Sedaxicenes: potential new antifungal Ferrocene-based Agents?

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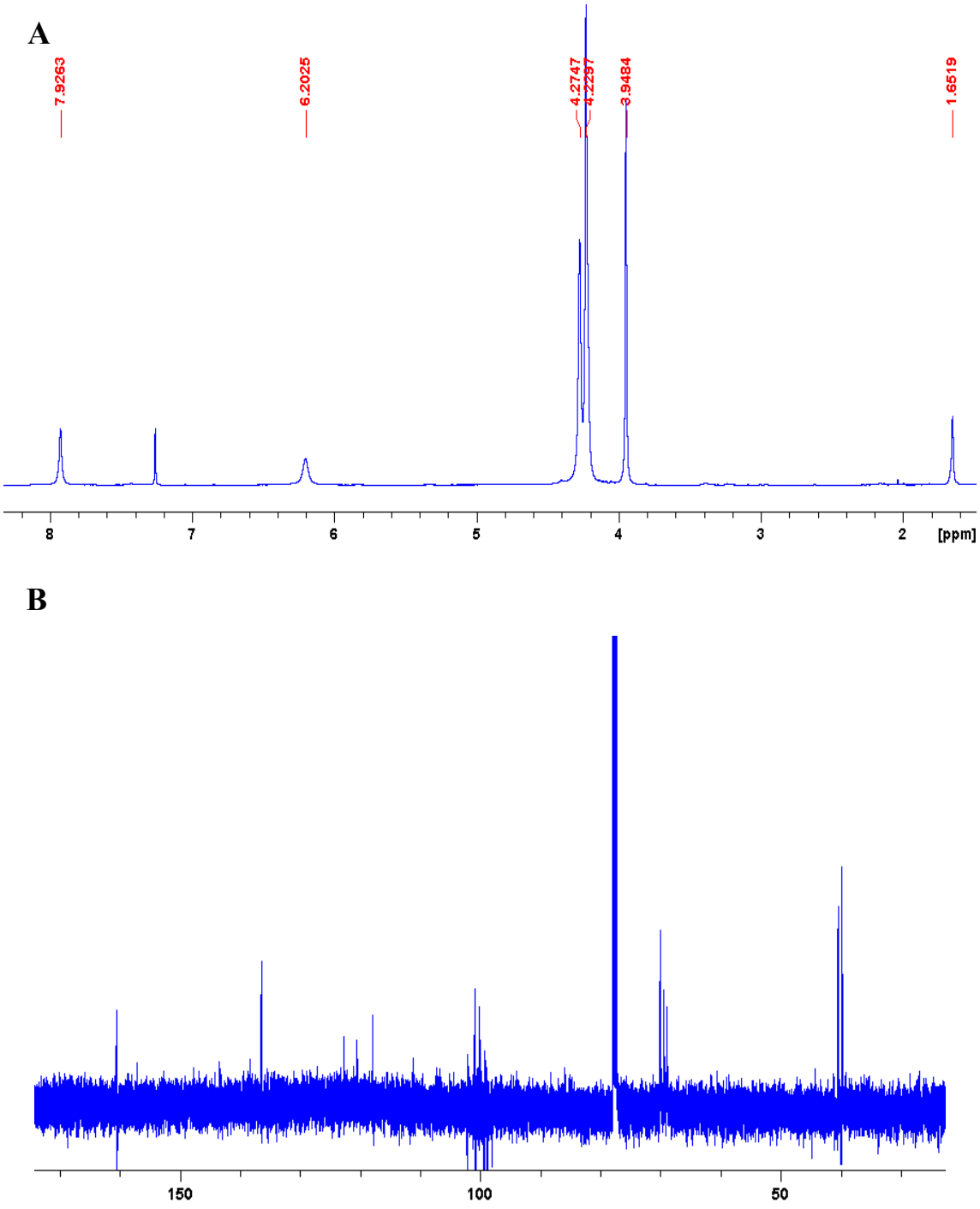
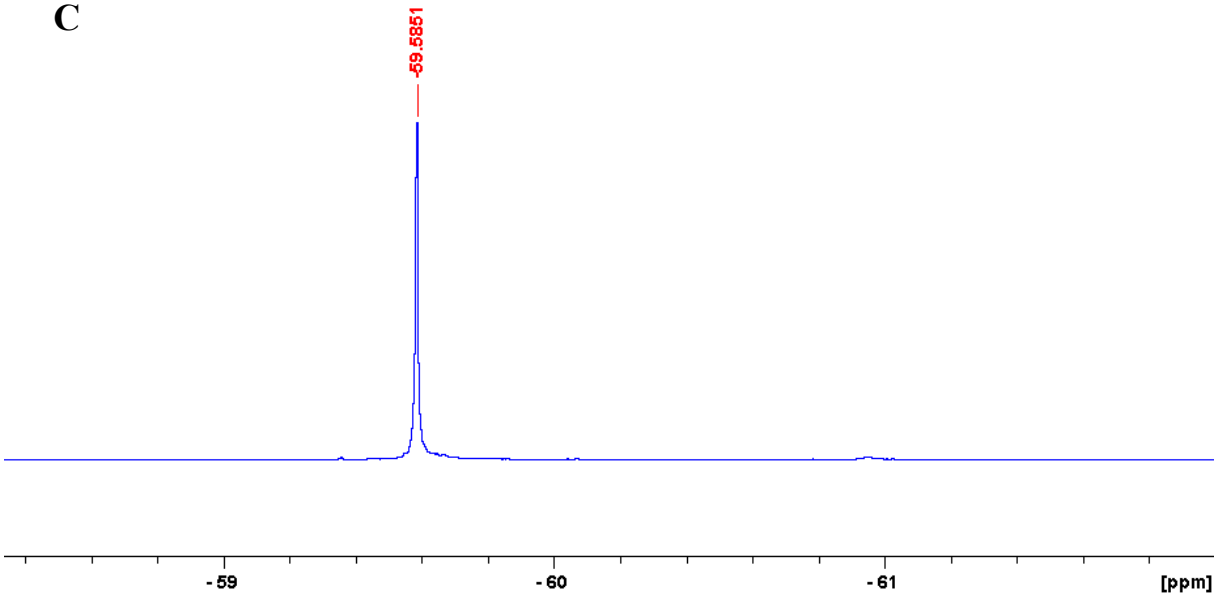
Supporting Information

Figure S1. Analytical data for complex **1a**: A) ^{1}H NMR ($CDCl_3$); B) ^{13}C NMR ($CDCl_3$); C) ^{19}F NMR ($CDCl_3$); D) MS



C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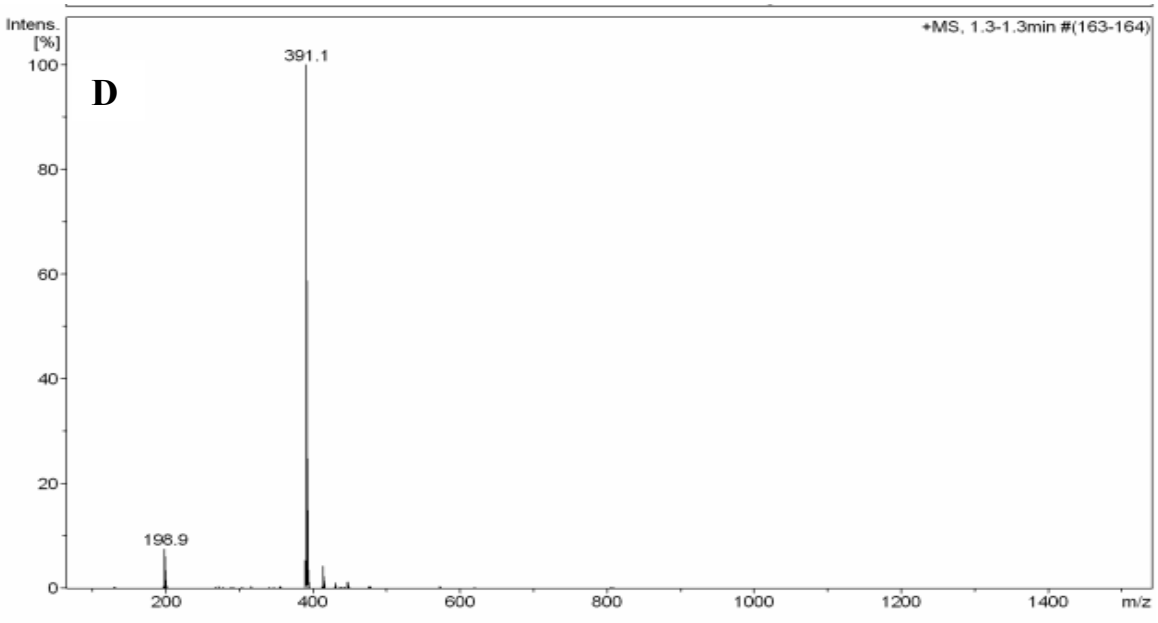
-60
-61
[ppm]

D


Intens.
[%]
+MS, 1.3-1.3min #(163-164)
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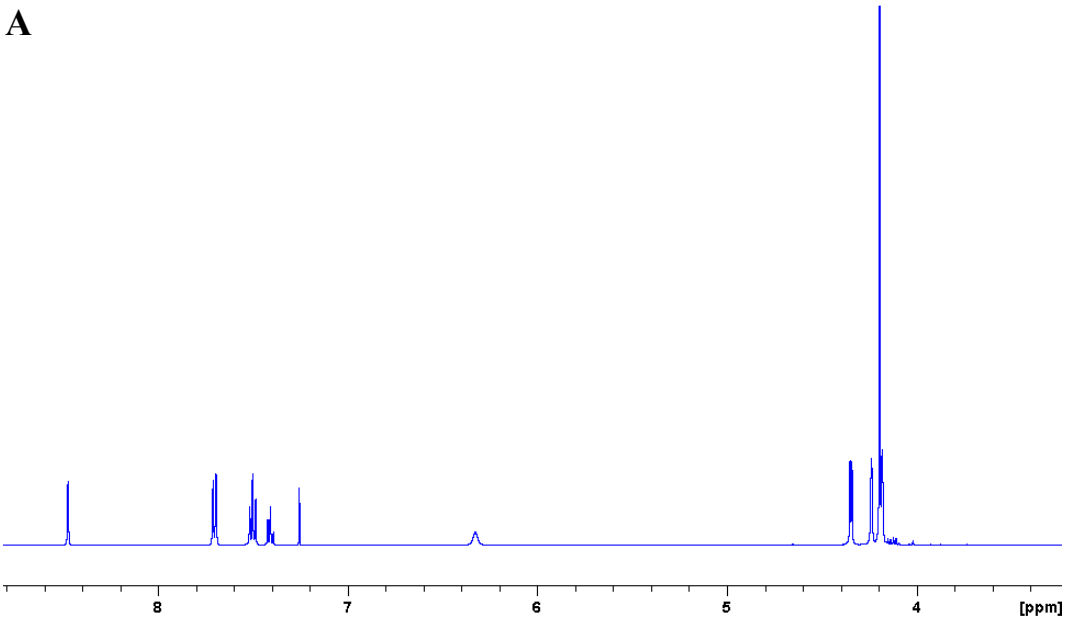
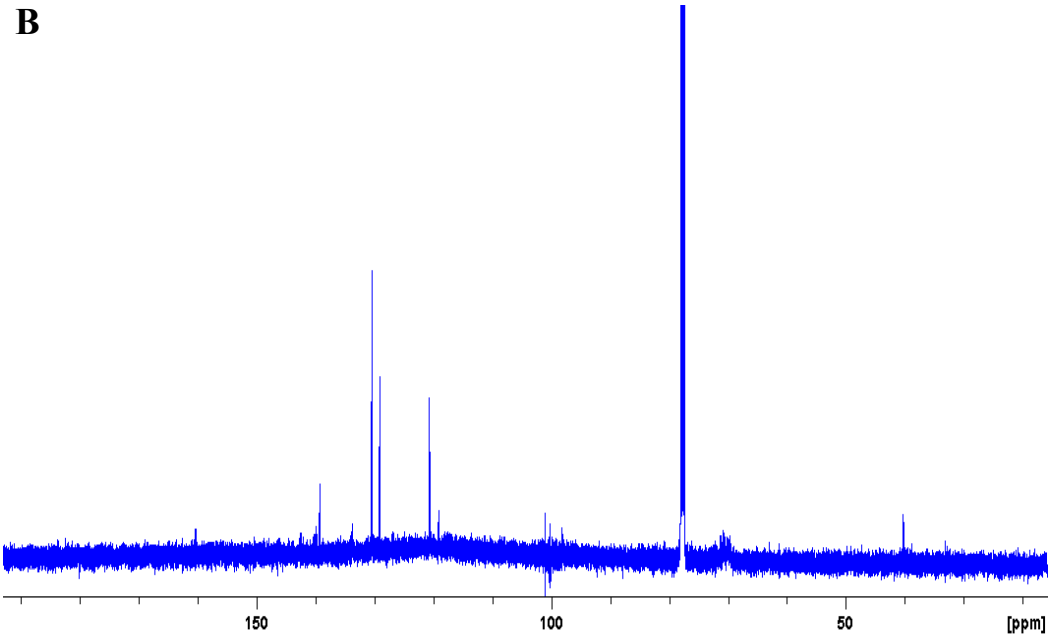
40
20
0
200
400
600
800
1000
1200
1400
m/z

