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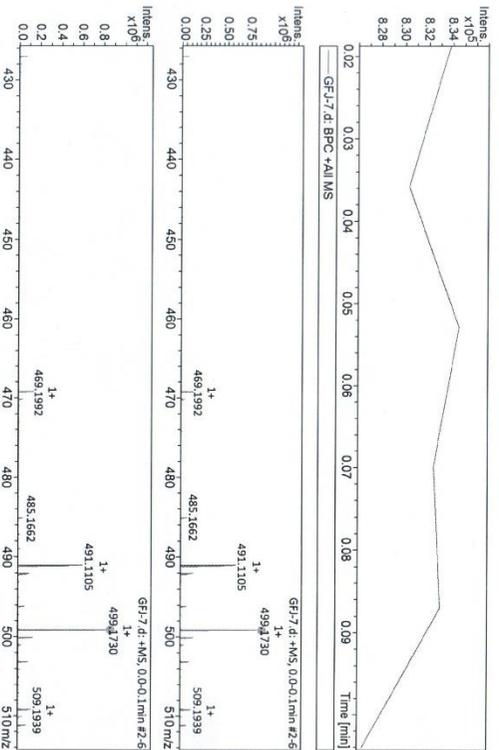
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Mass Spectrum SmartFormula Report

Analysis Info
Analysis Name: D:\Data\A501V\JZ2018.9.25\GF-J7.d
Method: Tune_pos_Mild.m
Sample Name: GF-J7
Comment:
Acquisition Date: 2018-09-25 16:14:50
Operator: Demo User
Instrument: compact 8255754.20156

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive
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Scan End	1800 m/z	Set Charging Voltage	2000 V
		Set Corona	0 nA
		Set Nebulizer	0.3 Bar
		Set Dry Gas Flow	2.0 l/min
		Set Dry Gas Source	3.0 l/min
		Set Divergent Valve	Source
		Set APCI Heater	0 °C



Mass, m/z	# Ion Formula	m/z	err [ppm]	Mean err [ppm]	rdB	N-Rule	e_Conf	mSigma	Adduct
499.172988	1	C28H42SNO7	499.172724	-0.5	-0.5	14.5	ok	even	M+Na

