Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

Heterobimetallic complexes with highly flexible 1,1'-bis(phospholanoalkyl)ferrocene ligands

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1. Electrochemistry

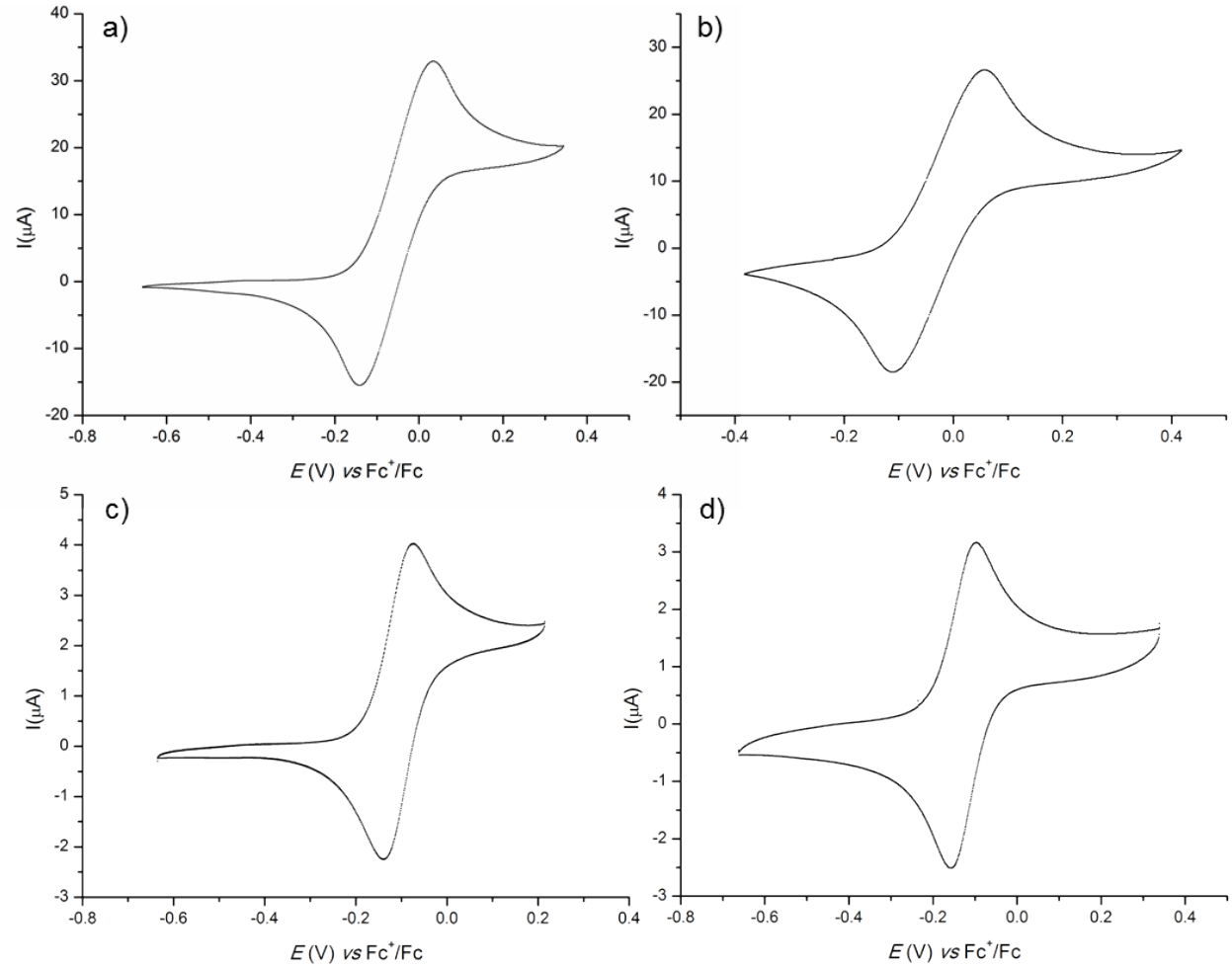

Fig. S1 Cyclic voltammograms of a) **8a**, b) **8b**, c) **7a** and d) **7b** in dichloromethane (50 mV·s^{-1}).

