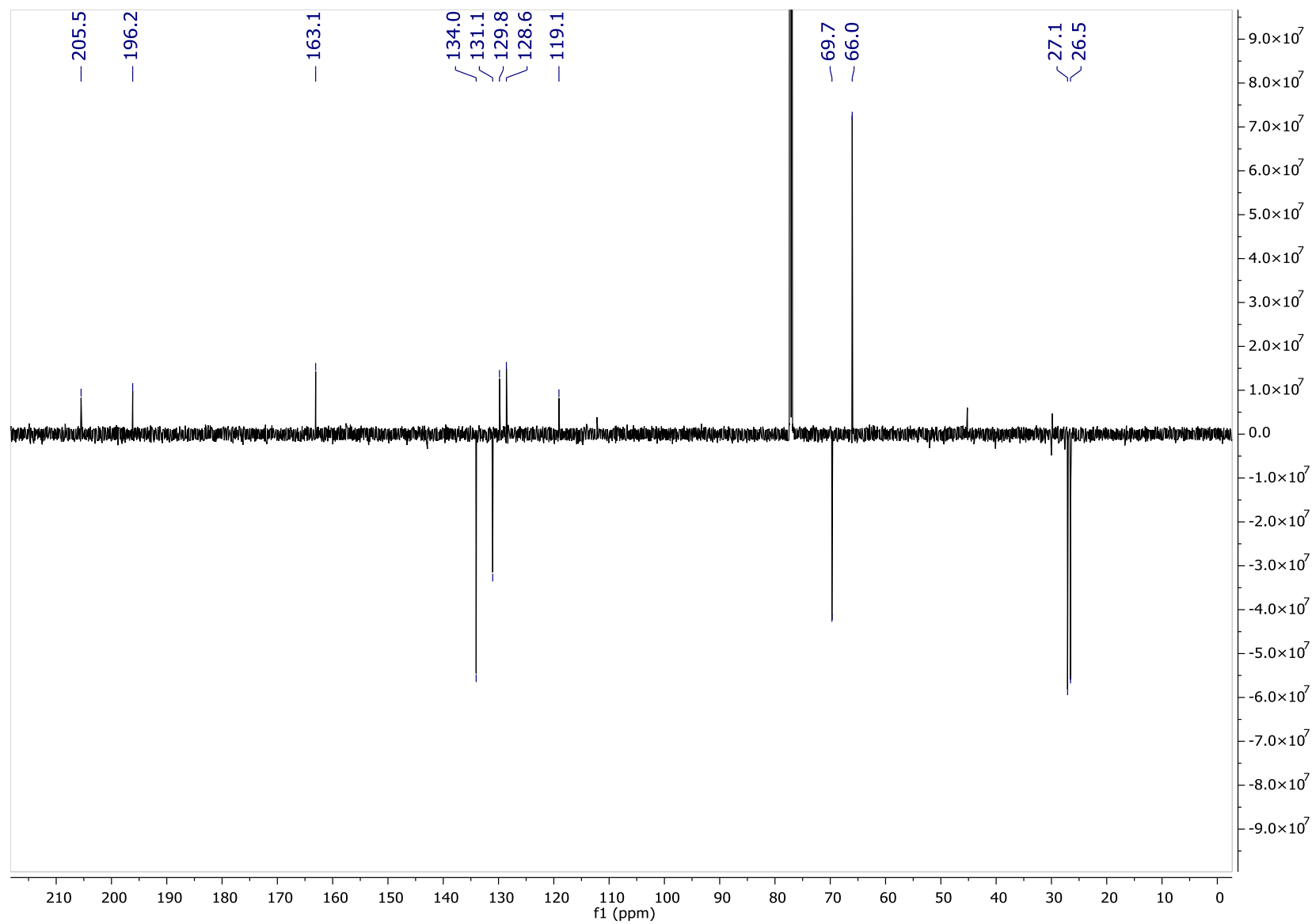


Figure S24. DEPTQ NMR spectrum of **3** in chloroform-*d* at 175 MHz.

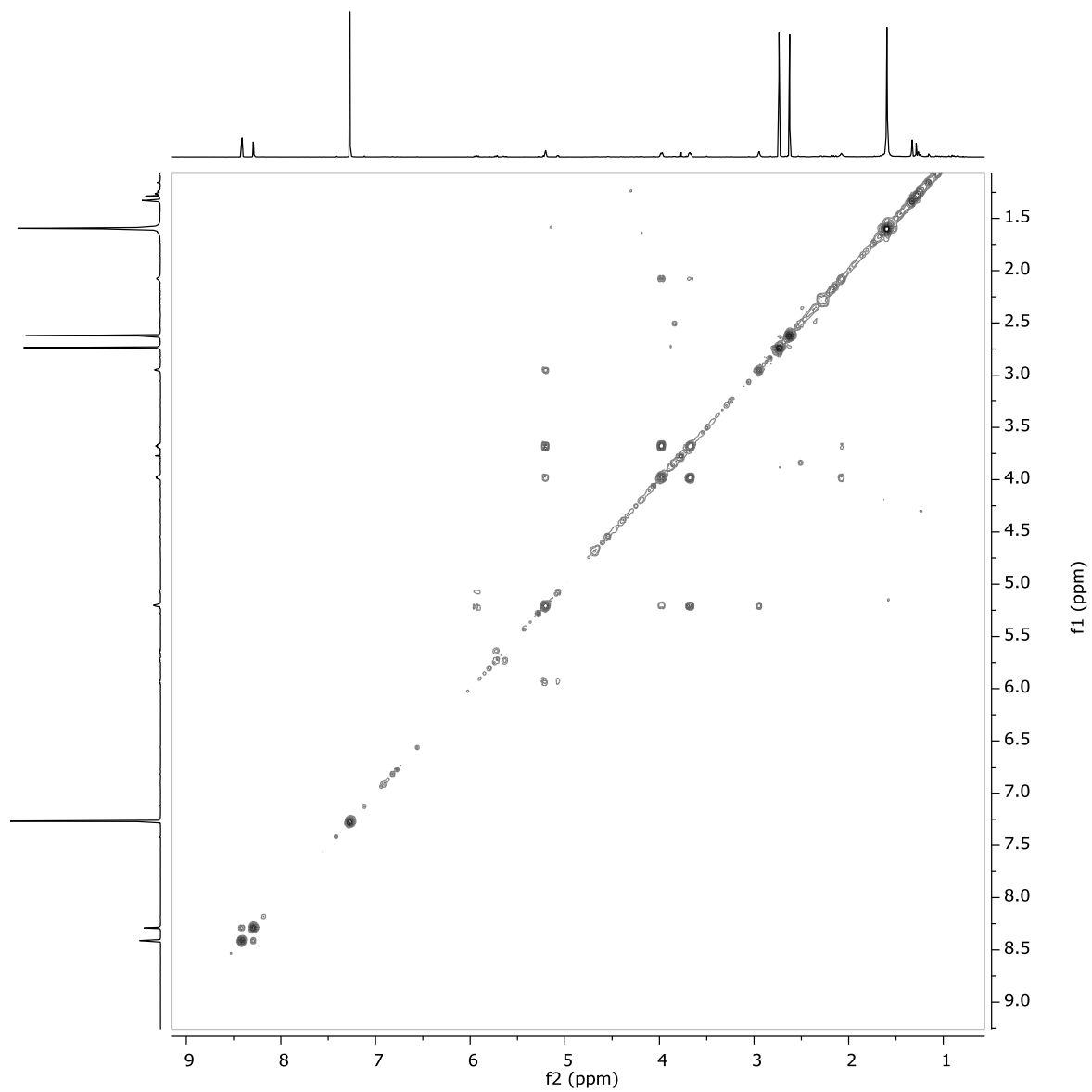


Figure S25. ^1H - ^1H COSY spectrum of **3** in chloroform-*d* at 700 MHz.

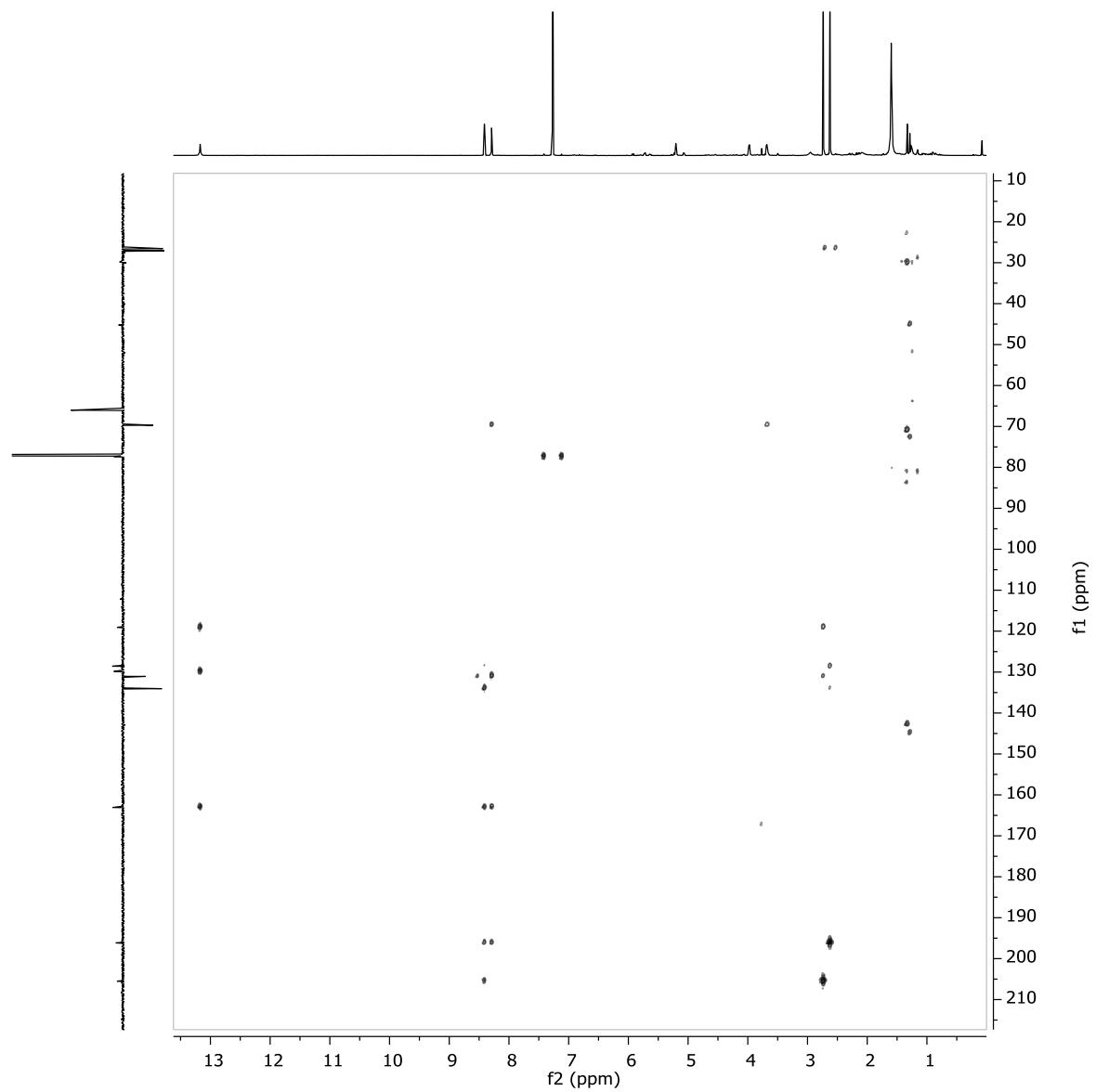


Figure S26. HMBC spectrum of **3** in chloroform-*d* at 700 MHz.