Figure S1. HRESIMS spectrum of 1

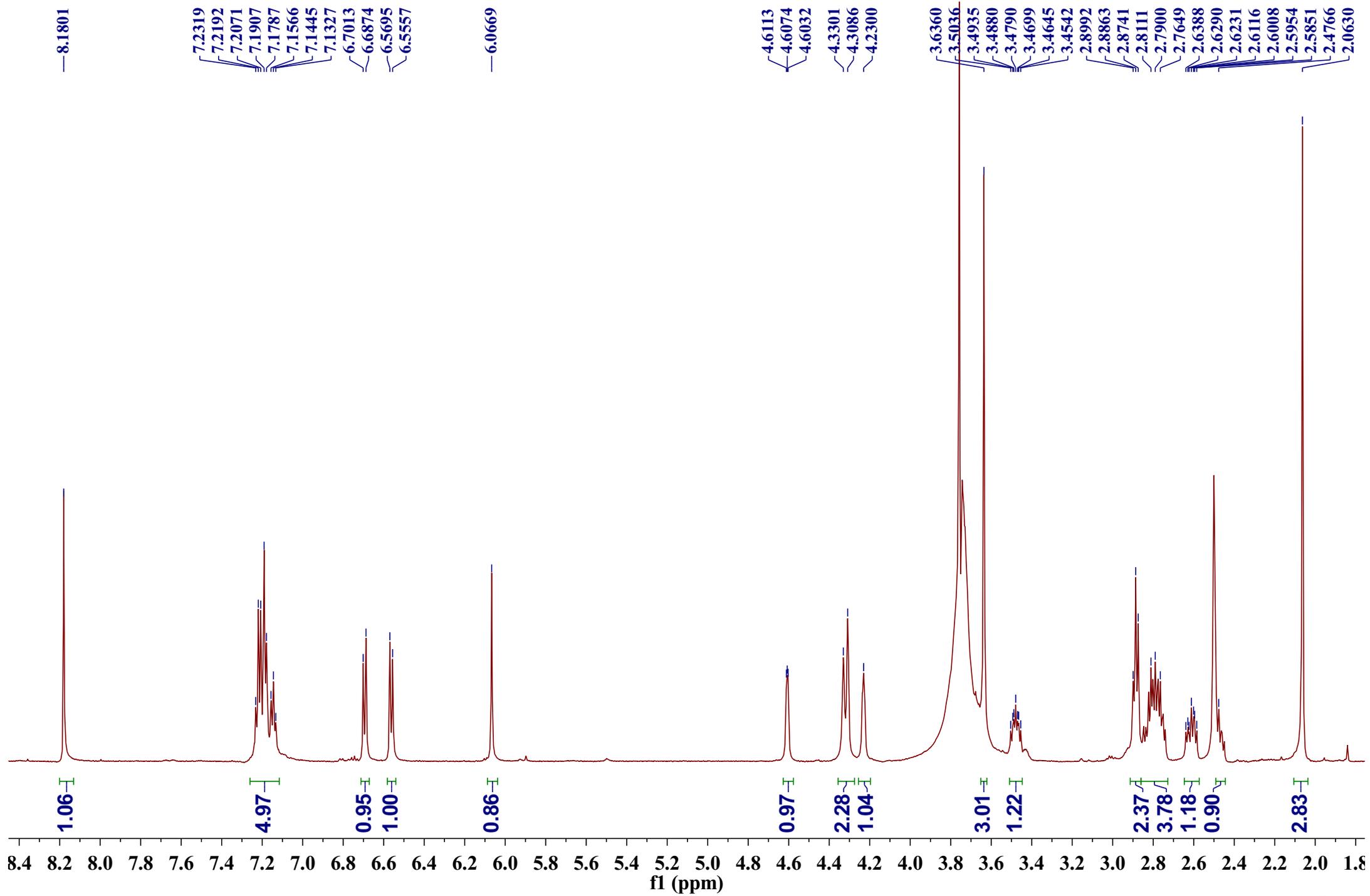


Figure S2. ^1H NMR (600 MHz, $\text{DMSO-}d_6$) spectrum of **1**

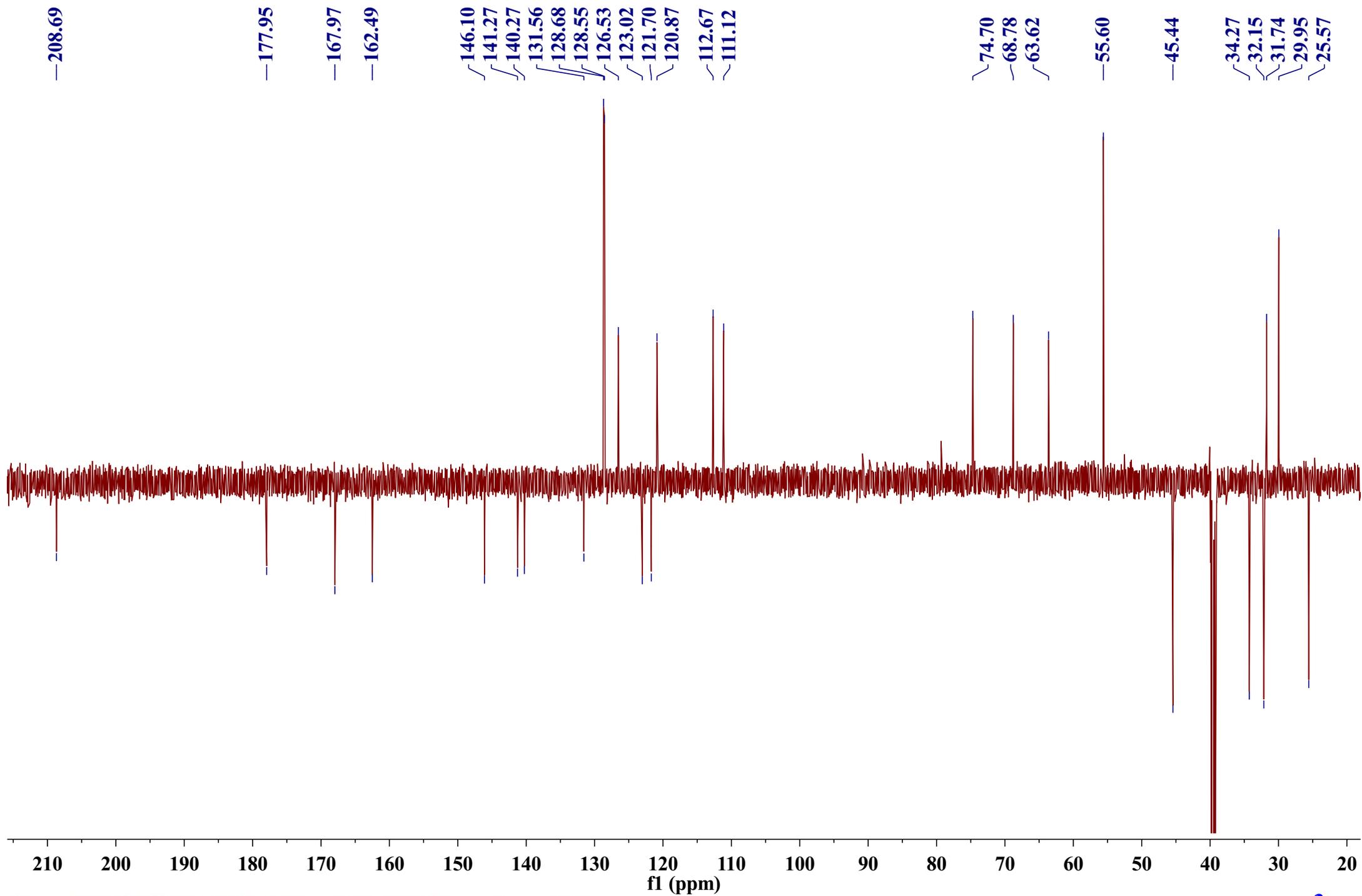


Figure S3. DEPTQ (150 MHz, DMSO- d_6) spectrum of **1**

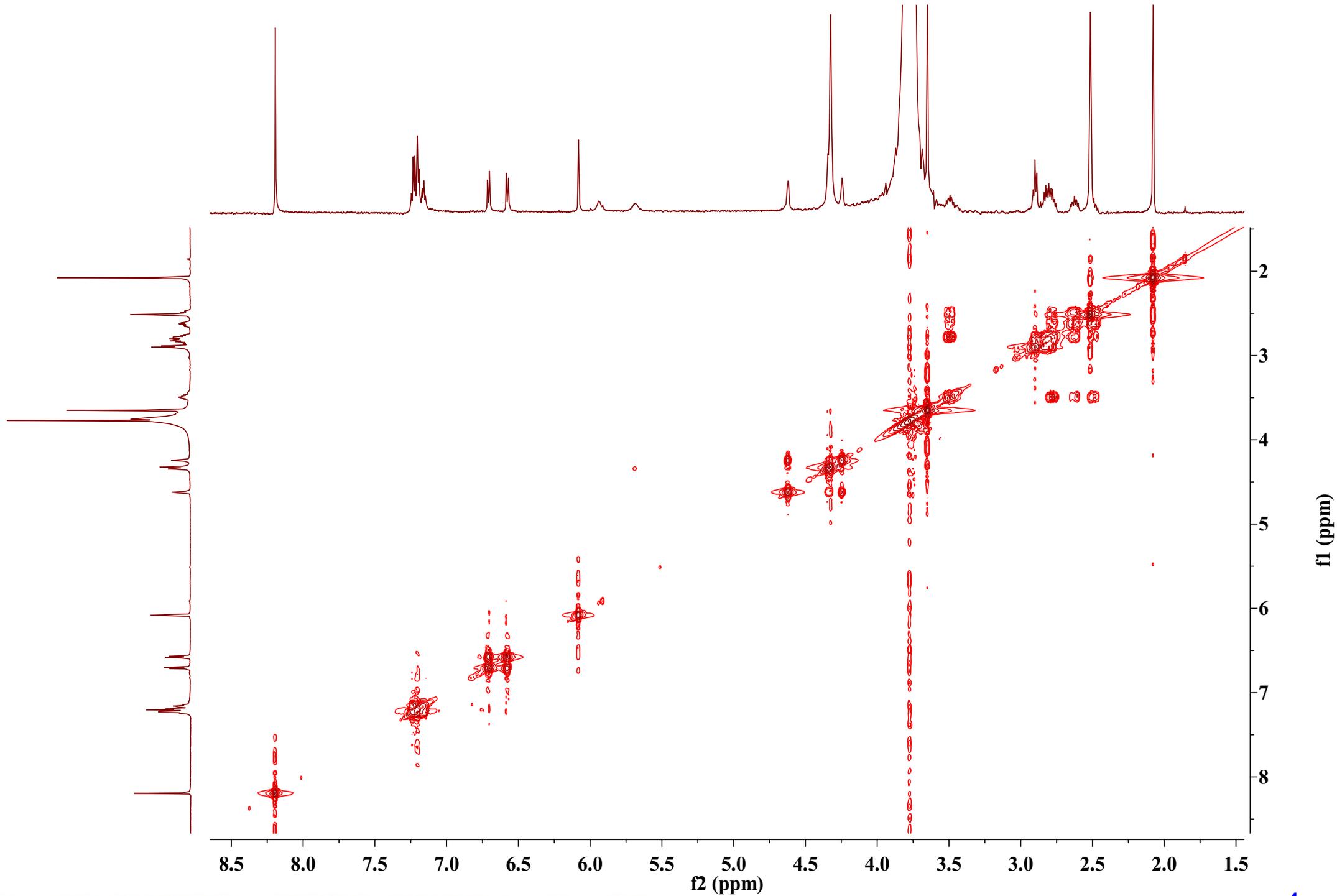


