

# Construction of five- and six-membered heterocycles on both Cp rings of ferrocene moiety of $\alpha$ -oxoketene-S,S-acetal and $\beta$ -oxodithioester via heteroaromatic annulation

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Department of Chemistry, Faculty of Science, Banaras Hindu University, Varanasi 221005, India

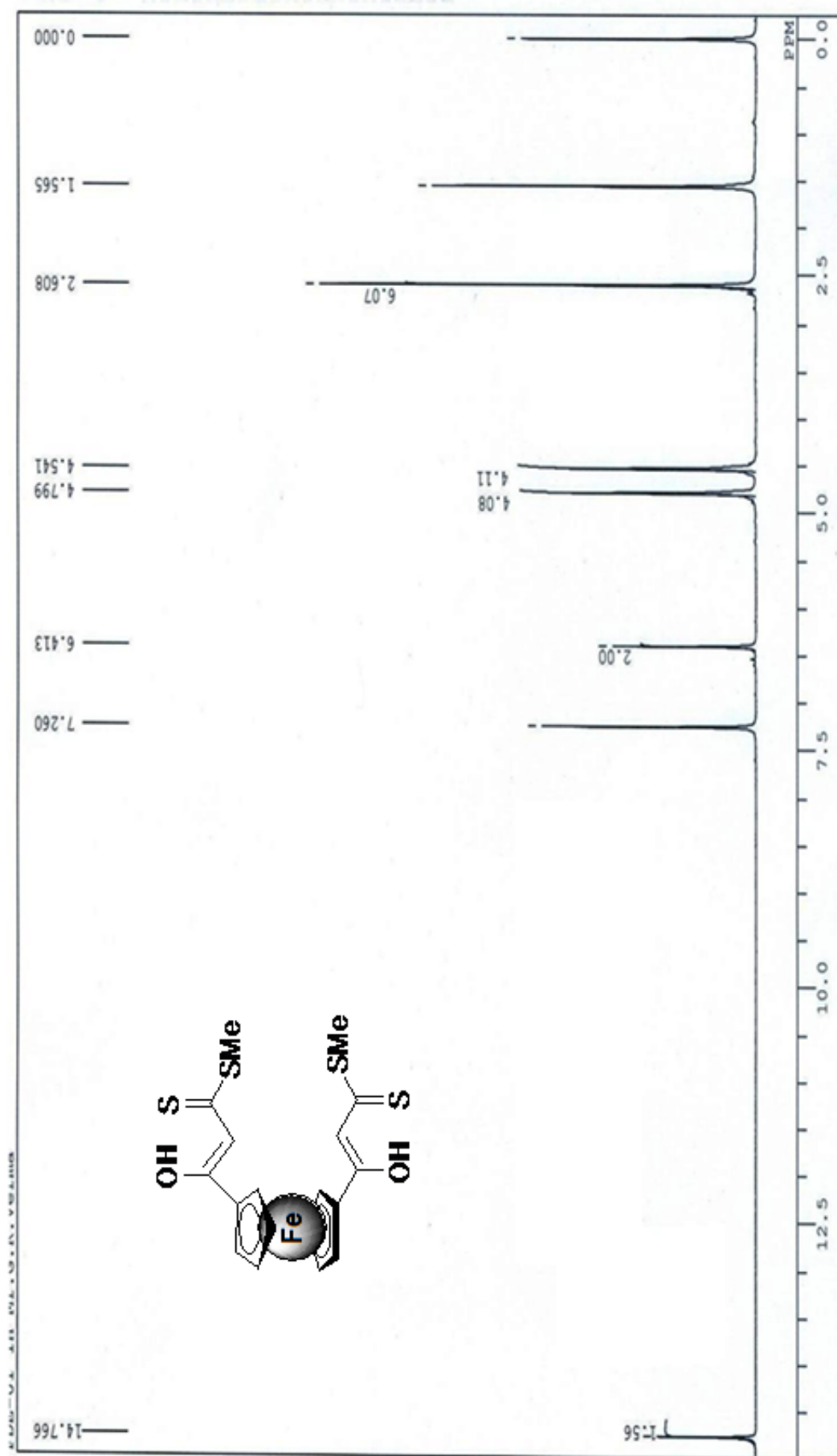
[mssinghbhu@yahoo.co.in](mailto:mssinghbhu@yahoo.co.in)

## *Supplementary Information*

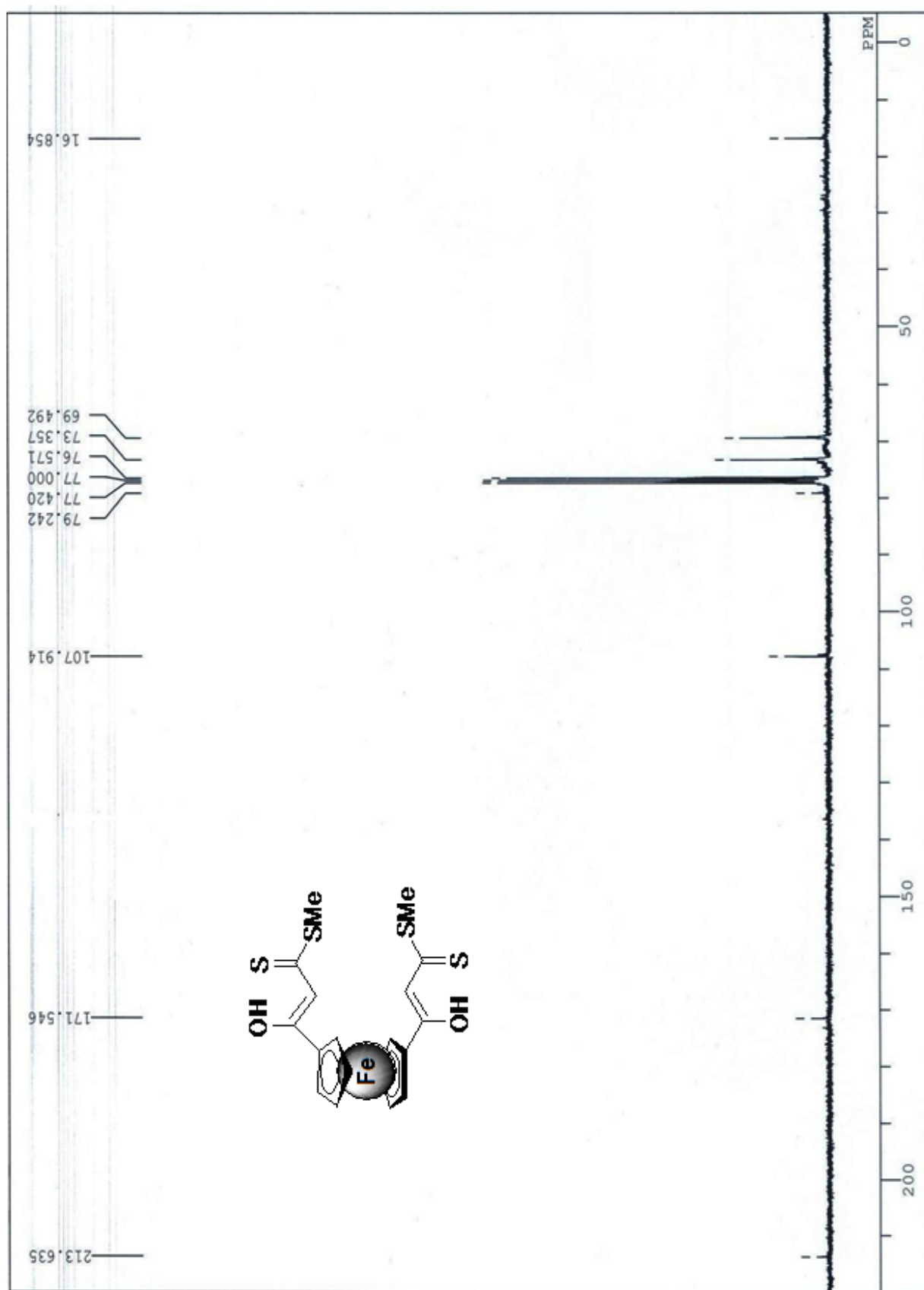
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$^1\text{H}$ , $^{13}\text{C}$ NMR, and HRMS Spectra of the starting materials and final products	S2
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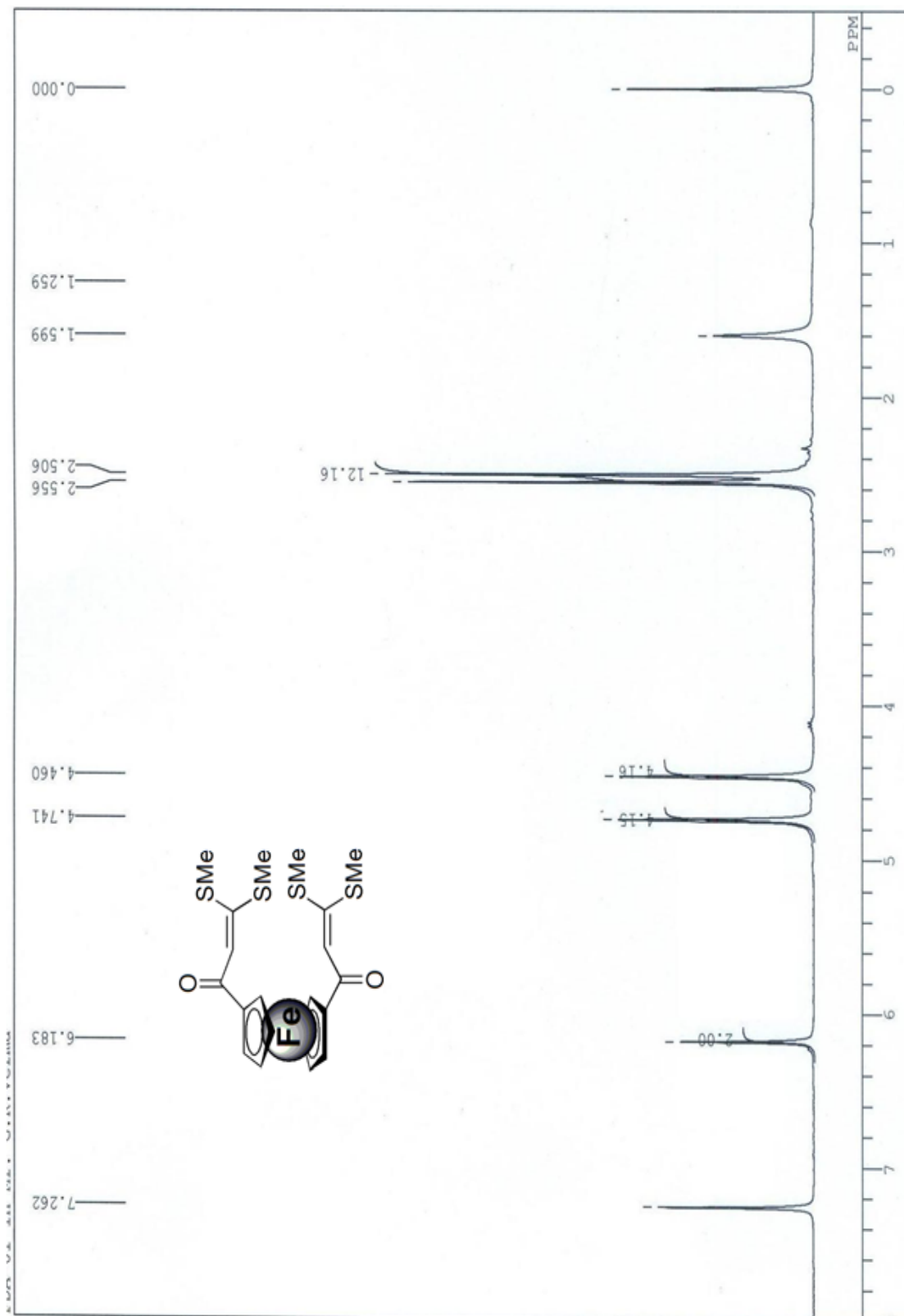
<sup>1</sup>H NMR Spectrum of 1,1'-Bis(methyl-3-hydroxy-prop-2-ene-dithioate)ferrocene 2



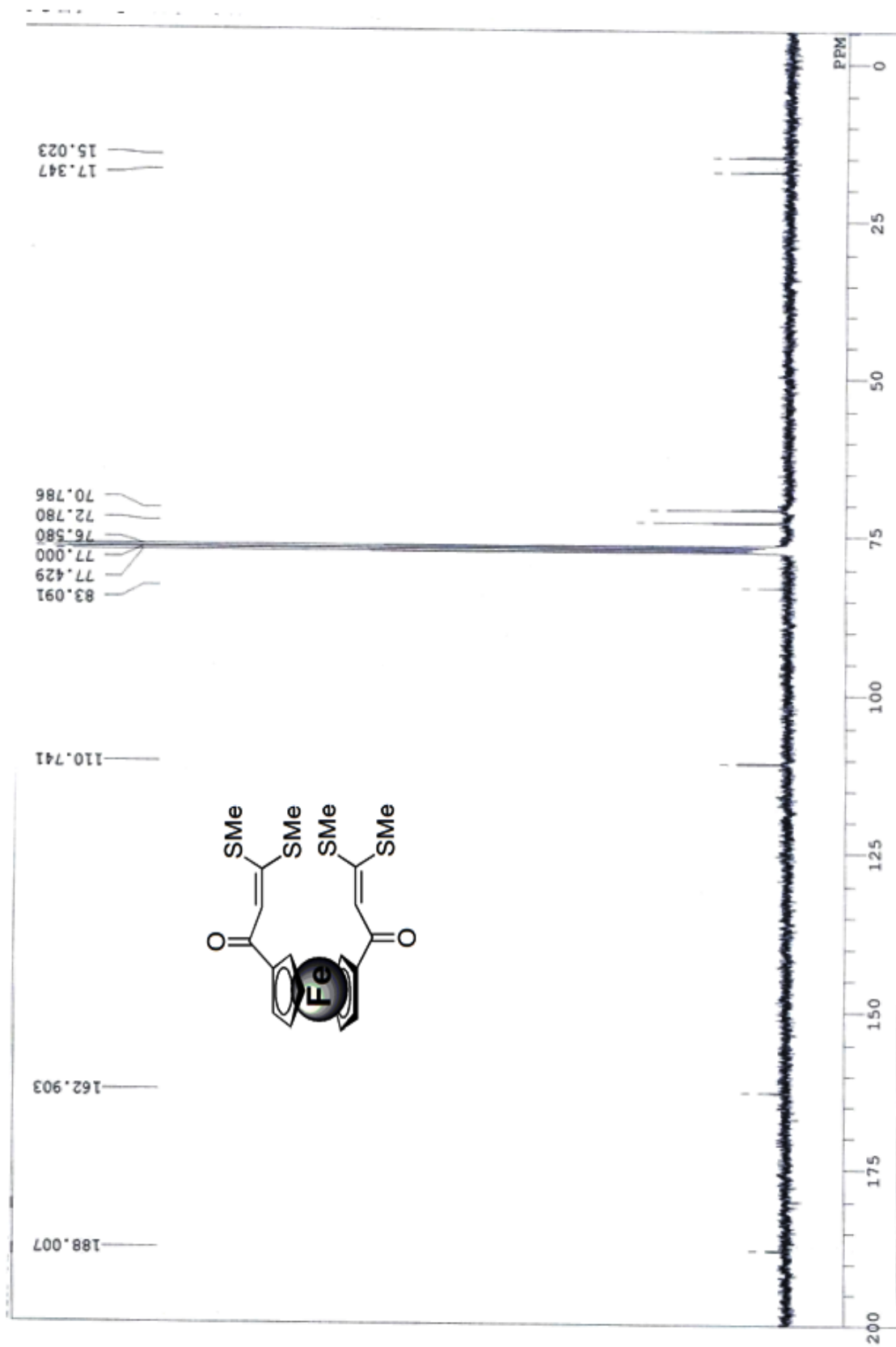
$^{13}\text{C}$  NMR Spectrum of 1,1'-Bis(methyl-3-hydroxy-prop-2-ene-dithioate)ferrocene 2



