

3-Nitroasterric Acid Derivatives from an Antarctic Sponge-derived *Pseudogymnoascus* sp. Fungus

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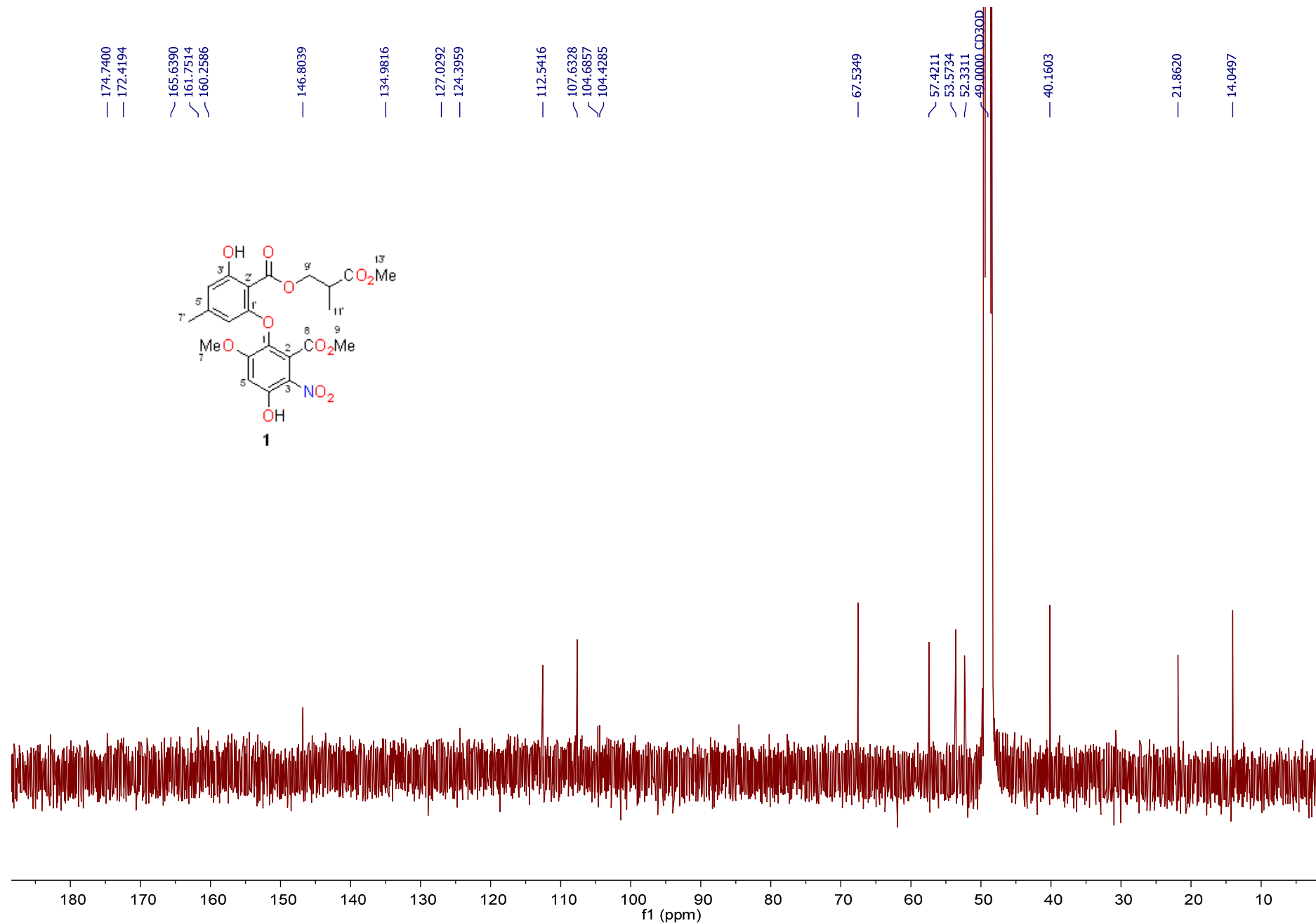
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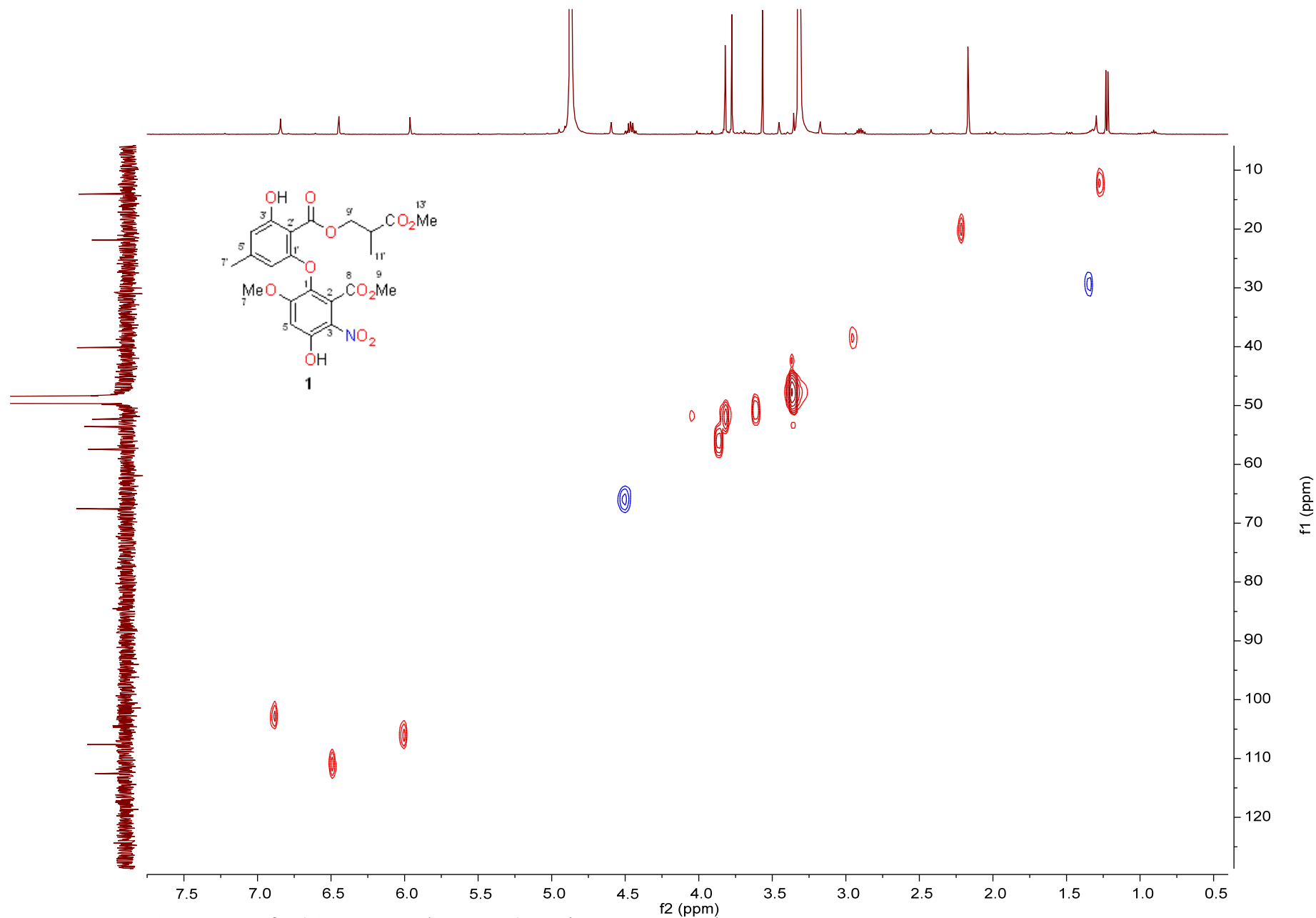
[⊥] Fundación MEDINA, Centro de Excelencia en Investigación de Medicamentos Innovadores en Andalucía, Avda. Del Conocimiento 34, Parque Tecnológico de Ciencias de la Salud, 18016 Armilla, Granada, Spain.

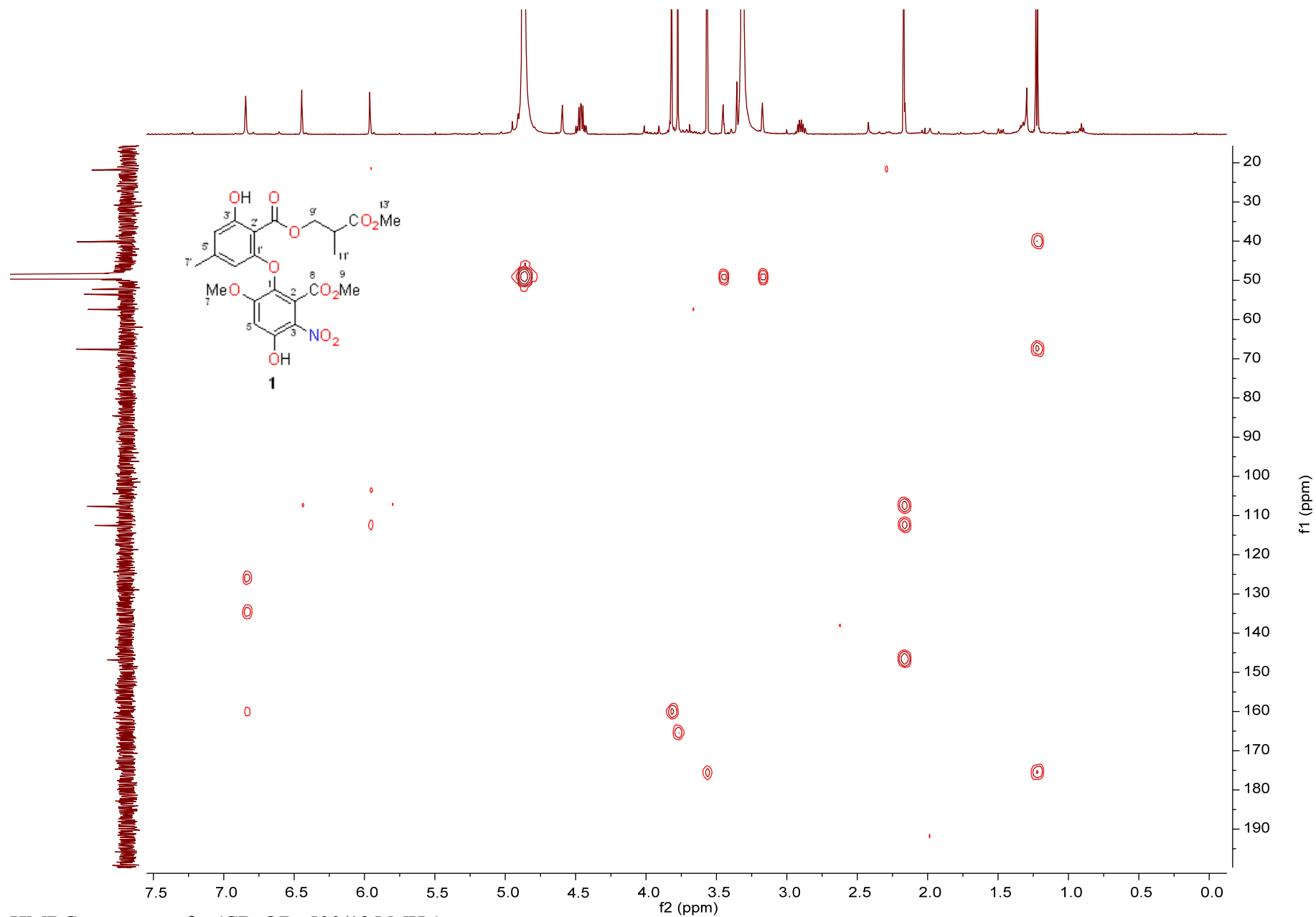
Supporting Information (31 pages)

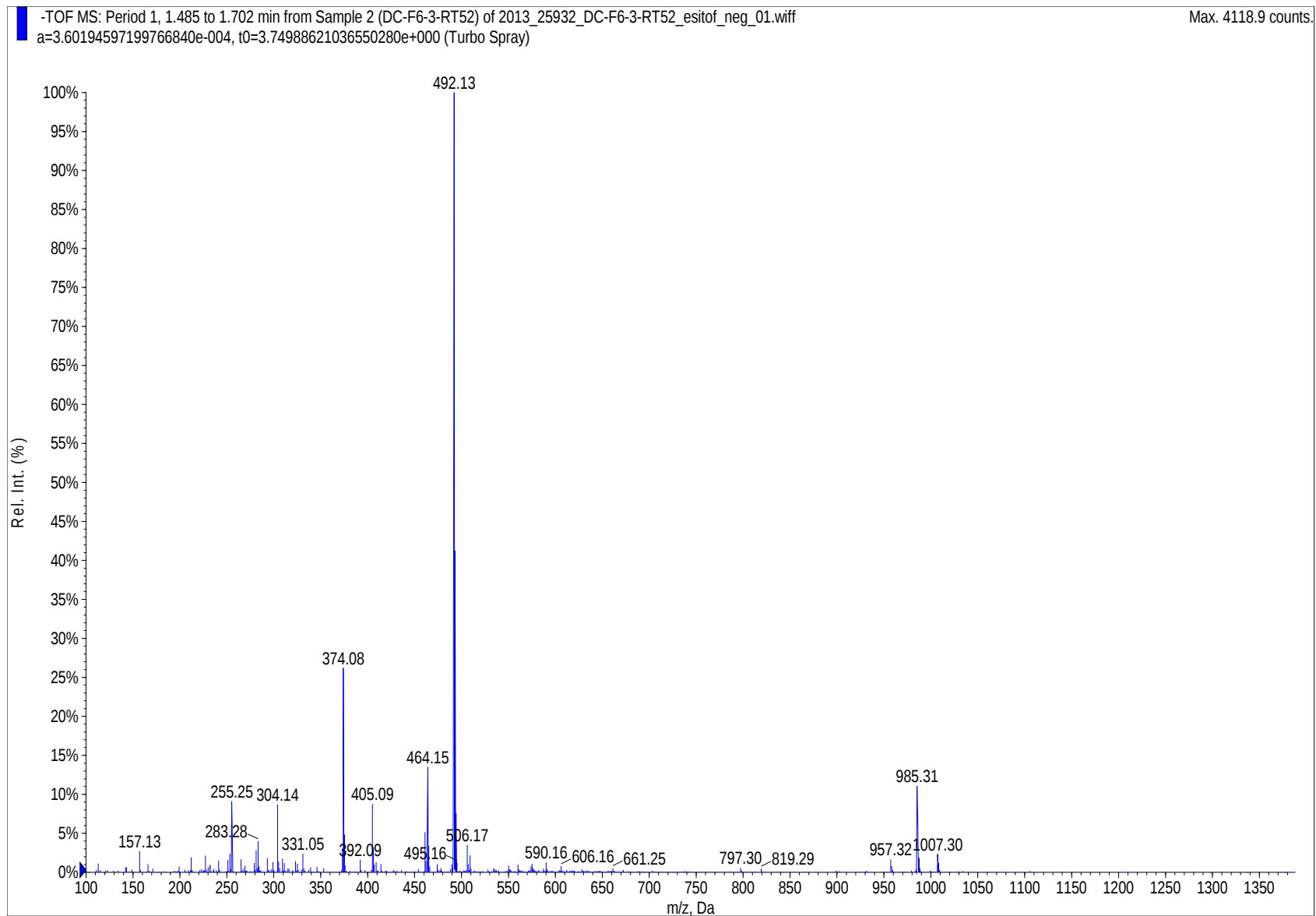
Compound 1 (¹ H, ¹³ C, Ed-HSCQ, HMBC, (-)-LRESIMS and (-)-HRESIMS)	SI2
Compound 2 (¹ H, ¹³ C, Ed-HSCQ, HMBC, (-)-LRESIMS, (-)-HRESIMS, and FT-IR)	SI8
Compound 3 (¹ H, ¹³ C, Ed-HSCQ, HMBC, ROESY, (-)-LRESIMS and (-)-HRESIMS)	SI19
Compound 4 (¹ H, ¹³ C, (-)-LRESIMS and (-)-HRESIMS)	SI28