Figure S2. Analytical data for complex **2**: A) ^{1}H NMR ($CDCl_3$); B) ^{13}C NMR ($CDCl_3$); C) ^{19}F NMR ($CDCl_3$); D) MS





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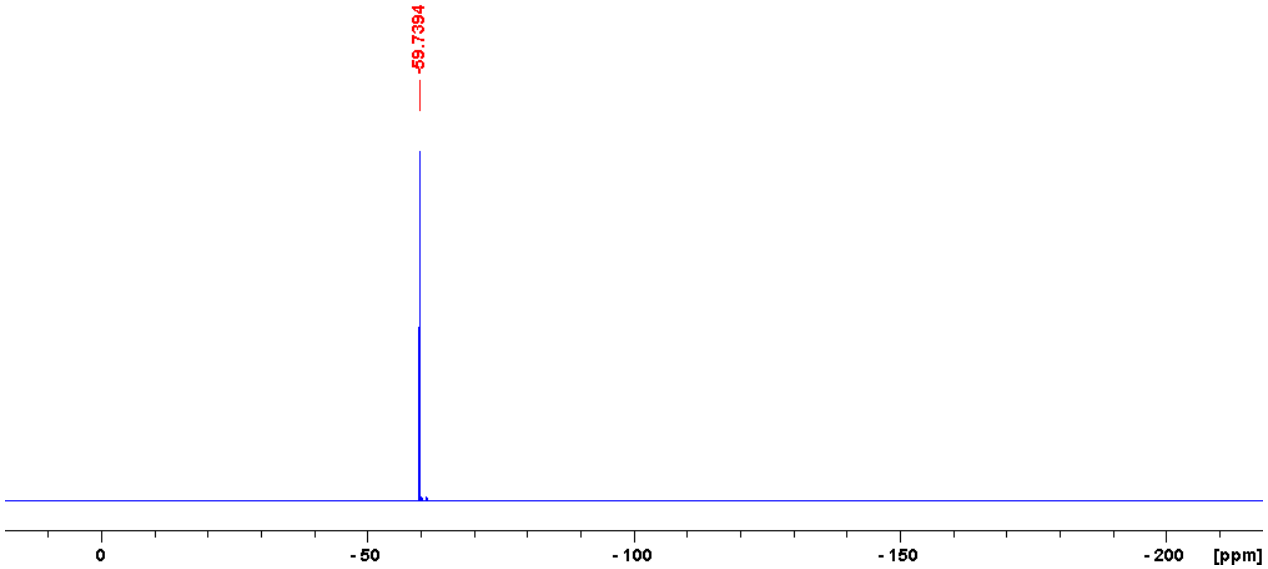
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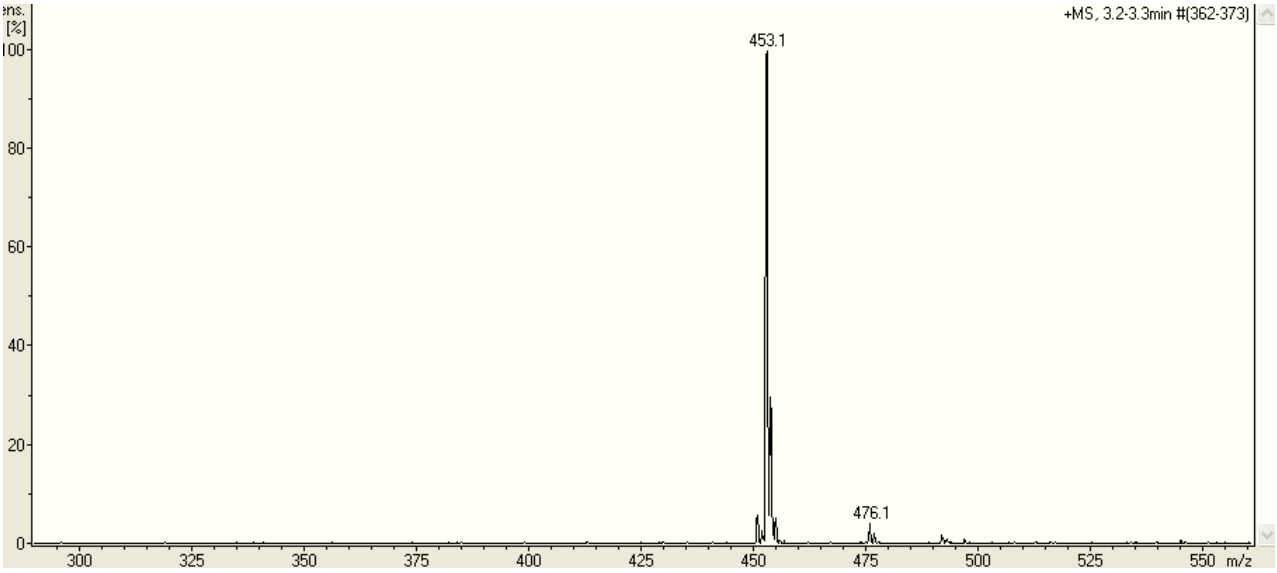
- 50
- 100
- 150
- 200
[ppm]

D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476.1
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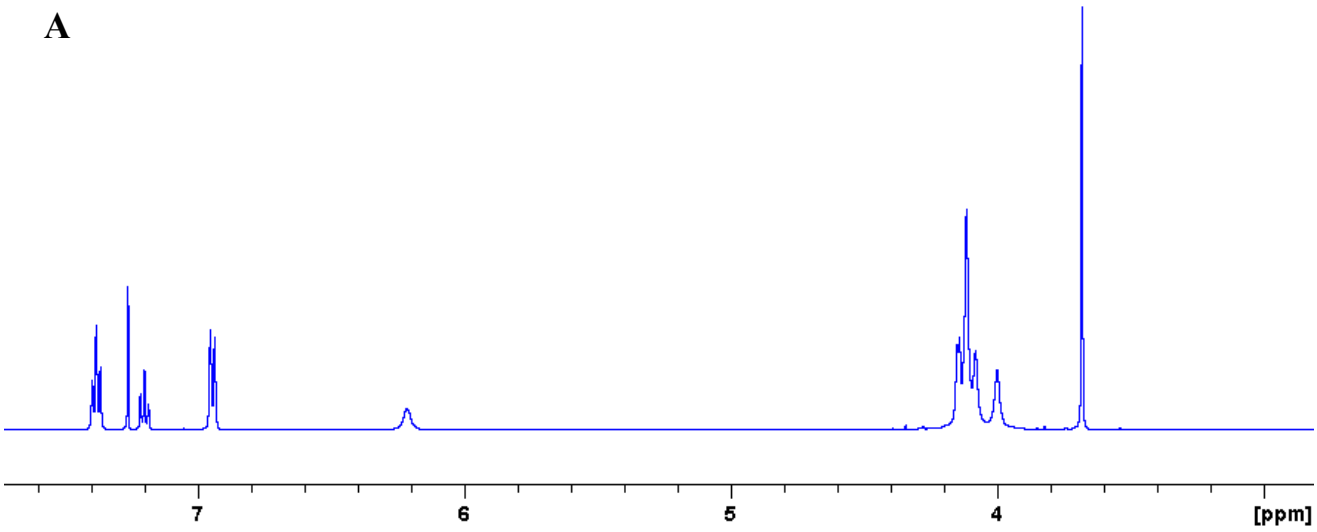
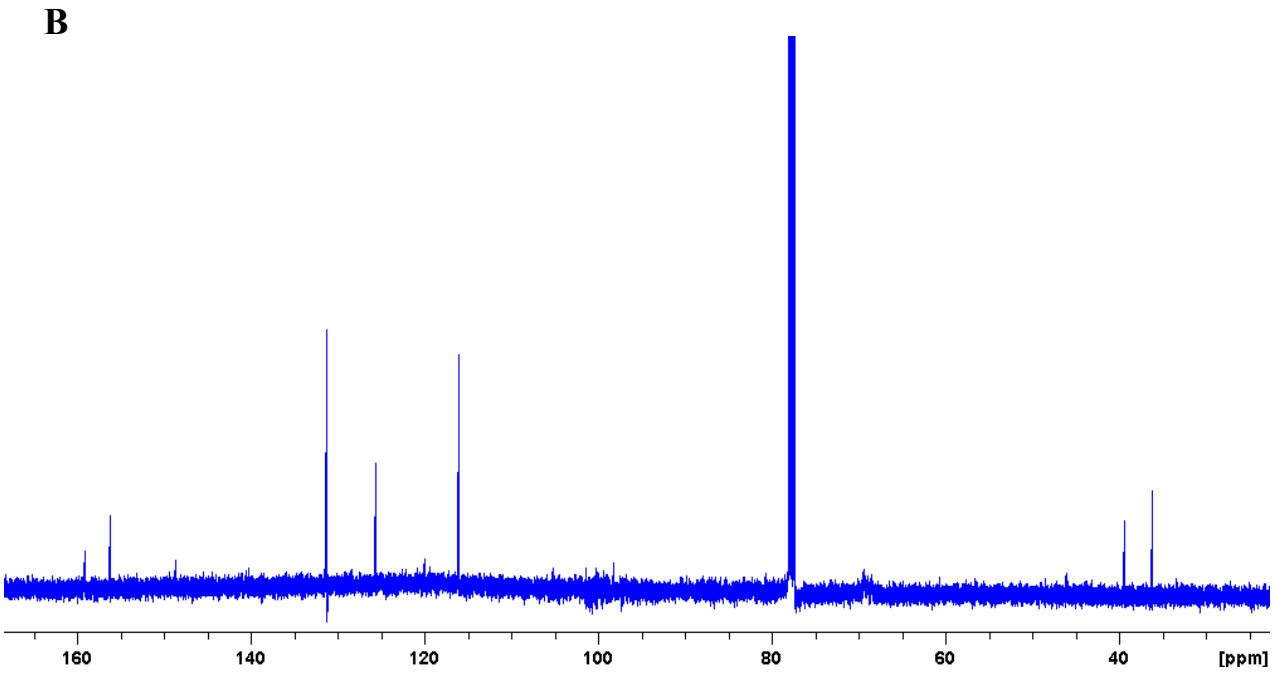
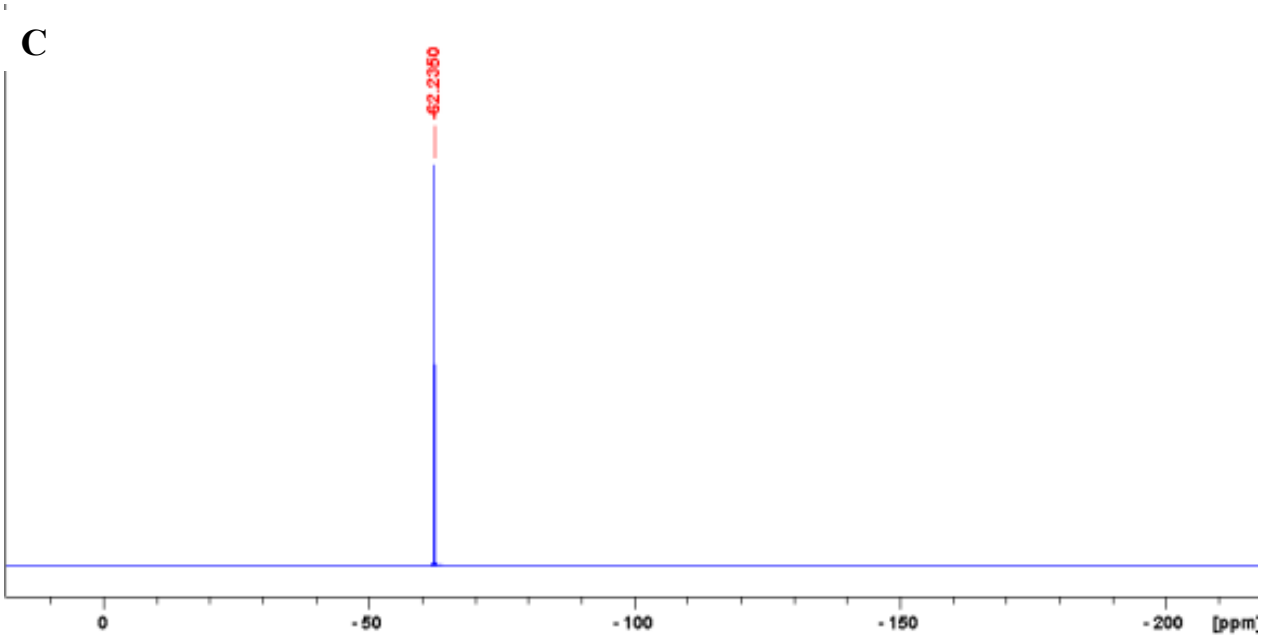
80
60
40
20
0
300
325
350
375
400
425
450
475
500
525
550
m/z