Figure S4. HSQC (600 and 150 MHz, DMSO-*d*₆) spectrum of **1**

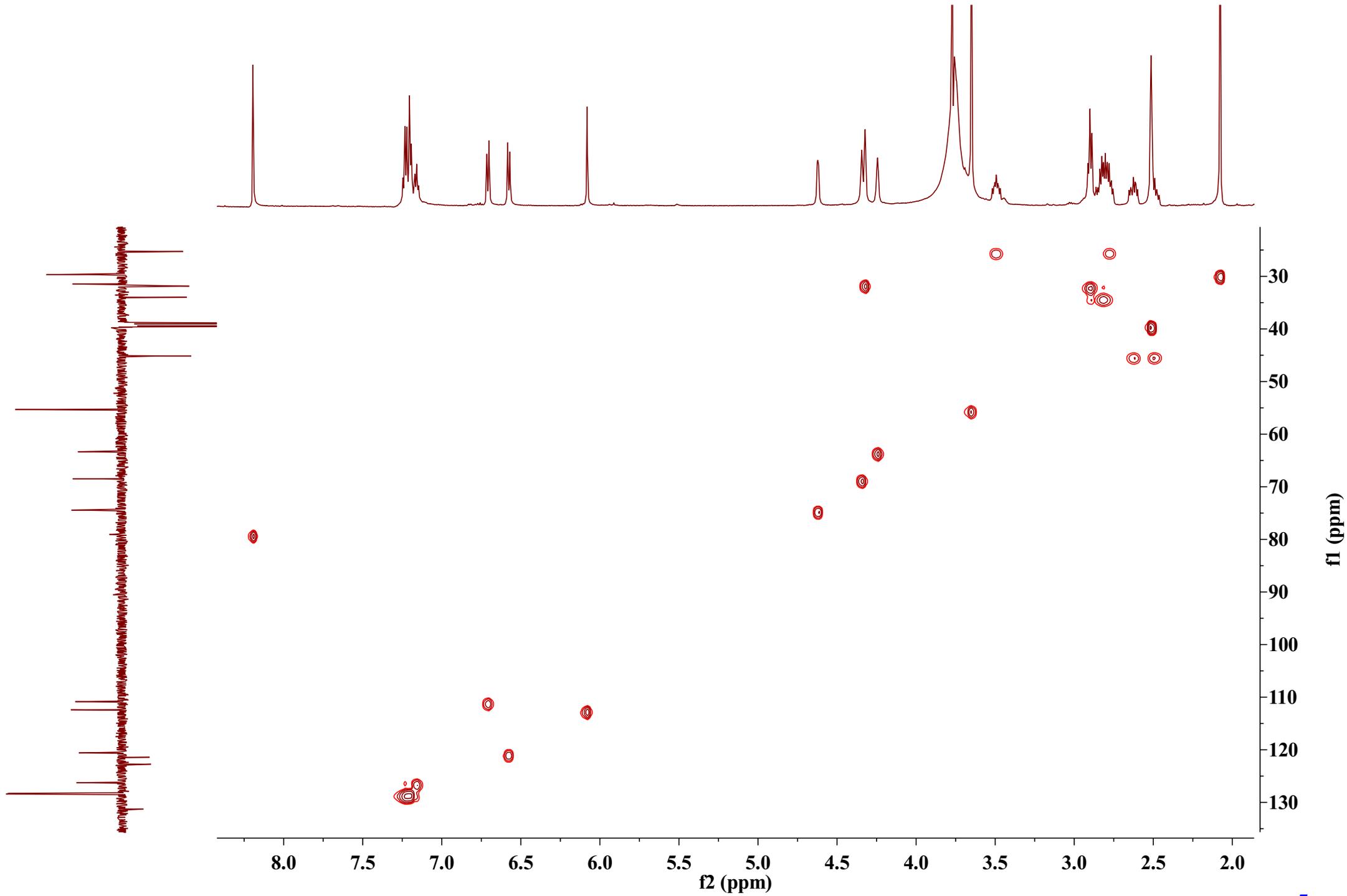


Figure S5. HSQC (600 and 150 MHz, $\text{DMSO-}d_6$) spectrum of **1**

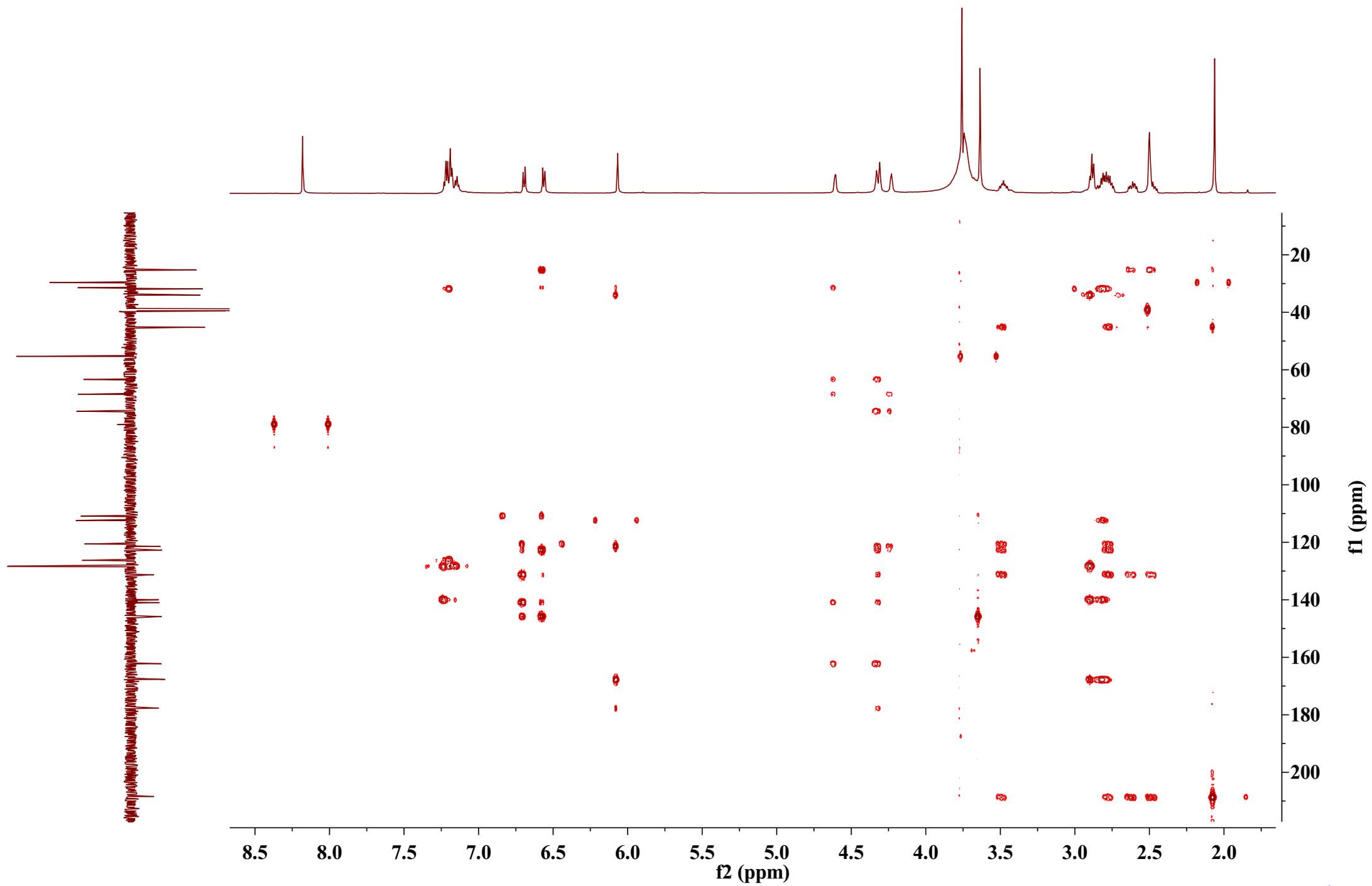


Figure S6. HMBC (600 and 150 MHz, DMSO-*d*₆) spectrum of 1

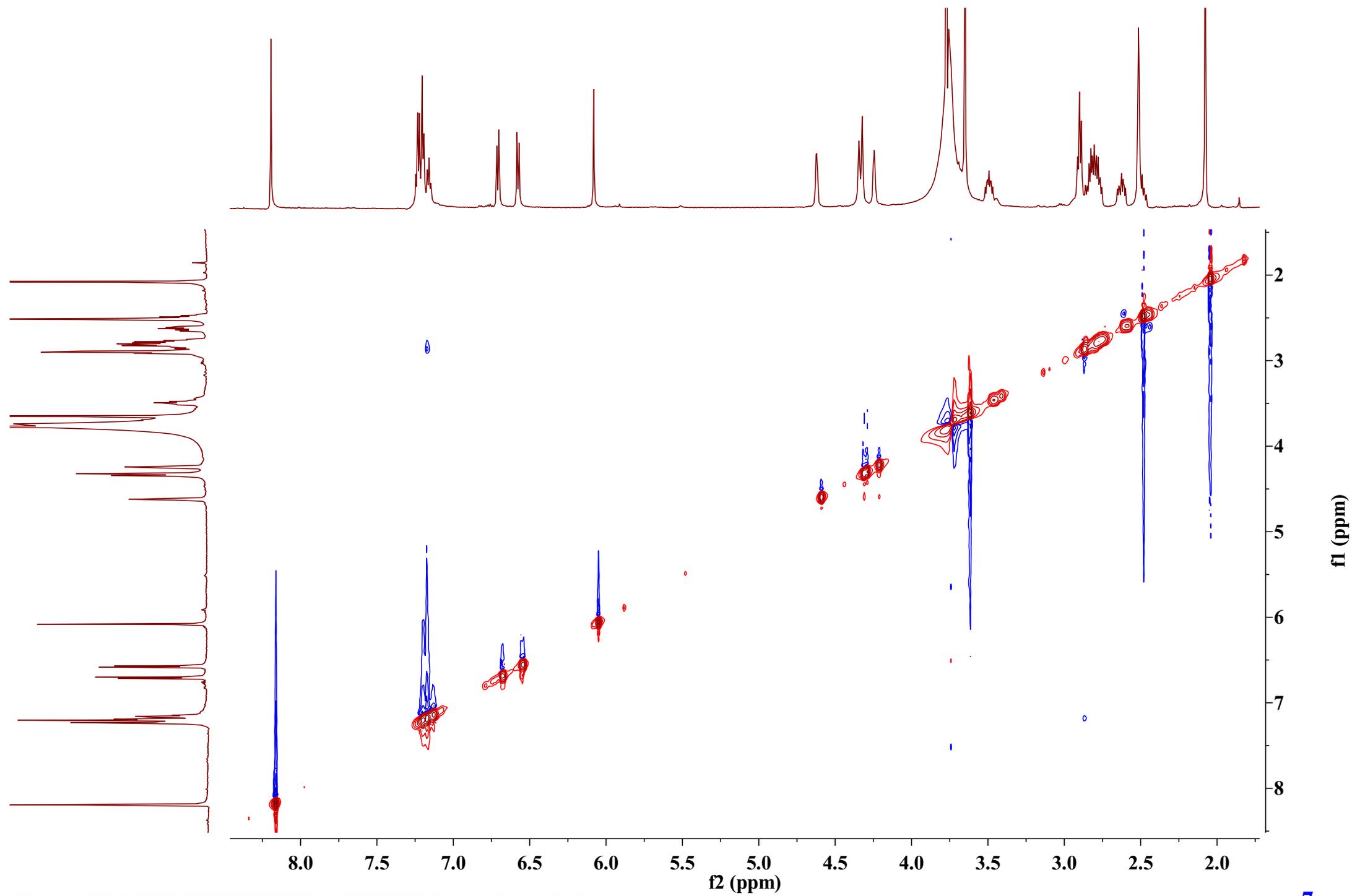