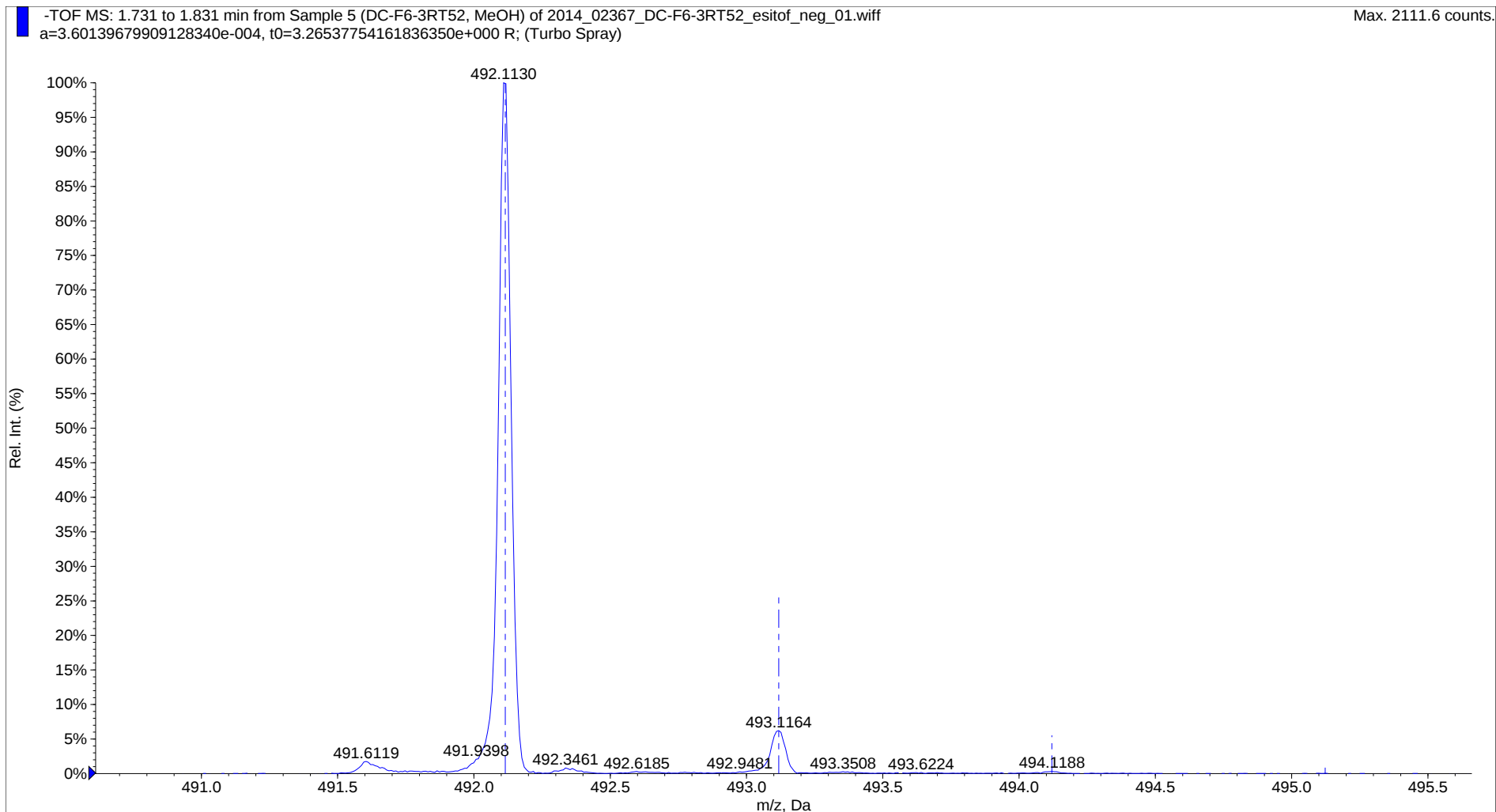
¹³C NMR spectrum of **1** (CD₃OD, 125 MHz)





