

## Carotane Sesquiterpenes from *Ferula vesceritensis*: *in silico* Analysis as SARS-CoV-2 Binding Inhibitors

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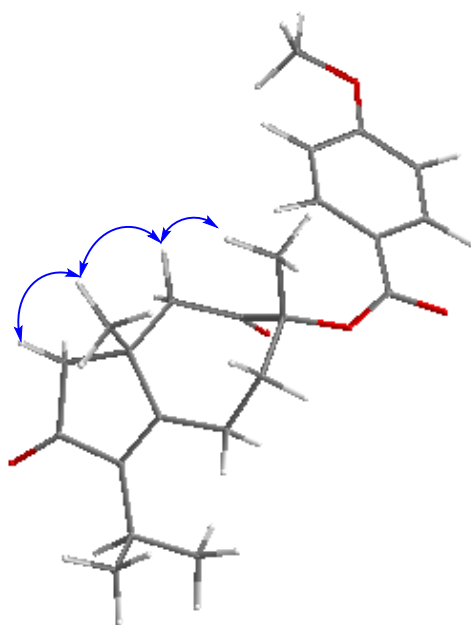
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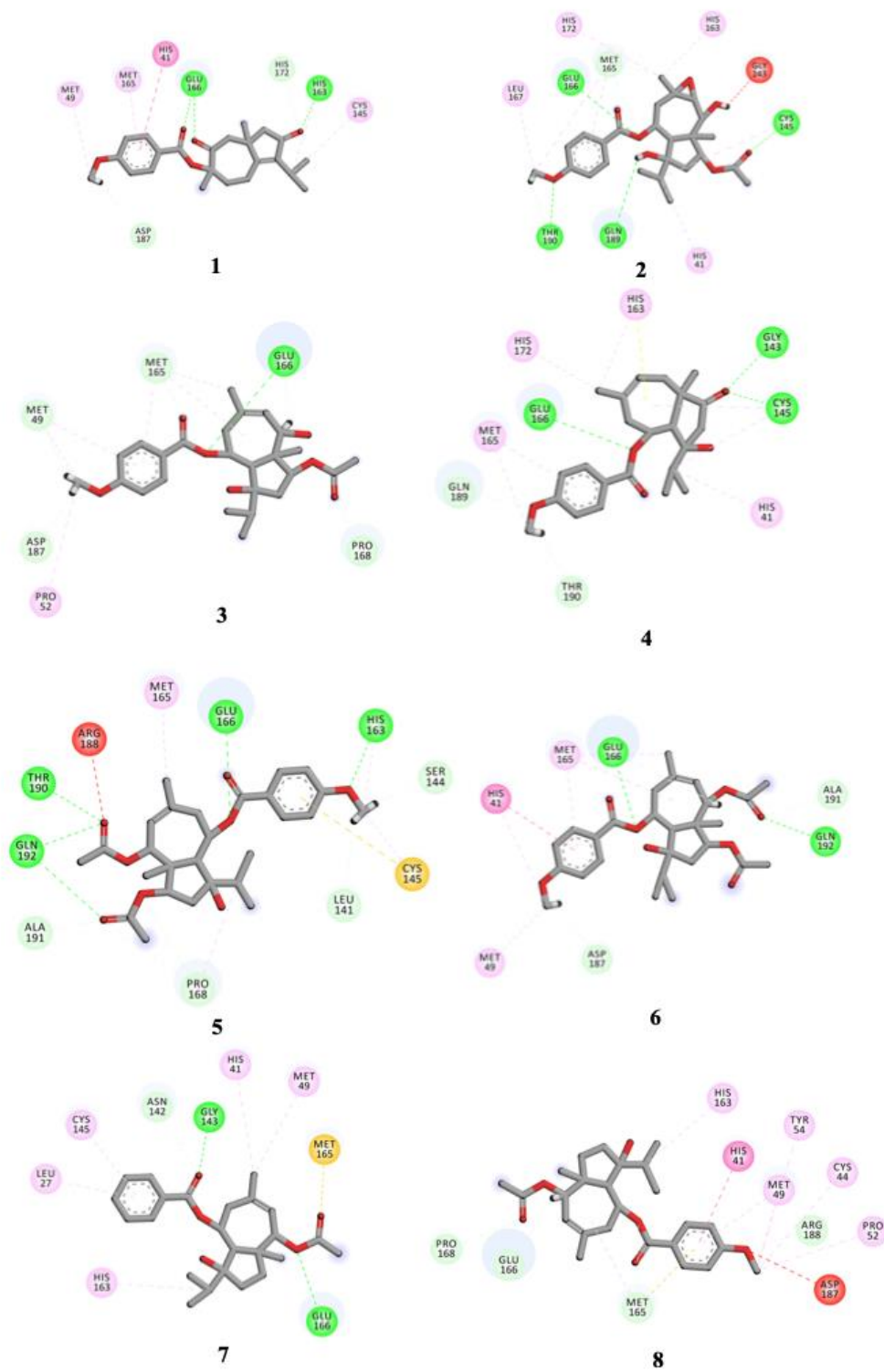
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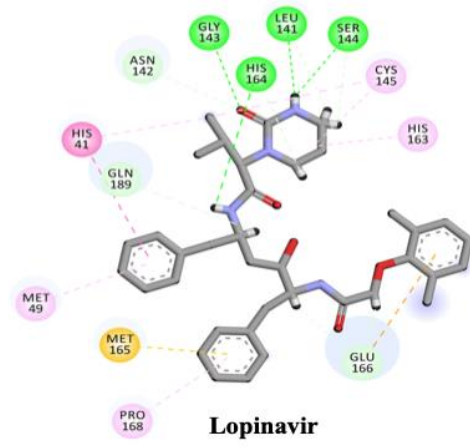
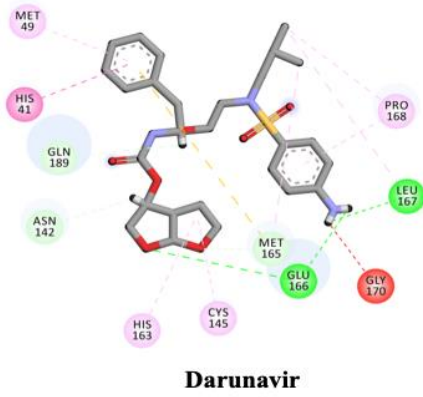
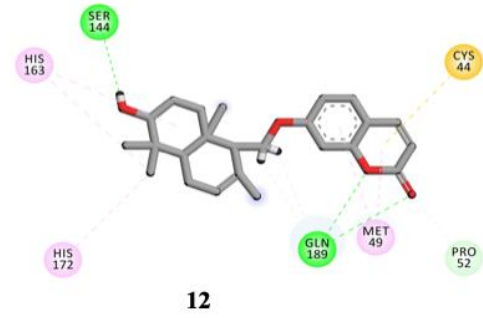
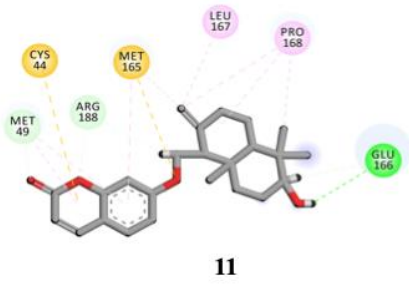
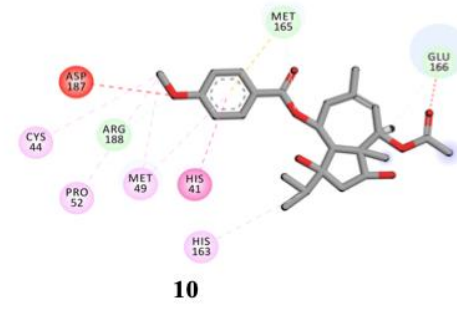
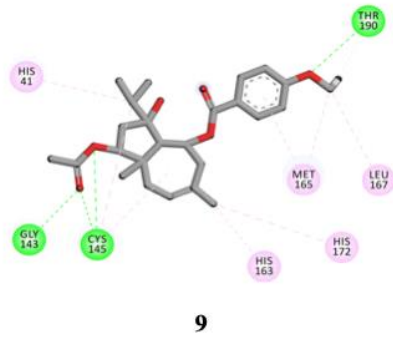
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**Figure S1.** NOESY correlations for **1**.