Figure S7. ROESY (600 MHz, DMSO- d_6) spectrum of **1**

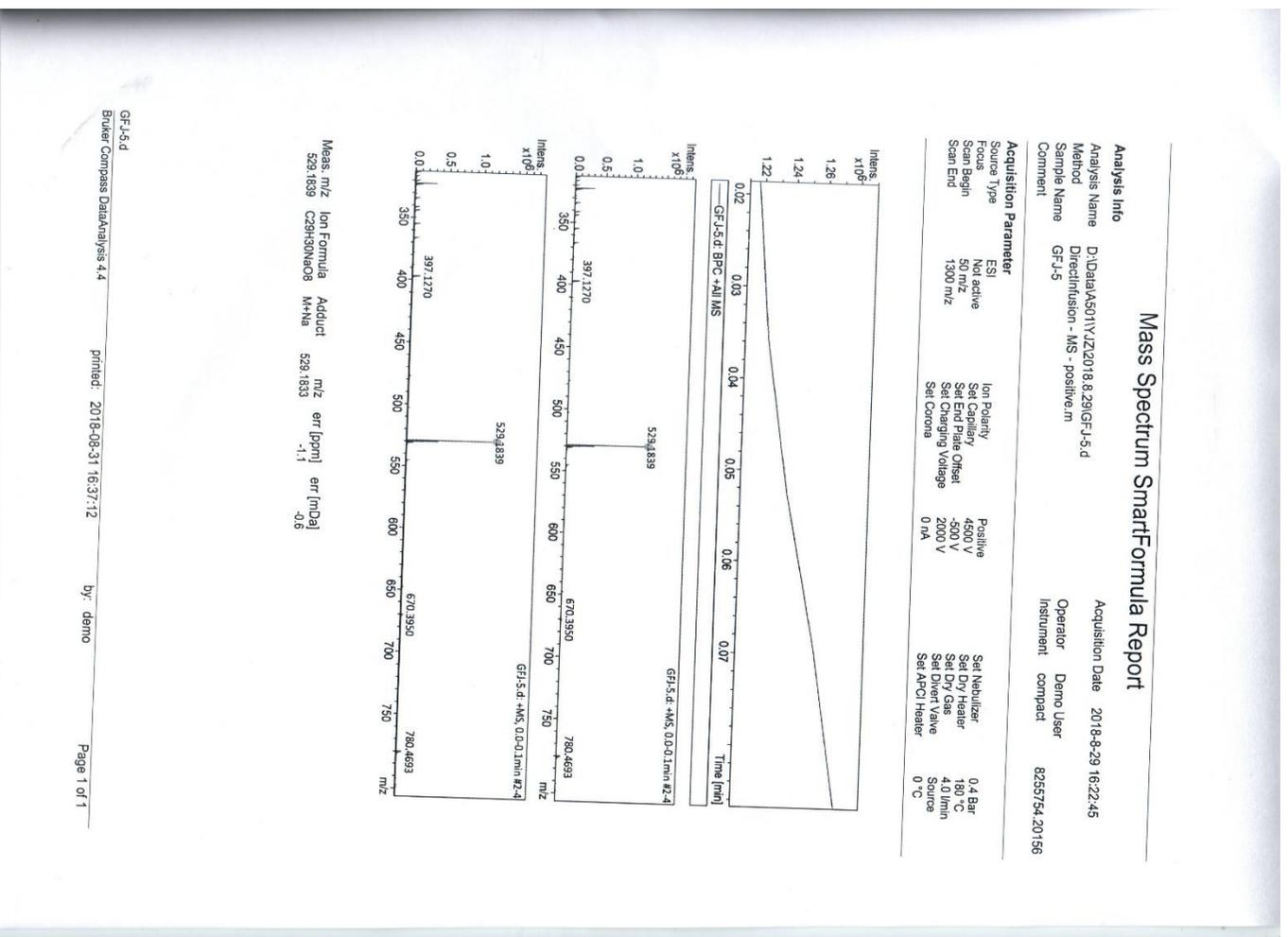


Figure S8. HRESIMS spectrum of 2

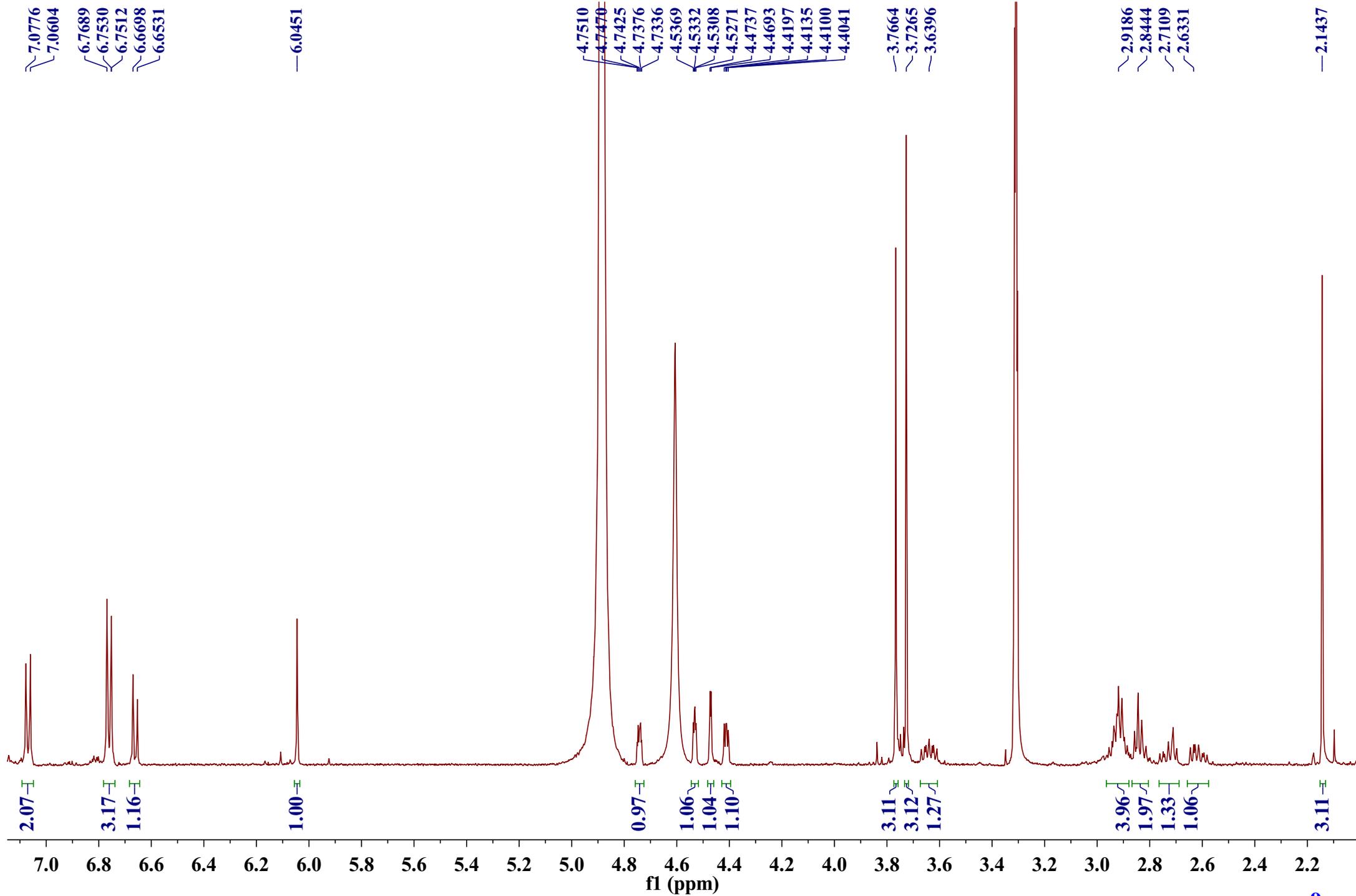


Figure S9. ¹H NMR (600 MHz, methanol-*d*₄) spectrum of **2**

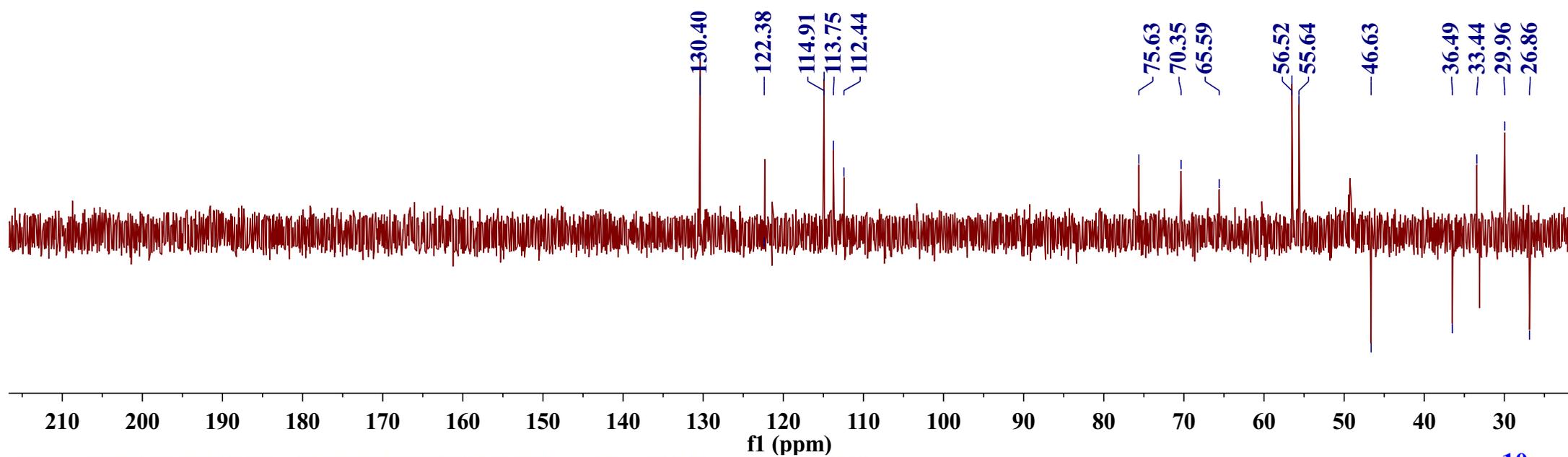
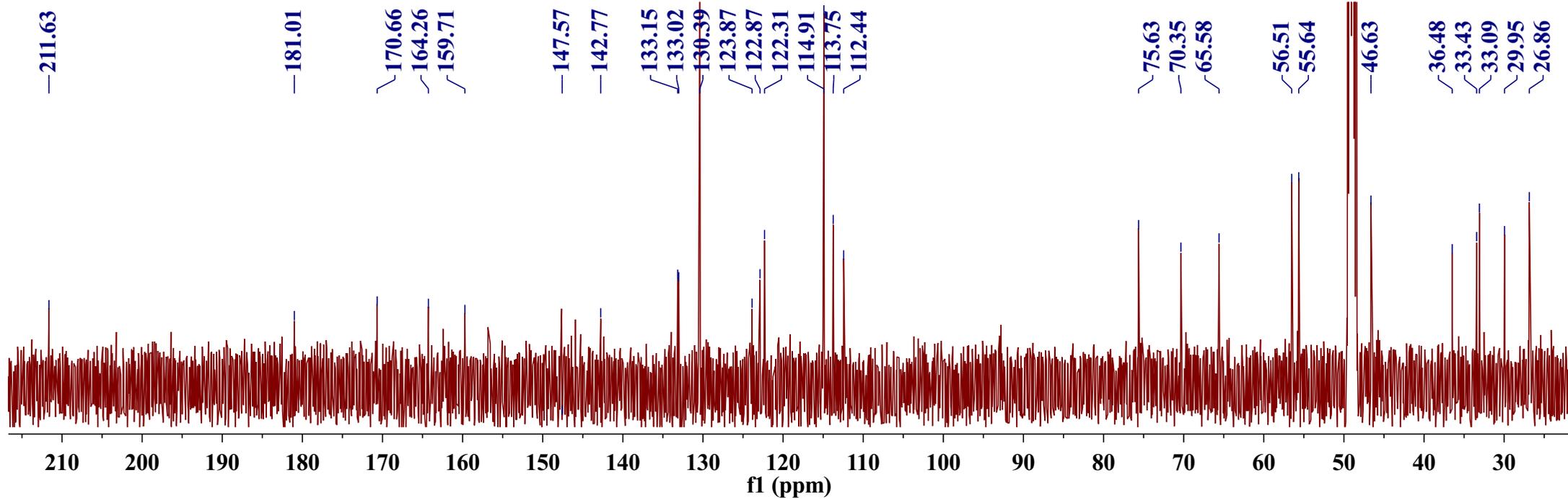


