Electronic Supplementary Information for Dalton Transactions

Synthesis and Characterization of New Ferrocene Peptide Conjugates

Supplementary Information

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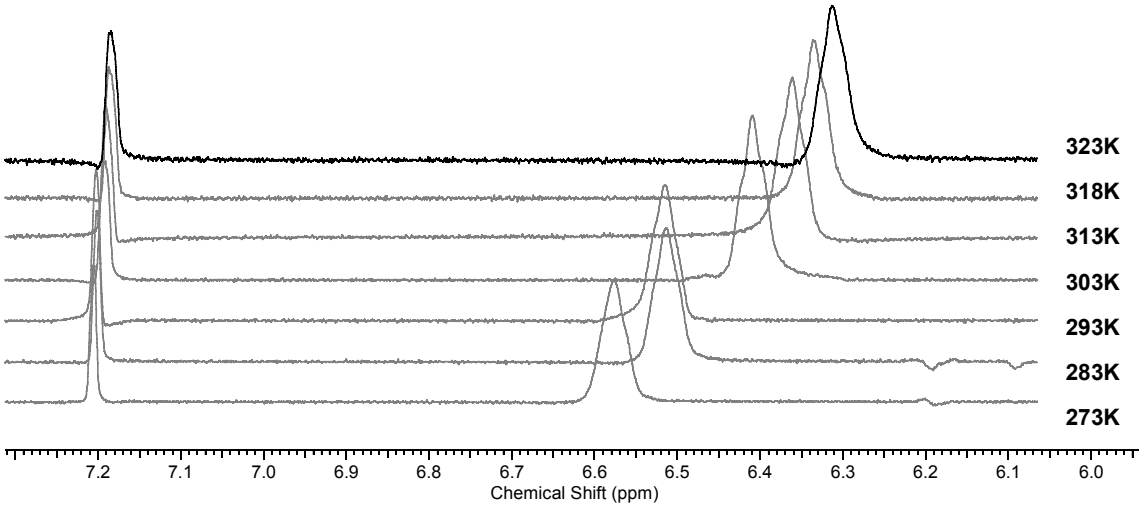


Figure S1 Variable temperature ^{1}H-NMR stack plots of compound **2** displaying the amide region in $CDCl_3$ from 273-323K.

Figure S2 Amide protons of compound **2** upfield shift with increasing temperature, giving a temperature coefficient of -5.2 ppb K^{-1}.

Figure S3 FT-IR spectrum of compound **6**, showing the amide A (3000-3500 cm^{-1}) regions.

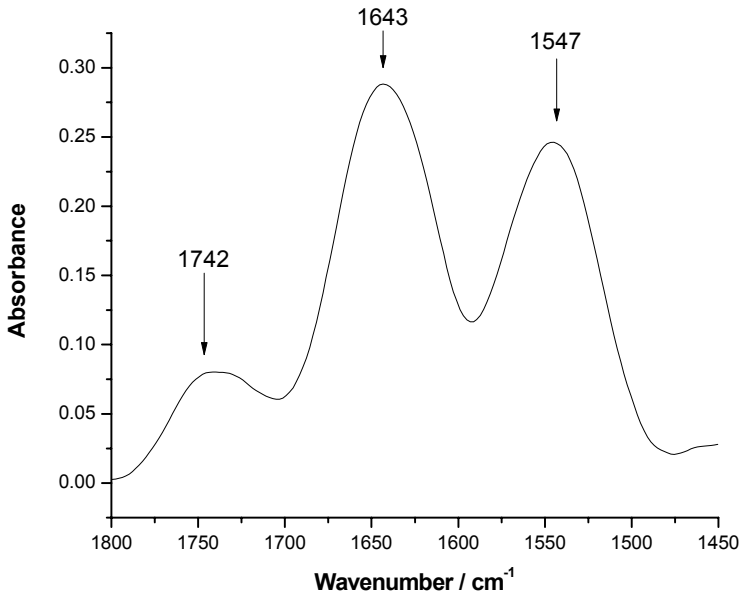


Figure S4 FT-IR spectrum of compound **6**, showing the amide I, amide II (1500-1800 cm^{1}) and methyl ester carbonyl absorption.

