N-arylation of ferrocenyl 2,4-thiazolidinedione conjugates via copper-catalysed Chan-Lam cross coupling reaction with aryl boronic acids and their optoelectronic properties

Dilip Nivrutti *Shinde,*[a,d] Rajiv Trivedi,*[a,d] Jonnadula V S Krishna,[a] L. Giribabu,[a,d] B. Sridhar[b], Parag S. Khursade,[c] R. S. Prakasham[c]

[a] Catalysis and Fine Chemicals Division, CSIR-Indian Institute of Chemical Technology, Hyderabad, 500007, Telangana, India, E-mail: trivedi@csiriict.in, trivedi.iict@gov.in; Fax: +91-40-27160921; Tel: +91-40-27191667

[b] Centre for X-ray Crystallography, CSIR-Indian Institute of Chemical Technology, Hyderabad 500007, Telangana, India

[c] Organic Synthesis and Process Chemistry Division, CSIR-Indian Institute of Chemical Technology, Hyderabad 500007, Telangana, India

[d] Academy of Scientific and Innovative Research (AcSIR), CSIR-IICT Campus, Hyderabad 500007, Telangana, India

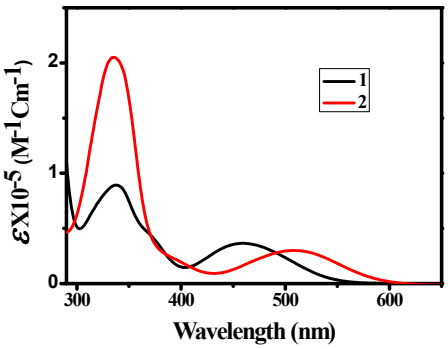


Figure 1: Absorption spectra of ferrocene carboxaldehyde andferrocenyl 2,4-thiazolidinedione conjugates (**1** and **2**) in CH_2Cl_2.

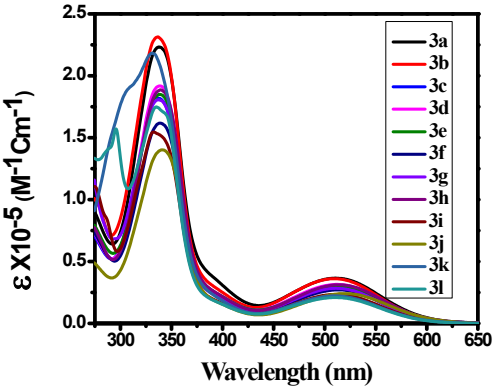


Figure 2: Absorption spectra of ferrocenyl 2,4-thiazolidinedione substituted N-aryl conjugates (**3a-l**) in CH_2Cl_2.

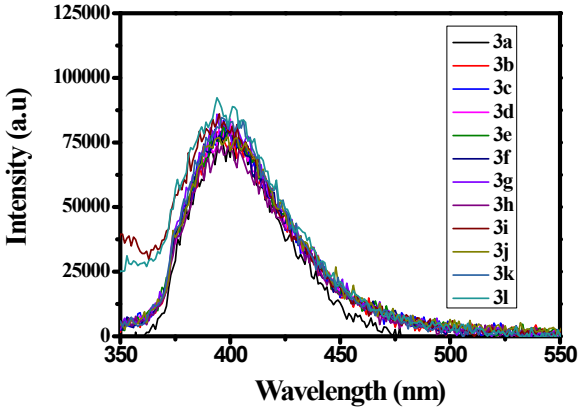


Figure 3: Fluorescence spectra of ferrocenyl 2,4-thiazolidinedione substituted aryl conjugates (**3a-l**) in CH_2Cl_2

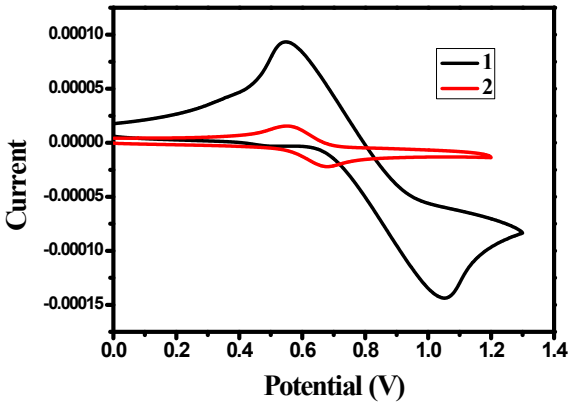


Figure 4: Electrochemical oxidative potential curves of (**1 and 2**) in CH_2Cl_2 at RT

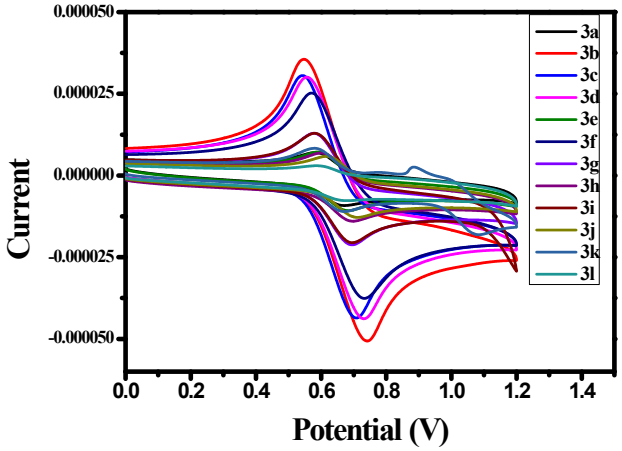
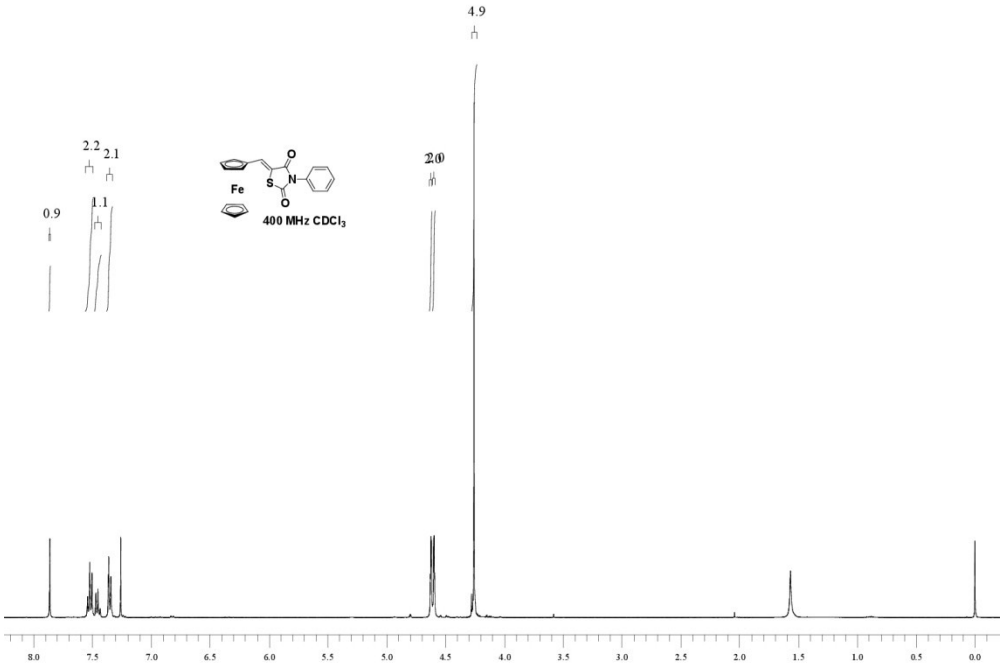
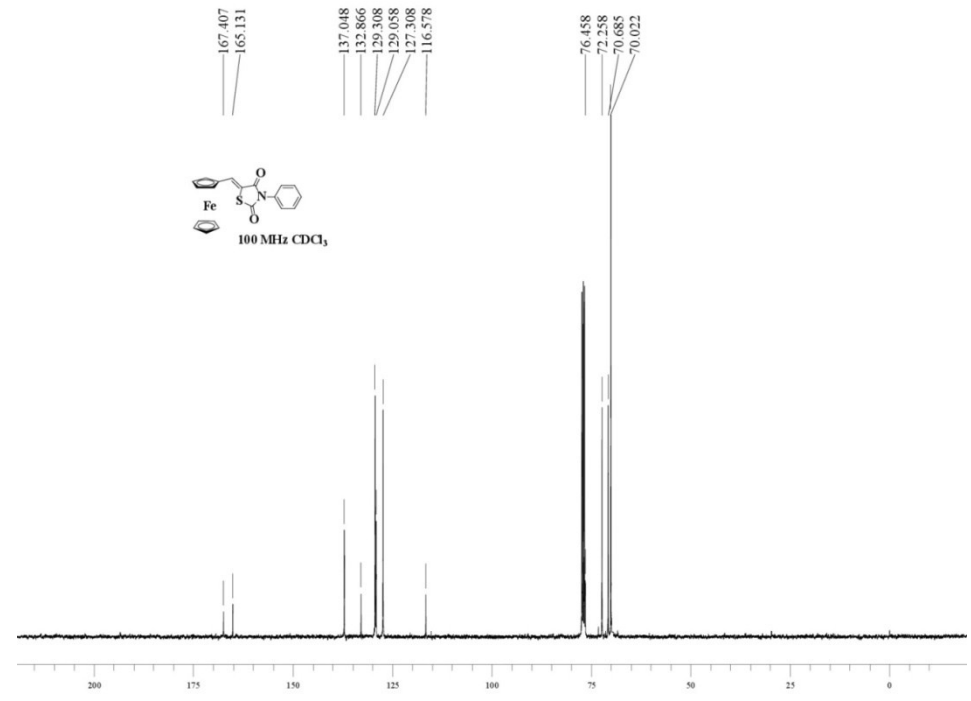


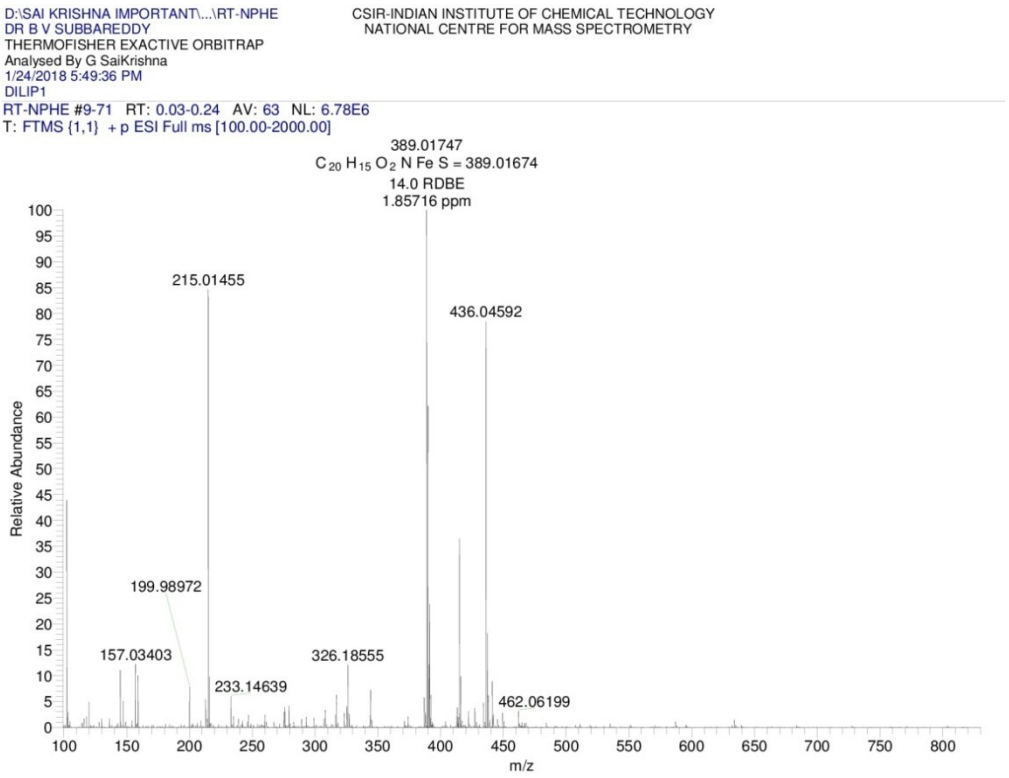
Figure 5: Electrochemical oxidative potential curves of (**3a-l**) in CH_2Cl_2 at RT