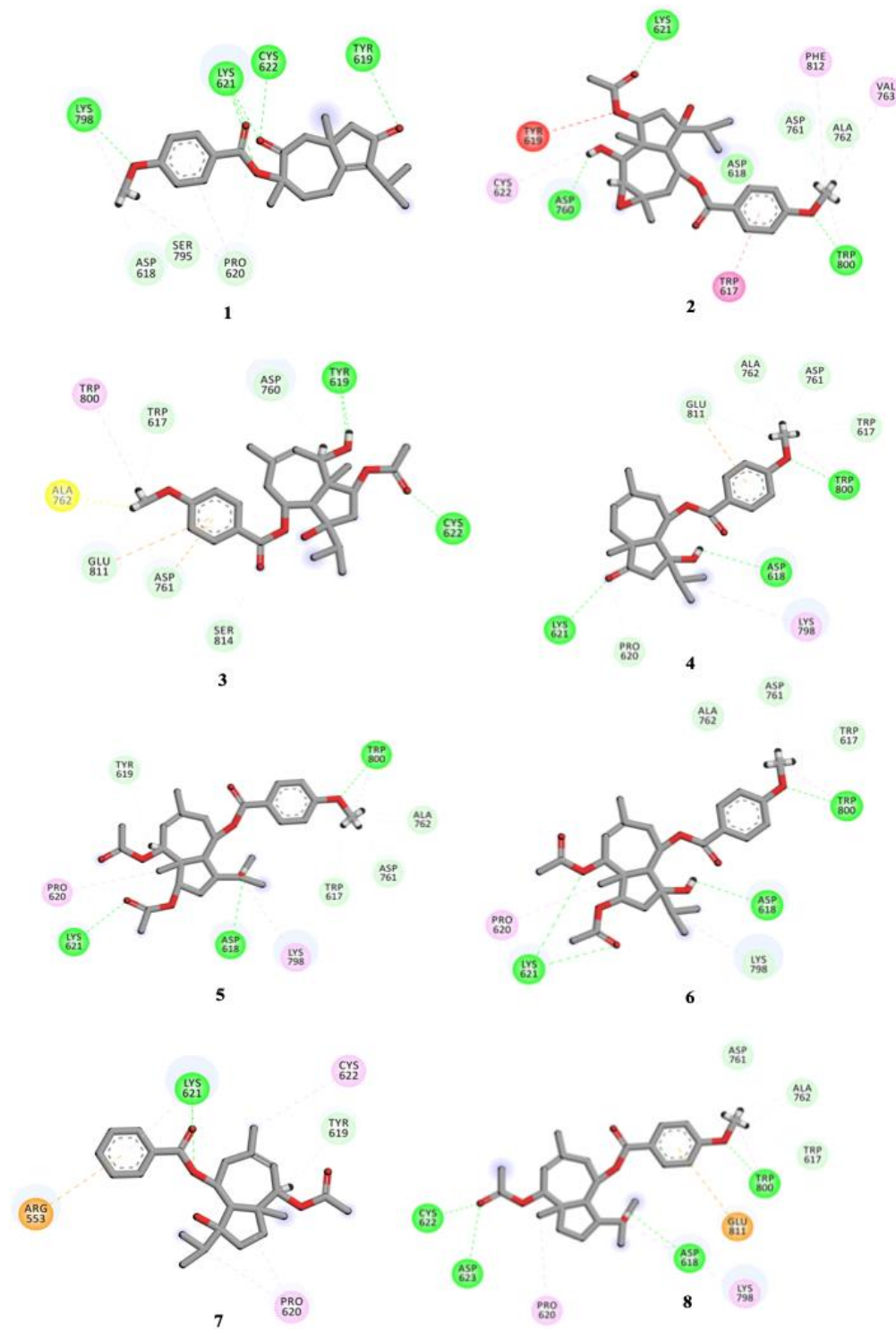
**Figure S2.** 2D representations of interactions of compounds 1-12, duranavir and lopinavir with important amino acid residues of SARS-CoV-2 main protease (M<sup>Pro</sup>).



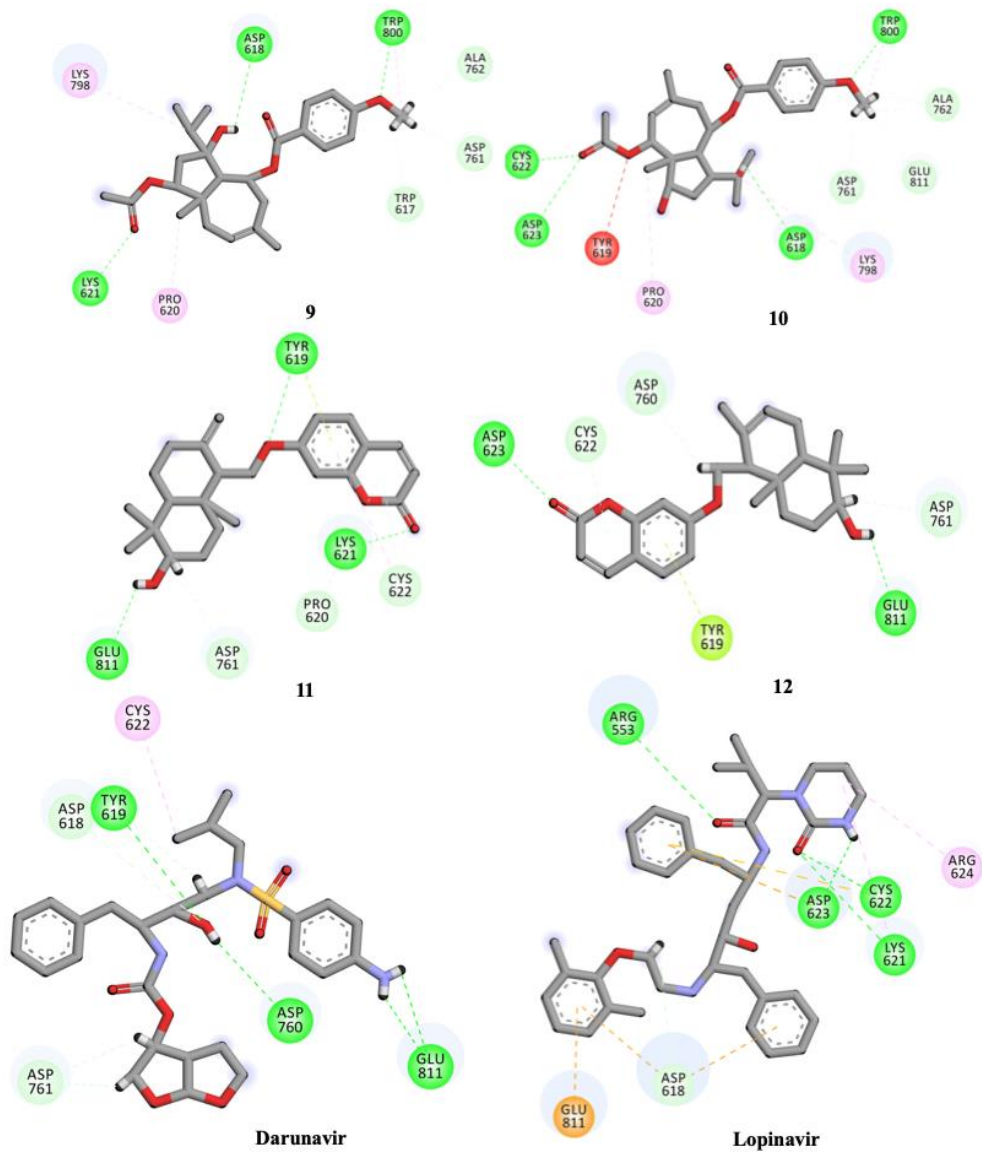
**Interactions**

- Conventional Hydrogen Bond
- Carbon Hydrogen Bond
- Unfavorable Acceptor-Acceptor
- Alkyl
- pi-Alkyl

**Figure S2.**Continued.



**Figure S3.** 2D representations of interactions of compounds **1-12**, duranavir and lopinavir with important amino acid residues of SARS-CoV-2 RNA-dependent RNA Polymerase (RdRp).



**Interactions**

- Conventional Hydrogen Bond
- Carbon Hydrogen Bond
- Unfavorable Acceptor-Acceptor
- Alkyl
- pi-Alkyl

**Figure S3.**Continued.



Monoisotopic Mass, Even Electron Ions  
152 formula(e) evaluated with 25 results within limits (up to 10 closest results for each mass)

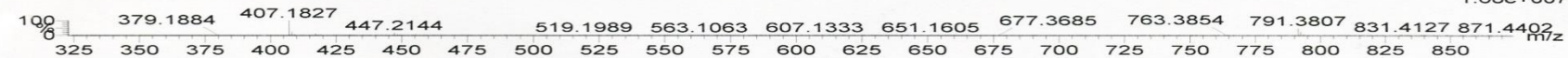
Elements Used:

C: 0-100 H: 0-250 O: 0-20 Na: 0-1

Fer-4-B

Shoyaku20160929\_03 73 (1.449) AM2 (Ar,10000.0,0.00,0.00)