Figure S5 CD spectrum of compound **7**displaying a positive Cotton effect at 483 nm, indicating *P*-helicity of the Fc core.

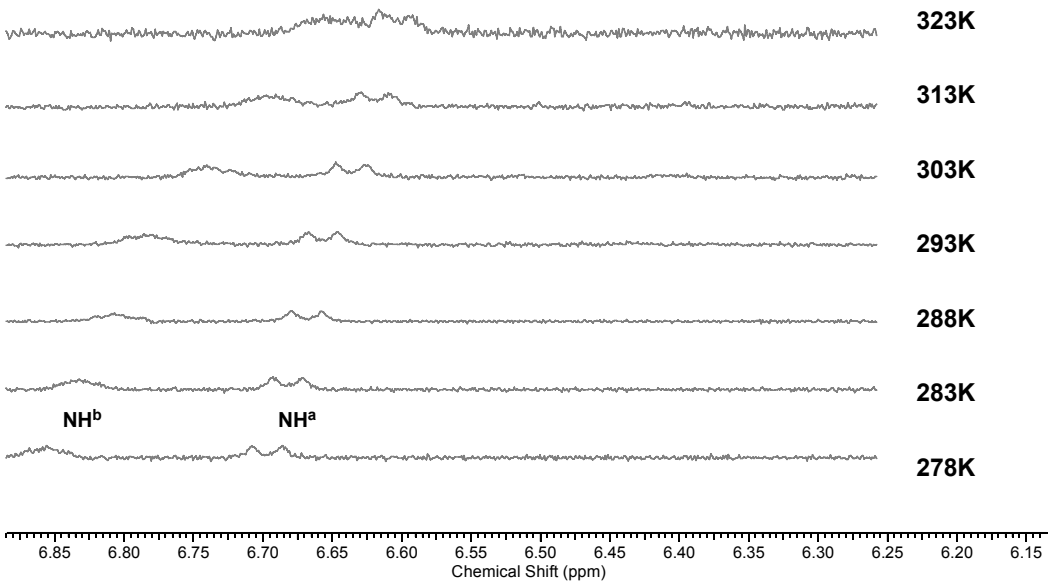
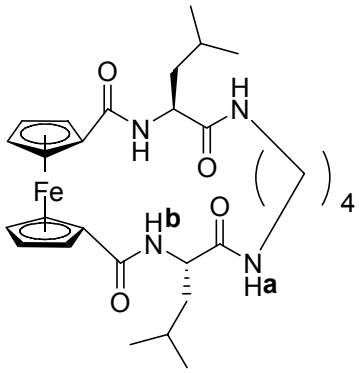


Figure S6 Variable temperature ^{1}H-NMR stack plots of compound **8**, displaying the amide region in $CDCl_3$ from 278-323K.



Scheme S1 Labelling scheme for amide protons of compound **8**.

Figure S7 Amide protons of compound **8** upfield shift with increasing temperature. Corresponding to Scheme S1, NH^a (circle data points) and NH^b (square data points) have temperature coefficients of -2.15 ppb K^{-1} and -4.67 ppb K^{-1}, respectively.

Figure S8 Concentration dependence of the amide protons of compound **8** with varying concentration. Corresponding to Scheme S1, NH^a are the circle data points and NH^b are the square data points.