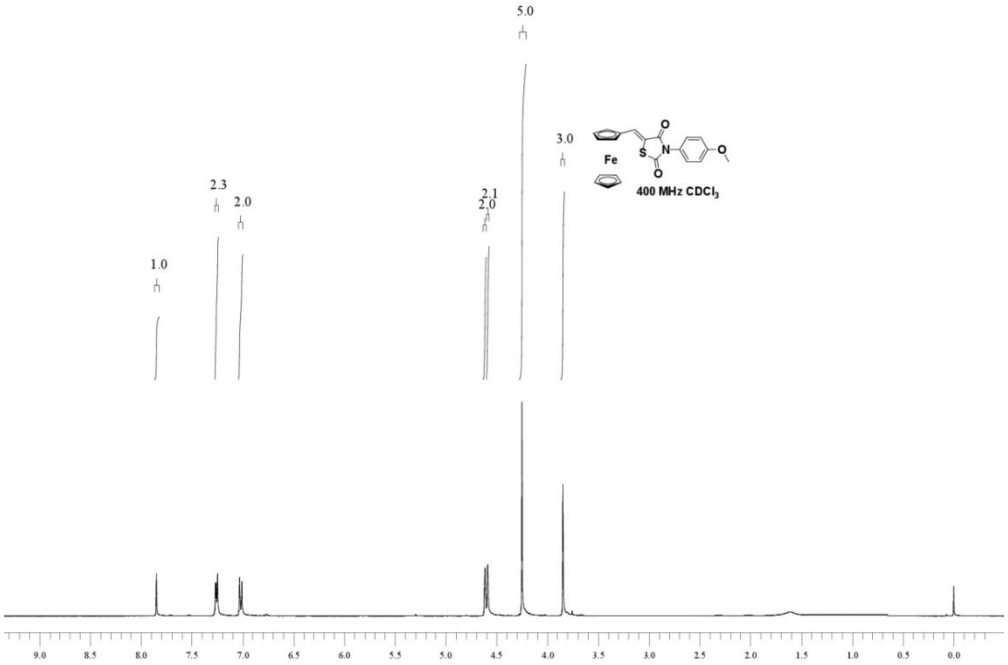
^{1}H NMR spectrum of compound **3a**



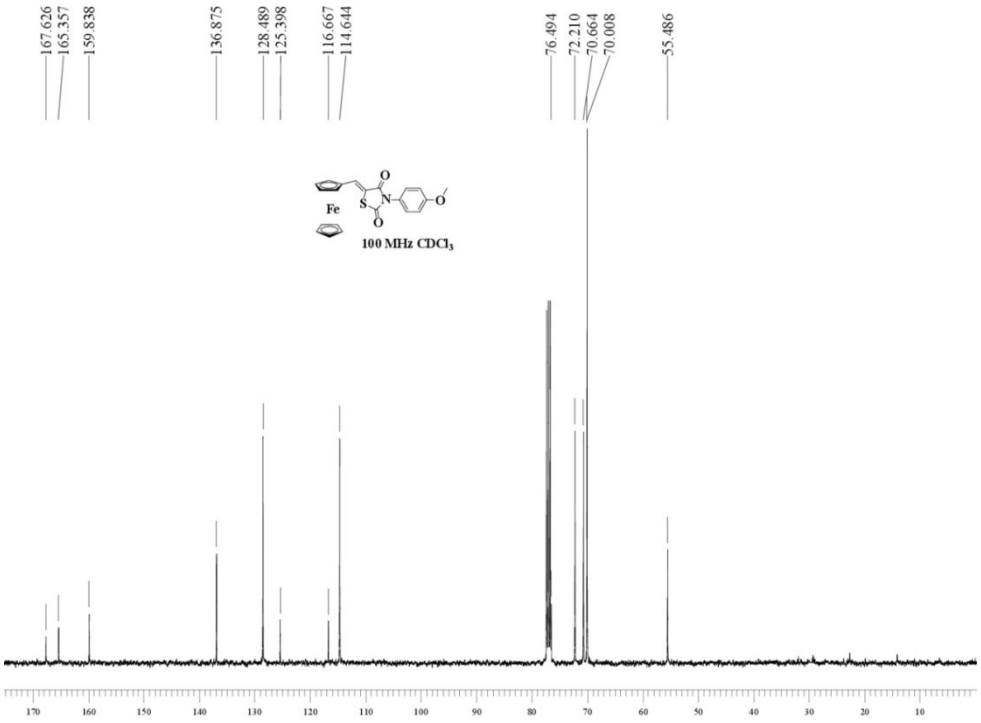
^{13}C NMR spectrum of compound **3a**



HRMS spectra of compound **3a**



^{1}H NMR spectrum of compound **3b**



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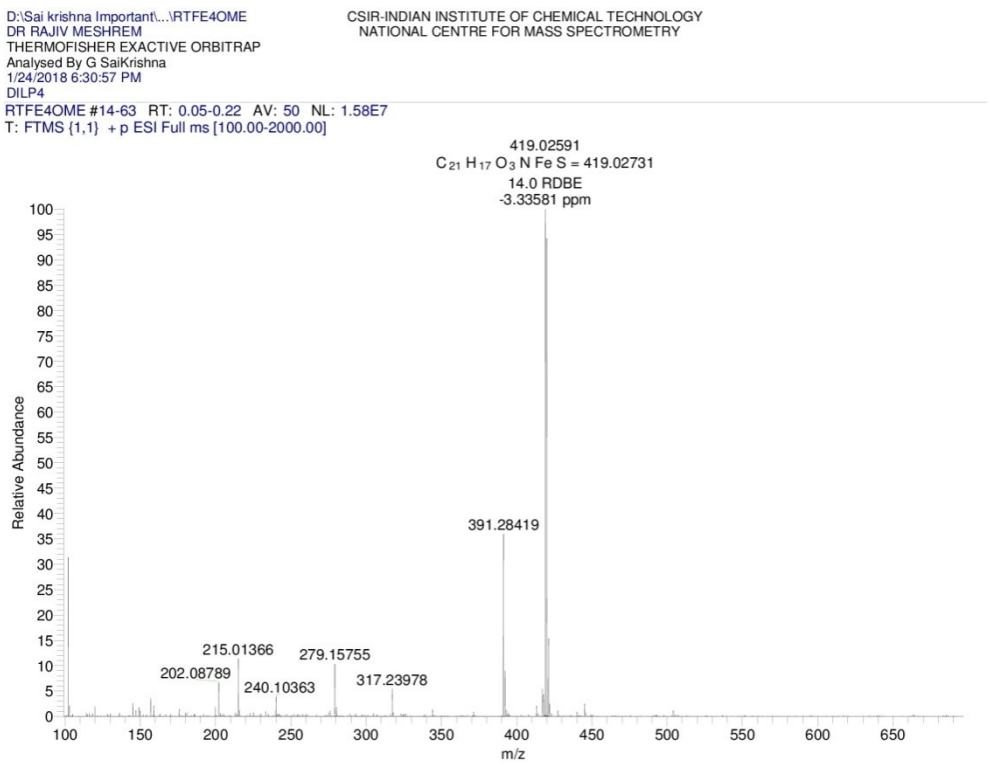
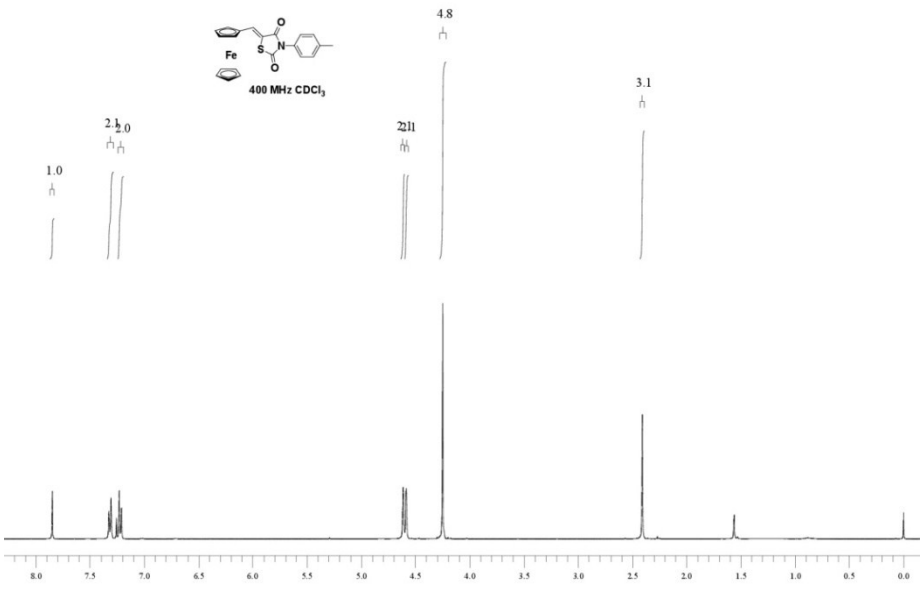
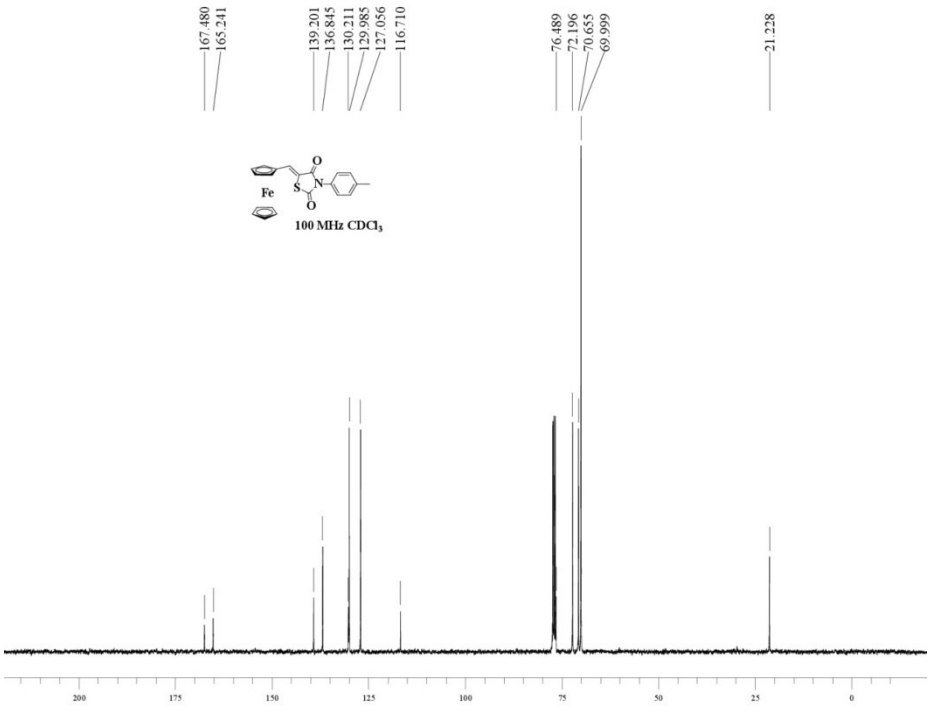