Figure S3. Analytical data for complex **3**: A) ^{1}H NMR ($CDCl_3$); B) ^{13}C NMR ($CDCl_3$); C) ^{19}F NMR ($CDCl_3$); D) MS



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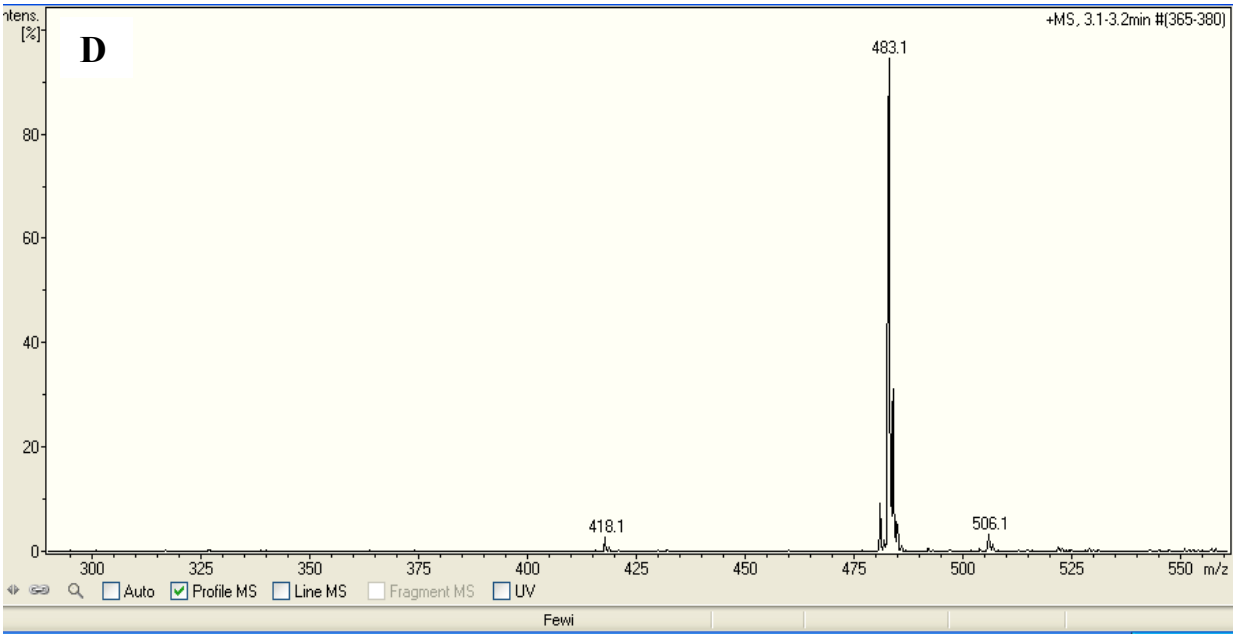
-50
-100
-150
-200
[ppm]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+MS, 3.1-3.2min #(365-380)
483.1
418.1
506.1
Intens. [%]
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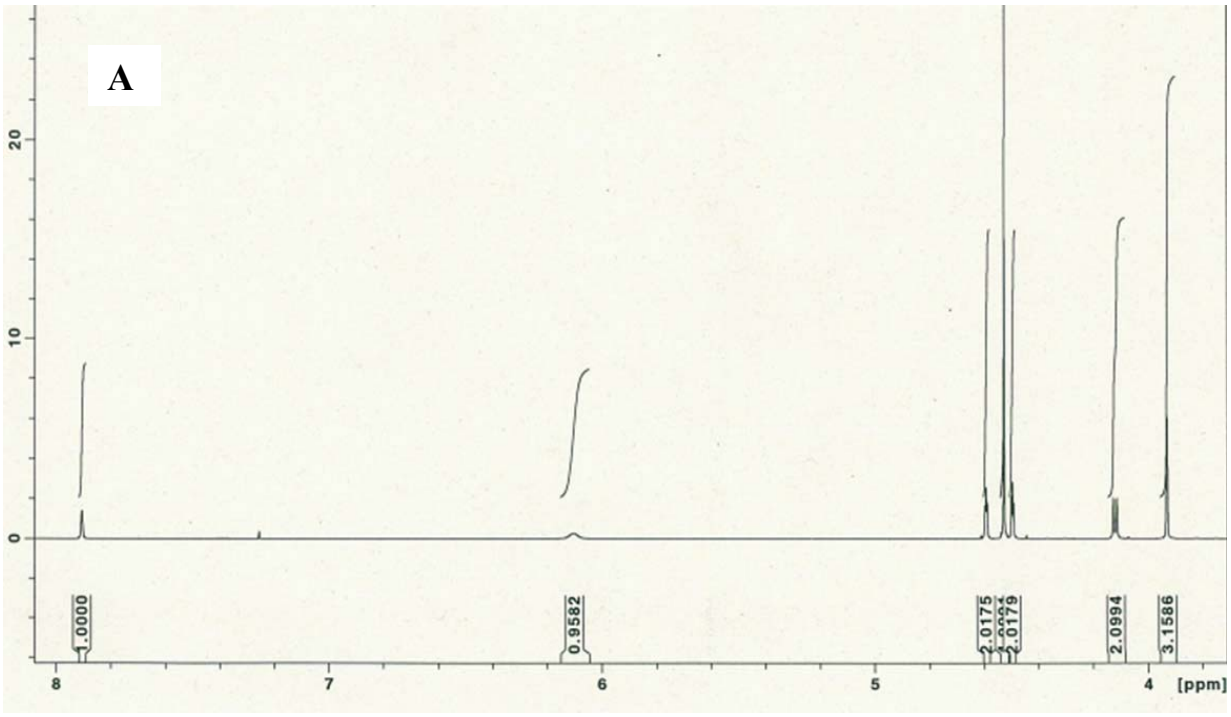
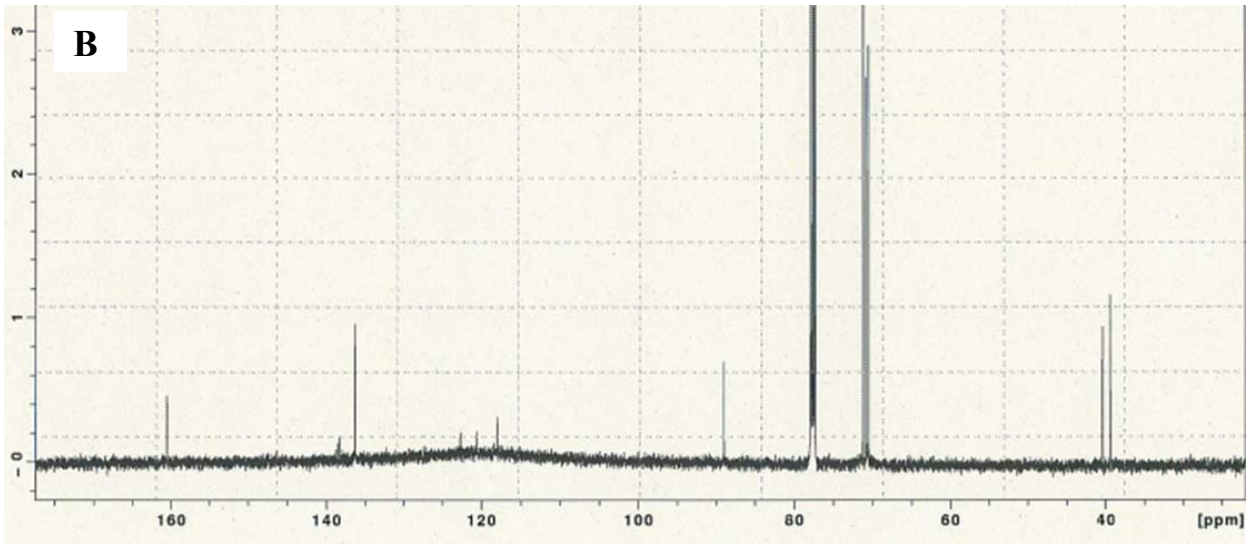
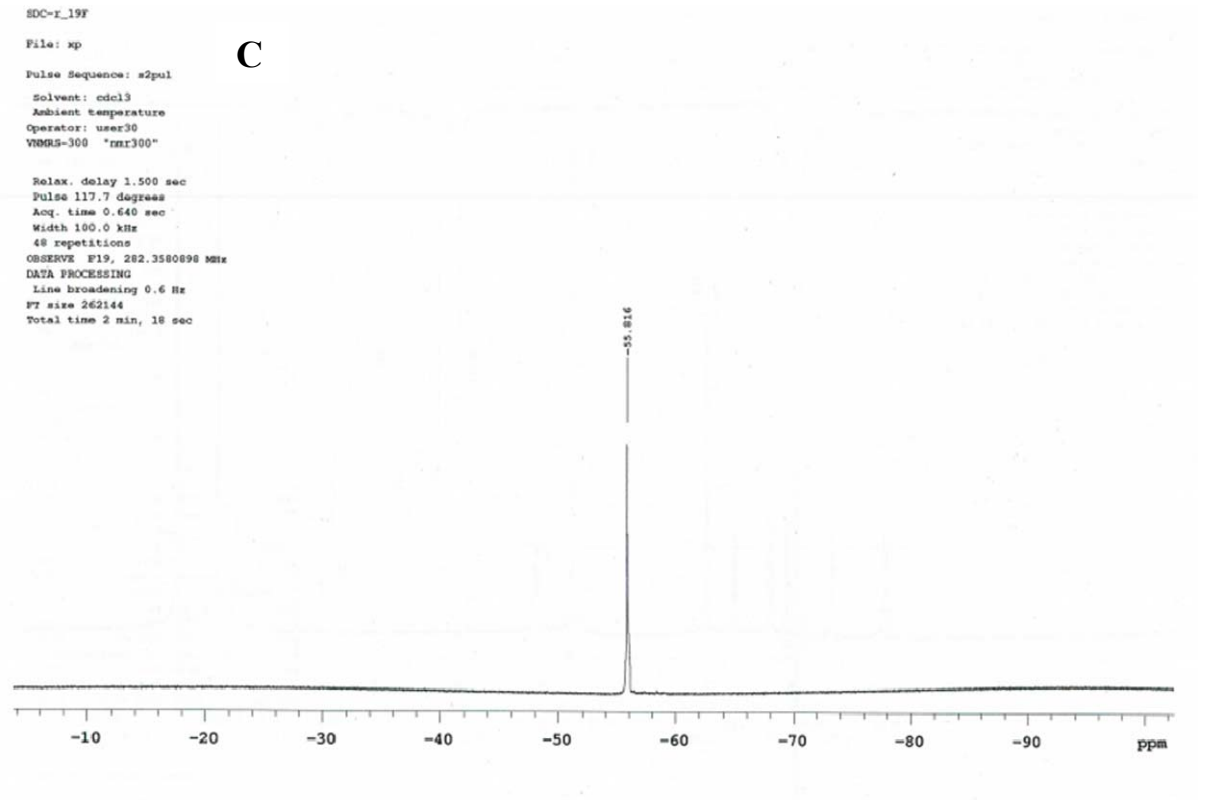
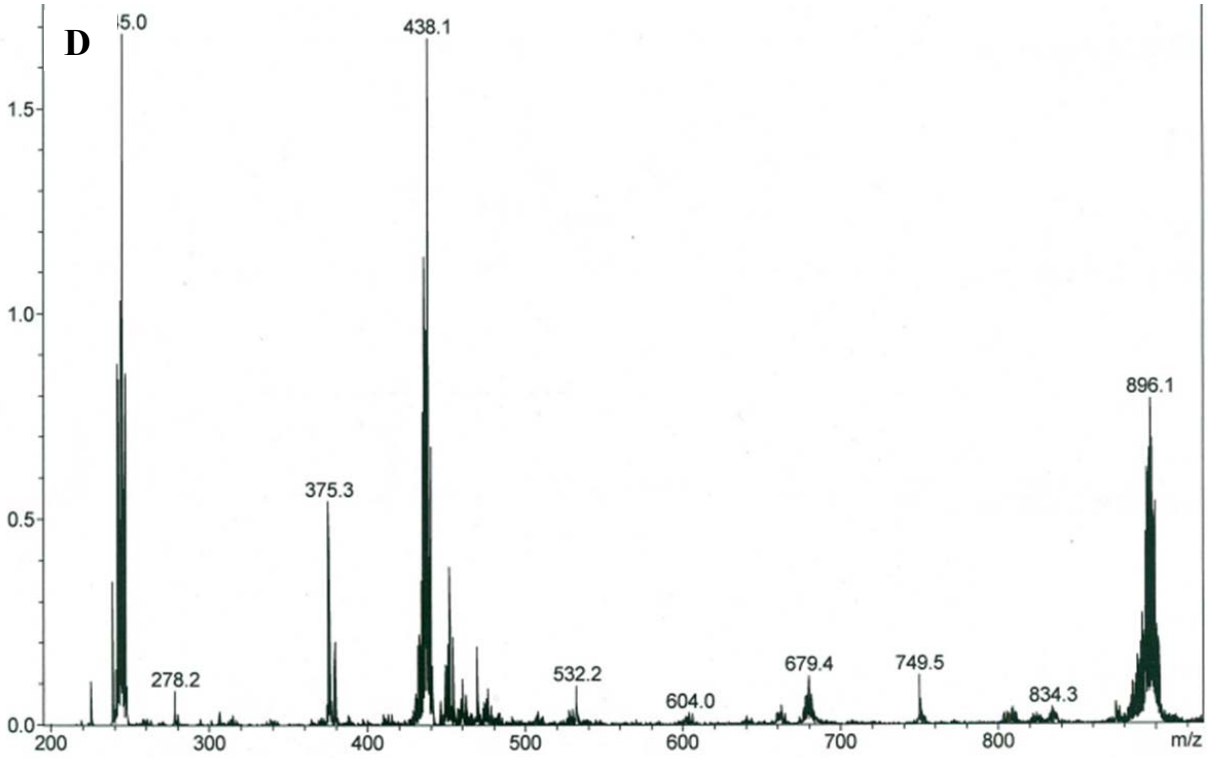
20
40
60
80
300
325
350
375
400
425
450
475
500
525
550 m/z
Auto
Profile MS
Line MS
Fragment MS
UV
Fewi