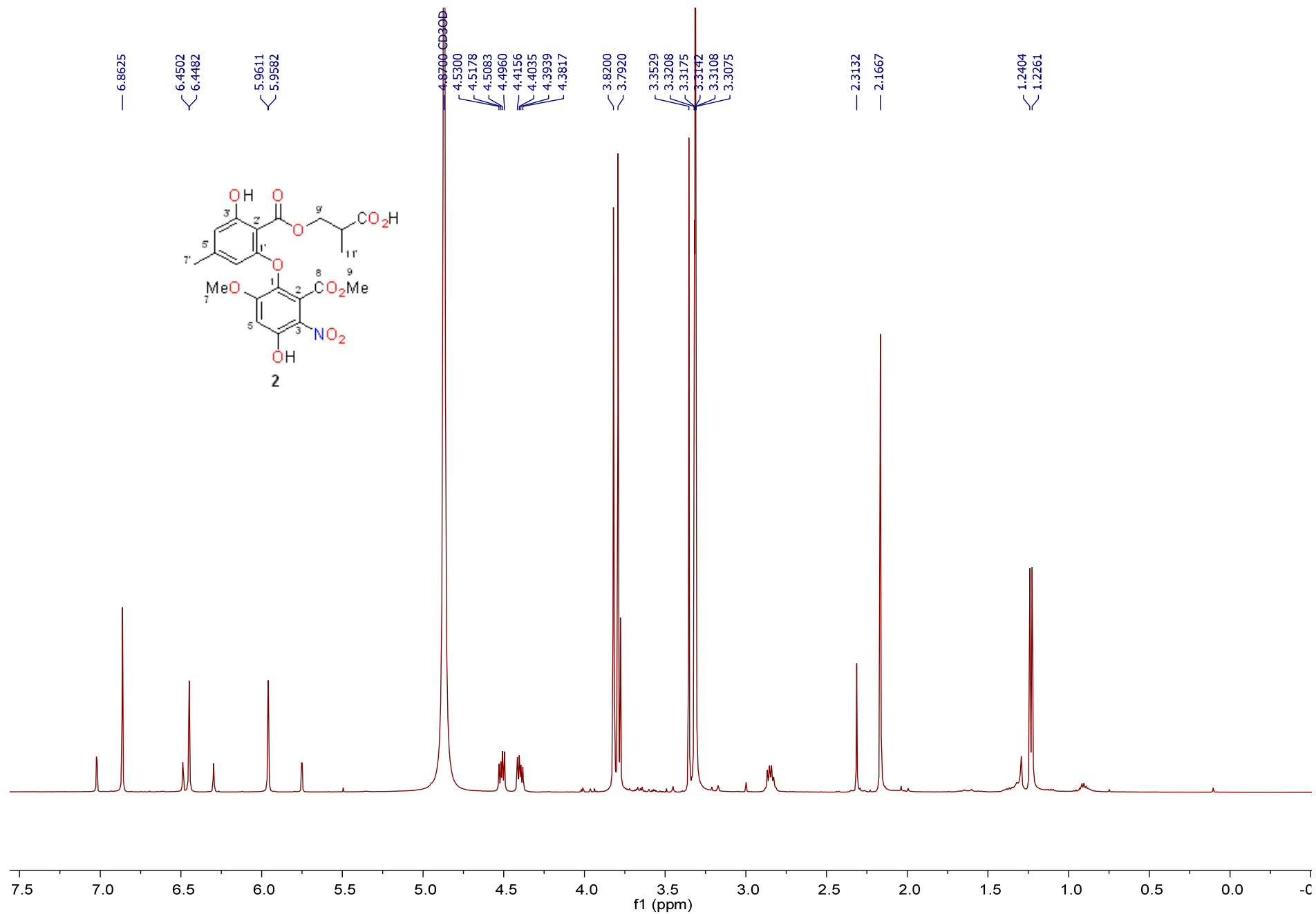


(-)-LRESIMS of **1**

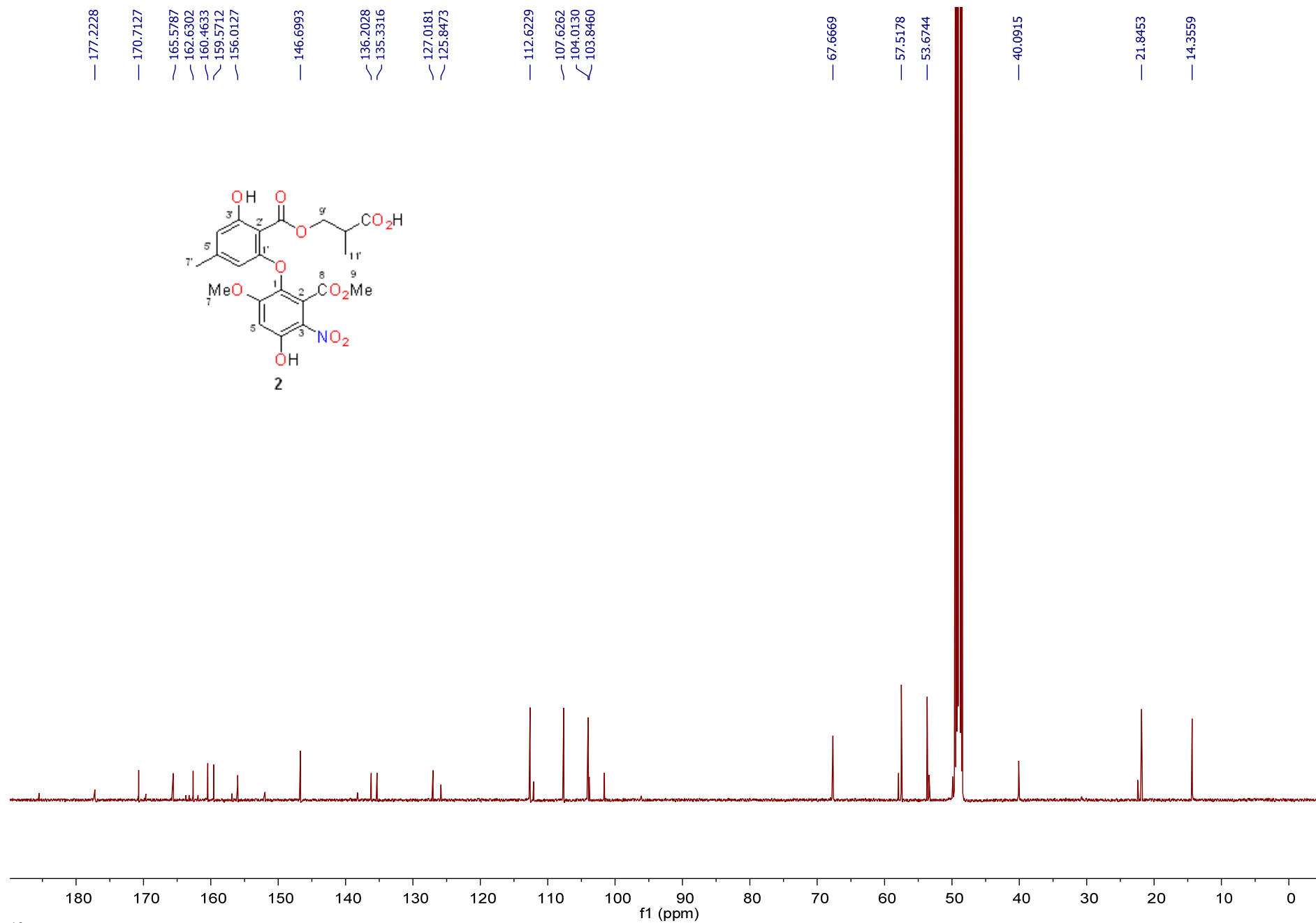


(-)-HRESIMS of **1**

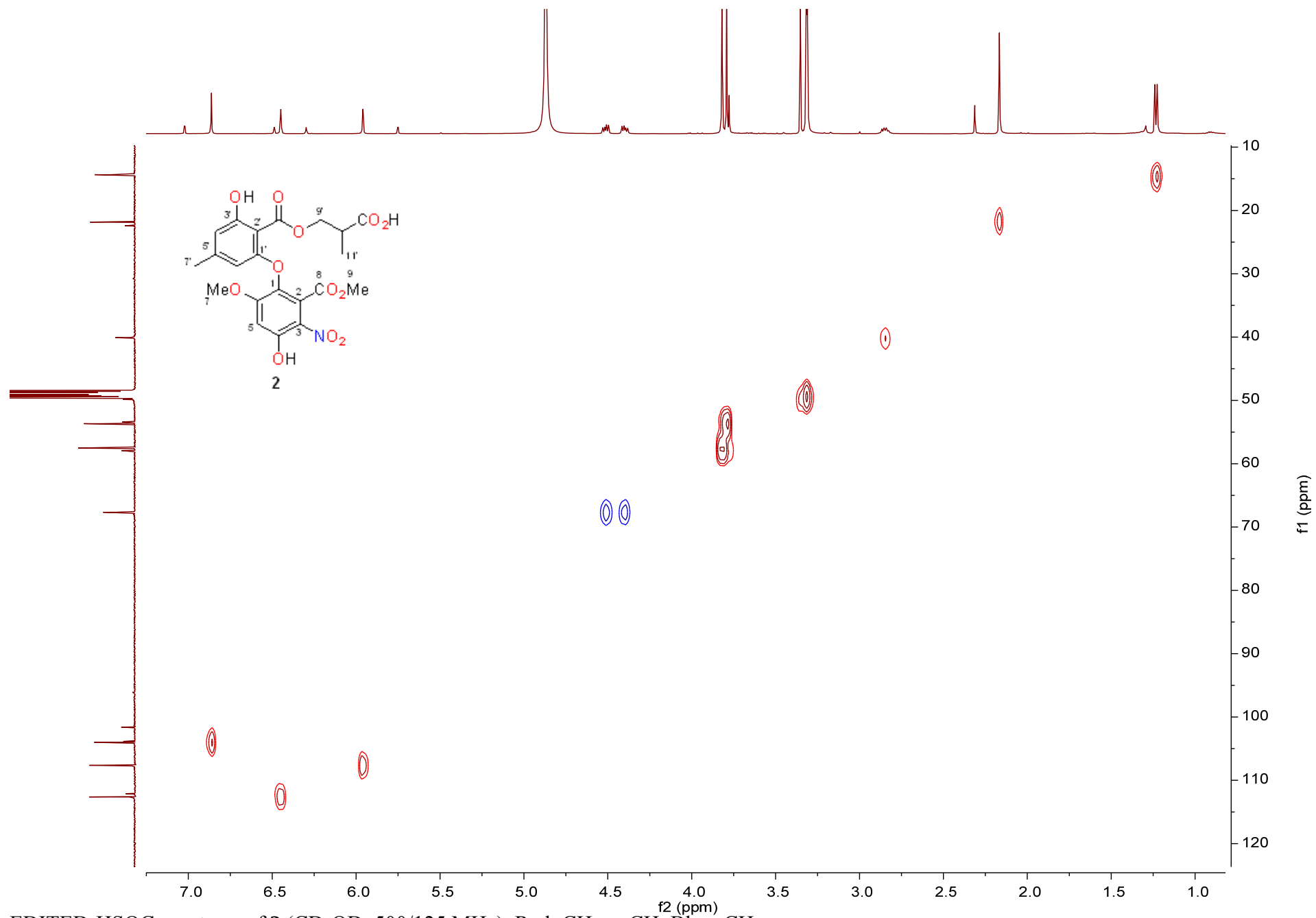
m/z experimental	492.1130			
MF	m/z	Error, mDa	Error in ppm	DBE
C22 H22 N O12	492.1147	-1.7491	-3.5543	12.5



¹H NMR spectrum of **2** (CD₃OD, 500 MHz)

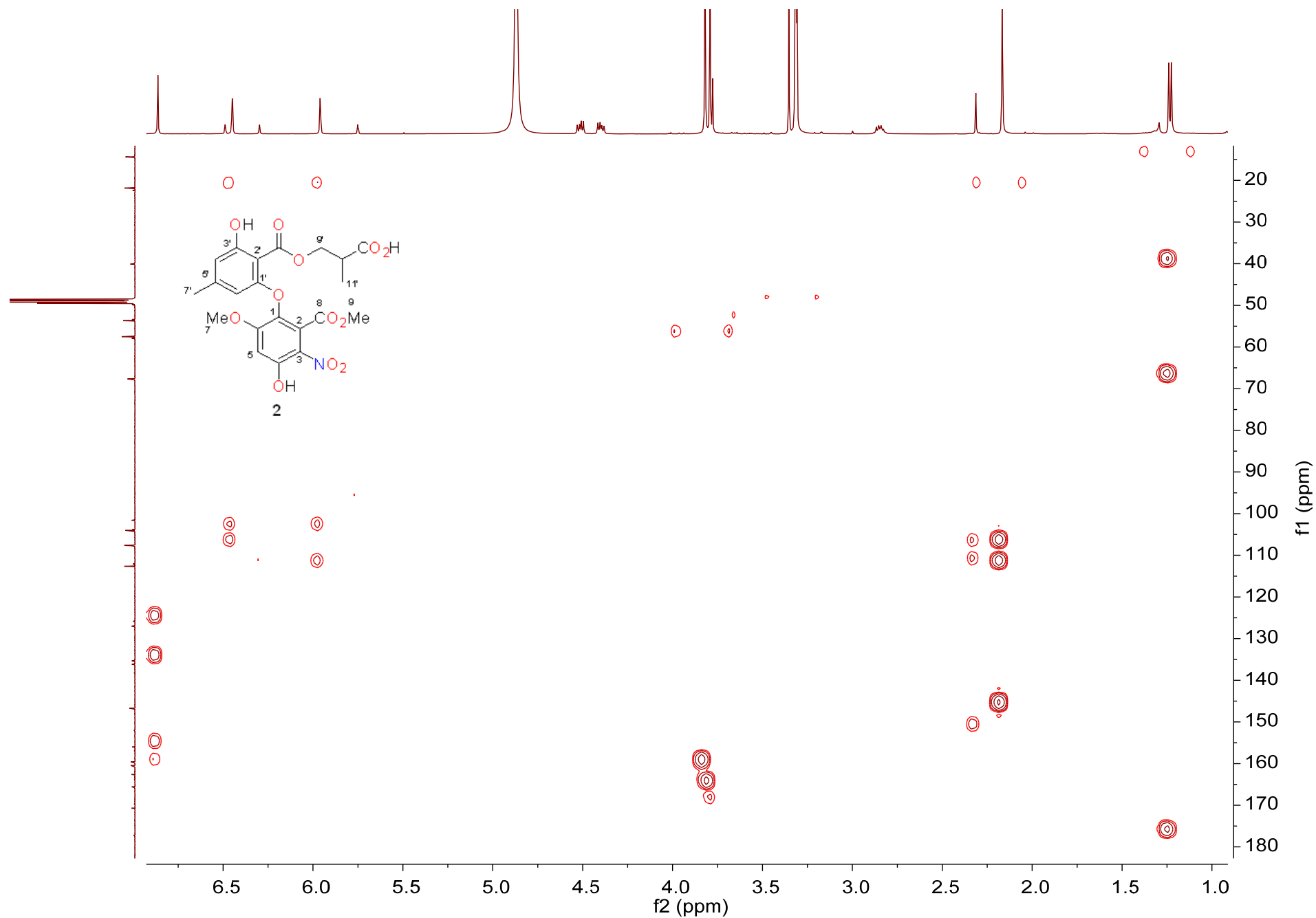


¹³C NMR spectrum of 2 (CD₃OD, 125 MHz)



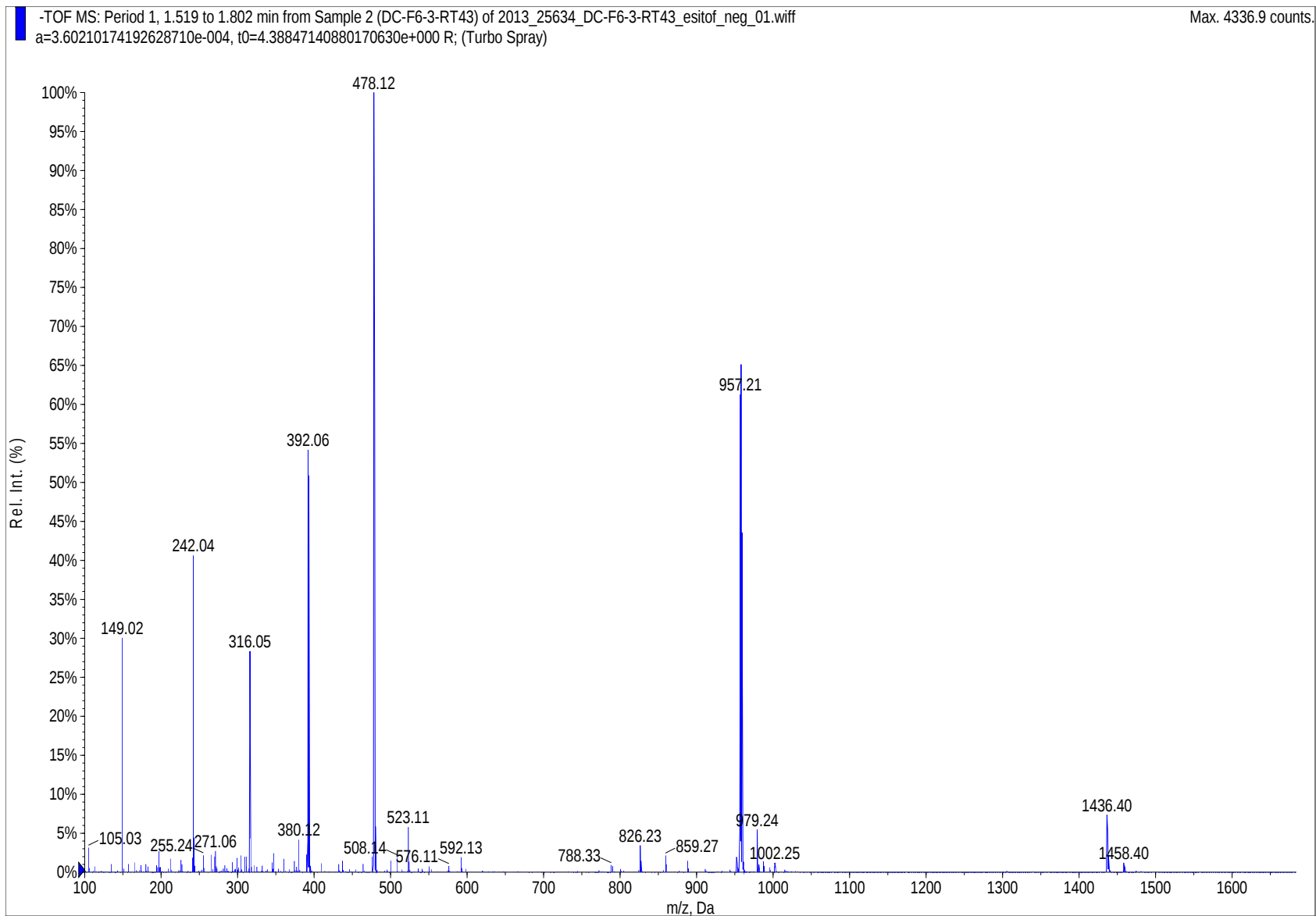
EDITED-HSQC spectrum of **2** (CD₃OD, 500/125 MHz). Red: CH₃ or CH, Blue: CH₂

SI10

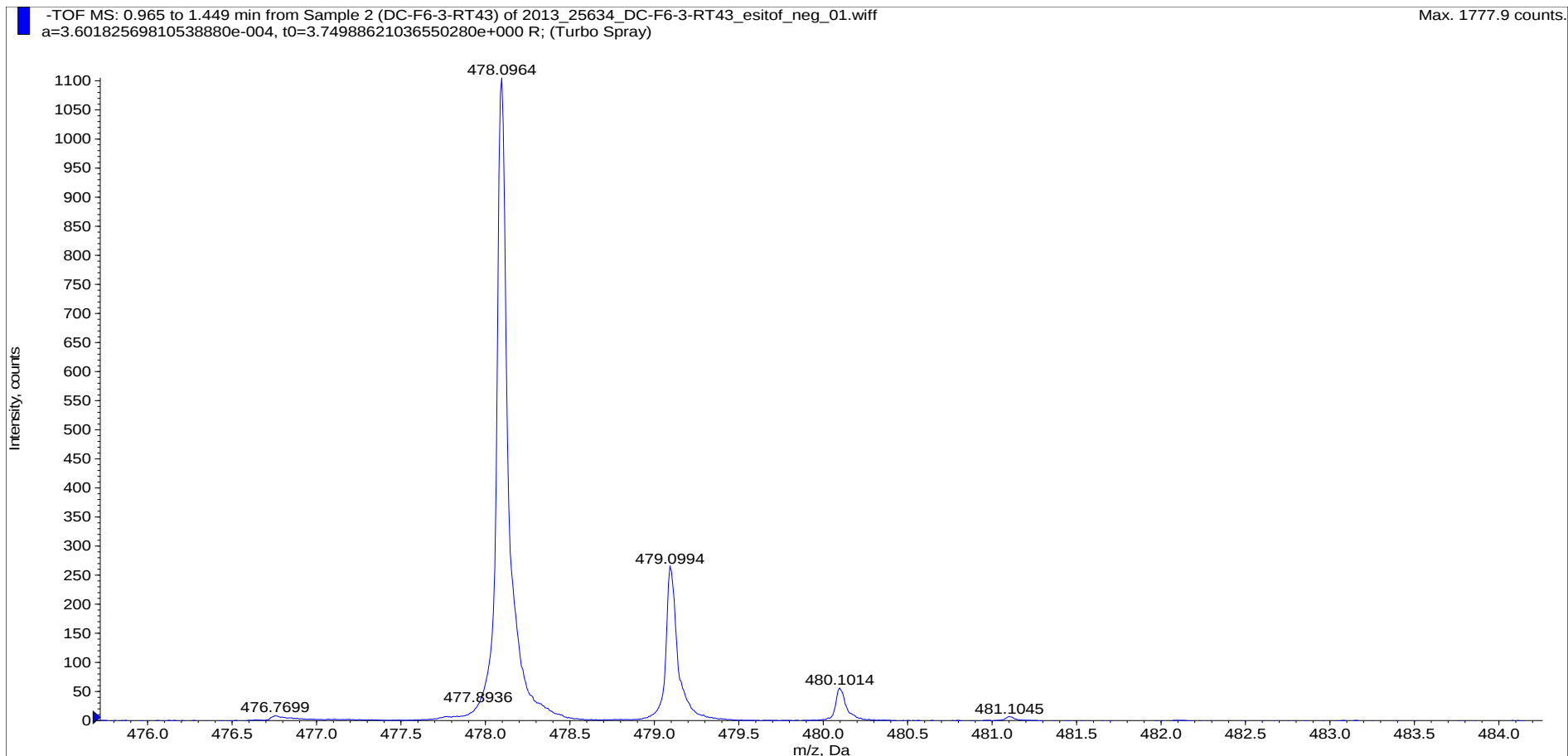


HMBC spectrum of **2** (CD₃OD, 500/125 MHz)