1: TOF MS ES+  
1.68e+007

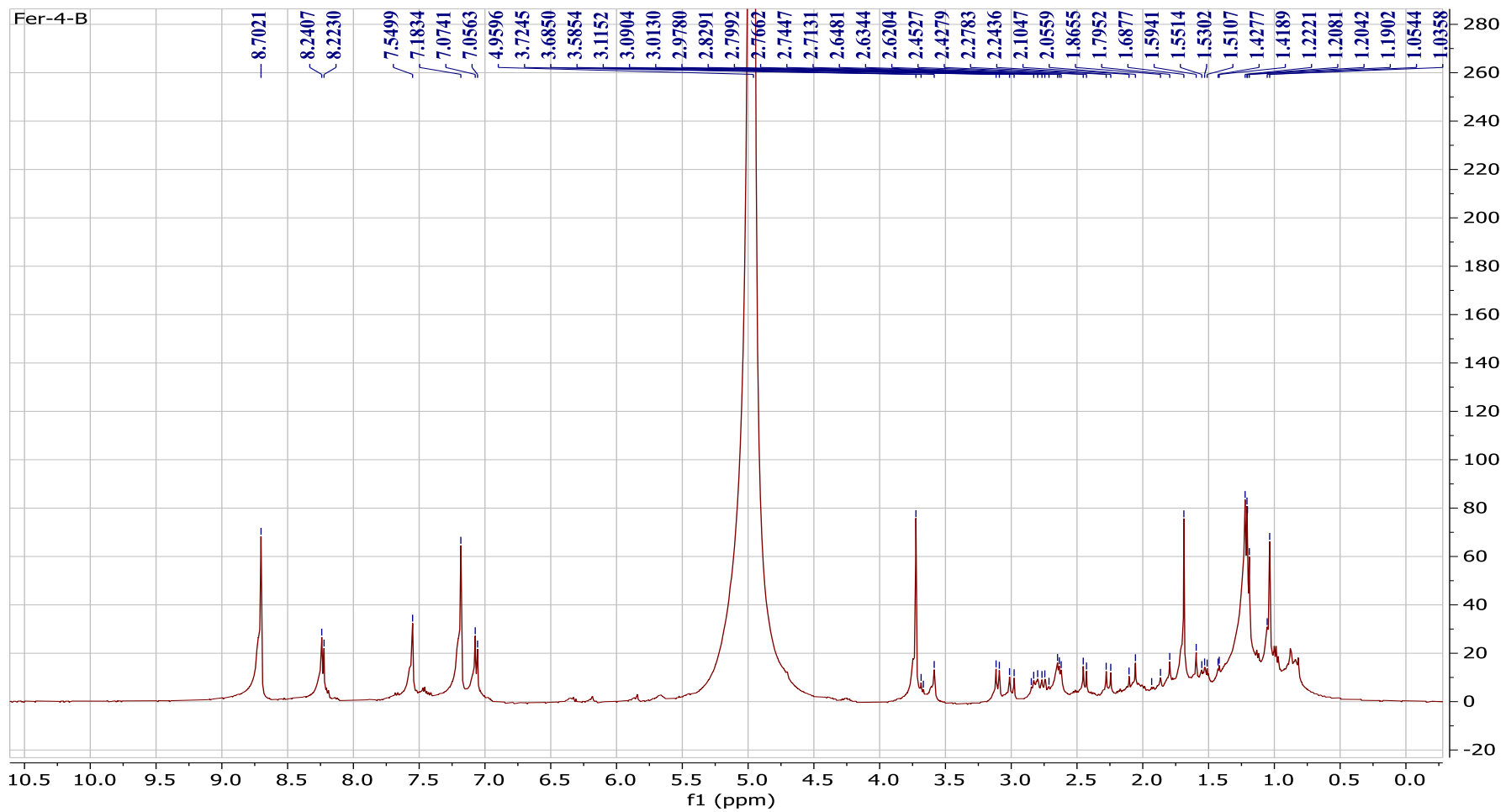


Minimum: 0.0  
Maximum: 50.0 10.0 30.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
407.1827	407.1834	-0.7	-1.7	9.5	394.7	1.655	19.11	C23 H28 O5 Na