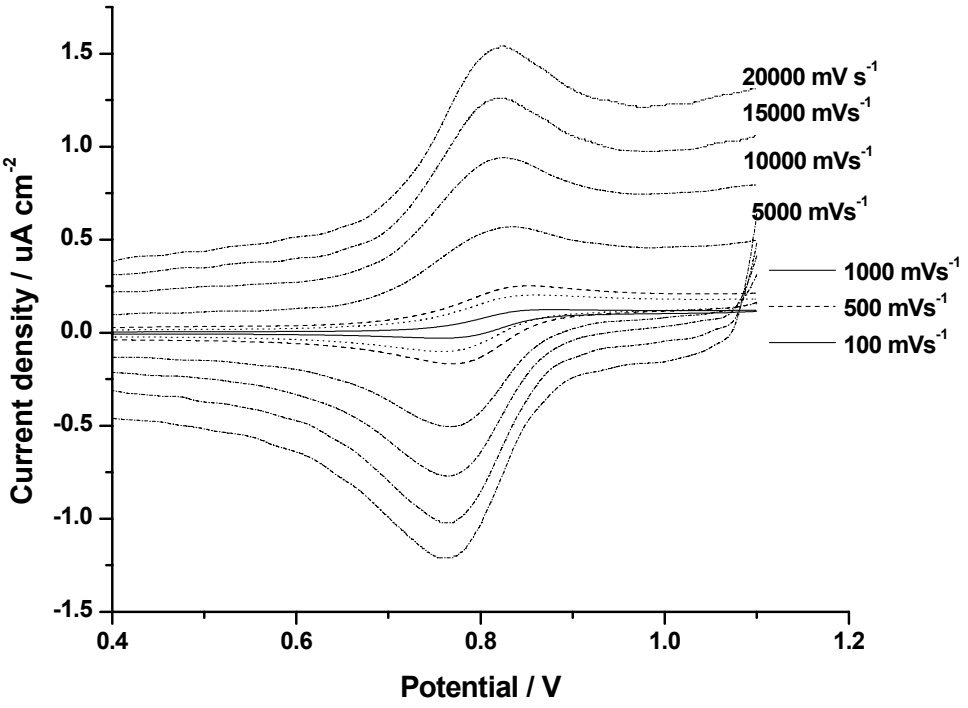


Figure S9 Representative cyclic voltammogram of compounds **1**-**7**, with **7** shown here. Scan rate was varied from 100 mV s^{-1} to 20000 mV s^{-1}.

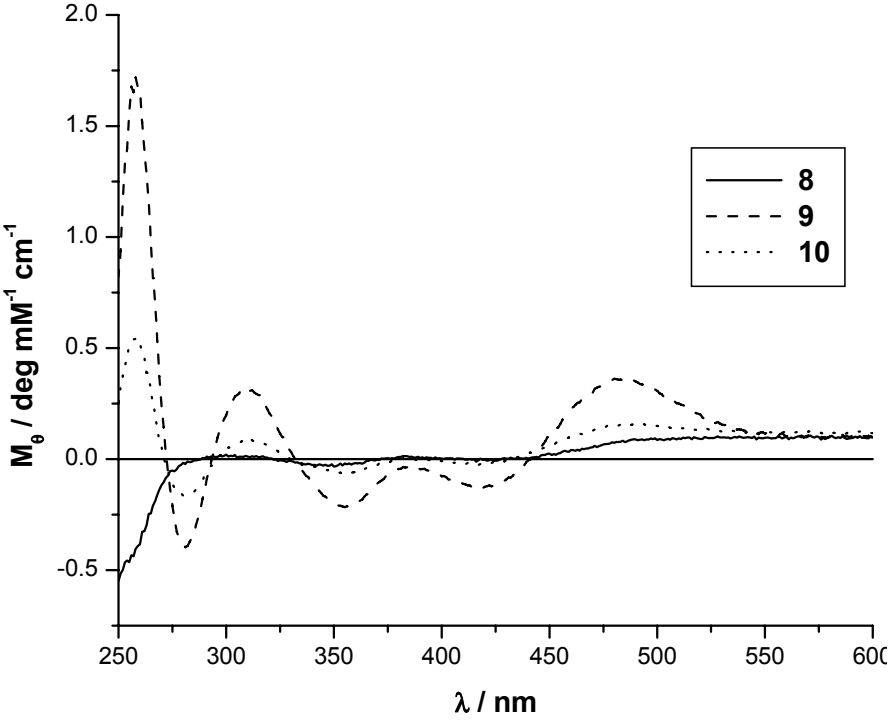


Figure S10 CD spectra of compounds **8** – **10** (0.2 mM, CH_2Cl_2)