Figure S10. ^{13}C NMR and DEPT-135 (150 MHz, methanol- d_4) spectrum of 2

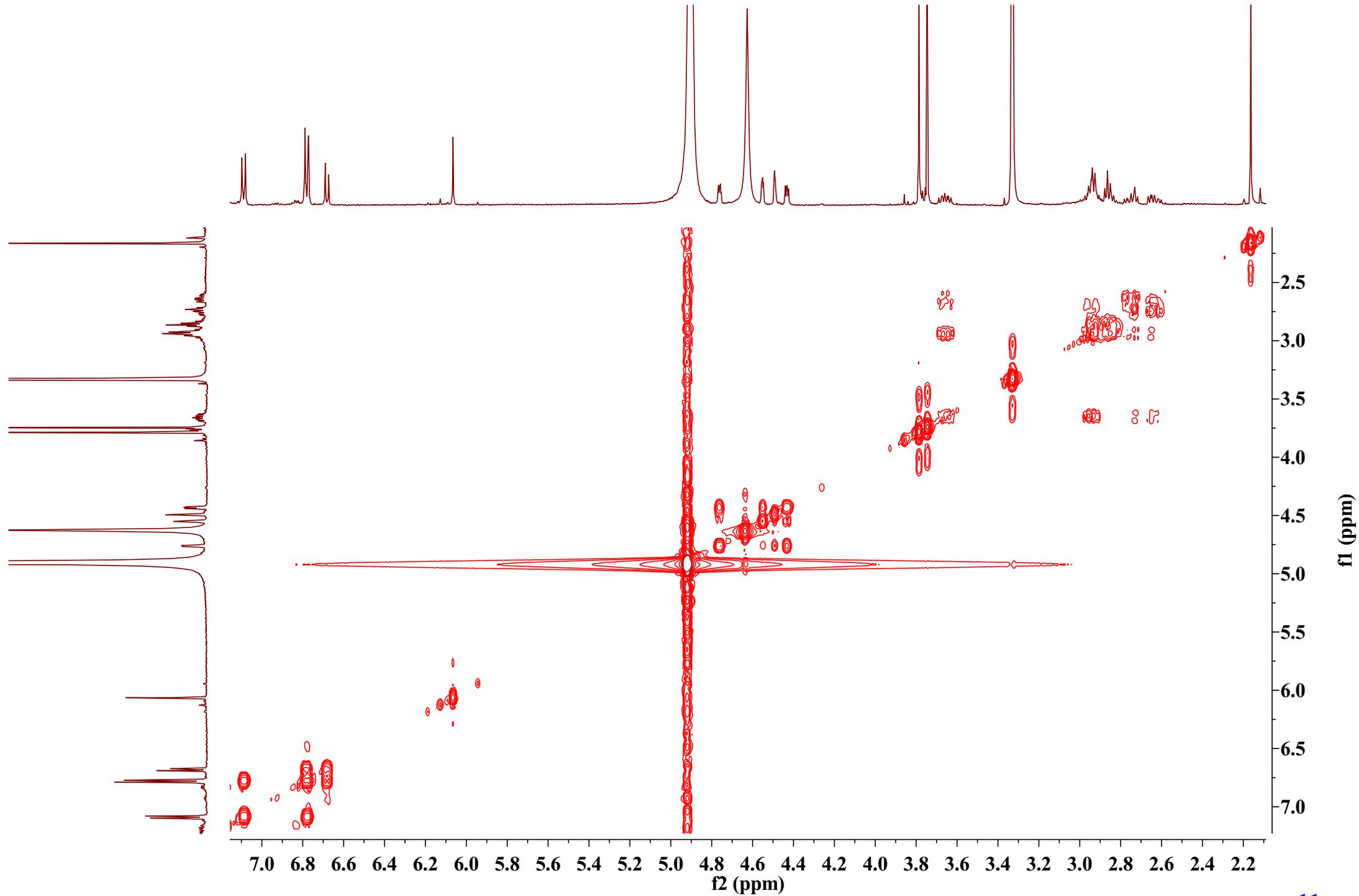


Figure S11. ^1H - ^1H COSY (600 MHz, methanol- d_4) spectrum of **2**

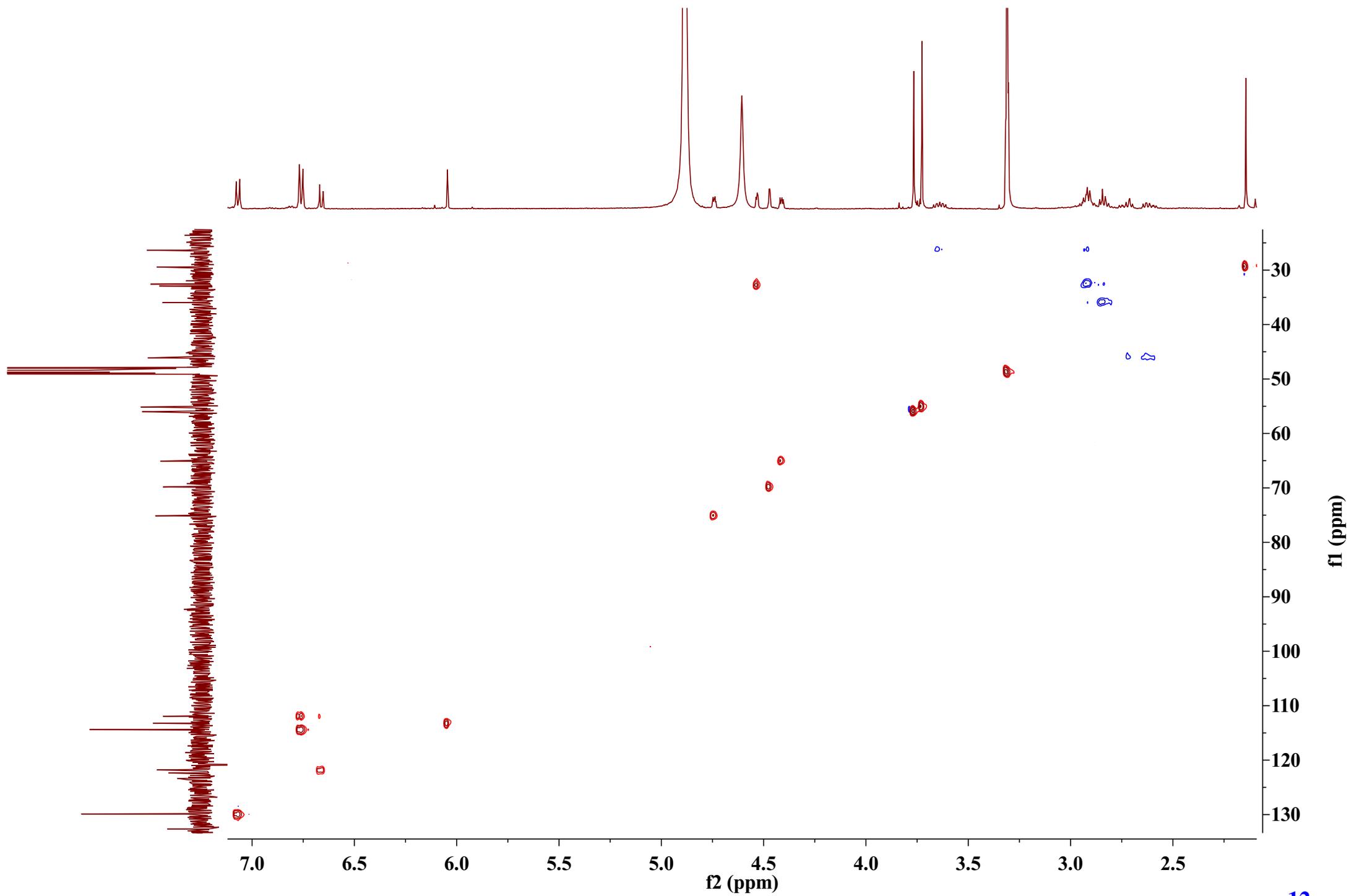


Figure S12. HSQC (600 and 150 MHz, methanol- d_4) spectrum of **2**

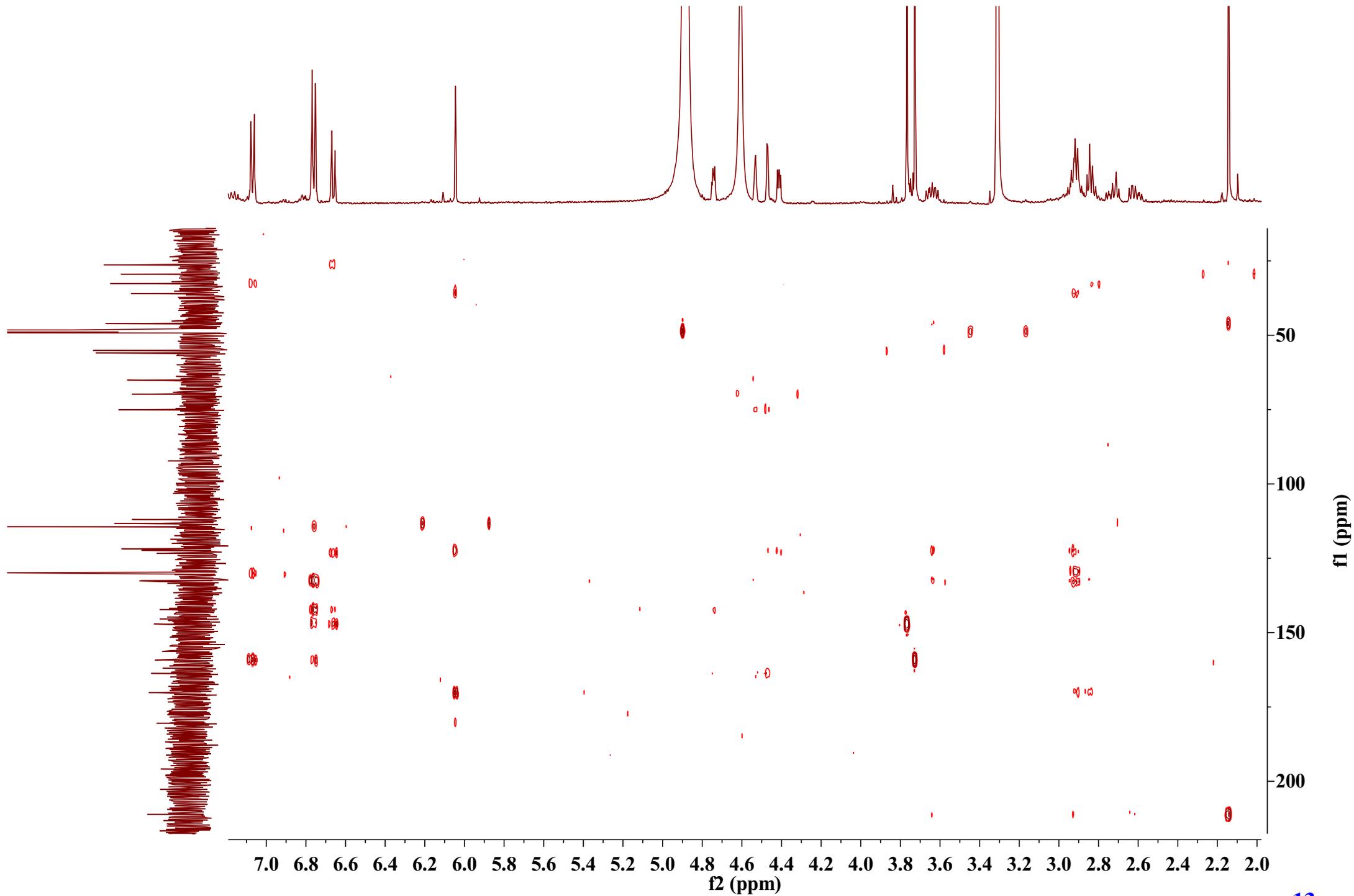


Figure S13. HMBC (600 and 150 MHz, methanol- d_4) spectrum of **2**

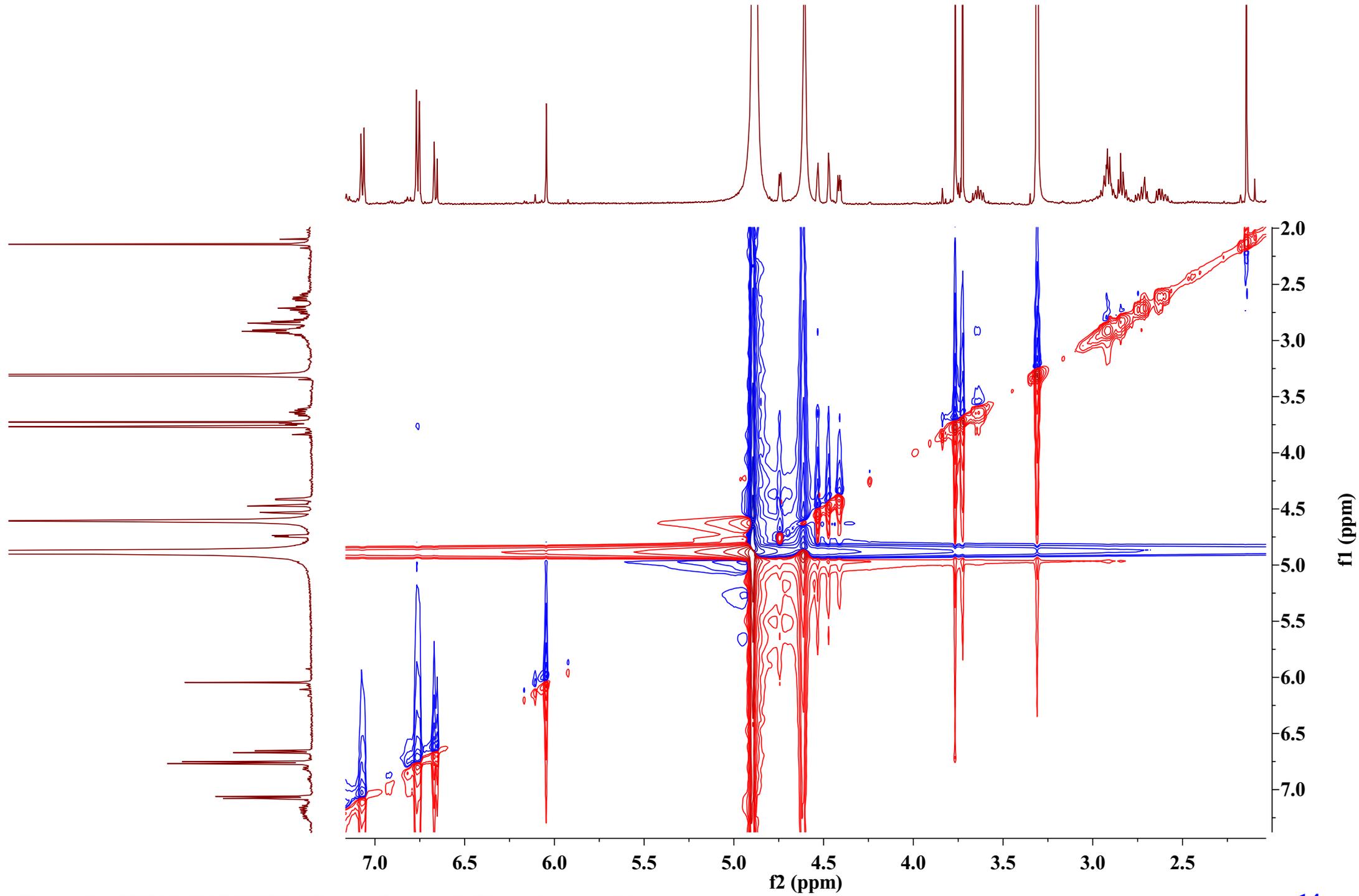
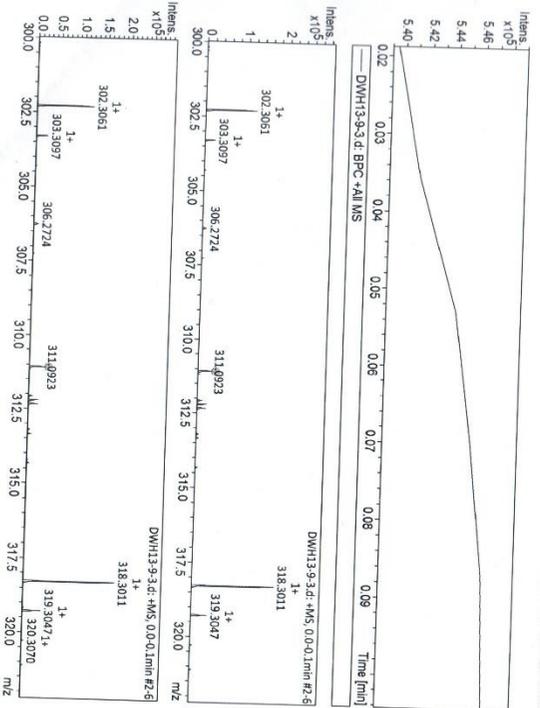


Figure S14. ROESY (600 MHz, methanol- d_4) spectrum of 2

Mass Spectrum SmartFormula Report

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Analysis Name	D:\Data\A501\YZJ2018_12_27\DW13-9-3.d	Operator	Demo User
Method	Tune_pos Mid.m	Instrument	compact
Sample Name	DWH13-9-3		8255754_20156
Comment			

Acquisition Parameter	
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Scan End	1800 m/z
Ion Polarity	Positive
Set Capillary	3500 V
Set End Plate Offset	-500 V
Set Changing Voltage	2000 V
Set Corona	0 nA
Set Nebulizer	0.3 Bar
Set Dry Heater	220 °C
Set Dry Gas	3.0 l/min
Set Divert Valve	Source
Set APCI Heater	0 °C



Mass m/z	#	Ion Formula	m/z	err [ppm]	Mean err [ppm]	rdp	N-Rule	e_Conf	mSigma	Adduct
311.092332	1	C18H15OS	311.091400	-3.0	-3.0	12.0	ok	even	3.5	M+H