FigureS4:(+ve) TOF-ESI-MS of 1





FigureS5:  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz) of **1**

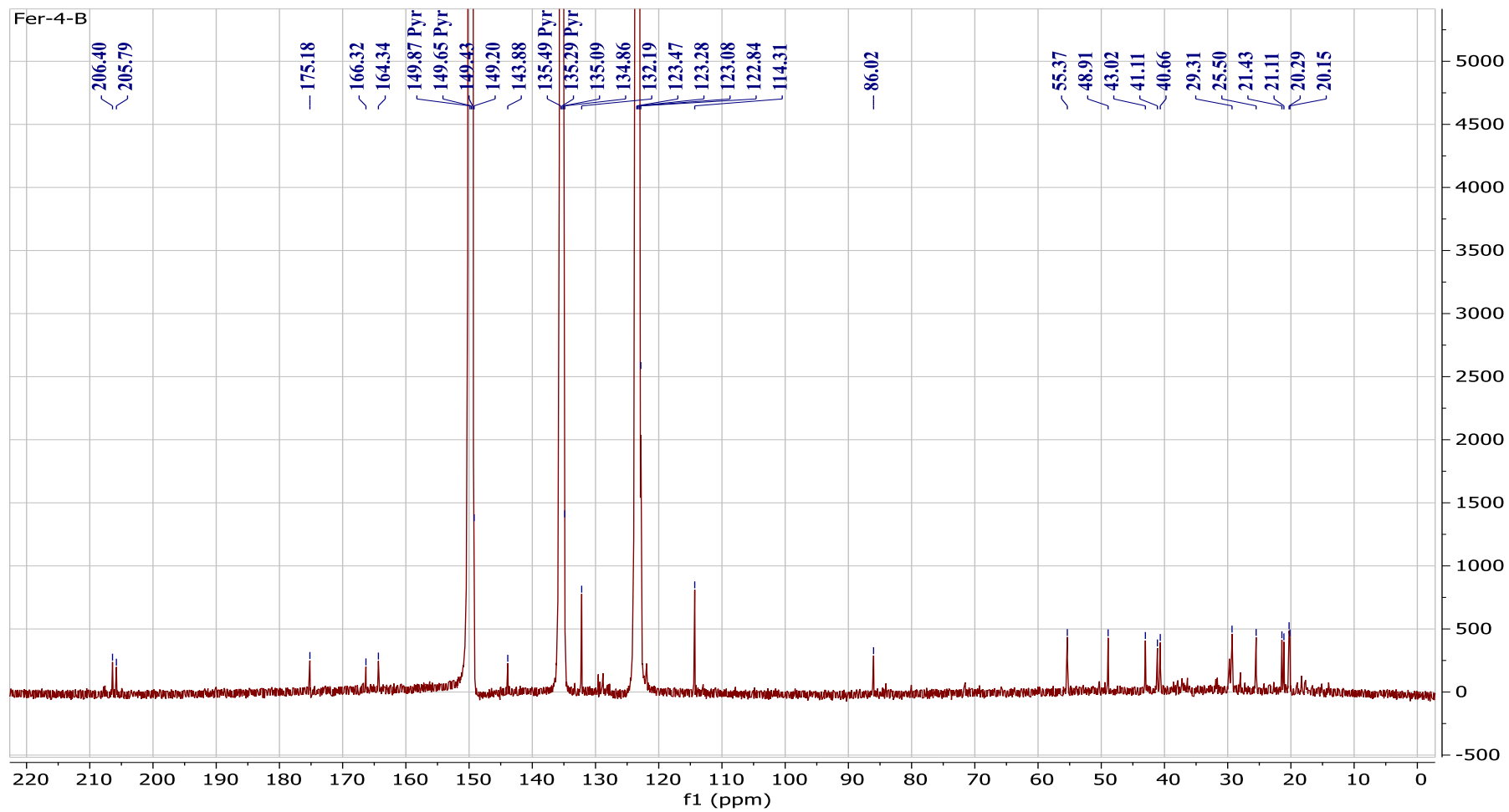
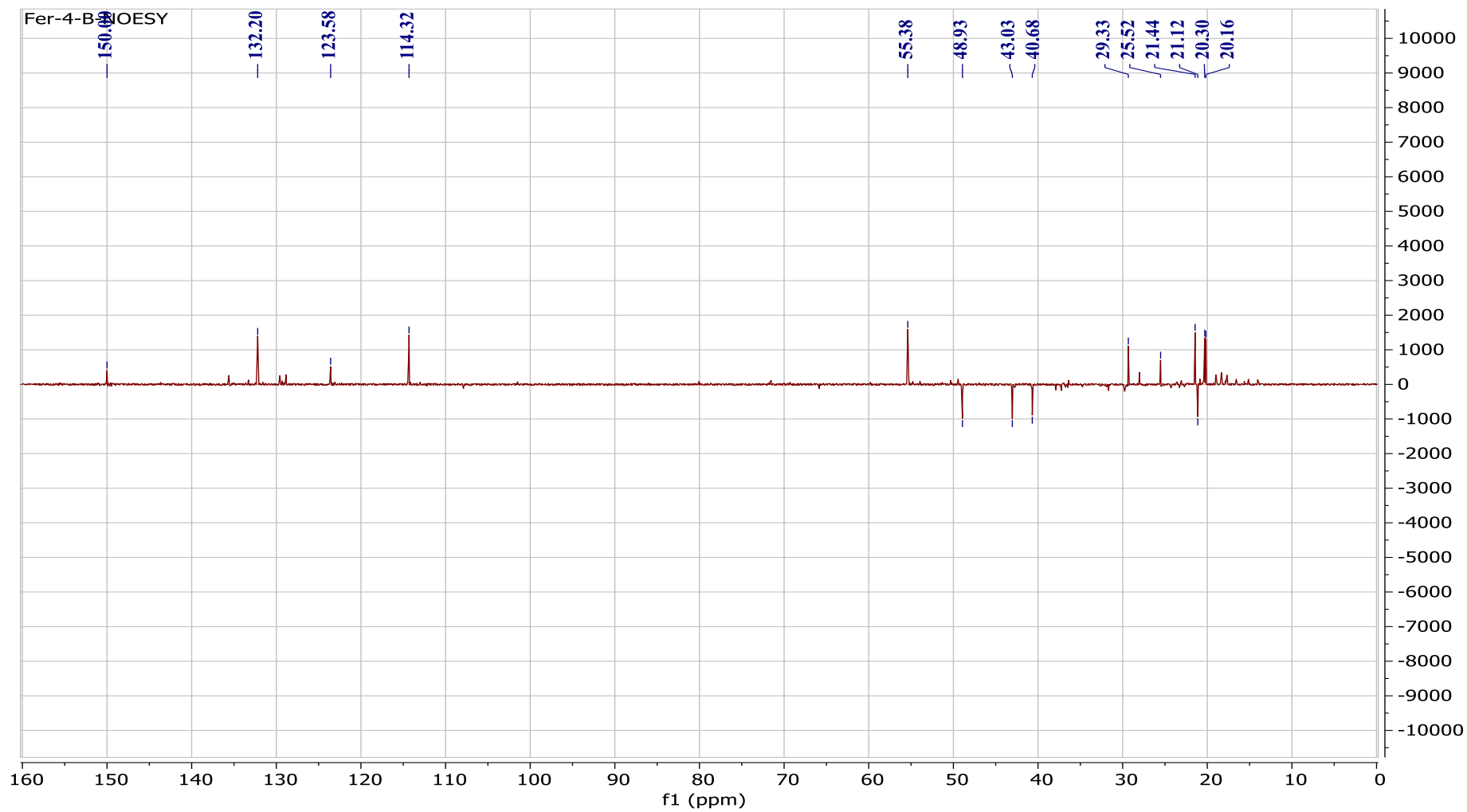