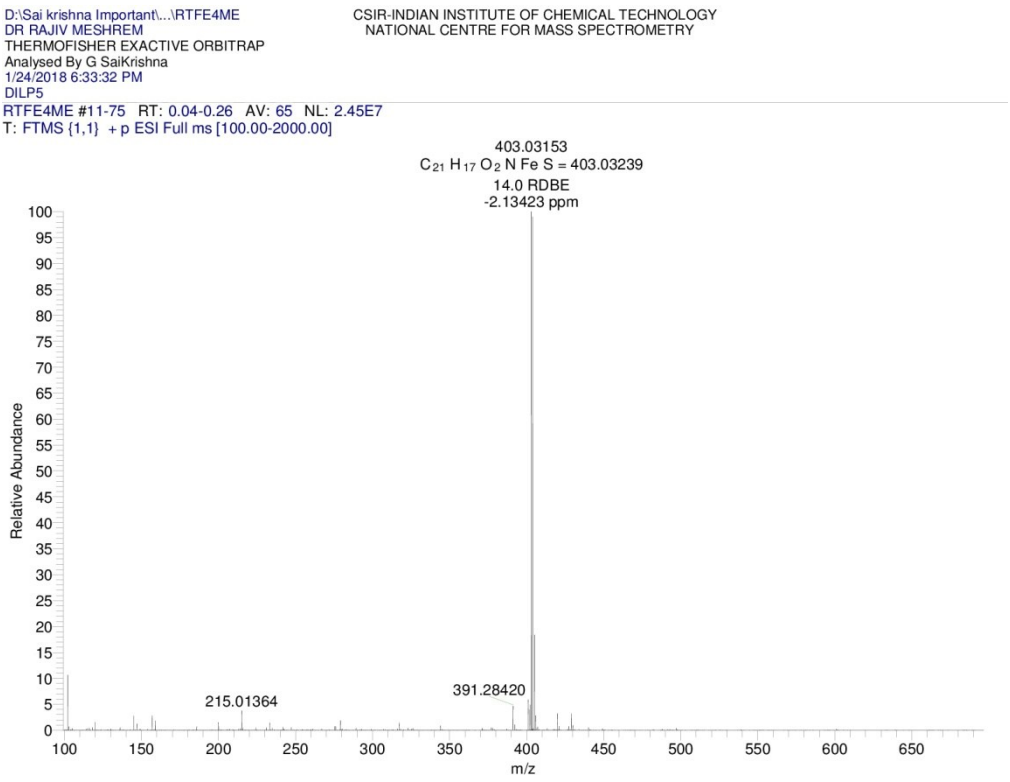
HRMS spectra of compound **3b**



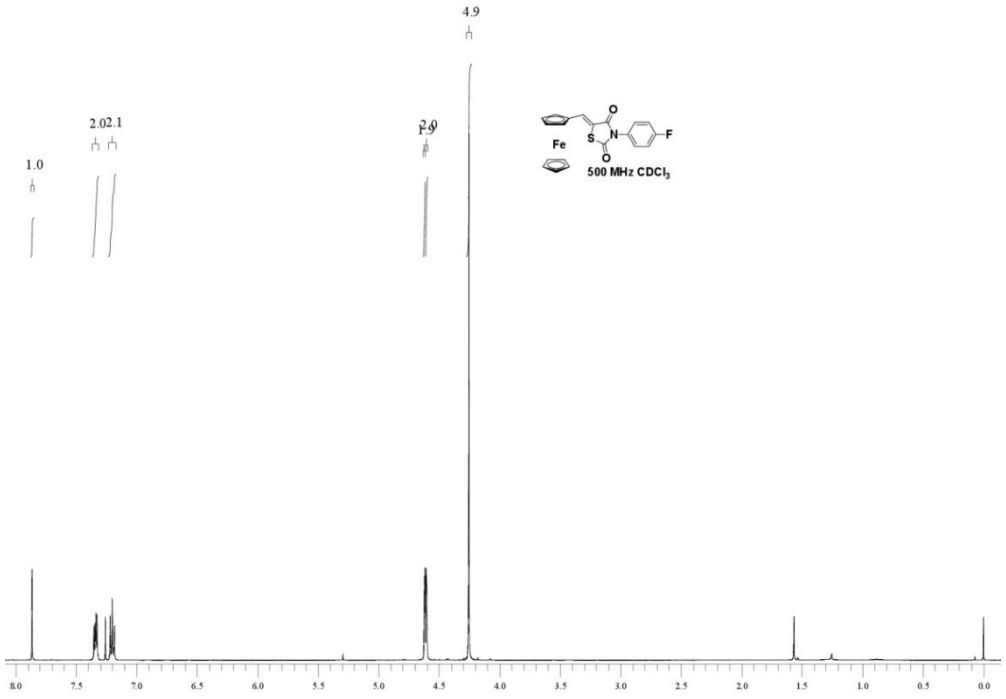
^{1}H NMR spectrum of compound **3c**



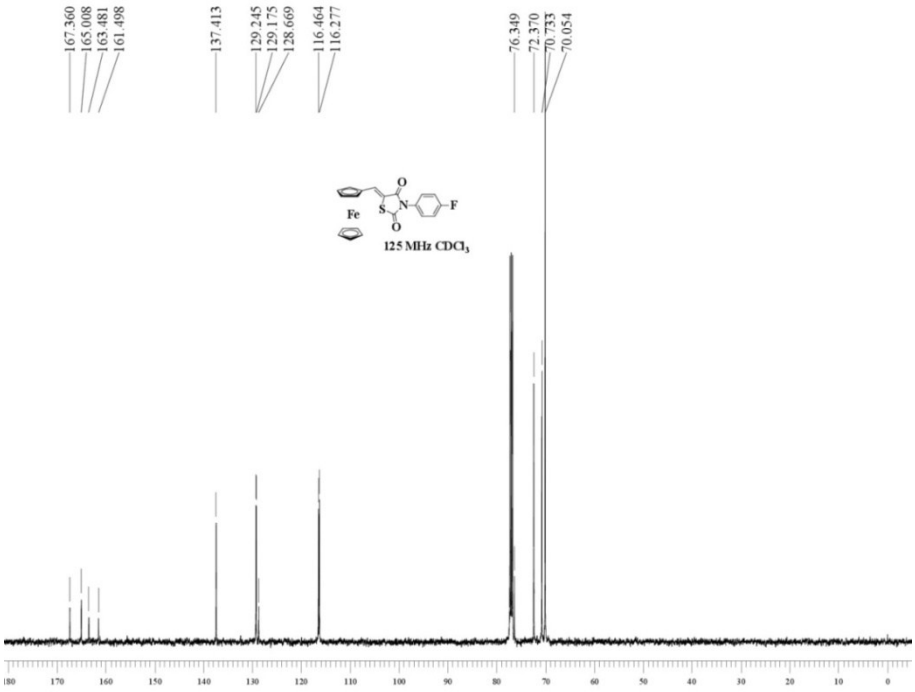
^{13}C NMR spectrum of compound **3c**



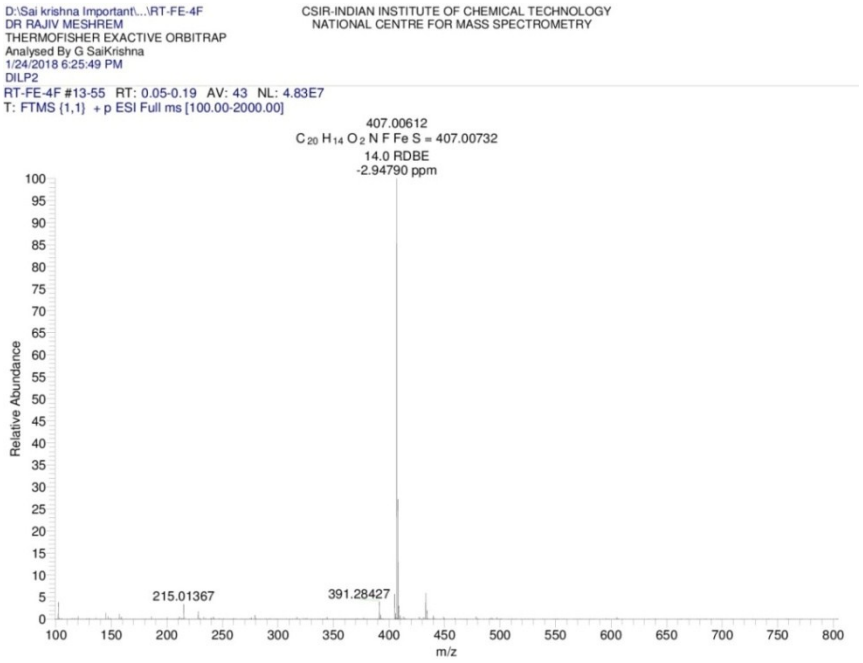
HRMS spectra of compound **3c**



^{1}H NMR spectrum of compound **3d**



^{13}C NMR spectrum of compound **3d**



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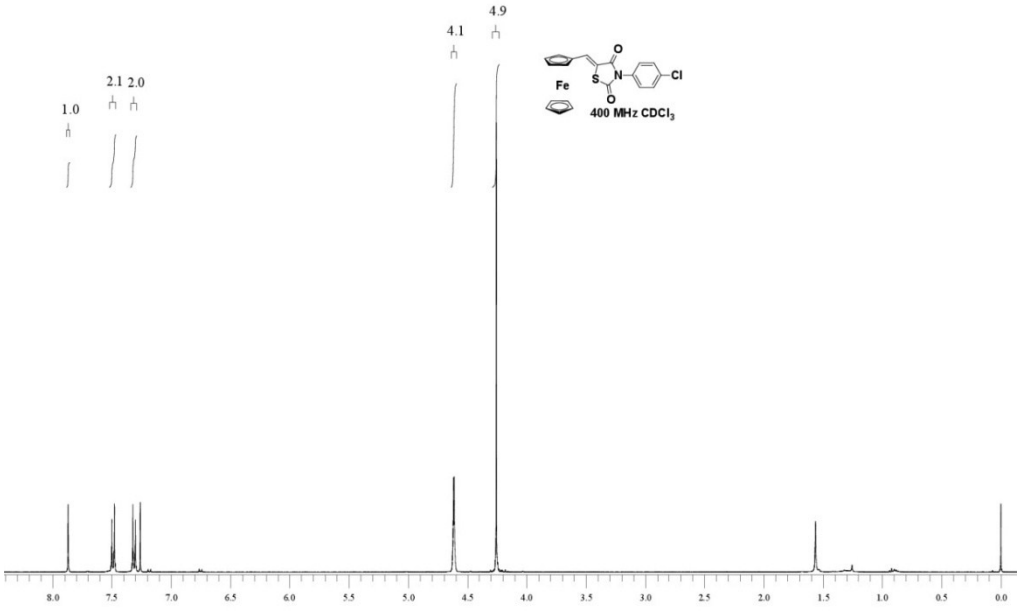

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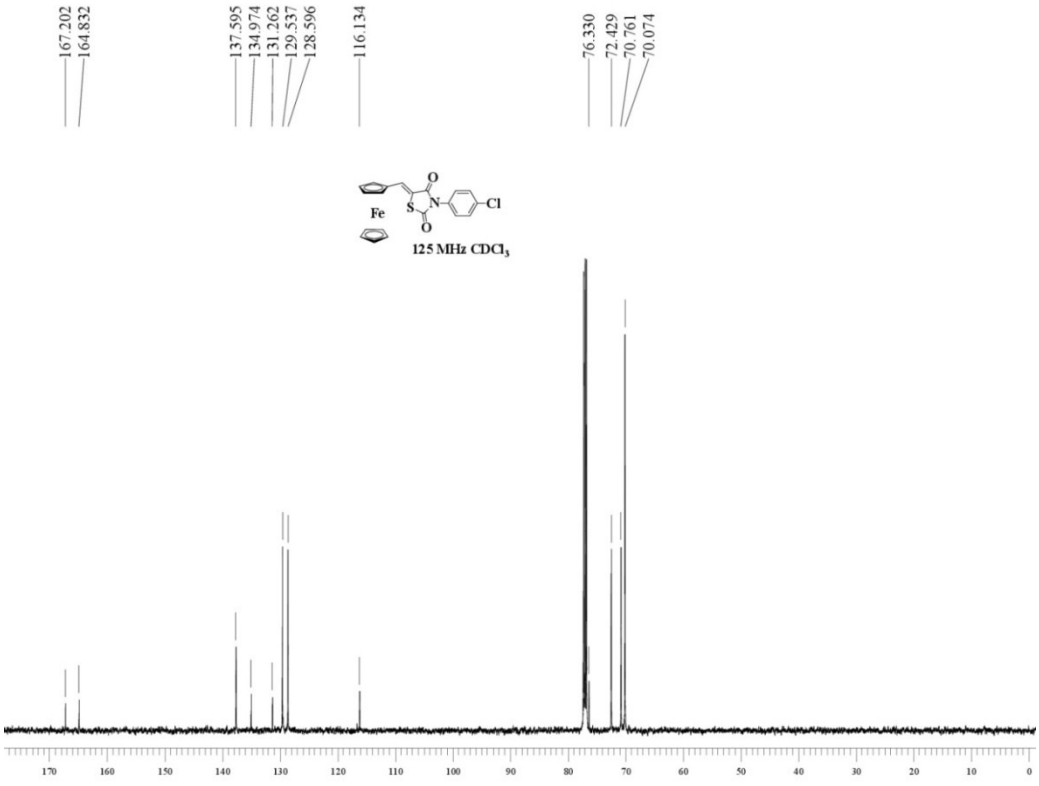

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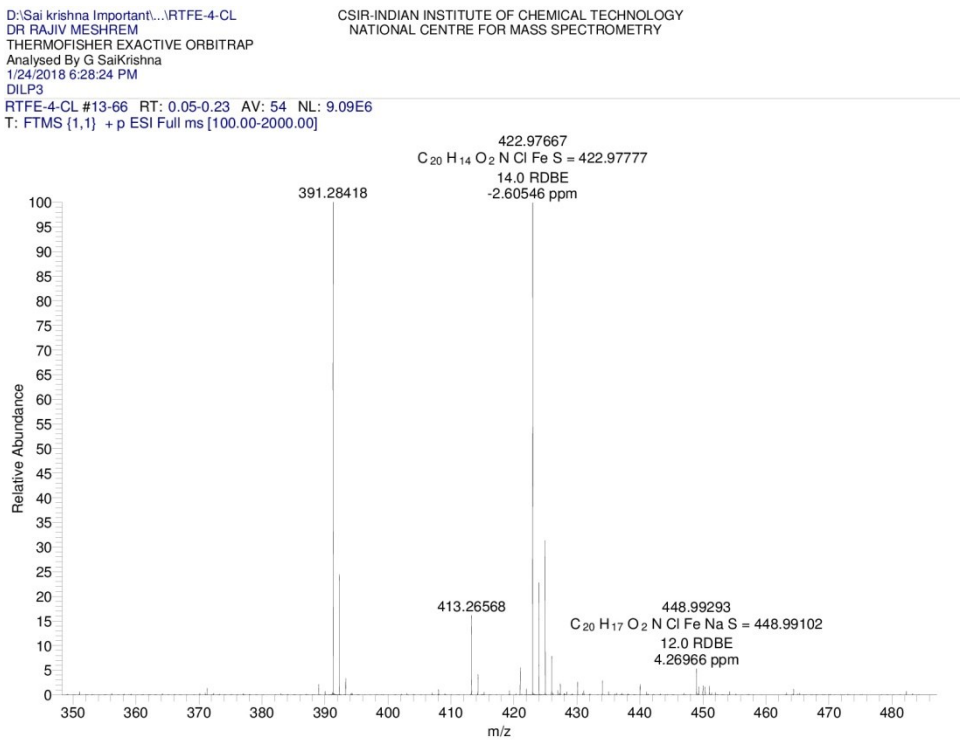
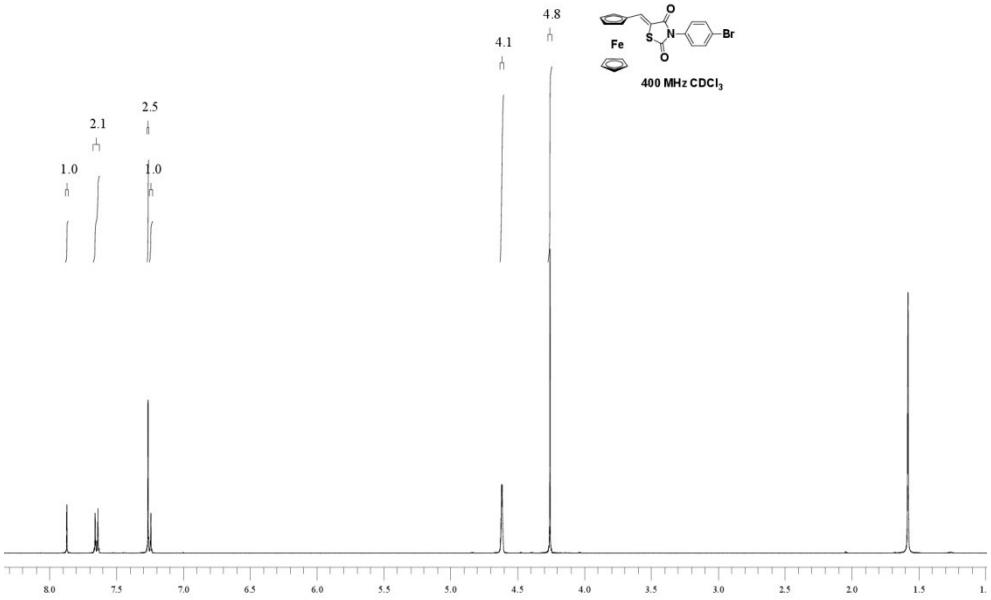
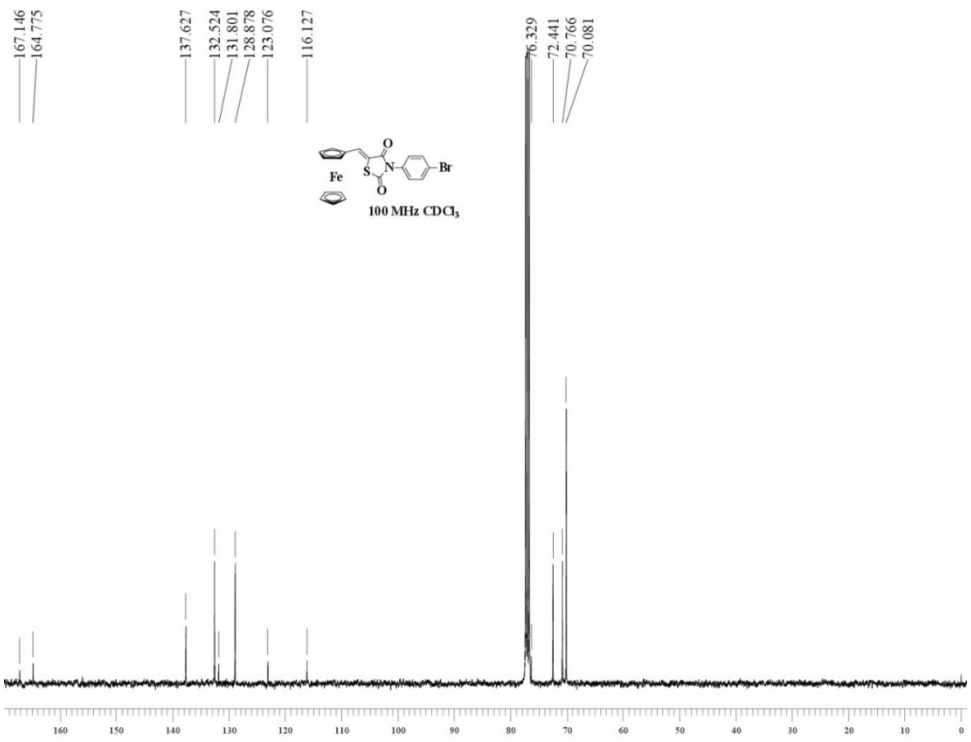