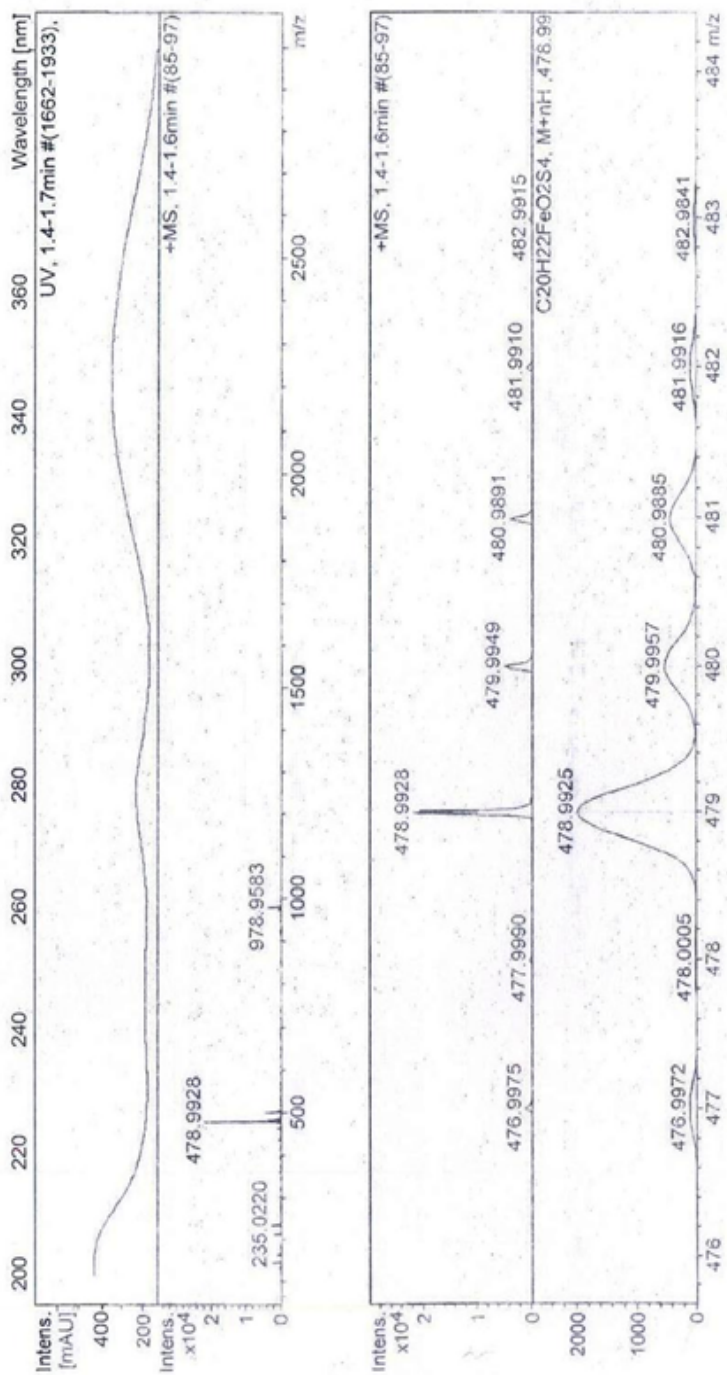
<sup>1</sup>H NMR Spectrum of 1,1'-Bis(1,1-dimethylsulfanyl-3-oxo-1-propene)ferrocene **3**



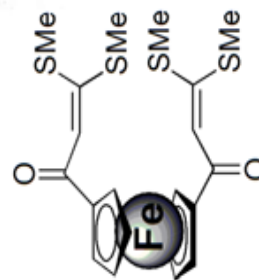
$^{13}\text{C}$  NMR Spectrum of 1,1'-Bis(1,1-dimethylsulfanyl-3-oxo-1-propene)ferrocene 3



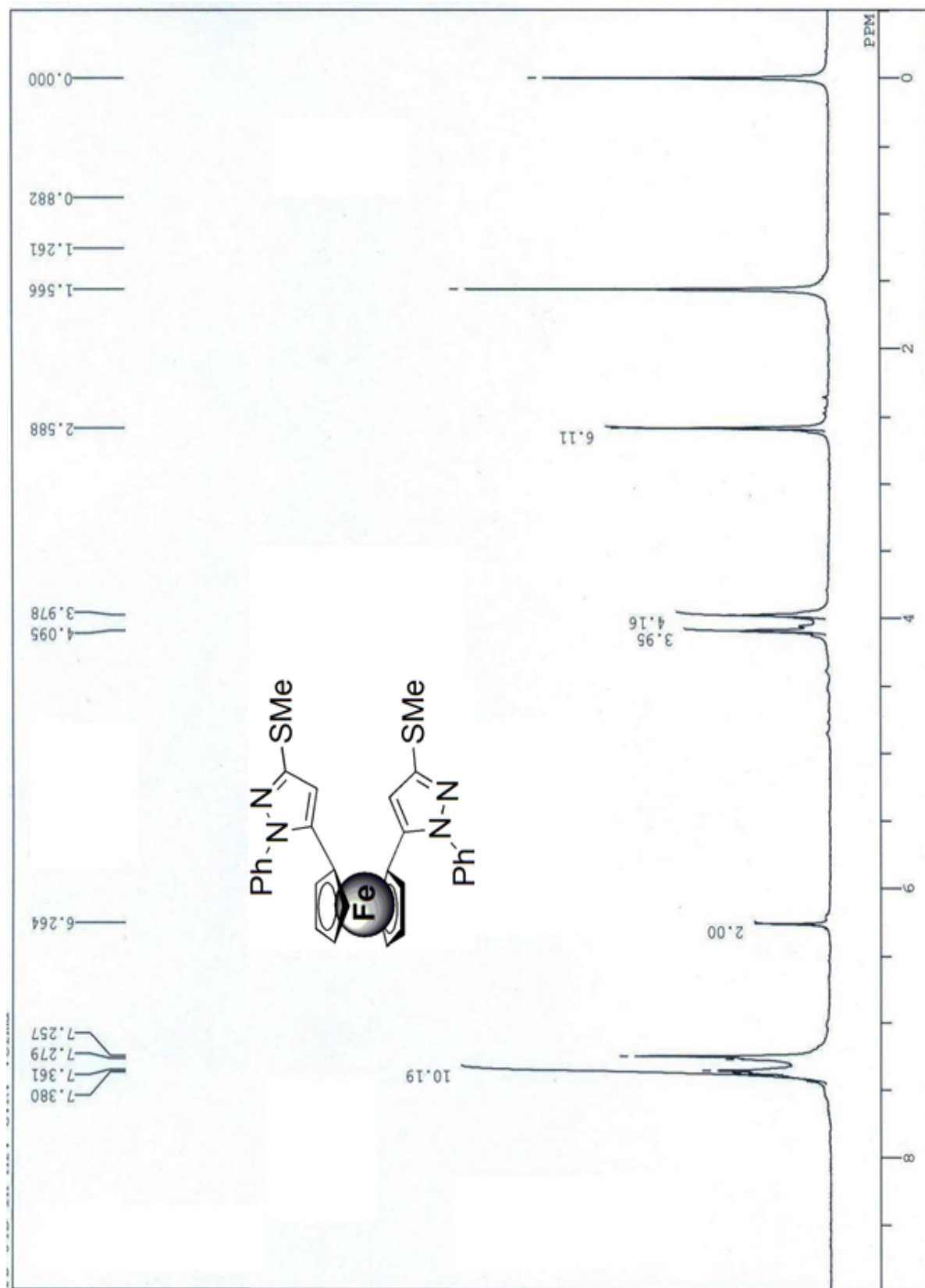
### LC-HRMS Spectrum of 1,1'-Bis(1,1-dimethylsulfanyl-3-oxo-1-propene)ferrocene 3



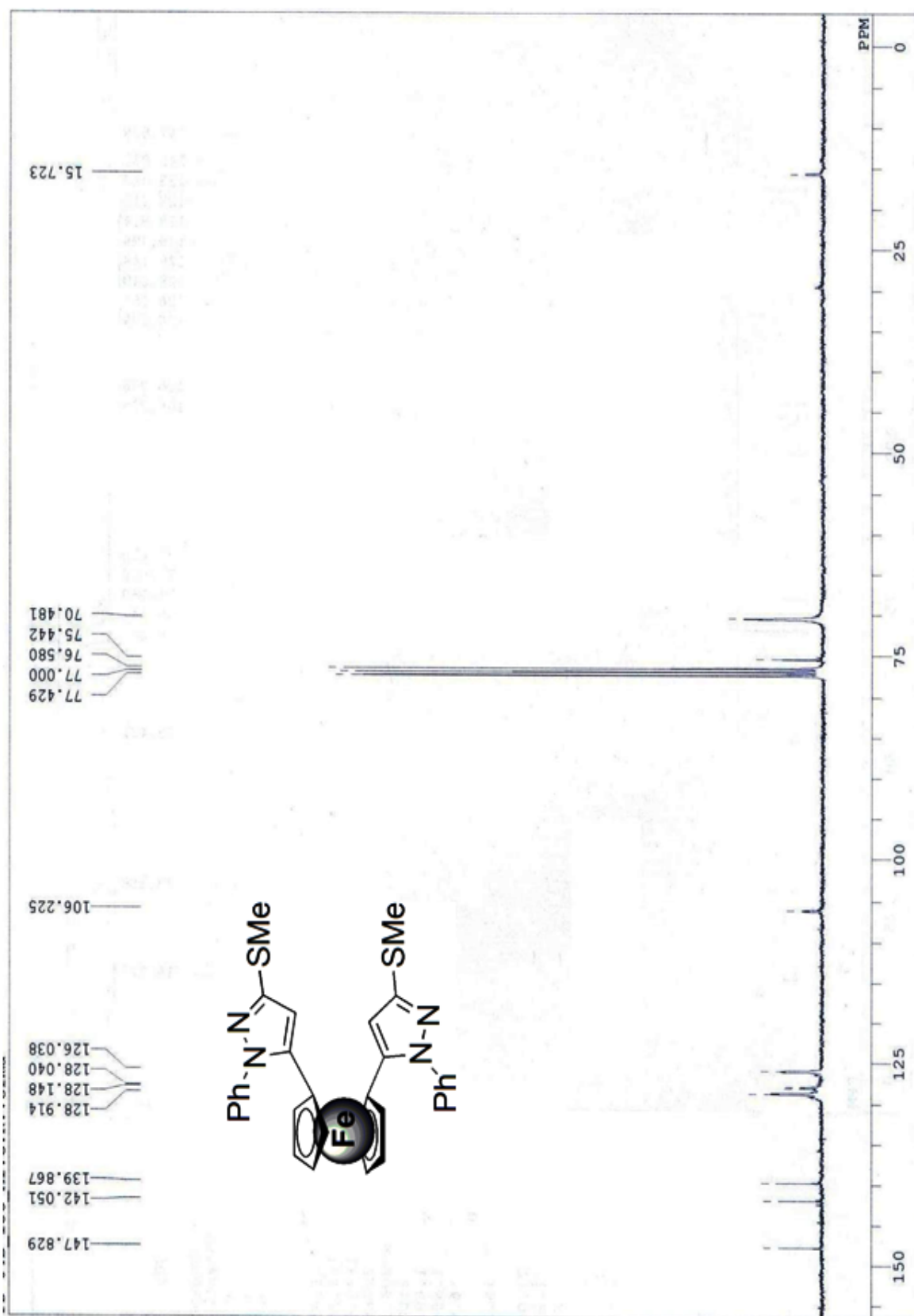
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<sup>1</sup>H NMR Spectrum of 1,1'-Bis(3-methylsulfanyl-1-phenyl-pyrazole-5-yl)ferrocene 4

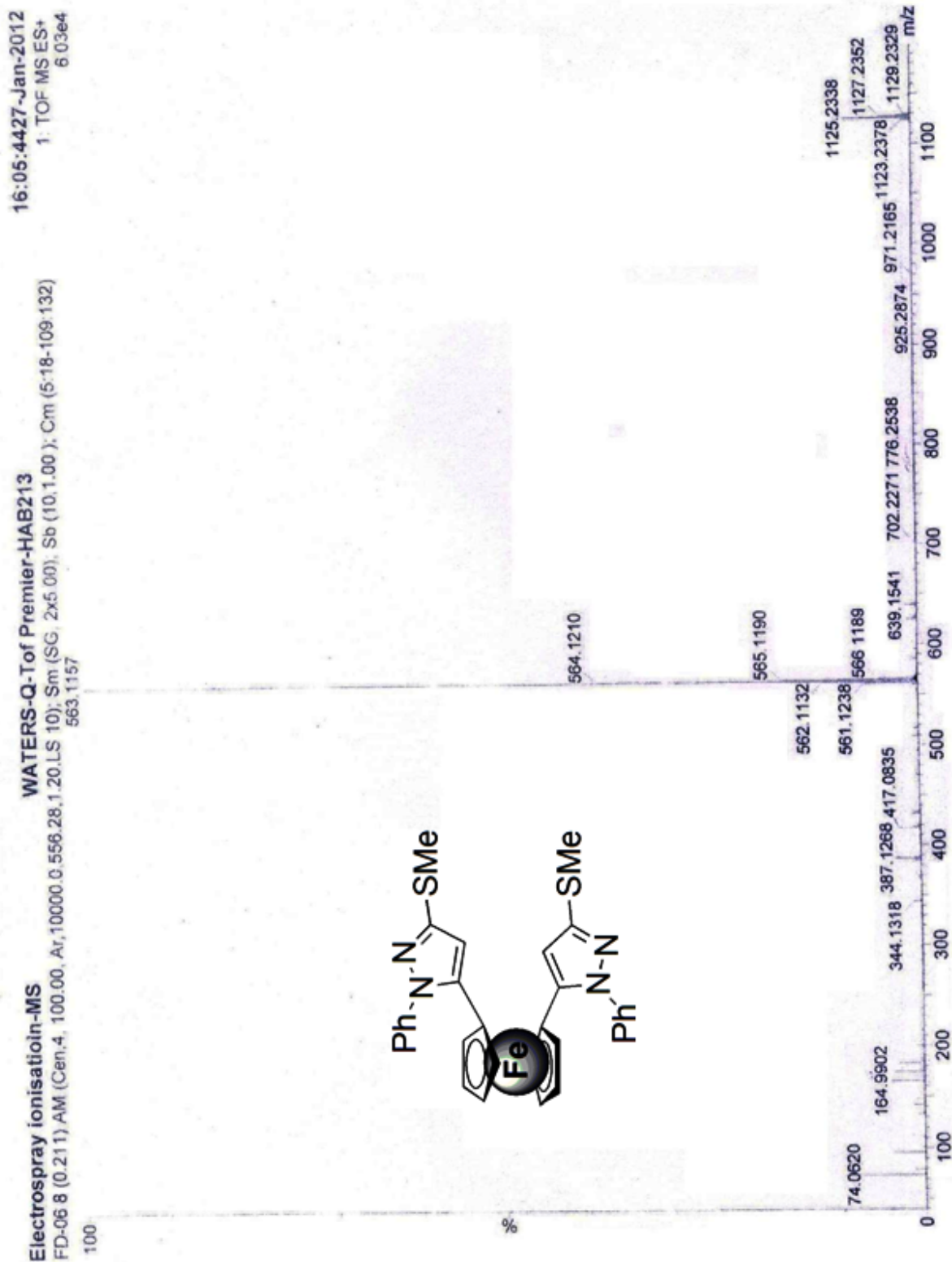


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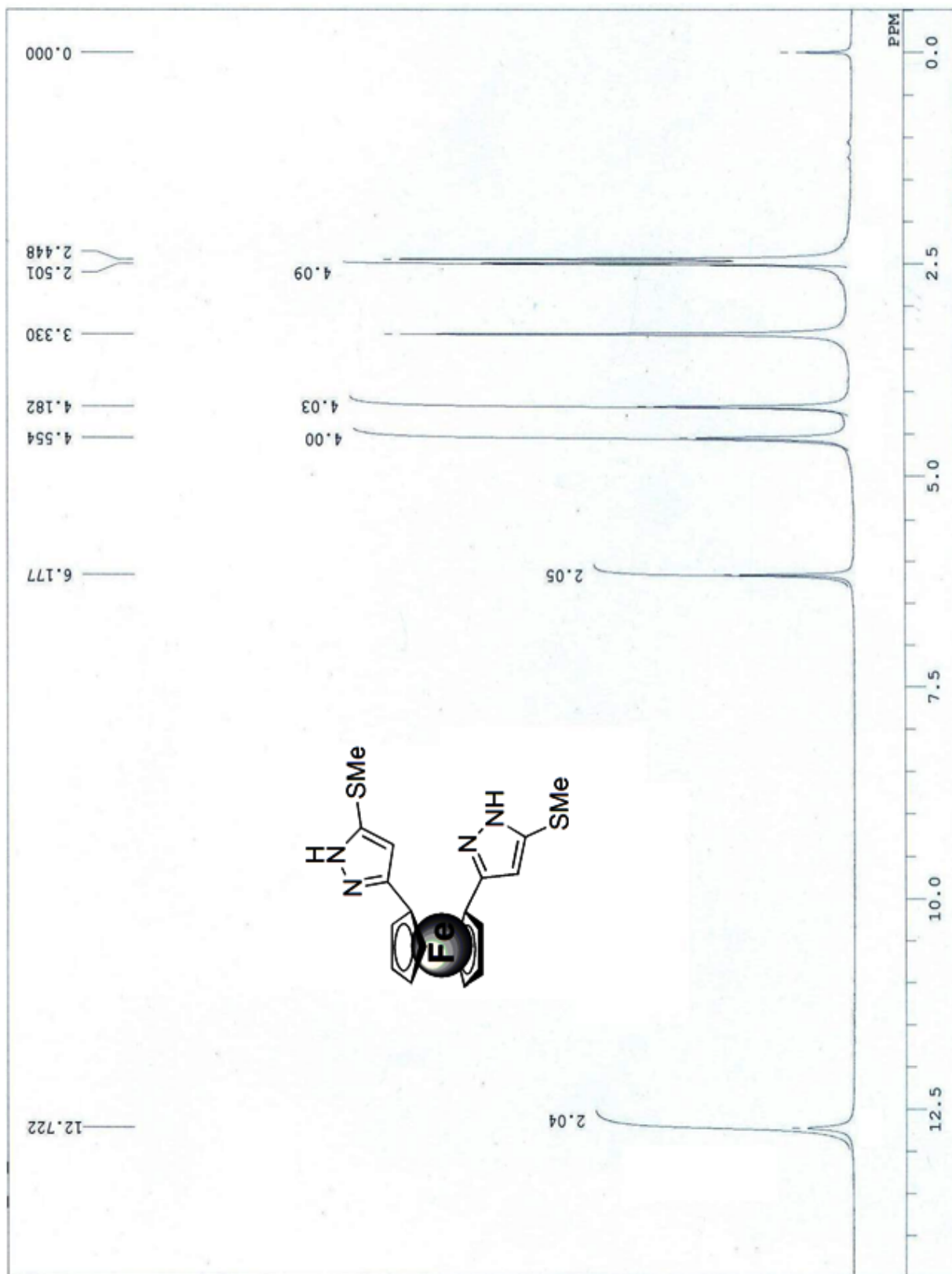