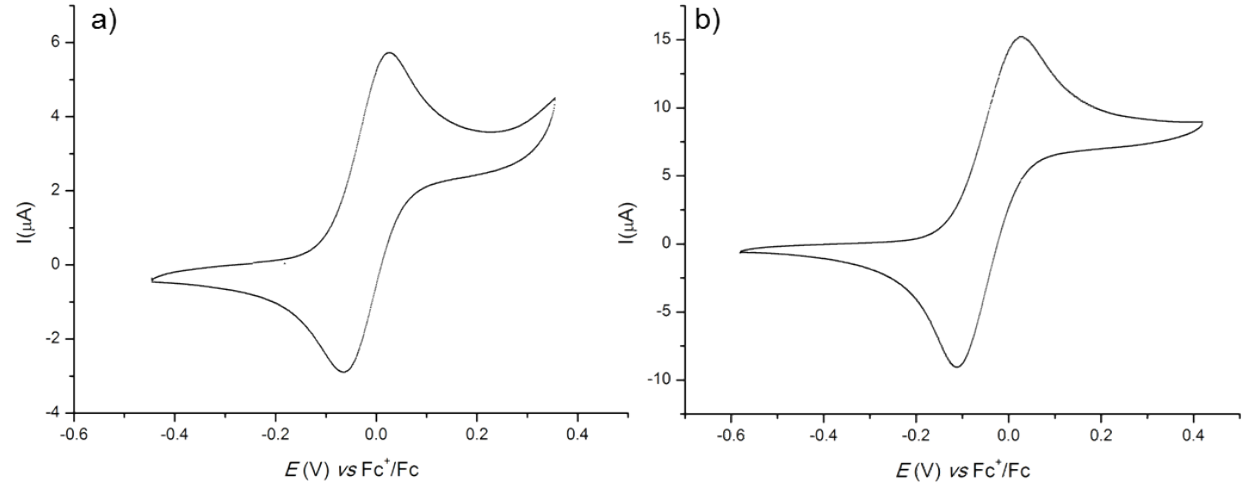

Fig. S2 Cyclic voltammograms of a) **5a** and b) **5b** in dichloromethane (50 mV·s^{-1}).

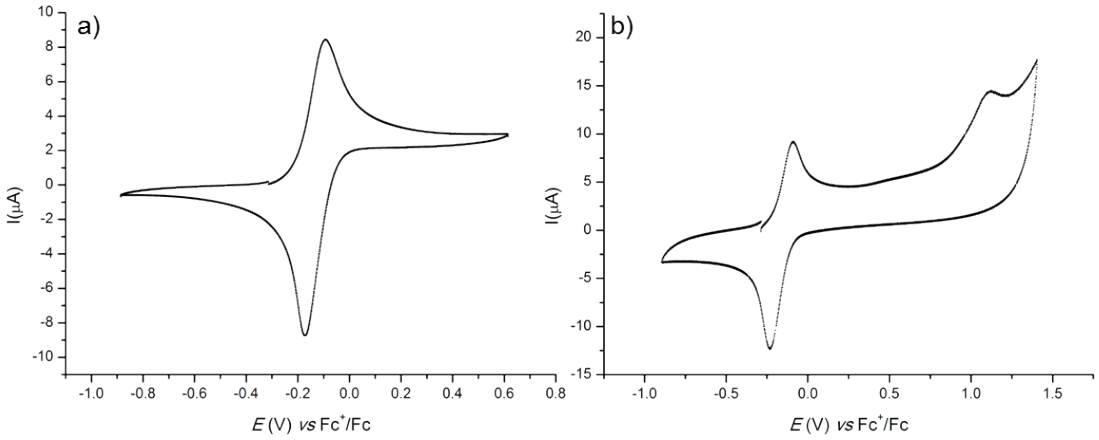

Fig. S3 Cyclic voltammograms of **9b** a) –0.9 to 0.6 V vs. Fc^+/FcH and (50 $mV \cdot s^{-1}$) b) –0.9 to 1.5 V vs. Fc^+/FcH (200 $mV \cdot s^{-1}$) in dichloromethane.

