Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Synthesis, characterization and antimicrobial evaluation of ferrocene-oxime ether benzyl 1*H*-1,2,3-triazole hybrids

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Contents

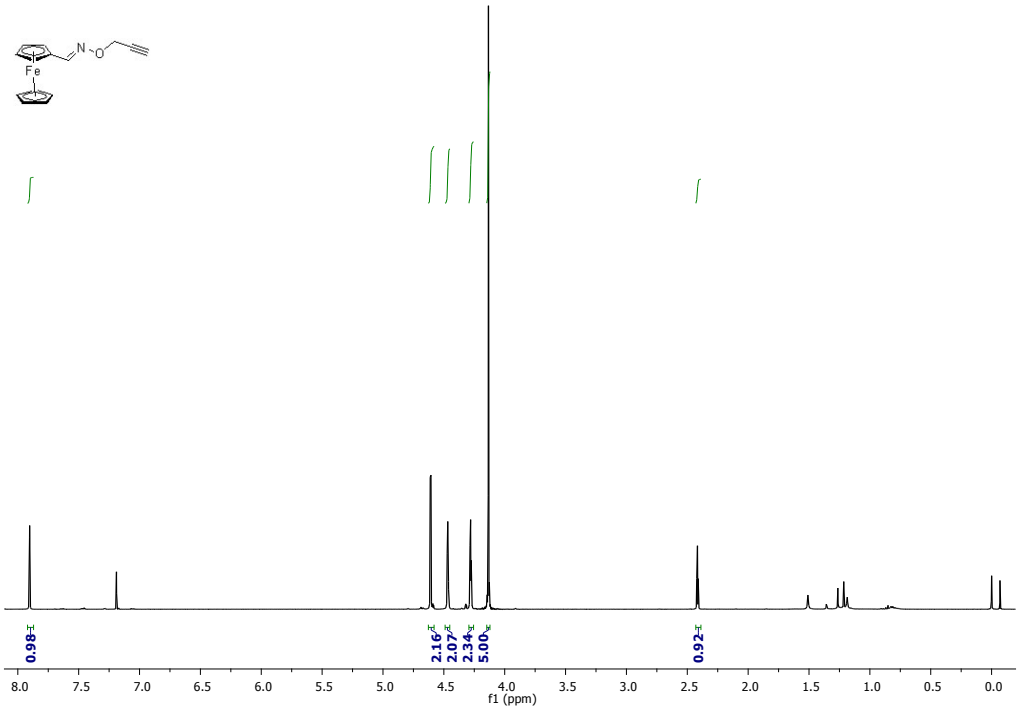

Figure S1: ^{1}H NMR spectra of 3

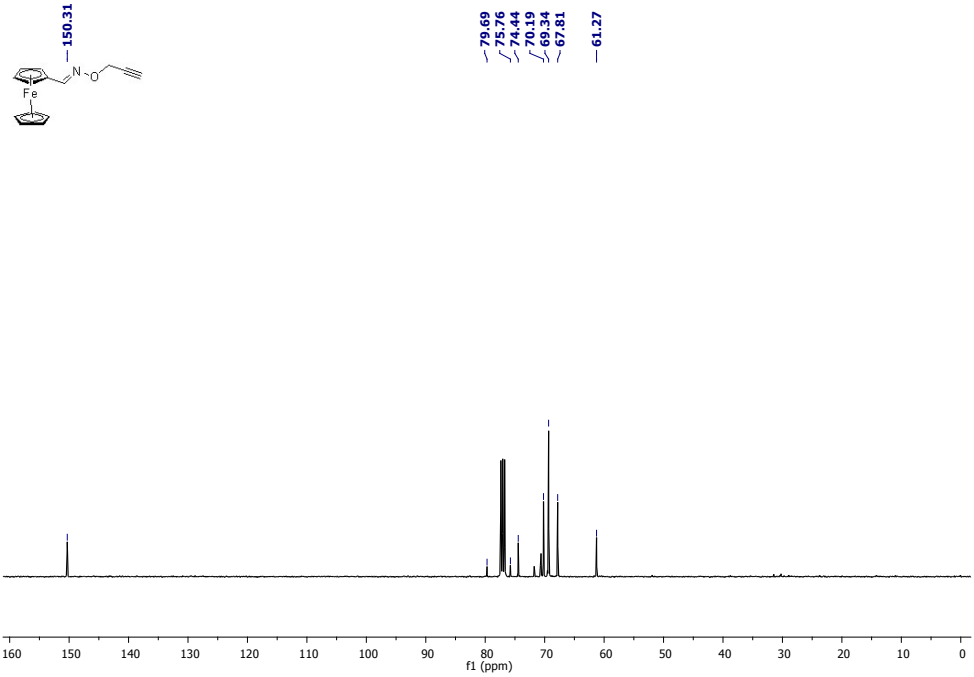

Figure S2: ^{13}C NMR spectra of 3

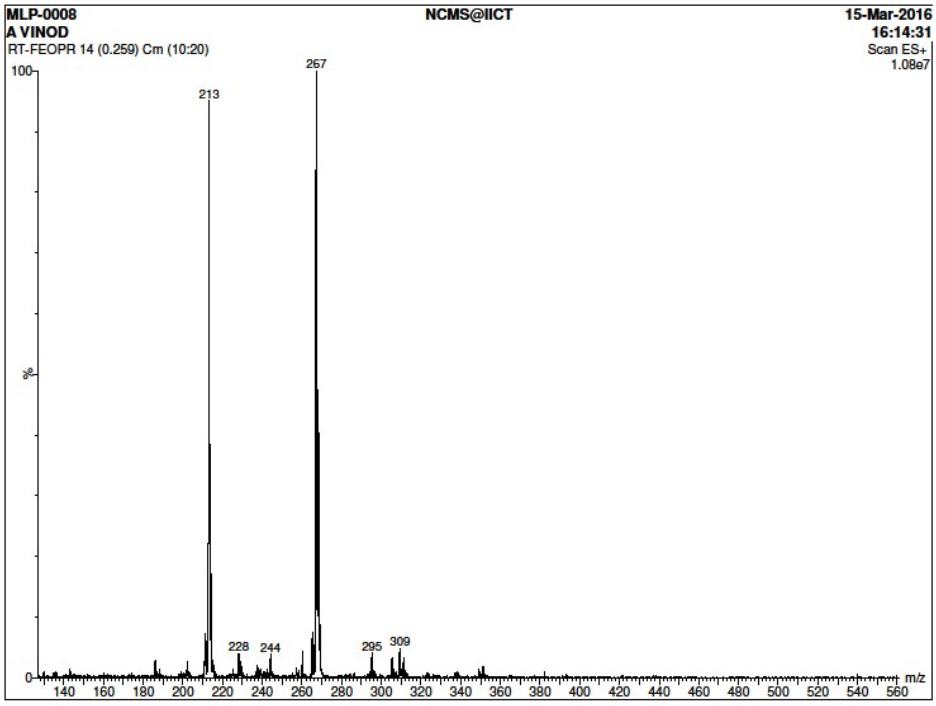

Figure S3: ESI-MS spectra of 3

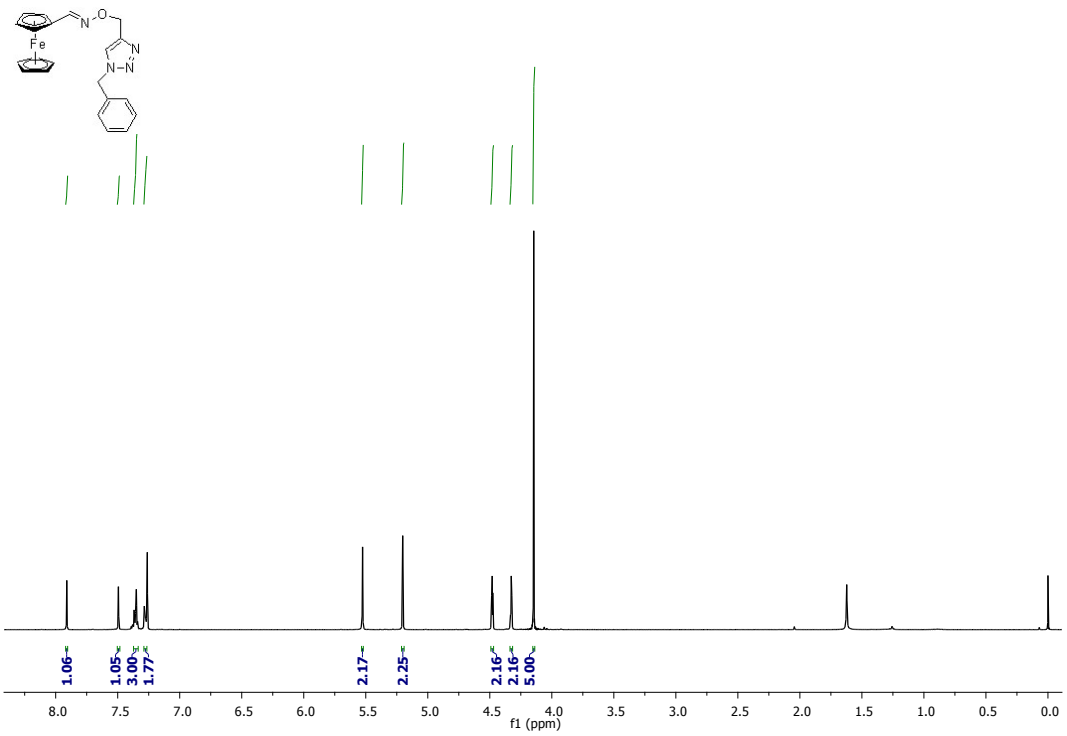