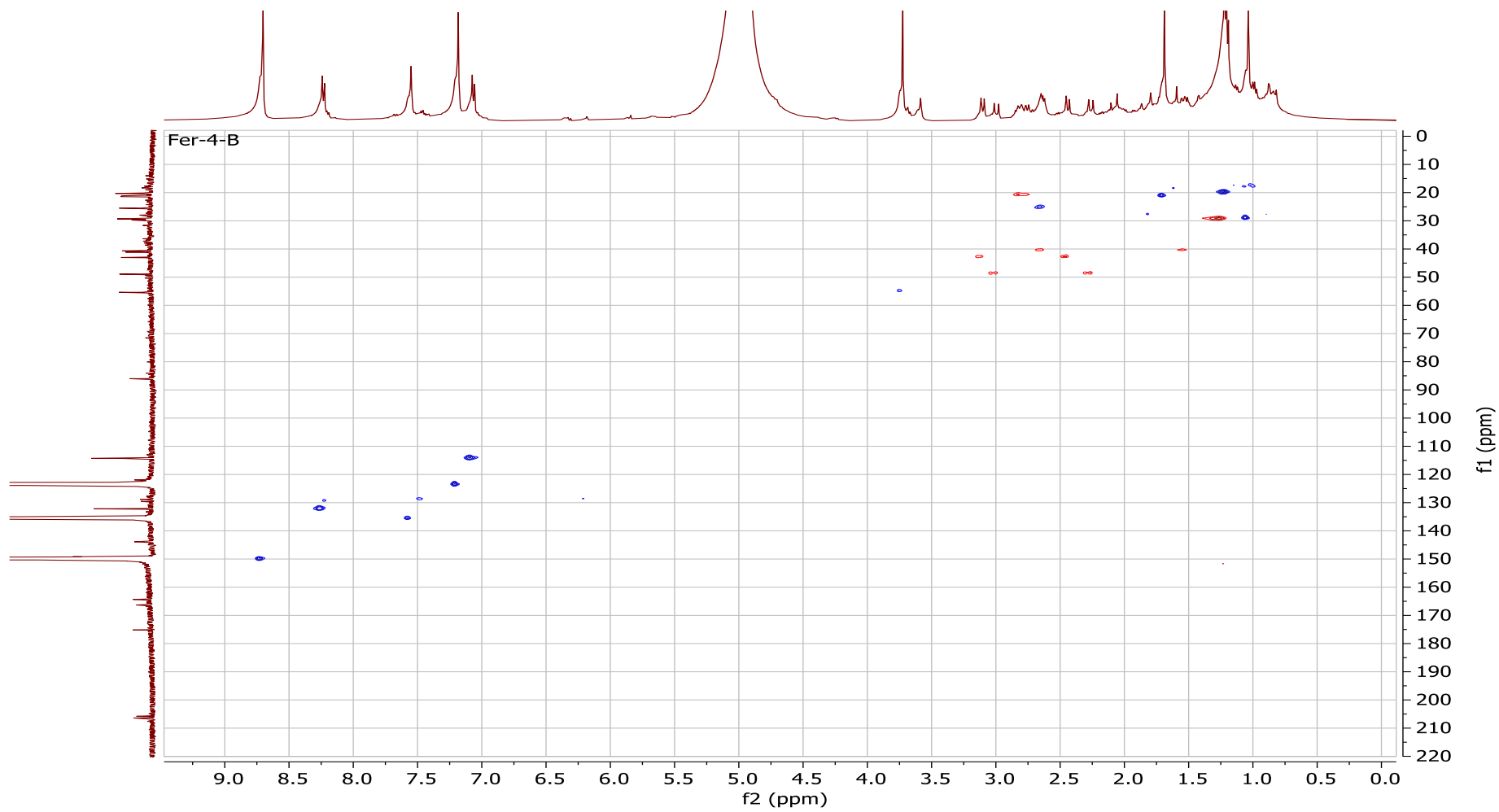


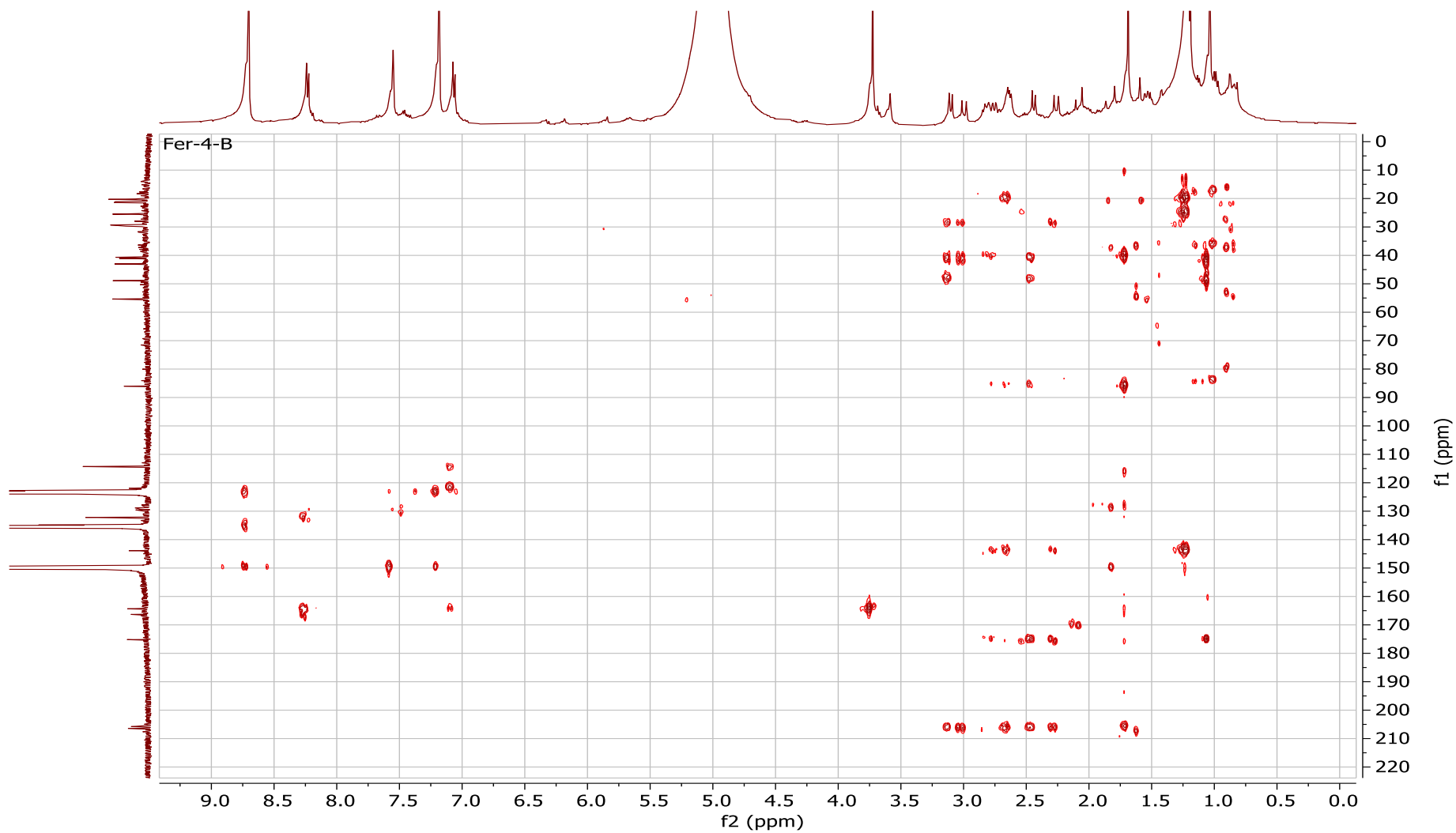
Figure S6:  $^{13}\text{C}$  NMR ( $\text{C}_5\text{D}_5\text{N}$ , 125 MHz) of **1**