Table S1 Electrochemical data (V vs. Fc^+/FcH). [a] Irreversible oxidation (scan rate 200 $mV \cdot s^{-1}$)

Compound	Scan rate ($mV \cdot s^{-1}$)	$E_{1/2}$	E_P
5a	50	–0.03	
5b	50	–0.04	
7a	50	–0.10	
7b	50	–0.13	
8a	50	–0.06	
8b	50	–0.06	
9a	50	–0.13	1.18[a]

2. Crystallographic Data

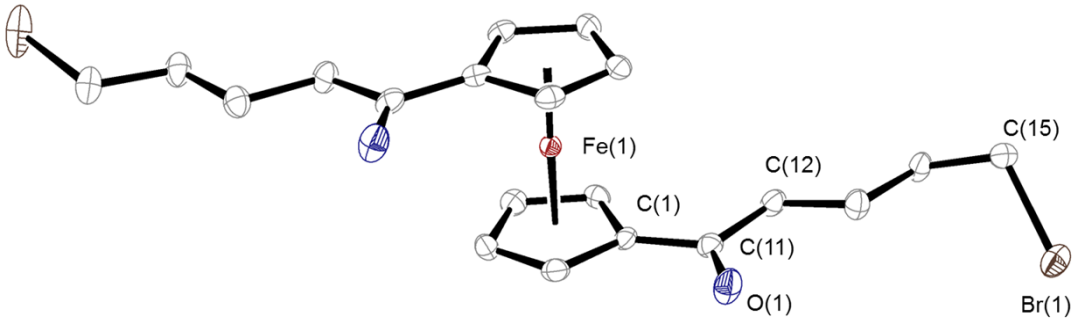

Fig. S4 Molecular structure of 1,1'-bis(5-bromobutanoyl)ferrocene (**1b**). Ellipsoids are drawn at the 50% probability level. Hydrogen atoms are omitted for clarity.

Table S2 Selected bond lengths (pm) and angles (°) for **1b**.

	Bond length(pm)		Bond angle (°)
C11–O1	122.1(4)	C1–C11–C12	117.7(3)
C1–C11	147.7(5)	C12–C11–O1	121.8(3)
C11–C12	150.4(5)	C11–C11–O1	120.5(3)
C15–Br1	195.6(3)		

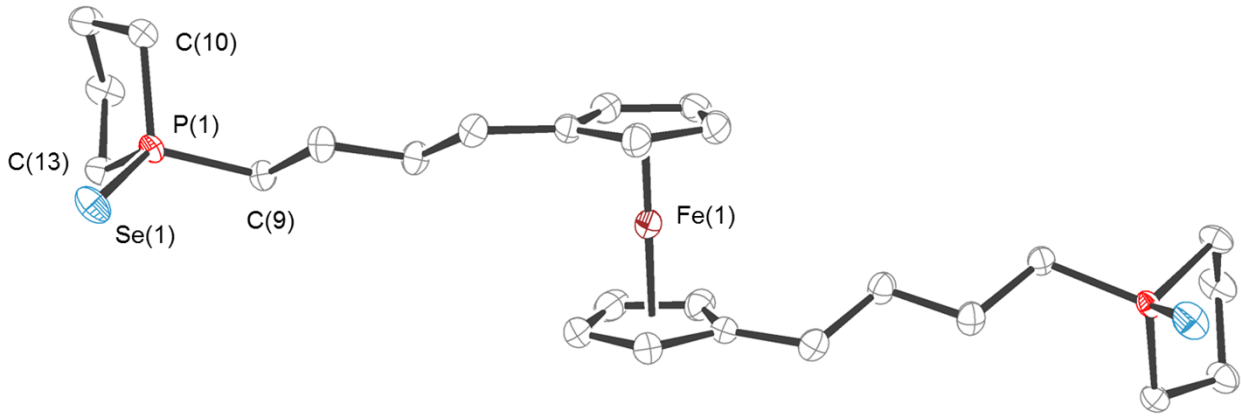

Fig. S5 Molecular structure of 1,1'-bis(4-(phospholanoselenide)butyl)ferrocene (**6a**). Ellipsoids are drawn at the 50% probability level. Hydrogen atoms are omitted for clarity.