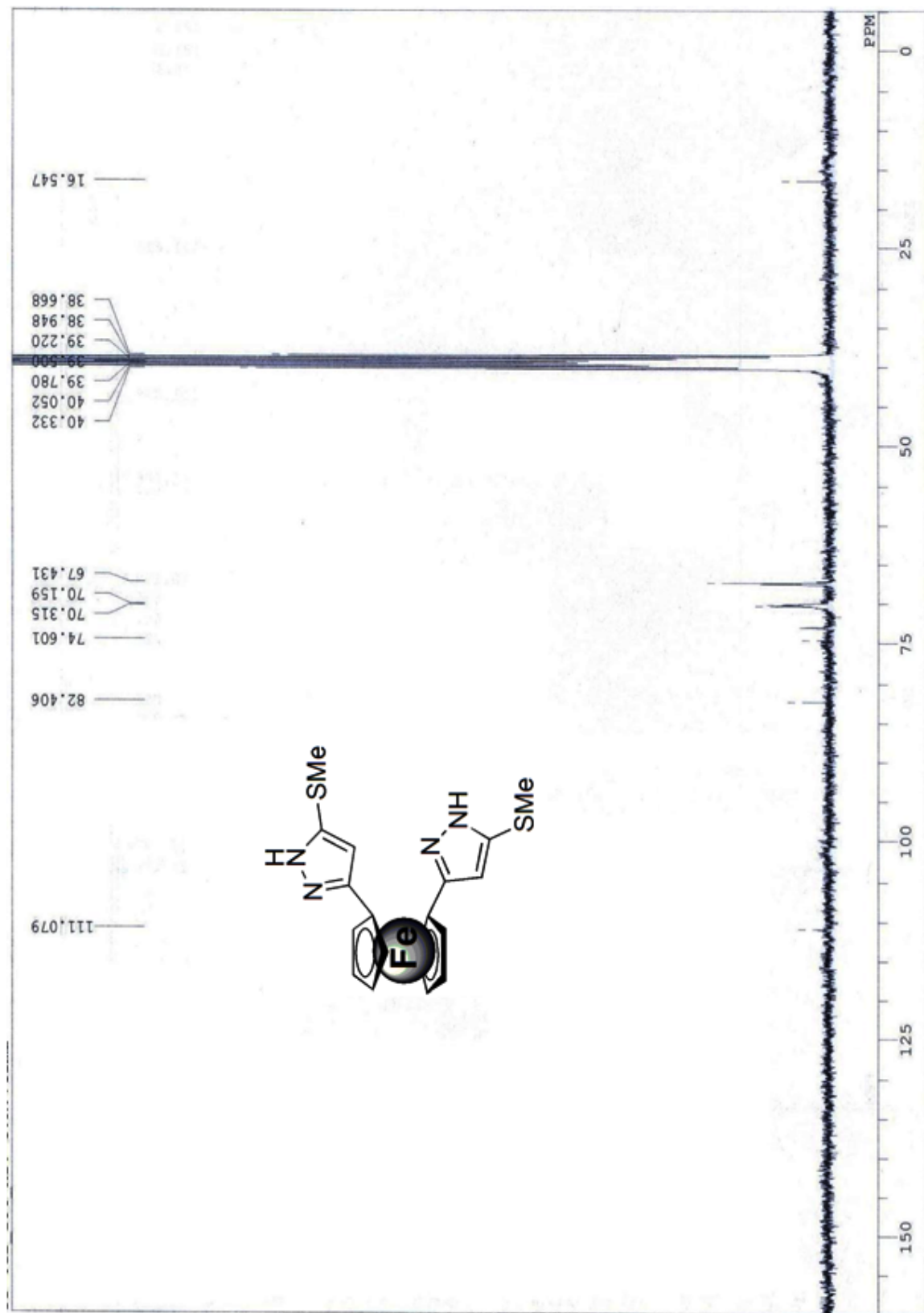
HRMS Spectrum of 1,1'-Bis(3-methylsulfanyl-1-phenyl-pyrazole-5-yl)ferrocene 4



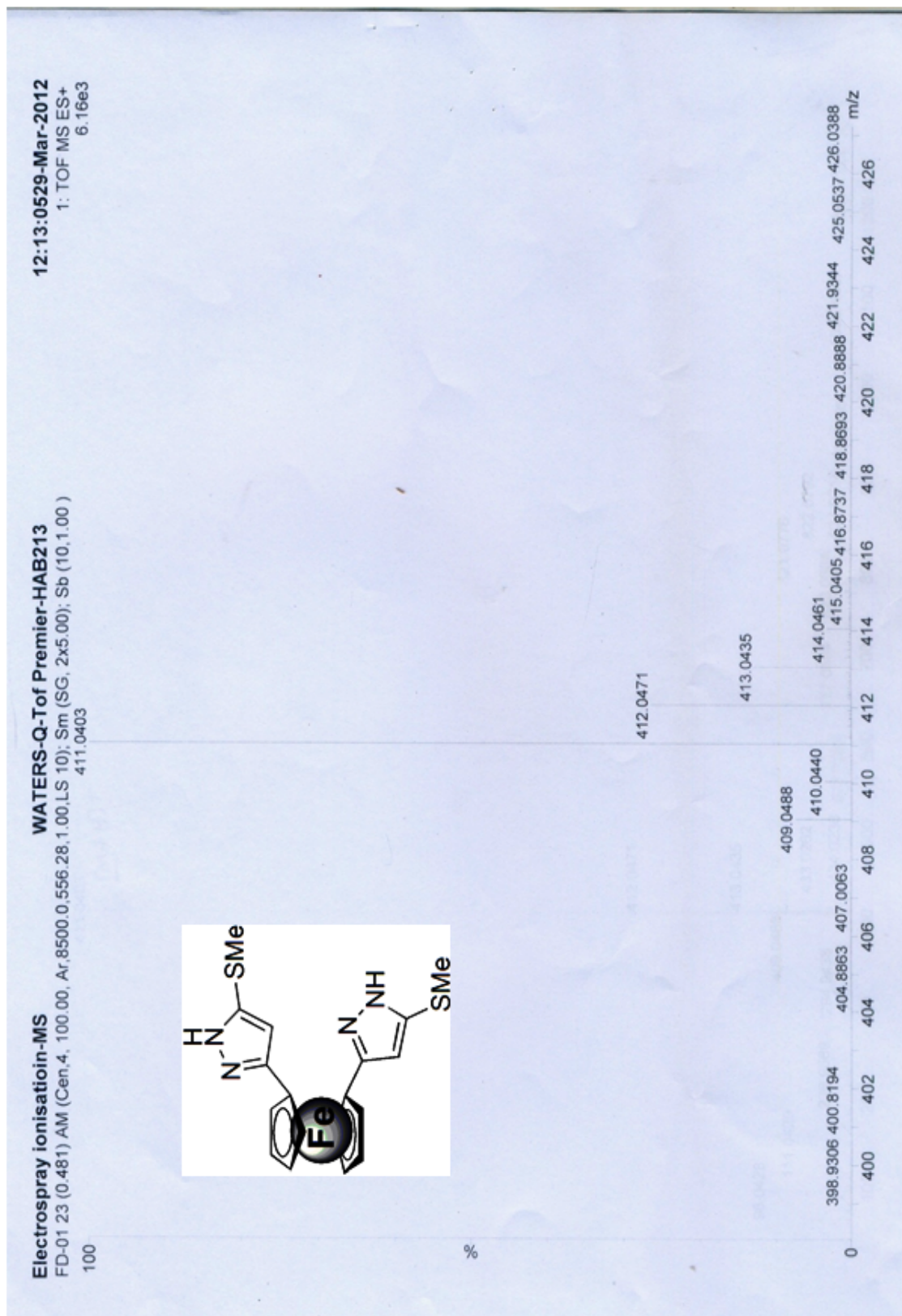
<sup>1</sup>H NMR Spectrum of 1,1'-Bis(3-methylsulfanyl-pyrazole-5-yl)ferrocene **5**



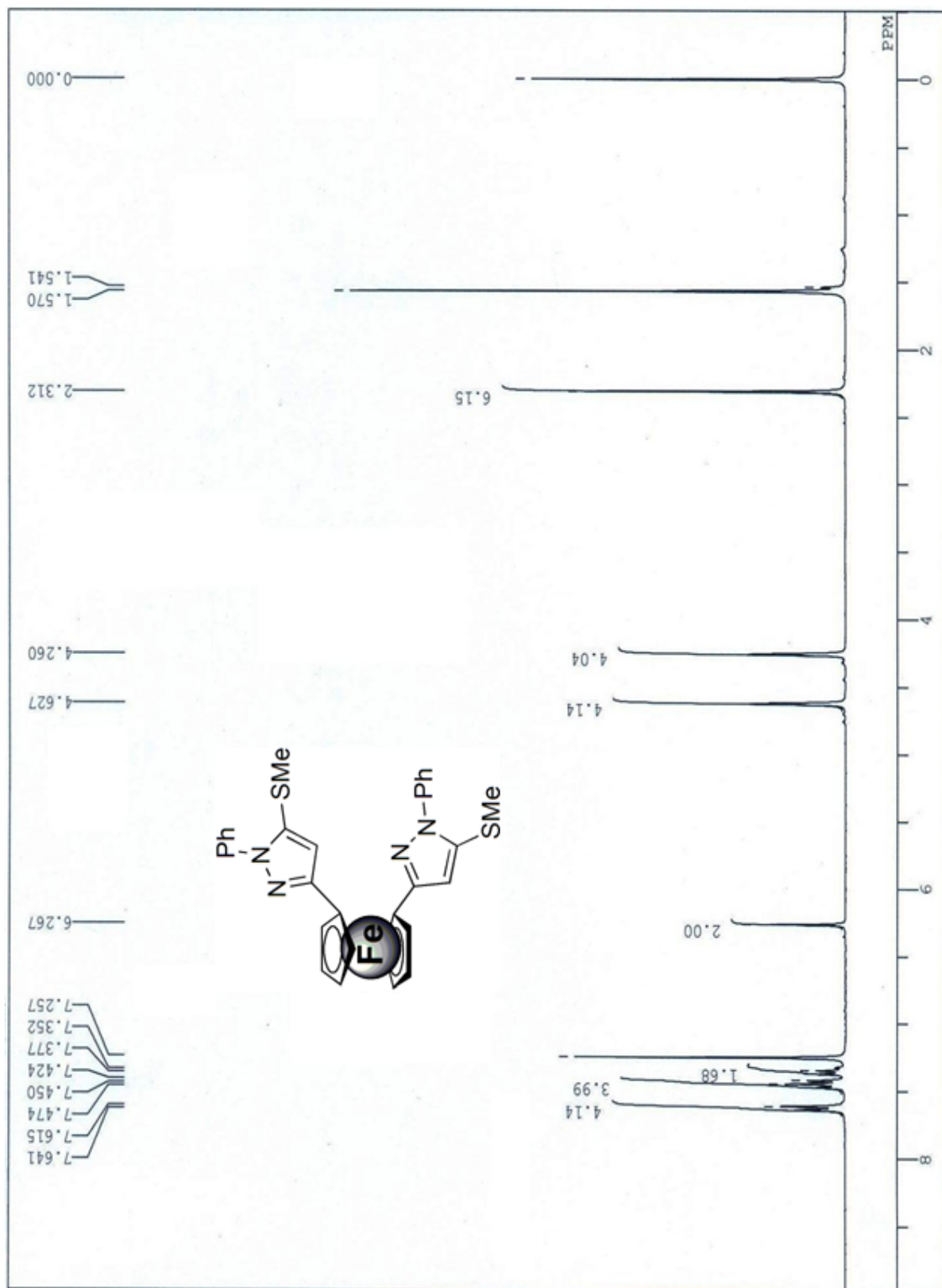
$^{13}\text{C}$  NMR Spectrum of 1,1'-Bis(3-methylsulfanyl-pyrazole-5-yl)ferrocene **5**



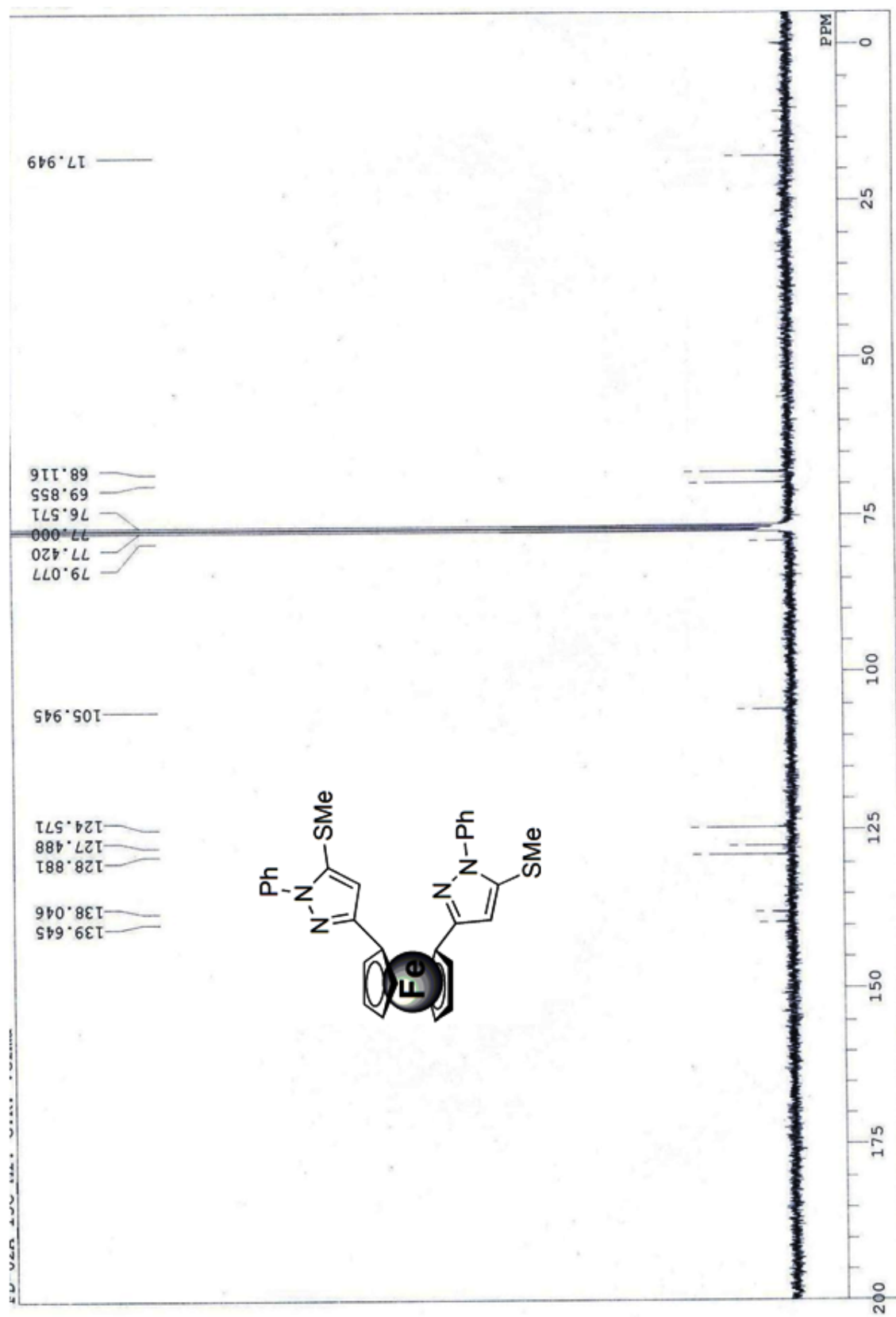
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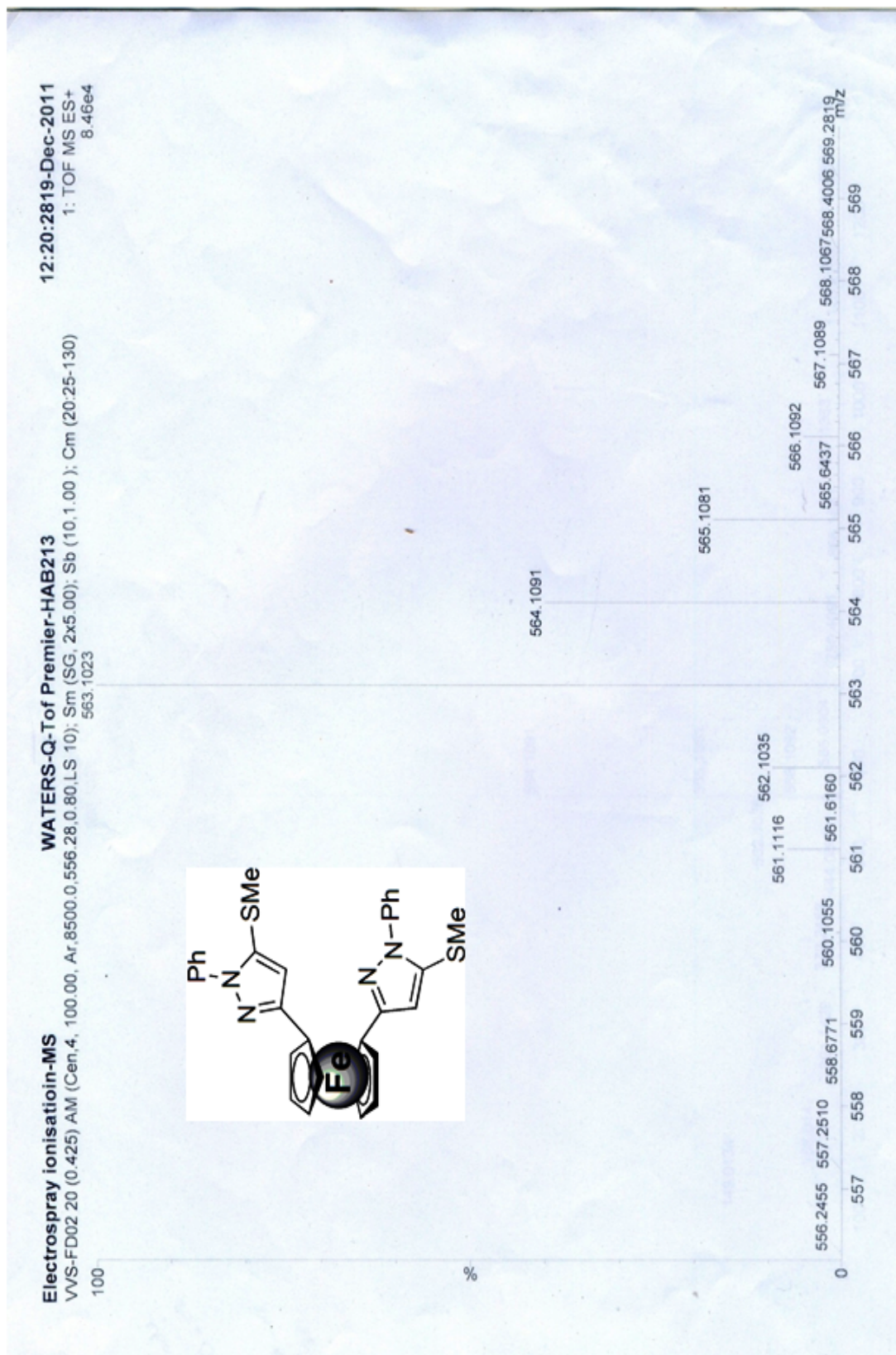
<sup>1</sup>H NMR Spectrum of 1,1'-Bis(5-methylsulfanyl-1-phenyl-pyrazole-3-yl)ferrocene 6