Figure S4: ^{1}H NMR spectra of 5a

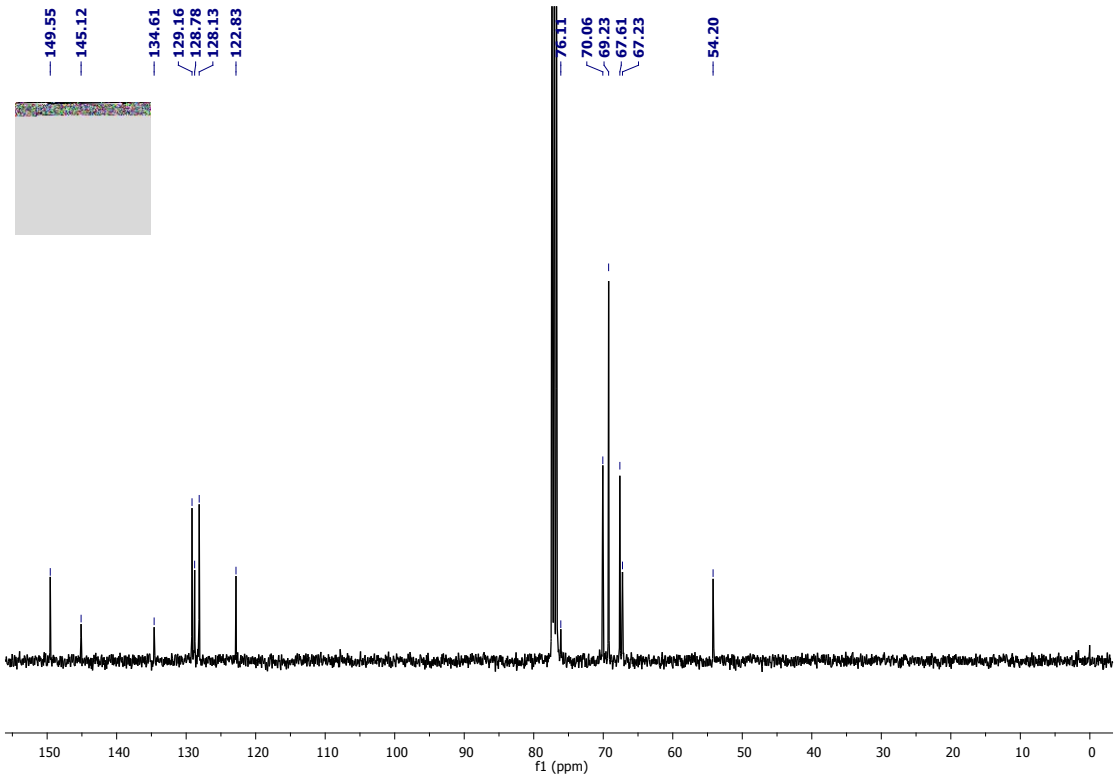

Figure S5: ^{13}C NMR spectra of 5a

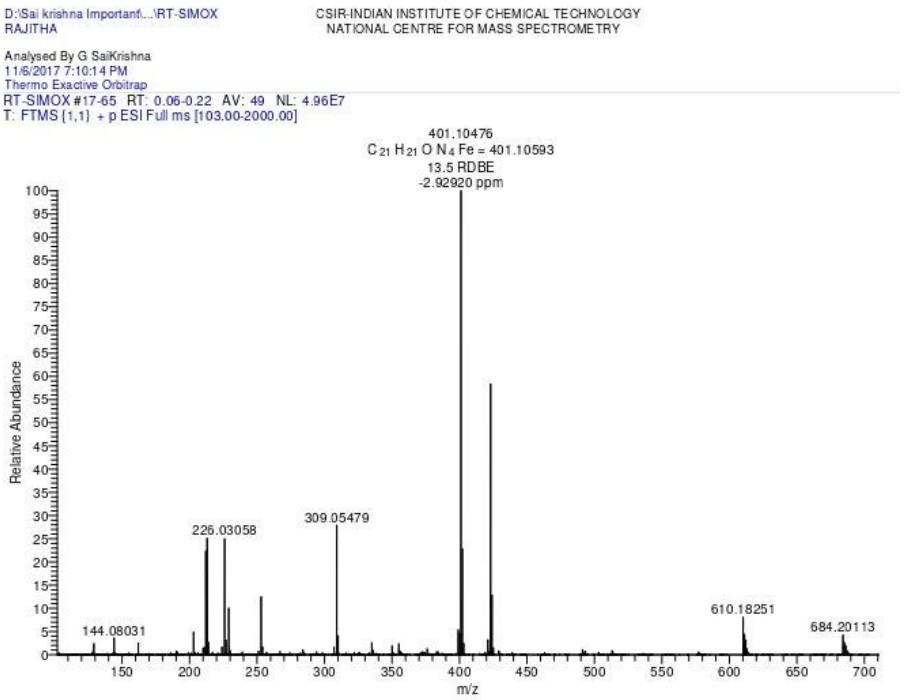

Figure S6: HRMS spectra of 5a

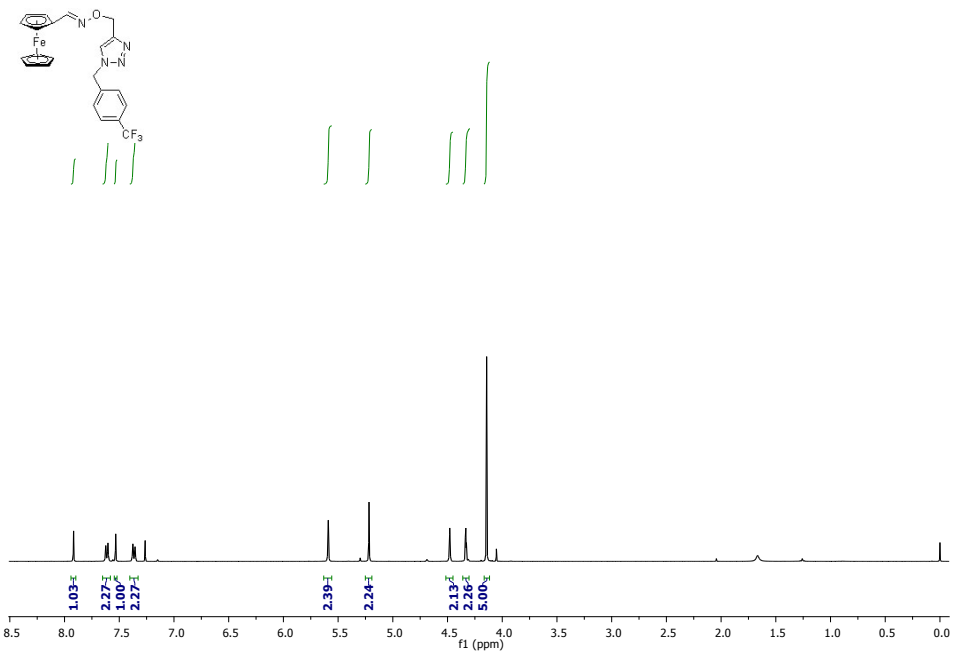

Figure S7: ^{1}H NMR spectra of 5b

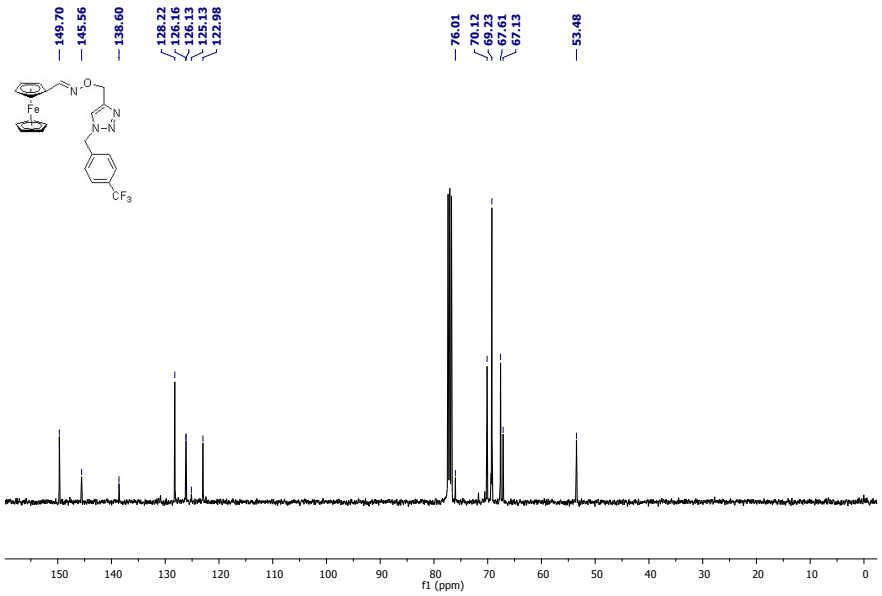

Figure S8: ^{13}C NMR spectra of 5b

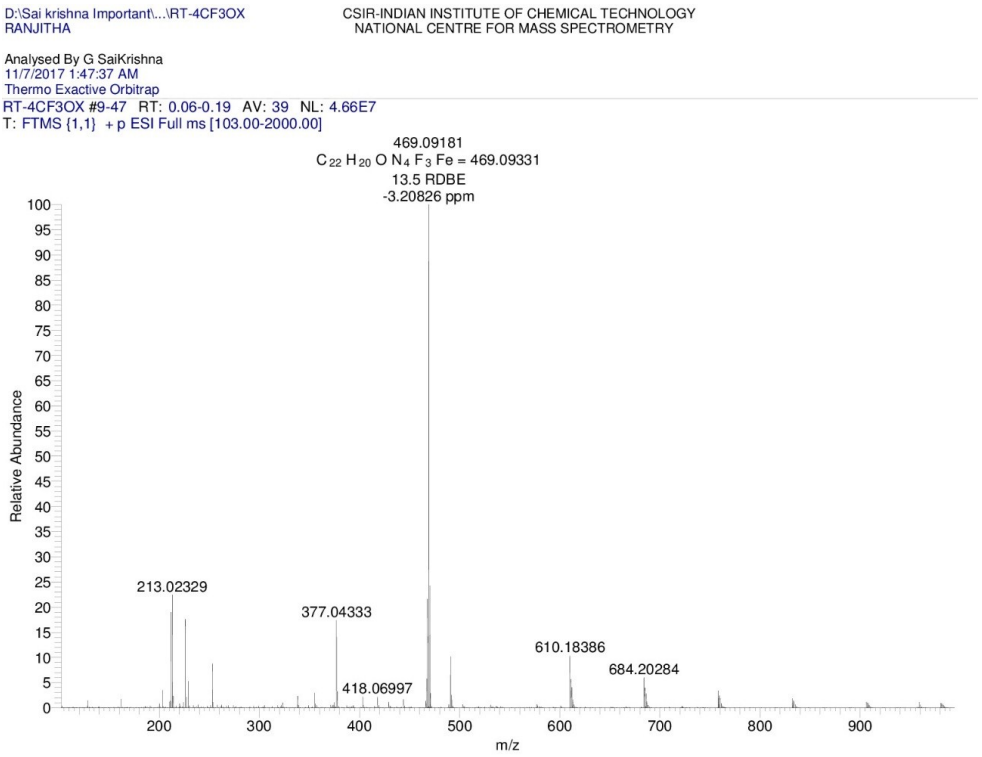

Figure S9: HRMS spectra of 5b

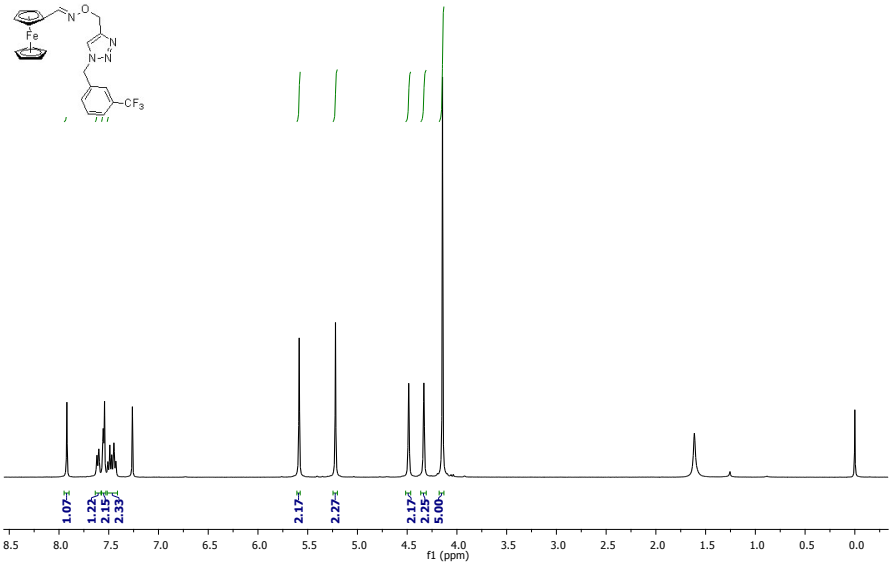

Figure S10: ^{1}H NMR spectra of 5c