Figure S4. Analytical data for complex **1b**: A) ^{1}H NMR ($CDCl_3$); B) ^{13}C NMR ($CDCl_3$); C) ^{19}F NMR ($CDCl_3$); D) MS






C
SDC-r_19F
File: xp
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
Operator: user30
VNMRS-300 "nmr300"
Relax. delay 1.500 sec
Pulse 117.7 degrees
Acq. time 0.640 sec
Width 100.0 kHz
48 repetitions
OBSERVE F19, 282.3580898 MHz
DATA PROCESSING
Line broadening 0.6 Hz
FT size 262144
Total time 2 min, 18 sec
-55.816
-10
-20
-30
-40
-50
-60
-70
-80
-90
ppm


D
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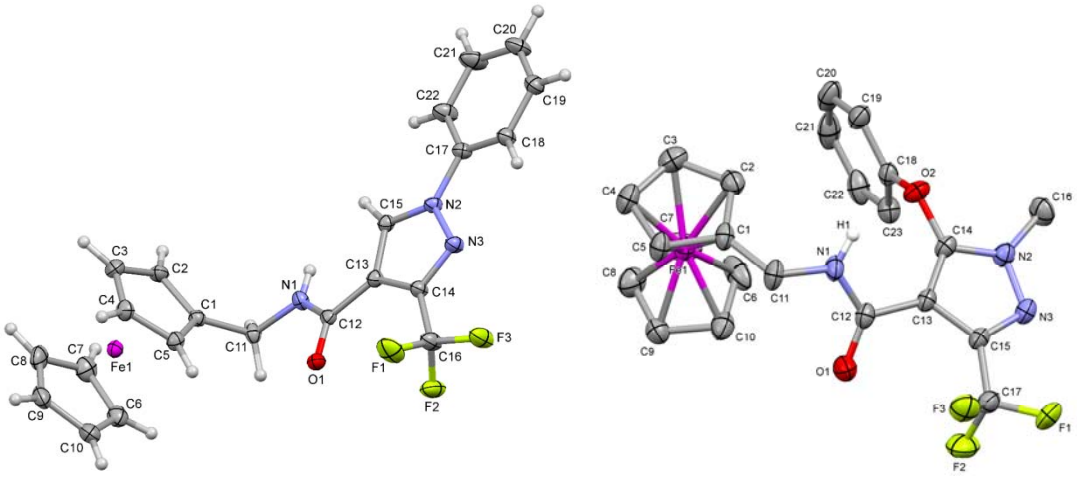
438.1
896.1
375.3
278.2
532.2
604.0
679.4
749.5
834.3
1.5
1.0
0.5
0.0
200
300
400
500
600
700
800
m/z

Figure S5. Crystal structures of complexes **2** and **3**. Thermal ellipsoids are drawn at the 30% probability level.



Crystal representation of complex **2** (left) and complex **3** (right).

Table S1. Crystal data and structure refinement for complex **1**.

Identification code	RR2011
Empirical formula	$C_{17}H_{16}F_3FeN_3O$
Formula weight	391.18
Temperature/K	183(1)
Crystal system	orthorhombic
Space group	Pbca
a/Å	10.3579(2)
b/Å	8.72054(14)
c/Å	36.8998(7)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	3333.04(10)
Z	8
ρ_{calc}g/cm^3	1.559
μ/mm^{-1}	0.946
F(000)	1600.0
Crystal size/mm^3	0.33 × 0.08 × 0.06
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.416 to 50.692
Index ranges	-12 ≤ h ≤ 12, -10 ≤ k ≤ 10, -44 ≤ l ≤ 44
Reflections collected	22551
Independent reflections	3034 [R_{int} = 0.0293, R_{sigma} = 0.0172]
Data/restraints/parameters	3034/60/231
Goodness-of-fit on F^2	1.086
Final R indexes [I>=2σ (I)]	R_1 = 0.0380, wR_2 = 0.0885
Final R indexes [all data]	R_1 = 0.0453, wR_2 = 0.0929
Largest diff. peak/hole / e Å^{-3}	0.60/-0.35

Table S2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for complex **1**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor

Atom	*x*	*y*	*z*	U(eq)
C1	1035(2)	5540(3)	3585.1(6)	32.6(5)
C2	1823(3)	5641(3)	3273.6(7)	42.9(6)
C3	1320(3)	6798(3)	3044.8(8)	48.0(7)
C4	236(3)	7429(3)	3214.4(8)	46.0(7)
C5	58(2)	6676(3)	3549.5(7)	37.9(6)
C6	-490(5)	2879(5)	3117.0(11)	86.2(12)
C7	-17(4)	3345(4)	2785.7(11)	78.8(11)
C8	-796(4)	4507(4)	2651.1(9)	73.9(10)
C9	-1776(4)	4790(5)	2898.2(13)	88.7(12)
C10	-1567(5)	3736(6)	3193.2(12)	93.5(13)
C11	1242(3)	4530(3)	3906.0(7)	40.7(6)
C12	3136(2)	4794(2)	4304.8(6)	26.9(5)
C13	3859(2)	5895(2)	4537.8(6)	25.7(5)
C14	3431(2)	6676(3)	4836.9(6)	28.6(5)
C15	5140(2)	6365(2)	4502.1(6)	26.4(5)
C16	4419(3)	8488(3)	5284.2(6)	36.8(6)
C17	6079(2)	5941(3)	4215.0(7)	35.9(6)
F1	5487.9(17)	5627(2)	3903.5(4)	56.1(5)
F2	6783.2(17)	4713.5(19)	4299.3(5)	59.2(5)
F3	6917.0(15)	7059.2(18)	4145.1(5)	54.3(5)
Fe1	-29.0(4)	5142.9(4)	3134.6(2)	37.45(14)
N1	2043(2)	5339(2)	4171.3(6)	33.7(5)
N2	4416.5(19)	7517(2)	4961.9(5)	29.3(4)
N3	5491.2(19)	7358(2)	4761.2(5)	29.7(4)
O1	3553.9(17)	3494.6(18)	4250.5(5)	40.4(4)

Table S3 Anisotropic Displacement Parameters (Å^2×10^3) for complex **1**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	38.2(13)	28.2(12)	31.3(12)	-4.4(10)	-10.4(11)	-4.8(11)
C2	36.3(14)	46.3(15)	46.0(15)	-3.2(13)	-3.0(12)	3.2(12)
C3	53.9(18)	51.0(17)	39.0(15)	10.1(13)	-3.4(13)	-8.6(14)
C4	60.1(18)	31.8(14)	46.3(16)	1.4(12)	-14.2(14)	6.3(13)
C5	42.2(15)	38.3(14)	33.1(13)	-7.8(11)	-5.4(11)	4.9(11)
C6	131(3)	53(2)	74(2)	5.5(18)	-51(2)	-34(2)
C7	118(3)	48.7(18)	69(2)	-22.2(17)	-32(2)	2.0(19)
C8	123(3)	51.1(18)	47.7(17)	-8.9(15)	-41.5(19)	-6(2)
C9	78(2)	87(3)	101(3)	-28(2)	-49(2)	-6(2)
C10	97(3)	110(3)	73(2)	-17(2)	-13(2)	-63(2)
C11	54.9(17)	28.5(13)	38.9(14)	-0.6(11)	-16.2(12)	-8.0(12)
C12	32.1(13)	20.8(11)	27.8(11)	1.7(9)	2.8(9)	-2.5(9)
C13	29.0(12)	20.3(10)	27.8(11)	2.1(9)	-3.0(9)	1.0(9)
C14	27.1(12)	27.3(12)	31.4(12)	1.4(10)	-0.2(10)	0.1(10)
C15	31.2(12)	20.8(11)	27.2(11)	2.0(9)	-2.3(9)	1.0(9)
C16	43.9(15)	35.6(14)	30.8(13)	-7.4(11)	-1.9(11)	3.1(11)