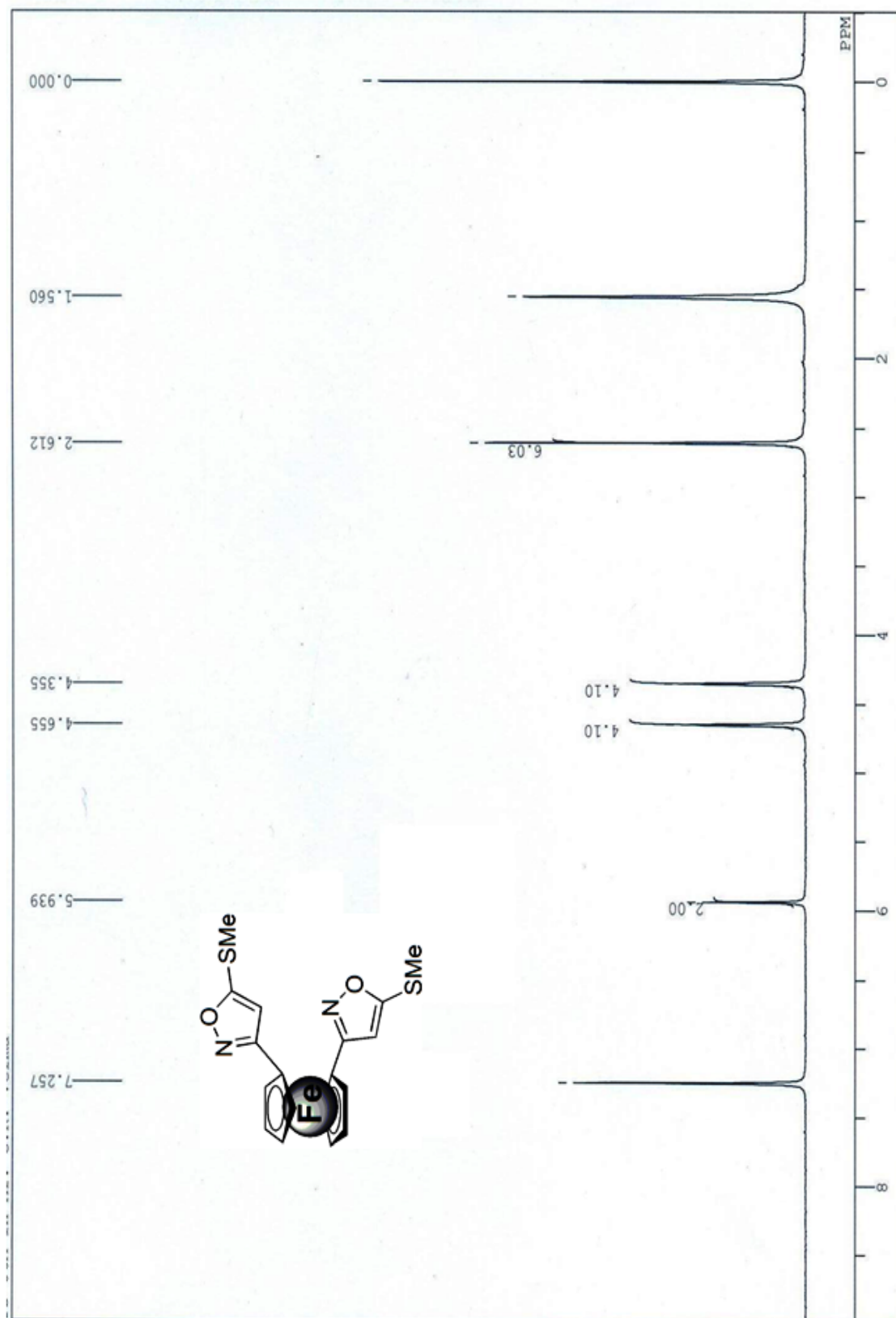
$^{13}\text{C}$  NMR Spectrum of 1,1'-Bis(5-methylsulfanyl-1-phenyl-pyrazole-3-yl)ferrocene **6**



HRMS Spectrum of 1,1'-Bis(5-methylsulfanyl-1-phenyl-pyrazole-3-yl)ferrocene **6**

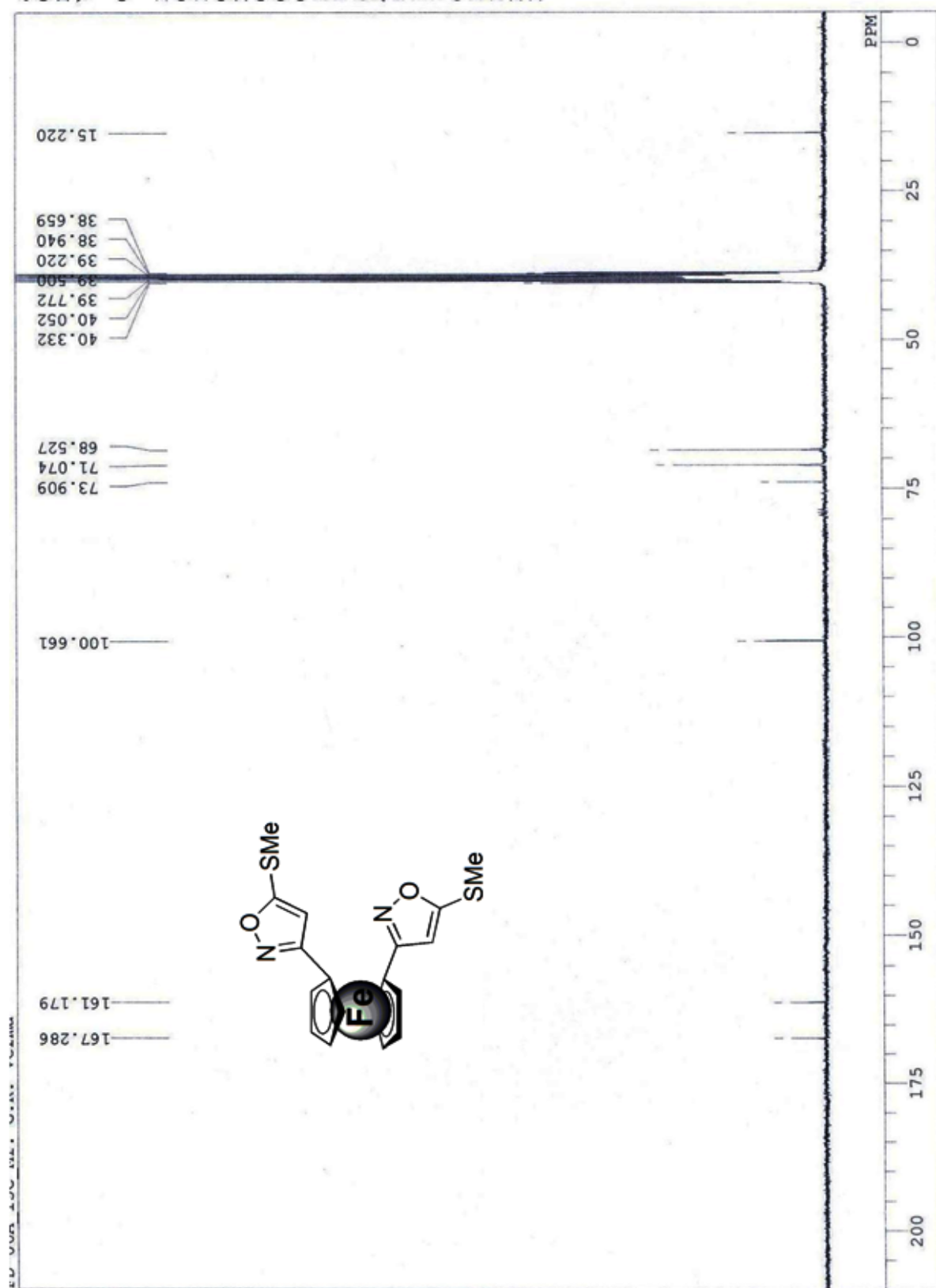


<sup>1</sup>H NMR Spectrum of 1,1'-Bis(5-methylsulfanyl-isoxazole-3-yl)ferrocene 7

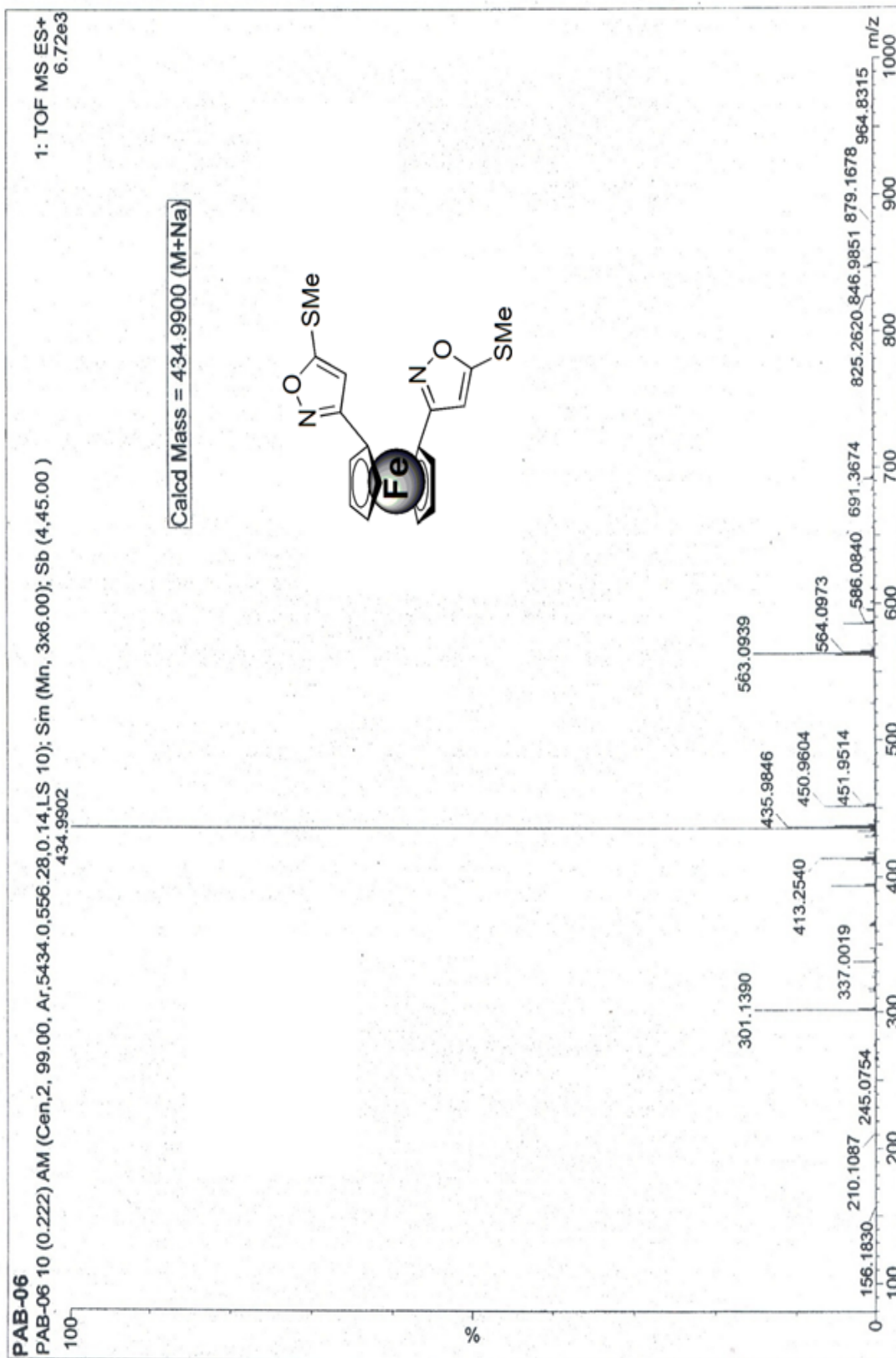




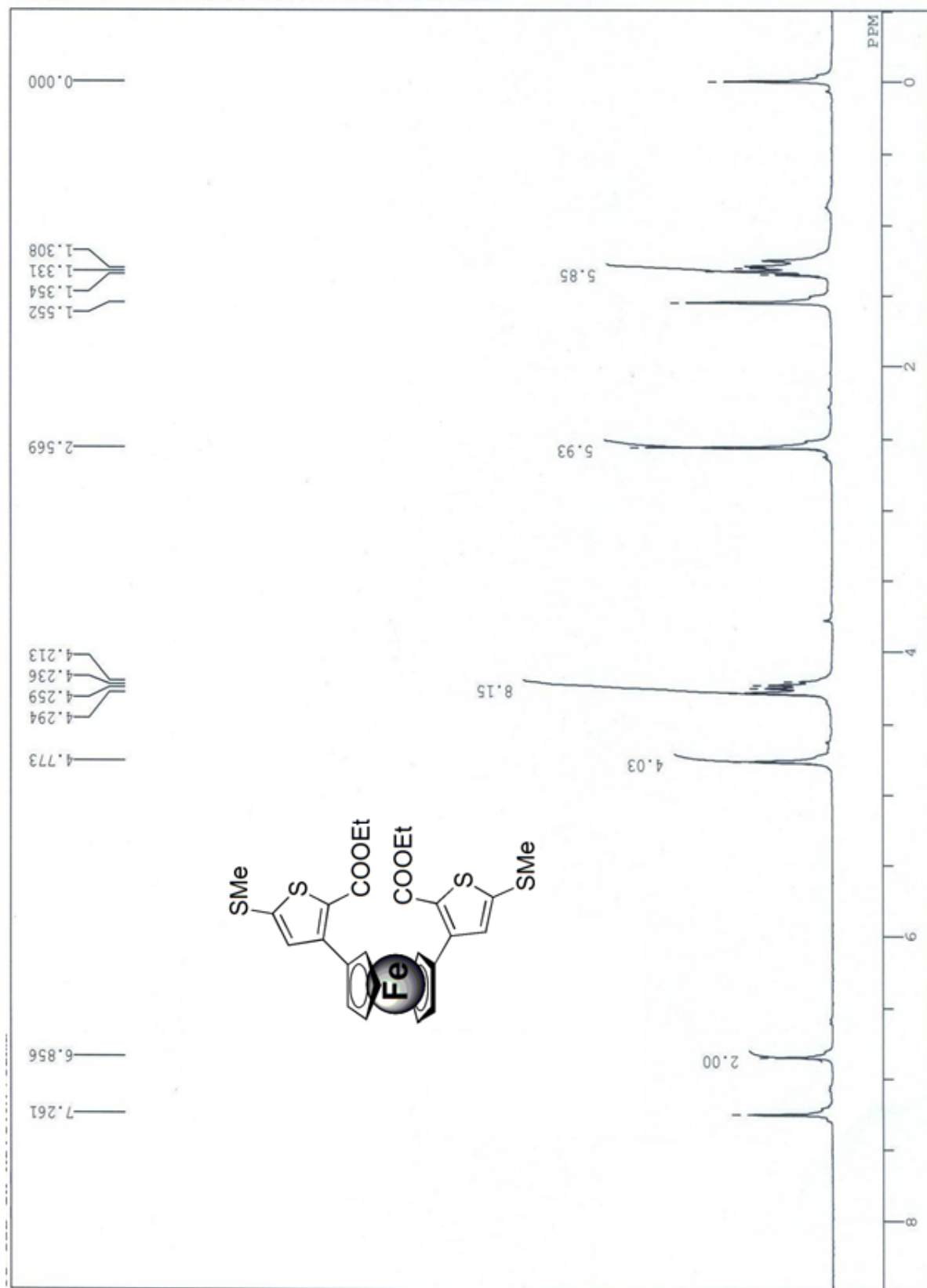
$^{13}\text{C}$  NMR Spectrum of 1,1'-Bis(5-methylsulfanyl-isoxazole-3-yl)ferrocene 7