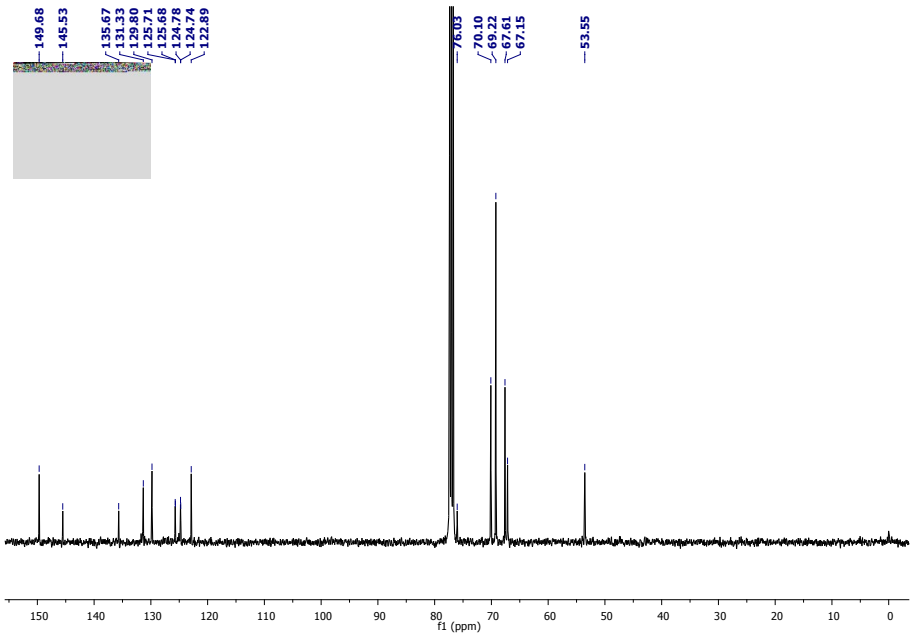

Figure S11: ^{13}C NMR spectra of 5c

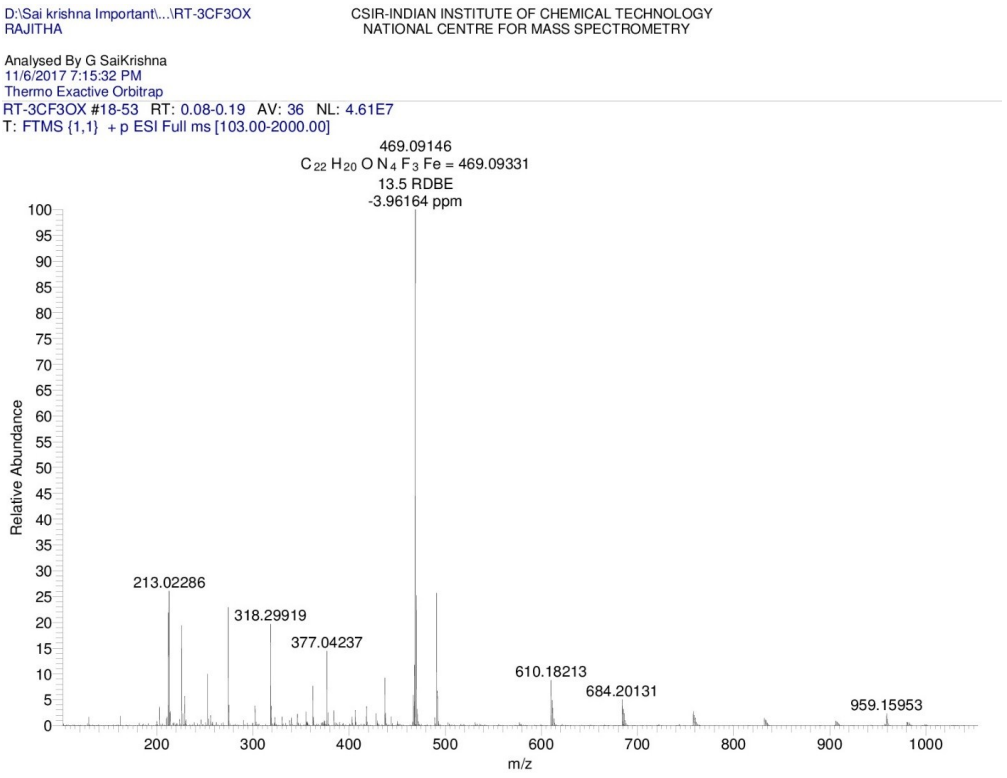

Figure S12: HRMS spectra of 5c

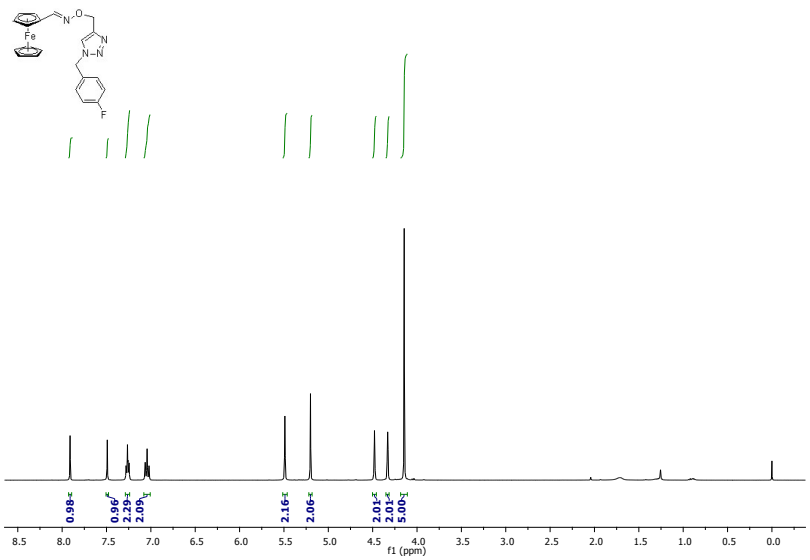

Figure S13: ^{1}H NMR spectra of 5d

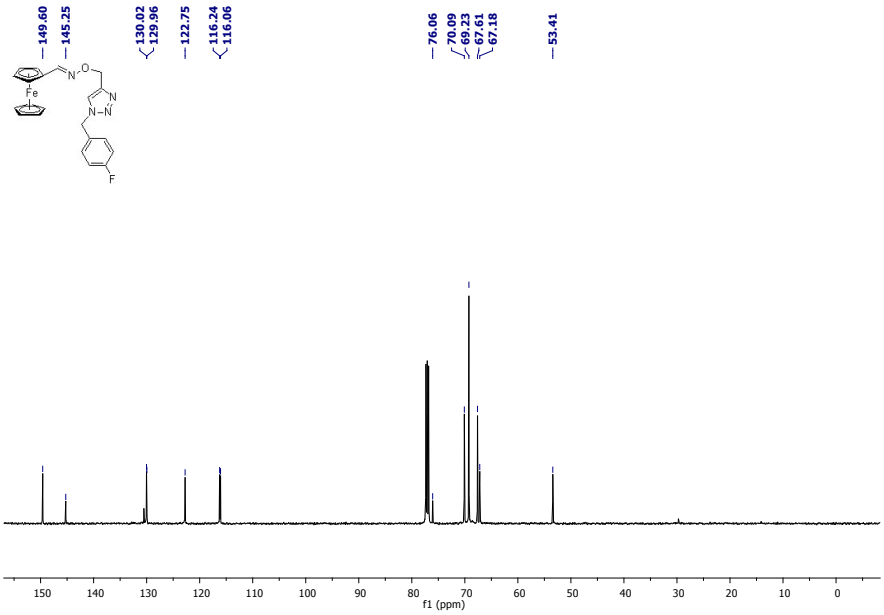

Figure S14: ^{13}C NMR spectra of 5d

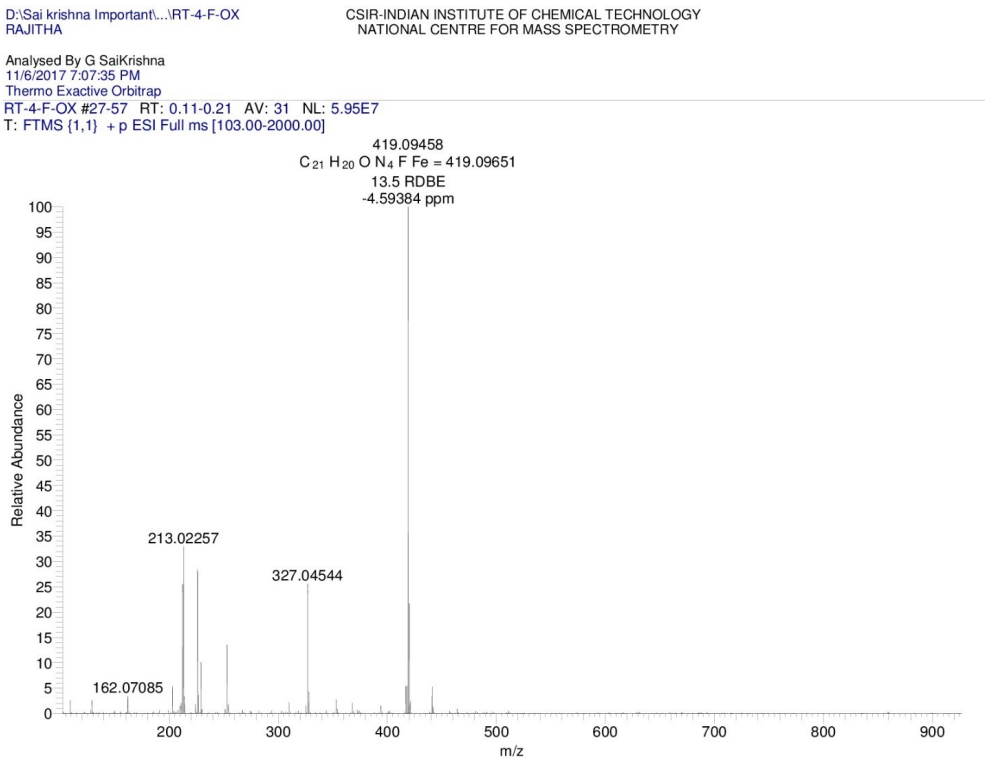

Figure S15: HRMS spectra of 5d

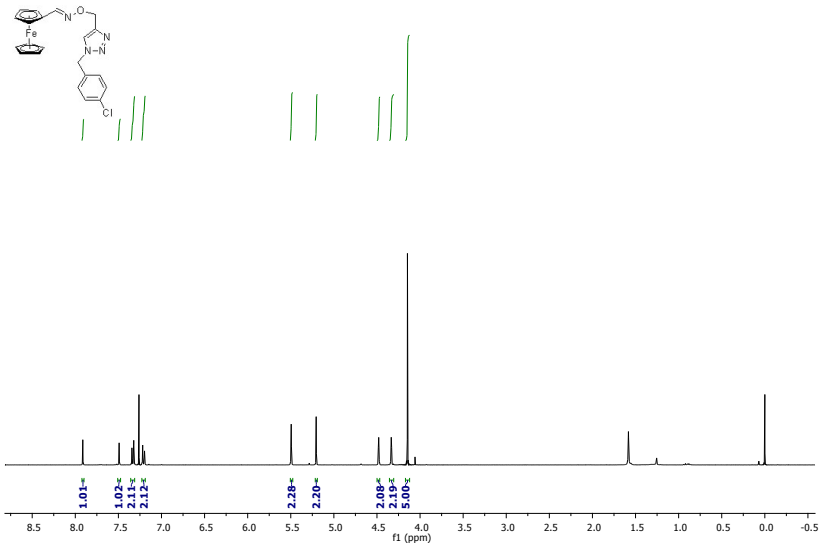

Figure S16: ^{1}H NMR spectra of 5e

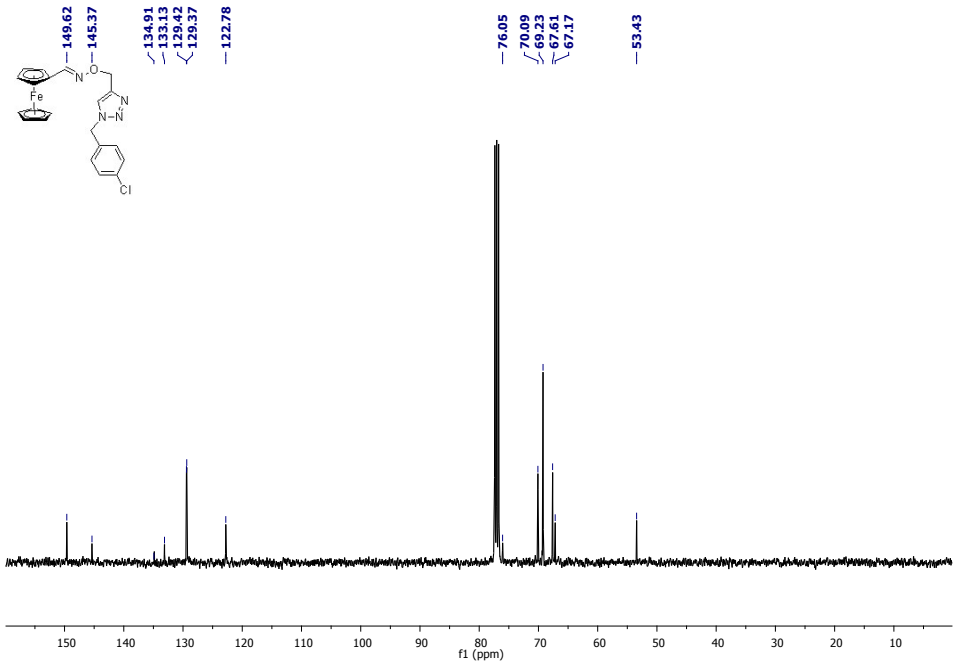