C17	37.5(14)	29.6(13)	40.6(14)	-4.2(11)	4.3(11)	-5.4(11)
F1	56.5(10)	75.8(12)	36.0(8)	-15.6(8)	8.8(8)	-14.2(9)
F2	60.5(11)	42.9(9)	74.3(12)	-0.1(8)	20.1(9)	21.5(8)
F3	51.7(10)	45.2(9)	66.0(11)	-9.6(8)	23.4(8)	-19.3(8)
Fe1	47.1(3)	35.2(2)	30.0(2)	-3.20(15)	-10.30(16)	-2.17(16)
N1	43.5(13)	20.5(10)	37.0(11)	-5.5(9)	-13.0(9)	0.7(9)
N2	31.9(11)	26.6(10)	29.5(10)	-2.1(8)	-2.8(8)	2.2(9)
N3	29.5(10)	26.6(10)	33.1(11)	-0.9(8)	-1.9(8)	-1.1(8)
O1	42.6(10)	21.4(9)	57.3(11)	-6.5(8)	-4.2(9)	1.8(7)

Table S4 Bond Lengths for complex **1**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	C2	1.413(4)	C9	C10	1.441(6)
C1	C5	1.422(3)	C9	Fe1	2.032(4)
C1	C11	1.492(3)	C10	Fe1	2.022(4)
C1	Fe1	2.024(2)	C11	N1	1.464(3)
C2	C3	1.415(4)	C12	C13	1.491(3)
C2	Fe1	2.033(3)	C12	N1	1.323(3)
C3	C4	1.398(4)	C12	O1	1.229(3)
C3	Fe1	2.037(3)	C13	C14	1.371(3)
C4	C5	1.412(4)	C13	C15	1.395(3)
C4	Fe1	2.034(3)	C14	N2	1.338(3)
C5	Fe1	2.034(3)	C15	C17	1.485(3)
C6	C7	1.378(6)	C15	N3	1.340(3)
C6	C10	1.372(6)	C16	N2	1.460(3)
C6	Fe1	2.032(4)	C17	F1	1.331(3)
C7	C8	1.388(5)	C17	F2	1.332(3)
C7	Fe1	2.029(3)	C17	F3	1.331(3)
C8	C9	1.386(6)	N2	N3	1.344(3)
C8	Fe1	2.030(3)			

Table S5 Bond Angles for complex **1**.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C2	C1	C5	107.0(2)	C1	Fe1	C2	40.76(10)
C2	C1	C11	126.8(2)	C1	Fe1	C3	68.82(10)
C2	C1	Fe1	69.96(14)	C1	Fe1	C4	68.88(10)
C5	C1	C11	126.0(2)	C1	Fe1	C5	41.01(10)
C5	C1	Fe1	69.88(14)	C1	Fe1	C6	108.69(13)
C11	C1	Fe1	129.00(17)	C1	Fe1	C7	130.55(13)
C1	C2	C3	108.5(2)	C1	Fe1	C8	168.95(15)
C1	C2	Fe1	69.28(14)	C1	Fe1	C9	149.67(16)
C3	C2	Fe1	69.79(16)	C2	Fe1	C3	40.70(11)
C2	C3	Fe1	69.51(16)	C2	Fe1	C4	68.07(12)
C4	C3	C2	108.0(2)	C2	Fe1	C5	68.16(11)
C4	C3	Fe1	69.79(17)	C4	Fe1	C3	40.19(12)

C3	C4	C5	108.3(2)	C4	Fe1	C5	40.62(11)
C3	C4	Fe1	70.02(16)	C5	Fe1	C3	68.06(12)
C5	C4	Fe1	69.72(15)	C6	Fe1	C2	115.94(17)
C1	C5	Fe1	69.11(14)	C6	Fe1	C3	147.65(19)
C4	C5	C1	108.2(2)	C6	Fe1	C4	171.33(18)
C4	C5	Fe1	69.66(15)	C6	Fe1	C5	132.28(15)
C7	C6	Fe1	70.1(2)	C6	Fe1	C9	68.28(18)
C10	C6	C7	108.1(4)	C7	Fe1	C2	108.64(15)
C10	C6	Fe1	69.8(2)	C7	Fe1	C3	116.13(16)
C6	C7	C8	109.0(4)	C7	Fe1	C4	148.07(15)
C6	C7	Fe1	70.3(2)	C7	Fe1	C5	170.09(14)
C8	C7	Fe1	70.0(2)	C7	Fe1	C6	39.68(17)
C7	C8	Fe1	69.97(19)	C7	Fe1	C8	39.98(14)
C9	C8	C7	108.7(4)	C7	Fe1	C9	67.41(17)
C9	C8	Fe1	70.12(19)	C8	Fe1	C2	130.50(16)
C8	C9	C10	105.9(4)	C8	Fe1	C3	108.61(14)
C8	C9	Fe1	70.0(2)	C8	Fe1	C4	116.60(13)
C10	C9	Fe1	68.8(2)	C8	Fe1	C5	149.10(13)
C6	C10	C9	108.3(4)	C8	Fe1	C6	67.35(15)
C6	C10	Fe1	70.6(2)	C8	Fe1	C9	39.91(17)
C9	C10	Fe1	69.6(2)	C9	Fe1	C2	168.81(17)
N1	C11	C1	109.1(2)	C9	Fe1	C3	130.44(16)
N1	C12	C13	114.41(19)	C9	Fe1	C4	109.33(15)
O1	C12	C13	120.7(2)	C9	Fe1	C5	117.52(15)
O1	C12	N1	124.9(2)	C10	Fe1	C1	116.41(14)
C14	C13	C12	128.5(2)	C10	Fe1	C2	147.79(18)
C14	C13	C15	103.7(2)	C10	Fe1	C3	171.14(19)
C15	C13	C12	127.8(2)	C10	Fe1	C4	133.27(19)
N2	C14	C13	107.6(2)	C10	Fe1	C5	110.66(16)
C13	C15	C17	128.1(2)	C10	Fe1	C6	39.56(18)
N3	C15	C13	112.4(2)	C10	Fe1	C7	66.66(19)
N3	C15	C17	119.5(2)	C10	Fe1	C8	67.68(17)
F1	C17	C15	111.5(2)	C10	Fe1	C9	41.64(18)
F1	C17	F2	106.8(2)	C12	N1	C11	124.1(2)
F2	C17	C15	113.1(2)	C14	N2	C16	126.9(2)
F3	C17	C15	112.5(2)	C14	N2	N3	112.65(19)
F3	C17	F1	106.5(2)	N3	N2	C16	120.5(2)
F3	C17	F2	106.1(2)	C15	N3	N2	103.60(18)

Table S6. Hydrogen Bonds for complex **1**.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
N1	H1	O1[1]	0.79(3)	2.05(3)	2.836(3)	177(3)

[1]1/2-X,1/2+Y,+Z

Table S7. Torsion Angles for complex **1**.

A	B	C	D	Angle/˚	A	B	C	D	Angle/˚
C1	C2	C3	C4	0.8(3)	C13	C14	N2	C16	-177.5(2)
C1	C2	C3	Fe1	-58.64(18)	C13	C14	N2	N3	0.6(3)

C1	C11	N1	C12	-124.9(3)	C13	C15	C17	F1	28.7(3)
C2	C1	C5	C4	1.5(3)	C13	C15	C17	F2	-91.6(3)
C2	C1	C5	Fe1	60.40(17)	C13	C15	C17	F3	148.2(2)
C2	C1	C11	N1	89.2(3)	C13	C15	N3	N2	-0.1(2)
C2	C3	C4	C5	0.2(3)	C14	C13	C15	C17	-177.3(2)
C2	C3	C4	Fe1	-59.2(2)	C14	C13	C15	N3	0.5(3)
C3	C4	C5	C1	-1.1(3)	C14	N2	N3	C15	-0.3(2)
C3	C4	C5	Fe1	-59.6(2)	C15	C13	C14	N2	-0.6(2)
C5	C1	C2	C3	-1.4(3)	C16	N2	N3	C15	178.0(2)
C5	C1	C2	Fe1	-60.35(17)	C17	C15	N3	N2	177.8(2)
C5	C1	C11	N1	-85.3(3)	Fe1	C1	C2	C3	58.95(19)
C6	C7	C8	C9	0.0(4)	Fe1	C1	C5	C4	-58.88(18)
C6	C7	C8	Fe1	59.7(3)	Fe1	C1	C11	N1	-177.60(18)
C7	C6	C10	C9	-0.3(4)	Fe1	C2	C3	C4	59.4(2)
C7	C6	C10	Fe1	-59.8(3)	Fe1	C3	C4	C5	59.42(19)
C7	C8	C9	C10	-0.2(4)	Fe1	C4	C5	C1	58.54(17)
C7	C8	C9	Fe1	59.6(2)	Fe1	C6	C7	C8	-59.5(2)
C8	C9	C10	C6	0.3(4)	Fe1	C6	C10	C9	59.5(2)
C8	C9	C10	Fe1	60.5(2)	Fe1	C7	C8	C9	-59.7(2)
C10	C6	C7	C8	0.2(4)	Fe1	C8	C9	C10	-59.8(2)
C10	C6	C7	Fe1	59.7(3)	Fe1	C9	C10	C6	-60.2(3)
C11	C1	C2	C3	-176.7(2)	N1	C12	C13	C14	54.6(3)
C11	C1	C2	Fe1	124.3(2)	N1	C12	C13	C15	-125.7(2)
C11	C1	C5	C4	176.9(2)	N3	C15	C17	F1	-148.9(2)
C11	C1	C5	Fe1	-124.2(2)	N3	C15	C17	F2	90.8(3)
C12	C13	C14	N2	179.2(2)	N3	C15	C17	F3	-29.4(3)
C12	C13	C15	C17	3.0(4)	O1	C12	C13	C14	-125.0(3)
C12	C13	C15	N3	-179.3(2)	O1	C12	C13	C15	54.8(3)
C13	C12	N1	C11	173.3(2)	O1	C12	N1	C11	-7.2(4)

Table S8. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for complex **1**.

Atom	***x***	***y***	***z***	**U(eq)**
H2	2550	5047	3227	51
H3	1653	7089	2821	58
H4	-279	8210	3122	55
H5	-587	6886	3718	45
H6	-140	2117	3263	103
H7	707	2944	2671	95
H8	-680	5013	2432	89
H9	-2433	5511	2878	106
H10	-2075	3652	3400	112
H11A	418	4264	4014	49
H11B	1667	3590	3832	49
H14	2605	6631	4935	34
H16A	4433	7856	5497	55
H16B	3656	9113	5286	55
H16C	5170	9134	5281	55
H1	1910(20)	6230(30)	4191(7)	33(7)

Table S9. Crystal data and structure refinement for complex **2**.