SI11

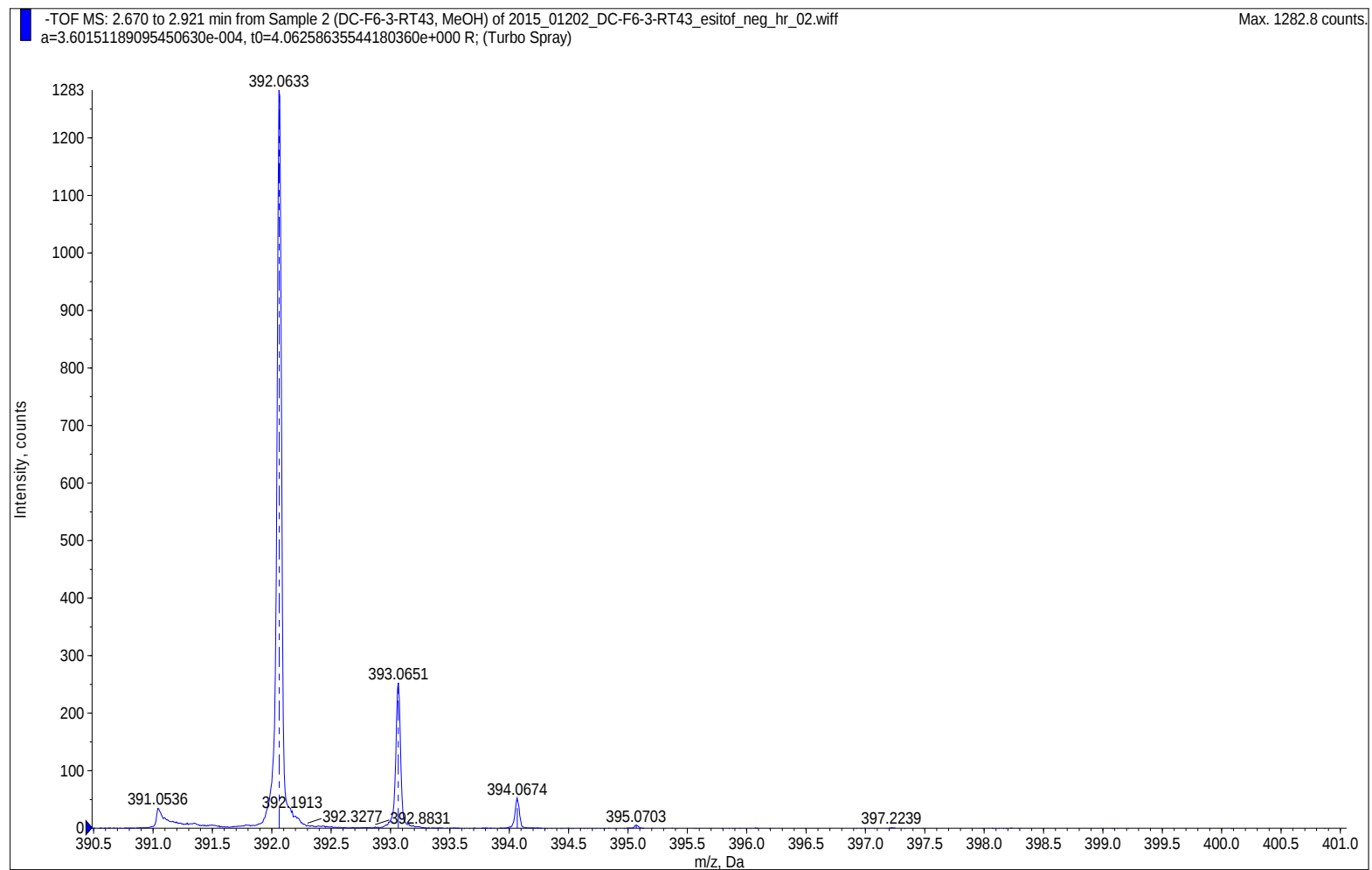


(-)-LRESIMS of 2



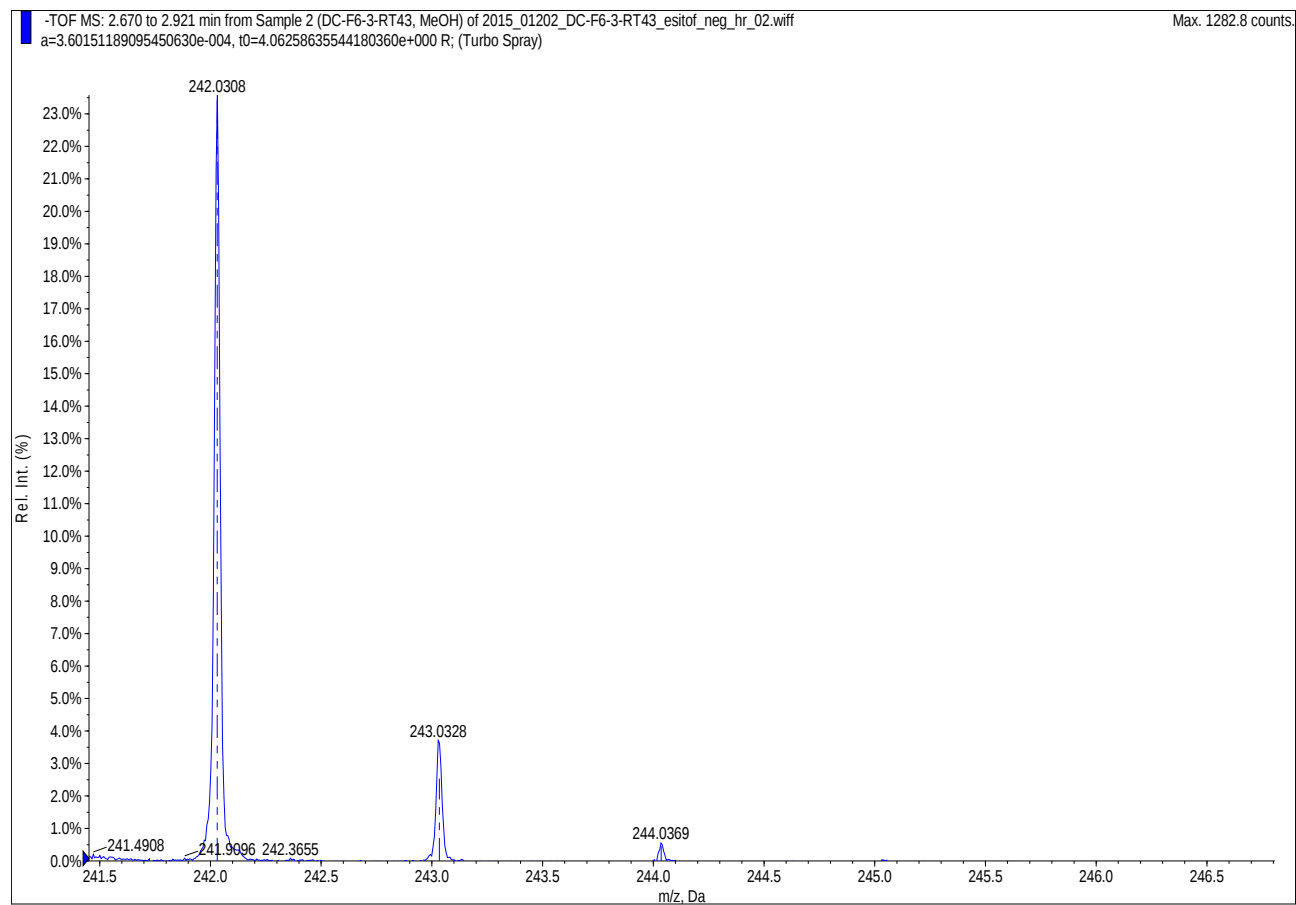
(-)-HRESIMS of 2

<i>m/z</i> experimental	478.0964			
MF	<i>m/z</i>	Error, mDa	Error in ppm	DBE
C21 H20 N O12	478.0991	-2.7	-5,64	12.5



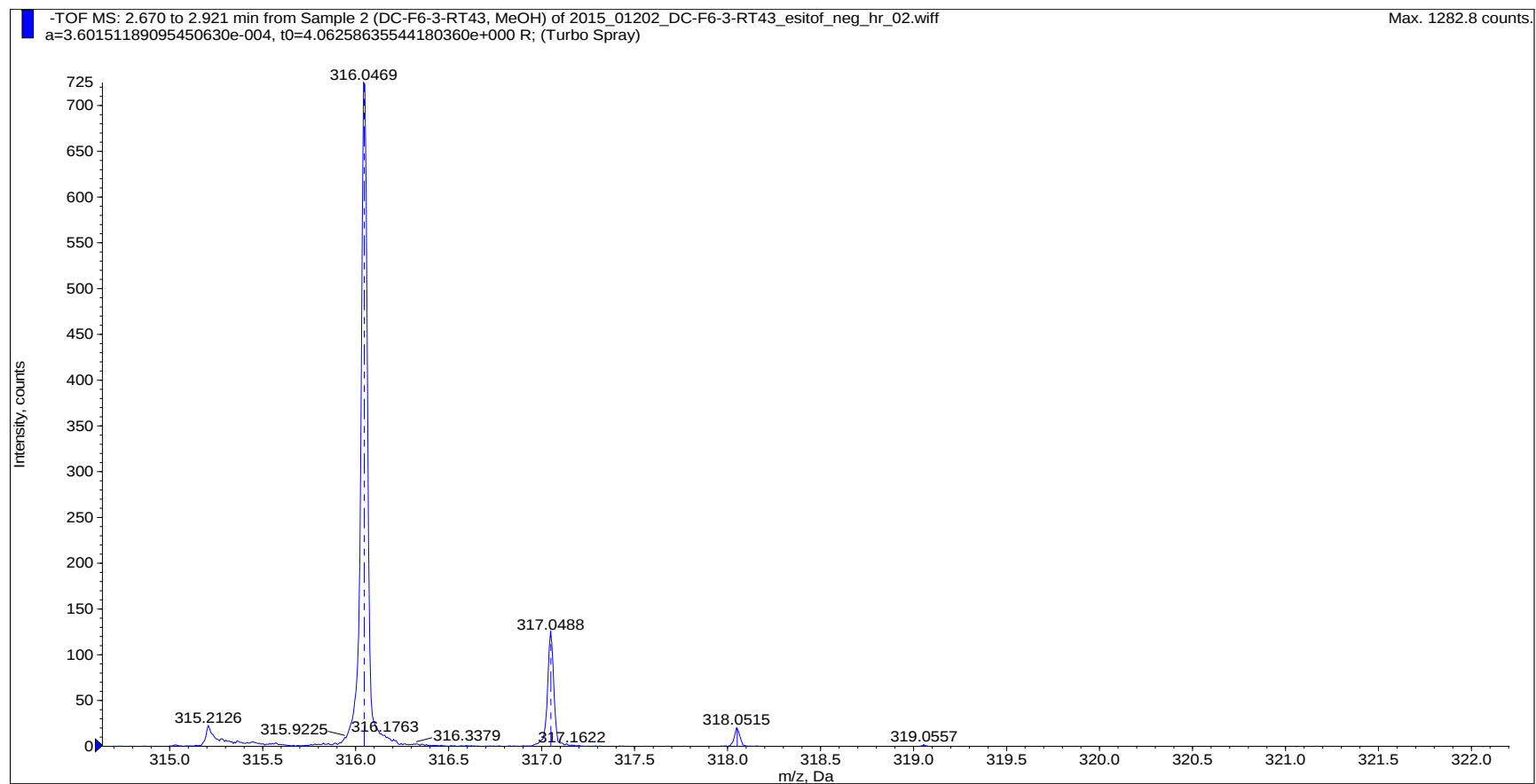
(-)-HRESIMS of the fragment at m/z 392 of **2**

m/z experimental	392.0633			
MF	m/z	Error, mDa	Error in ppm	DBE s
C17 H14 N O10	392.0623	0.9804	2.5007	11.5



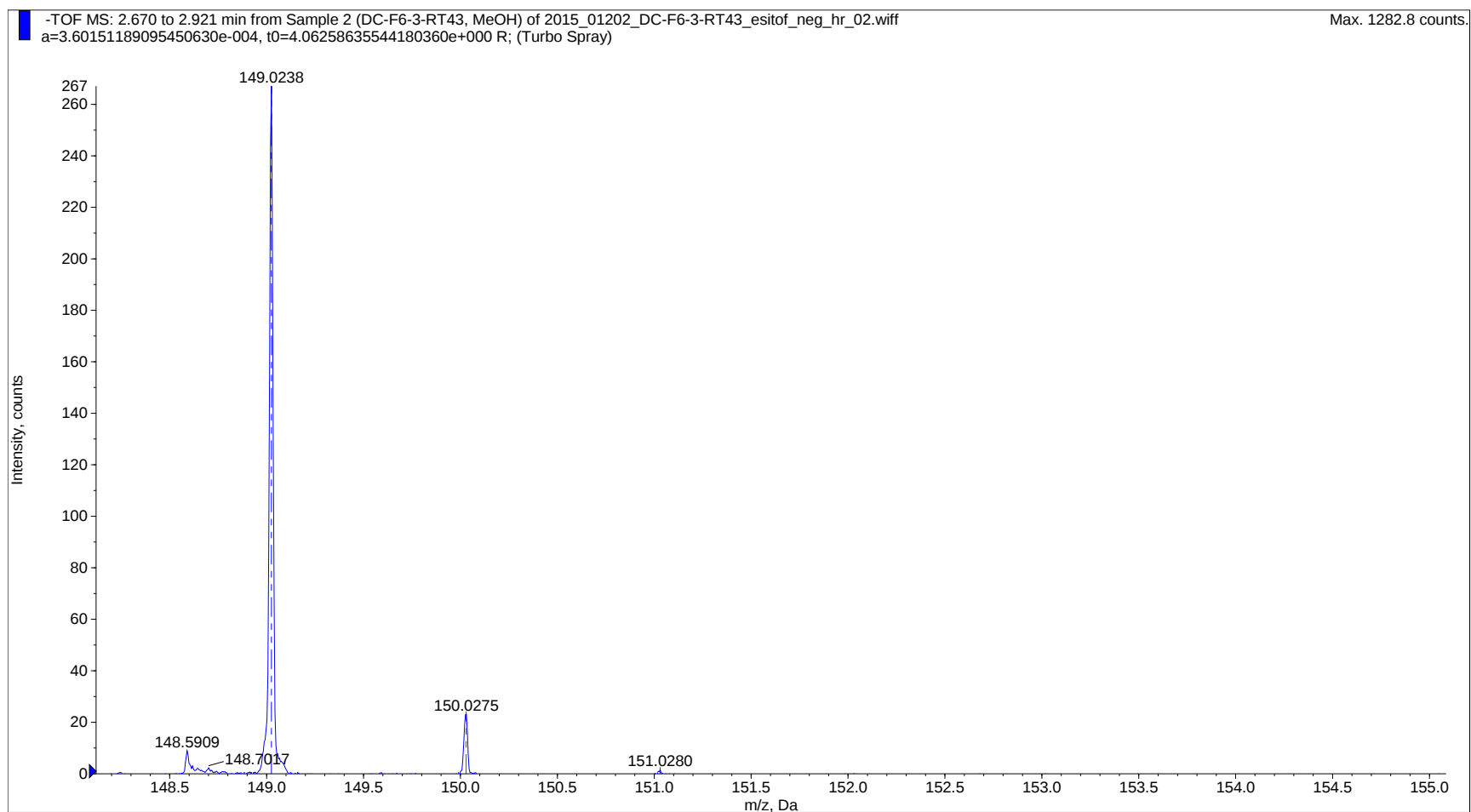
(-)-HRESIMS of the fragment at m/z 242 of **2**

m/z experimental	242.0308			
MF	m/z	Error in mDa	Error in ppm	DBE
C9 H8 N O7	242.0306	-0.0253	-0.1048	6.5