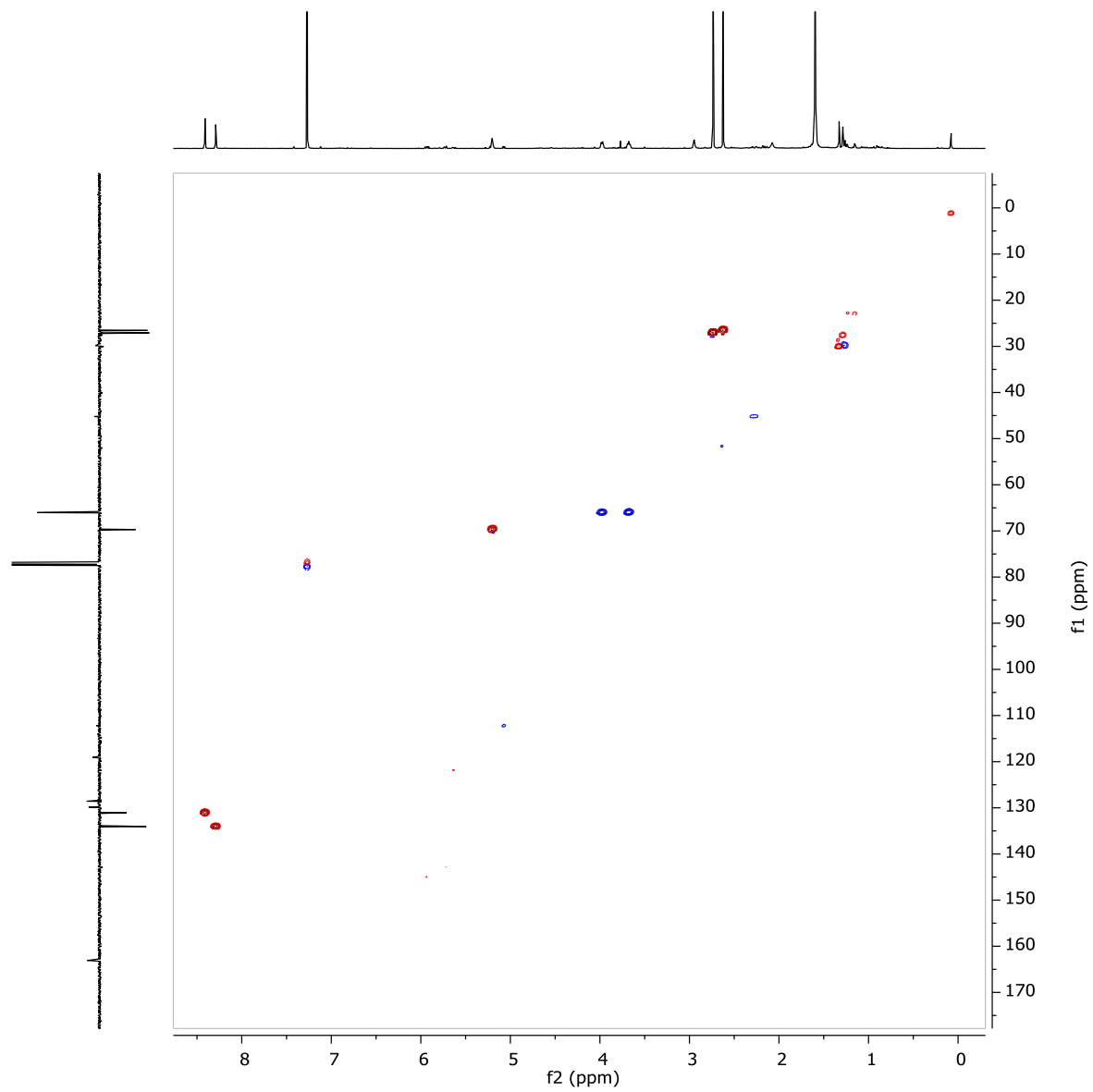


Figure S27. HSQC spectrum of **3** in chloroform-*d* at 700 MHz.

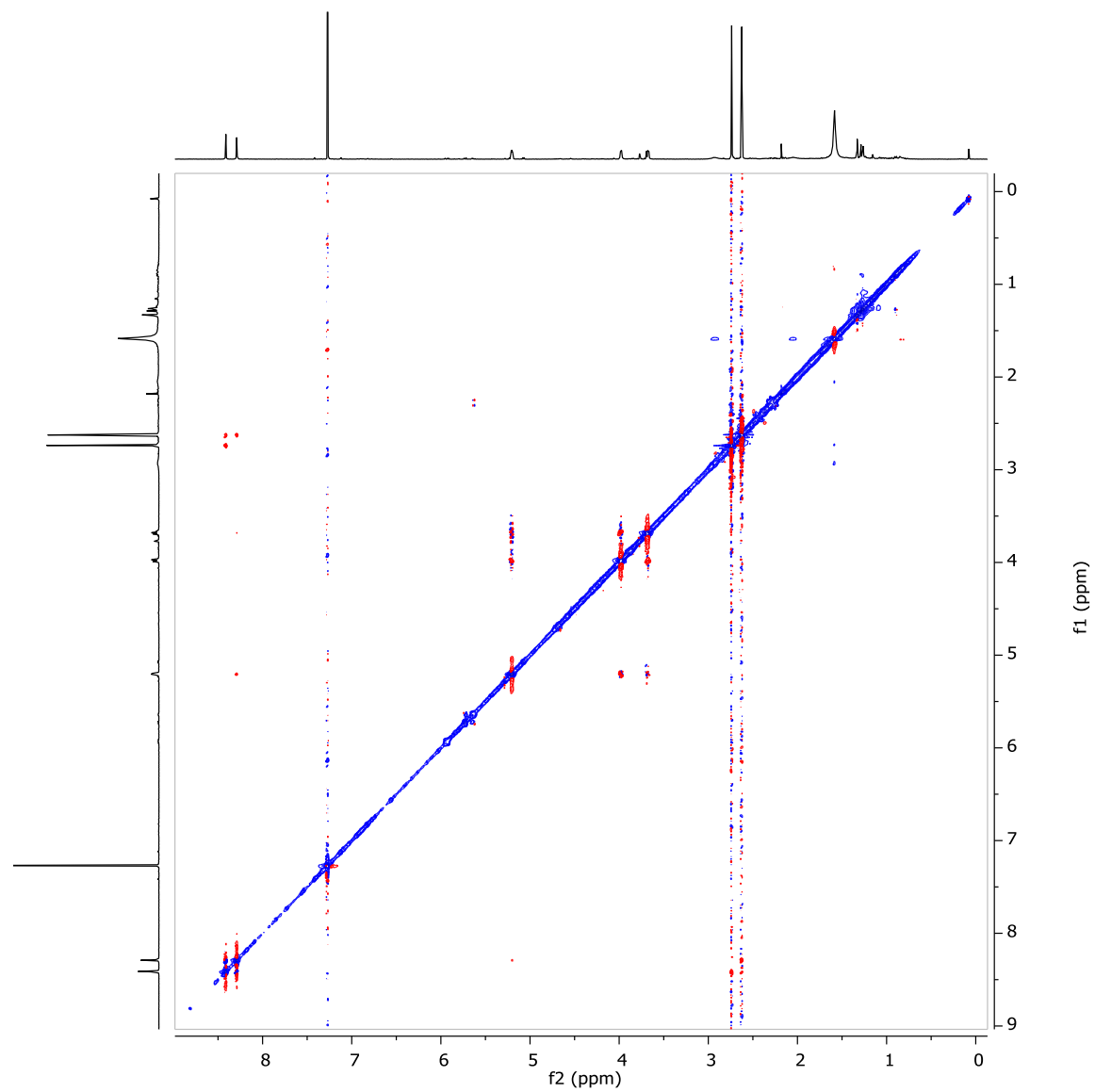


Figure S28. ROESY spectrum of **3** in chloroform-*d* at 700 MHz.

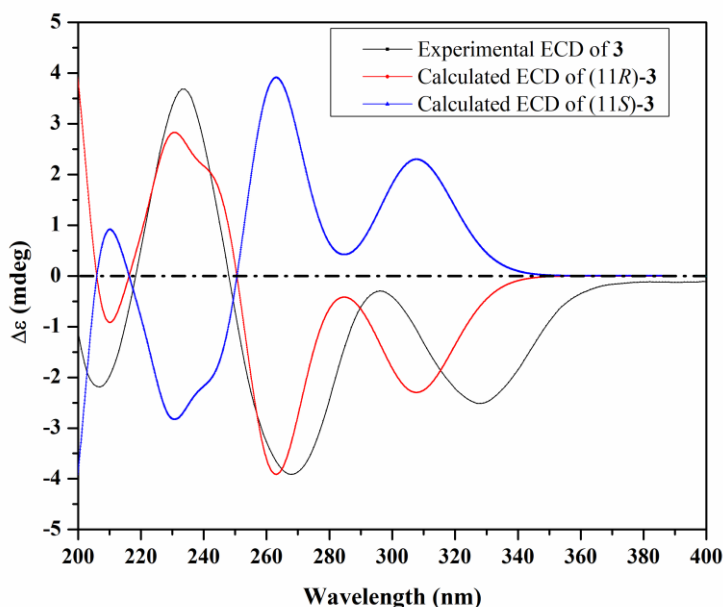
Table S1. 1D (^1H and ^{13}C) NMR data of **3** and dentipellinol.^[1]

pos.	3		Dentipellinol ^[1]	
	$\delta_{\text{C}},^a$ type	$\delta_{\text{H}},^b$ (multi, J [Hz])	$\delta_{\text{C}},^c$ type	$\delta_{\text{H}},^d$ (multi, J [Hz])
1	163.1, C		163.9, C	
2	119.1, C		119.9, C	
3	131.1, CH	8.40 d (2.2)	132.5, CH	8.49 d (2.2)
4	128.6, C		129.4, C	
5	134.0, CH	8.28 d (2.2)	134.9, CH	8.28 d (2.2)
6	129.8, C		132.4, C	
7	205.5, CO		207.1, CO	
8	27.1, CH ₃	2.73 s	27.0, CH ₃	2.74 s
9	196.2, CO		198.7, CO	
10	26.5, CH ₃	2.61 s	26.4, CH ₃	2.61 s
11	69.7, CH	5.19 dd (7.2, 3.5)	69.6, CH	5.15 dd (6.8, 3.3)
12	66.0, CH ₂	α 3.67 dd (11.2, 7.2) β 3.97 dd (11.2, 3.5)	66.7, CH ₂	α 3.55 dd (11.4, 6.8) β 3.79 dd (11.4, 3.3)
1-OH	-	13.16 br s		

Measured in chloroform-*d* at ^a 175 / ^b 700 MHz.