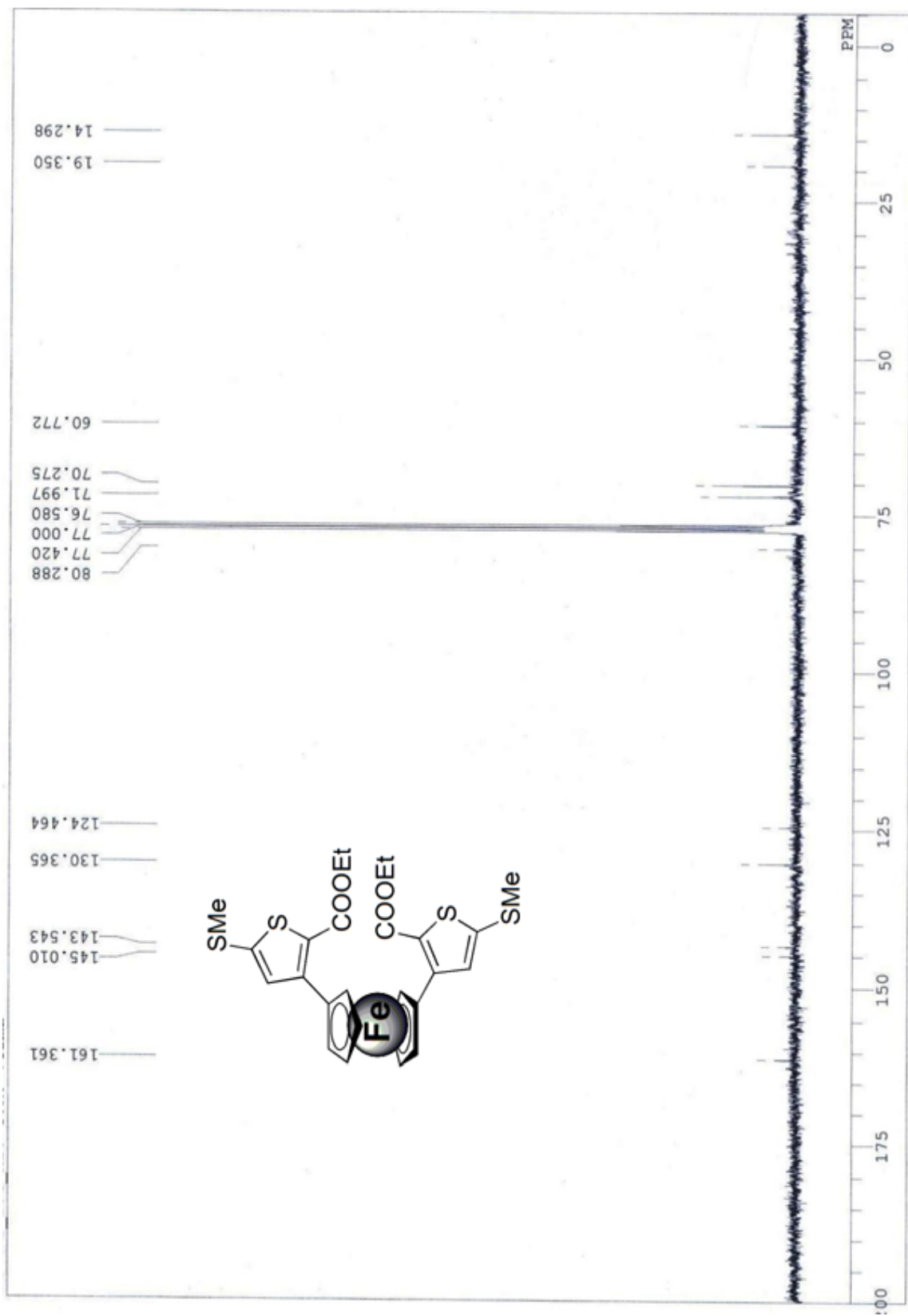
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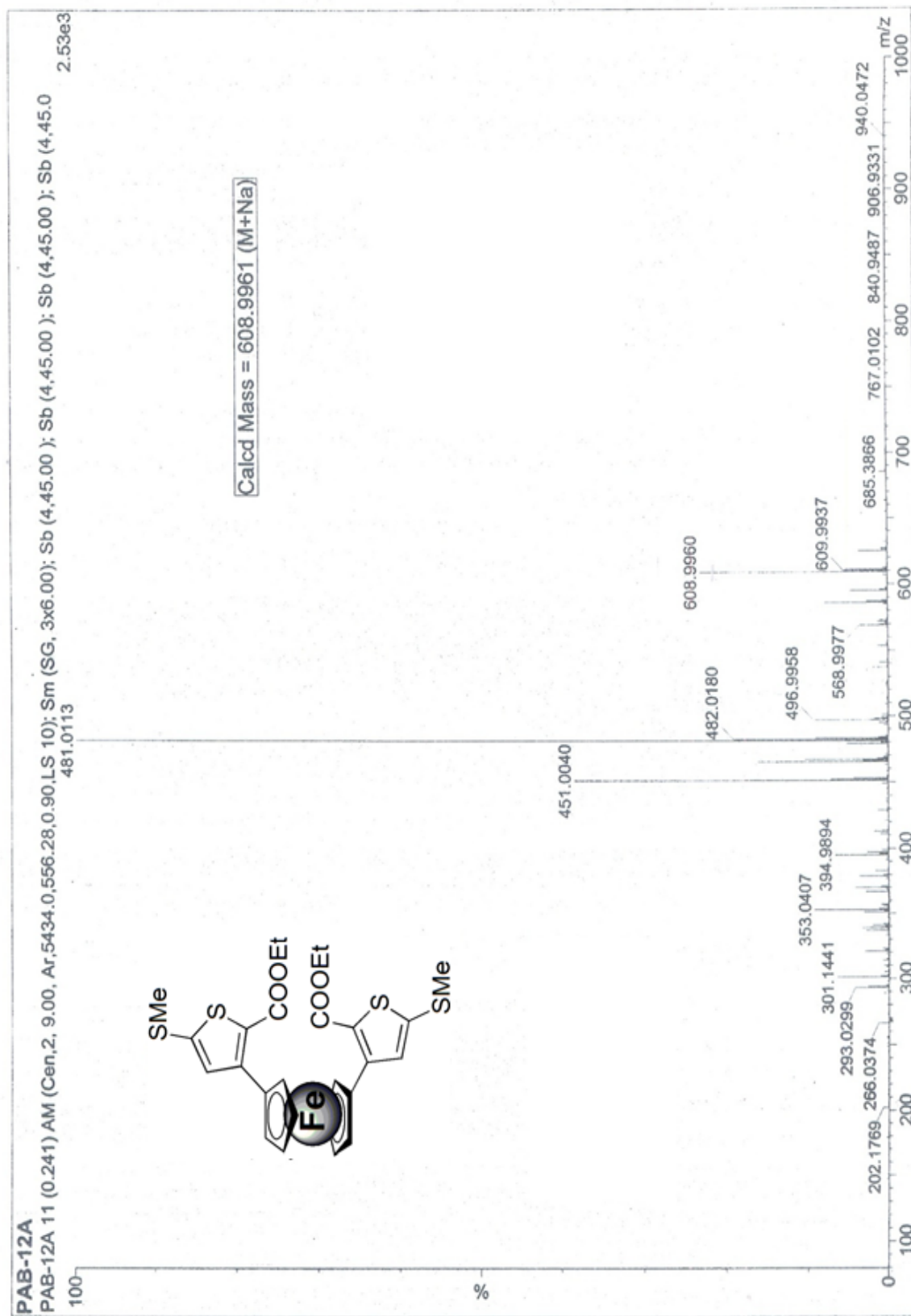
<sup>1</sup>H NMR Spectrum of 1,1'-Bis(5-methylsulfanyl-2-carboethoxy-thiophene-3-yl)ferrocene 9



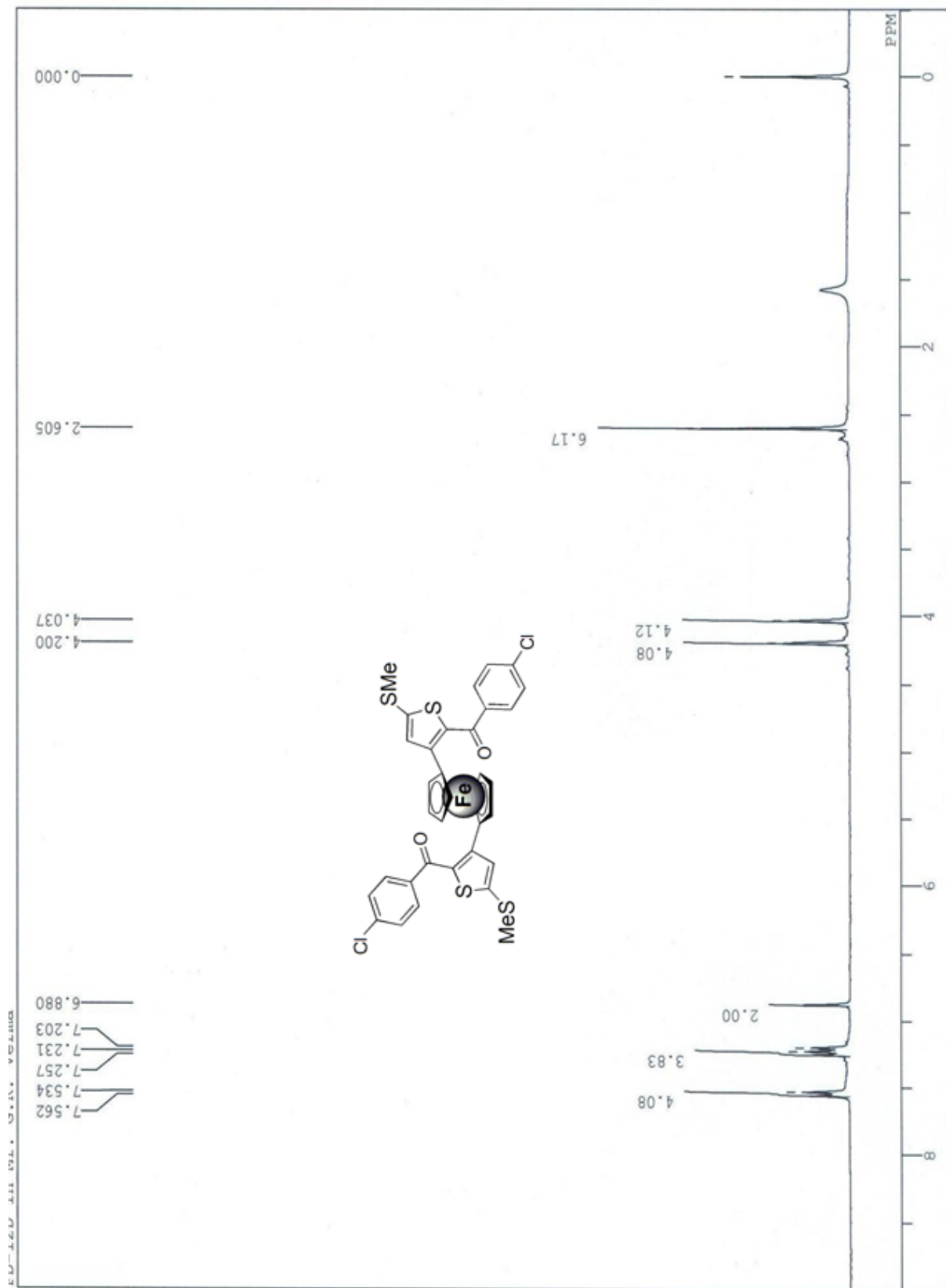
$^{13}\text{C}$  NMR Spectrum of 1,1'-Bis(5-methylsulfanyl-2-carboethoxy-thiophene-3-yl)ferrocene **9**



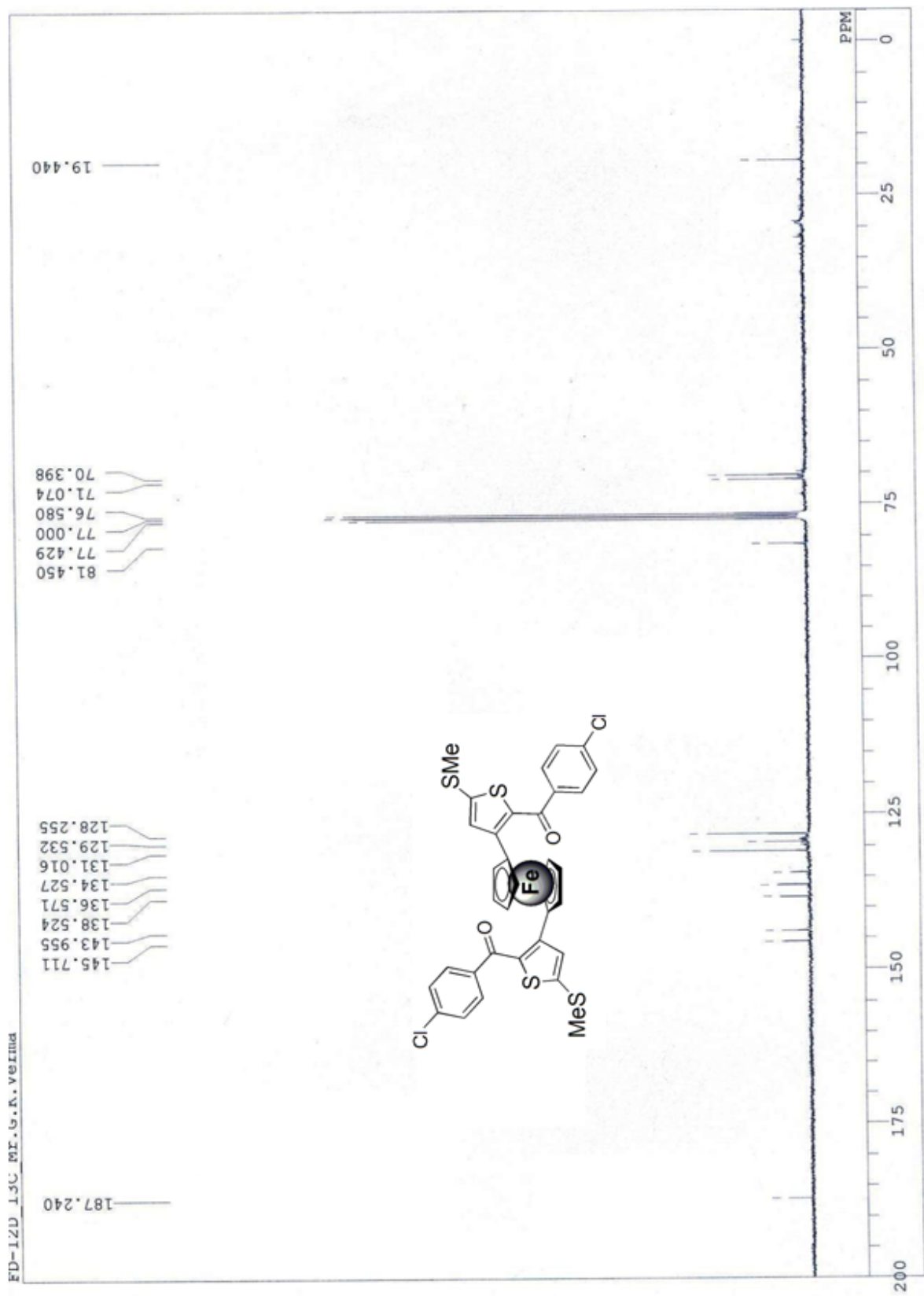
HRMS Spectrum of 1,1'-Bis(5-methylsulfanyl-2-carboethoxy-thiophene-3-yl)ferrocene 9



<sup>1</sup>H NMR Spectrum of 1,1'-Bis(2-(4-Chlorobenzoyl)-5-methylsulfanyl-thiophene-3-yl)ferrocene 10



$^{13}\text{C}$  NMR Spectrum of 1,1'-Bis(2-(4-Chlorobenzoyl)-5-methylsulfanyl-thiophene-3-yl)ferrocene 10



Elemental Composition Report

Single Mass Analysis (displaying only valid results)