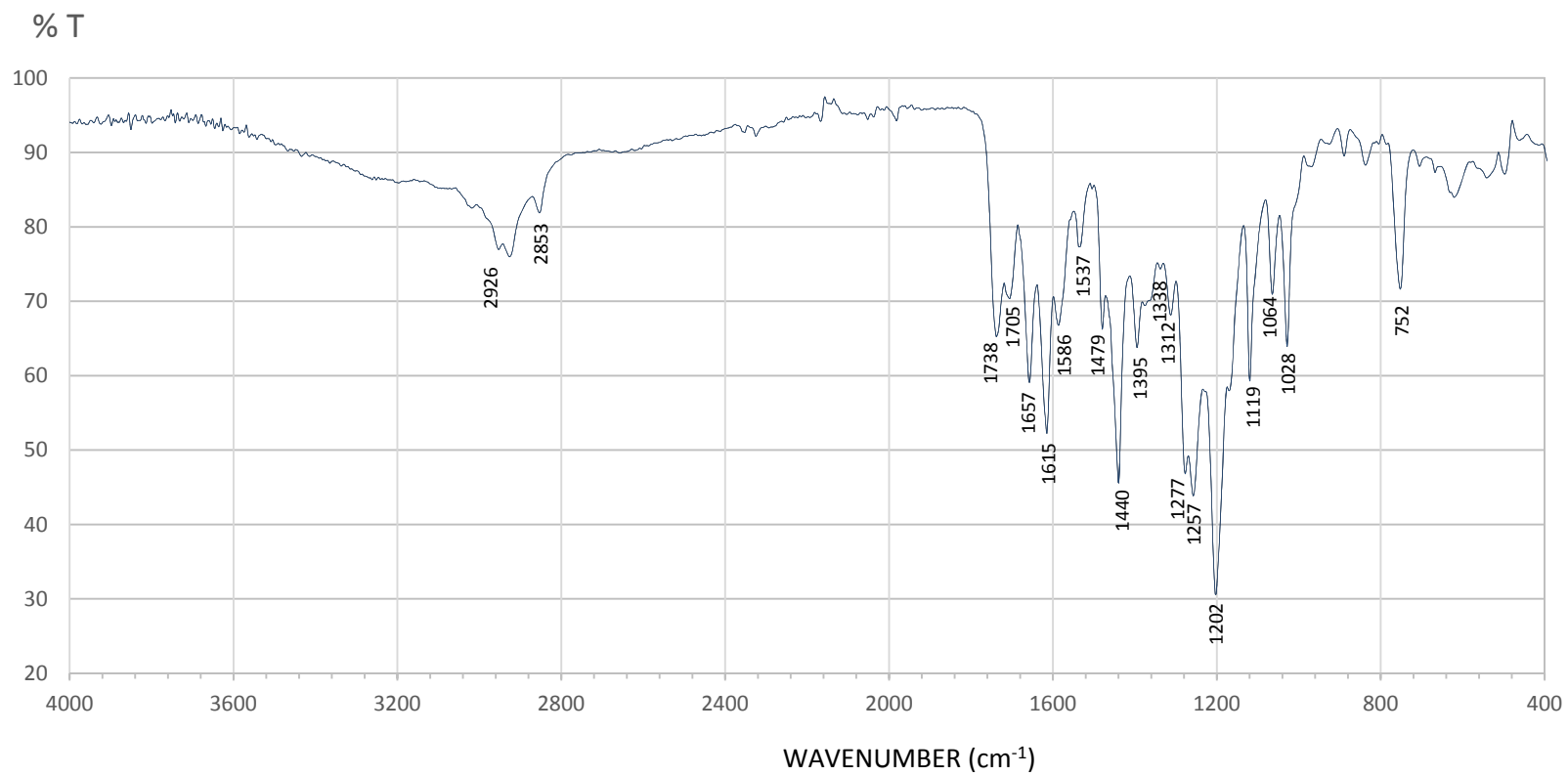
(-)-HRESIMS of the fragment at m/z 316 of **2**

m/z experimental	316.0469			
MF	<i>m/z</i>	Error in mDa	Error in ppm	DBE
C₁₅H₁₀N O₇	316.0462	0.6245	1.976	11.5

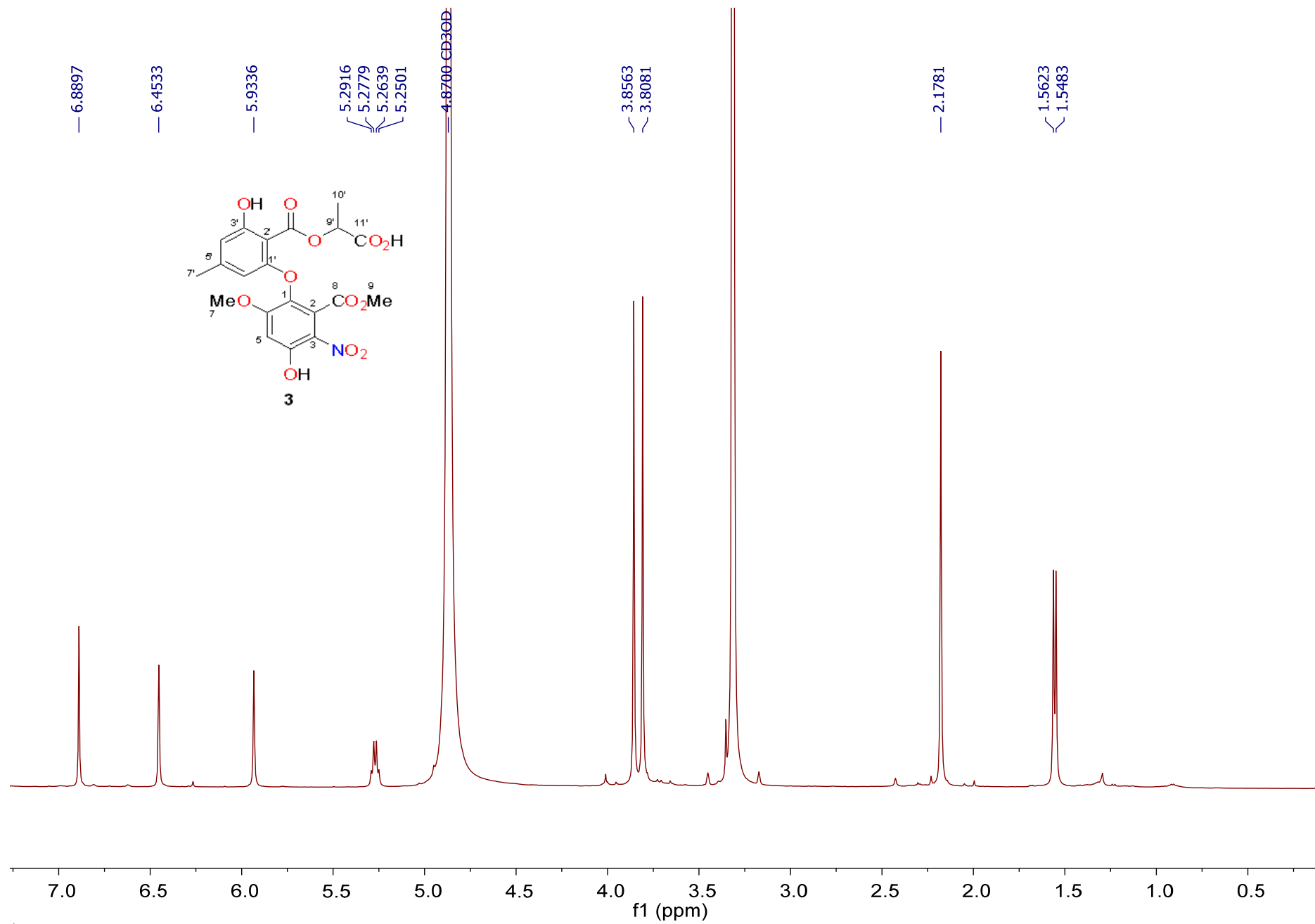


(-)-HRESIMS of the fragment at m/z 149 of 2

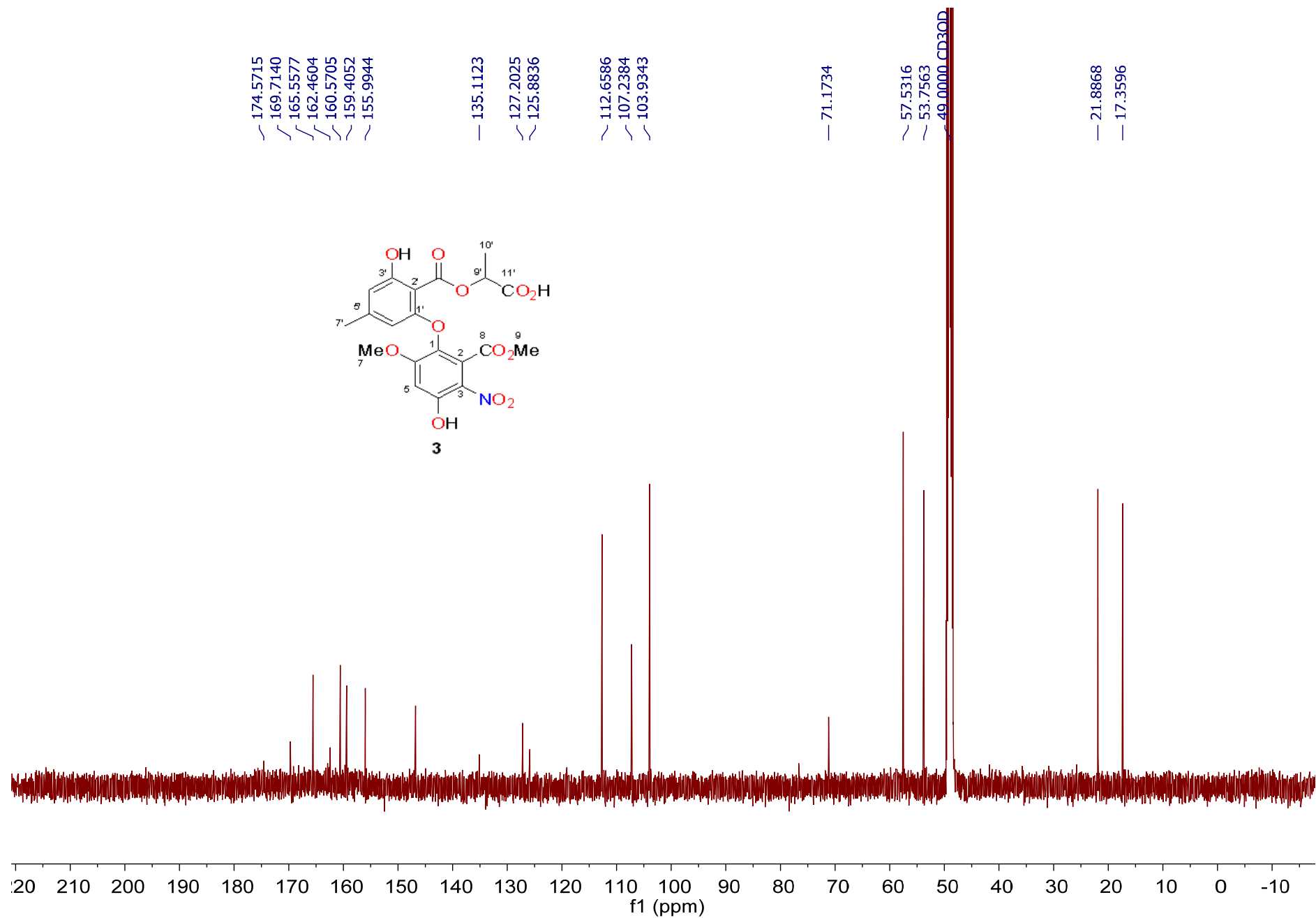
m/z experimental	149.0238			
MF	m/z	Error in mDa	Error in ppm	DBE
C8 H5 O3	149.0244	-0.6176	-4.1449	6.5