Measured in methanol-*d*₄ at ^c 150 / ^d 600 MHz.

[1] Ki, D.-W.; Kim, C.-W.; Choi, D.-C.; Oh, G.-W.; Doan, T.-P.; Kim, J.-Y.; Oh, W.-K.; Lee, I.-K.; Yun, B.-S. Chemical constituents of the culture broth of *Dentipellis fragilis* and their anti-inflammatory activities. *Phytochemistry* 2023, 214, 113828.

**Figure S29.** Experimental and calculated ECD spectra of **3**.

Display Report

Analysis Info

Analysis Name F:\Volume D\HZI Projects\Winnie\11-Dentipellis fragilis\Amazon\Dent Rice F13_RC3_01_10235.d
Method Screening_Set-05iso-uv210_10235.m
Sample Name Dent Rice F13
Comment

Acquisition Date 18.02.2022 18:35:02

Operator lab
Instrument amaZon speed

Acquisition Parameter

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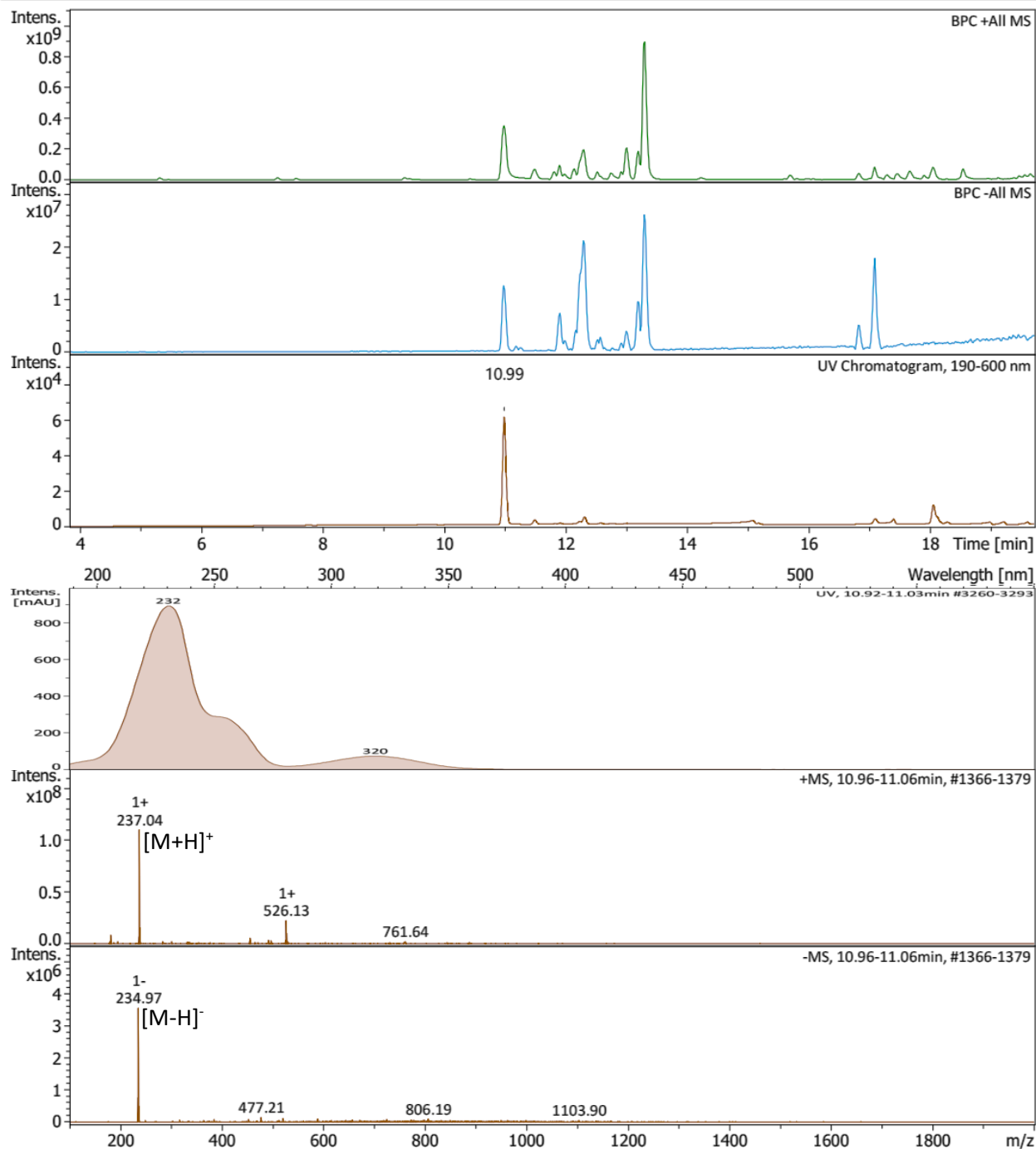


Figure S30. LR-ESI-MS of 4.

Display Report

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Comment Screening01
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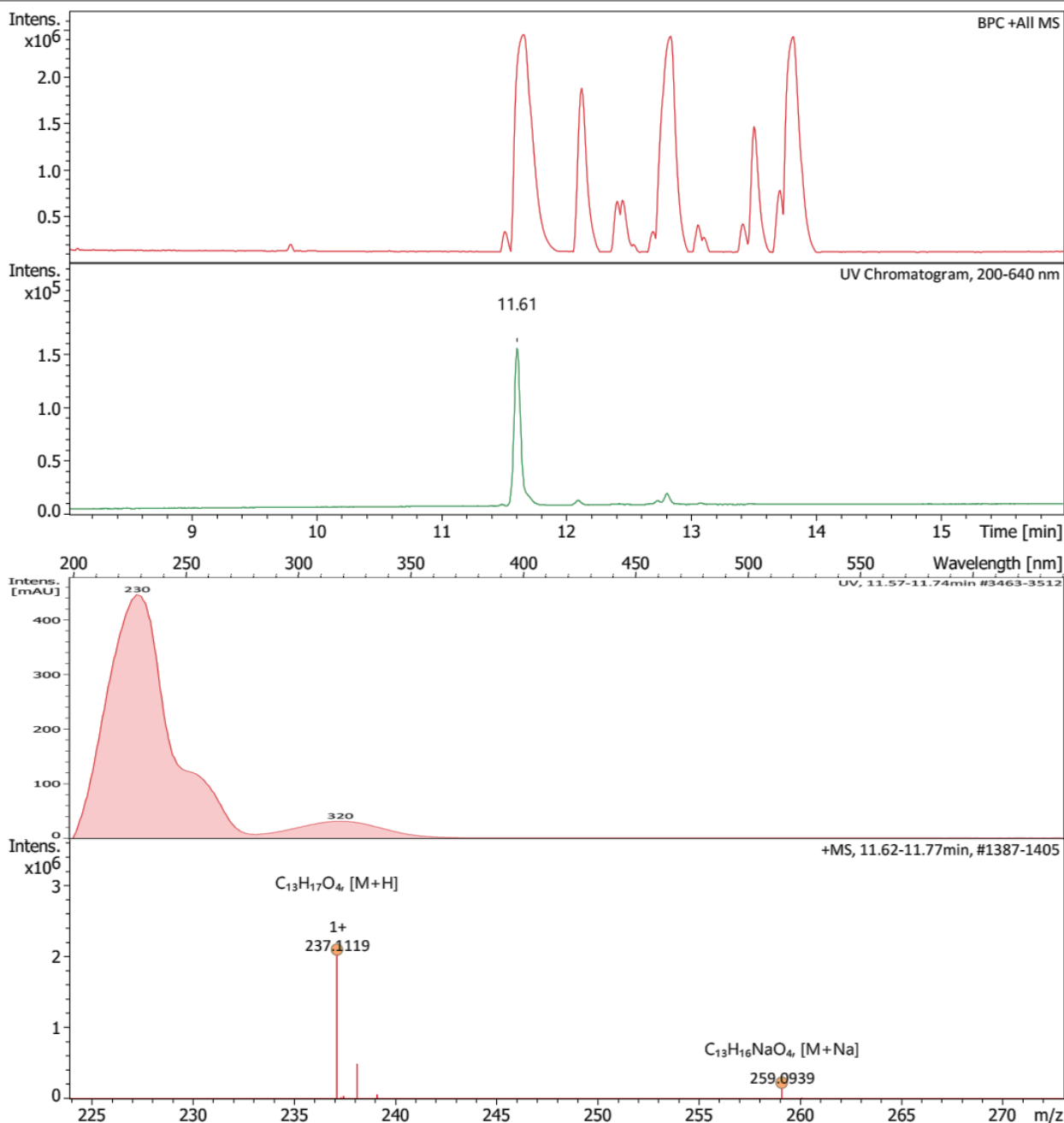
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Operator ate06

Instrument maXis 255552.00037

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Scan End	2500 m/z	Set Charging Voltage	0 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Dent Rice F13_P1-B-4_01_9611.d

Bruker Compass DataAnalysis 6.1

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by: sel22

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Figure S31. HR-ESI-MS of 4.