Figure S17: ^{13}C NMR spectra of 5e

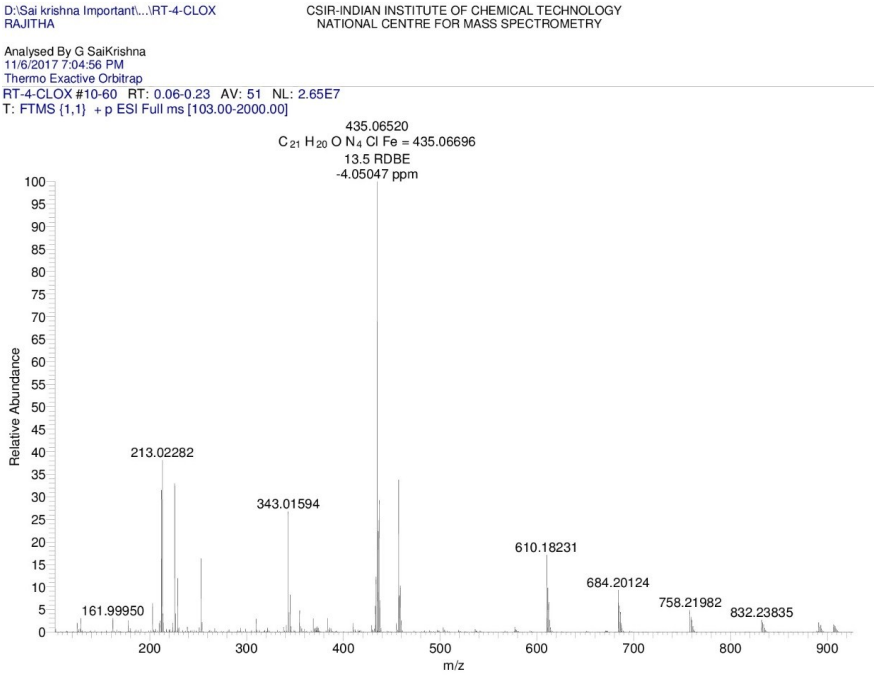

Figure S18: HRMS spectra of 5e

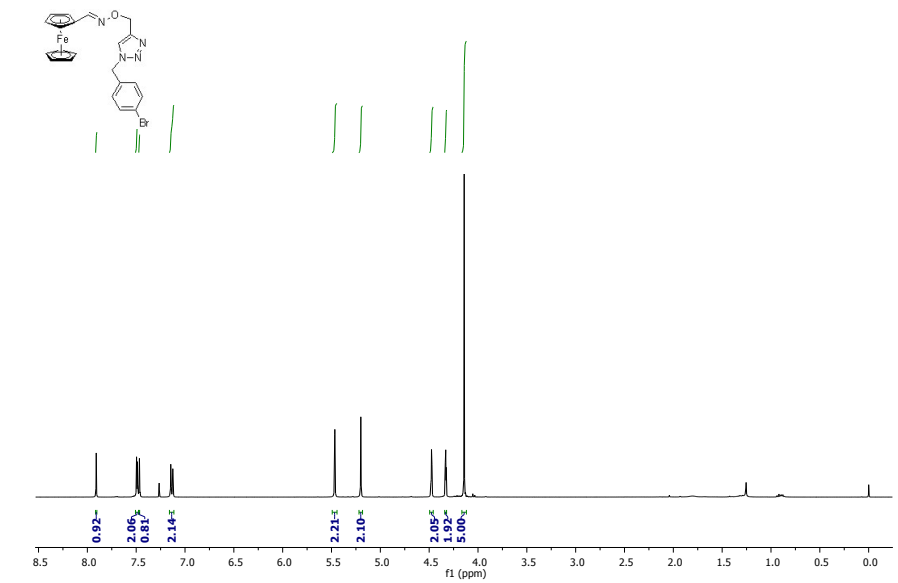

Figure S19: ^{1}H NMR spectra of 5f

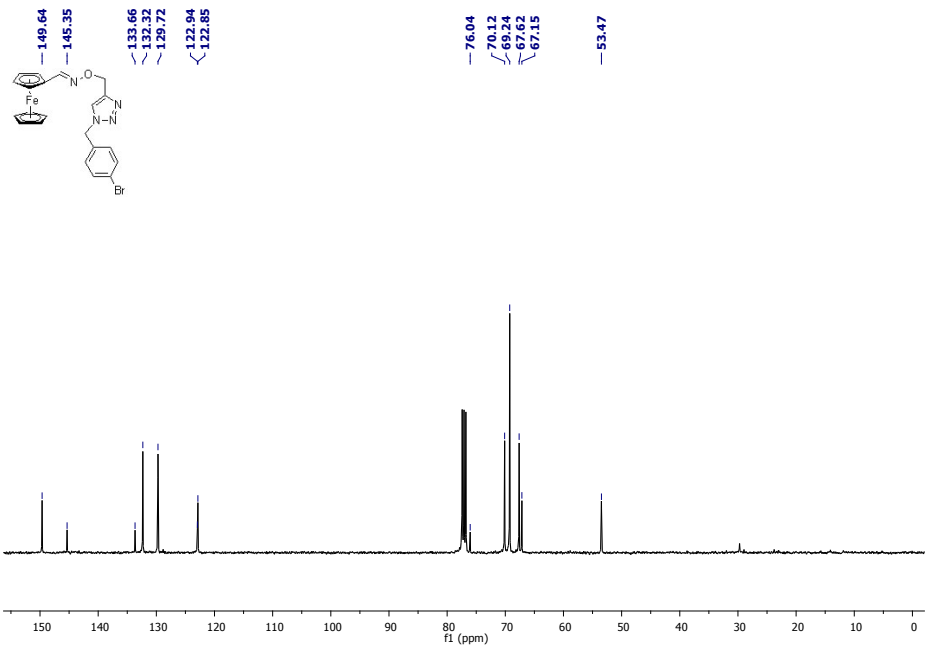

Figure S20: ^{13}C NMR spectra of 5f

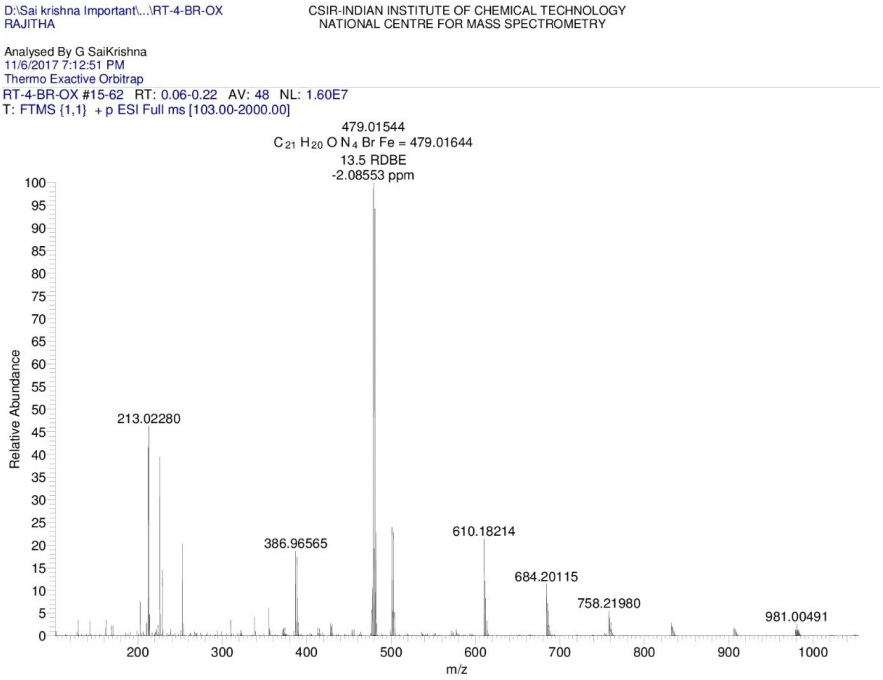

Figure S21: HRMS spectra of 5f

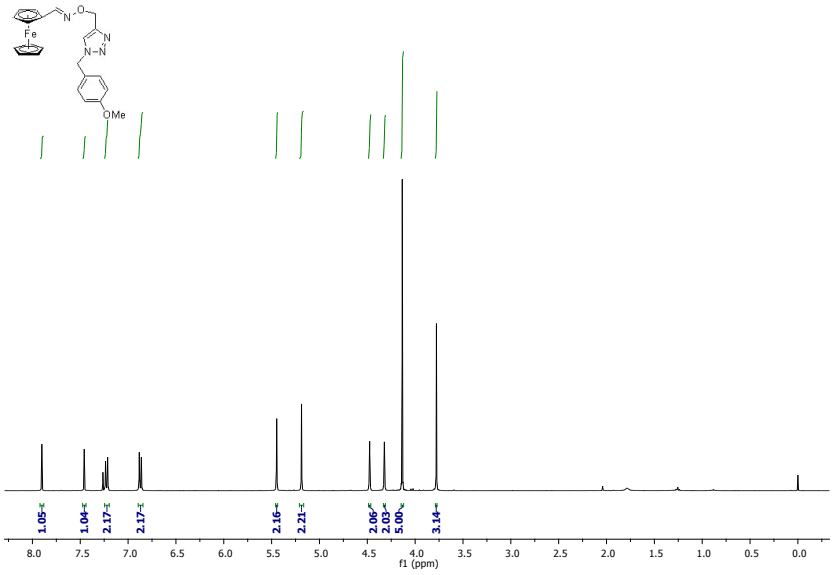

Figure S22: ^{1}H NMR spectra of 5g

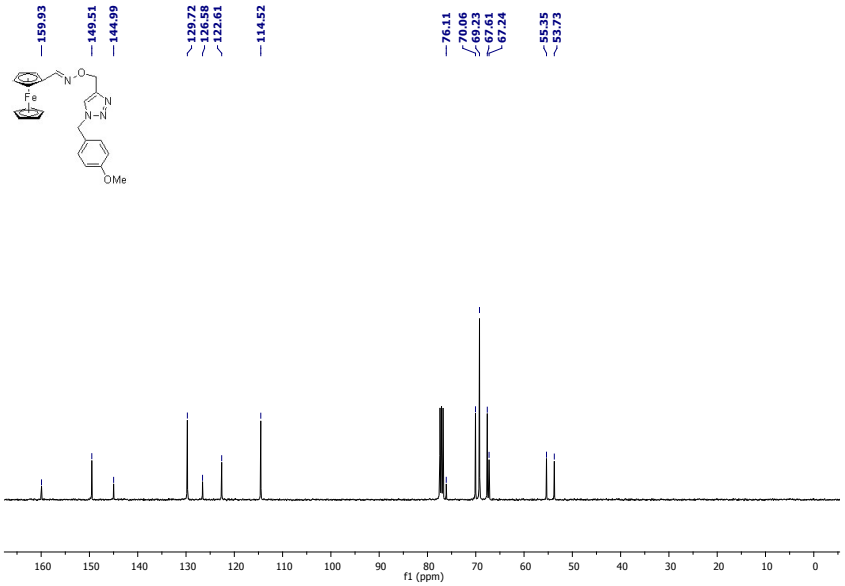

Figure S23: ^{13}C NMR spectra of 5g