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0

Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions

84 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

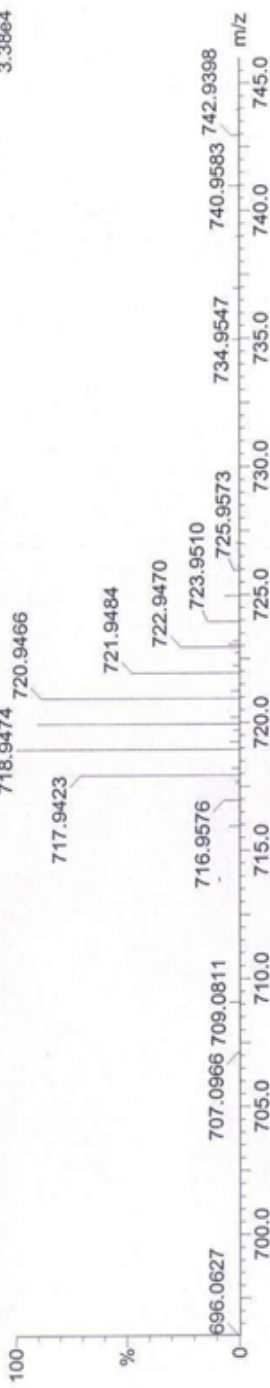
Micromass : Q-ToF micro (YA-105)  
 C34H24Cl2FeO2S4

Dept. Of Chemistry I.I.T.(B)

11-Feb-2012 16:20:45

INN-FD-12D 17 (0.170) AM (Cen.5, 80.00, Ar.5000.0,556.28,1.00); Sb (5,40.00 ); Cm (10:44)

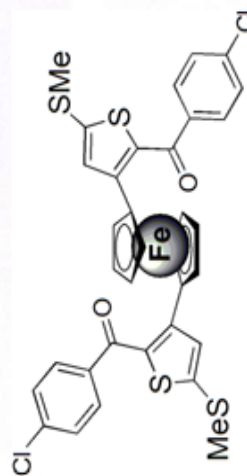
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Minimum:  
 Maximum:

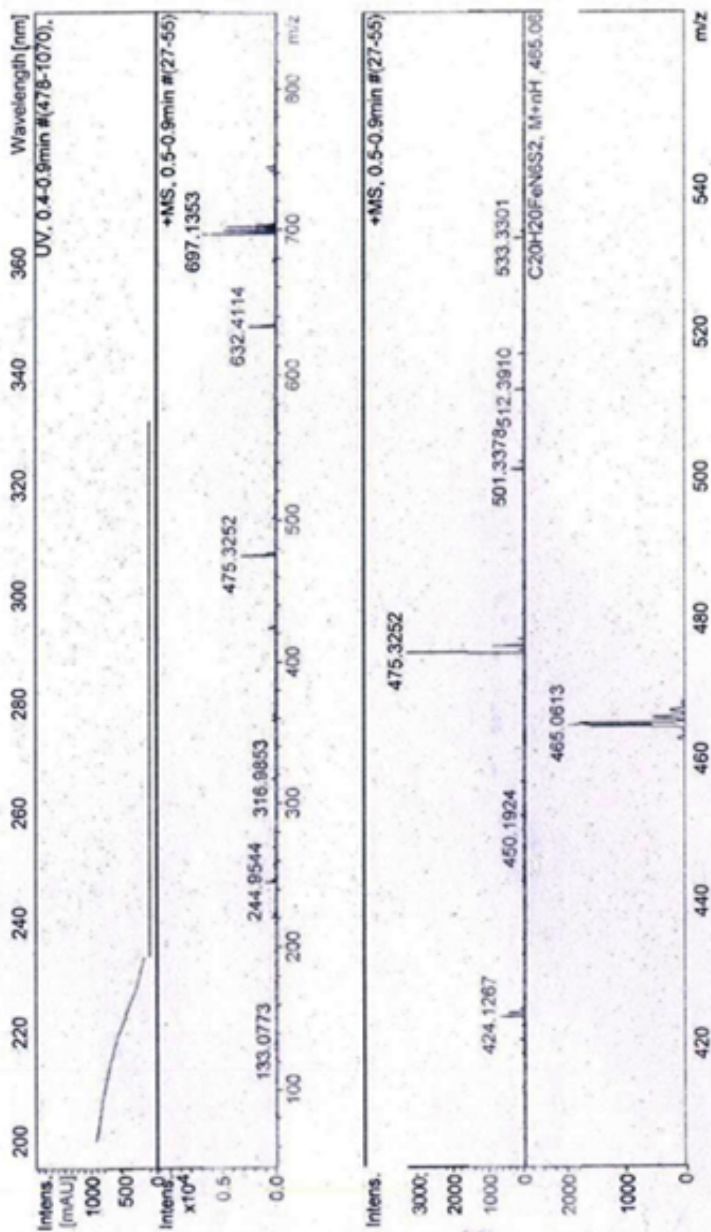
-1.5  
 100.0

Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
718.9474	718.9464	1.0	1.4	21.5	1	C34 H25 O2 Cl2 S4 Fe

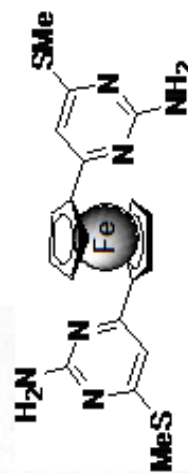




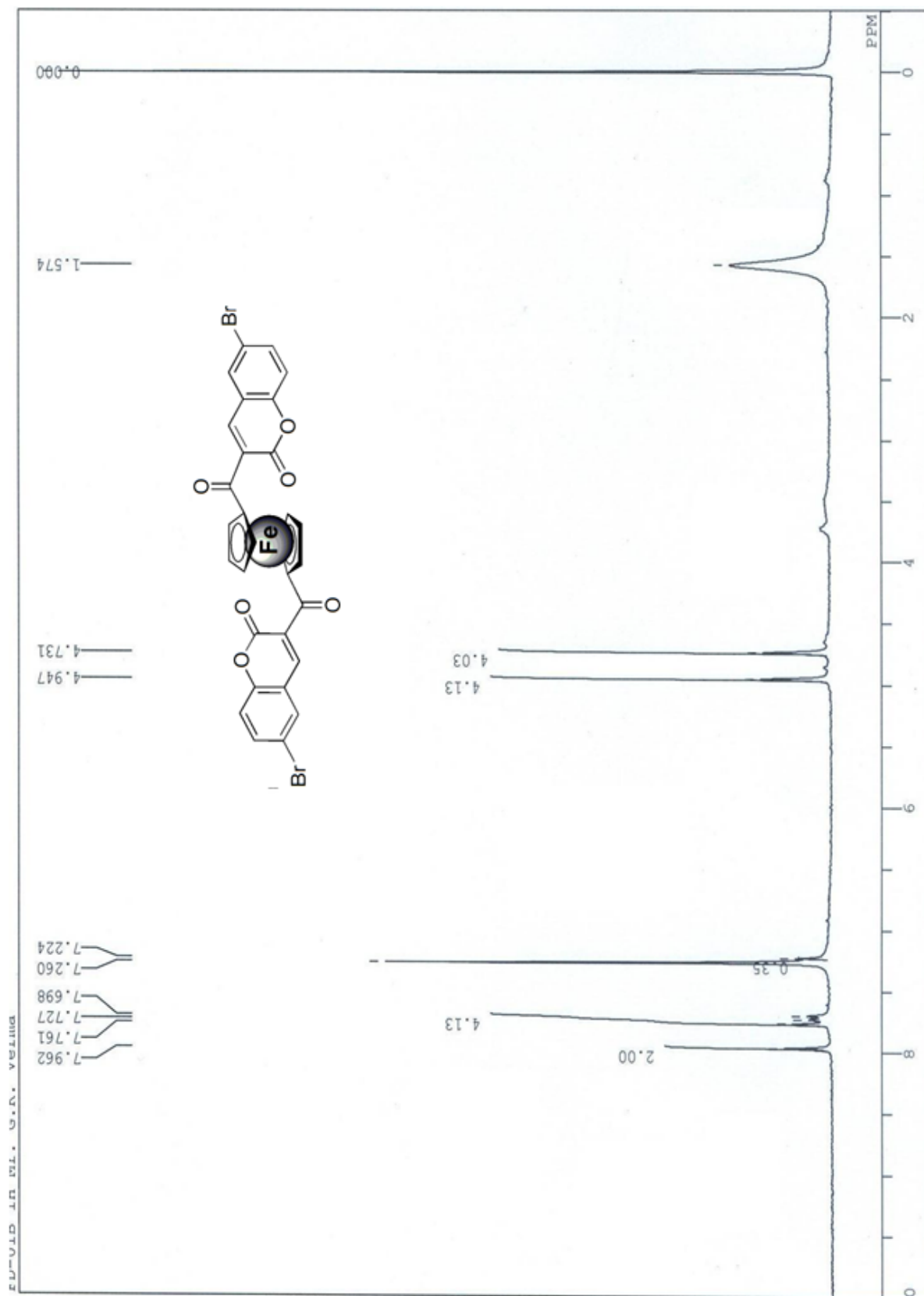
# LC-HRMS Spectrum of 1,1'-Bis(2-amino-4-methylsulfanyl-pyrimidine-6-yl)ferrocene 11



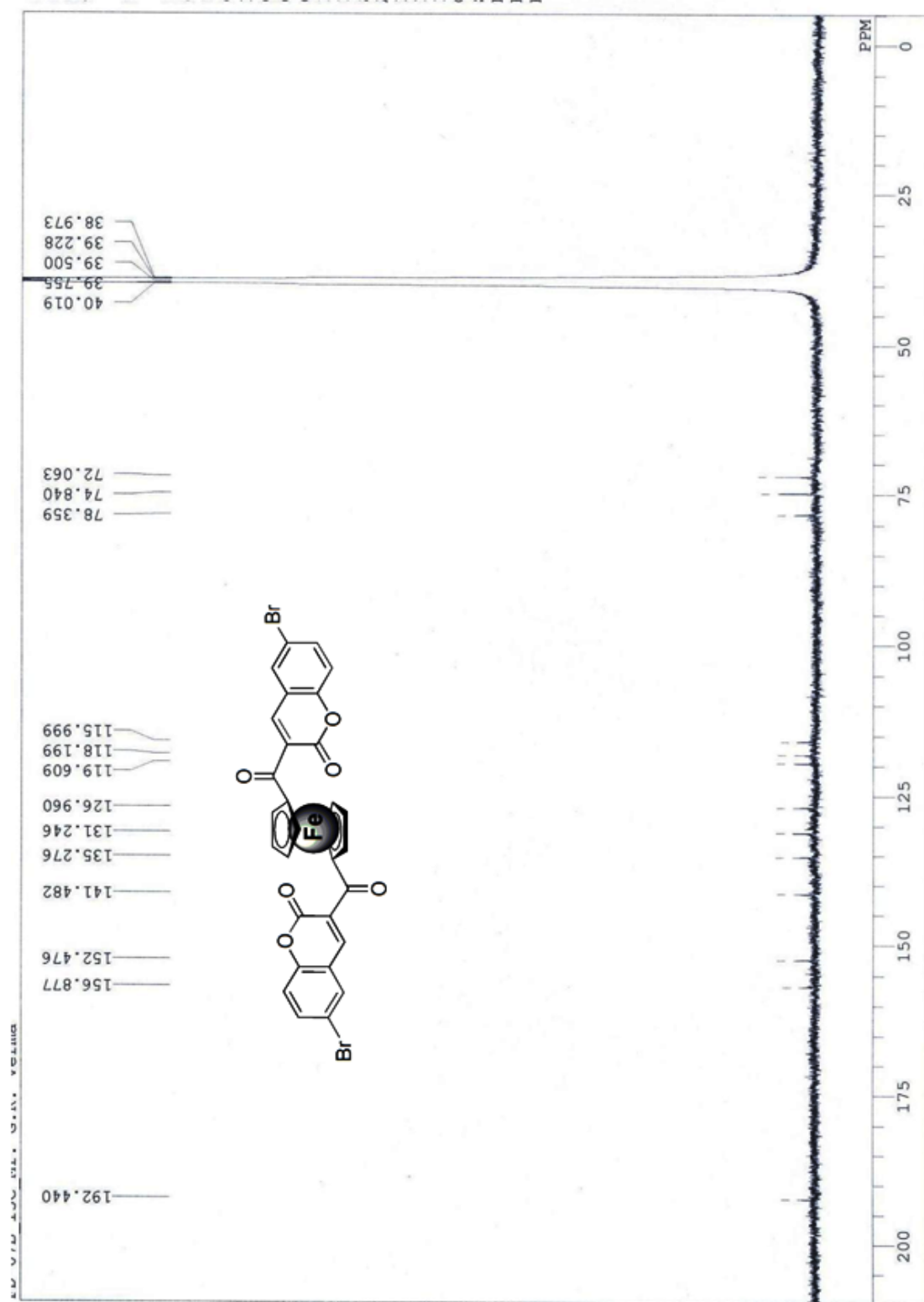
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<sup>1</sup>H NMR Spectrum of 1,1'-Bis(6-bromochromene-3-carbonyl)ferrocene 12



$^{13}\text{C}$  NMR Spectrum of 1,1'-Bis(6-bromochromene-3-carbonyl)ferrocene 12