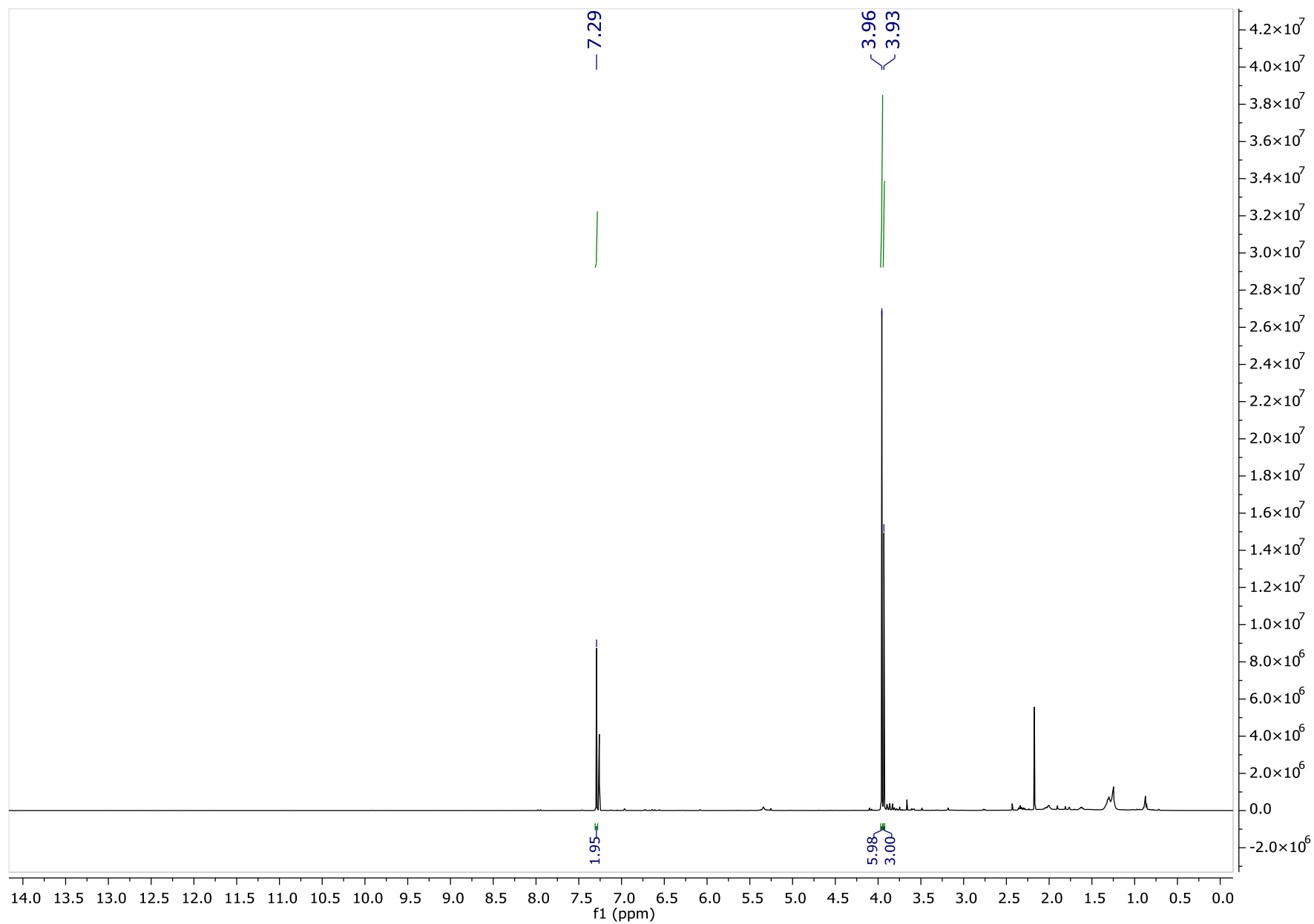


Figure S32. ^1H NMR spectrum of **4** in chloroform-*d* at 500 MHz.

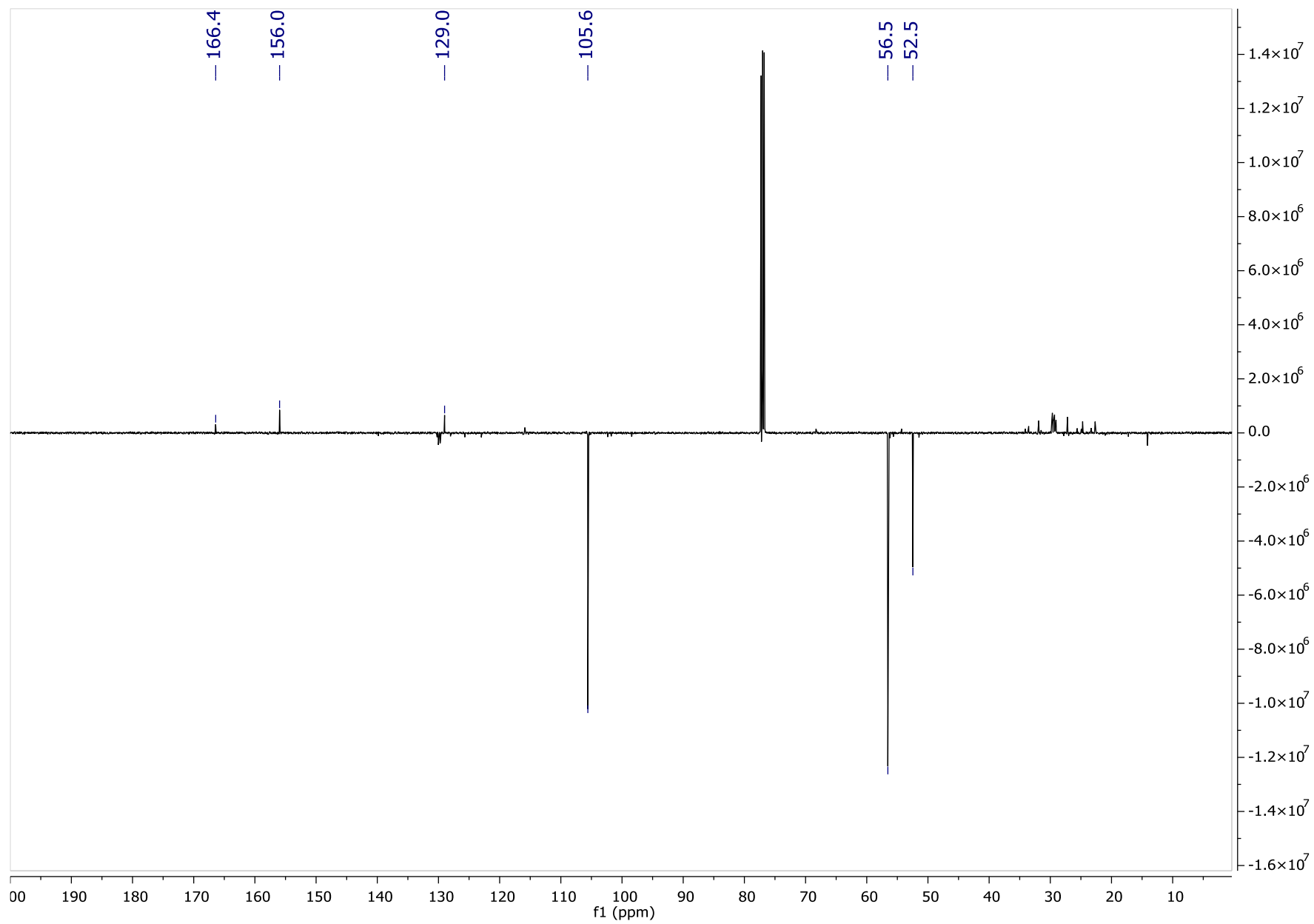


Figure S33. DEPTQ spectrum of **4** in chloroform-*d* at 125 MHz.

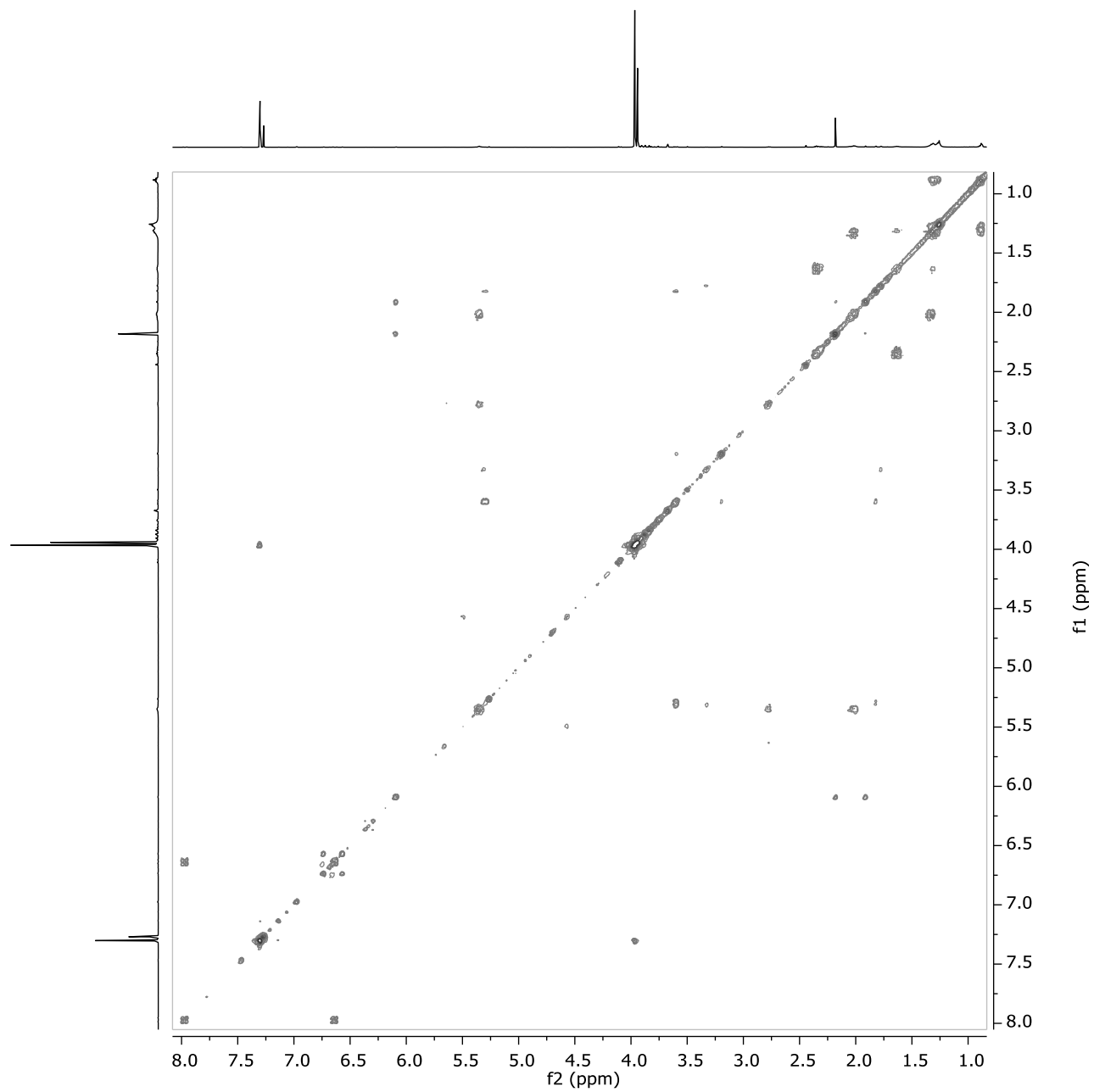


Figure S34. ^1H - ^1H COSY spectrum of **4** in chloroform-*d* at 500 MHz.