Table S2 Selected bond lengths (pm) and angles (°) for **6a**.

	Bond length(pm)		Bond angle (°)
P1–Se1	210.9(2)	C10–P1–C13	95.9(2)
P1–C13	181.9(5)	C10–P1–Se1	115.3(2)
P1–C10	182.5(5)	C13–P1–Se1	115.6(2)

Table S4 Crystallographic data for 1,1'-bis(5-bromobutanoyl)ferrocene (**1b**)

Empirical formula		$C_{20}H_{24}Br_2FeO_2$
Formula weight		512.06 g·mol^{-1}
Temperature		130(2) K
Wavelength		0.71073 Å
Crystal system		triclinic
Space group		$P\bar{1}$
Unit cell dimensions	a	562.19(3) pm
	b	871.07(4) pm
	c	2056.47(15) pm
	α	83.135(5)°
	β	84.840(5)°
	γ	74.380(4)°
Volume		961.2(1) Å^3
Z		2
Calculated density		1.769 g·cm^{-3}
Absorption coefficient		4.952 mm^{-1}
F(000)		512
Crystal size		0.30 x 0.25 x 0.08 mm
θ range for data collection		2.44 to 25.35°
Limiting indices		$-6 \le h \le 5$ $-10 \le k \le 9$ $-24 \le l \le 21$
Reflections collected/ unique		6379 / 3526
R(int)		0.0285
Completeness to θ = 25.35		99.9 %
Refinement method		Full-matrix least-squares on F^2
Data / restraints / parameters		3526 / 0 / 258
Goodness-of-fit on F^2		0.956
Final R indices [I>2σ(I)]		R_1 = 0.0337, wR_2 = 0.0763
R indices (all data)		R_1 = 0.0428, wR_2 = 0.0814
Largest diff. peak and hole		0.783 and –0.873 e·Å^{-3}
Crystal description		orange plate

Table S5 Crystallographic data for 1,1'-bis(4-(phospholanoselenide)butyl)ferrocene (**6a**)

Empirical formula		$C_{26}H_{40}FeP_2Se$
Formula weight		628.29 $g \cdot mol^{-1}$
Temperature		130(2) K
Wavelength		0.71073 Å
Crystal system		monoclinic
Space group		C2/c
Unit cell dimensions	a	795.8(5) pm
	b	1019.5(5) pm
	c	3298.6(5) pm
	α	90°
	β	92.871(5)°
	γ	90°
Volume		2673(2) $Å^3$
Z		4
Calculated density		1.561 $g \cdot cm^{-3}$
Absorption coefficient		3.420 mm^{-1}
F(000)		1280
Crystal size		0.40 x 0.20 x 0.02 mm
θ range for data collection		2.47 to 26.37 °
Limiting indices		$-8 \leq h \leq 9$ $-12 \leq k \leq 12$ $-39 \leq l \leq 41$
Reflections collected/ unique		9149 / 2724
R(int)		0.0586
Completeness to θ = 26.37		100.0 %
Refinement method		Full-matrix least-squares on F^2
Data / restraints / parameters		2724 / 0 / 157
Goodness-of-fit on F^2		1.294
Final R indices [I>2σ(I)]		$R_1 = 0.0670$, $wR_2 = 0.1126$
R indices (all data)		$R_1 = 0.0766$, $wR_2 = 0.1156$
Largest diff. peak and hole		0.870 and –0.927 $e \cdot Å^{-3}$
Crystal description		yellow plate