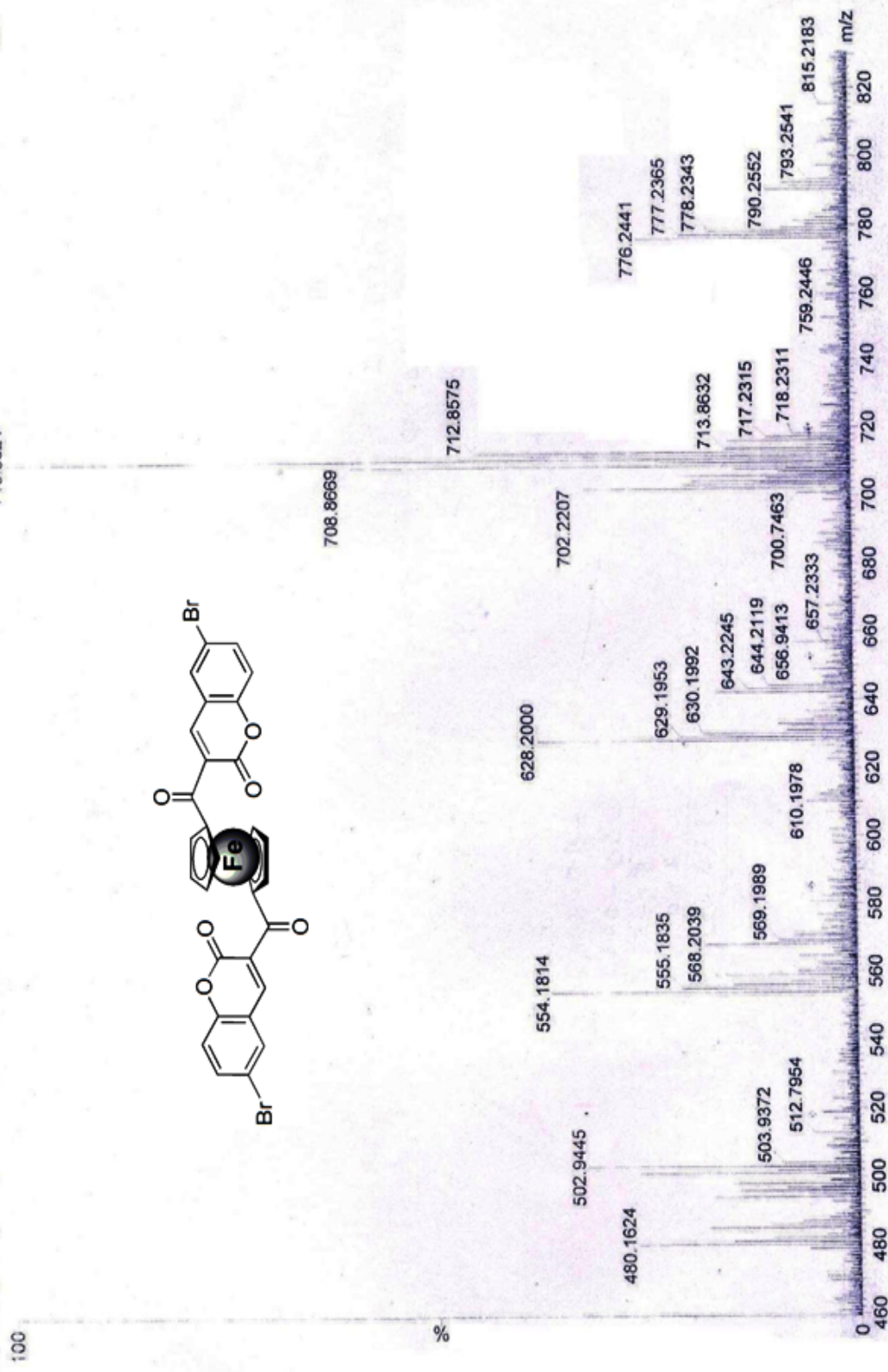
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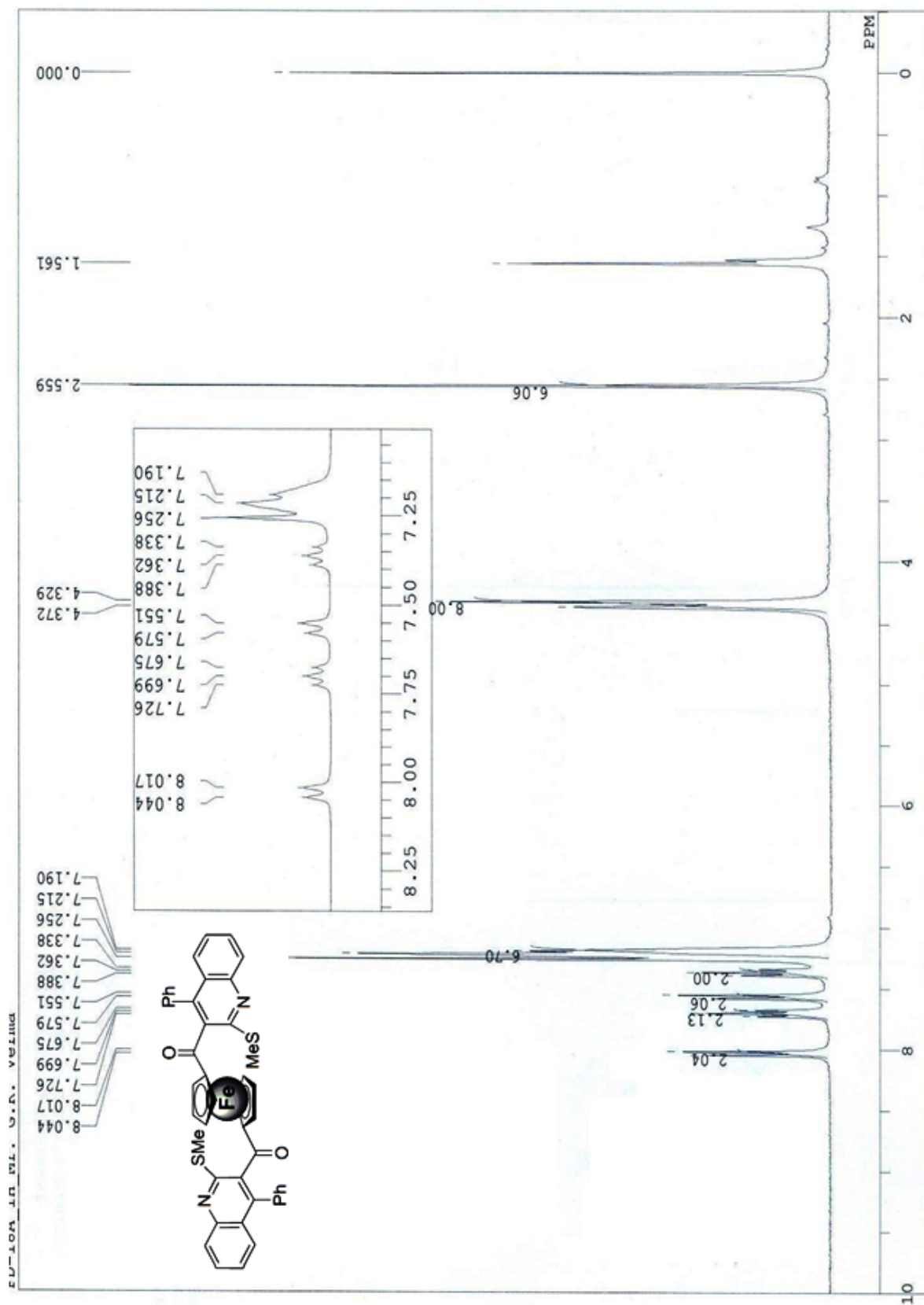
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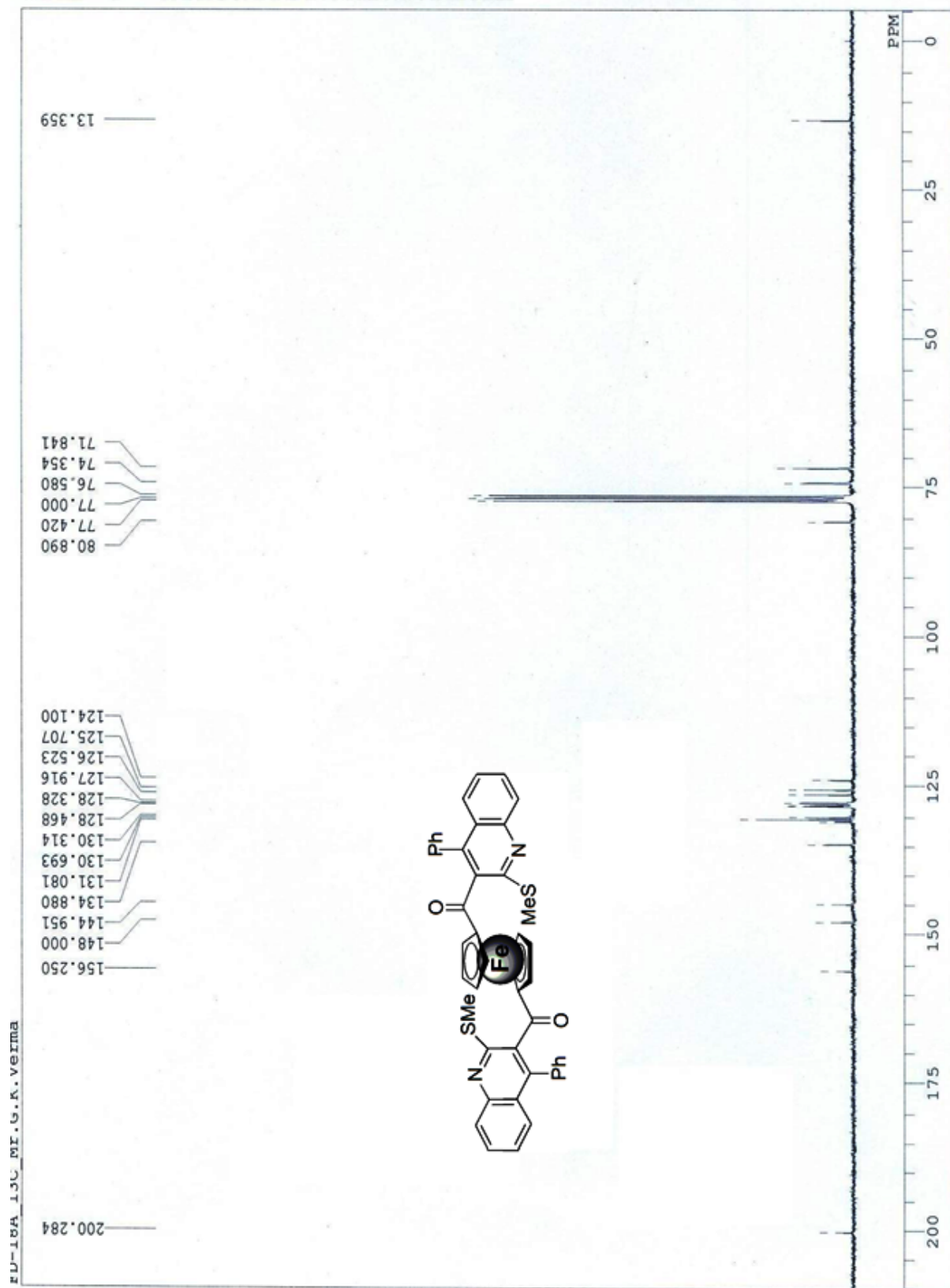
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<sup>1</sup>H NMR Spectrum of 1,1'-Bis(2-methylsulfanyl-4-phenyl-quinoline-3-carbonyl)ferrocene 13a



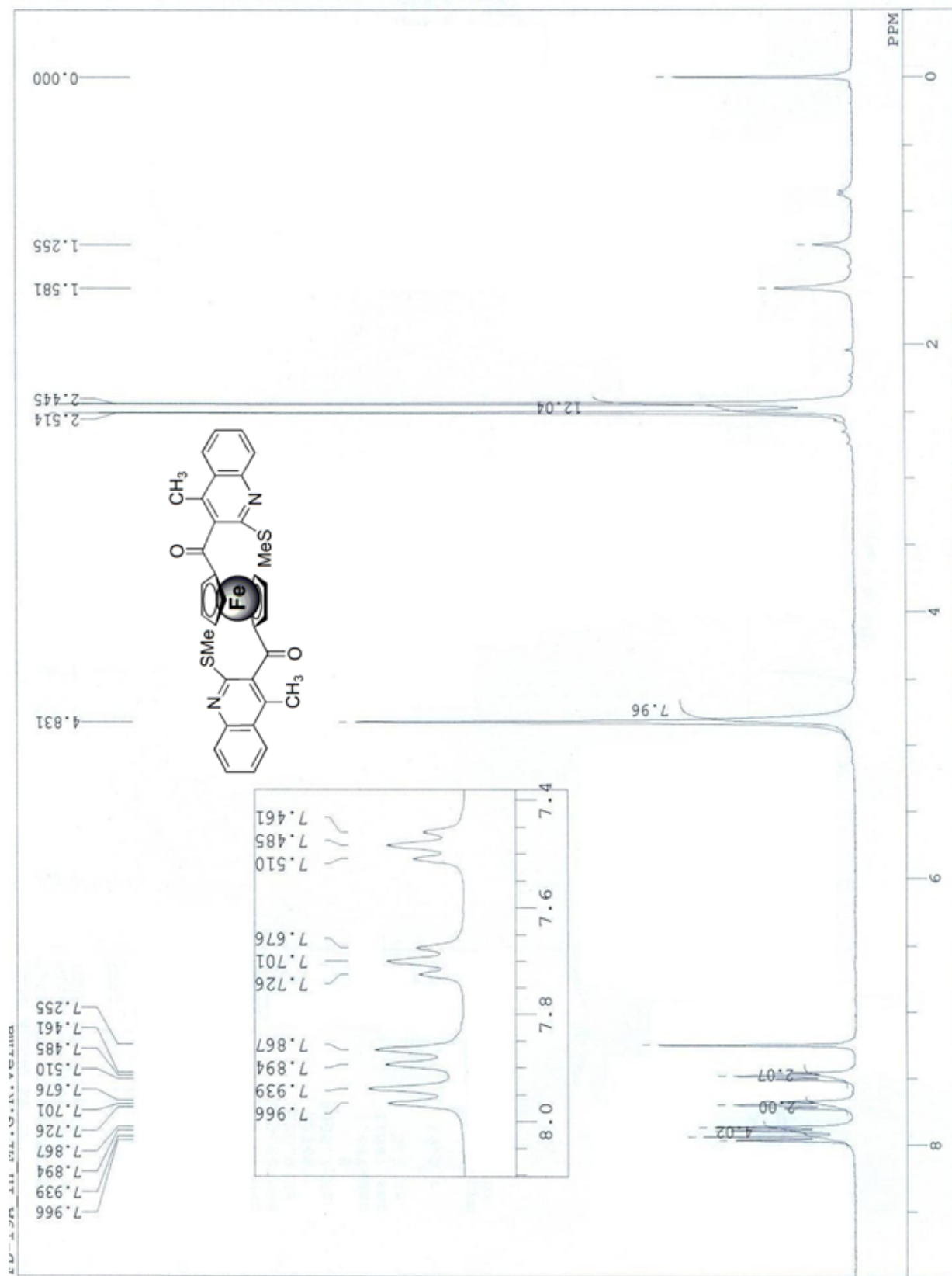
<sup>13</sup>C NMR Spectrum of 1,1'-Bis(2-methylsulfonyl-4-phenyl-quinoline-3-carbonyl)ferrocene 13a



HRMS Spectrum of 1,1'-Bis(2-methylsulfonyl-4-phenyl-quinoline-3-carbonyl)ferrocene 13a

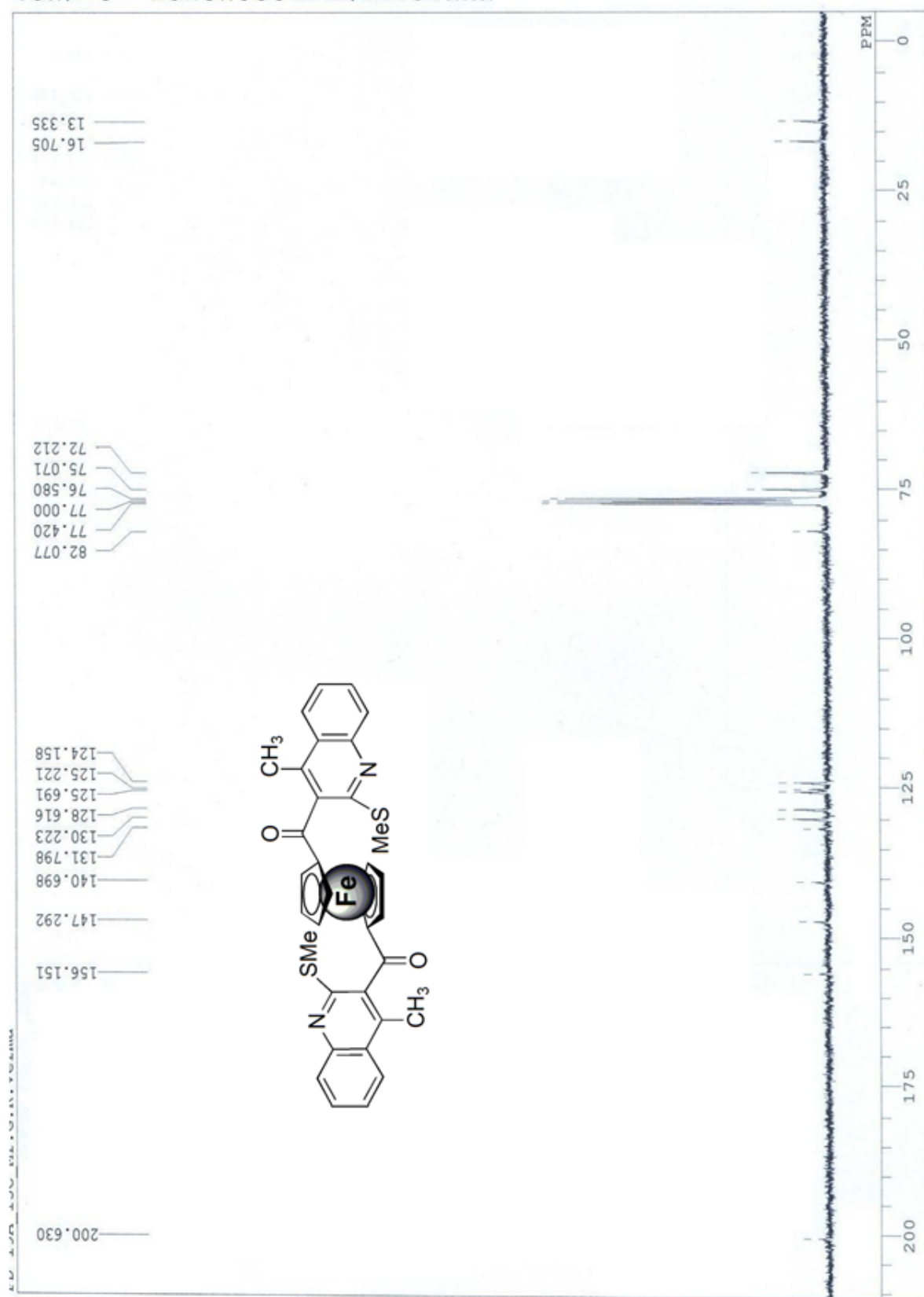


<sup>1</sup>H NMR Spectrum of 1,1'-Bis(2-methylsulfanyl-4-methyl-quinoline-3-carbonyl)ferrocene 13b

