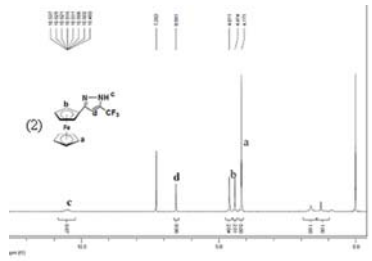
Supporting information

Table S1 Crystallographic data for the ferrocence derivatives

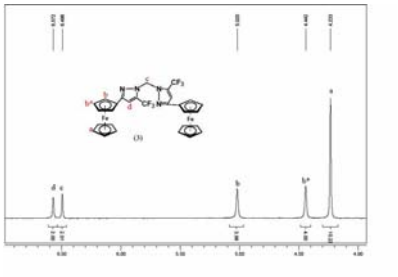
complex	2	3
Empirical formula	$C_{14}H_{11}F_3FeN_2$	$C_{29}H_{22}F_6Fe_2N_4$
Formula weight	320.10	652.21
Crystal system, space group	Tetragonal, $I4_1/a$	Orthorhombic, Pbca
Unit cell dimensions	a = 21.247(5) Å	*a* = 12.2286(9) Å
	b = 21.247(5) Å	*b* = 17.4493(13) Å
	c = 60.721(5) Å	*c* = 25.3574(19) Å
Volume	27412(9) $Å^3$	5410.8(7) $Å^3$
Z, Calculated density	80, 1.551 Mg/m^3	8, 1.601 Mg/m^3
Theta range for data collection	1.02 to 25.00	2.19 to 25.00°
Reflections collected / unique	64581 / 12078 [R (int) = 0.0985]	27043 / 4770 [R (int) = 0.0385]
Completeness to theta =25.01	100.0 %	100.0 %
Max. and min. transmission	0.8959 and 0.8495	0.8945 and 0.7260
Data / restraints / parameters	12078 / 204 / 1036	4770 / 558 / 426
Goodness-of-fit on F^2	0.994	1.170
Final R indices [I>2sigma(I)]	R1 = 0.0607, wR2 = 0.1430	R_1 = 0.0424, wR_2 = 0.1417
R indices (all data)	R1 = 0.1632, wR2 = 0.2141	R_1 = 0.0572, wR_2 = 0.1563
Largest diff. peak and hole	0.624 and -0.366 $e.A^{-3}$	0.542 and -0.398 $e.A^{-3}$

Table S2 Selected bond distances (Å) and bond angles (°) for the ferrocene derivatives

Compound 2			
C(1)-Fe(1)	2.033(10)	C(10)-C(6)-Fe(1)	70.0(4)
C(17)-Fe(2)	2.012(11)	N(2)-C(11)-C(7)	111.3(15)
C(30)-Fe(3)	2.013(11)	C(16)-C(15)-Fe(2)	70.5(7)
C(44)-Fe(4)	2.016(9)	N(4)-C(27)-C(26)	108.2(17)
C(57)-Fe(5)	2.057(12)	C(33)-C(29)-Fe(3)	73.3(9)
C(12)-N(1)	1.270(11)	N(6)-C(39)-C(40)	105.1(6)
Compound 3			
C(1)-C(2)	1.485(7)	N(3)-C(5)-N(1)	111.9(4)
C(16)-C(17)	1.489(8)	C(3)-C(4)-C(6)	127.9(4)
N(1)-C(5)	1.454(5)	N(1)-C(4)-C(6)	127.9(4)
N(3)-C(5)	1.445(6)	N(3)-C(19)-C(20)	124.6(4)
C(4)-C(6)	1.453(6)	C(21)-C(20)-C(19)	130.2(3)
C(19)-C(20)	1.449(6)	N(4)-N(3)-C(5)	118.5(4)
N(3)-N(4)	1.351(5)	C(4)-N(1)-C(5)	128.8(3)
N(2)-N(1)	1.354(4)	C(8)-C(7)-C(6)	108.6(5)
Fe(1)-C(15)	2.016(5)	C(21)-C(20)-C(19)	130.2(3)
Fe(2)-C(22)	2.030(4)	C(16)-F(4)	1.284(9)



(a)



(b)

Fig. S1. ^{1}H NMR spectrum of (2) and (3).

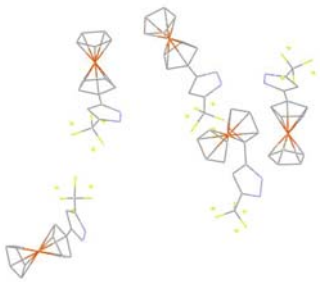


Fig. S2 The molecular structure of (2). All hydrogen atoms are ommitted for clarity.

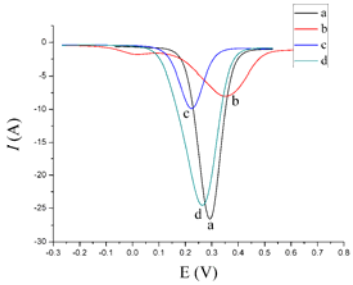


Fig. S3. DPV of 1 mM solution of (a) $FcCOCH_3$, (b) (1), (c) (2) and (d) (3) in 0.3 M TBAP/CH_3CN CH_3CN(vs. Fc/Fc^{+}). Scan rate, 100 mV s^{-1}.