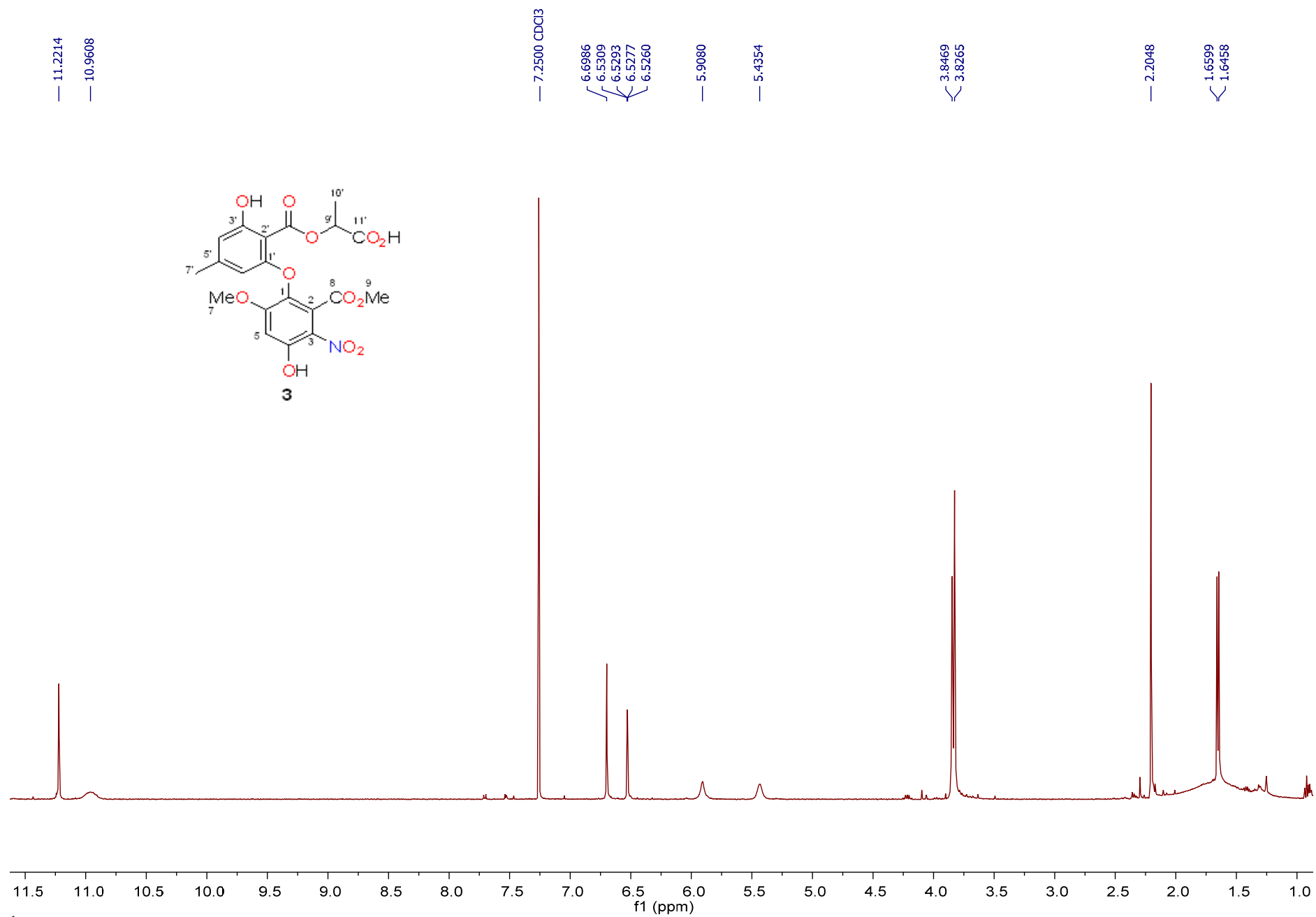
FT-IR spectrum of **2**



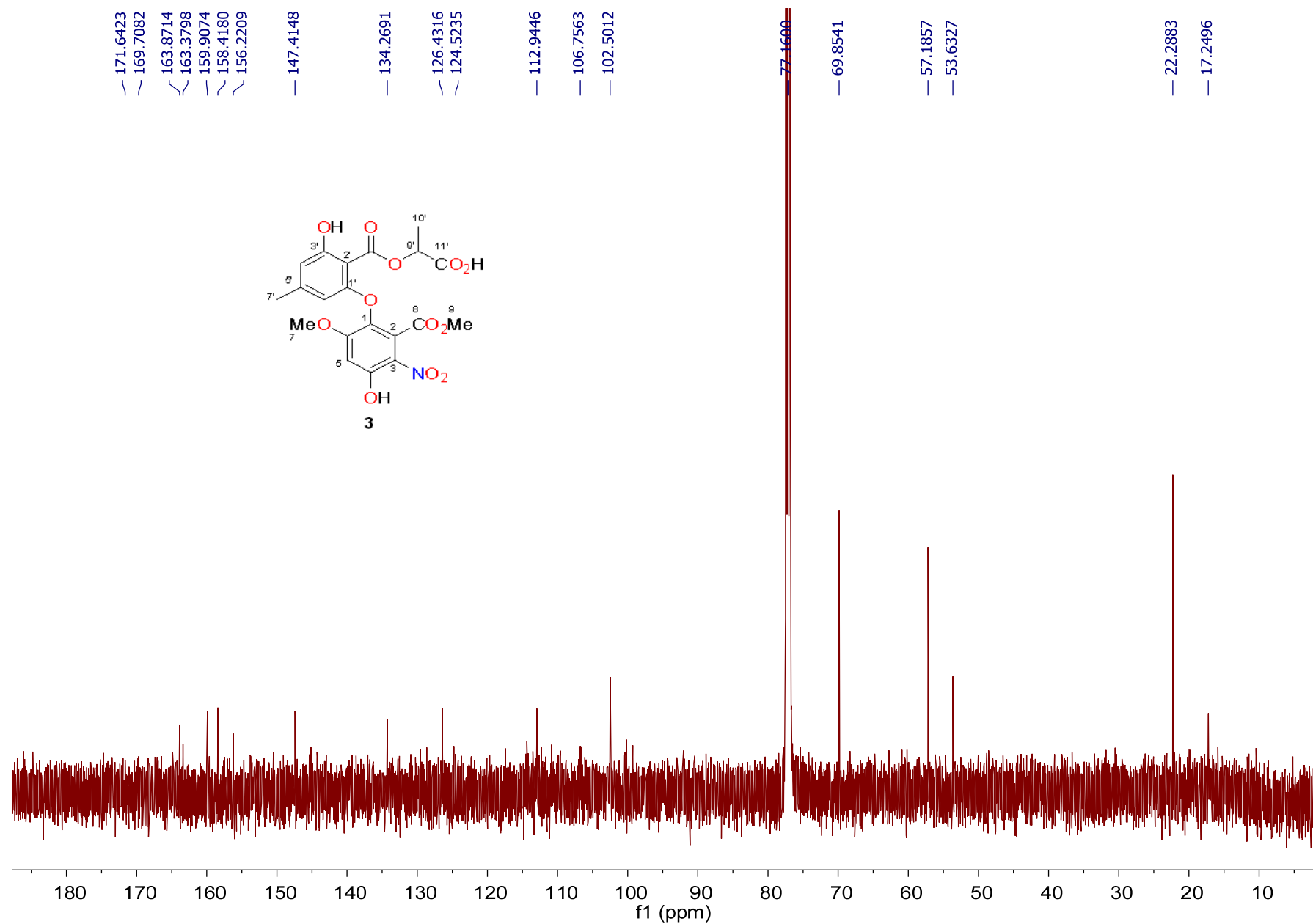
¹H NMR spectrum of **3** (CD₃OD, 500 MHz)



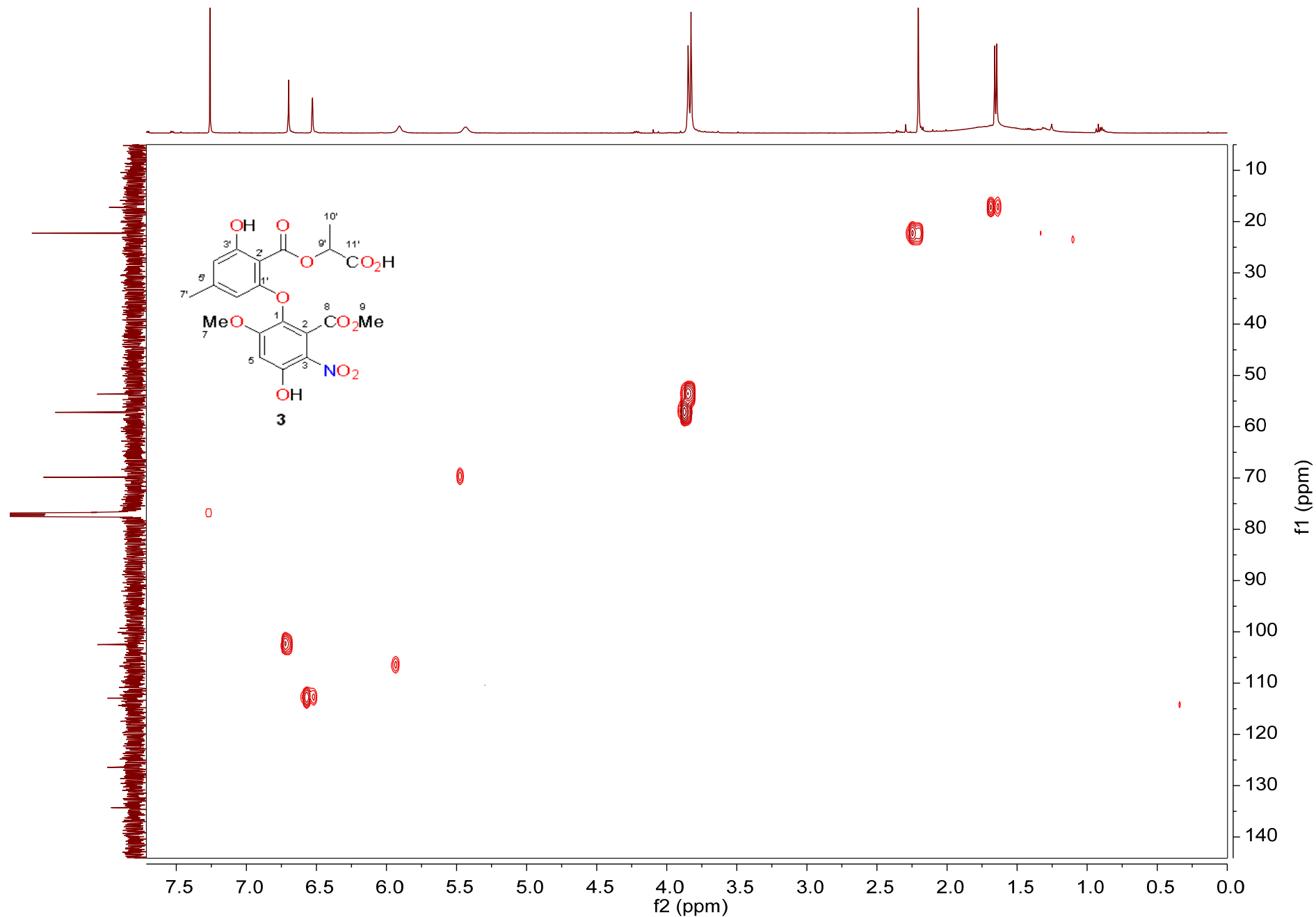
¹³C NMR spectrum of **3** (CD₃OD, 125 MHz)



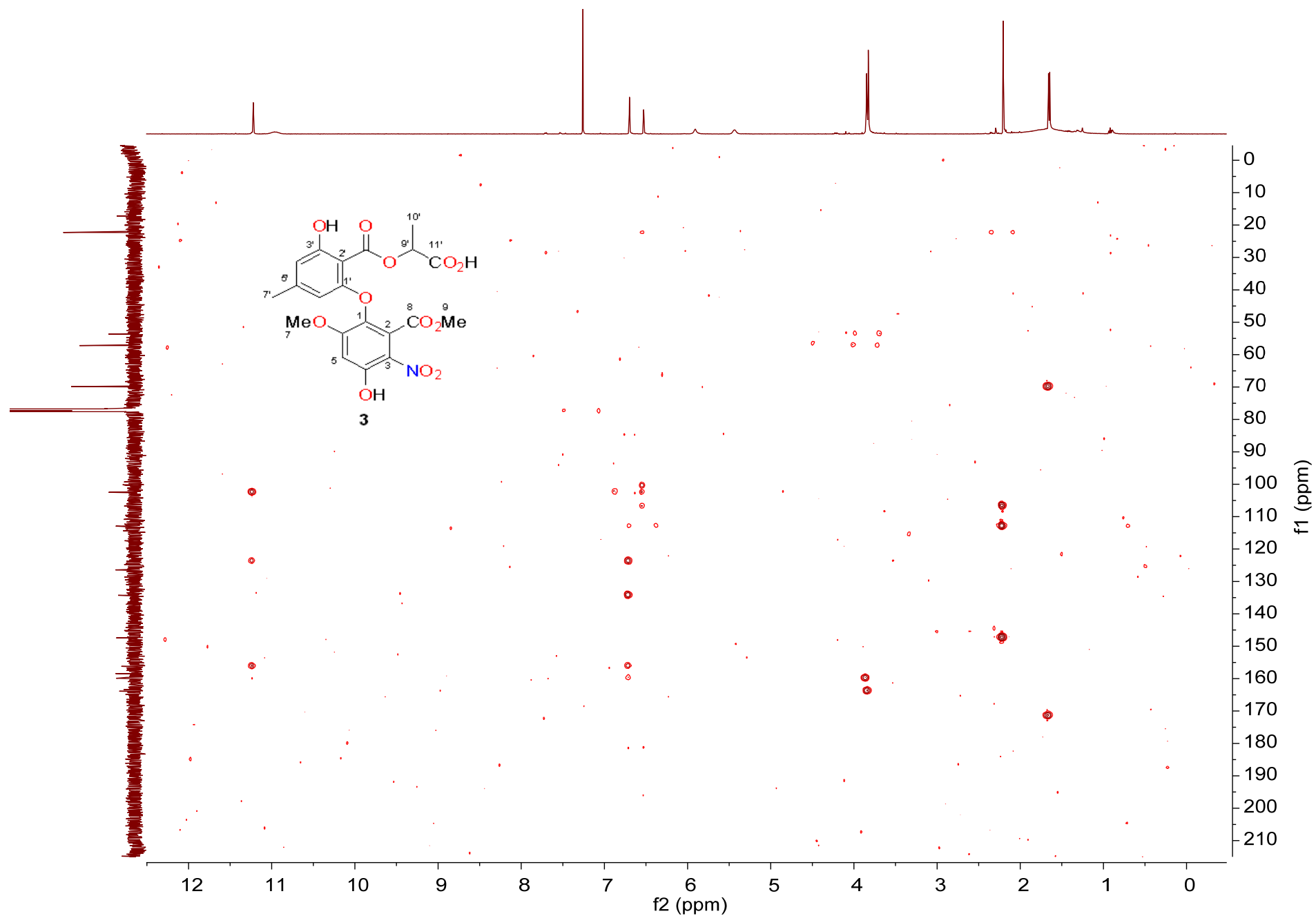
¹H NMR spectrum of **3** (CDCl₃, 500 MHz)