HRMS spectra of compound **3e**



^{1}H NMR spectrum of compound **3f**



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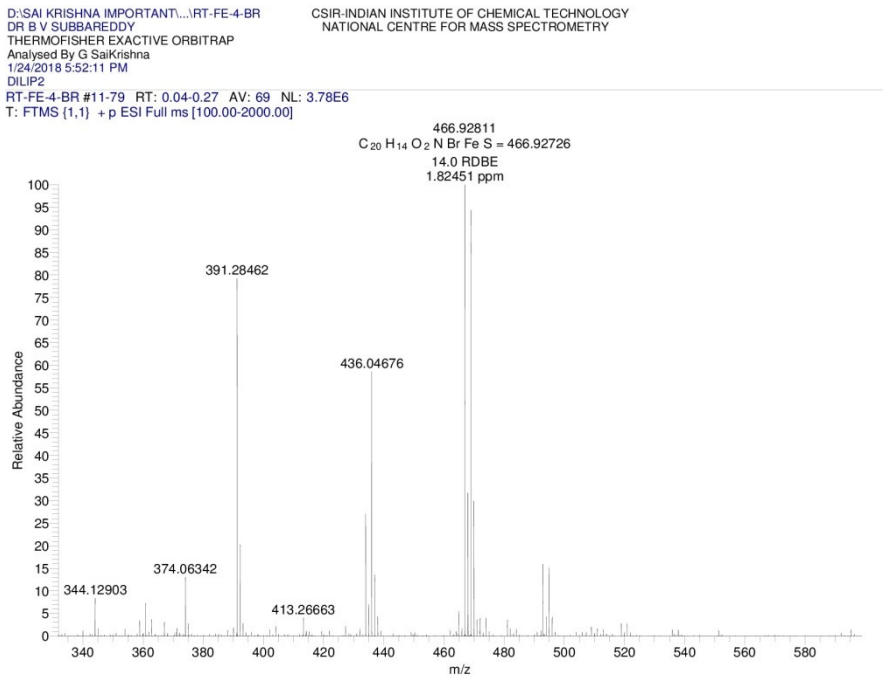

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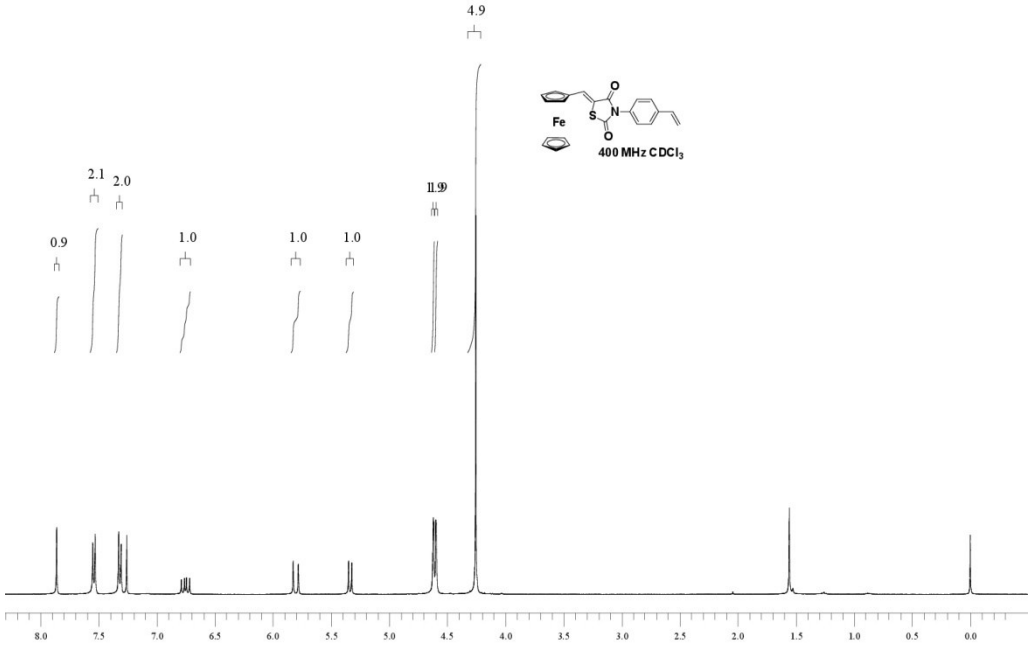
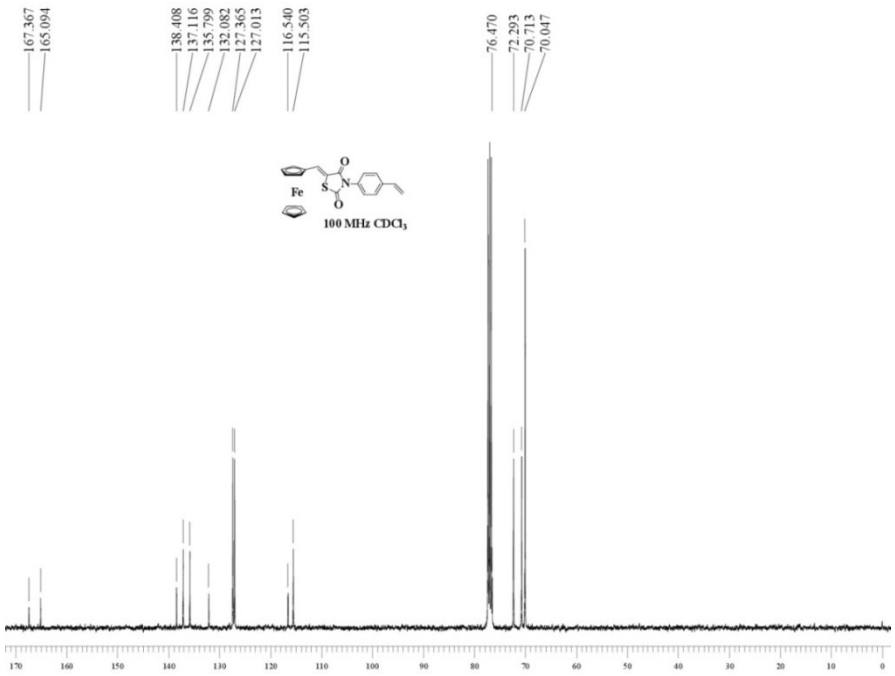


^{1}H NMR spectrum of compound **3g**



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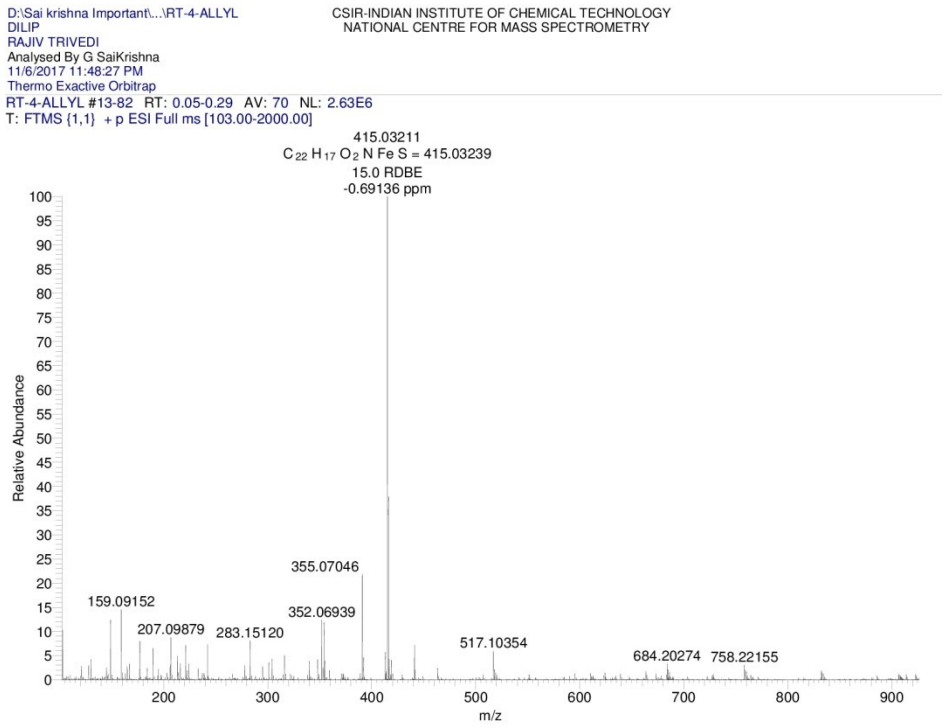

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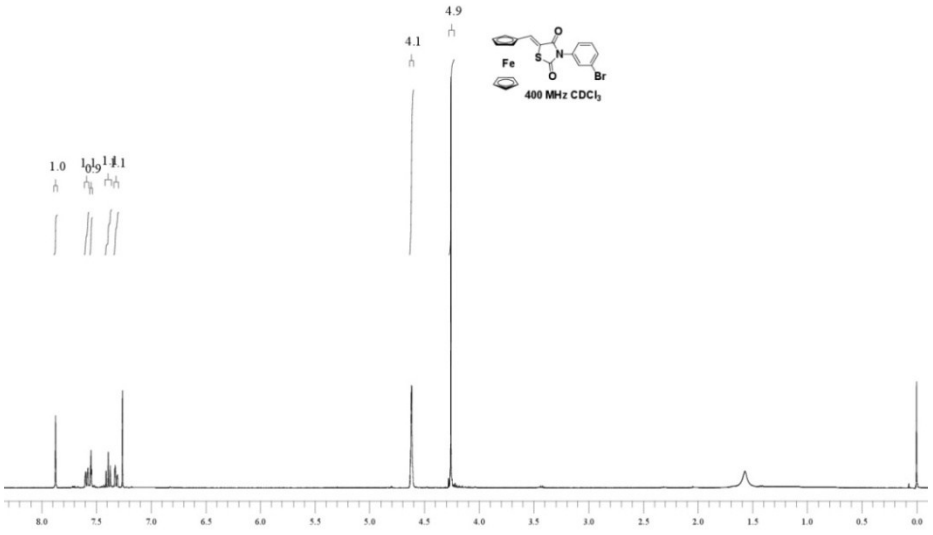

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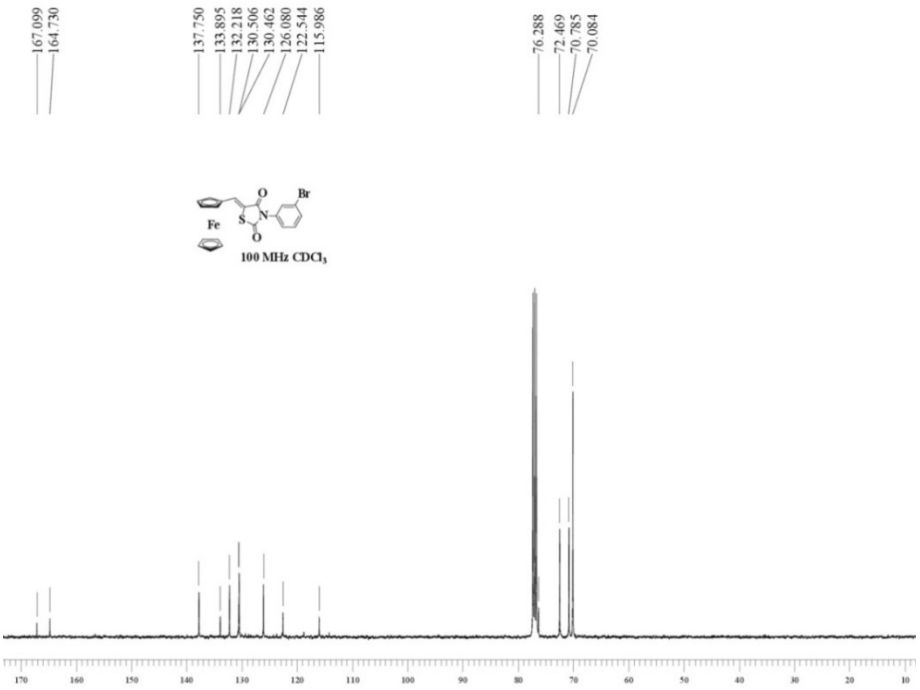