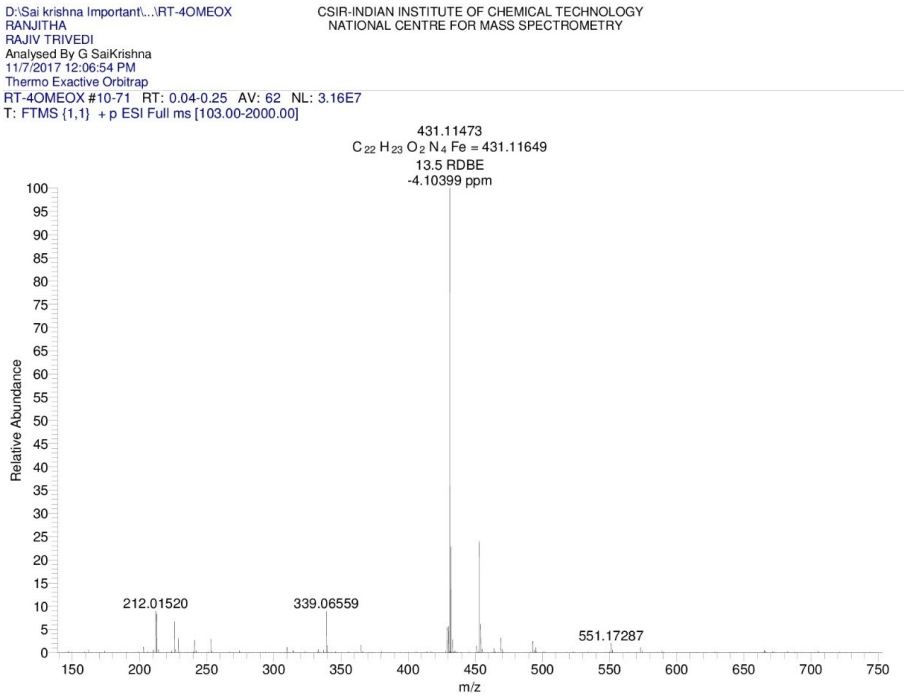

Figure S24: HRMS spectra of 5g

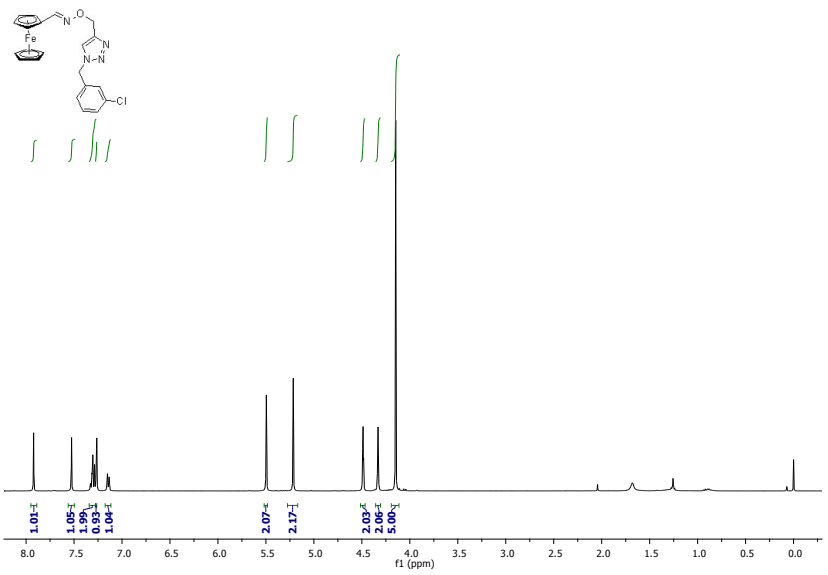

Figure S25: ^{1}H NMR spectra of 5h

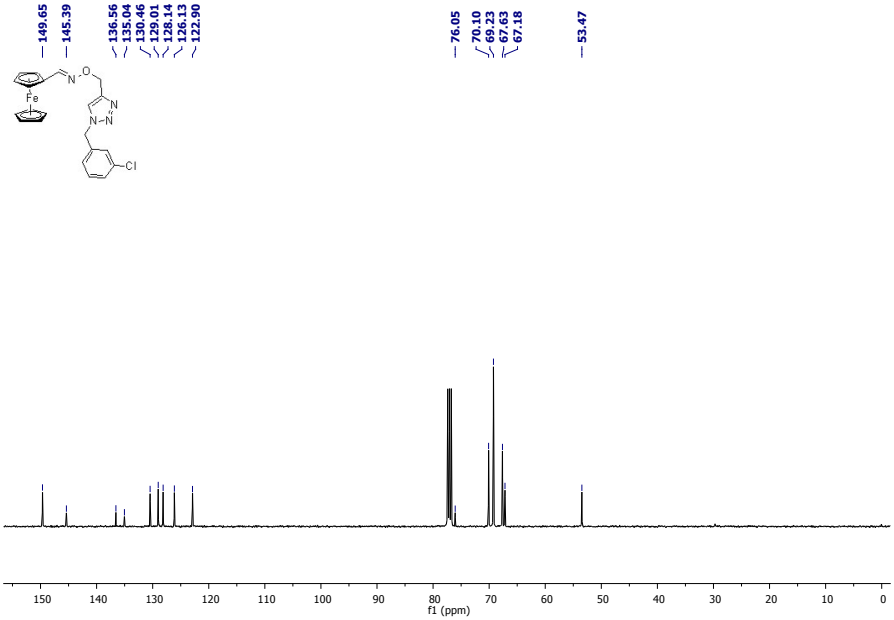

Figure S26: ^{13}C NMR spectra of 5h

D:\Sai krishna Important\...\RT-3-CLOX
RANJITHA
RAJIV TRIVEDI
Analysed By G SaiKrishna
11/7/2017 12:04:11 PM
Thermo Exactive Orbitrap

CSIR-INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY
NATIONAL CENTRE FOR MASS SPECTROMETRY