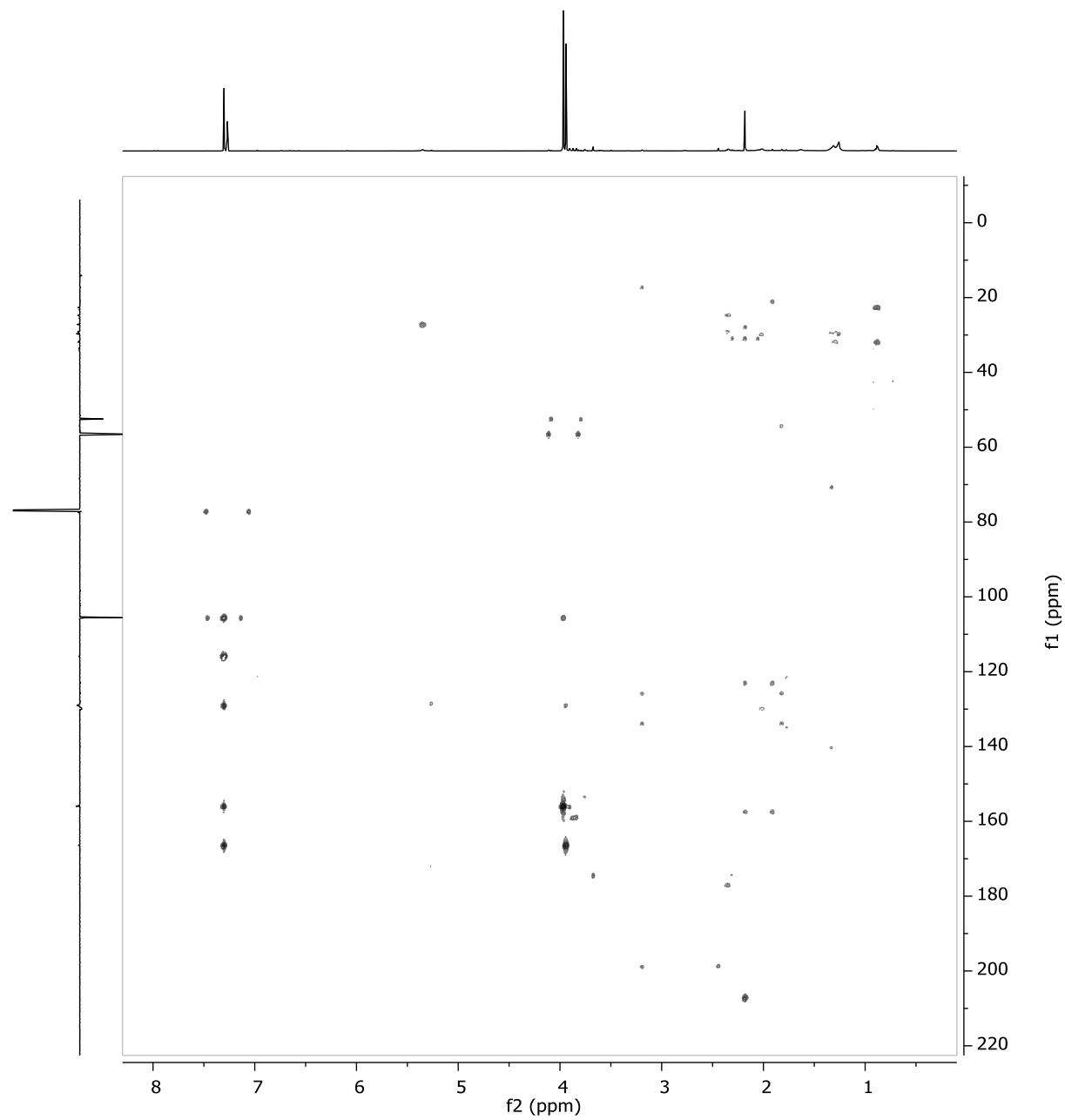


Figure S35. HMBC spectrum of **4** in chloroform-*d* at 500 MHz.

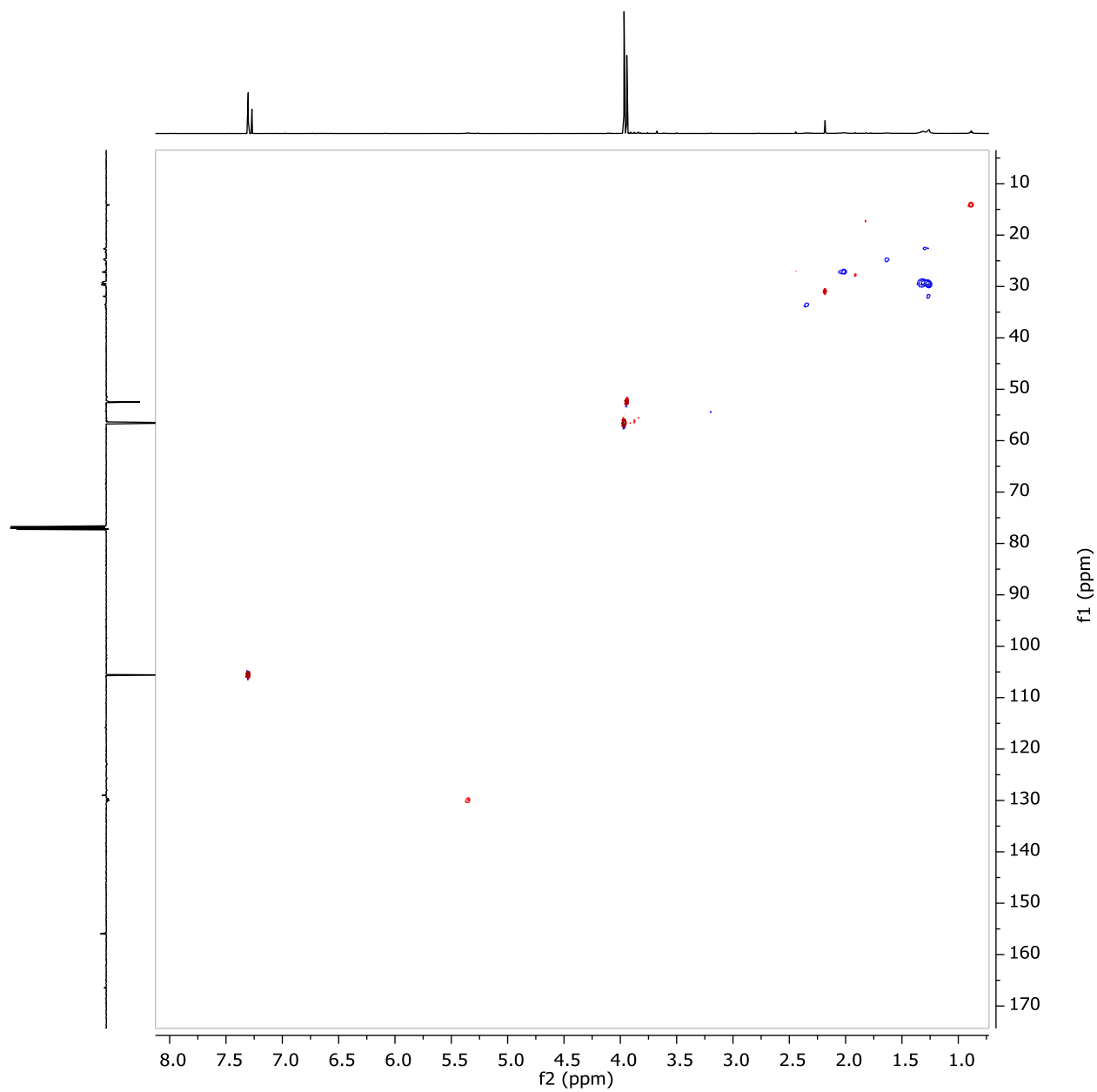


Figure S36. HSQC spectrum of **4** in chloroform-*d* at 500 MHz.

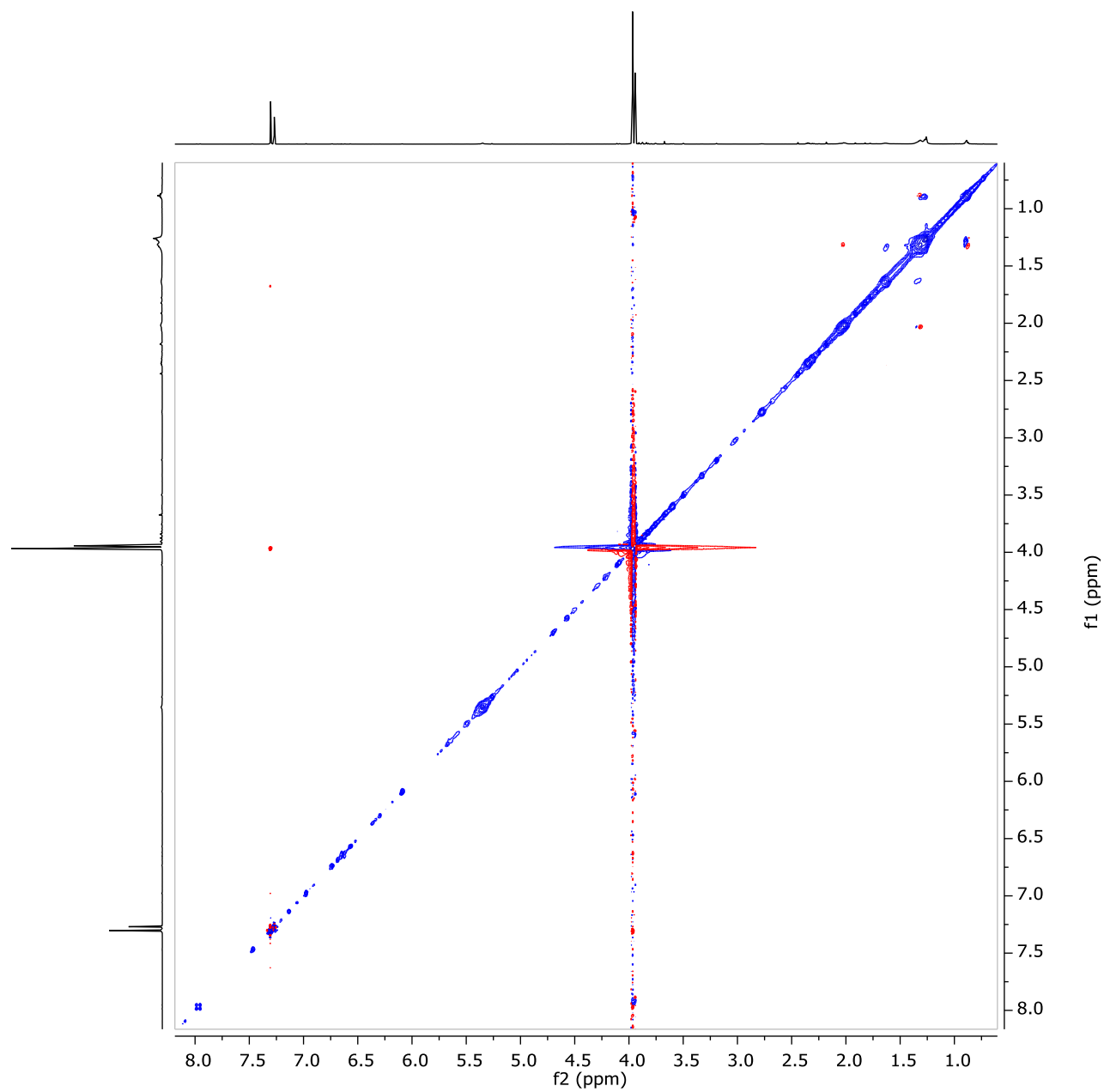


Figure S37. ROESY spectrum of **4** in chloroform-*d* at 500 MHz.