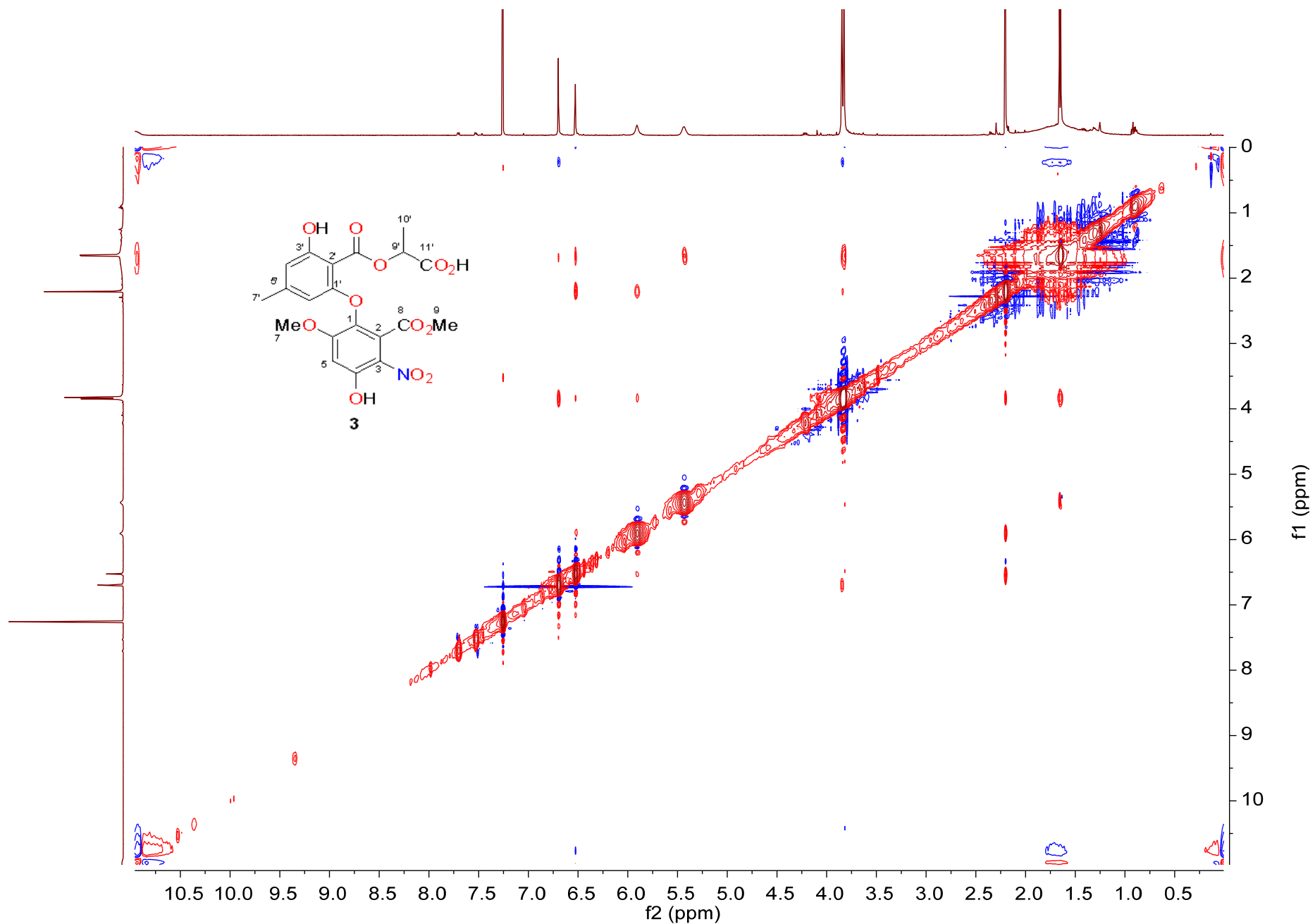


¹³C NMR spectrum of **3** (CDCl₃, 500 MHz)



EDITED-HSQC spectrum of **3** (CDCl₃, 500/125 MHz)

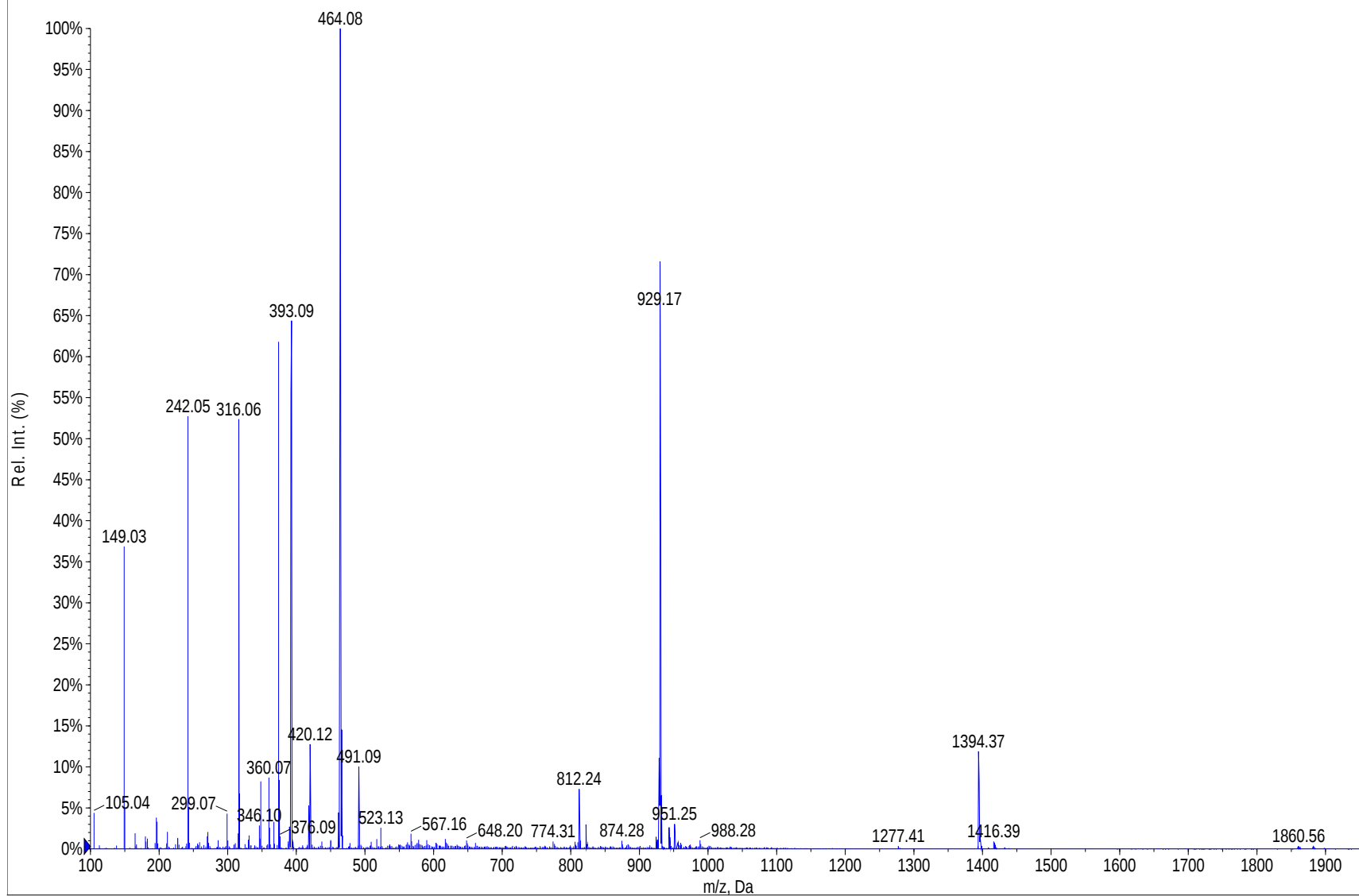




ROESY spectrum of **3** (CDCl₃ 500 MHz)

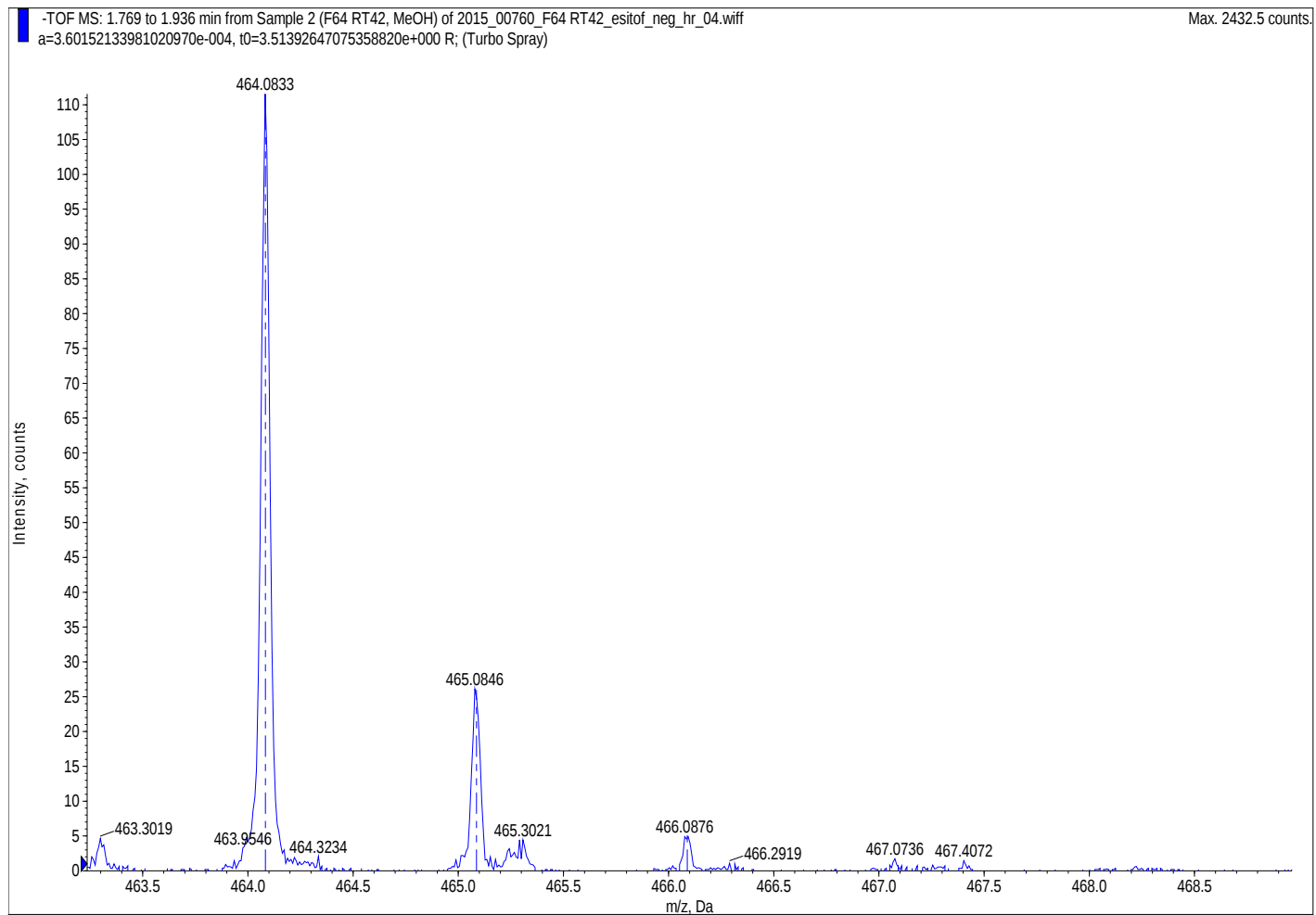
-TOF MS: 1.469 to 1.655 min from Sample 2 (DC-F6-4-RT42) of 2013_25635_DC-F6-4-RT42_esitof_neg_01.wiff
a=3.60201012737532860e-004, t0=3.74988621036550280e+000 R; (Turbo Spray)

Max. 3287.4 counts.