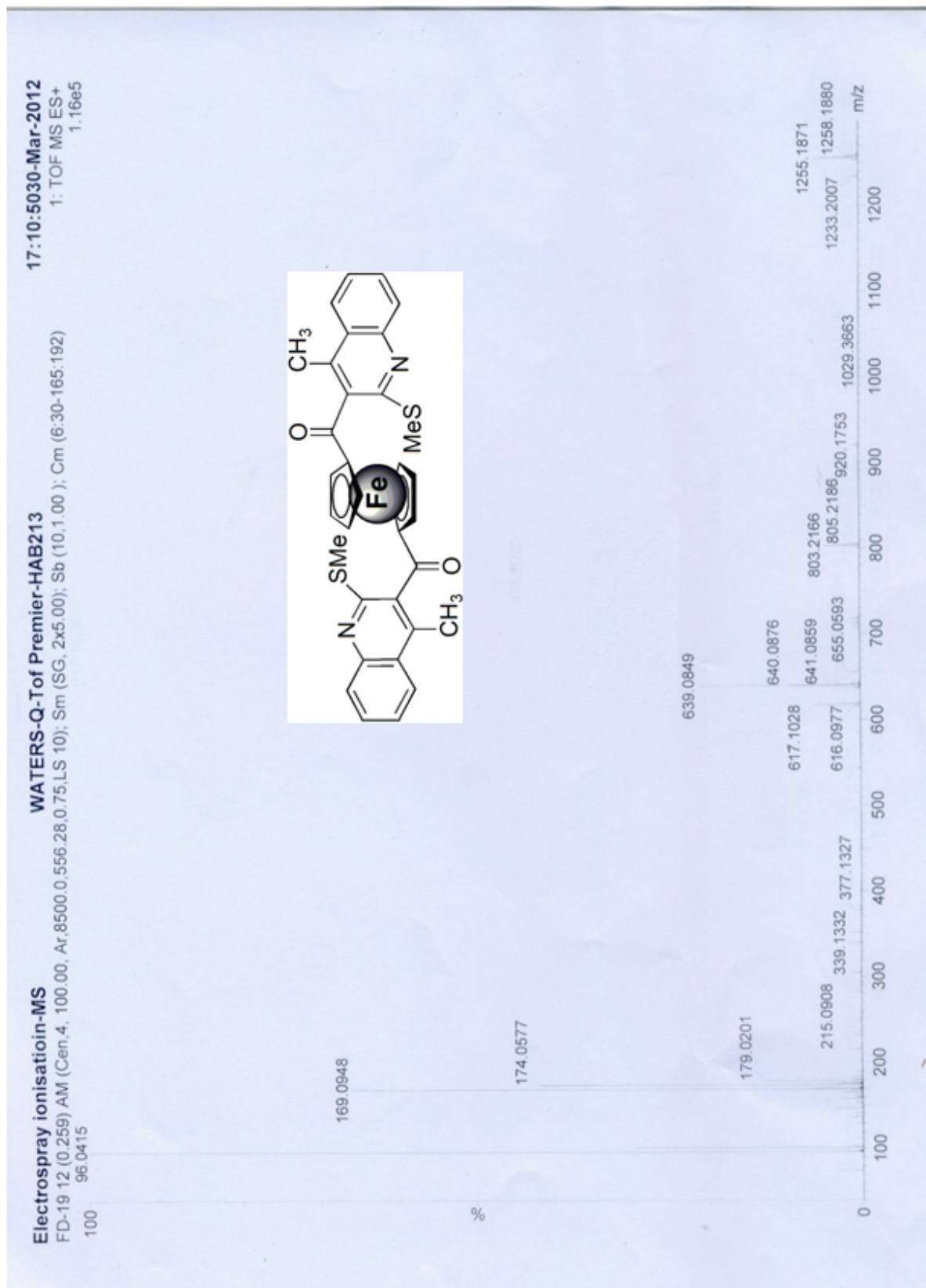




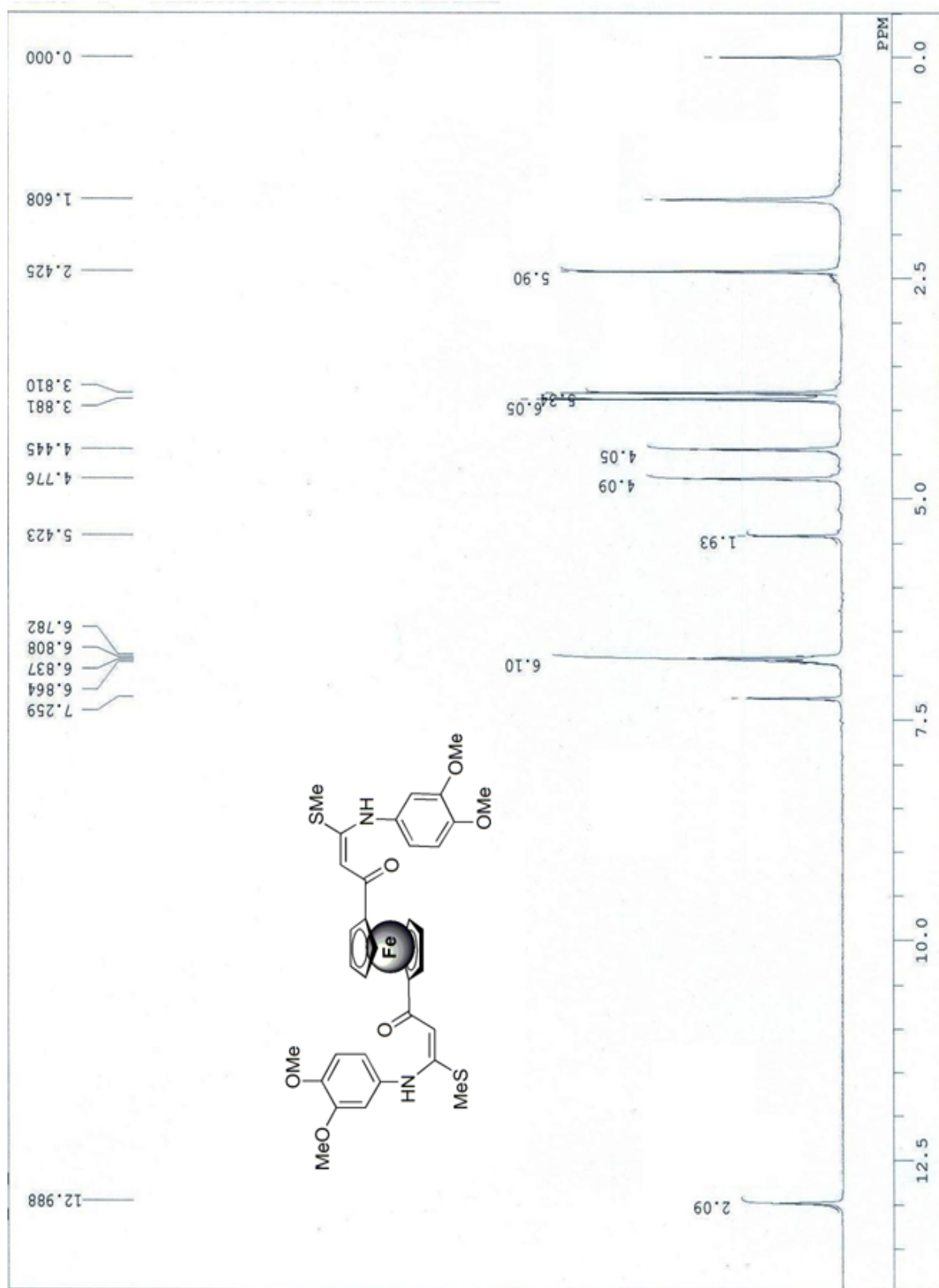
<sup>13</sup>C NMR Spectrum of 1,1'-Bis(2-methylsulfanyl-4-methyl-quinoline-3-carbonyl)ferrocene 13b



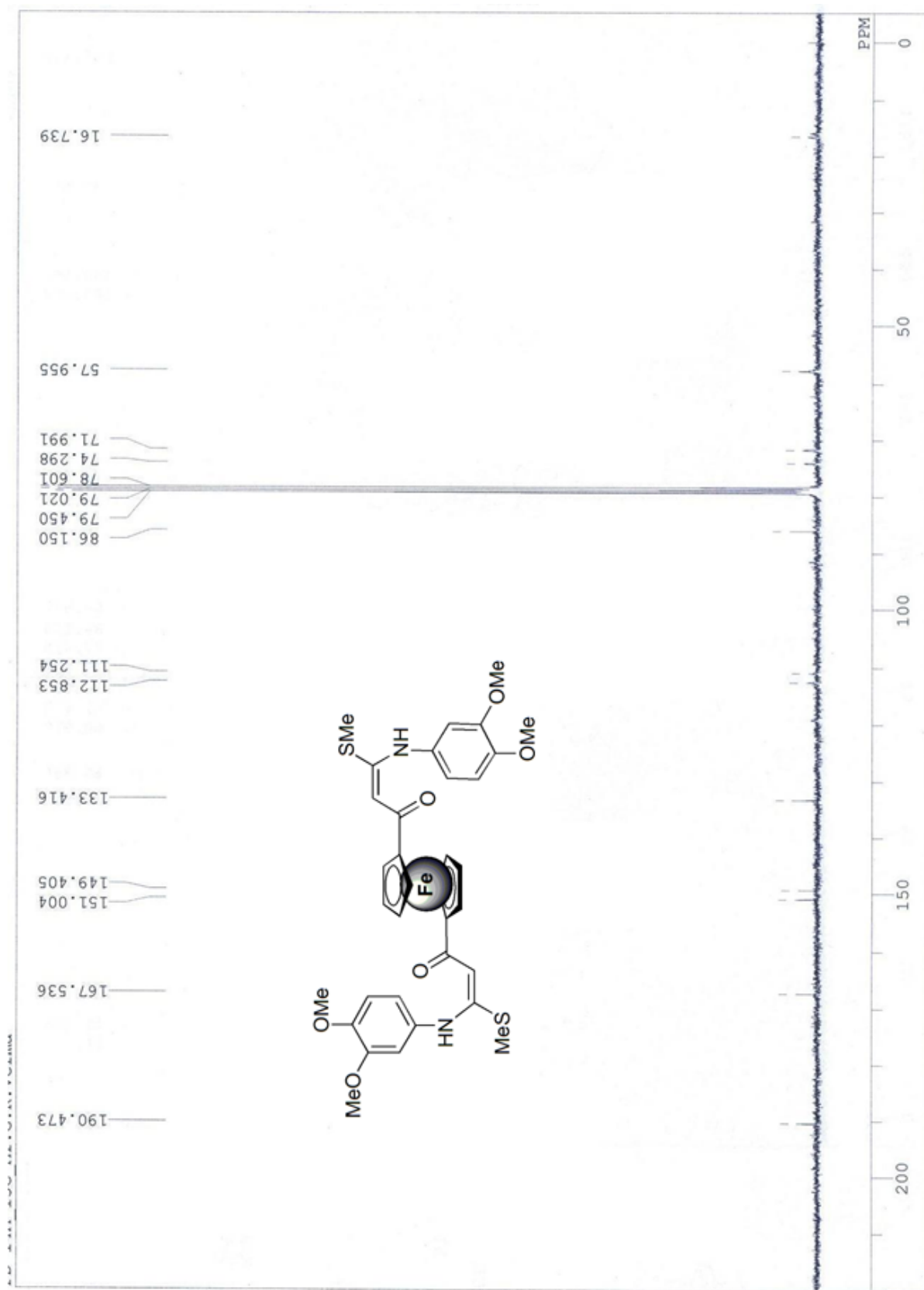
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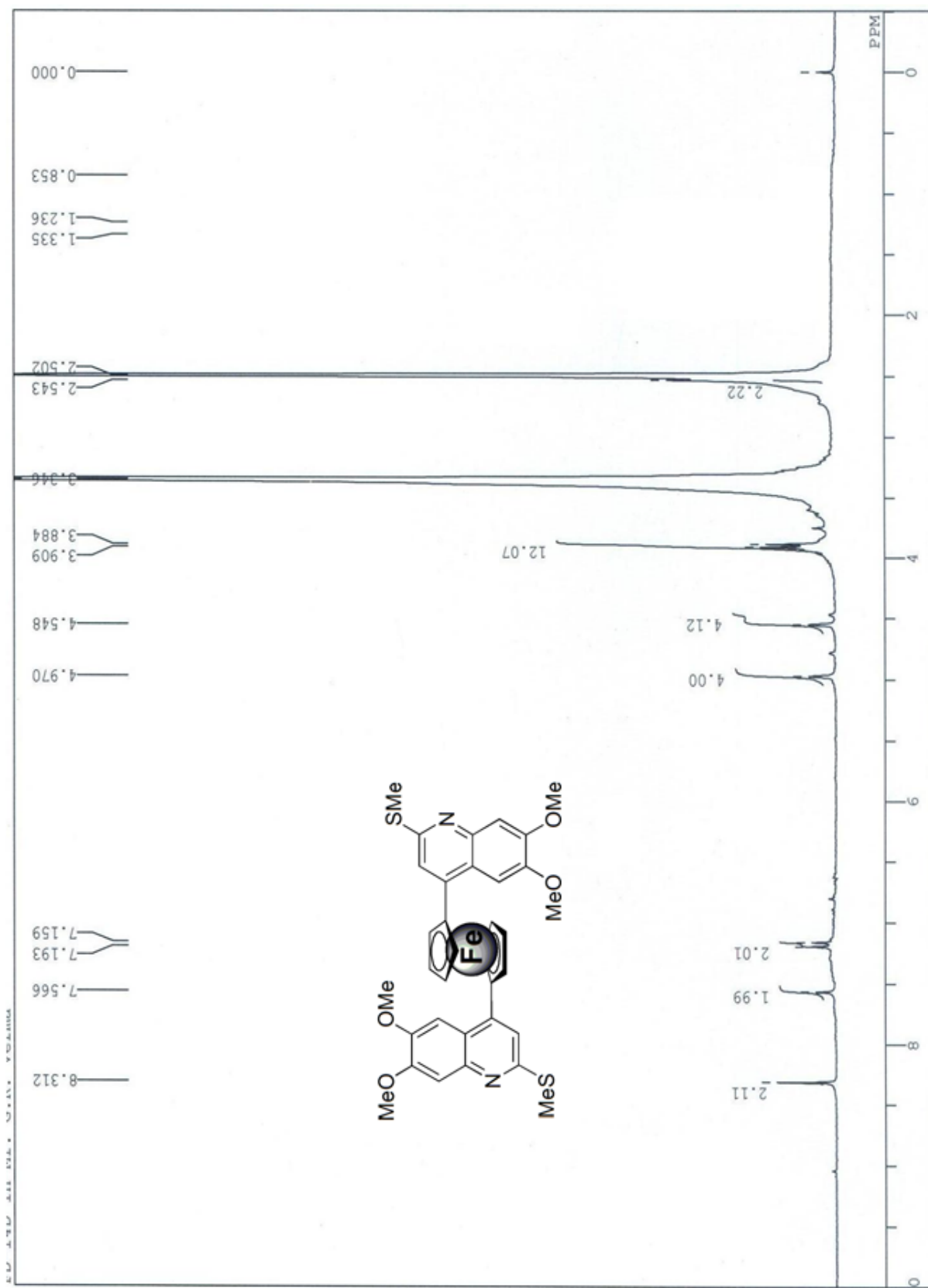
<sup>1</sup>H NMR Spectrum of 1,1'-Bis(1-(3,4-dimethoxyamino)-1-methylsulfonyl-3-oxo-1-propene)ferrocene 14



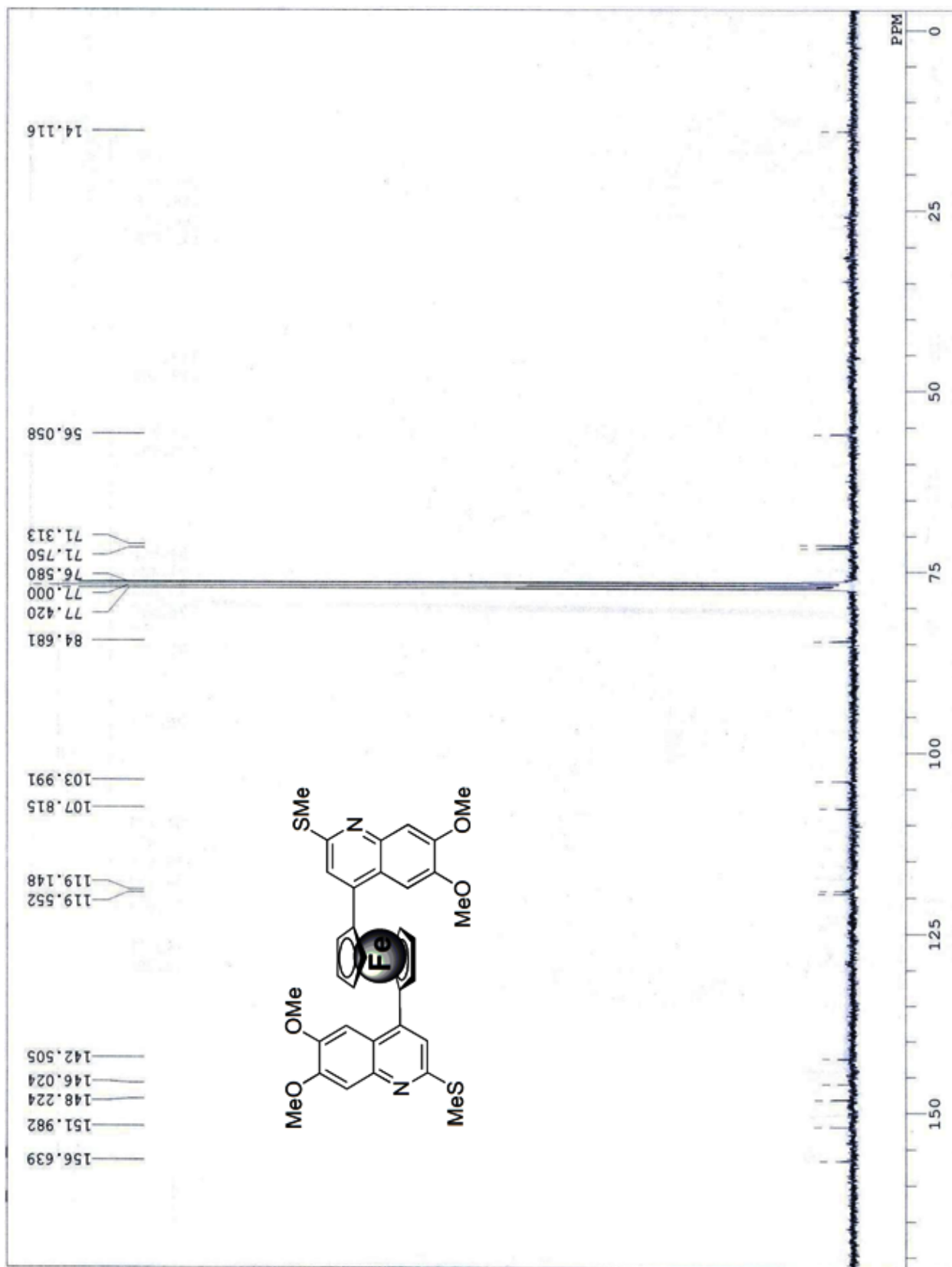
$^{13}\text{C}$  NMR Spectrum of **1,1'-Bis(1-(3,4-dimethoxyamino)-1-methylsulfonyl-3-oxo-1-propene)ferrocene** **14**



<sup>1</sup>H NMR Spectrum of 1,1'-Bis(6,7-dimethoxy-2-methylsulfanyl-quinoline-4-yl)ferrocene 15



$^{13}\text{C}$  NMR Spectrum of 1,1'-Bis(6,7-dimethoxy-2-methylsulfanyl-quinoline-4-yl)ferrocene 15



# HRMS Spectrum of 1,1'-Bis(6,7-dimethoxy-2-methylsulfanyl-quinoline-4-yl)ferrocene 15