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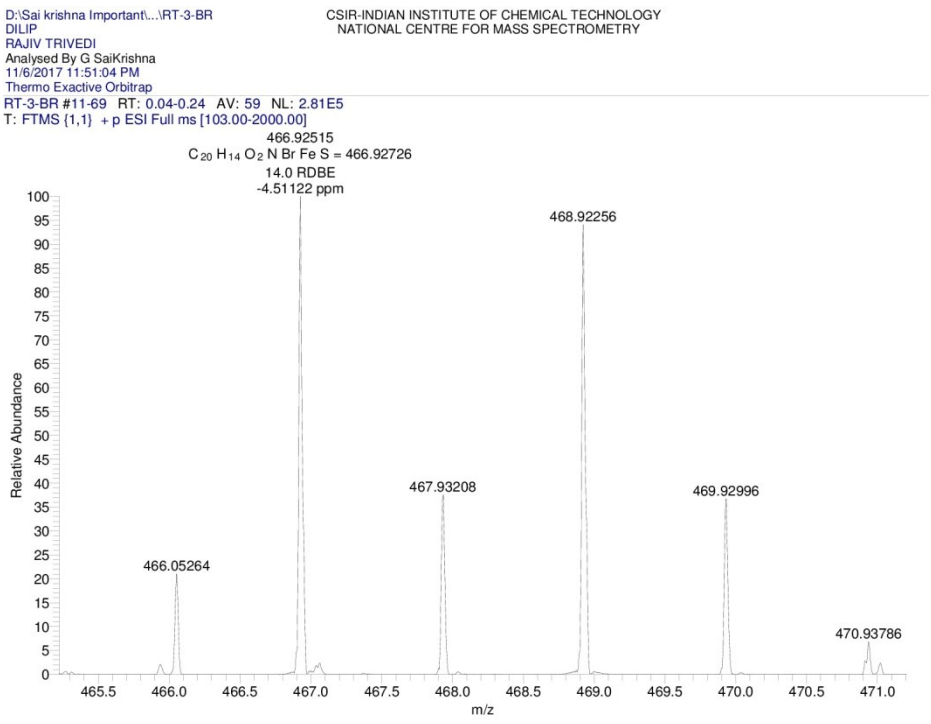
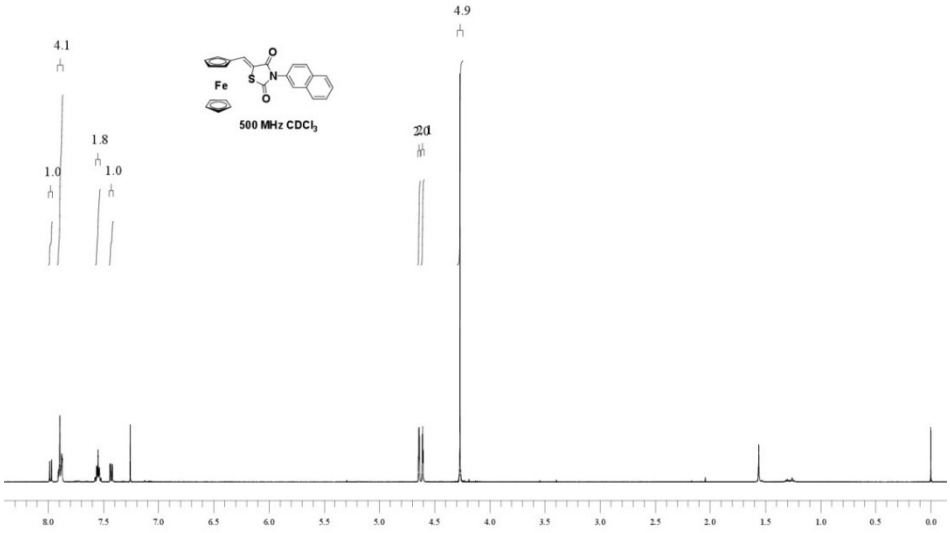
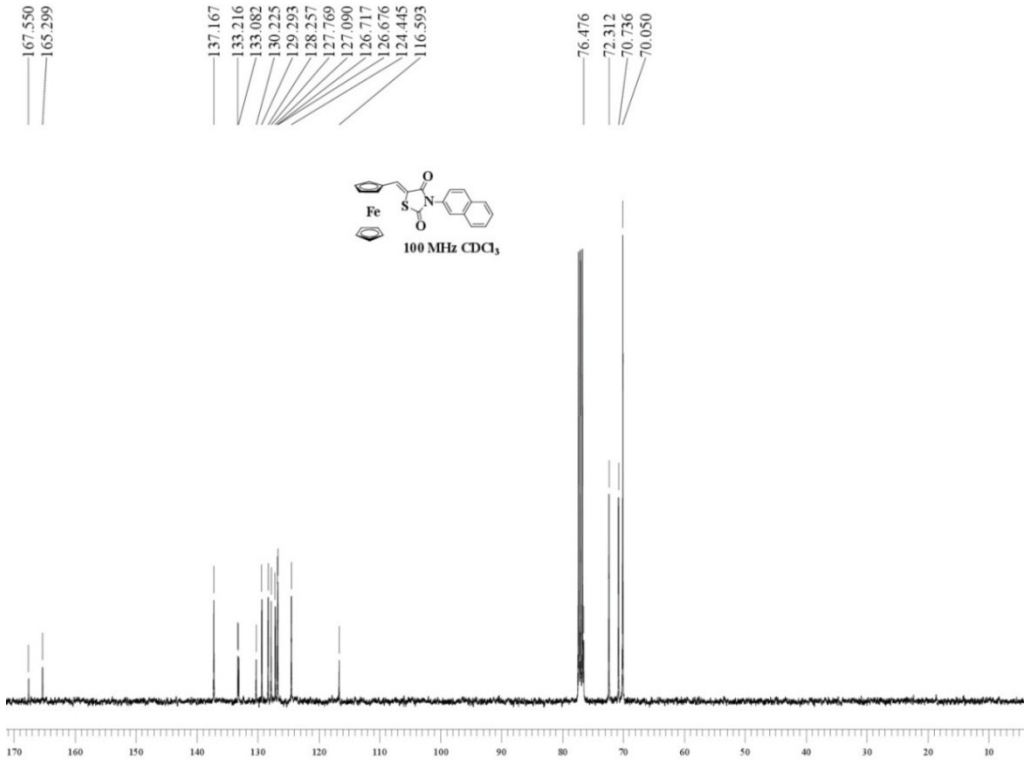


HRMS spectra of compound **3h**



^{1}H NMR spectrum of compound **3i**



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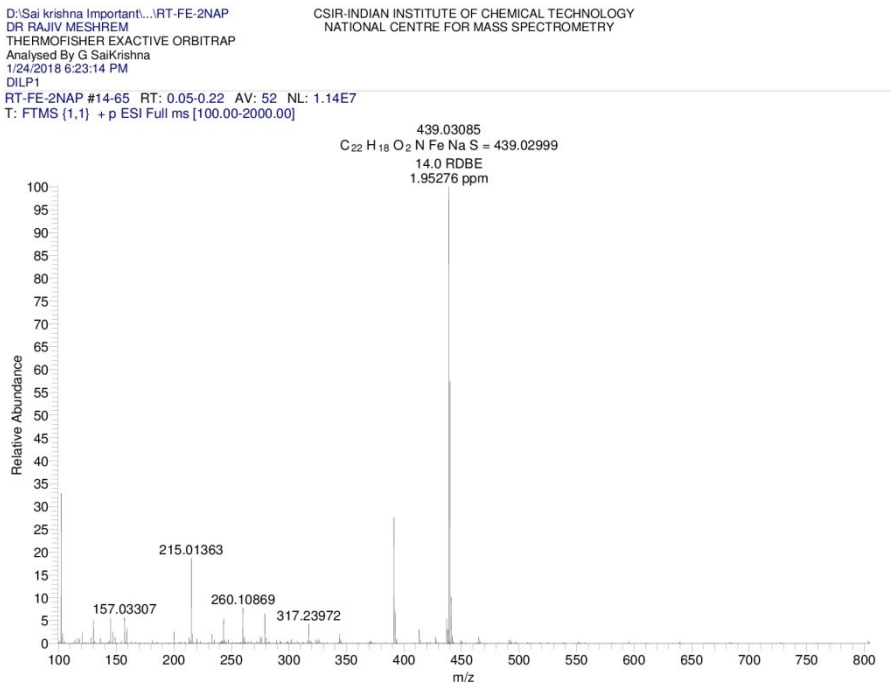

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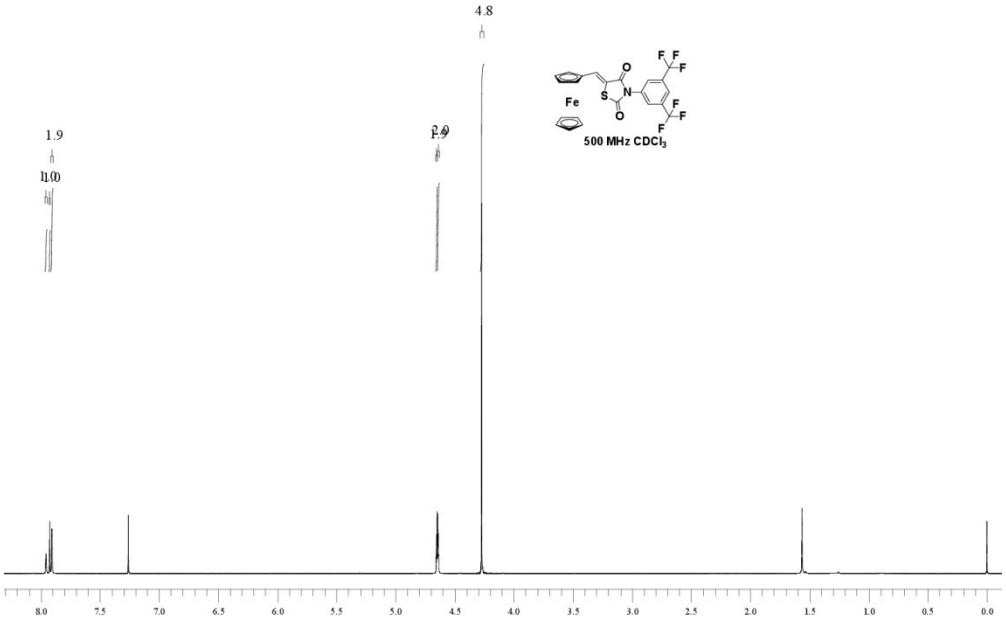

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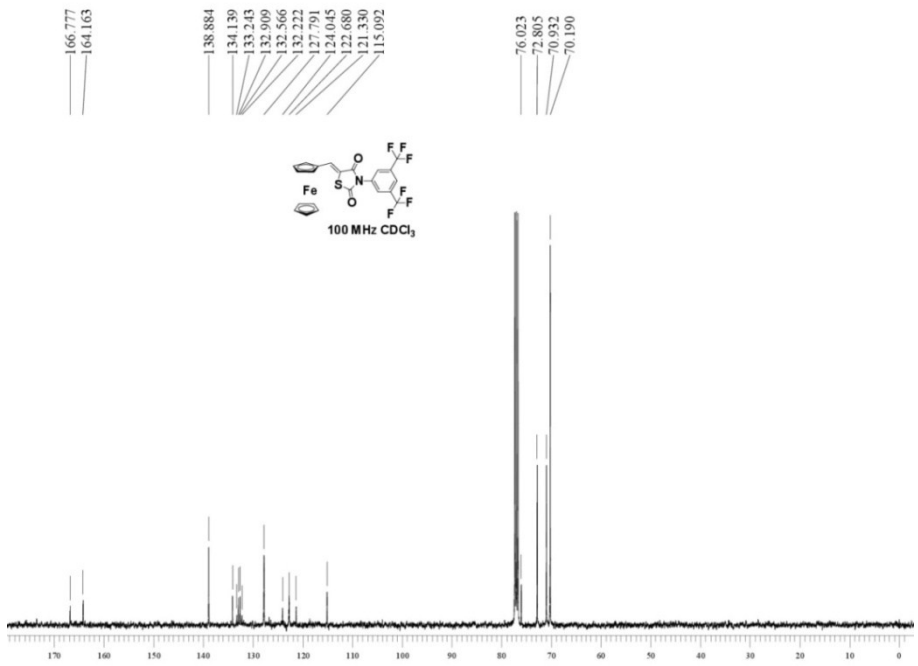