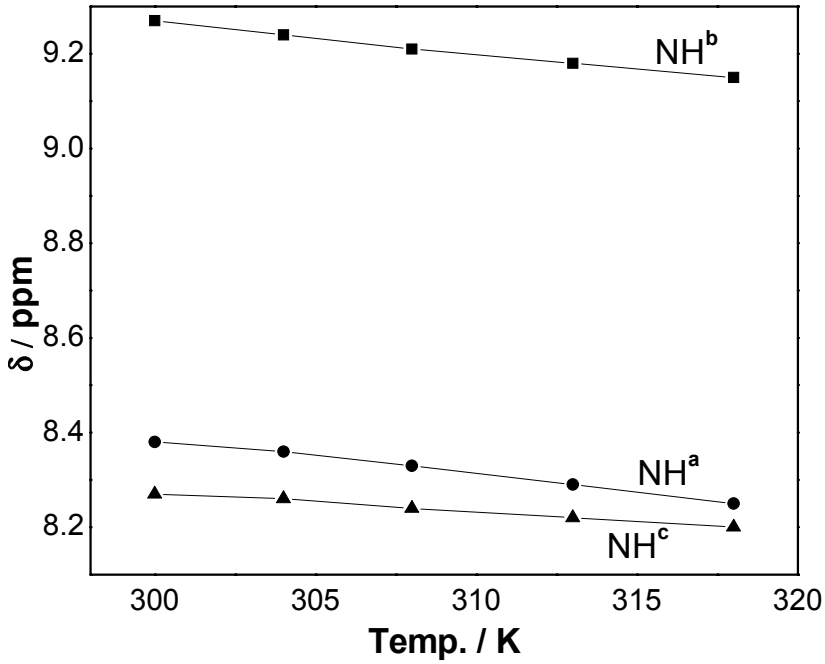


Figure S11: Temperature dependence of amides NHs of compound **6**. The diamine linker NH^{a} and Gly $NH^{b,c}$ protons shift upfield with increasing temperature (with circles, squares and triangle labels, respectively)

Table S1 Selected Spectroscopic data for Fc conjugates **1 – 10**

Compound	*^{1}H-NMR* δ / ppm				*^{13}C-NMR* δ / ppm			*FT-IR* cm^{-1}			
	NH[a]	NH[b]	NH[c]	αH	$C{=}O_{Fc}$	$C{=}O_{R}$	$C{=}O_{ester}$	Amide A	Amide I	$C{=}O_{ester}$	Amide II
1	7.14	n/a	n/a	n/a	169.8	n/a	172.1	3328	1629	1716	1531
2	6.48	n/a	n/a	n/a	169.5	n/a	172.2	3313	1628	1715	1540
3	6.31	n/a	n/a	n/a	169.4	n/a	172.1	3335	1627	1713	1537
4	6.19	n/a	n/a	n/a	169.2	n/a	172.2	3338	1628	1713	1539
5	6.14	n/a	n/a	n/a	169.2	n/a	172.2	3398	1637	1717	1532
6	8.34	9.23	8.26	4.08 3.86	169.5	173.8	171.2	3298	1643	1742	1547
7	8.55	8.97	7.95	4.82 4.95	170.0	175.9	171.1	3289	1636	1732	1543
8	7.06	6.62	n/a	4.52	171.4	172.8	n/a	3310	1638	n/a	1528
9	7.38 7.25	7.15 7.00	n/a	4.55	170.7	172.6	n/a	3289	1638	n/a	1528
10	6.94 6.88	6.74 6.46	n/a	4.68	170.5	172.2	n/a	3292	1639	n/a	1533

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