Display Report

Analysis Info

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Sample Name Dent Rice F15
Comment

Acquisition Date 18.02.2022 19:47:25

Operator lab

Instrument amaZon speed

Acquisition Parameter

Ion Source Type	ESI	Ion Polarity	Negative	Alternating Ion Polarity	on
Mass Range Mode	UltraScan	Scan Begin	100 m/z	Scan End	2000 m/z
Accumulation Time	4000 μ s	RF Level	100 %	Trap Drive	68.9
SPS Target Mass	1000 m/z	Averages	6 Spectra		

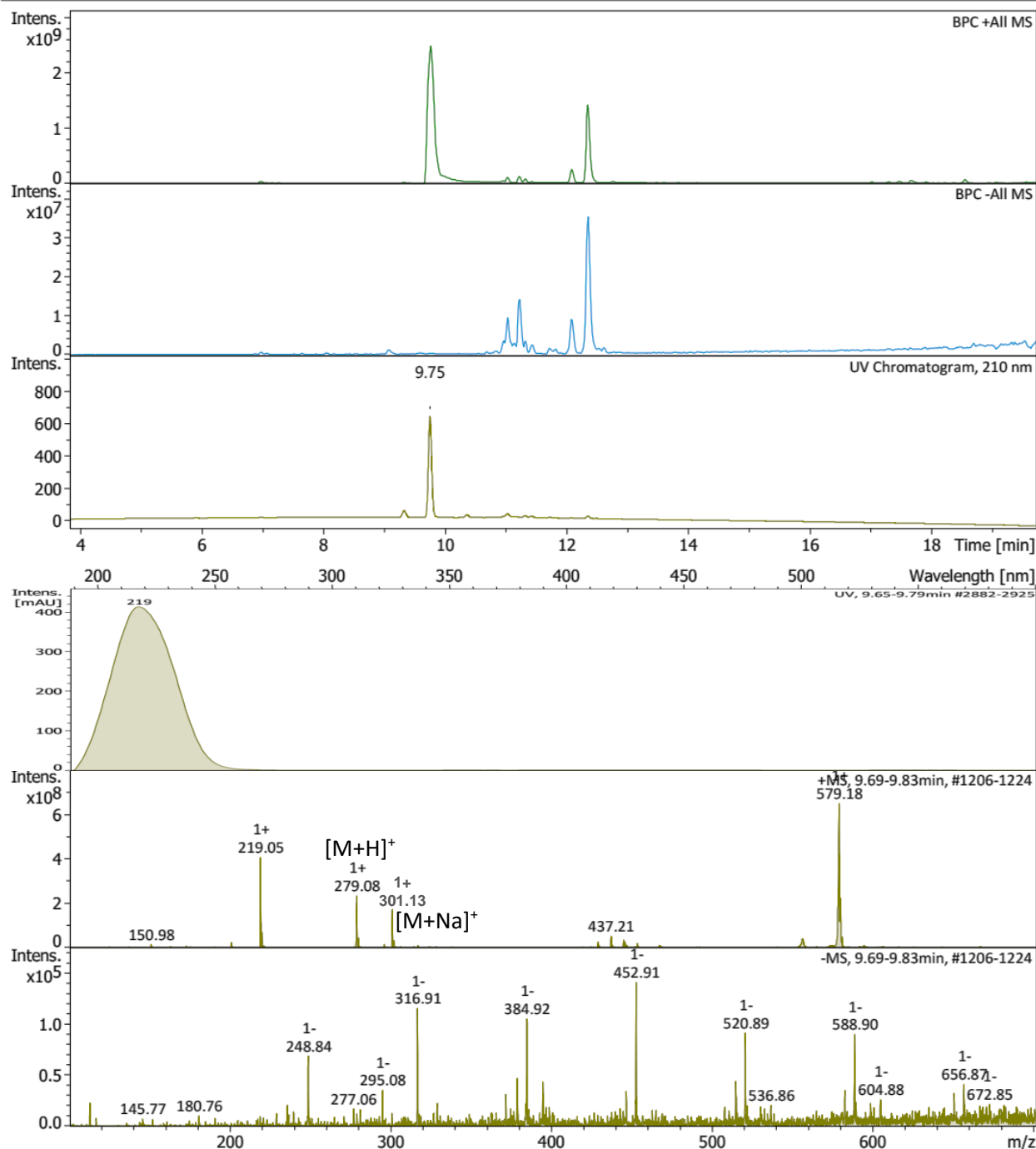


Figure S38. LR-ESI-MS of 5.

Display Report

Analysis Info

Analysis Name S:\DATA\Maxis\wsu20_Winnie Sum Chemutai\22_02\Dent Rice F15_P1-B-5_01_9612.d
 Method pos_säure_10000_screening_ms_100_2500_line.m
 Sample Name Dent Rice F15
 Comment Screening01
 Waters Acquity UPLC BEH C₁₈ 1,7um 2.1x50mm

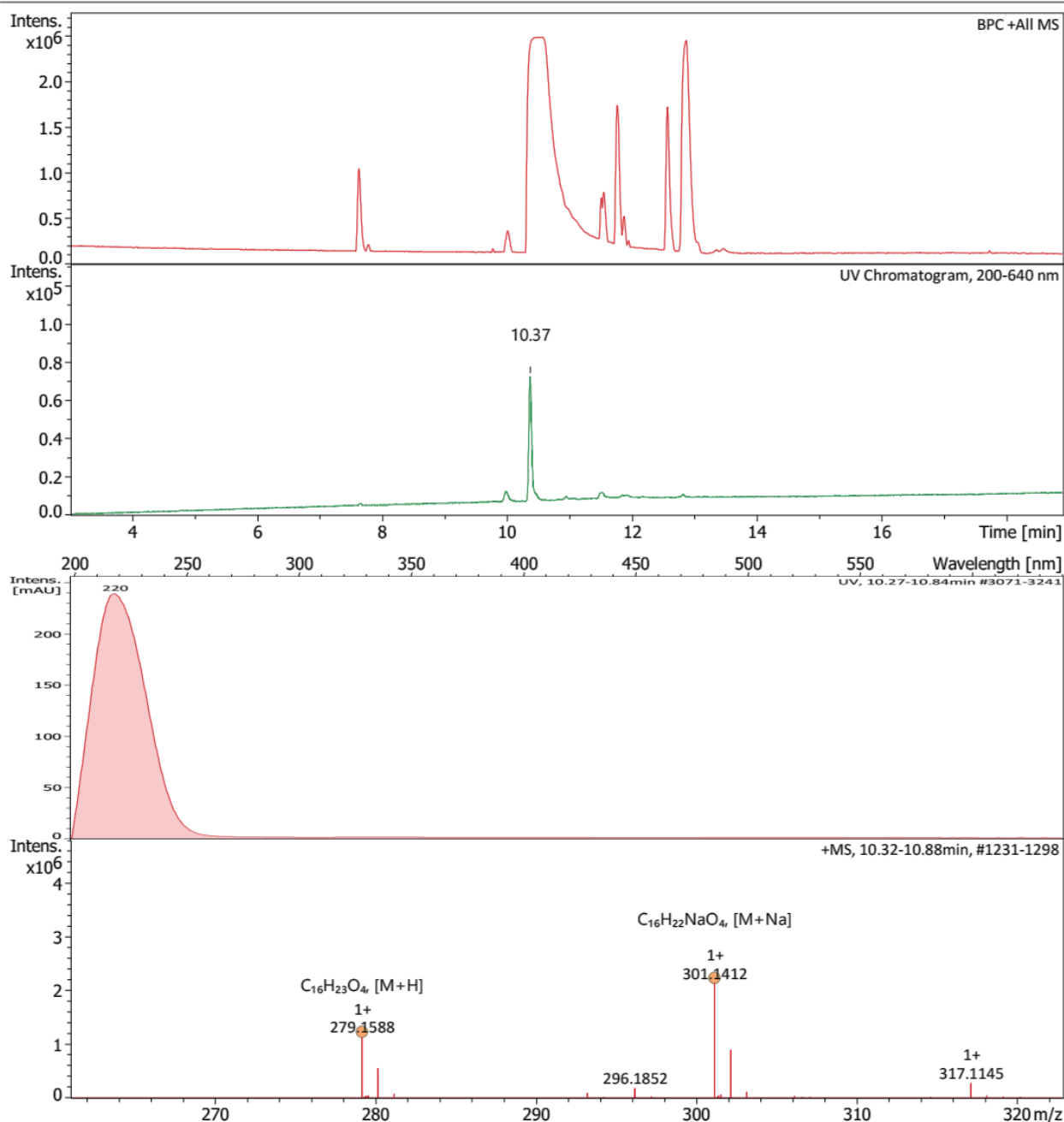
Acquisition Date 23.02.2022 13:40:10

Operator ate06

Instrument maxis 255552.00037

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.0 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	10.0 l/min
Scan End	2500 m/z	Set Charging Voltage	0 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Dent Rice F15_P1-B-5_01_9612.d

Bruker Compass DataAnalysis 6.1

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by: sel22

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Figure S39. HR-ESI-MS of 5.