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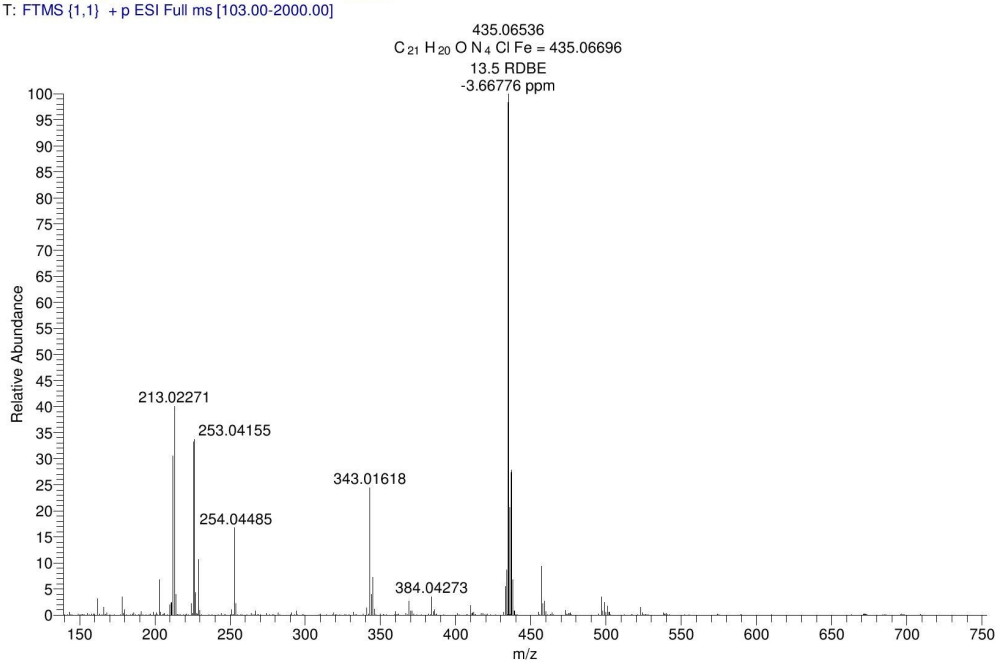
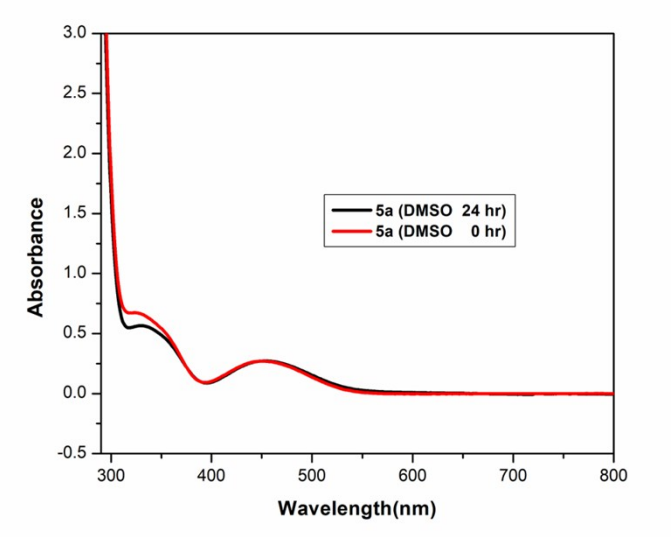


Figure S27: HRMS spectra of 5h

Stability Studies

(a)



(b)

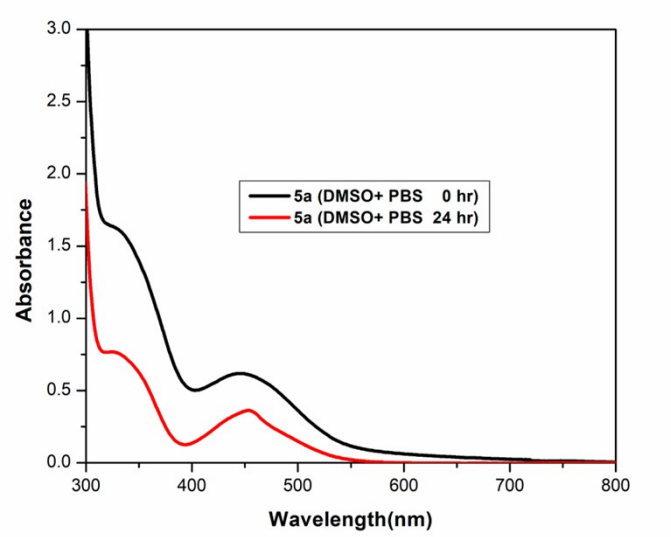


Figure S28: UV-visible spectroscopy of compound **5a** in (a) DMSO and (b) 10% DMSO in PBS solution (pH 7.4).

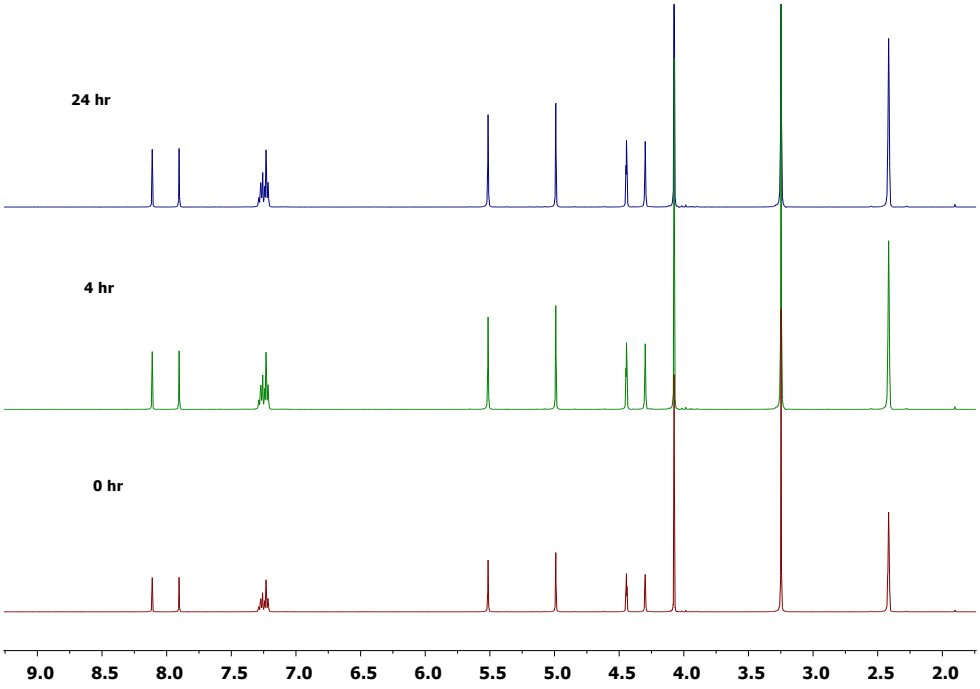


Figure 29: Stacked ^{1}H-NMR spectrum of compound **5a** in DMSO-d_6 at different time intervals (0, 4 and 24 hr.).