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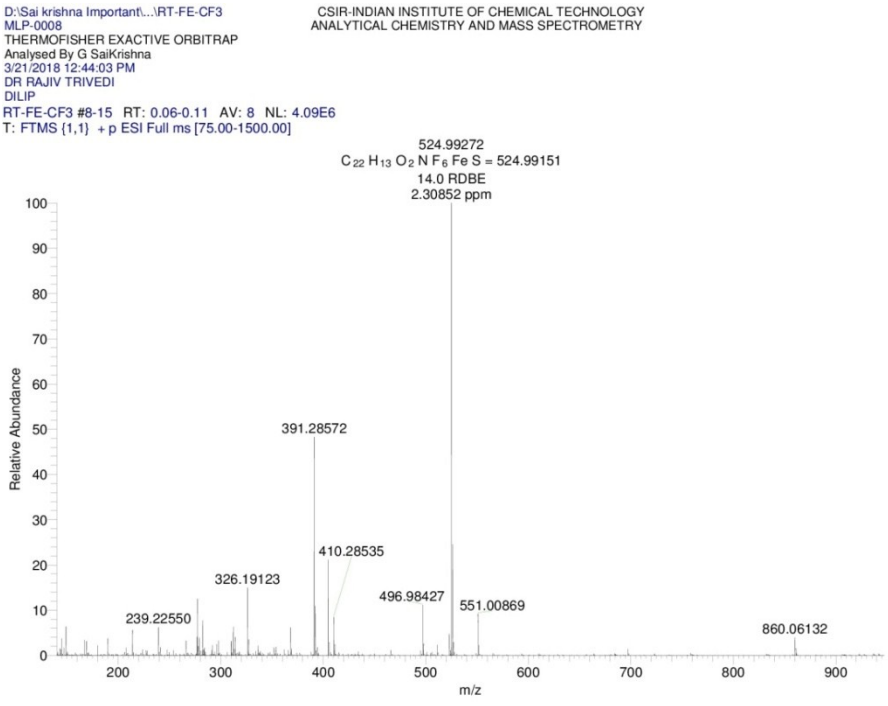
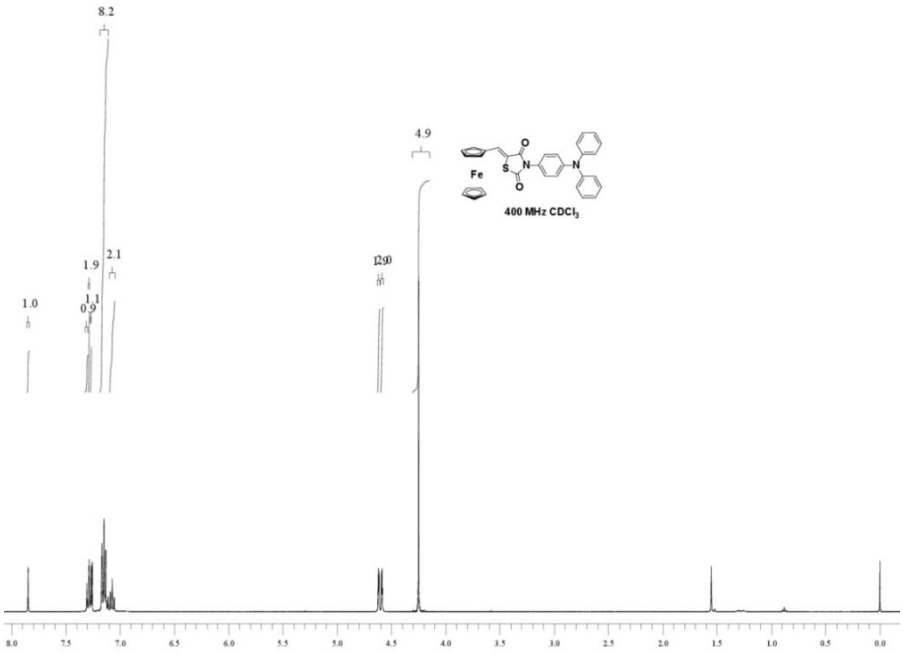
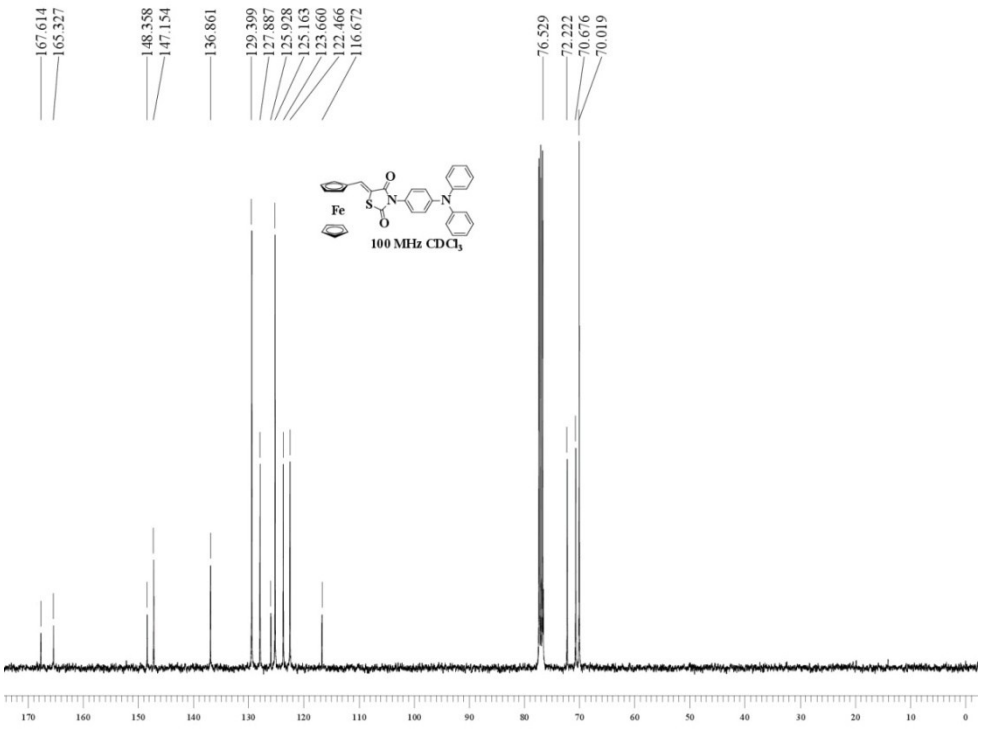


HRMS spectra of compound **3j**



^{1}H NMR spectrum of compound **3k**



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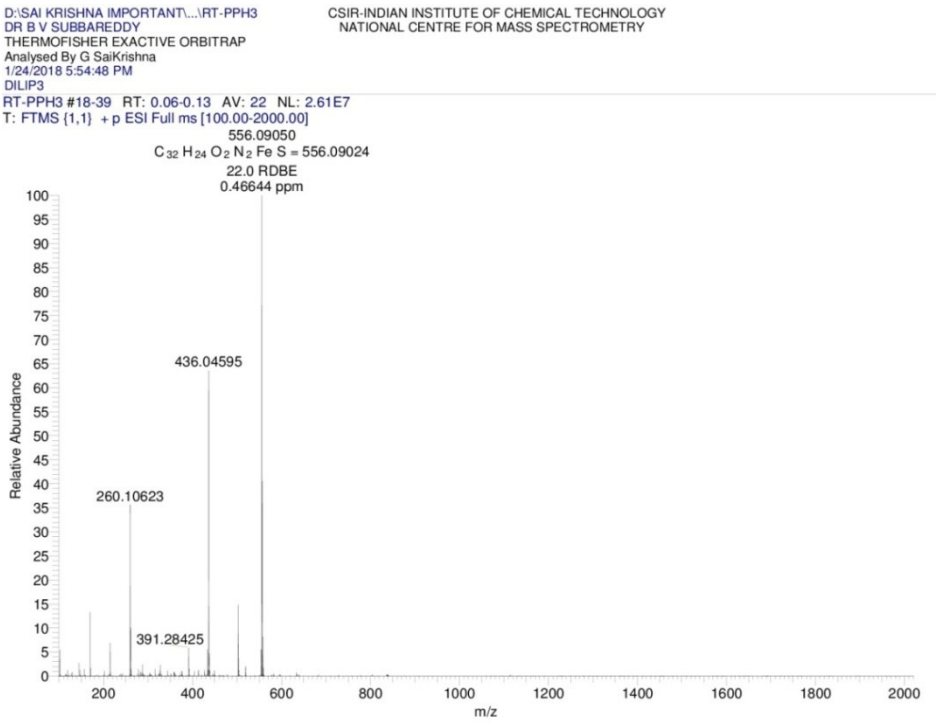
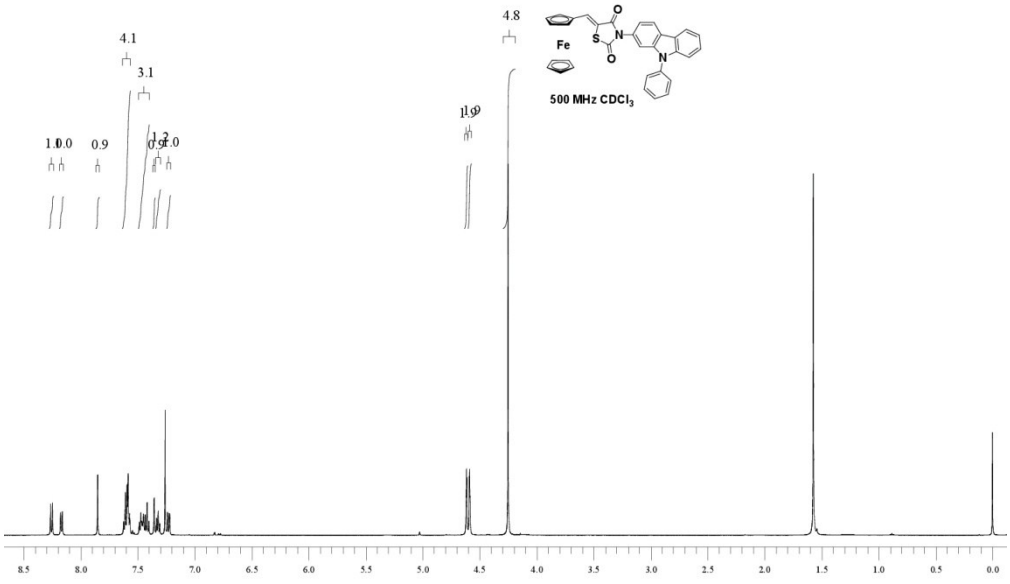
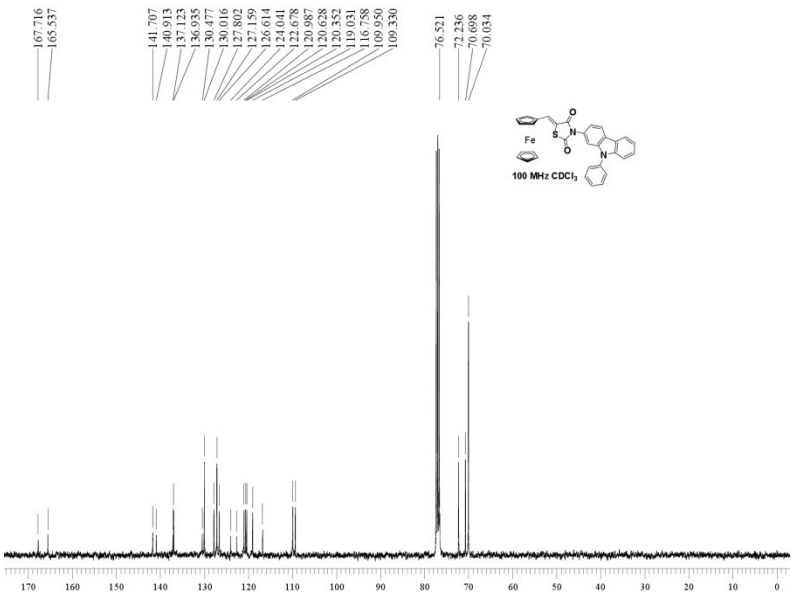


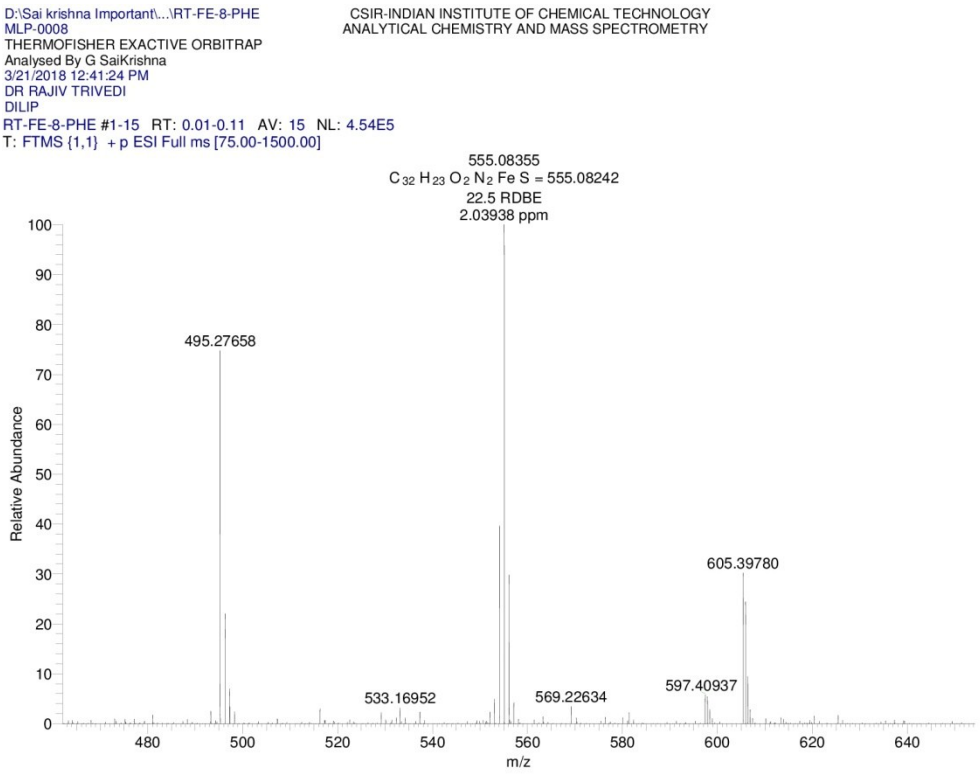
HRMS spectra of compound **3k**



^{1}H NMR spectrum of compound **3l**



^{13}C NMR spectrum of compound **3l**



HRMS spectra of compound **3l**

Crystal structure Data (3b)

Data for the compound (**3b**)was collected on Bruker D8 QUEST instrument at 100 K with an IμS Mo micro source (λ = 0.7107 A) and a PHOTON-100 detector. The raw data frames were reduced and corrected for absorption effects using the Bruker Apex 3 software suite programs [1].The structure was solved using intrinsic phasing method [2] and further refined with the SHELXL [2] program and expanded using Fourier techniques. Anisotropic displacement parameters were included for all non-hydrogen atoms. All C bound H atoms were positioned geometrically and treated as riding on their parent C atoms [C-H = 0.93-0.97 Å and $U_{iso}(H) = 1.2U_{eq}(C)$ for other H atoms].

Crystal Data for(3b): $C_{21}H_{17}FeNO_3S$ (M =419.29 g/mol): orthorhombic, space group $P2_12_12_1$ (no. 19), a = 6.7825(1) Å, b = 12.1423(2) Å, c = 22.2710(4) Å, V = 1834.13(5) Å^3, Z = 4, T = 100.15 K, μ(Mo Kα) = 0.958 mm^{-1}, $Dcalc$ = 1.5183 g/cm^3, 19852 reflections measured (4.96° ≤ 2Θ ≤ 61.06°), 5603 unique (R_{int} = 0.1029, R_{sigma} = 0.1306) which were used in all calculations. The final $R_1$was 0.0609 (I>2σ(I)) and wR_2 was 0.1098 (all data). CCDC1815428 contains supplementary Crystallographic data for the structure. These data can be obtained free of charge at www.ccdc.cam.ac.uk/conts/retrieving.html [or from the Cambridge Crystallographic Data Centre (CCDC), 12 Union Road, Cambridge CB2 1EZ, UK; fax: +44(0) 1223 336 033; email: deposit@ccdc.cam.ac.uk].