Figure S15. HRESIMS spectrum of **3**

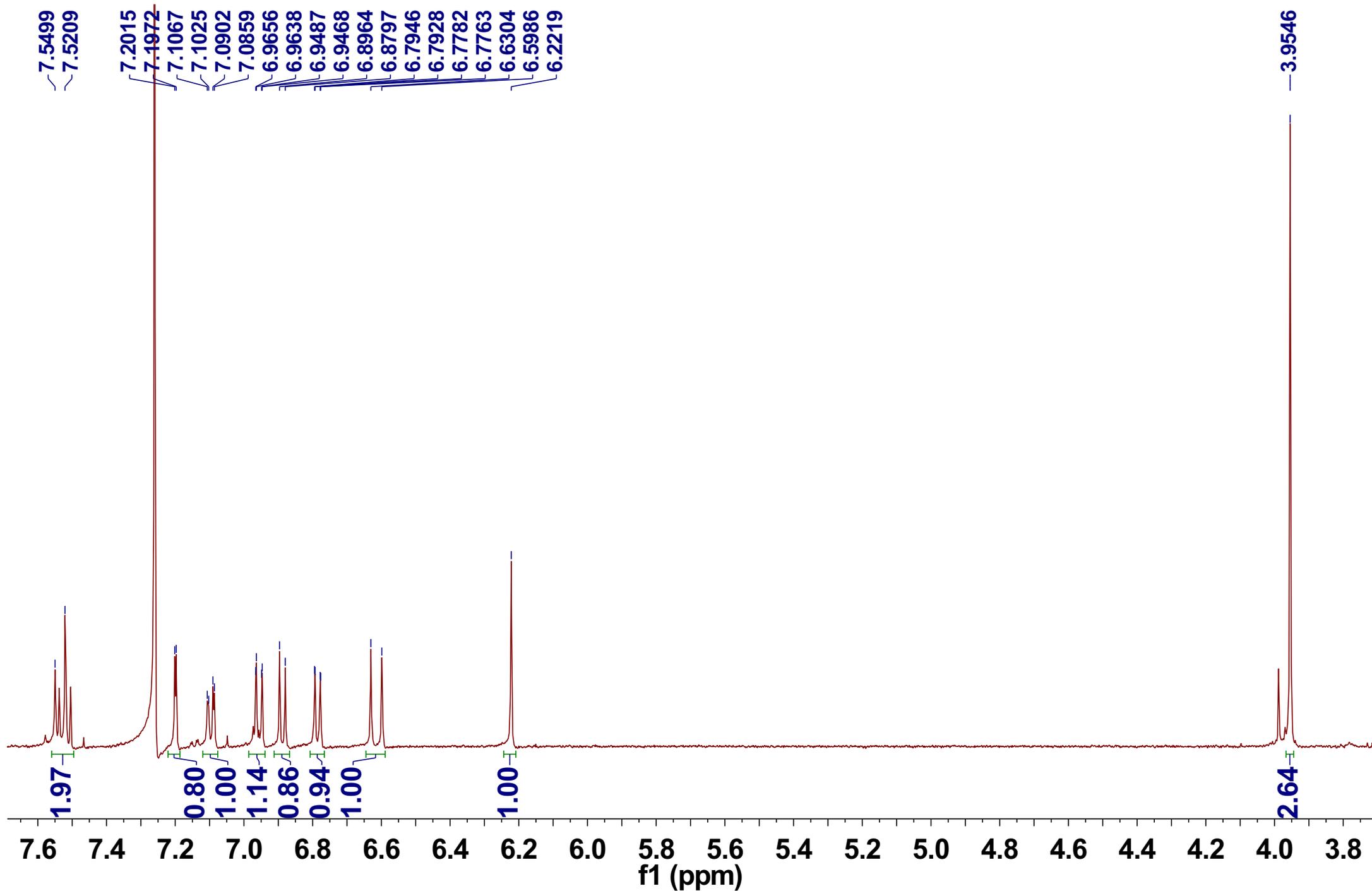


Figure S16. ¹H NMR (500 MHz, CDCl₃) spectrum of 3

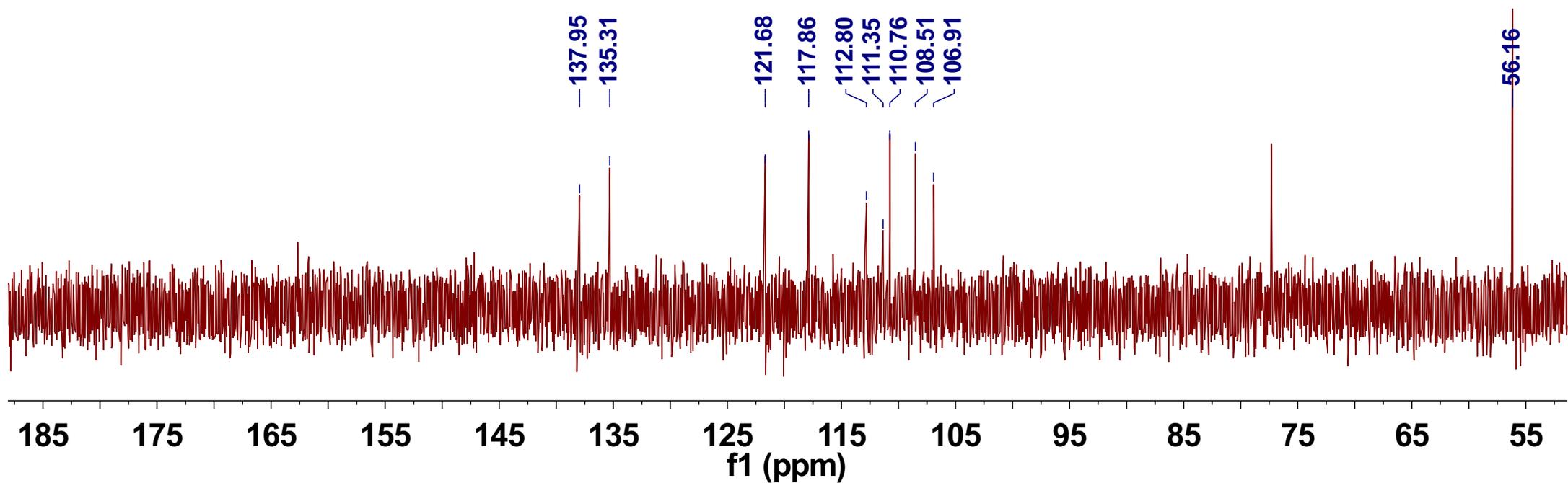
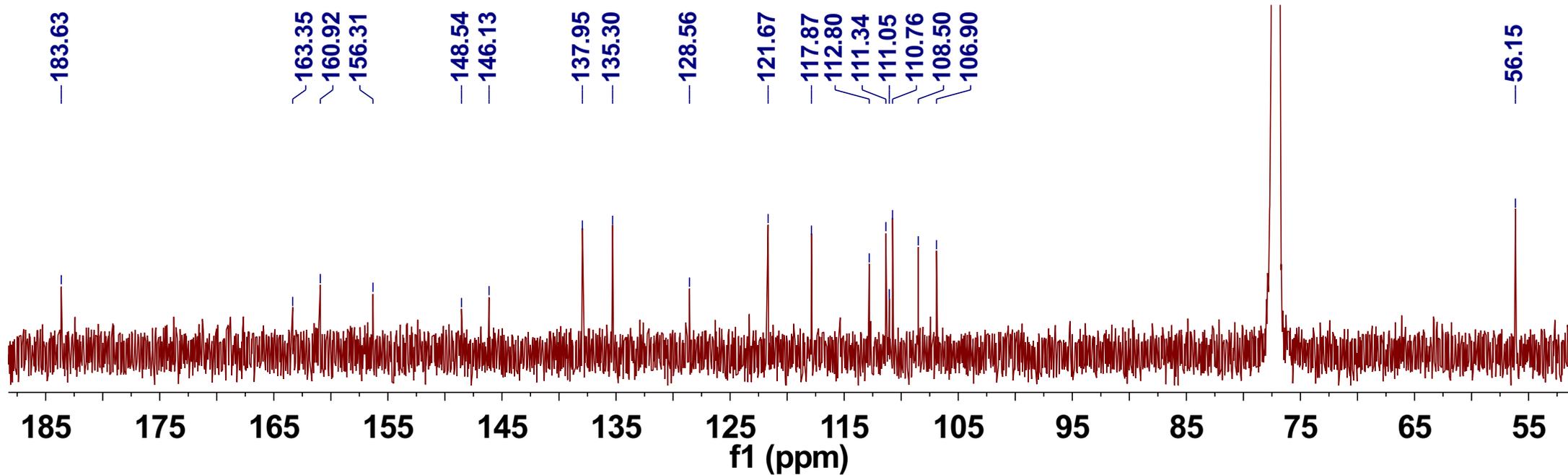