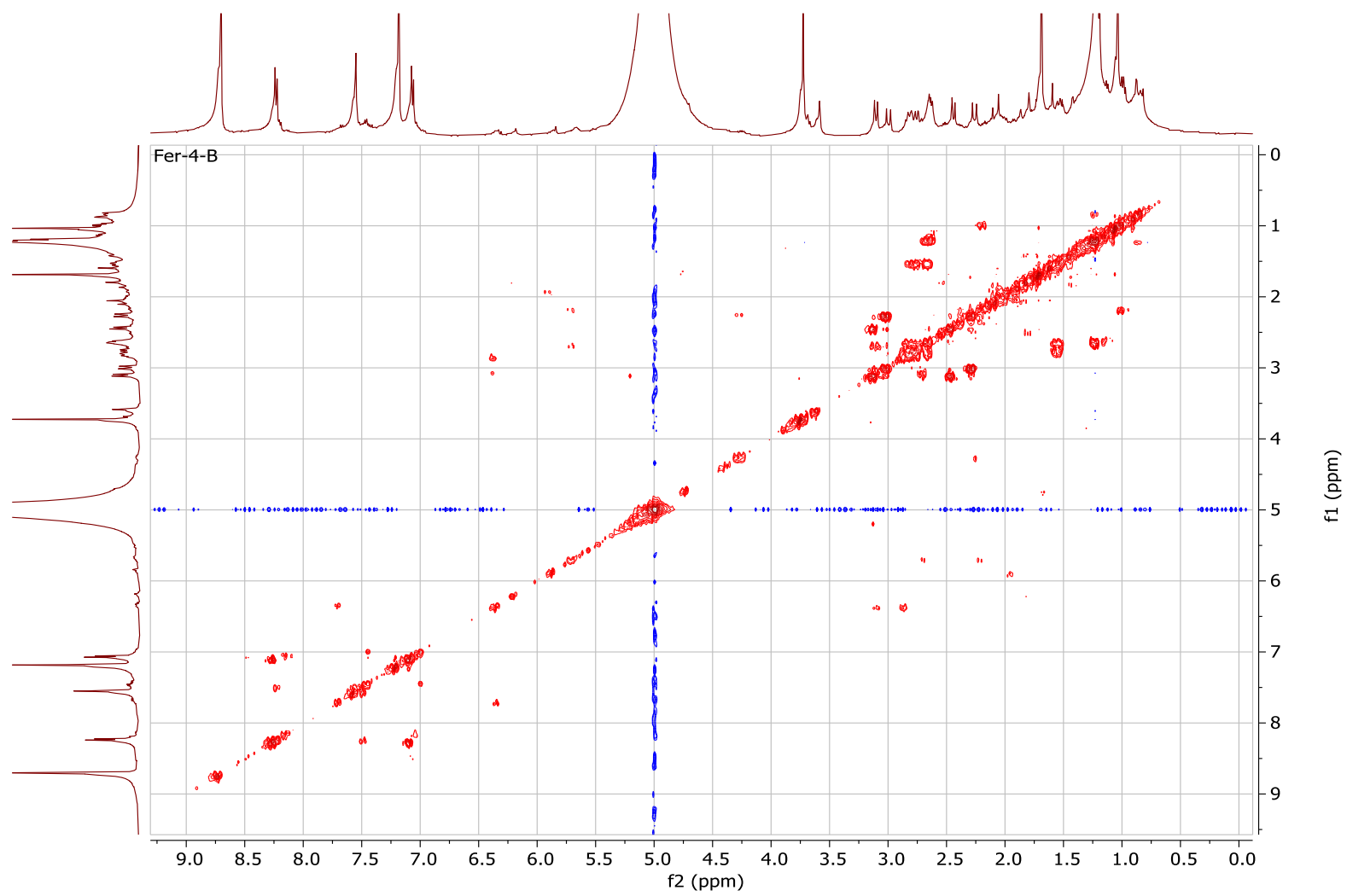
FigureS7:DEPT of 1



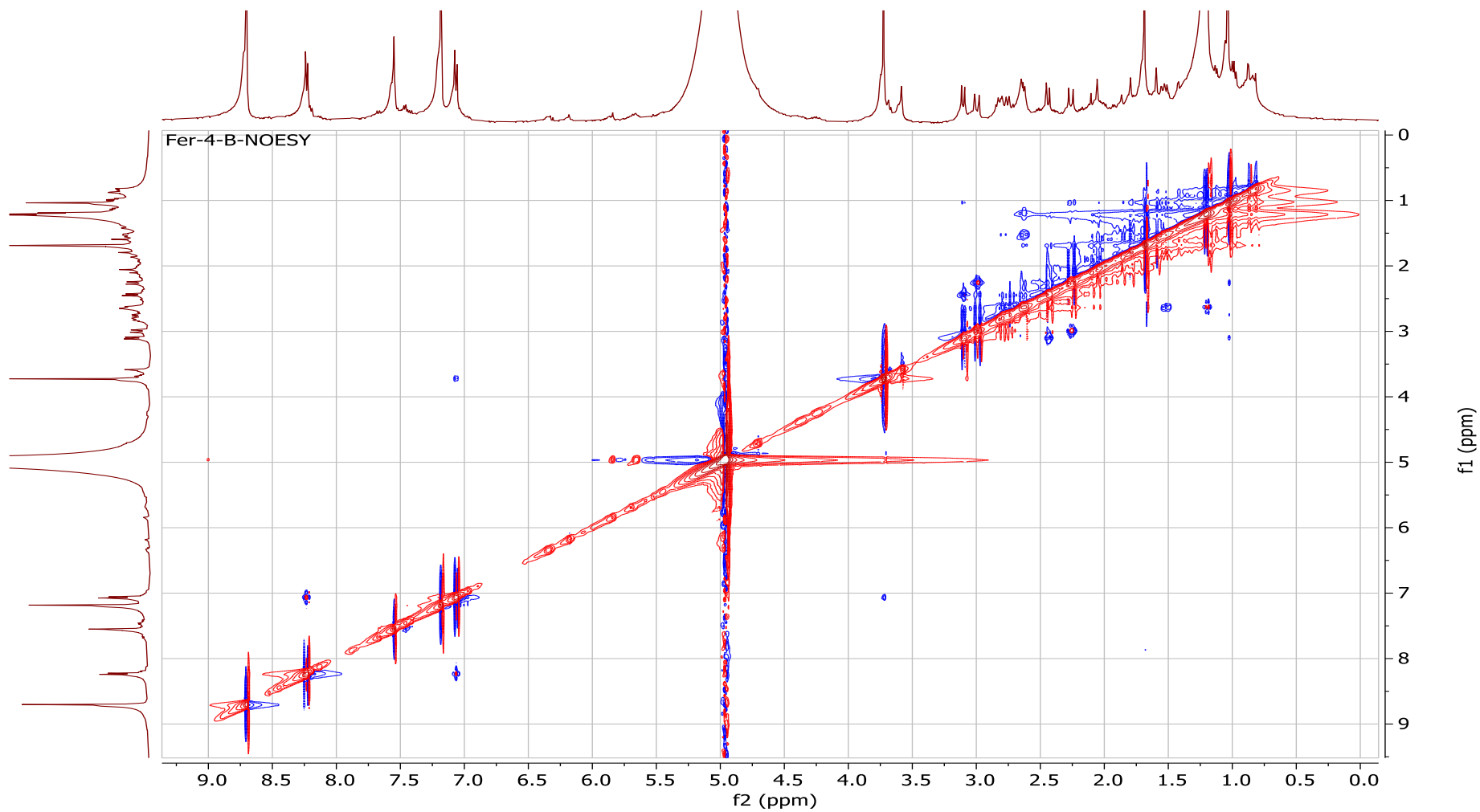
FigureS8:HSQC of 1



FigureS9:HMBC of 1



FigureS10:  $^1\text{H}$   $^1\text{H}$  COSY of **1**



FigureS11:NOESY of 1

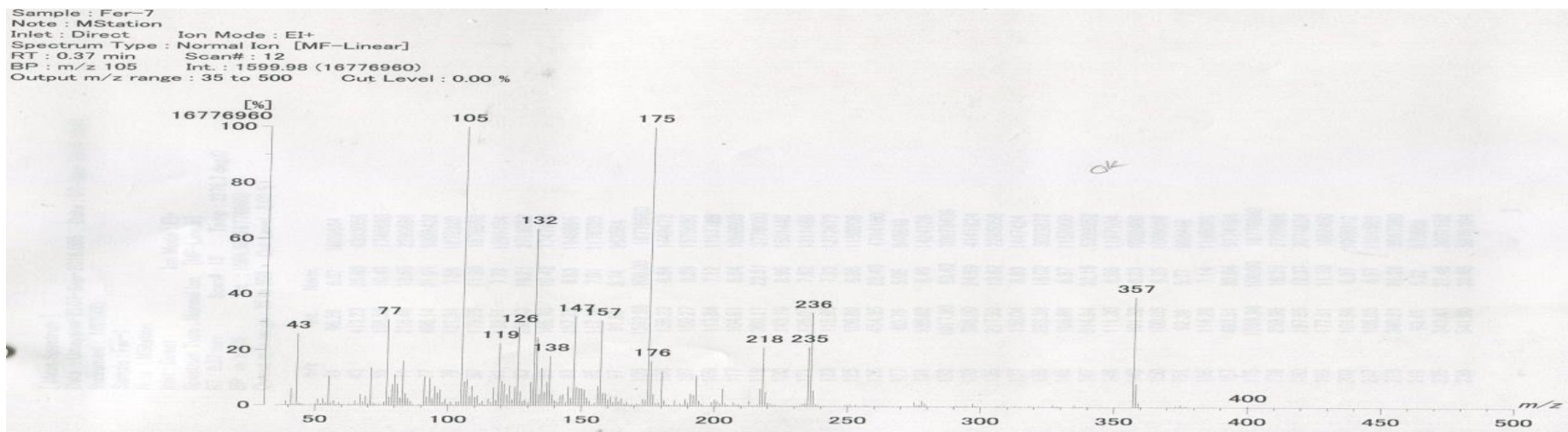


Figure S12: LREIMS of 2

Date : 23-Mar-2019 12:11  
 Instrument: MS700D  
 Sample: Fer-7  
 Note: MStation  
 Inlet: Direct Ion Mode: EI+  
 RT: 1.69 min Scan#: 19  
 Elements: C 150/0, H 250/0, O 50/0  
 Mass Tolerance: 5mmu  
 Unsaturation (U.S.): 0.0 - 15.0

Observed	m/z	Int %	Err. [ppm I mmu]	U.S	Compos
1	400.2249	100.00	-0.1 / -0.6	13.5	C24 H32