1. Bruker (2016). APEX3, SAINT and SADABS. Bruker AXS, Inc., Madison, Wisconsin, USA.
2. Sheldrick G. M. (2015**)** Acta Crystallogr C71: 3-8.

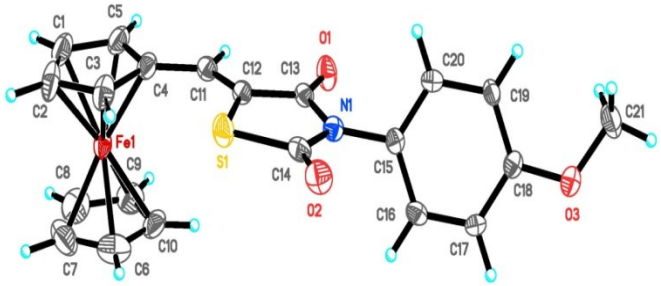


Figure 6: A view of (**3b**), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are represented by circles of arbitrary radii.

Table 1: Crystal data and structure refinement for (**3b**)

Identification code	3b	
Empirical formula	$C_{21}H_{17}FeNO_3S$	
Formula weight	419.27	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 6.78250(10) Å	α= 90°.
	b = 12.1423(2) Å	β= 90°.
	c = 22.2710(4) Å	γ = 90°.
Volume	1834.13(5) $Å^3$	
Z	4	
Density (calculated)	1.518 Mg/m^3	
Absorption coefficient	0.958 mm^{-1}	
F(000)	864	
Crystal size	0.280 x 0.260 x 0.120 mm^3	
θ range for data collection	2.482 to 30.534°.	
Index ranges	-9<=h<=9, -16<=k<=17, -31<=l<=31	
Reflections collected	19852	
Independent reflections	5603 [R(int) = 0.1029]	
Completeness to θ = 25.242°	99.9 %	

Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5603 / 0 / 246
Goodness-of-fit on F^2	0.981
Final R indices [I>2σ(I)]	R1 = 0.0607, wR2 = 0.0909
R indices (all data)	R1 = 0.1520, wR2 = 0.1108
Absolute structure parameter	0.06(3)
Largest diff. peak and hole	0.268 and -0.273 e.Å^{-3}

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for ka293_0m_a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	7962(10)	8888(5)	6920(3)	68(2)
C(2)	9529(10)	8697(5)	6526(3)	65(2)
C(3)	8931(9)	7917(4)	6093(2)	55(1)
C(4)	6935(7)	7620(4)	6222(2)	45(1)
C(5)	6375(10)	8241(4)	6740(2)	56(2)
C(6)	10547(11)	5937(6)	6918(3)	79(2)
C(7)	11125(11)	6678(7)	7364(4)	90(2)
C(8)	9596(14)	6805(6)	7770(3)	84(2)
C(9)	8074(10)	6134(6)	7574(3)	70(2)
C(10)	8686(11)	5600(5)	7052(3)	65(2)
C(11)	5682(7)	6812(4)	5946(2)	40(1)
C(12)	6010(7)	6172(4)	5463(2)	36(1)
C(13)	4567(7)	5327(4)	5271(2)	35(1)
C(14)	7155(7)	5060(4)	4566(2)	39(1)
C(15)	4292(6)	3825(4)	4517(2)	32(1)
C(16)	5084(6)	2781(4)	4532(2)	36(1)
C(17)	4086(6)	1921(4)	4278(2)	34(1)
C(18)	2262(7)	2098(4)	4009(2)	35(1)
C(19)	1471(7)	3144(4)	3990(2)	36(1)
C(20)	2499(6)	4011(4)	4246(2)	38(1)
C(21)	-458(8)	1356(5)	3457(3)	67(2)
Fe(1)	8734(1)	7254(1)	6926(1)	42(1)
N(1)	5328(5)	4722(3)	4793(2)	35(1)
O(1)	2965(5)	5175(3)	5487(2)	53(1)
O(2)	7957(5)	4684(3)	4138(2)	55(1)

O(3)	1357(5)	1193(3)	3773(2)	52(1)
S(1)	8113(2)	6140(1)	5012(1)	50(1)

Table 3. Bond lengths [Å] and angles [°] for **3b**_

C(1)-C(5)	1.391(8)
C(1)-C(2)	1.397(8)
C(1)-Fe(1)	2.051(6)
C(1)-H(1)	1.0000
C(2)-C(3)	1.412(7)
C(2)-Fe(1)	2.038(6)
C(2)-H(2)	1.0000
C(3)-C(4)	1.430(7)
C(3)-Fe(1)	2.026(5)
C(3)-H(3)	1.0000
C(4)-C(5)	1.429(7)
C(4)-C(11)	1.437(6)
C(4)-Fe(1)	2.035(5)
C(5)-Fe(1)	2.041(6)
C(5)-H(5)	1.0000
C(6)-C(10)	1.360(9)
C(6)-C(7)	1.396(10)
C(6)-Fe(1)	2.017(6)
C(6)-H(6)	1.0000
C(7)-C(8)	1.385(9)
C(7)-Fe(1)	2.018(6)
C(7)-H(7)	1.0000
C(8)-C(9)	1.386(9)
C(8)-Fe(1)	2.043(6)
C(8)-H(8)	1.0000
C(9)-C(10)	1.393(8)
C(9)-Fe(1)	2.034(6)
C(9)-H(9)	1.0000
C(10)-Fe(1)	2.029(6)
C(10)-H(10)	1.0000
C(11)-C(12)	1.345(6)
C(11)-H(11)	0.9500
C(12)-C(13)	1.481(6)

C(12)-S(1)	1.745(5)
C(13)-O(1)	1.202(5)
C(13)-N(1)	1.395(6)
C(14)-O(2)	1.189(5)
C(14)-N(1)	1.399(6)
C(14)-S(1)	1.769(5)
C(15)-C(20)	1.377(6)
C(15)-C(16)	1.378(6)
C(15)-N(1)	1.434(6)
C(16)-C(17)	1.367(6)
C(16)-H(16)	0.9500
C(17)-C(18)	1.391(6)
C(17)-H(17)	0.9500
C(18)-O(3)	1.363(5)
C(18)-C(19)	1.379(7)
C(19)-C(20)	1.386(6)
C(19)-H(19)	0.9500
C(20)-H(20)	0.9500
C(21)-O(3)	1.433(6)
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800

C(5)-C(1)-C(2)	108.3(5)
C(5)-C(1)-Fe(1)	69.7(3)
C(2)-C(1)-Fe(1)	69.5(4)
C(5)-C(1)-H(1)	125.8
C(2)-C(1)-H(1)	125.8
Fe(1)-C(1)-H(1)	125.8
C(1)-C(2)-C(3)	108.8(5)
C(1)-C(2)-Fe(1)	70.5(3)
C(3)-C(2)-Fe(1)	69.2(3)
C(1)-C(2)-H(2)	125.6
C(3)-C(2)-H(2)	125.6
Fe(1)-C(2)-H(2)	125.6
C(2)-C(3)-C(4)	107.6(5)
C(2)-C(3)-Fe(1)	70.1(3)
C(4)-C(3)-Fe(1)	69.7(3)

C(2)-C(3)-H(3)	126.2
C(4)-C(3)-H(3)	126.2
Fe(1)-C(3)-H(3)	126.2
C(5)-C(4)-C(3)	106.3(5)
C(5)-C(4)-C(11)	123.3(5)
C(3)-C(4)-C(11)	130.2(5)
C(5)-C(4)-Fe(1)	69.7(3)
C(3)-C(4)-Fe(1)	69.1(3)
C(11)-C(4)-Fe(1)	122.4(3)
C(1)-C(5)-C(4)	108.9(6)
C(1)-C(5)-Fe(1)	70.5(4)
C(4)-C(5)-Fe(1)	69.2(3)
C(1)-C(5)-H(5)	125.5
C(4)-C(5)-H(5)	125.5
Fe(1)-C(5)-H(5)	125.5
C(10)-C(6)-C(7)	107.4(7)
C(10)-C(6)-Fe(1)	70.8(4)
C(7)-C(6)-Fe(1)	69.8(4)
C(10)-C(6)-H(6)	126.3
C(7)-C(6)-H(6)	126.3
Fe(1)-C(6)-H(6)	126.3
C(8)-C(7)-C(6)	109.0(6)
C(8)-C(7)-Fe(1)	71.0(4)
C(6)-C(7)-Fe(1)	69.7(4)
C(8)-C(7)-H(7)	125.5
C(6)-C(7)-H(7)	125.5
Fe(1)-C(7)-H(7)	125.5
C(9)-C(8)-C(7)	106.7(6)
C(9)-C(8)-Fe(1)	69.8(3)
C(7)-C(8)-Fe(1)	69.1(4)
C(9)-C(8)-H(8)	126.7
C(7)-C(8)-H(8)	126.7
Fe(1)-C(8)-H(8)	126.7
C(8)-C(9)-C(10)	108.3(6)
C(8)-C(9)-Fe(1)	70.5(4)
C(10)-C(9)-Fe(1)	69.7(3)
C(8)-C(9)-H(9)	125.8
C(10)-C(9)-H(9)	125.8

Fe(1)-C(9)-H(9)	125.8
C(6)-C(10)-C(9)	108.6(6)
C(6)-C(10)-Fe(1)	69.9(4)
C(9)-C(10)-Fe(1)	70.1(3)
C(6)-C(10)-H(10)	125.7
C(9)-C(10)-H(10)	125.7
Fe(1)-C(10)-H(10)	125.7
C(12)-C(11)-C(4)	129.7(5)
C(12)-C(11)-H(11)	115.1
C(4)-C(11)-H(11)	115.1
C(11)-C(12)-C(13)	121.4(4)
C(11)-C(12)-S(1)	127.5(4)
C(13)-C(12)-S(1)	111.1(3)
O(1)-C(13)-N(1)	124.0(5)
O(1)-C(13)-C(12)	126.1(5)
N(1)-C(13)-C(12)	109.9(4)
O(2)-C(14)-N(1)	125.5(5)
O(2)-C(14)-S(1)	124.5(4)
N(1)-C(14)-S(1)	109.9(4)
C(20)-C(15)-C(16)	120.4(5)
C(20)-C(15)-N(1)	119.8(4)
C(16)-C(15)-N(1)	119.8(4)
C(17)-C(16)-C(15)	120.0(4)
C(17)-C(16)-H(16)	120.0
C(15)-C(16)-H(16)	120.0
C(16)-C(17)-C(18)	120.1(4)
C(16)-C(17)-H(17)	120.0
C(18)-C(17)-H(17)	120.0
O(3)-C(18)-C(19)	123.7(4)
O(3)-C(18)-C(17)	116.2(4)
C(19)-C(18)-C(17)	120.1(5)
C(18)-C(19)-C(20)	119.4(4)
C(18)-C(19)-H(19)	120.3
C(20)-C(19)-H(19)	120.3
C(15)-C(20)-C(19)	120.1(5)
C(15)-C(20)-H(20)	120.0
C(19)-C(20)-H(20)	120.0
O(3)-C(21)-H(21A)	109.5

O(3)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
O(3)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(6)-Fe(1)-C(7)	40.5(3)
C(6)-Fe(1)-C(3)	105.5(3)
C(7)-Fe(1)-C(3)	121.8(3)
C(6)-Fe(1)-C(10)	39.3(3)
C(7)-Fe(1)-C(10)	66.6(3)
C(3)-Fe(1)-C(10)	121.4(2)
C(6)-Fe(1)-C(9)	67.0(3)
C(7)-Fe(1)-C(9)	66.5(3)
C(3)-Fe(1)-C(9)	158.4(3)
C(10)-Fe(1)-C(9)	40.1(2)
C(6)-Fe(1)-C(4)	122.1(3)
C(7)-Fe(1)-C(4)	158.4(3)
C(3)-Fe(1)-C(4)	41.2(2)
C(10)-Fe(1)-C(4)	108.3(2)
C(9)-Fe(1)-C(4)	124.1(2)
C(6)-Fe(1)-C(2)	121.1(3)
C(7)-Fe(1)-C(2)	107.3(3)
C(3)-Fe(1)-C(2)	40.7(2)
C(10)-Fe(1)-C(2)	156.4(3)
C(9)-Fe(1)-C(2)	160.7(3)
C(4)-Fe(1)-C(2)	68.6(2)
C(6)-Fe(1)-C(5)	160.3(3)
C(7)-Fe(1)-C(5)	158.7(3)
C(3)-Fe(1)-C(5)	68.5(2)
C(10)-Fe(1)-C(5)	126.6(3)
C(9)-Fe(1)-C(5)	111.4(3)
C(4)-Fe(1)-C(5)	41.05(19)
C(2)-Fe(1)-C(5)	67.3(3)
C(6)-Fe(1)-C(8)	67.8(3)
C(7)-Fe(1)-C(8)	39.9(3)
C(3)-Fe(1)-C(8)	158.4(3)
C(10)-Fe(1)-C(8)	67.2(3)
C(9)-Fe(1)-C(8)	39.7(3)