Figure S17. ^{13}C NMR and DEPT-135 (125 MHz, CDCl_3) spectrum of 3

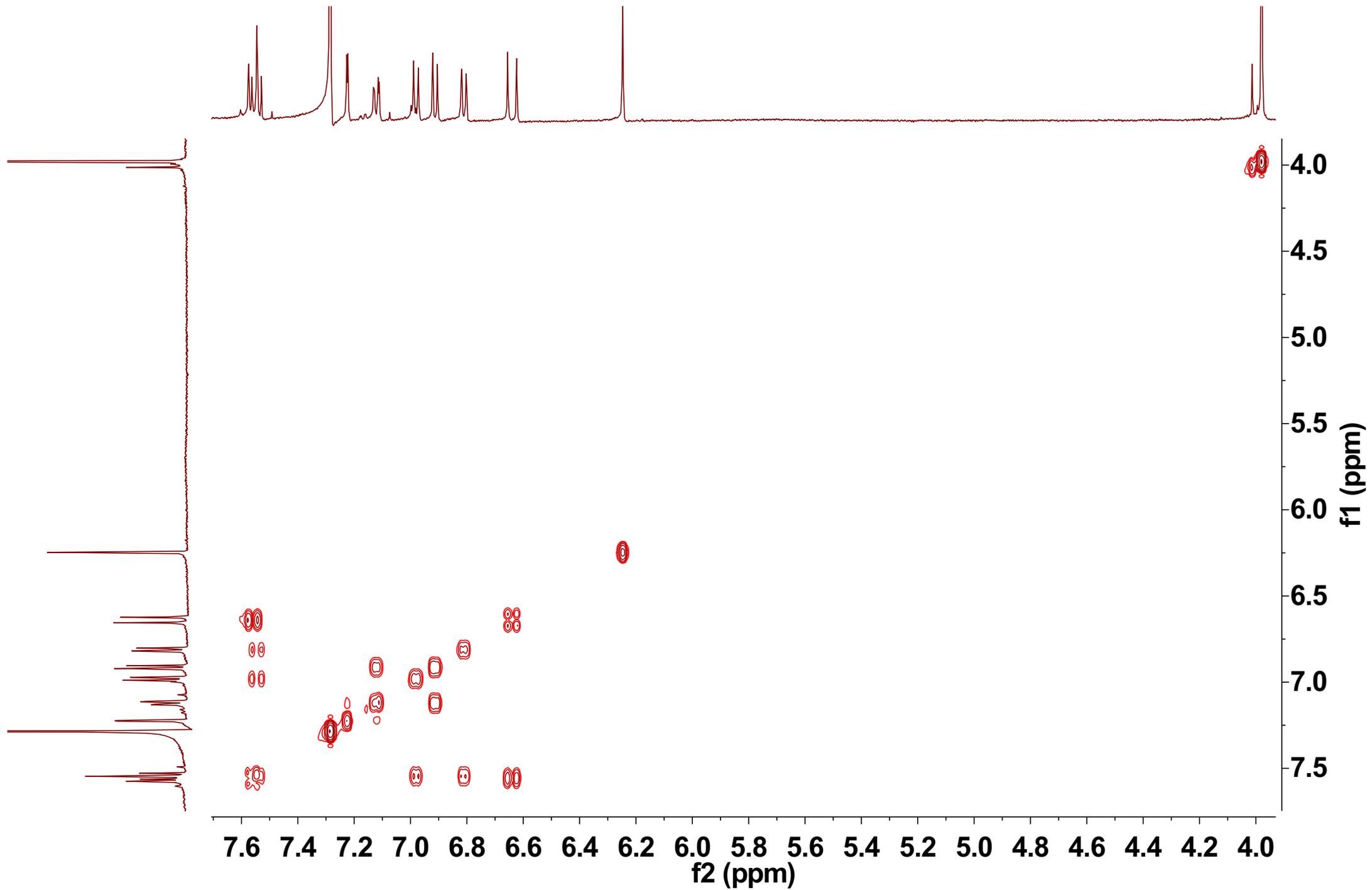


Figure S18. ^1H - ^1H COSY (500 MHz, CDCl_3) spectrum of 3

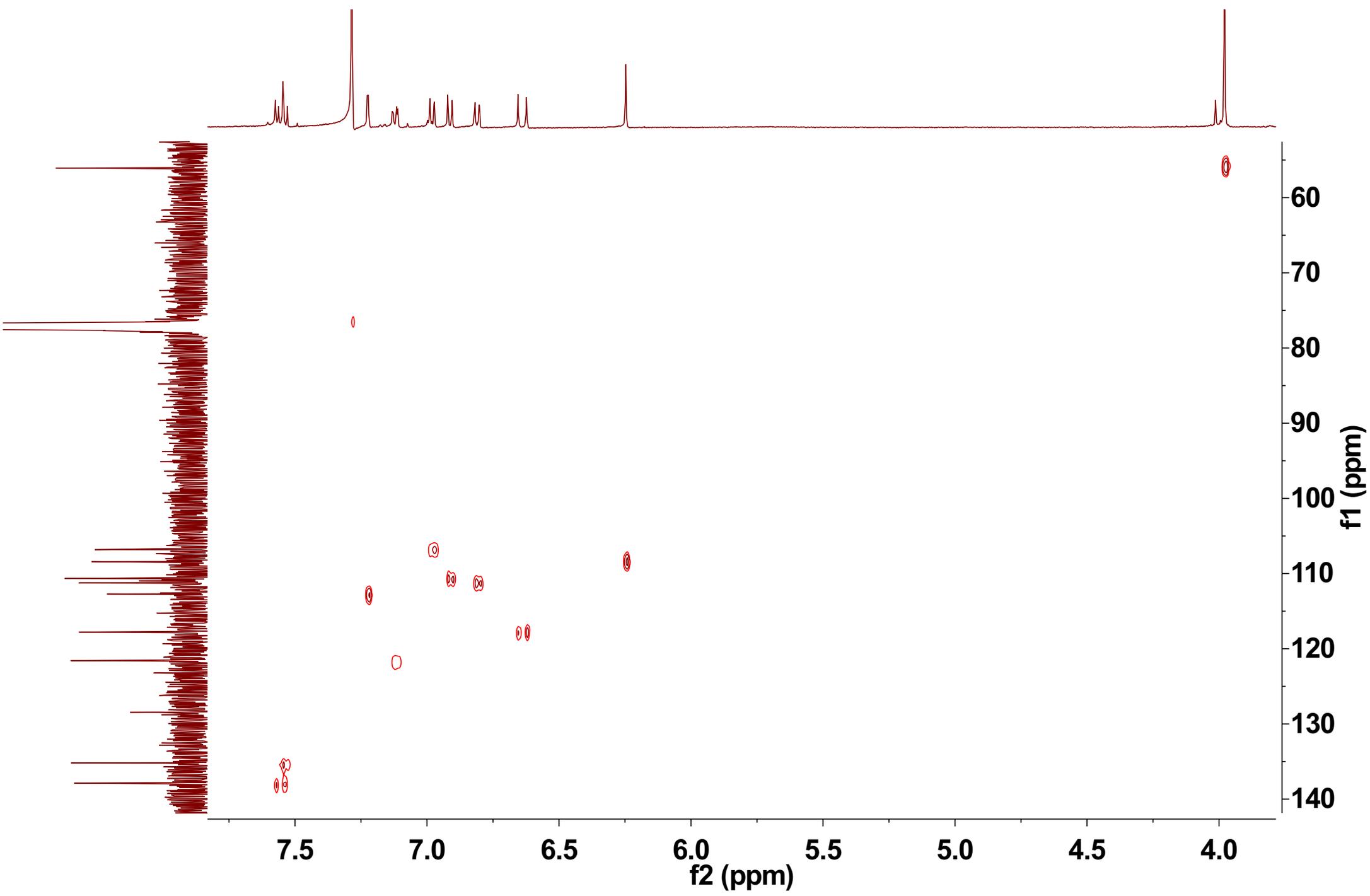


Figure S19. HSQC (500 and 125 MHz, CDCl₃) spectrum of 3

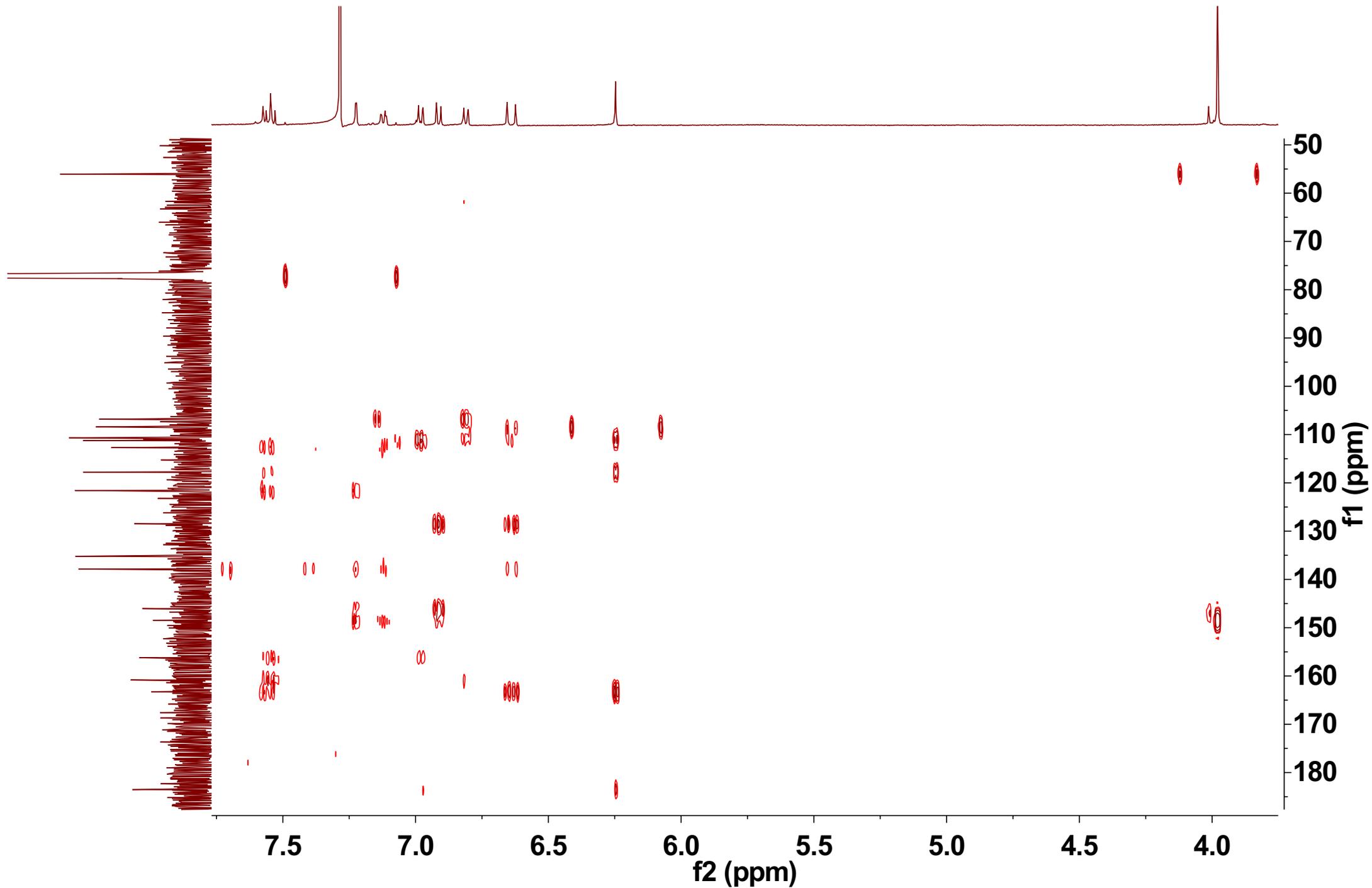


Figure S20. HMBC (500 and 125 MHz, CDCl₃) spectrum of 3

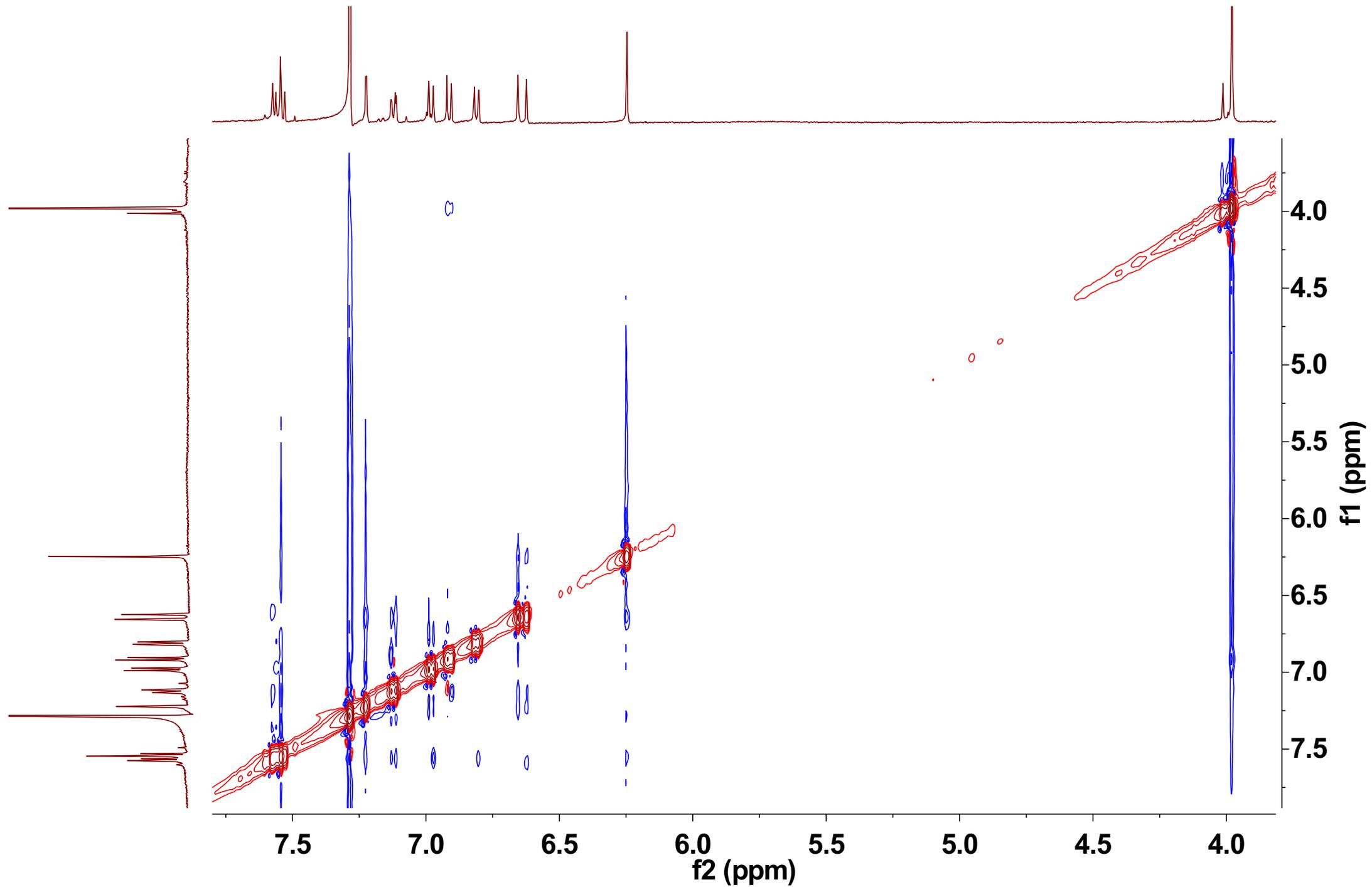


Figure S21. ROESY (500 MHz, CDCl₃) spectrum of 3