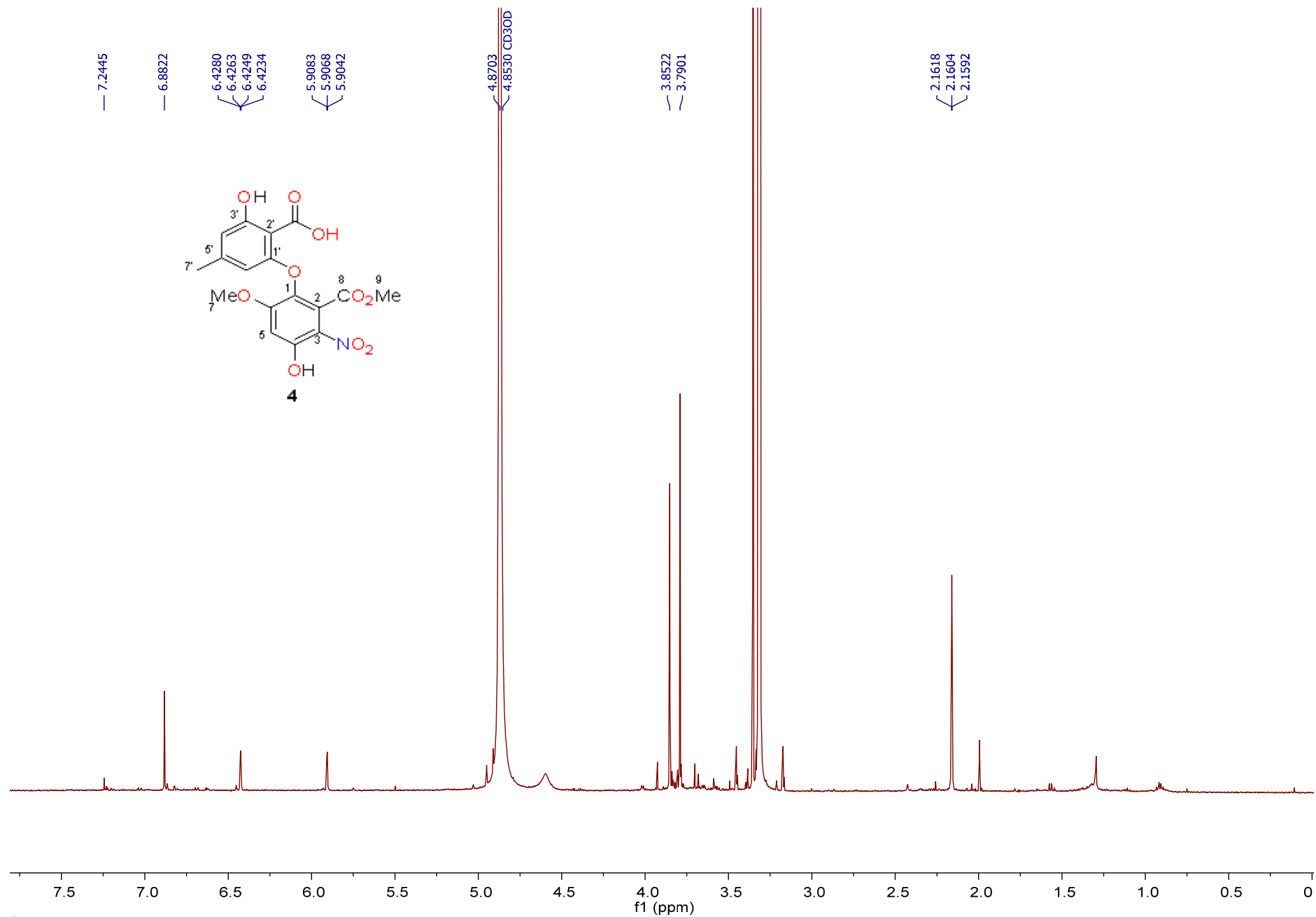
(-)-LRESIMS of **3**

SI26

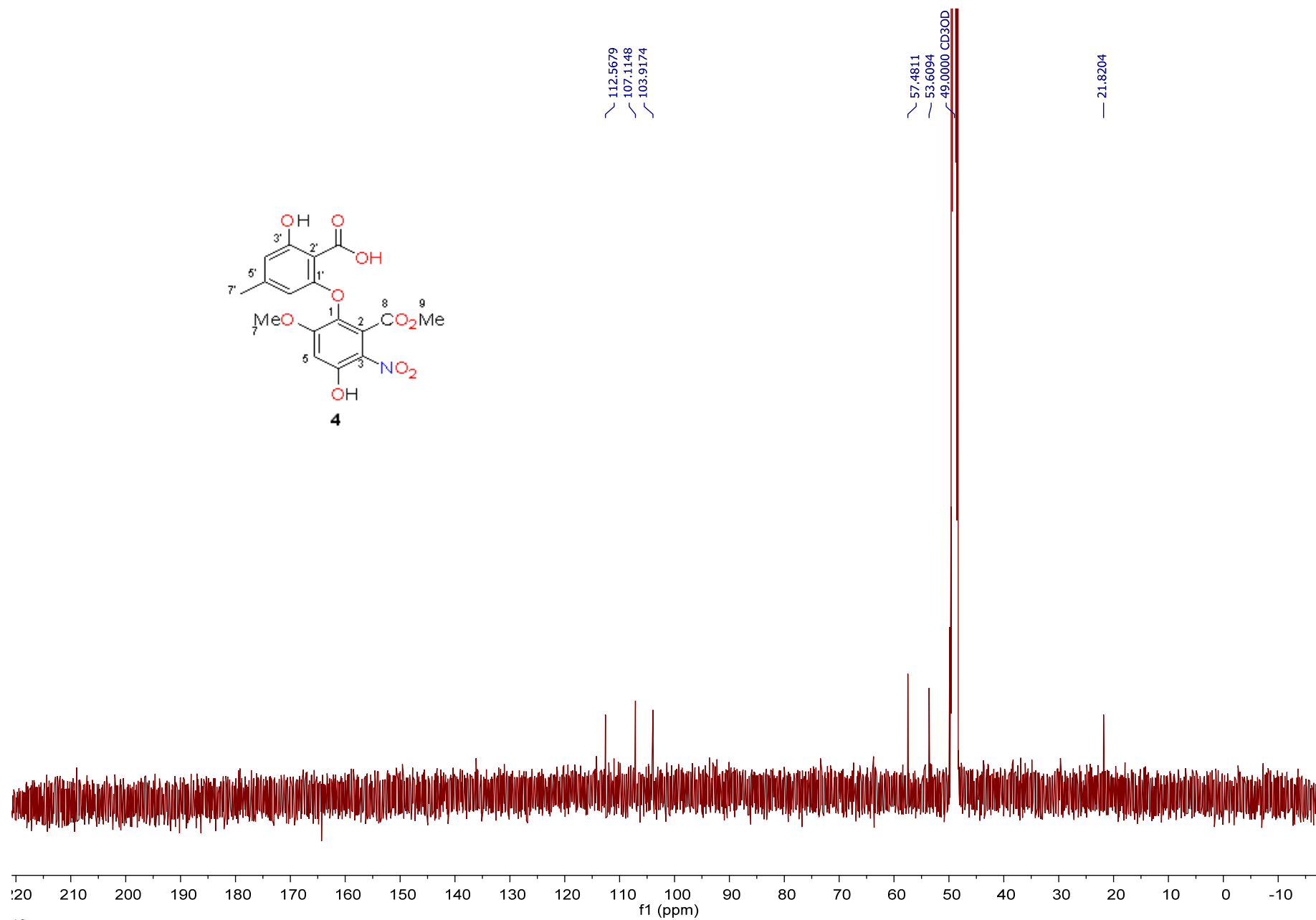
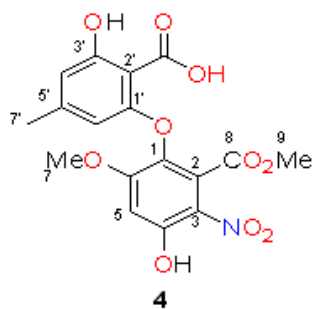


(-)-HRESIMS of **3**

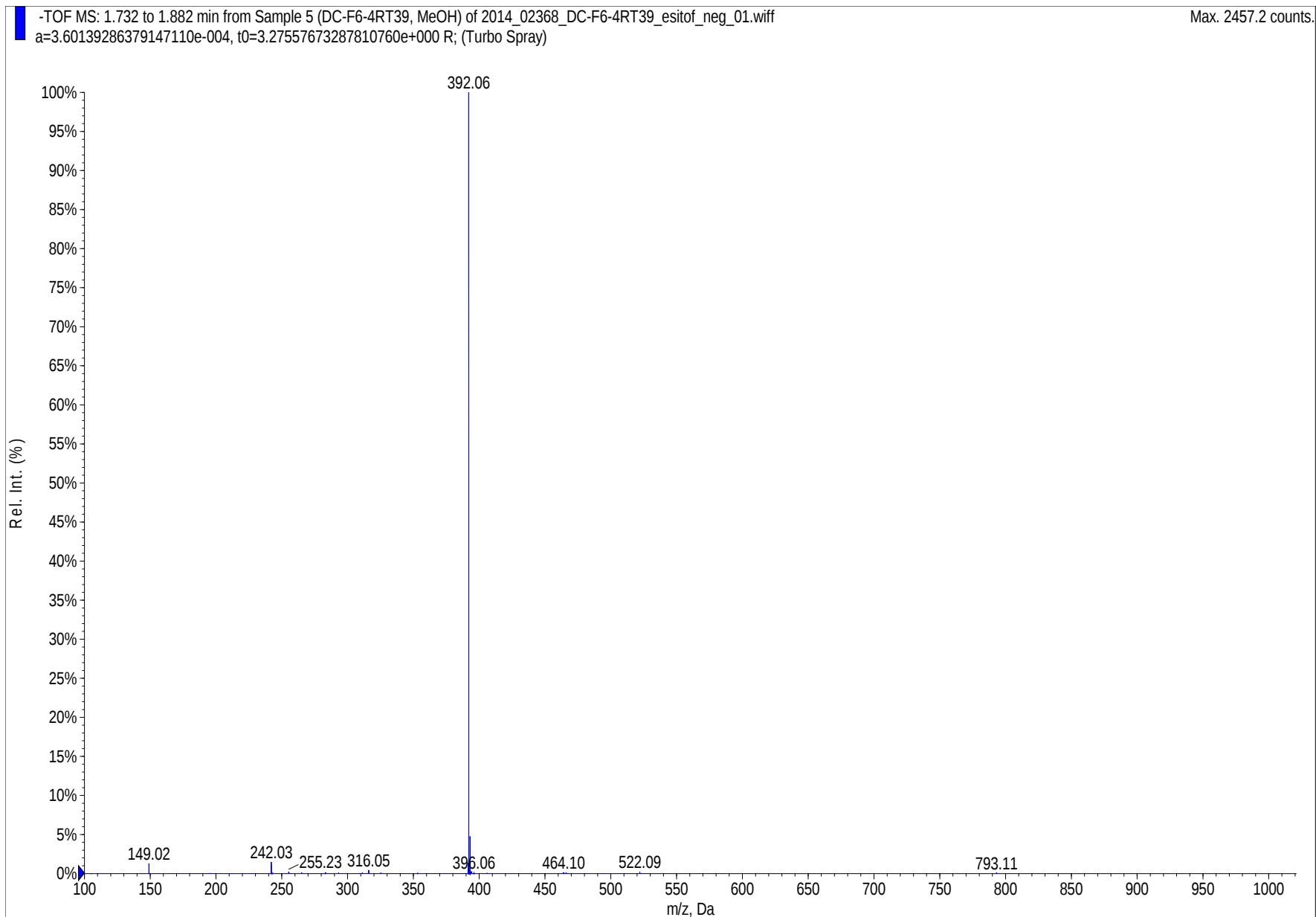
m/z experimental	464.0833			
MF	m/z	Error, mDa	Error in ppm	DBE
C20 H18 N O12	464.0834	-0.1489	-0.321	12.5



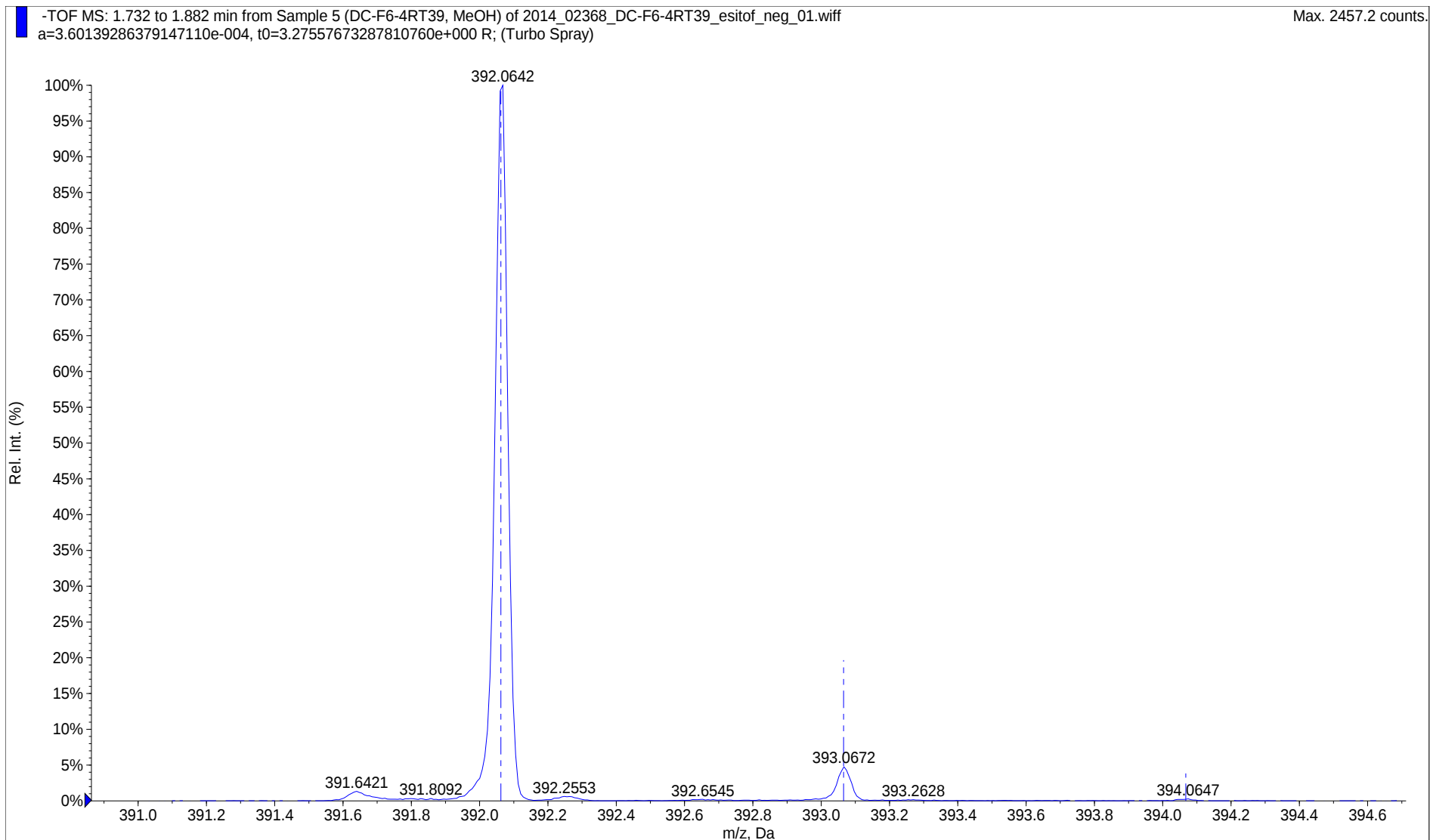
¹H NMR spectrum of **4** (CD₃OD, 500 MHz)



^{13}C NMR spectrum of **4** (CD_3OD , 125 MHz)



(-)-LRESIMS of **4**



(-)-HRESIMS of **4**

m/z experimental	392.0642			
MF	m/z	Error, mDa	Error in ppm	DBE
C17 H14 N O10	392.0623	1.8804	4.7962	11.5