Crystallographic data of compound 5a

Table S1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **5a**. U (eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

__	x	y	z	U(eq)
C(1)	5399(1)	3549(2)	5987(2)	47(1)
C(2)	4930(1)	2649(3)	5382(3)	70(1)
C(3)	4252(2)	2516(4)	5779(4)	96(1)
C(4)	4036(2)	3290(4)	6784(4)	105(1)
C(5)	4495(2)	4201(4)	7379(3)	100(1)
C(6)	5180(2)	4337(3)	6998(2)	70(1)
C(7)	6133(1)	3763(2)	5543(2)	52(1)
C(8)	6767(1)	2131(2)	4096(2)	41(1)
C(9)	7054(1)	851(2)	4314(2)	38(1)
C(10)	7449(1)	-64(2)	3449(2)	51(1)
C(11)	8428(1)	2420(2)	2039(2)	38(1)
C(12)	9010(1)	3392(2)	2271(2)	36(1)
C(13)	9441(1)	3609(2)	3448(2)	42(1)
C(14)	9934(1)	4672(2)	3220(2)	49(1)
C(15)	9811(1)	5122(2)	1920(2)	50(1)
C(16)	9241(1)	4346(2)	1333(2)	43(1)
C(17)	8312(1)	5934(2)	4402(2)	50(1)
C(18)	7879(1)	5733(2)	3251(2)	47(1)
C(19)	8098(1)	6659(2)	2310(2)	46(1)
C(20)	8668(1)	7433(2)	2873(2)	47(1)
C(21)	8806(1)	6989(2)	4165(2)	49(1)
Fe(1)	8917(1)	5379(1)	2916(1)	32(1)
N(1)	6485(1)	2479(2)	5206(1)	39(1)
N(2)	6589(1)	1471(2)	6086(2)	50(1)
N(3)	6936(1)	475(2)	5542(2)	46(1)
N(4)	8292(1)	1517(2)	2882(2)	43(1)
O(1)	7710(1)	679(1)	2392(1)	47(1)

Table S2. Bond lengths [Å] and angles [°] for compound **5a**.

C(1)-C(2)	1.361(3)
C(1)-C(6)	1.376(3)
C(1)-C(7)	1.502(3)
C(2)-C(3)	1.376(4)
C(2)-H(2)	0.9300
C(3)-C(4)	1.362(5)
C(3)-H(3)	0.9300
C(4)-C(5)	1.353(5)
C(4)-H(4)	0.9300
C(5)-C(6)	1.381(4)
C(5)-H(5)	0.9300
C(6)-H(6)	0.9300
C(7)-N(1)	1.461(2)
C(7)-H(7A)	0.9700
C(7)-H(7B)	0.9700
C(8)-N(1)	1.337(2)
C(8)-C(9)	1.363(3)
C(8)-H(8)	0.9300
C(9)-N(3)	1.350(2)
C(9)-C(10)	1.492(3)
C(10)-O(1)	1.420(2)
C(10)-H(10A)	0.9700
C(10)-H(10B)	0.9700
C(11)-N(4)	1.270(2)
C(11)-C(12)	1.452(2)
C(11)-H(11)	0.9300
C(12)-C(16)	1.427(3)
C(12)-C(13)	1.429(3)
C(12)-Fe(1)	2.0445(17)
C(13)-C(14)	1.416(3)
C(13)-Fe(1)	2.0322(18)
C(13)-H(13)	0.9300
C(14)-C(15)	1.413(3)
C(14)-Fe(1)	2.0395(18)

C(14)-H(14)	0.9300
C(15)-C(16)	1.412(3)
C(15)-Fe(1)	2.0484(19)
C(15)-H(15)	0.9300
C(16)-Fe(1)	2.0422(18)
C(16)-H(16)	0.9300
C(17)-C(18)	1.408(3)
C(17)-C(21)	1.414(3)
C(17)-Fe(1)	2.0429(19)
C(17)-H(17)	0.9300
C(18)-C(19)	1.402(3)
C(18)-Fe(1)	2.0396(18)
C(18)-H(18)	0.9300
C(19)-C(20)	1.401(3)
C(19)-Fe(1)	2.0431(18)
C(19)-H(19)	0.9300
C(20)-C(21)	1.407(3)
C(20)-Fe(1)	2.0399(19)
C(20)-H(20)	0.9300
C(21)-Fe(1)	2.0399(19)
C(21)-H(21)	0.9300
N(1)-N(2)	1.337(2)
N(2)-N(3)	1.311(2)
N(4)-O(1)	1.428(2)

C(2)-C(1)-C(6)	118.8(2)
C(2)-C(1)-C(7)	122.1(2)
C(6)-C(1)-C(7)	119.0(2)
C(1)-C(2)-C(3)	120.7(3)
C(1)-C(2)-H(2)	119.6
C(3)-C(2)-H(2)	119.6
C(4)-C(3)-C(2)	120.5(3)
C(4)-C(3)-H(3)	119.7
C(2)-C(3)-H(3)	119.7
C(5)-C(4)-C(3)	119.1(3)
C(5)-C(4)-H(4)	120.5

C(3)-C(4)-H(4)	120.5
C(4)-C(5)-C(6)	121.0(3)
C(4)-C(5)-H(5)	119.5
C(6)-C(5)-H(5)	119.5
C(1)-C(6)-C(5)	119.9(3)
C(1)-C(6)-H(6)	120.1
C(5)-C(6)-H(6)	120.1
N(1)-C(7)-C(1)	113.46(17)
N(1)-C(7)-H(7A)	108.9
C(1)-C(7)-H(7A)	108.9
N(1)-C(7)-H(7B)	108.9
C(1)-C(7)-H(7B)	108.9
H(7A)-C(7)-H(7B)	107.7
N(1)-C(8)-C(9)	105.25(16)
N(1)-C(8)-H(8)	127.4
C(9)-C(8)-H(8)	127.4
N(3)-C(9)-C(8)	108.09(16)
N(3)-C(9)-C(10)	121.47(17)
C(8)-C(9)-C(10)	130.43(17)
O(1)-C(10)-C(9)	111.82(16)
O(1)-C(10)-H(10A)	109.3
C(9)-C(10)-H(10A)	109.3
O(1)-C(10)-H(10B)	109.3
C(9)-C(10)-H(10B)	109.3
H(10A)-C(10)-H(10B)	107.9
N(4)-C(11)-C(12)	121.20(17)
N(4)-C(11)-H(11)	119.4
C(12)-C(11)-H(11)	119.4
C(16)-C(12)-C(13)	107.33(16)
C(16)-C(12)-C(11)	124.75(17)
C(13)-C(12)-C(11)	127.90(17)
C(16)-C(12)-Fe(1)	69.49(10)
C(13)-C(12)-Fe(1)	69.02(10)
C(11)-C(12)-Fe(1)	125.52(12)
C(14)-C(13)-C(12)	107.90(18)
C(14)-C(13)-Fe(1)	69.93(11)

C(12)-C(13)-Fe(1)	69.94(10)
C(14)-C(13)-H(13)	126.0
C(12)-C(13)-H(13)	126.0
Fe(1)-C(13)-H(13)	125.7
C(15)-C(14)-C(13)	108.31(18)
C(15)-C(14)-Fe(1)	70.12(11)
C(13)-C(14)-Fe(1)	69.38(10)
C(15)-C(14)-H(14)	125.8
C(13)-C(14)-H(14)	125.8
Fe(1)-C(14)-H(14)	126.2
C(16)-C(15)-C(14)	108.27(18)
C(16)-C(15)-Fe(1)	69.58(10)
C(14)-C(15)-Fe(1)	69.44(11)
C(16)-C(15)-H(15)	125.9
C(14)-C(15)-H(15)	125.9
Fe(1)-C(15)-H(15)	126.7
C(15)-C(16)-C(12)	108.18(18)
C(15)-C(16)-Fe(1)	70.05(11)
C(12)-C(16)-Fe(1)	69.65(10)
C(15)-C(16)-H(16)	125.9
C(12)-C(16)-H(16)	125.9
Fe(1)-C(16)-H(16)	126.0
C(18)-C(17)-C(21)	107.79(18)
C(18)-C(17)-Fe(1)	69.71(11)
C(21)-C(17)-Fe(1)	69.63(11)
C(18)-C(17)-H(17)	126.1
C(21)-C(17)-H(17)	126.1
Fe(1)-C(17)-H(17)	126.1
C(19)-C(18)-C(17)	108.24(18)
C(19)-C(18)-Fe(1)	70.04(11)
C(17)-C(18)-Fe(1)	69.96(11)
C(19)-C(18)-H(18)	125.9
C(17)-C(18)-H(18)	125.9
Fe(1)-C(18)-H(18)	125.7
C(20)-C(19)-C(18)	107.97(18)
C(20)-C(19)-Fe(1)	69.80(11)

C(18)-C(19)-Fe(1)	69.78(11)
C(20)-C(19)-H(19)	126.0
C(18)-C(19)-H(19)	126.0
Fe(1)-C(19)-H(19)	126.0
C(19)-C(20)-C(21)	108.46(18)
C(19)-C(20)-Fe(1)	70.06(11)
C(21)-C(20)-Fe(1)	69.82(11)
C(19)-C(20)-H(20)	125.8
C(21)-C(20)-H(20)	125.8
Fe(1)-C(20)-H(20)	125.9
C(20)-C(21)-C(17)	107.53(18)
C(20)-C(21)-Fe(1)	69.82(11)
C(17)-C(21)-Fe(1)	69.86(11)
C(20)-C(21)-H(21)	126.2
C(17)-C(21)-H(21)	126.2
Fe(1)-C(21)-H(21)	125.7
C(13)-Fe(1)-C(14)	40.69(8)
C(13)-Fe(1)-C(20)	158.80(8)
C(14)-Fe(1)-C(20)	122.85(8)
C(13)-Fe(1)-C(21)	122.74(8)
C(14)-Fe(1)-C(21)	107.13(8)
C(20)-Fe(1)-C(21)	40.35(8)
C(13)-Fe(1)-C(18)	123.37(8)
C(14)-Fe(1)-C(18)	158.95(9)
C(20)-Fe(1)-C(18)	67.54(8)
C(21)-Fe(1)-C(18)	67.94(8)
C(13)-Fe(1)-C(16)	68.75(8)
C(14)-Fe(1)-C(16)	68.23(8)
C(20)-Fe(1)-C(16)	122.63(8)
C(21)-Fe(1)-C(16)	157.91(9)
C(18)-Fe(1)-C(16)	124.09(8)
C(13)-Fe(1)-C(17)	107.75(8)
C(14)-Fe(1)-C(17)	122.68(9)
C(20)-Fe(1)-C(17)	67.74(8)
C(21)-Fe(1)-C(17)	40.51(9)
C(18)-Fe(1)-C(17)	40.34(8)