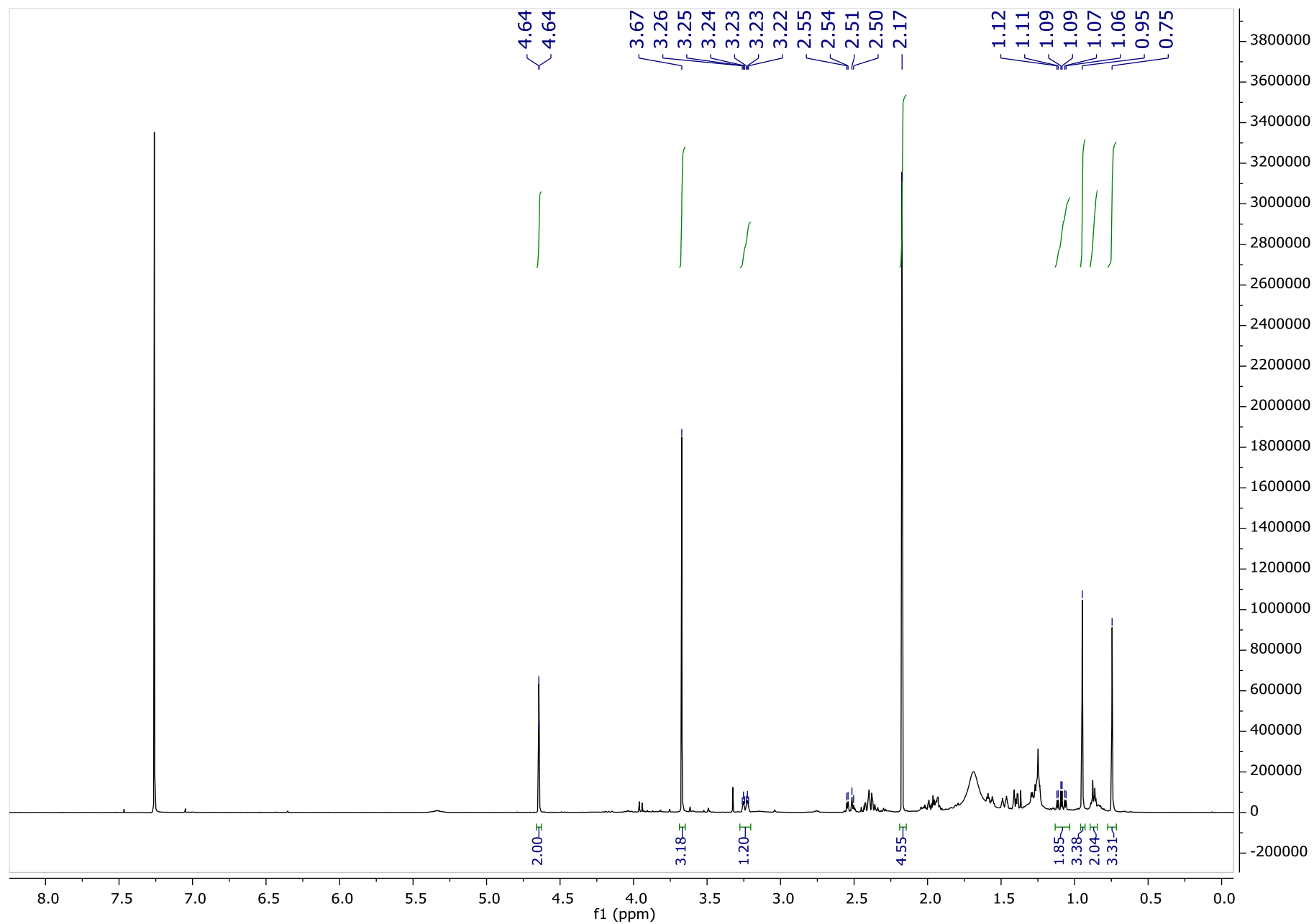


Figure S40. ^1H NMR spectrum of **5** in chloroform-*d* at 500 MHz.

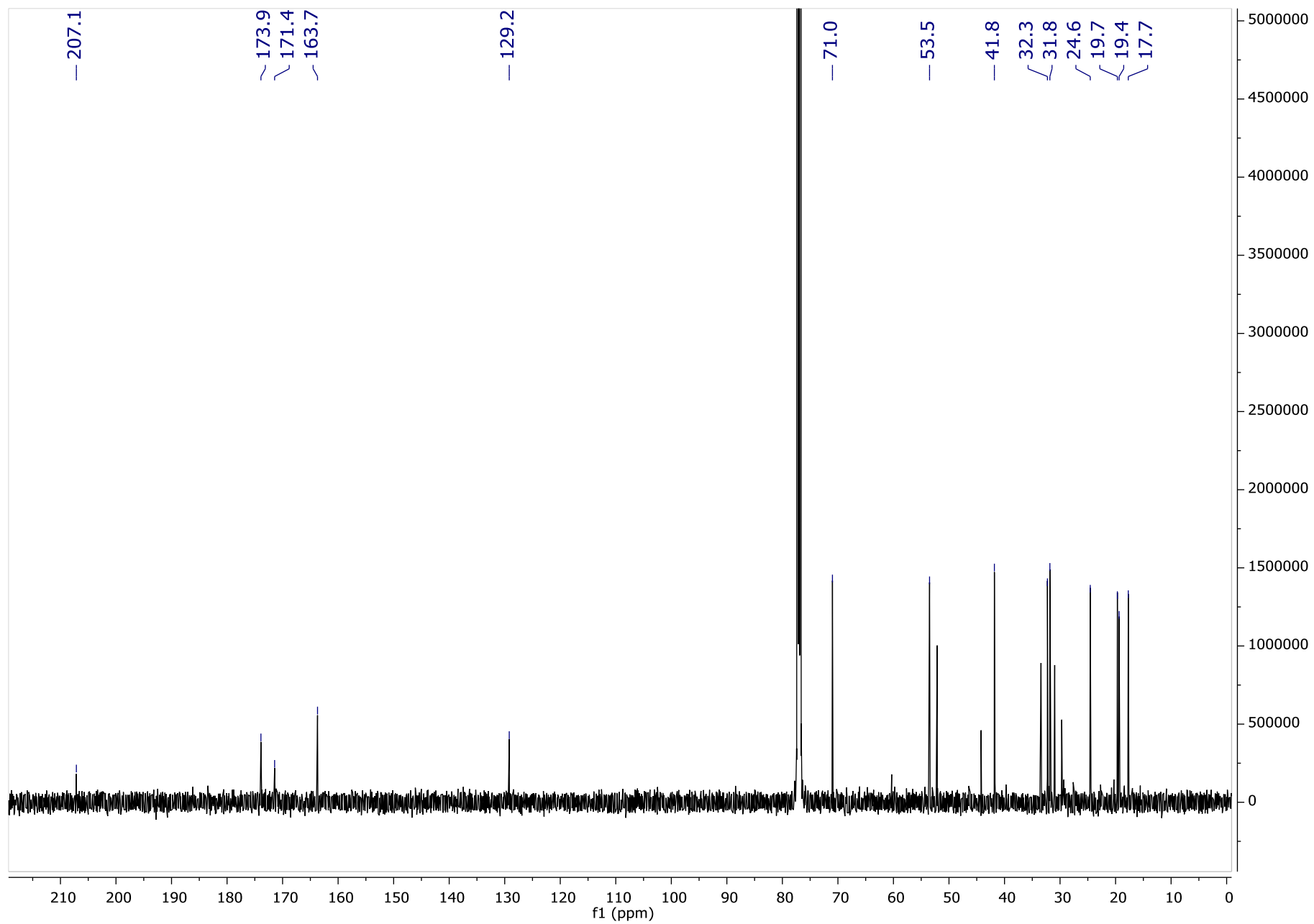


Figure S41. ^{13}C NMR spectrum of **5** in chloroform-*d* at 125 MHz.

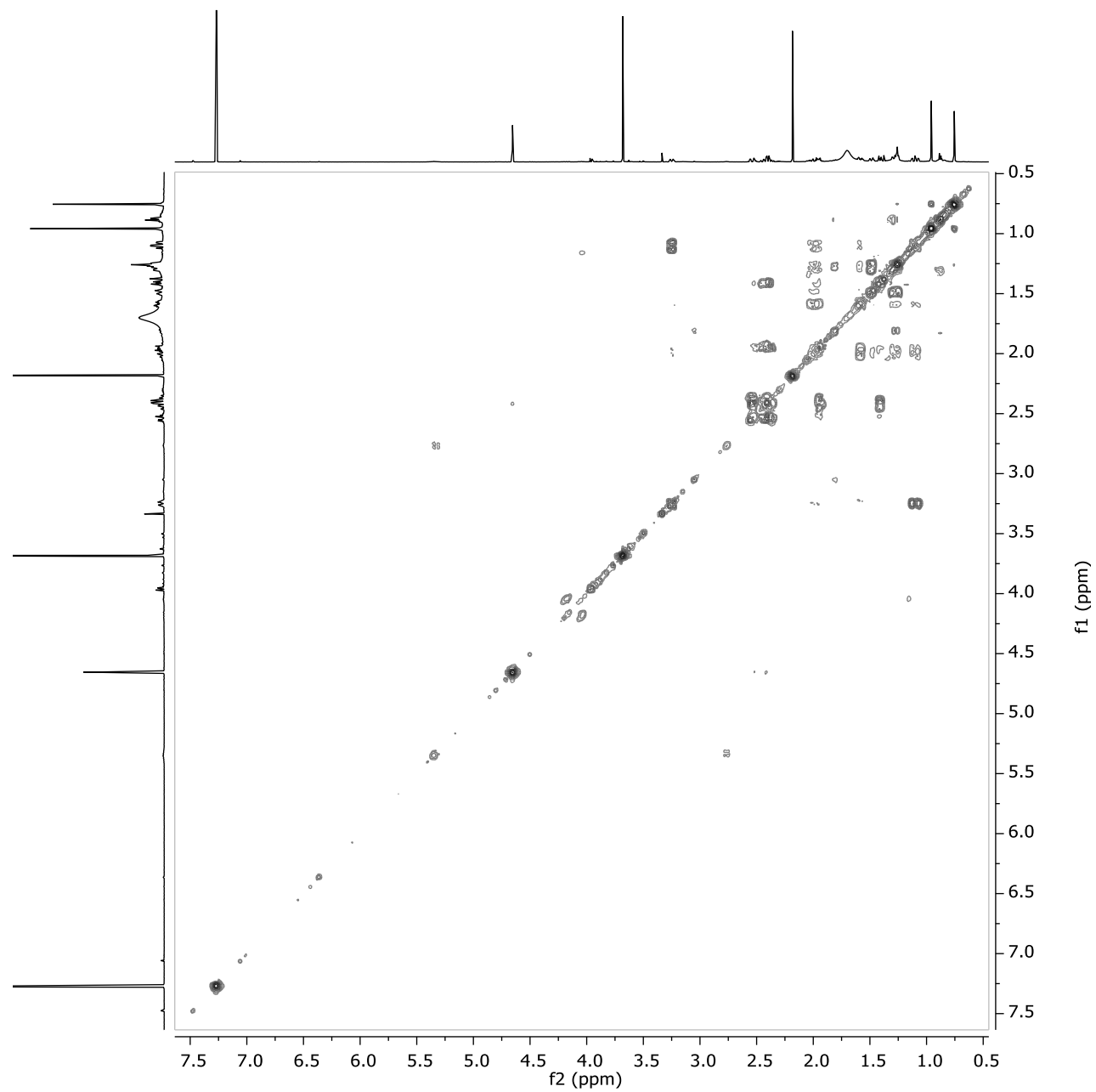


Figure S42. ^1H - ^1H COSY spectrum of **5** in chloroform-*d* at 500 MHz.