Figure S13: HREIMS of 2



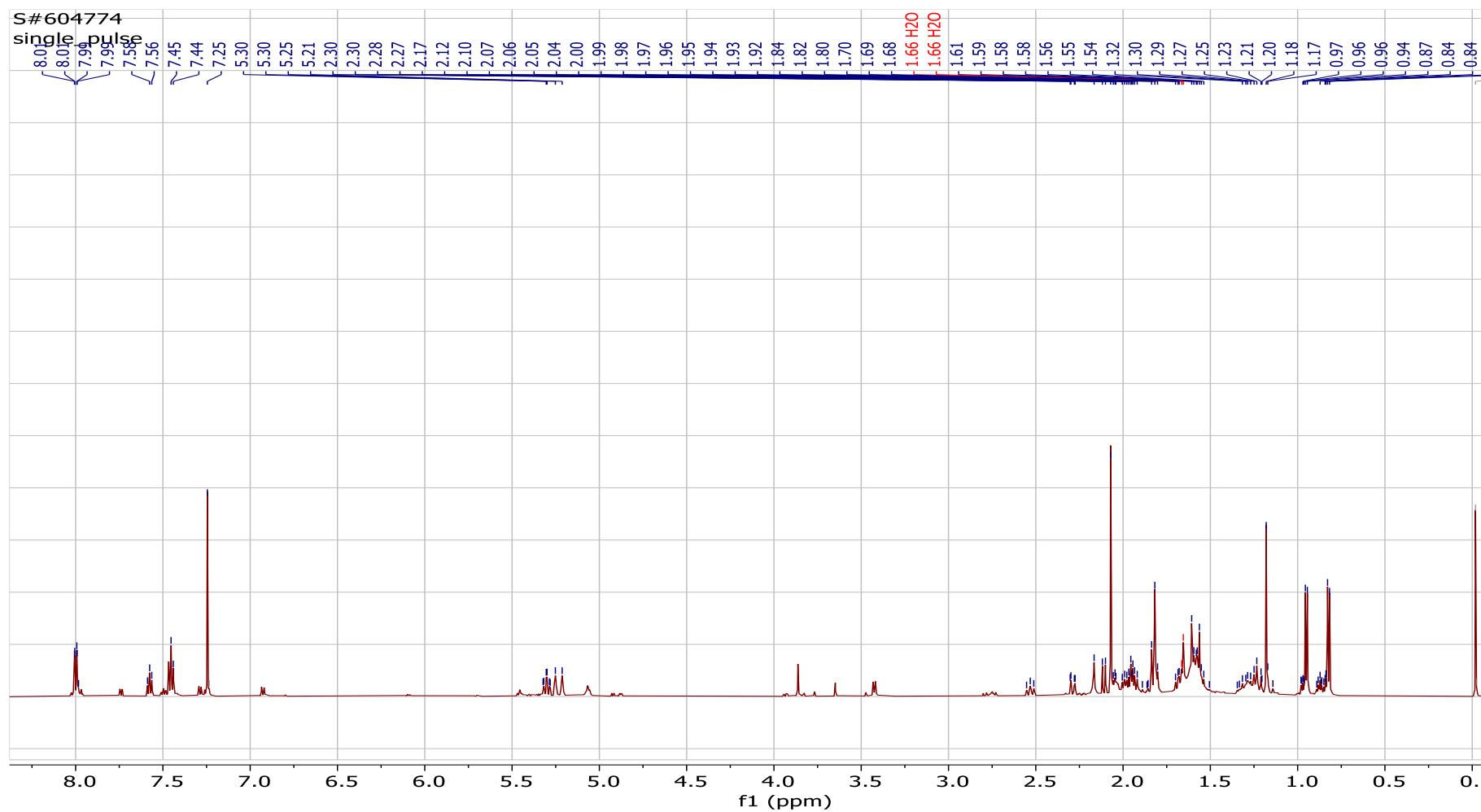
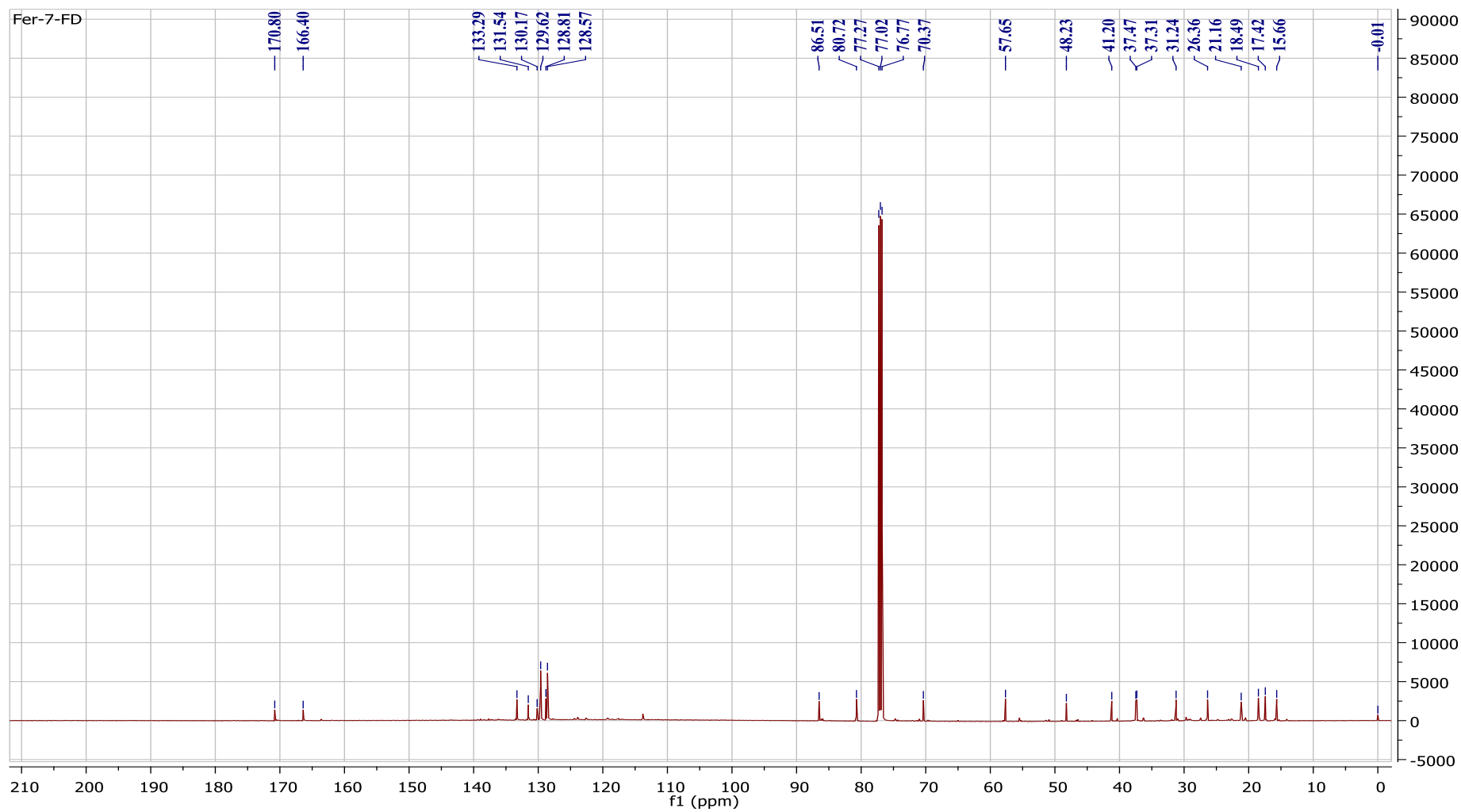
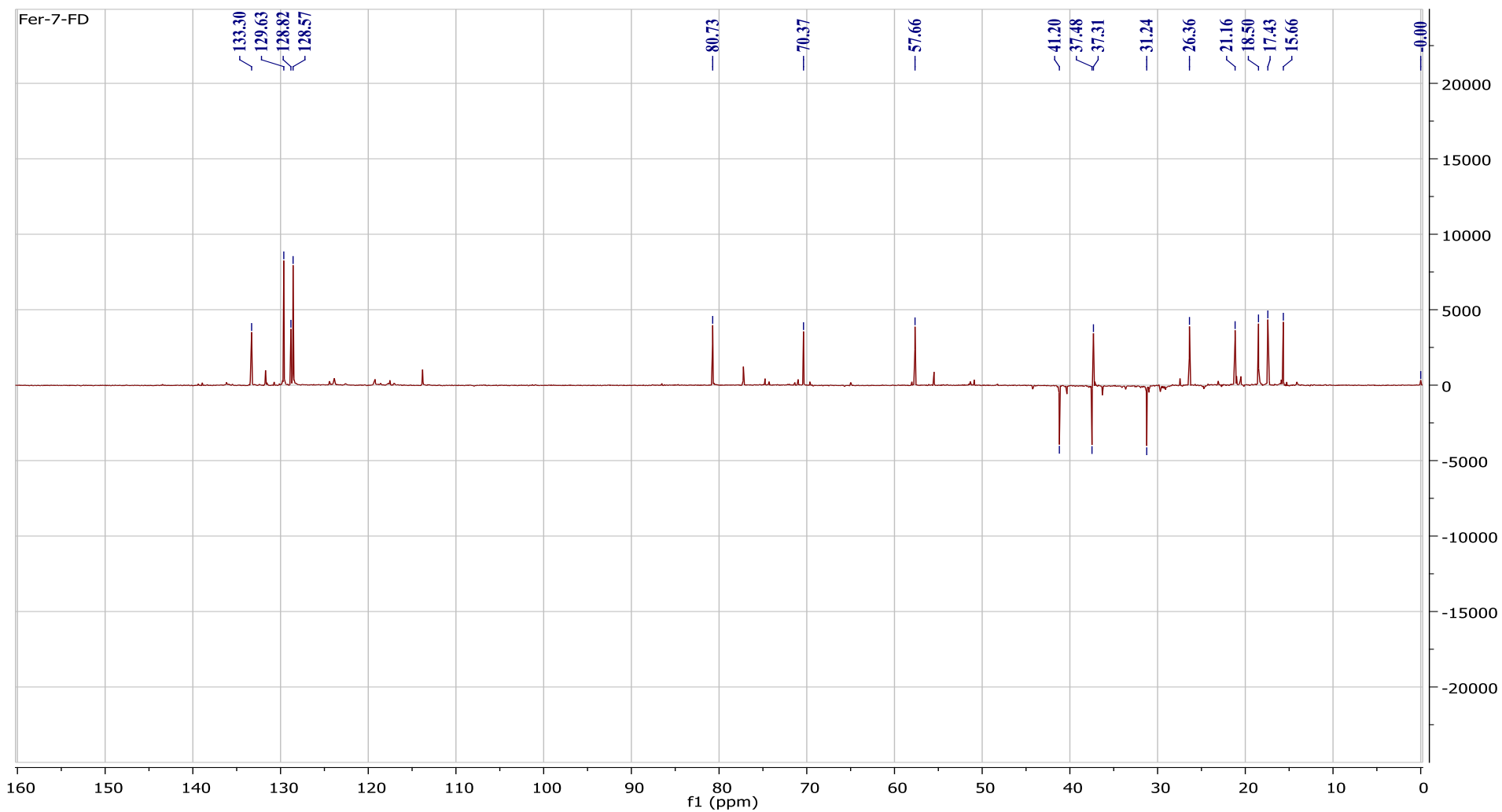


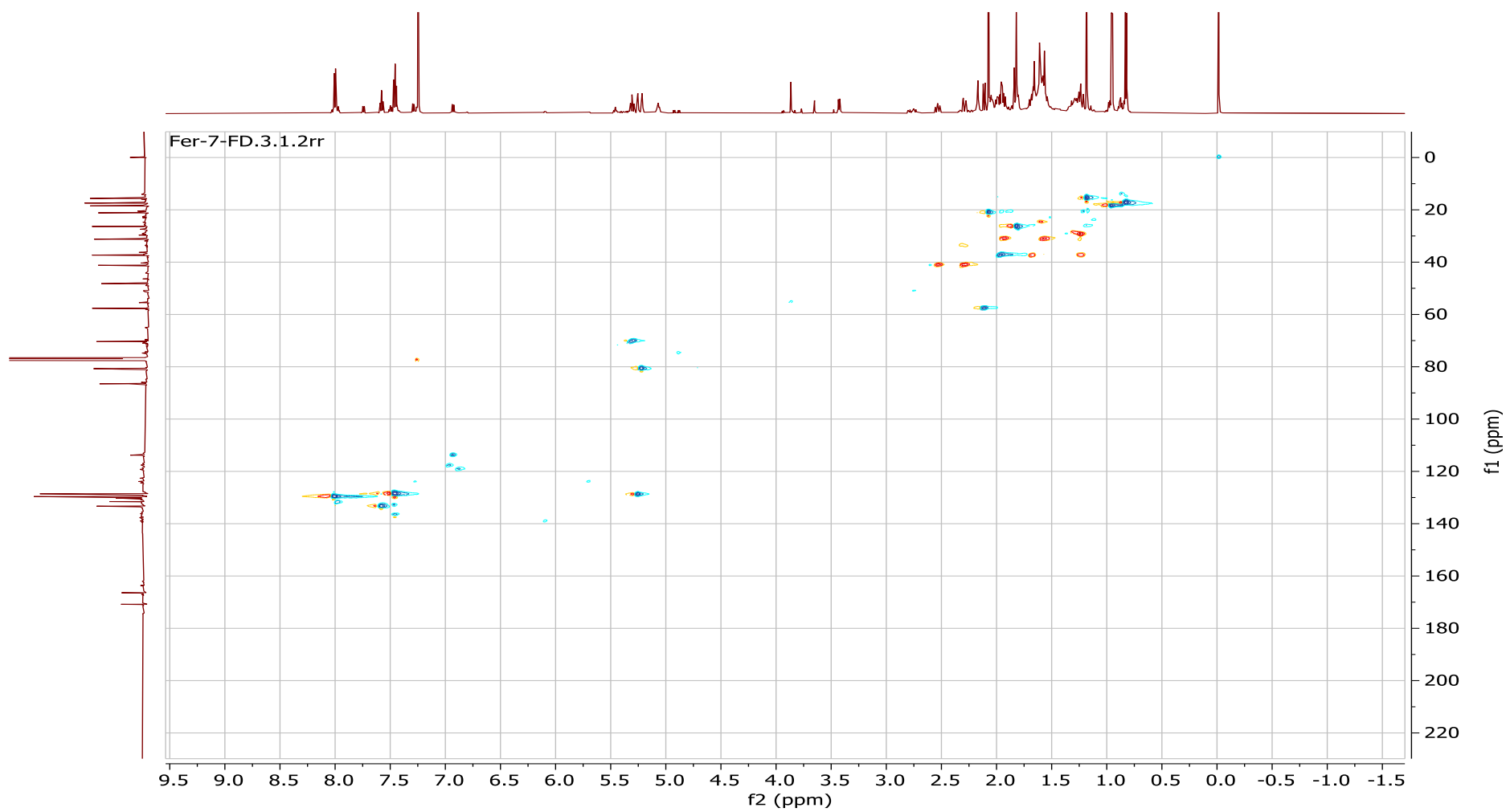
Figure S14:  $^1\text{H}$  NMR of **2** ( $\text{CDCl}_3$ , 500 Hz)