Identification code	rr2711_sq
Empirical formula	$C_{23}H_{19}Cl_3F_3FeN_3O$
Formula weight	572.61
Temperature/K	183(1)
Crystal system	monoclinic
Space group	I2/a
a/Å	10.6241(2)
b/Å	15.1983(4)
c/Å	29.6784(7)
α/°	90
β/°	90.352(2)
γ/°	90
Volume/Å^3	4792.03(19)
Z	8
ρ_{calc}g/cm^3	1.587
μ/mm^{-1}	8.534
F(000)	2320.0
Crystal size/mm^3	0.26 × 0.08 × 0.05
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	5.956 to 136.496
Index ranges	-12 ≤ h ≤ 12, -17 ≤ k ≤ 18, -35 ≤ l ≤ 35
Reflections collected	16614
Independent reflections	4393 [R_{int} = 0.0432, R_{sigma} = 0.0284]
Data/restraints/parameters	4393/0/275
Goodness-of-fit on F^2	1.030
Final R indexes [I>=2σ (I)]	R_1 = 0.0370, wR_2 = 0.0949
Final R indexes [all data]	R_1 = 0.0444, wR_2 = 0.0994
Largest diff. peak/hole / e Å^{-3}	0.29/-0.40

Table S10. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for complex **2**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor

Atom	***x***	***y***	***z***	**U(eq)**
C1	4217.2(19)	4232.9(14)	3751.9(7)	28.5(4)
C2	3221(2)	4334.0(16)	4065.7(8)	35.2(5)
C3	3692(2)	4785.3(16)	4448.0(8)	39.0(5)
C4	4994(2)	4959.5(16)	4375.3(8)	36.6(5)
C5	5316(2)	4615.6(14)	3947.4(7)	31.4(5)
C6	5080(3)	2344.9(17)	4233.4(9)	45.6(6)
C7	3963(3)	2415.5(18)	4491.4(10)	50.7(6)
C8	4265(3)	2859.4(19)	4897.8(9)	53.2(7)
C9	5557(3)	3065.0(19)	4888.2(9)	49.3(6)
C10	6062(3)	2750.8(18)	4481.2(9)	46.5(6)
C11	4095(2)	3876.1(14)	3281.0(7)	31.3(5)
C12	4730.6(19)	5075.8(13)	2774.2(7)	26.9(4)
C13	4292.9(19)	5766.5(13)	2457.8(7)	27.6(4)
C14	4992(2)	6265.4(14)	2146.3(8)	30.8(4)
C15	3078.7(19)	6064.2(14)	2397.6(7)	27.2(4)

C16	6365(2)	6244.1(17)	2045.0(9)	43.4(6)
C17	2071.3(19)	7165.8(14)	1883.2(8)	30.3(4)
C18	2303(2)	7848.2(15)	1586.1(8)	34.9(5)
C19	1298(2)	8308.6(17)	1402.5(9)	41.8(5)
C20	83(2)	8097.6(19)	1519.7(11)	50.9(7)
C21	-138(2)	7432(2)	1823.3(11)	55.6(7)
C22	852(2)	6955.8(17)	2007(1)	45.7(6)
F1	7066.6(14)	6561.7(13)	2385.9(7)	63.3(5)
F2	6784.5(14)	5435.4(11)	1965.9(6)	58.5(5)
F3	6644.3(13)	6725.9(12)	1682.1(6)	57.5(5)
Fe1	4646.2(3)	3636.5(2)	4353.8(2)	28.94(11)
N1	3822.7(18)	4582.0(12)	2958.3(6)	30.1(4)
N2	3106.0(15)	6685.5(12)	2073.6(6)	27.7(4)
N3	4283.2(16)	6820.9(12)	1912.4(6)	32.0(4)
O1	5859.2(14)	4962.8(10)	2856.4(5)	34.5(3)

Table S11 Anisotropic Displacement Parameters ($Å^2×10^3$) for complex **2**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
C1	28.6(10)	27.8(11)	29.1(10)	4.7(8)	-0.3(8)	1.4(8)
C2	25.4(10)	42.5(13)	37.7(12)	4.8(10)	1.5(9)	5.5(9)
C3	39.5(12)	44.4(14)	33.2(12)	-2.5(10)	5.2(9)	9.6(10)
C4	39.3(12)	37.9(12)	32.6(11)	-2.4(9)	-2.3(9)	-2.6(10)
C5	30.8(10)	31.7(11)	31.7(11)	1.9(9)	1.9(8)	-2.5(9)
C6	58.6(16)	37.3(13)	41.0(13)	4.0(11)	0.0(11)	5.9(12)
C7	57.2(16)	43.3(15)	51.5(15)	13.0(12)	3.6(12)	-8.6(12)
C8	71.2(19)	53.2(16)	35.5(13)	15.7(12)	14.1(12)	3.3(14)
C9	63.1(17)	49.4(15)	35.3(13)	7.6(11)	-9.5(11)	10.0(13)
C10	46.3(14)	50.1(15)	43.0(14)	6.3(11)	-3.3(11)	13.8(12)
C11	40.9(12)	26.3(11)	26.8(10)	4.1(8)	-1.7(9)	-3.4(9)
C12	30.7(10)	26(1)	24.0(9)	-1.3(8)	2.1(8)	2.2(8)
C13	27.1(10)	27(1)	28.6(10)	1.7(8)	2.2(8)	-0.6(8)
C14	25.9(10)	31.1(11)	35.3(11)	7.5(9)	2.3(8)	1.2(8)
C15	26.4(10)	26.7(10)	28.3(10)	1.9(8)	3.0(8)	-1.3(8)
C16	29.7(12)	47.2(14)	53.2(15)	20.6(12)	8.1(10)	4.3(10)
C17	25.3(10)	28.4(11)	37.1(11)	-0.1(9)	-0.7(8)	2.8(8)
C18	29.7(11)	35.7(12)	39.2(12)	7(1)	1.3(9)	2.1(9)
C19	42.4(13)	39.4(13)	43.5(13)	7.4(11)	-1.4(10)	7.6(10)
C20	32.8(13)	50.0(16)	69.8(18)	9.7(13)	-8.7(12)	11.0(11)
C21	26.6(12)	57.3(17)	83(2)	14.1(15)	1.3(12)	3.3(11)
C22	28.5(11)	42.0(14)	66.7(17)	17.0(12)	4.4(11)	-1.5(10)
F1	29.2(7)	83.1(12)	77.5(12)	19(1)	-10.7(7)	-8.0(7)
F2	45.6(8)	60(1)	70.2(11)	24.4(8)	25.2(8)	22.7(7)
F3	31.9(7)	69.2(10)	71.5(11)	39.7(9)	15.9(7)	8.0(7)
Fe1	26.62(17)	35.3(2)	24.95(17)	4.05(14)	1.91(12)	0.69(13)
N1	30.6(10)	31.2(10)	28.3(9)	5.4(7)	-3.5(7)	-2.9(7)
N2	21.2(8)	28.2(9)	33.9(9)	4.8(7)	3.3(7)	-0.8(7)

N3	23.7(8)	33.9(10)	38.3(10)	9.7(8)	4.7(7)	0.1(7)
O1	28.6(8)	39.9(9)	35.0(8)	5.2(7)	4.8(6)	7.3(6)

Table S12 Bond Lengths for complex **2**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	C2	1.423(3)	C11	N1	1.466(3)
C1	C5	1.425(3)	C12	C13	1.481(3)
C1	C11	1.504(3)	C12	N1	1.341(3)
C1	Fe1	2.052(2)	C12	O1	1.234(3)
C2	C3	1.415(3)	C13	C14	1.410(3)
C2	Fe1	2.033(2)	C13	C15	1.378(3)
C3	C4	1.426(3)	C14	C16	1.491(3)
C3	Fe1	2.039(2)	C14	N3	1.325(3)
C4	C5	1.417(3)	C15	N2	1.348(3)
C4	Fe1	2.045(2)	C16	F1	1.343(3)
C5	Fe1	2.046(2)	C16	F2	1.329(3)
C6	C7	1.420(4)	C16	F3	1.337(3)
C6	C10	1.415(4)	C17	C18	1.384(3)
C6	Fe1	2.048(3)	C17	C22	1.385(3)
C7	C8	1.417(4)	C17	N2	1.433(3)
C7	Fe1	2.035(3)	C18	C19	1.385(3)
C8	C9	1.408(4)	C19	C20	1.377(4)
C8	Fe1	2.043(3)	C20	C21	1.376(4)
C9	C10	1.409(4)	C21	C22	1.385(4)
C9	Fe1	2.046(2)	N2	N3	1.357(2)
C10	Fe1	2.052(3)			

Table S13 Bond Angles for complex **2**.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C2	C1	C5	107.49(19)	C20	C19	C18	120.3(2)
C2	C1	C11	125.9(2)	C21	C20	C19	120.0(2)
C2	C1	Fe1	68.90(12)	C20	C21	C22	120.6(2)
C5	C1	C11	126.28(19)	C17	C22	C21	118.9(2)
C5	C1	Fe1	69.43(12)	C1	Fe1	C10	127.50(10)
C11	C1	Fe1	131.85(15)	C2	Fe1	C1	40.76(9)
C1	C2	Fe1	70.34(12)	C2	Fe1	C3	40.66(10)
C3	C2	C1	108.4(2)	C2	Fe1	C4	68.54(9)
C3	C2	Fe1	69.91(13)	C2	Fe1	C5	68.52(9)
C2	C3	C4	107.9(2)	C2	Fe1	C6	126.46(11)
C2	C3	Fe1	69.43(13)	C2	Fe1	C7	107.12(11)
C4	C3	Fe1	69.80(14)	C2	Fe1	C8	118.89(11)
C3	C4	Fe1	69.34(14)	C2	Fe1	C9	153.49(11)
C5	C4	C3	107.9(2)	C2	Fe1	C10	164.36(10)

C5	C4	Fe1	69.76(13)	C3	Fe1	C1	68.48(9)
C1	C5	Fe1	69.88(12)	C3	Fe1	C4	40.86(10)
C4	C5	C1	108.26(19)	C3	Fe1	C5	68.48(9)
C4	C5	Fe1	69.70(13)	C3	Fe1	C6	163.16(11)
C7	C6	Fe1	69.14(15)	C3	Fe1	C8	106.59(11)
C10	C6	C7	107.6(2)	C3	Fe1	C9	119.36(11)
C10	C6	Fe1	69.97(15)	C3	Fe1	C10	154.28(11)
C6	C7	Fe1	70.16(15)	C4	Fe1	C1	68.40(9)
C8	C7	C6	108.0(3)	C4	Fe1	C5	40.53(9)
C8	C7	Fe1	69.97(16)	C4	Fe1	C6	155.08(11)
C7	C8	Fe1	69.36(15)	C4	Fe1	C9	107.98(11)
C9	C8	C7	107.7(2)	C4	Fe1	C10	120.47(11)
C9	C8	Fe1	69.99(15)	C5	Fe1	C1	40.69(8)
C8	C9	C10	108.6(3)	C5	Fe1	C6	120.98(10)
C8	C9	Fe1	69.73(15)	C5	Fe1	C9	126.94(11)
C10	C9	Fe1	70.13(14)	C5	Fe1	C10	109.17(10)
C6	C10	Fe1	69.67(15)	C6	Fe1	C1	108.69(10)
C9	C10	C6	108.0(3)	C6	Fe1	C10	40.36(11)
C9	C10	Fe1	69.67(15)	C7	Fe1	C1	120.00(10)
N1	C11	C1	111.03(17)	C7	Fe1	C3	125.11(11)
N1	C12	C13	115.54(18)	C7	Fe1	C4	162.71(11)
O1	C12	C13	121.65(19)	C7	Fe1	C5	155.14(11)
O1	C12	N1	122.80(19)	C7	Fe1	C6	40.71(12)
C14	C13	C12	129.19(19)	C7	Fe1	C8	40.67(12)
C15	C13	C12	127.22(19)	C7	Fe1	C9	67.97(12)
C15	C13	C14	103.58(18)	C7	Fe1	C10	68.09(12)
C13	C14	C16	129.8(2)	C8	Fe1	C1	154.08(11)
N3	C14	C13	112.73(19)	C8	Fe1	C4	125.48(11)
N3	C14	C16	117.49(19)	C8	Fe1	C5	163.27(11)
N2	C15	C13	107.35(18)	C8	Fe1	C6	68.27(11)
F1	C16	C14	112.3(2)	C8	Fe1	C9	40.28(12)
F2	C16	C14	112.7(2)	C8	Fe1	C10	67.90(12)
F2	C16	F1	106.3(2)	C9	Fe1	C1	164.52(10)
F2	C16	F3	106.7(2)	C9	Fe1	C6	67.83(11)
F3	C16	C14	111.89(19)	C9	Fe1	C10	40.20(11)
F3	C16	F1	106.6(2)	C12	N1	C11	122.45(18)
C18	C17	C22	120.8(2)	C15	N2	C17	128.19(17)
C18	C17	N2	119.62(19)	C15	N2	N3	112.43(17)
C22	C17	N2	119.6(2)	N3	N2	C17	119.35(17)
C17	C18	C19	119.3(2)	C14	N3	N2	103.92(17)

Table S14: Hydrogen Bonds for complex **2**.

A	B	C	D	Angle/˚	A	B	C	D	Angle/˚
C1	C2	C3	C4	-0.6(3)	C14	C13	C15	N2	0.1(2)
C1	C2	C3	Fe1	-60.03(15)	C15	C13	C14	C16	-179.3(2)
C1	C11	N1	C12	84.6(2)	C15	C13	C14	N3	-0.2(3)
C2	C1	C5	C4	-0.8(2)	C15	N2	N3	C14	-0.1(2)

C2	C1	C5	Fe1	58.57(15)	C16	C14	N3	N2	179.4(2)
C2	C1	C11	N1	89.5(3)	C17	C18	C19	C20	1.0(4)
C2	C3	C4	C5	0.1(3)	C17	N2	N3	C14	-178.04(19)
C2	C3	C4	Fe1	-59.19(17)	C18	C17	C22	C21	1.0(4)
C3	C4	C5	C1	0.4(3)	C18	C17	N2	C15	173.0(2)
C3	C4	C5	Fe1	-59.05(17)	C18	C17	N2	N3	-9.4(3)
C5	C1	C2	C3	0.9(3)	C18	C19	C20	C21	0.5(5)
C5	C1	C2	Fe1	-58.91(15)	C19	C20	C21	C22	-1.3(5)
C5	C1	C11	N1	-83.3(3)	C20	C21	C22	C17	0.6(5)
C6	C7	C8	C9	0.4(3)	C22	C17	C18	C19	-1.7(4)
C6	C7	C8	Fe1	60.10(18)	C22	C17	N2	C15	-5.4(4)
C7	C6	C10	C9	0.2(3)	C22	C17	N2	N3	172.2(2)
C7	C6	C10	Fe1	-59.09(18)	Fe1	C1	C2	C3	59.76(16)
C7	C8	C9	C10	-0.2(3)	Fe1	C1	C5	C4	-59.34(16)
C7	C8	C9	Fe1	59.33(19)	Fe1	C1	C11	N1	-177.49(15)
C8	C9	C10	C6	0.0(3)	Fe1	C2	C3	C4	59.42(17)
C8	C9	C10	Fe1	59.32(19)	Fe1	C3	C4	C5	59.32(16)
C10	C6	C7	C8	-0.4(3)	Fe1	C4	C5	C1	59.45(15)
C10	C6	C7	Fe1	59.61(18)	Fe1	C6	C7	C8	-59.98(19)
C11	C1	C2	C3	-173.1(2)	Fe1	C6	C10	C9	59.32(18)
C11	C1	C2	Fe1	127.1(2)	Fe1	C7	C8	C9	-59.73(19)
C11	C1	C5	C4	173.2(2)	Fe1	C8	C9	C10	-59.56(19)
C11	C1	C5	Fe1	-127.5(2)	Fe1	C9	C10	C6	-59.31(18)
C12	C13	C14	C16	0.0(4)	N1	C12	C13	C14	-165.9(2)
C12	C13	C14	N3	179.2(2)	N1	C12	C13	C15	13.2(3)
C12	C13	C15	N2	-179.2(2)	N2	C17	C18	C19	179.9(2)
C13	C12	N1	C11	-179.43(18)	N2	C17	C22	C21	179.4(3)
C13	C14	C16	F1	-69.3(3)	N3	C14	C16	F1	111.6(2)
C13	C14	C16	F2	50.7(4)	N3	C14	C16	F2	-128.5(2)
C13	C14	C16	F3	170.9(2)	N3	C14	C16	F3	-8.2(3)
C13	C14	N3	N2	0.1(3)	O1	C12	C13	C14	13.3(3)
C13	C15	N2	C17	177.7(2)	O1	C12	C13	C15	-167.5(2)
C13	C15	N2	N3	0.0(2)	O1	C12	N1	C11	1.3(3)

Table S15: Torsion Angles for complex **2**.

Atom	***x***	***y***	***z***	**U(eq)**
H2	2381	4133	4025	42
H3	3224	4944	4707	47
H4	5547	5254	4578	44
H5	6126	4637	3814	38
H6	5154	2074	3946	55
H7	3155	2203	4406	61
H8	3698	2994	5134	64
H9	6012	3365	5118	59
H10	6914	2802	4389	56
H11A	4887	3578	3196	38
H11B	3409	3435	3271	38

H15	2356	5868	2555	33
H18	3142	7999	1509	42
H19	1448	8772	1195	50
H20	-604	8412	1391	61
H21	-977	7297	1908	67
H22	698	6493	2214	55
H1	3080(30)	4675(17)	2896(9)	35(7)

Table S16. Crystal data and structure refinement for complex **3**.

Identification code	RR1401
Empirical formula	$C_{23}H_{20}F_3FeN_3O_2$
Formula weight	483.27
Temperature/K	183(1)
Crystal system	triclinic
Space group	P-1
a/Å	9.4458(3)
b/Å	10.3520(4)
c/Å	11.0470(4)
α/°	96.727(3)
β/°	102.651(3)
γ/°	100.958(3)
Volume/Å^3	1020.46(6)
Z	2
ρ_{calc}g/cm^3	1.573
μ/mm^{-1}	0.793
F(000)	496.0
Crystal size/mm^3	0.41 × 0.25 × 0.21
Radiation	MoKα (λ = 0.71073)
Absorption correction	analytical
Transmission (max/min)	0.892 and 0.814
2Θ range for data collection/°	4.534 to 61.016
Index ranges	-13 ≤ h ≤ 13, -14 ≤ k ≤ 14, -15 ≤ l ≤ 15
Reflections collected	24870
Independent reflections	6226 [R_{int} = 0.0381, R_{sigma} = 0.0276]
Data/restraints/parameters	6226/0/294
Goodness-of-fit on F^2	1.047
Final R indexes [I>=2σ (I)]	R_1 = 0.0344, wR_2 = 0.0892
Final R indexes [all data]	R_1 = 0.0411, wR_2 = 0.0941
Largest diff. peak/hole / e Å^{-3}	0.42/-0.29

Table S17. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for complex **3**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
Fe1	5614.1(2)	6568.3(2)	3157.1(2)	25.50(7)

F1	10120.2(12)	13669.6(9)	751.4(11)	43.5(2)
F2	8782.3(15)	13309.2(10)	2059.8(11)	50.5(3)
F3	7975.9(11)	12329.1(10)	143.4(10)	41.6(2)
O1	6787.7(13)	10392.6(11)	1643.0(12)	38.2(3)
O2	10367.4(12)	8359.3(9)	1729.6(9)	27.8(2)
N1	7103.0(14)	8399.0(12)	791.3(12)	28.9(2)
N2	11644.8(13)	10579.1(11)	1827.2(11)	26.1(2)
N3	11358.1(13)	11775.6(11)	1630.9(11)	26.7(2)
C1	5373.3(16)	6532.5(14)	1269.8(13)	27.1(3)
C2	6458.9(17)	5813.4(15)	1743.1(15)	32.4(3)
C3	5775(2)	4765.4(15)	2294.9(16)	37.2(3)
C4	4256.3(19)	4815.8(15)	2146.4(15)	35.7(3)
C5	4008.7(16)	5902.7(15)	1516.2(14)	30.7(3)
C6	7305.3(19)	7923(2)	4384.0(18)	47.7(5)
C7	6771(2)	6866(2)	4994.4(17)	50.3(5)
C8	5257(2)	6817.8(18)	4926.7(16)	40.8(4)
C9	4850.0(18)	7845.1(16)	4286.4(15)	33.4(3)
C10	6102(2)	8531.5(16)	3940.4(15)	36.2(3)
C11	5561.1(16)	7685.3(15)	566.0(14)	31.1(3)
C12	7580.5(15)	9698.8(13)	1297.3(12)	25.0(3)
C13	9187.7(15)	10264.1(12)	1433.5(12)	22.1(2)
C14	10374.6(15)	9663.0(12)	1702.4(12)	23.1(2)
C15	9890.0(15)	11585.4(12)	1398.0(12)	23.5(2)
C16	13176.4(17)	10413.5(17)	2170.7(16)	36.0(3)
C17	9188.9(18)	12719.3(14)	1089.4(15)	31.0(3)
C18	10711.6(14)	7924.0(13)	2890.4(13)	23.7(2)
C19	10648.4(17)	6565.3(14)	2793.5(16)	31.1(3)
C20	10955.3(19)	6036.5(17)	3889.9(18)	41.1(4)
C21	11323.1(19)	6838(2)	5044.8(17)	44.8(4)
C22	11390.0(18)	8196.2(19)	5121.7(15)	37.9(4)
C23	11081.1(16)	8757.1(15)	4031.3(13)	28.9(3)

Table S18. Anisotropic Displacement Parameters ($Å^2×10^3$) for complex **3**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe1	21.32(10)	26.97(11)	27.40(11)	6.54(8)	5.41(7)	2.87(7)
F1	52.3(6)	22.3(4)	61.3(6)	17.4(4)	21.8(5)	5.6(4)
F2	73.7(8)	37.3(5)	52.7(6)	4.6(5)	32.9(6)	23.3(5)
F3	38.1(5)	40.0(5)	48.5(6)	16.8(4)	4.1(4)	14.9(4)
O1	30.8(6)	32.3(5)	53.4(7)	4.0(5)	17.5(5)	5.0(4)
O2	38.8(6)	20.1(4)	23.2(4)	5.0(3)	4.7(4)	6.5(4)
N1	26.0(6)	25.8(6)	32.9(6)	1.4(5)	12.7(5)	-3.6(5)
N2	23.3(5)	25.0(5)	28.3(6)	7.0(4)	3.7(4)	2.6(4)
N3	27.5(6)	21.7(5)	28.2(6)	5.6(4)	5.6(5)	-0.3(4)
C1	23.9(6)	26.7(6)	26.4(6)	3.4(5)	5.6(5)	-3.5(5)
C2	27.9(7)	32.9(7)	35.2(7)	1.1(6)	9.5(6)	4.5(6)
C3	43.5(9)	27.6(7)	39.2(8)	5.9(6)	6.8(7)	8.3(6)
C4	35.4(8)	28.7(7)	38.0(8)	8.5(6)	7.1(6)	-4.6(6)

C5	22.9(6)	32.3(7)	32.2(7)	9.3(6)	3.0(5)	-3.3(5)
C6	22.6(7)	62.8(12)	44.7(9)	-18.5(8)	5.8(7)	-2.8(7)
C7	56.8(12)	60.2(12)	31.8(8)	1.4(8)	-5.7(8)	30.9(10)
C8	53.5(11)	40.6(9)	32.6(8)	12.4(7)	15.8(7)	11.0(7)
C9	30.9(7)	36.0(8)	36.0(8)	7.1(6)	12.8(6)	8.2(6)
C10	41.0(9)	30.0(7)	35.0(8)	2.0(6)	14.0(7)	-1.8(6)
C11	26.2(7)	31.7(7)	29.6(7)	8.0(5)	4.6(5)	-6.4(5)
C12	26.0(6)	25.2(6)	22.7(6)	6.6(5)	7.0(5)	0.3(5)
C13	23.9(6)	20.1(5)	21.4(5)	4.9(4)	6.4(5)	0.8(4)
C14	27.2(6)	19.6(5)	21.5(5)	5.5(4)	5.0(5)	2.6(5)
C15	27.2(6)	18.7(5)	23.8(6)	5.0(4)	6.9(5)	1.7(5)
C16	22.8(7)	42.3(8)	41.4(8)	10.3(7)	3.5(6)	6.5(6)
C17	38.9(8)	22.0(6)	34.8(7)	7.6(5)	13.7(6)	6.6(5)
C18	20.4(6)	24.9(6)	26.8(6)	9.9(5)	6.0(5)	3.6(5)
C19	28.5(7)	24.9(6)	39.7(8)	10.9(6)	6.5(6)	4.1(5)
C20	34.2(8)	34.8(8)	55.1(10)	24.9(7)	6.7(7)	4.1(6)
C21	31.3(8)	62.9(11)	43.0(9)	33.9(9)	7.1(7)	4.0(7)
C22	27.6(7)	57.4(10)	25.9(7)	10.8(7)	6.6(6)	0.5(7)
C23	25.4(6)	32.7(7)	27.7(6)	5.8(5)	7.2(5)	2.9(5)

Table S19. Bond Lengths for complex **3**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Fe1	C1	2.0422(14)	C1	C2	1.423(2)
Fe1	C2	2.0455(16)	C1	C5	1.4271(19)
Fe1	C3	2.0415(16)	C1	C11	1.5025(19)
Fe1	C4	2.0485(15)	C2	C3	1.424(2)
Fe1	C5	2.0411(14)	C3	C4	1.419(2)
Fe1	C6	2.0273(17)	C4	C5	1.420(2)
Fe1	C7	2.0404(17)	C6	C7	1.421(3)
Fe1	C8	2.0508(17)	C6	C10	1.424(3)
Fe1	C9	2.0482(16)	C7	C8	1.407(3)
Fe1	C10	2.0369(16)	C8	C9	1.411(2)
F1	C17	1.3349(17)	C9	C10	1.412(2)
F2	C17	1.3363(18)	C12	C13	1.4871(19)
F3	C17	1.3299(19)	C13	C14	1.3766(19)
O1	C12	1.2199(18)	C13	C15	1.4112(17)
O2	C14	1.3522(15)	C15	C17	1.4910(19)
O2	C18	1.4006(15)	C18	C19	1.3868(19)
N1	C11	1.4554(18)	C18	C23	1.376(2)
N1	C12	1.3450(18)	C19	C20	1.383(2)
N2	N3	1.3488(16)	C20	C21	1.373(3)
N2	C14	1.3499(17)	C21	C22	1.387(3)
N2	C16	1.4613(19)	C22	C23	1.396(2)
N3	C15	1.3251(18)			

Table S20. Bond Angles for complex **3**.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C1	Fe1	C2	40.75(6)	C11	C1	Fe1	128.73(10)

C1	Fe1	C4	68.84(6)	C1	C2	Fe1	69.50(9)
C1	Fe1	C8	162.07(7)	C1	C2	C3	108.42(14)
C1	Fe1	C9	124.56(6)	C3	C2	Fe1	69.46(9)
C2	Fe1	C4	68.36(7)	C2	C3	Fe1	69.77(9)
C2	Fe1	C8	156.42(7)	C4	C3	Fe1	69.96(9)
C2	Fe1	C9	161.54(6)	C4	C3	C2	108.01(14)
C3	Fe1	C1	68.87(6)	C3	C4	Fe1	69.43(9)
C3	Fe1	C2	40.77(6)	C3	C4	C5	107.80(13)
C3	Fe1	C4	40.60(7)	C5	C4	Fe1	69.40(8)
C3	Fe1	C8	121.72(7)	C1	C5	Fe1	69.58(8)
C3	Fe1	C9	156.36(7)	C4	C5	Fe1	69.95(9)
C4	Fe1	C8	108.83(7)	C4	C5	C1	108.60(14)
C5	Fe1	C1	40.91(5)	C7	C6	Fe1	70.05(10)
C5	Fe1	C2	68.28(6)	C7	C6	C10	107.89(16)
C5	Fe1	C3	68.38(7)	C10	C6	Fe1	69.85(9)
C5	Fe1	C4	40.65(6)	C6	C7	Fe1	69.06(10)
C5	Fe1	C8	125.85(7)	C8	C7	Fe1	70.28(10)
C5	Fe1	C9	107.86(7)	C8	C7	C6	108.08(16)
C6	Fe1	C1	119.26(7)	C7	C8	Fe1	69.49(10)
C6	Fe1	C2	107.16(7)	C7	C8	C9	107.98(16)
C6	Fe1	C3	125.42(8)	C9	C8	Fe1	69.76(9)
C6	Fe1	C4	162.96(8)	C8	C9	Fe1	69.96(10)
C6	Fe1	C5	154.68(8)	C8	C9	C10	108.79(15)
C6	Fe1	C7	40.89(9)	C10	C9	Fe1	69.35(9)
C6	Fe1	C8	68.28(8)	C6	C10	Fe1	69.13(10)
C6	Fe1	C9	68.15(7)	C9	C10	Fe1	70.22(9)
C6	Fe1	C10	41.03(8)	C9	C10	C6	107.26(15)
C7	Fe1	C1	155.32(8)	N1	C11	C1	113.22(12)
C7	Fe1	C2	121.19(7)	O1	C12	N1	124.06(13)
C7	Fe1	C3	108.54(7)	O1	C12	C13	120.63(12)
C7	Fe1	C4	126.15(8)	N1	C12	C13	115.31(13)
C7	Fe1	C5	162.86(8)	C14	C13	C12	129.14(12)
C7	Fe1	C8	40.23(8)	C14	C13	C15	102.37(11)
C7	Fe1	C9	67.77(7)	C15	C13	C12	128.38(12)
C9	Fe1	C4	121.30(7)	O2	C14	C13	128.95(12)
C9	Fe1	C8	40.28(6)	N2	C14	O2	121.88(12)
C10	Fe1	C1	105.90(6)	N2	C14	C13	108.87(11)
C10	Fe1	C2	124.40(6)	N3	C15	C13	112.91(12)
C10	Fe1	C3	162.18(7)	N3	C15	C17	118.62(12)
C10	Fe1	C4	155.10(7)	C13	C15	C17	128.42(13)
C10	Fe1	C5	119.55(7)	F1	C17	F2	106.36(12)
C10	Fe1	C7	68.69(8)	F1	C17	C15	111.49(13)
C10	Fe1	C8	68.31(7)	F2	C17	C15	112.80(12)
C10	Fe1	C9	40.43(6)	F3	C17	F1	107.13(12)
C14	O2	C18	119.46(10)	F3	C17	F2	106.91(14)
C12	N1	C11	122.92(14)	F3	C17	C15	111.79(12)
N3	N2	C14	111.10(11)	C19	C18	O2	113.96(12)
N3	N2	C16	120.62(12)	C23	C18	O2	123.62(12)
C14	N2	C16	128.25(12)	C23	C18	C19	122.41(13)

C15	N3	N2	104.75(10)	C20	C19	C18	118.31(16)
C2	C1	Fe1	69.75(8)	C21	C20	C19	120.83(15)
C2	C1	C5	107.16(12)	C20	C21	C22	119.98(15)
C2	C1	C11	127.68(13)	C21	C22	C23	120.46(16)
C5	C1	Fe1	69.50(8)	C18	C23	C22	118.00(14)
C5	C1	C11	125.05(14)				

Table S21. Torsion Angles for complex **3**.

A	B	C	D	Angle/˚	A	B	C	D	Angle/˚
Fe1	C1	C2	C3	58.71(11)	C7	C6	C10	C9	0.17(19)
Fe1	C1	C5	C4	-59.26(11)	C7	C8	C9	Fe1	59.19(12)
Fe1	C1	C11	N1	70.56(18)	C7	C8	C9	C10	0.6(2)
Fe1	C2	C3	C4	59.75(12)	C8	C9	C10	Fe1	59.00(12)
Fe1	C3	C4	C5	58.99(11)	C8	C9	C10	C6	-0.45(19)
Fe1	C4	C5	C1	59.03(10)	C10	C6	C7	Fe1	59.84(12)
Fe1	C6	C7	C8	-59.68(13)	C10	C6	C7	C8	0.2(2)
Fe1	C6	C10	C9	60.15(11)	C11	N1	C12	O1	1.9(2)
Fe1	C7	C8	C9	-59.36(12)	C11	N1	C12	C13	-178.84(12)
Fe1	C8	C9	C10	-58.63(12)	C11	C1	C2	Fe1	123.89(15)
Fe1	C9	C10	C6	-59.45(11)	C11	C1	C2	C3	-177.40(14)
O1	C12	C13	C14	144.90(15)	C11	C1	C5	Fe1	-123.61(14)
O1	C12	C13	C15	-30.6(2)	C11	C1	C5	C4	177.13(14)
O2	C18	C19	C20	-179.33(14)	C12	N1	C11	C1	-119.60(16)
O2	C18	C23	C22	179.54(13)	C12	C13	C14	O2	10.8(2)
N1	C12	C13	C14	-34.4(2)	C12	C13	C14	N2	-175.53(13)
N1	C12	C13	C15	150.12(14)	C12	C13	C15	N3	175.99(12)
N2	N3	C15	C13	-0.16(15)	C12	C13	C15	C17	-6.7(2)
N2	N3	C15	C17	-177.77(12)	C13	C15	C17	F1	-159.74(14)
N3	N2	C14	O2	173.16(11)	C13	C15	C17	F2	80.67(19)
N3	N2	C14	C13	-1.05(16)	C13	C15	C17	F3	-39.9(2)
N3	C15	C17	F1	17.45(19)	C14	O2	C18	C19	179.24(12)
N3	C15	C17	F2	-102.14(16)	C14	O2	C18	C23	-0.8(2)
N3	C15	C17	F3	137.34(13)	C14	N2	N3	C15	0.74(15)
C1	C2	C3	Fe1	-58.74(11)	C14	C13	C15	N3	-0.44(15)
C1	C2	C3	C4	1.01(18)	C14	C13	C15	C17	176.89(13)
C2	C1	C5	Fe1	59.86(10)	C15	C13	C14	O2	-172.81(13)
C2	C1	C5	C4	0.60(17)	C15	C13	C14	N2	0.86(14)
C2	C1	C11	N1	-22.8(2)	C16	N2	N3	C15	-177.27(13)
C2	C3	C4	Fe1	-59.62(11)	C16	N2	C14	O2	-9.0(2)
C2	C3	C4	C5	-0.63(19)	C16	N2	C14	C13	176.77(14)
C3	C4	C5	Fe1	-59.01(11)	C18	O2	C14	N2	82.07(16)
C3	C4	C5	C1	0.02(18)	C18	O2	C14	C13	-104.98(16)
C5	C1	C2	Fe1	-59.70(10)	C18	C19	C20	C21	-0.4(2)
C5	C1	C2	C3	-0.99(17)	C19	C18	C23	C22	-0.5(2)
C5	C1	C11	N1	161.38(14)	C19	C20	C21	C22	0.0(3)
C6	C7	C8	Fe1	58.92(12)	C20	C21	C22	C23	0.2(3)
C6	C7	C8	C9	-0.4(2)	C21	C22	C23	C18	0.0(2)
C7	C6	C10	Fe1	-59.97(12)	C23	C18	C19	C20	0.7(2)

Table 22. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for complex **3**.

Atom	*x*	*y*	*z*	U(eq)
H2	7469	6001	1698	39
H3	6251	4142	2693	45
H4	3534	4228	2420	43
H5	3088	6166	1296	37
H6	8290	8179	4288	57
H7	7338	6292	5381	60
H8	4620	6202	5254	49
H9	3891	8042	4116	40
H10	6137	9263	3495	43
H11A	5163	7349	-346	37
H11B	4968	8315	817	37
H16A	13728	10803	1597	54
H16B	13176	9461	2110	54
H16C	13652	10865	3035	54
H19	10401	6012	1994	37
H20	10911	5107	3843	49
H21	11532	6463	5791	54
H22	11648	8748	5922	45
H23	11125	9686	4076	35
H1	7700(20)	8020(19)	519(19)	37(5)

Figure S6. Examples of plate for fungal toxicity determination for complex **1b**, **2**, complex **3** and for the positive control Clotrimazole.