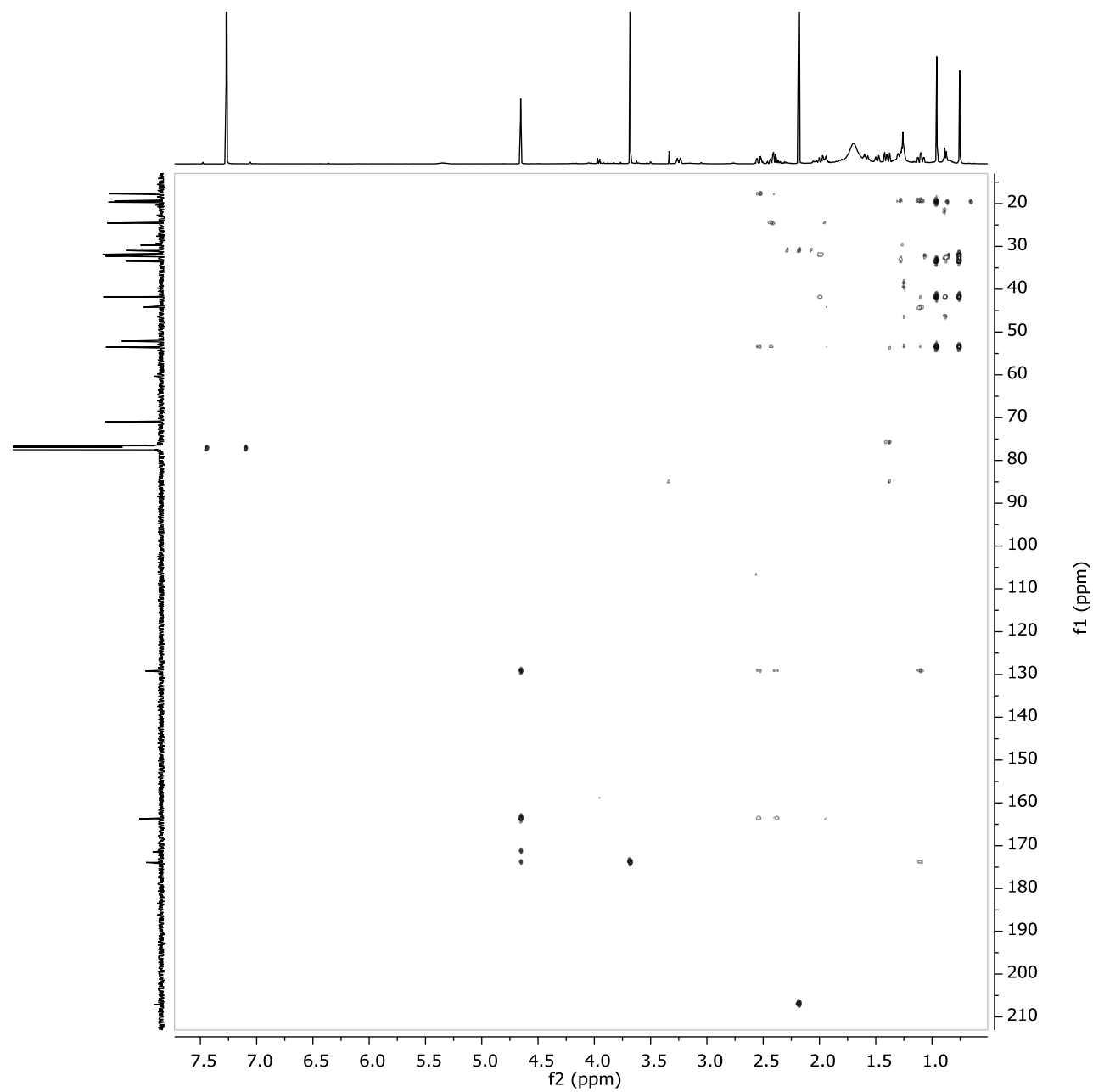


Figure S43. HMBC spectrum of **5** in chloroform-*d* at 500 MHz.

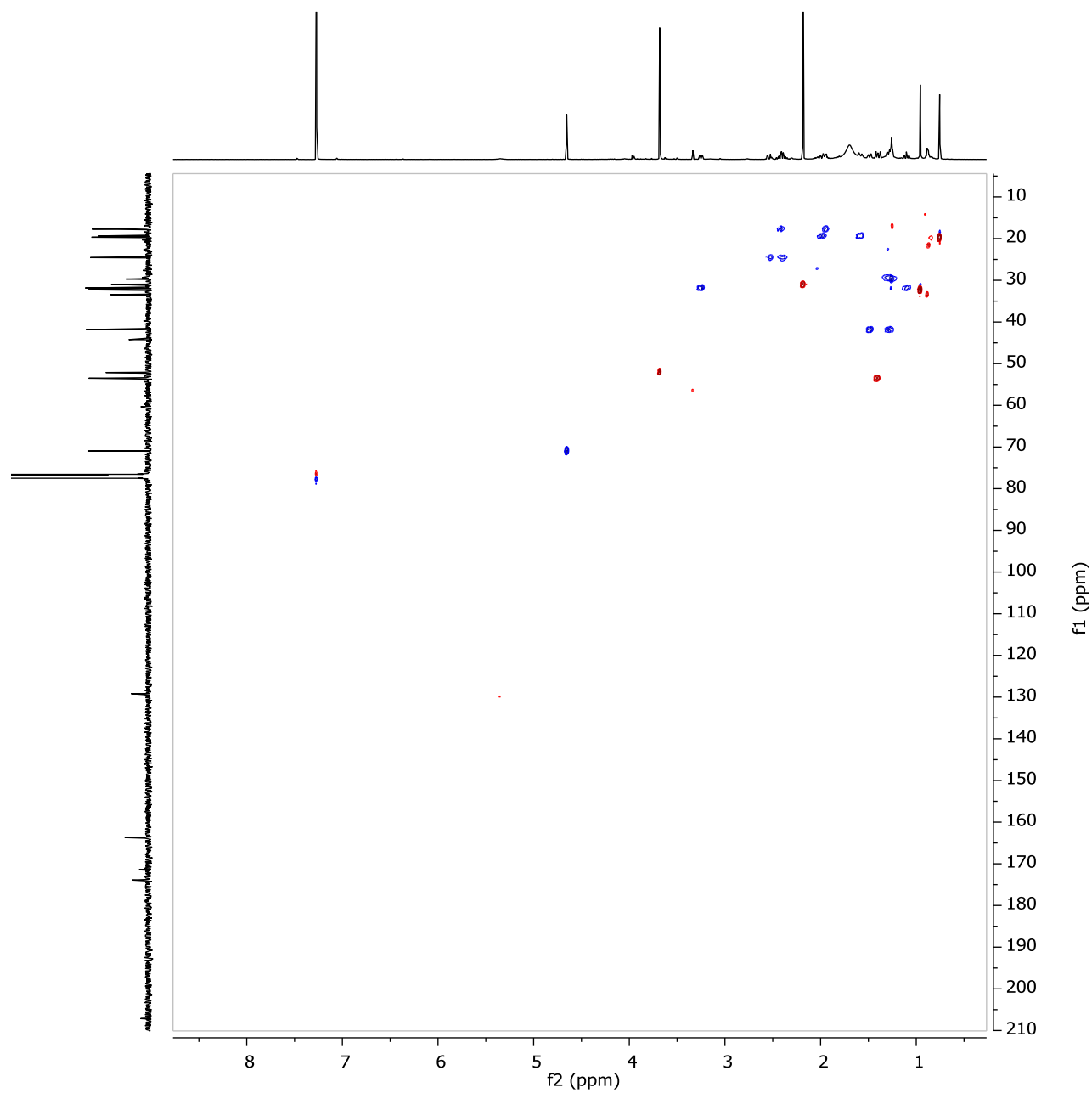


Figure S44. HSQC spectrum of **5** in chloroform-*d* at 500 MHz.

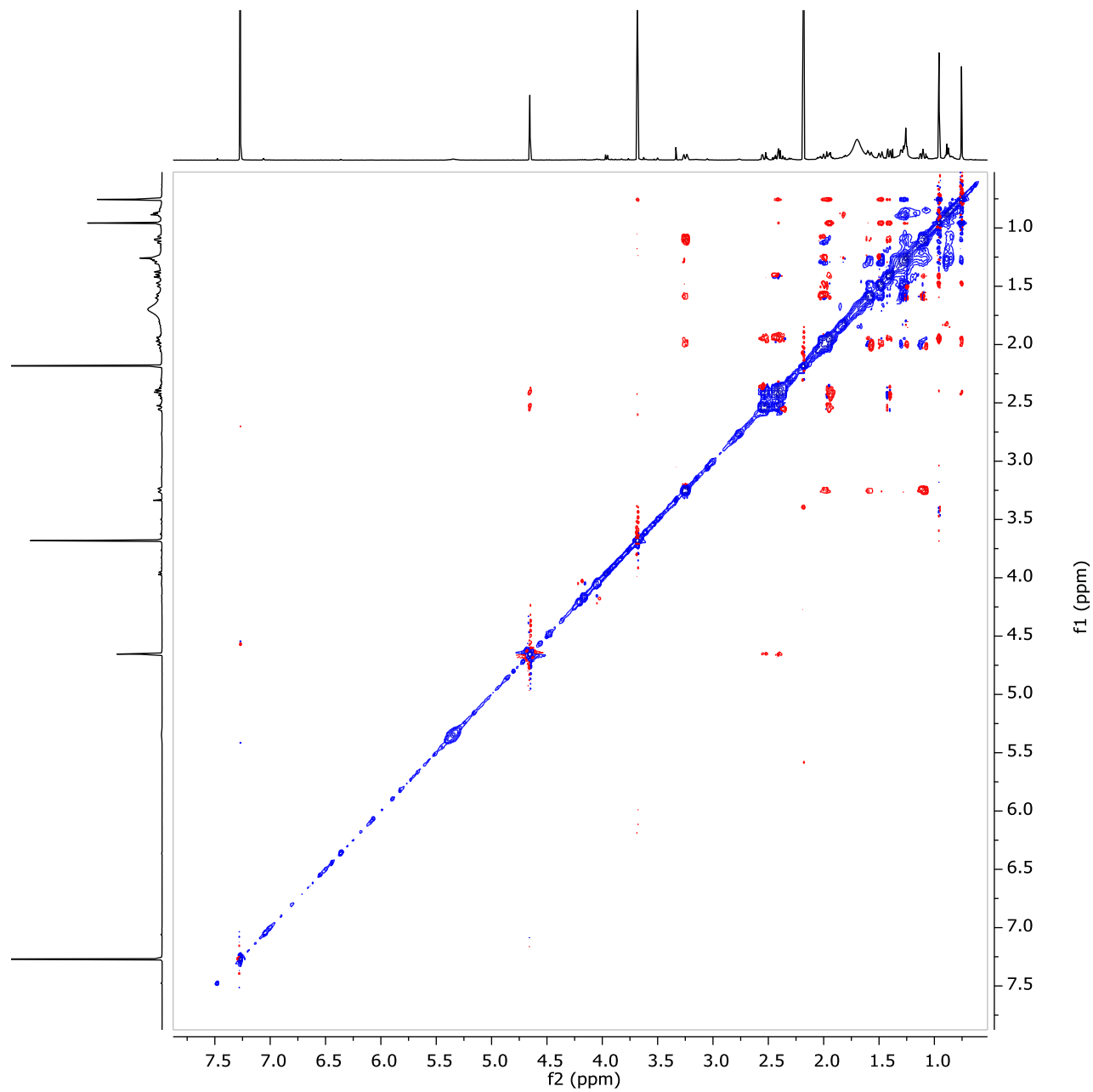


Figure S45. ROESY spectrum of **5** in chloroform-*d* at 500 MHz.