C(16)-Fe(1)-C(17)	160.16(9)
C(13)-Fe(1)-C(19)	159.35(8)
C(14)-Fe(1)-C(19)	158.90(9)
C(20)-Fe(1)-C(19)	40.14(8)
C(21)-Fe(1)-C(19)	67.84(8)
C(18)-Fe(1)-C(19)	40.18(8)
C(16)-Fe(1)-C(19)	108.26(8)
C(17)-Fe(1)-C(19)	67.73(8)
C(13)-Fe(1)-C(12)	41.04(7)
C(14)-Fe(1)-C(12)	68.55(8)
C(20)-Fe(1)-C(12)	158.76(8)
C(21)-Fe(1)-C(12)	159.57(8)
C(18)-Fe(1)-C(12)	108.50(8)
C(16)-Fe(1)-C(12)	40.86(7)
C(17)-Fe(1)-C(12)	123.74(8)
C(19)-Fe(1)-C(12)	123.34(8)
C(13)-Fe(1)-C(15)	68.38(8)
C(14)-Fe(1)-C(15)	40.45(9)
C(20)-Fe(1)-C(15)	107.67(8)
C(21)-Fe(1)-C(15)	122.17(9)
C(18)-Fe(1)-C(15)	159.63(9)
C(16)-Fe(1)-C(15)	40.38(8)
C(17)-Fe(1)-C(15)	158.22(9)
C(19)-Fe(1)-C(15)	123.45(9)
C(12)-Fe(1)-C(15)	68.34(8)
N(2)-N(1)-C(8)	110.45(16)
N(2)-N(1)-C(7)	120.41(16)
C(8)-N(1)-C(7)	129.08(16)
N(3)-N(2)-N(1)	107.40(15)
N(2)-N(3)-C(9)	108.82(15)
C(11)-N(4)-O(1)	109.52(15)
C(10)-O(1)-N(4)	108.29(15)

Symmetry transformations used to generate equivalent atoms:

Table S3. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for compound **5a**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	53(1)	45(1)	42(1)	4(1)	8(1)	12(1)
C(2)	61(2)	66(2)	86(2)	-11(1)	13(1)	-5(1)
C(3)	59(2)	83(2)	145(3)	24(2)	10(2)	-4(2)
C(4)	63(2)	110(3)	148(3)	67(3)	44(2)	41(2)
C(5)	106(3)	115(3)	85(2)	25(2)	49(2)	68(2)
C(6)	81(2)	74(2)	55(1)	-5(1)	9(1)	35(1)
C(7)	61(1)	37(1)	58(1)	-6(1)	11(1)	2(1)
C(8)	52(1)	39(1)	33(1)	5(1)	10(1)	-1(1)
C(9)	37(1)	36(1)	40(1)	1(1)	8(1)	-5(1)
C(10)	55(1)	36(1)	63(1)	-3(1)	22(1)	-2(1)
C(11)	39(1)	35(1)	41(1)	-9(1)	8(1)	5(1)
C(12)	36(1)	33(1)	41(1)	-5(1)	10(1)	6(1)
C(13)	39(1)	38(1)	50(1)	0(1)	4(1)	10(1)
C(14)	32(1)	48(1)	66(1)	-10(1)	4(1)	4(1)
C(15)	42(1)	44(1)	66(1)	-5(1)	26(1)	-2(1)
C(16)	46(1)	43(1)	42(1)	-3(1)	17(1)	4(1)
C(17)	61(1)	48(1)	43(1)	2(1)	20(1)	14(1)
C(18)	35(1)	42(1)	65(1)	-9(1)	13(1)	3(1)
C(19)	47(1)	45(1)	45(1)	-3(1)	0(1)	15(1)
C(20)	51(1)	31(1)	61(1)	0(1)	14(1)	4(1)
C(21)	50(1)	46(1)	50(1)	-19(1)	-1(1)	8(1)
Fe(1)	31(1)	30(1)	36(1)	-3(1)	7(1)	3(1)
N(1)	44(1)	37(1)	37(1)	5(1)	9(1)	1(1)
N(2)	64(1)	48(1)	39(1)	9(1)	11(1)	4(1)
N(3)	55(1)	41(1)	43(1)	7(1)	6(1)	6(1)
N(4)	38(1)	41(1)	50(1)	-6(1)	9(1)	-2(1)
O(1)	49(1)	44(1)	50(1)	-10(1)	17(1)	-10(1)

Table S4. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for compound **5a**.

	x	y	z	U(eq)
H(2)	5070	2117	4692	84
H(3)	3938	1894	5358	115
H(4)	3578	3192	7058	127
H(5)	4348	4745	8054	120
H(6)	5492	4959	7423	84
H(7A)	6103	4367	4789	62
H(7B)	6421	4226	6228	62
H(8)	6767	2652	3337	49
H(10A)	7845	-490	3951	61
H(10B)	7136	-797	3113	61
H(11)	8150	2459	1260	46
H(13)	9404	3136	4227	50
H(14)	10279	5015	3823	58
H(15)	10062	5810	1520	60
H(16)	9050	4442	482	52
H(17)	8280	5458	5180	60
H(18)	7511	5095	3134	56
H(19)	7900	6745	1463	55
H(20)	8913	8122	2461	56
H(21)	9159	7328	4757	59

Table S5. Torsion angles [°] for compound **5a**.

C(6)-C(1)-C(2)-C(3)	-0.7(4)
C(7)-C(1)-C(2)-C(3)	-177.3(2)
C(1)-C(2)-C(3)-C(4)	0.3(5)
C(2)-C(3)-C(4)-C(5)	0.7(5)
C(3)-C(4)-C(5)-C(6)	-1.3(5)
C(2)-C(1)-C(6)-C(5)	0.1(4)
C(7)-C(1)-C(6)-C(5)	176.9(2)
C(4)-C(5)-C(6)-C(1)	0.9(4)
C(2)-C(1)-C(7)-N(1)	-42.5(3)
C(6)-C(1)-C(7)-N(1)	140.8(2)
N(1)-C(8)-C(9)-N(3)	0.0(2)
N(1)-C(8)-C(9)-C(10)	-179.04(19)
N(3)-C(9)-C(10)-O(1)	-161.09(17)
C(8)-C(9)-C(10)-O(1)	17.8(3)
N(4)-C(11)-C(12)-C(16)	173.69(17)
N(4)-C(11)-C(12)-C(13)	-8.1(3)
N(4)-C(11)-C(12)-Fe(1)	-98.0(2)
C(16)-C(12)-C(13)-C(14)	-0.73(19)
C(11)-C(12)-C(13)-C(14)	-179.22(17)
Fe(1)-C(12)-C(13)-C(14)	-59.88(13)
C(16)-C(12)-C(13)-Fe(1)	59.15(12)
C(11)-C(12)-C(13)-Fe(1)	-119.34(17)
C(12)-C(13)-C(14)-C(15)	0.4(2)
Fe(1)-C(13)-C(14)-C(15)	-59.52(13)
C(12)-C(13)-C(14)-Fe(1)	59.88(12)
C(13)-C(14)-C(15)-C(16)	0.1(2)
Fe(1)-C(14)-C(15)-C(16)	-58.91(13)
C(13)-C(14)-C(15)-Fe(1)	59.06(13)
C(14)-C(15)-C(16)-C(12)	-0.6(2)
Fe(1)-C(15)-C(16)-C(12)	-59.43(12)
C(14)-C(15)-C(16)-Fe(1)	58.83(13)
C(13)-C(12)-C(16)-C(15)	0.8(2)
C(11)-C(12)-C(16)-C(15)	179.37(16)
Fe(1)-C(12)-C(16)-C(15)	59.68(13)

C(13)-C(12)-C(16)-Fe(1)	-58.85(12)
C(11)-C(12)-C(16)-Fe(1)	119.69(16)
C(21)-C(17)-C(18)-C(19)	-0.4(2)
Fe(1)-C(17)-C(18)-C(19)	-59.82(13)
C(21)-C(17)-C(18)-Fe(1)	59.44(13)
C(17)-C(18)-C(19)-C(20)	0.2(2)
Fe(1)-C(18)-C(19)-C(20)	-59.58(13)
C(17)-C(18)-C(19)-Fe(1)	59.76(13)
C(18)-C(19)-C(20)-C(21)	0.1(2)
Fe(1)-C(19)-C(20)-C(21)	-59.47(14)
C(18)-C(19)-C(20)-Fe(1)	59.56(13)
C(19)-C(20)-C(21)-C(17)	-0.3(2)
Fe(1)-C(20)-C(21)-C(17)	-59.94(13)
C(19)-C(20)-C(21)-Fe(1)	59.62(13)
C(18)-C(17)-C(21)-C(20)	0.4(2)
Fe(1)-C(17)-C(21)-C(20)	59.92(13)
C(18)-C(17)-C(21)-Fe(1)	-59.49(13)
C(9)-C(8)-N(1)-N(2)	0.1(2)
C(9)-C(8)-N(1)-C(7)	177.35(18)
C(1)-C(7)-N(1)-N(2)	-58.5(2)
C(1)-C(7)-N(1)-C(8)	124.6(2)
C(8)-N(1)-N(2)-N(3)	-0.2(2)
C(7)-N(1)-N(2)-N(3)	-177.68(17)
N(1)-N(2)-N(3)-C(9)	0.2(2)
C(8)-C(9)-N(3)-N(2)	-0.1(2)
C(10)-C(9)-N(3)-N(2)	179.04(17)
C(12)-C(11)-N(4)-O(1)	-178.41(14)
C(9)-C(10)-O(1)-N(4)	72.8(2)
C(11)-N(4)-O(1)-C(10)	-164.92(15)

Symmetry transformations used to generate equivalent atoms: