Supporting Information

Tuning of chain chirality by interchain stacking forces and structure-property relationship in coordination systems constructed by *meridional* Fe^{III} cyanide and Mn^{III} Schiff bases

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Table S1. Crystallographic Details of **1** – **8**.

	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**
formula	$C_{42}H_{29}ClFeN_6OP$	$C_{42}H_{29}BrFeN_6OP$	$C_{34}H_{22}ClFeMnN_8O_4$	$C_{34}H_{17}Br_2ClFeMnN_8O_3$	$C_{34}H_{23}BrFeMnN_8O_3$	$C_{34}H_{21}BrF_2FeMnN_8O_3$	$C_{34}H_{21}BrCl_2FeMnN_8O_3$	$C_{34}H_{21}Br_3FeMnN_8O_3$
Mr	755.98	800.44	752.84	891.62	782.30	828.29	851.19	940.11
T (K)	100(2)	100(2)	100(2)	296(2)	100(2)	296(2)	296(2)	296(2)
crystal system	Monoclinic	Triclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic
space group	P2(1)/c	P-1	P2(1)/n	P2(1)/n	P2(1)/c	C2/c	P2(1)/n	P2(1)/n
a (Å)	8.4720(17)	8.9170(18)	13.013(3)	10.4997(8)	10.680(2)	27.1284(8)	10.4825(2)	10.4788(4)
b (Å)	15.523(3)	14.417(3)	10.537(2)	12.8619(10)	12.549(3)	12.7388(4)	12.7551(3)	12.8922(4)
c (Å)	28.037(6)	14.577(3)	25.601(5)	26.645(2)	27.054(5)	20.6433(8)	26.6716(6)	26.6392(9)
α (°)	90	109.84(3)	90	90	90	90	90	90
β (°)	92.32(3)	96.49(3)	101.91(3)	96.843(2)	98.62(3)	95.7050(10)	96.7840(10)	96.718(2)
γ (°)	90	98.10(3)	90	90	90	90	90	90
V (Å^3)	3684.1(13)	1718.9(6)	3434.8(12)	3572.7(5)	3584.9(12)	7098.6(4)	3541.17(13)	3574.1(2)
Z	4	2	4	4	4	8	4	4
ρ_{calc} (g cm^{-3})	1.363	1.547	1.456	1.658	1.449	1.531	1.597	1.747
μ (mm^{-1})	0.568	1.693	0.918	3.117	1.916	1.946	2.092	4.160
F(000)	1556	814	1528	1756	1572	3272	1700	1844
total reflections	5316	4225	2828	3899	4562	6080	6414	2361
GOF	1.049	1.092	1.075	1.028	1.052	1.042	1.026	1.053
R1[a] (I≥2σ(I))	0.0955	0.0992	0.0678	0.0635	0.0536	0.0570	0.0679	0.0535
wR2[b] (I≥2σ(I))	0.2487	0.2535	0.1973	0.2151	0.1555	0.1640	0.1900	0.1324

[a] $R1=\Sigma||F_O|-|F_C||/\Sigma|F_C|$, [b] $wR2 = [\Sigma w(F_O^2 - F_C^2)^2/\Sigma w(F_O^2)^2]^{1/2}$

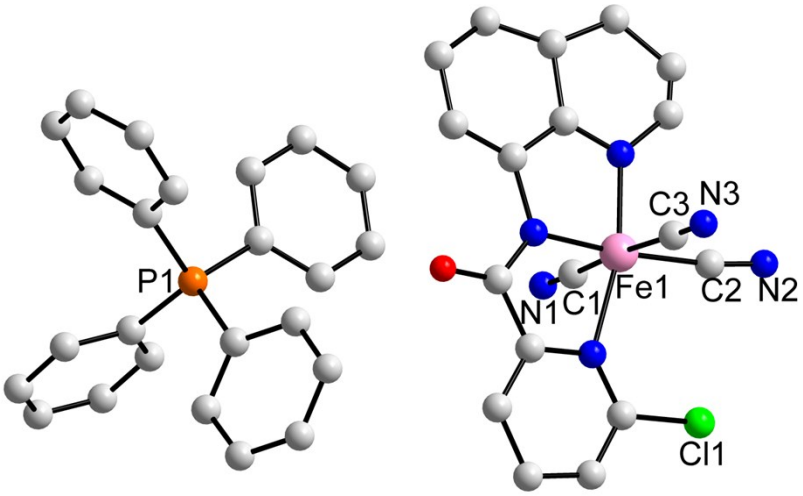

Fig. S1 Crystal structure of **1**.

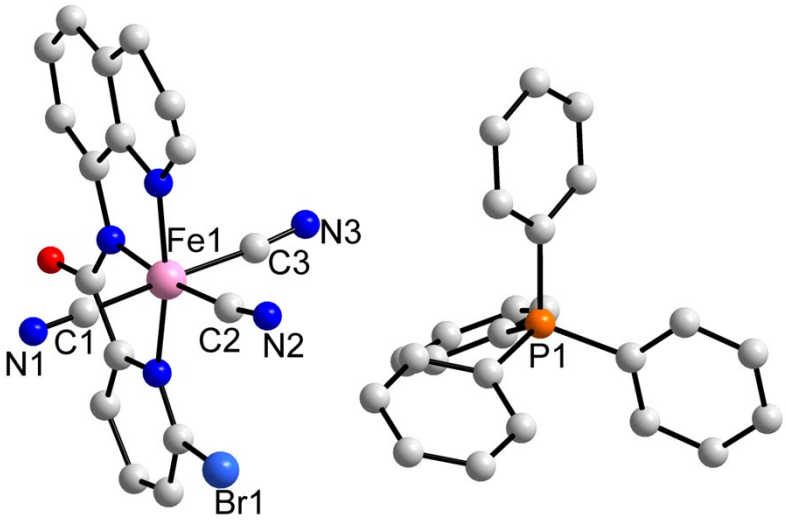

Fig. S2 Crystal structure of **2**.

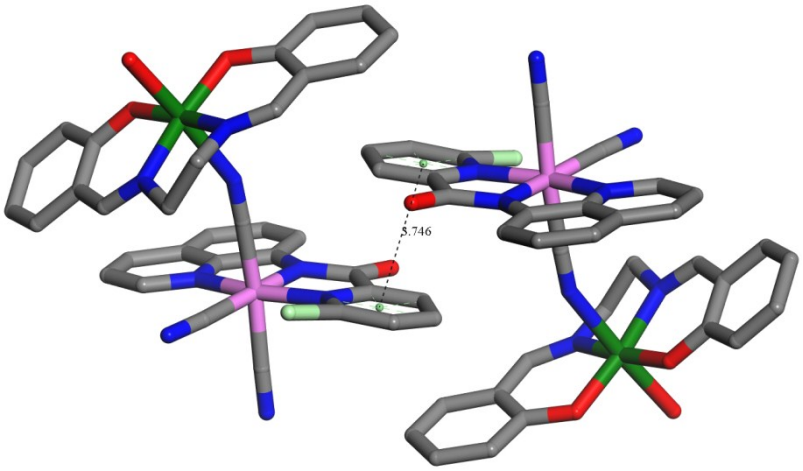

Fig. S3 Extended view of **3** displaying π-π stacking forces between pyridyl rings of Clqpa (centroid distance = 3.746 Å).

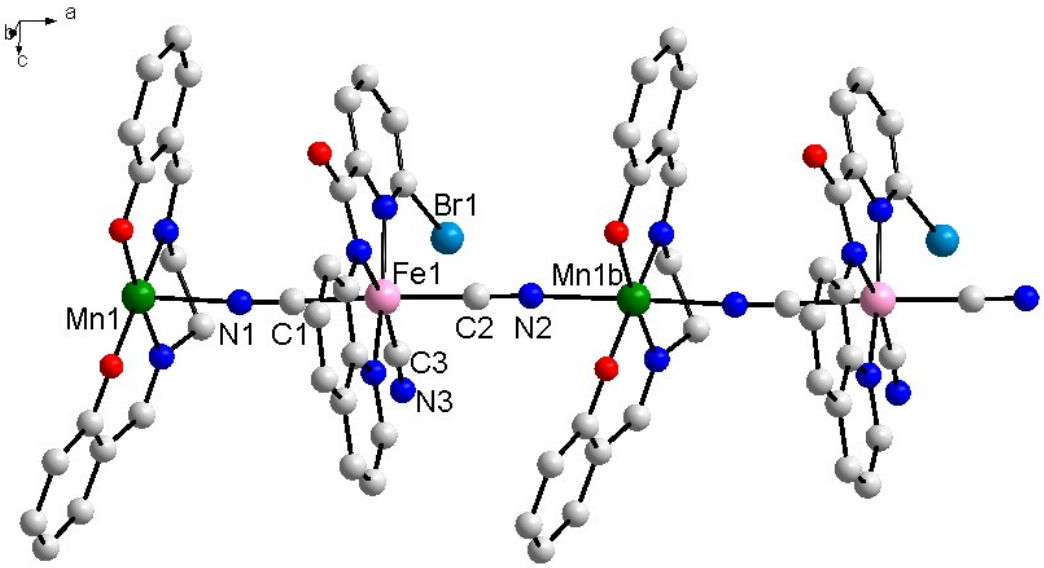

Fig. S4 Molecular structure of **5** with symmetry codes of b = 1+x, y, z.

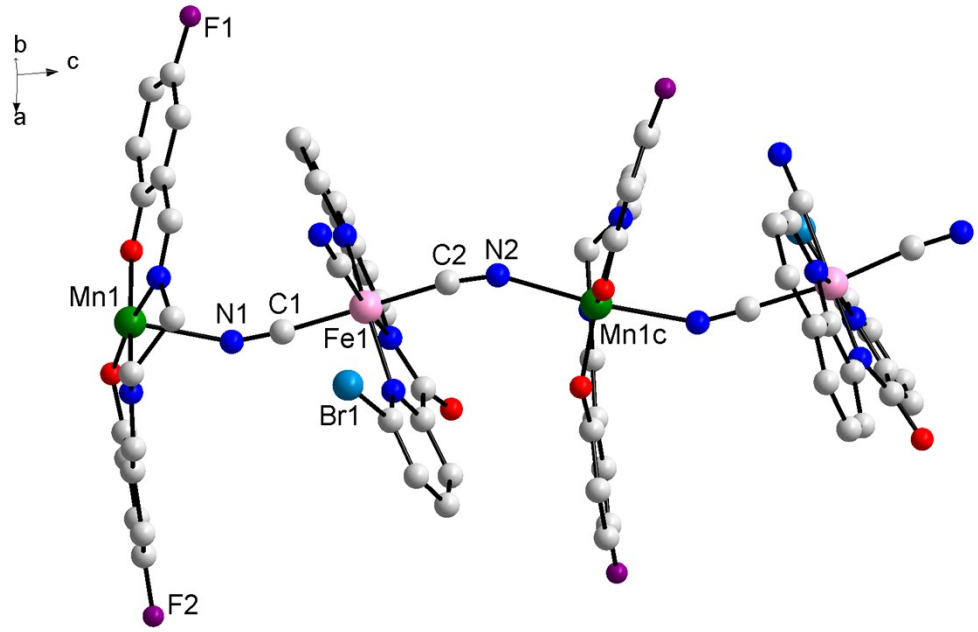

Fig. S5 Molecular structure of **6** with symmetry codes of c = x, -y, 0.5+z.

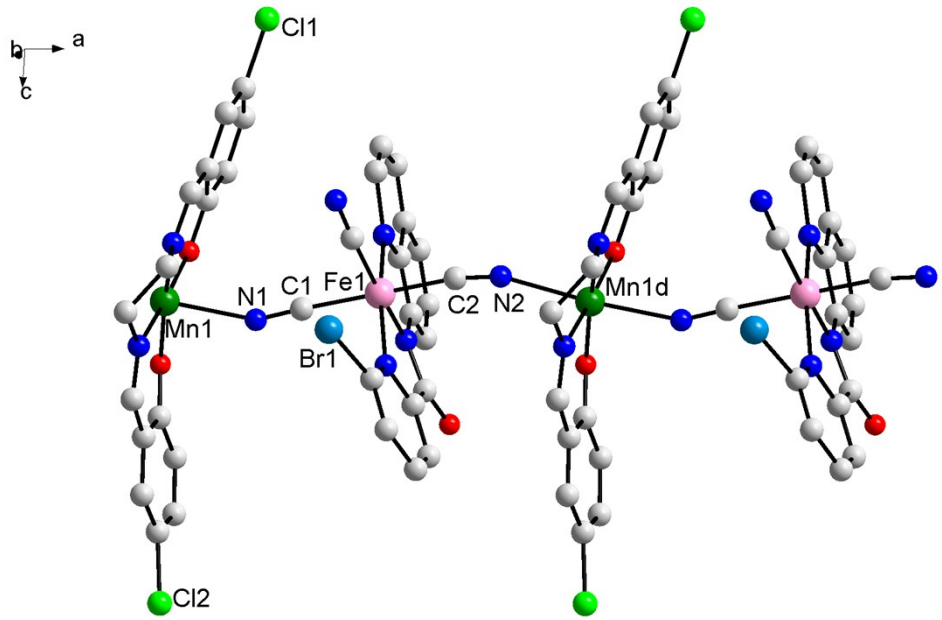

Fig. S6 Molecular structure of **7** with symmetry codes of d = 1+x, y, z.

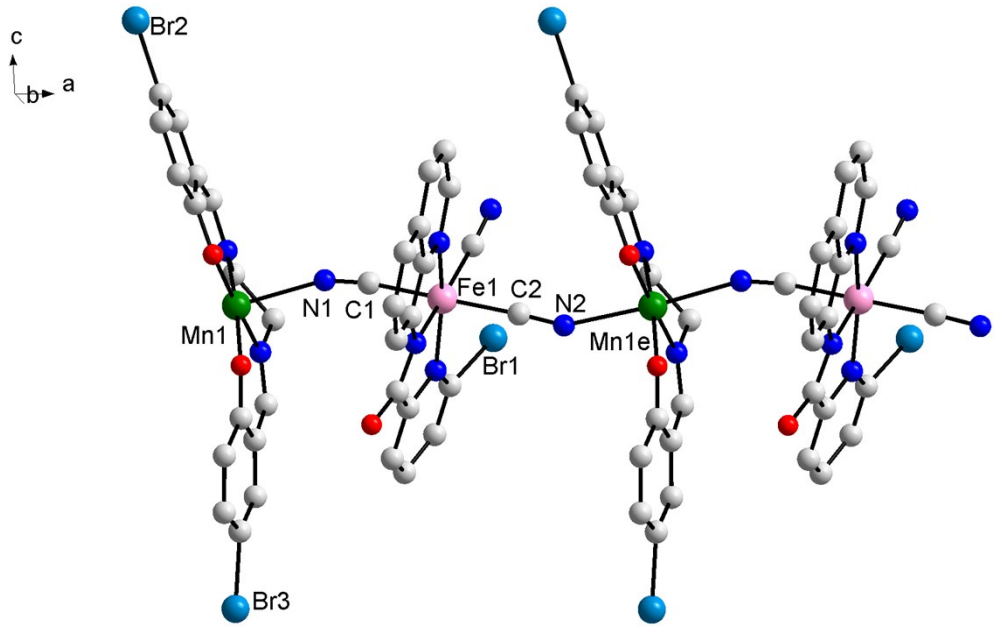

Fig. S7 Molecular structure of **8** with symmetry codes of e = 1+x, y, z.

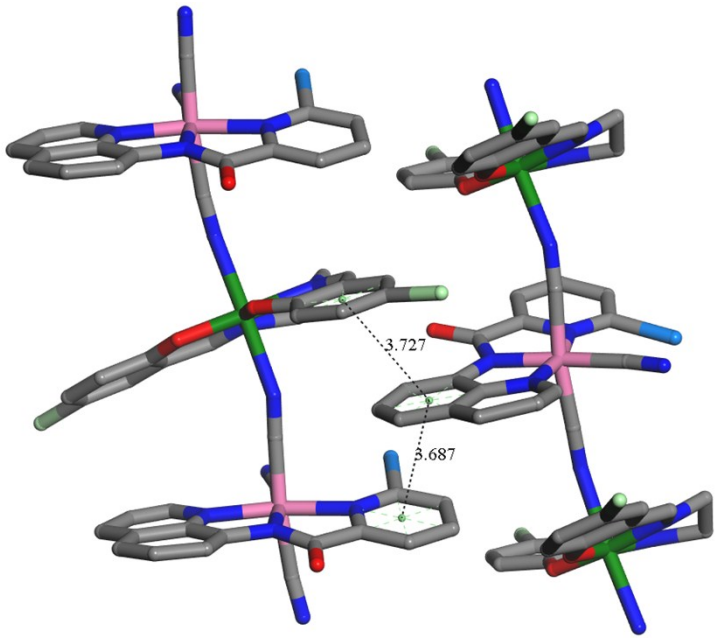

Fig. S8 Extended view of **7** showing that the quinolone benzene ring interacts with the phenoxide ring of Clsalen and the pyridyl ring of Brqpa via π-π stacking (centroid distance = 3.727 and 3.687 Å, respectively).

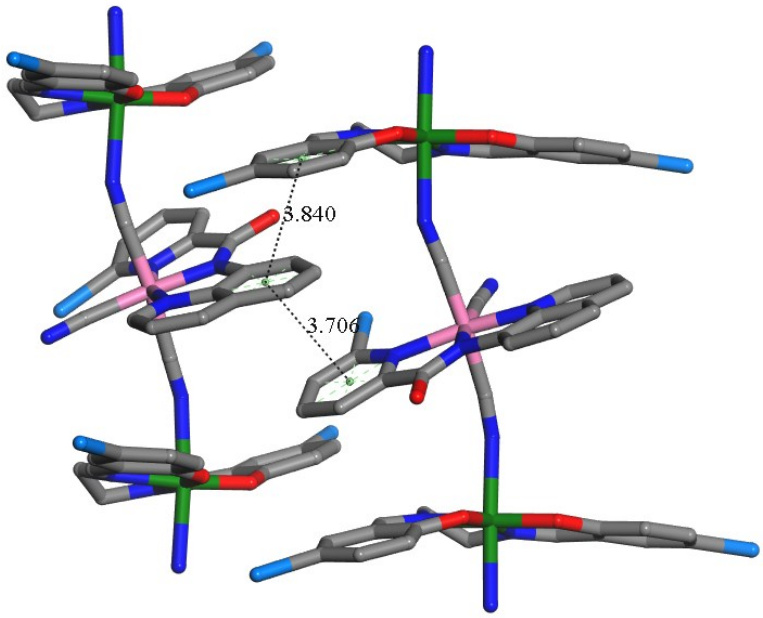

Fig. S9 Extended view of **8** showing that the quinolone benzene ring interacts with the phenoxide ring of Brsalen and the pyridyl ring of Brqpa via π-π stacking (centroid distance = 3.840 and 3.706 Å, respectively).

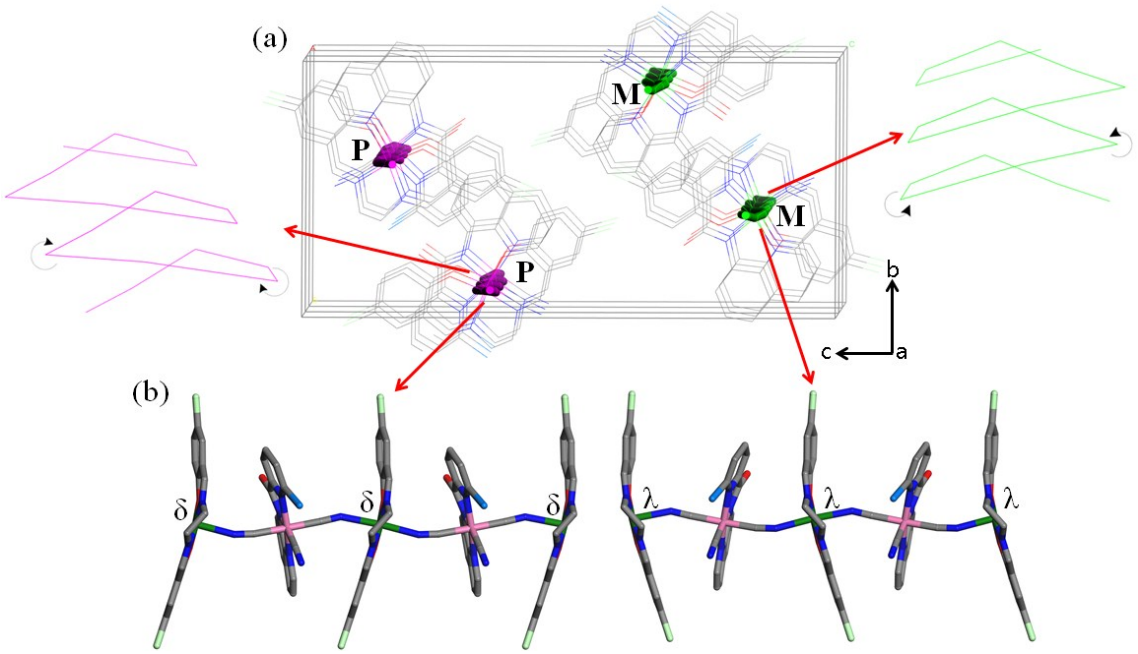

Fig. S10 (a) Illustration of a right-handed (P-) and a left-handed (M-) helical chain of **7**. (b) -δ-δ-δ- and -λ-λ-λ-conformational sequences of chelate rings formed by ethylenediamines of **7**.

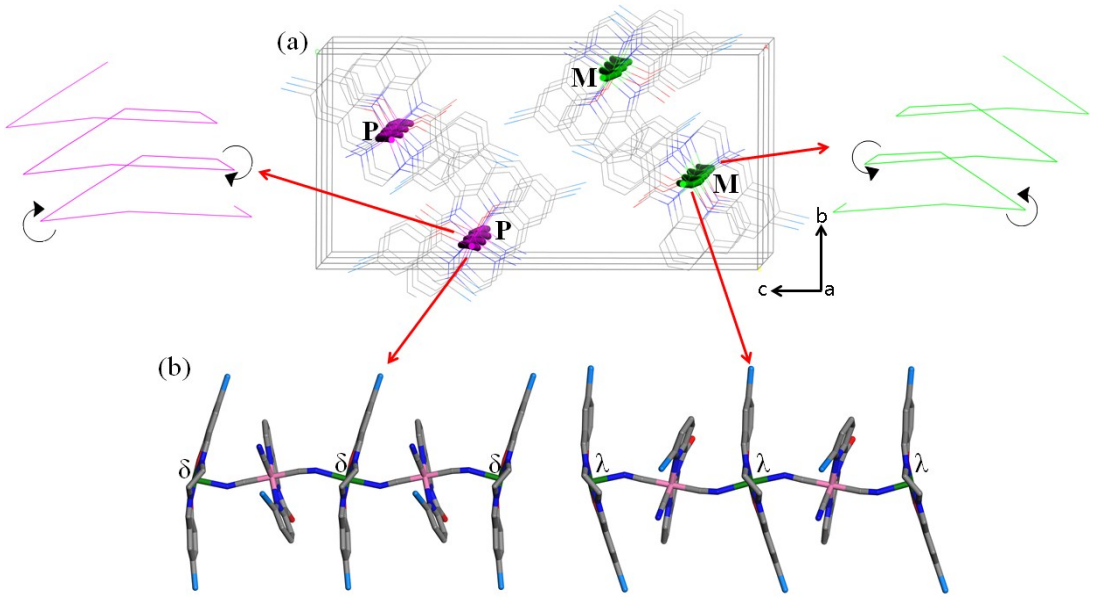

Fig. S11 (a) Illustration of a right-handed (P-) and a left-handed (M-) helical chain of **8**. (b) -δ-δ-δ- and -λ-λ-λ-conformational sequences of chelate rings formed by ethylenediamines of **8**.

Table S2. Selected Bond Distances (Å) of complexes **3** – **8.**.

		3	
Fe1-C1	1.942(8)	Fe1-C2	1.961(9)
Fe1-C3	1.934(9)	Fe1-N5	1.876(6)
Mn1-N1	2.307(7)	Mn1-O4	2.288(5)
Mn1-O2	1.883(5)	Mn1-O3	1.879(5)
Mn1-N7	1.990(6)	Mn1-N8	1.988(6)
		4	
Fe1-C1	1.971(7)	Fe1-C2	1.938(7)
Fe1-C3	1.955(7)	Fe1-N5	1.856(5)
Mn1-N1	2.276(6)	Mn1a-N2	2.285(5)
Mn1-O2	1.891(4)	Mn1-O3	1.833(4)
Mn1-N7	1.975(5)	Mn1-N8	1.998(5)
		5	
Fe1-C1	1.953(5)	Fe1-C2	1.962(5)
Fe1-C3	1.964(4)	Fe1-N5	1.891(3)
Mn1-N1	2.228(4)	Mn1b-N2	2.299(4)
Mn1-O2	1.895(3)	Mn1-O3	1.891(3)
Mn1-N7	2.002(3)	Mn1-N8	1.994(3)
		6	
Fe1-C1	1.942(4)	Fe1-C2	1.950(4)
Fe1-C3	1.950(5)	Fe1-N5	1.868(4)
Mn1-N1	2.307(3)	Mn1c-N2	2.269(3)
Mn1-O2	1.880(3)	Mn1-O3	1.891(3)
Mn1-N7	1.995(5)	Mn1-N8	2.005(3)
		7	
Fe1-C1	1.949(5)	Fe1-C2	1.952(4)
Fe1-C3	1.940(5)	Fe1-N5	1.879(4)
Mn1-N1	2.271(4)	Mn1d-N2	2.256(4)

Mn1-O2	1.890(3)	Mn1-O3	1.885(3)
Mn1-N7	1.987(4)	Mn1-N8	1.996(4)
		8	
Fe1-C1	1.950(15)	Fe1-C2	1.956(18)
Fe1-C3	1.952(19)	Fe1-N5	1.873(12)
Mn1-N1	2.264(12)	Mn1e-N2	2.270(13)
Mn1-O2	1.893(10)	Mn1-O3	1.887(9)
Mn1-N7	1.994(11)	Mn1-N8	1.985(11)

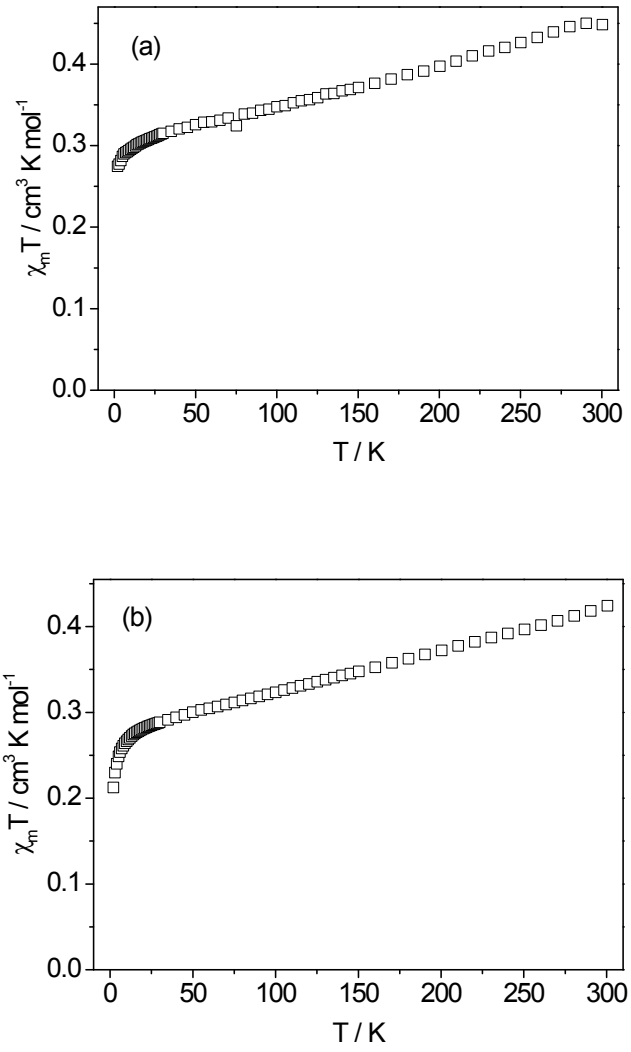

Fig. S12 Plot of $\chi_m T$ versus T of **1** (a) and **2** (b).

The magnetic data of **1** and **2** were collected in the temperature range 2-300 K and 1000 G. The $\chi_m T$ value is equal to 0.45 and 0.43 cm^3 K mol^{-1} at 300 K, respectively, which are larger than the spin-only value (0.375 cm^3 K mol^{-1}) for a noncoupled S_{Fe} = 1/2 but similar to those reported for low-spin Fe(III) analogues.[s1] The $\chi_m T$ behavior on lowering the temperature is due to the presence of an octahedral low-spin Fe(III) ion with the $^2T_{2g}$ ground term and/or temperature-independent paramagnetism.[s1]

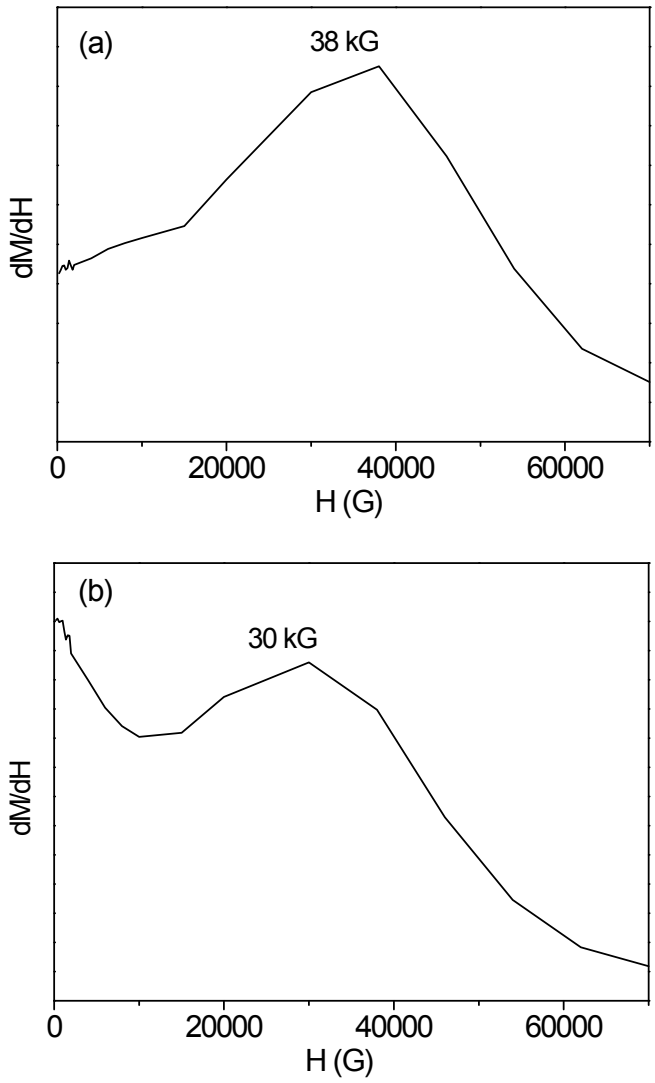

Fig. S13 Plots of d*M*/d*H* versus *H* for **4** (a) and **7** (b).

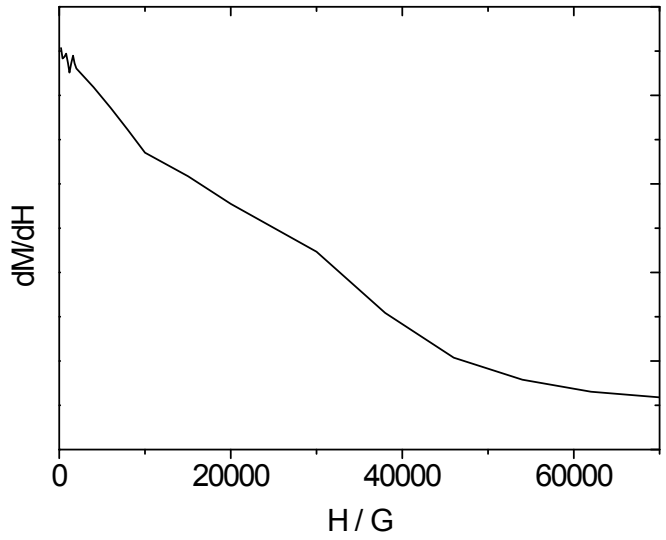

Fig. S14 Plot of d*M*/d*H* versus *H* for **5**. The dM/dH curve shows no special anomaly.

Table S3. Effective spin density of $[Fe(Brqpa)(CN)_3]^-$.

	effective spin density
Fe1	0.9960
C1	-0.03285
N1	0.03783
C2	-0.02582
N2	0.02362
C3	-0.03347
N3	0.02246

References

(s1) (a) Lescouëzec, R.; Lloret, F.; Julve, M.; Vaissermann, J.; Verdaguer, M.; Llusar, R.; Uriel, S. *Inorg. Chem.* **2001**, *40*, 2065. (b) Toma, L. M.; Lescouëzec, R.; Toma, L. D.; Lloret, F.; Julve, M.; Vaissermann, J.; Andruh, M. *J. Chem. Soc. Dalton Trans.* **2002**, 3171.