**Figure S15:**  $^{13}\text{C}$  NMR of **2** ( $\text{CDCl}_3$ , 125 Hz)



**FigureS16:** DEPT of 2



FigureS17: HSQC of 2

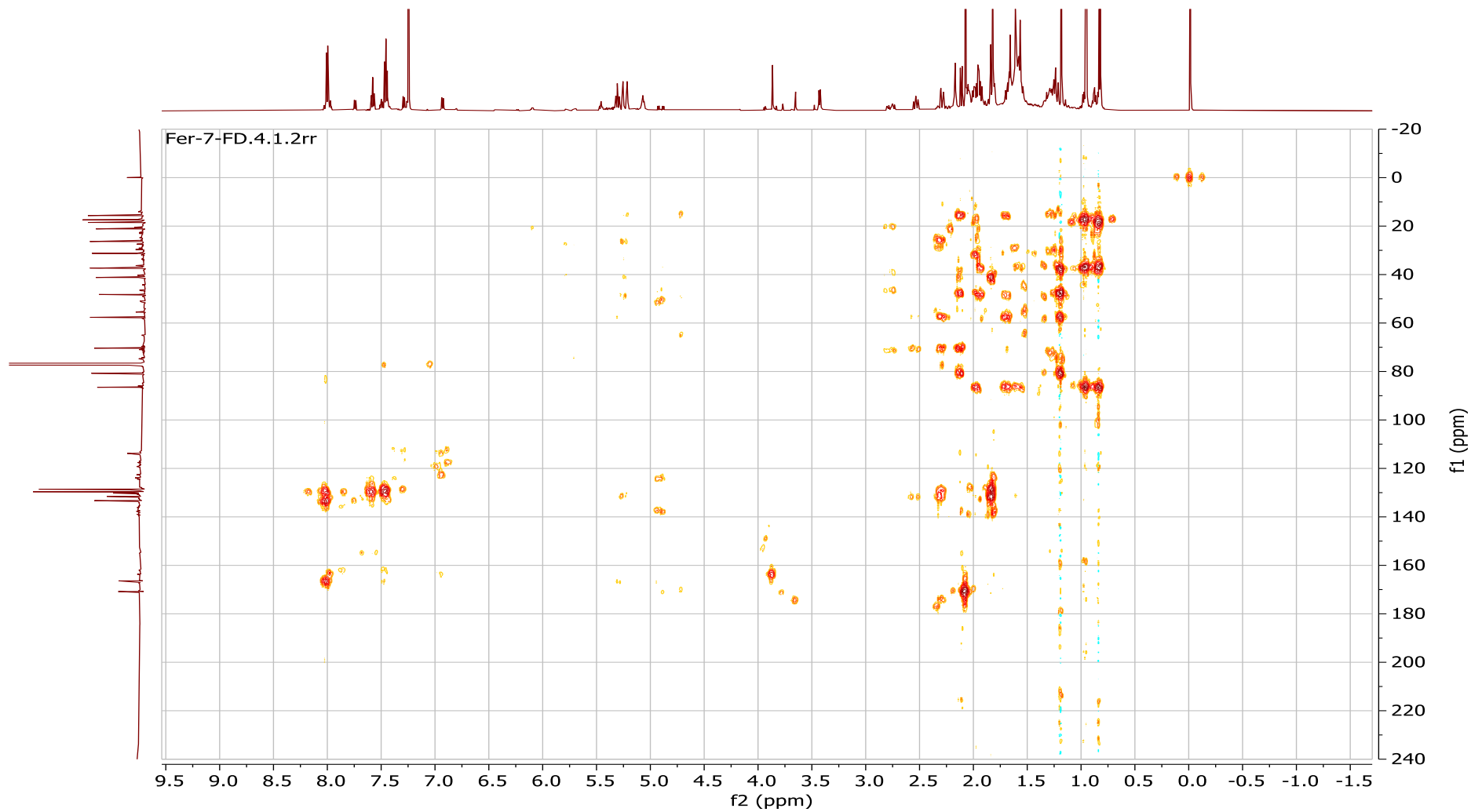
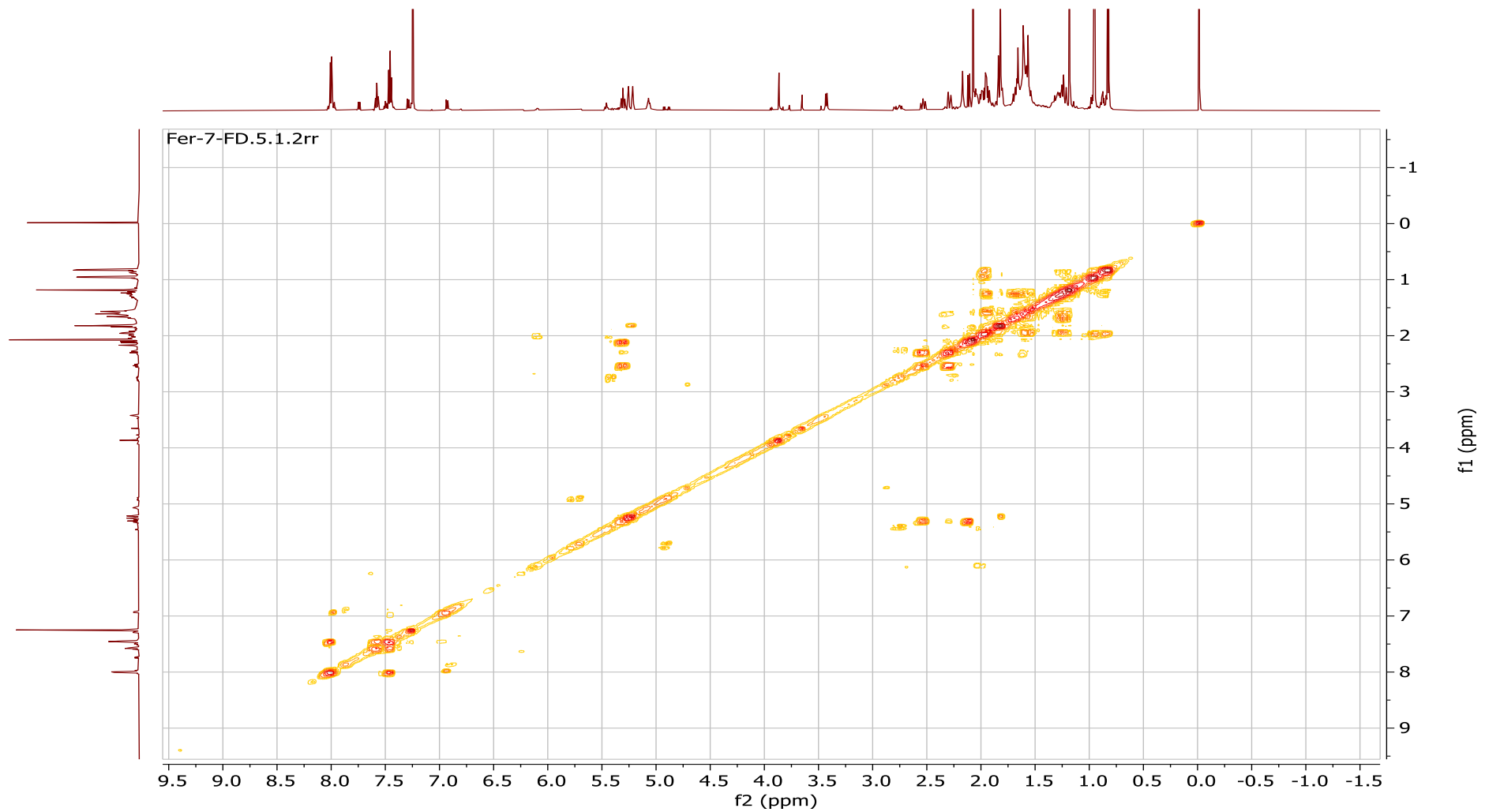


Figure S18: HMBC of 2



FigureS19:  $^1\text{H}$ - $^1\text{H}$  COSY of 2