C(4)-Fe(1)-C(8)	159.8(3)
C(2)-Fe(1)-C(8)	123.8(3)
C(5)-Fe(1)-C(8)	124.6(3)
C(6)-Fe(1)-C(1)	157.2(3)
C(7)-Fe(1)-C(1)	122.9(3)
C(3)-Fe(1)-C(1)	68.1(2)
C(10)-Fe(1)-C(1)	162.6(3)
C(9)-Fe(1)-C(1)	126.6(3)
C(4)-Fe(1)-C(1)	68.3(2)
C(2)-Fe(1)-C(1)	40.0(2)
C(5)-Fe(1)-C(1)	39.7(2)
C(8)-Fe(1)-C(1)	109.7(3)
C(13)-N(1)-C(14)	116.7(4)
C(13)-N(1)-C(15)	123.1(4)
C(14)-N(1)-C(15)	120.2(4)
C(18)-O(3)-C(21)	117.7(4)
C(12)-S(1)-C(14)	92.3(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for(**3b)**The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	102(5)	38(4)	65(4)	-8(4)	-23(4)	-10(3)
C(2)	91(4)	50(4)	55(4)	4(3)	-11(3)	-38(4)
C(3)	80(4)	48(4)	37(3)	9(3)	-3(3)	-20(3)
C(4)	61(3)	33(3)	41(3)	4(2)	-10(2)	-5(3)
C(5)	78(4)	35(3)	55(3)	-7(3)	-9(3)	1(3)
C(6)	84(5)	86(6)	67(4)	15(5)	8(4)	28(4)
C(7)	62(4)	100(6)	107(6)	39(5)	-35(5)	-17(4)
C(8)	135(7)	76(5)	42(4)	4(3)	-35(4)	5(5)
C(9)	77(4)	72(5)	62(4)	29(4)	3(4)	-4(4)
C(10)	94(5)	35(3)	65(4)	7(3)	-24(4)	1(4)
C(11)	44(3)	40(3)	35(3)	2(2)	-6(2)	2(2)
C(12)	39(3)	35(3)	34(2)	1(2)	-6(2)	2(2)
C(13)	37(3)	38(3)	31(3)	-1(2)	-6(2)	2(2)
C(14)	29(2)	45(3)	42(3)	5(3)	1(2)	5(2)
C(15)	34(3)	37(3)	24(2)	-2(2)	2(2)	0(2)
C(16)	30(2)	46(3)	33(2)	0(3)	0(2)	7(3)
C(17)	36(3)	29(3)	37(2)	2(2)	1(2)	7(2)
C(18)	41(3)	35(3)	28(2)	-3(2)	5(2)	-1(2)
C(19)	30(2)	41(3)	37(3)	-7(2)	-8(2)	-1(2)
C(20)	38(3)	36(3)	39(3)	5(2)	-2(2)	7(2)
C(21)	66(4)	65(4)	71(4)	0(3)	-32(3)	-14(3)
Fe(1)	54(1)	38(1)	34(1)	0(1)	-7(1)	-11(1)
N(1)	36(2)	38(3)	32(2)	-1(2)	0(2)	3(2)
O(1)	38(2)	69(3)	51(2)	-15(2)	7(2)	-12(2)
O(2)	38(2)	69(3)	57(2)	-12(2)	12(2)	6(2)
O(3)	52(2)	39(2)	64(2)	-9(2)	-8(2)	-5(2)
S(1)	39(1)	53(1)	57(1)	-4(1)	2(1)	-10(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for ka293_0m_a.

	x	y	z	U(eq)
H(1)	7984	9394	7274	82
H(2)	10860	9049	6550	78
H(3)	9749	7630	5753	66
H(5)	5063	8207	6944	67
H(6)	11367	5682	6572	95
H(7)	12435	7054	7387	108
H(8)	9596	7281	8136	101
H(9)	6764	6043	7774	84
H(10)	7888	5061	6815	78
H(11)	4433	6716	6132	48
H(16)	6323	2658	4719	43
H(17)	4638	1202	4284	41
H(19)	232	3268	3803	43
H(20)	1965	4734	4234	45
H(21A)	-1450	1656	3732	101
H(21B)	-920	651	3296	101
H(21C)	-246	1874	3125	101

Table 6. Torsion angles [°] for (**3b**)

C(5)-C(1)-C(2)-C(3)	-0.3(7)
Fe(1)-C(1)-C(2)-C(3)	58.9(4)
C(5)-C(1)-C(2)-Fe(1)	-59.1(4)
C(1)-C(2)-C(3)-C(4)	0.2(7)
Fe(1)-C(2)-C(3)-C(4)	59.9(4)
C(1)-C(2)-C(3)-Fe(1)	-59.7(4)
C(2)-C(3)-C(4)-C(5)	-0.1(6)
Fe(1)-C(3)-C(4)-C(5)	60.0(3)
C(2)-C(3)-C(4)-C(11)	-175.5(5)
Fe(1)-C(3)-C(4)-C(11)	-115.3(5)
C(2)-C(3)-C(4)-Fe(1)	-60.1(4)
C(2)-C(1)-C(5)-C(4)	0.2(7)
Fe(1)-C(1)-C(5)-C(4)	-58.8(4)
C(2)-C(1)-C(5)-Fe(1)	59.0(4)
C(3)-C(4)-C(5)-C(1)	-0.1(6)
C(11)-C(4)-C(5)-C(1)	175.7(5)
Fe(1)-C(4)-C(5)-C(1)	59.6(4)
C(3)-C(4)-C(5)-Fe(1)	-59.6(3)
C(11)-C(4)-C(5)-Fe(1)	116.1(5)
C(10)-C(6)-C(7)-C(8)	-0.7(8)
Fe(1)-C(6)-C(7)-C(8)	60.4(5)
C(10)-C(6)-C(7)-Fe(1)	-61.1(4)
C(6)-C(7)-C(8)-C(9)	0.3(8)
Fe(1)-C(7)-C(8)-C(9)	60.0(5)
C(6)-C(7)-C(8)-Fe(1)	-59.6(5)
C(7)-C(8)-C(9)-C(10)	0.2(7)
Fe(1)-C(8)-C(9)-C(10)	59.7(4)
C(7)-C(8)-C(9)-Fe(1)	-59.5(5)
C(7)-C(6)-C(10)-C(9)	0.8(7)
Fe(1)-C(6)-C(10)-C(9)	-59.7(4)
C(7)-C(6)-C(10)-Fe(1)	60.5(5)
C(8)-C(9)-C(10)-C(6)	-0.6(7)
Fe(1)-C(9)-C(10)-C(6)	59.5(4)
C(8)-C(9)-C(10)-Fe(1)	-60.2(4)
C(5)-C(4)-C(11)-C(12)	-179.9(5)
C(3)-C(4)-C(11)-C(12)	-5.2(9)

Fe(1)-C(4)-C(11)-C(12)	-94.2(6)
C(4)-C(11)-C(12)-C(13)	175.7(4)
C(4)-C(11)-C(12)-S(1)	-0.6(8)
C(11)-C(12)-C(13)-O(1)	5.2(8)
S(1)-C(12)-C(13)-O(1)	-177.9(4)
C(11)-C(12)-C(13)-N(1)	-175.2(4)
S(1)-C(12)-C(13)-N(1)	1.7(5)
C(20)-C(15)-C(16)-C(17)	-0.1(7)
N(1)-C(15)-C(16)-C(17)	179.0(4)
C(15)-C(16)-C(17)-C(18)	-0.7(7)
C(16)-C(17)-C(18)-O(3)	-179.2(4)
C(16)-C(17)-C(18)-C(19)	1.1(7)
O(3)-C(18)-C(19)-C(20)	179.6(4)
C(17)-C(18)-C(19)-C(20)	-0.7(7)
C(16)-C(15)-C(20)-C(19)	0.5(7)
N(1)-C(15)-C(20)-C(19)	-178.7(4)
C(18)-C(19)-C(20)-C(15)	-0.1(7)
O(1)-C(13)-N(1)-C(14)	175.3(5)
C(12)-C(13)-N(1)-C(14)	-4.3(5)
O(1)-C(13)-N(1)-C(15)	-1.9(7)
C(12)-C(13)-N(1)-C(15)	178.5(4)
O(2)-C(14)-N(1)-C(13)	-175.0(5)
S(1)-C(14)-N(1)-C(13)	4.9(5)
O(2)-C(14)-N(1)-C(15)	2.3(7)
S(1)-C(14)-N(1)-C(15)	-177.8(3)
C(20)-C(15)-N(1)-C(13)	61.3(6)
C(16)-C(15)-N(1)-C(13)	-117.9(5)
C(20)-C(15)-N(1)-C(14)	-115.8(5)
C(16)-C(15)-N(1)-C(14)	65.0(6)
C(19)-C(18)-O(3)-C(21)	4.0(7)
C(17)-C(18)-O(3)-C(21)	-175.8(4)
C(11)-C(12)-S(1)-C(14)	177.5(5)
C(13)-C(12)-S(1)-C(14)	0.8(4)
O(2)-C(14)-S(1)-C(12)	176.8(5)
N(1)-C(14)-S(1)-C(12)	-3.1(4)

Symmetry transformations used to generate equivalent atoms:

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) **(3b)**

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No syntax errors found. CIF dictionary interpreting this report

Datablock: (3b)

Bond precision: C-C = 0.0078 A Wavelength=0.71073

Cell: a=6.7825(1) b=12.1423(2) c=22.2710(4)

alpha=90 beta=90 gamma=90

Temperature: 100 K

Calculated Reported

Volume 1834.13(5) 1834.13(5)

Space group P 21 21 21 P 21 21 21

Hall group P 2ac 2ab P 2ac 2ab

Moiety formula C21 H17 Fe N O3 S C21 H17 Fe N O3 S

Sum formula C21 H17 Fe N O3 S C21 H17 Fe N O3 S

Mr 419.27 419.27

Dx,g cm-3 1.518 1.518

Z 4 4

Mu (mm-1) 0.958 0.958

F000 864.0 864.0

F000’ 866.18

h,k,lmax 9,17,31 9,17,31

Nref 5614[3197] 5603

Tmin,Tmax 0.765,0.891 0.655,0.746

Tmin’ 0.765

Correction method= # Reported T Limits: Tmin=0.655 Tmax=0.746

AbsCorr = MULTI-SCAN

Data completeness= 1.75/1.00 Theta(max)= 30.534

R(reflections)= 0.0609(3010) wR2(reflections)= 0.1080(5603)

S = 1.004 Npar= 246

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.

Alert level C

PLAT241_ALERT_2_C High ’MainMol’ Ueq as Compared to Neighbors of C7 Check

PLAT241_ALERT_2_C High ’MainMol’ Ueq as Compared to Neighbors of C8 Check

PLAT242_ALERT_2_C Low ’MainMol’ Ueq as Compared to Neighbors of Fe1 Check

PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00784 Ang.

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 4.493 Check

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.022 Check

PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.0 Info

Alert level G

PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 2 Note

PLAT912_ALERT_4_G Missing # of FCF Reflections AboveSTh/L= 0.600 6 Note

0 **ALERT level A** = Most likely a serious problem - resolve or explain

0 **ALERT level B** = A potentially serious problem, consider carefully

7 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

2 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

4 ALERT type 2 Indicator that the structure model may be wrong or deficient

4 ALERT type 3 Indicator that the structure quality may be low

1 ALERT type 4 Improvement, methodology, query or suggestion

0 ALERT type 5 Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

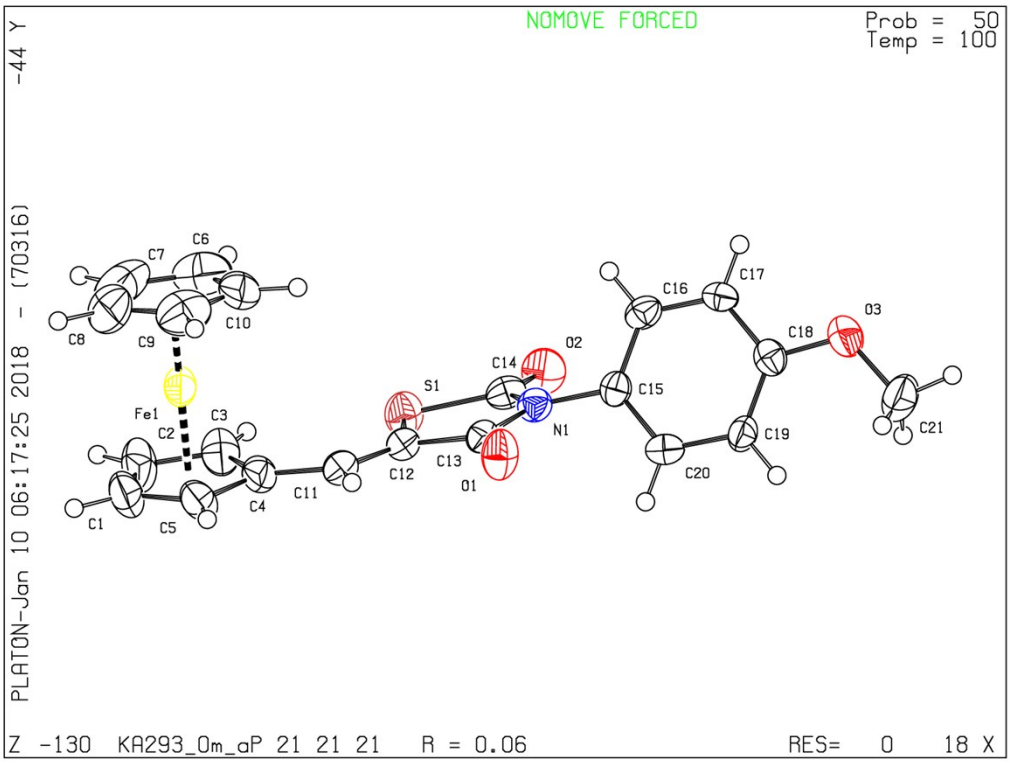
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 13/12/2017; check.def file version of 12/12/2017

Datablock(3b)ellipsoid plot



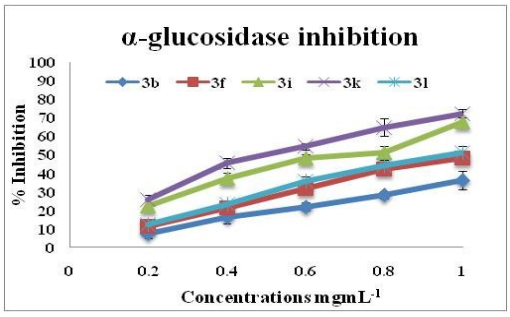


Figure 7: Anti-diabetic activity by α-glucosidase inhibition (**3b, 3f, 3i, 3k, 3l**).