Supporting Information for

Magnetic Circular Dichroism Studies of Iron(II) Binding to Human Calprotectin

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1. Supplementary Data

1.1 Sample Concentrations

Table S1. Protein and Metal Concentrations of MCD Samples

| Protein	[Protein] (mM)	[Fe(II)] (mM)	[Ca(II)] (mM)	Glassing agent[a]
CP-Ser	1.36	1.22	27.2	Glycerol
CP-Ser	1.68	1.51	33.6	Sucrose
H103A	1.44	1.30	28.8	Glycerol
H103A	1.84	1.66	36.8	Sucrose
AHA	1.81	1.63	36.2	Glycerol
AHA	1.74	1.57	34.8	Sucrose
AAA	1.36	1.22	27.2	Glycerol
AAA	2.24	2.01	44.8	Sucrose
$\Delta His_3 Asp$	1.11	1.00	22.2	Glycerol
$\Delta His_3 Asp$	1.54	1.39	30.8	Sucrose
$\Delta His_3 Asp$-H103A	1.61	1.45	32.2	Sucrose
CP-Ser	1.68	0.50	33.6	Sucrose
CP-Ser	1.68	1.01	33.6	Sucrose
CP-Ser	1.68	2.02	33.6	Sucrose
ΔHis_4	1.59	1.43	29.8	Glycerol
ΔHis_4	1.58	1.42	31.2	Sucrose
$\Delta His_3 Asp$	2.26	3.39	45.2	Sucrose
CP-Ser	1.85	1.11	0	Sucrose
$\Delta His_3 Asp$	1.42	0.85	0	Sucrose

[a] Glycerol samples were prepared with 40% (v/v) 150 HEPES, 200 mM NaCl, pD 7.4 60% (v/v) glycerol-d_8 in D_2O. Sucrose samples were prepared with 150 mM HEPES, 200 mM NaCl, pD 7.4 saturated with sucrose in D_2O.

1.2 MCD Spectra
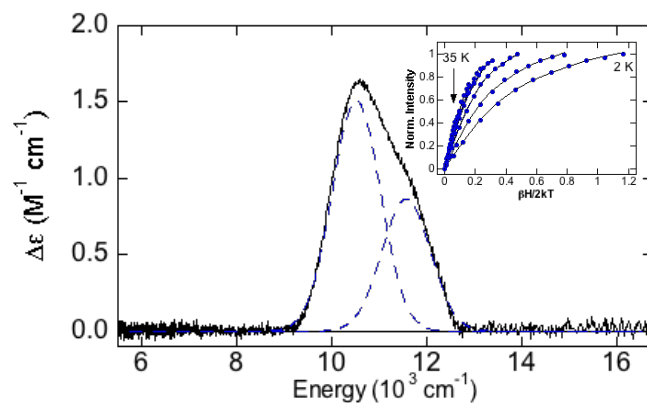
Figure S1. 5 K, 7 T NIR MCD spectra of $\Delta His_3Asp/Ca(II)/Fe(II)$ in a glycerol glass. Gaussian fits are shown as dashed blue lines. Inset: Saturation magnetization data (dots) and best fit (lines) for $\Delta His_3Asp/Ca(II)/Fe(II)$ in glycerol collected at 10310 cm^{-1}.
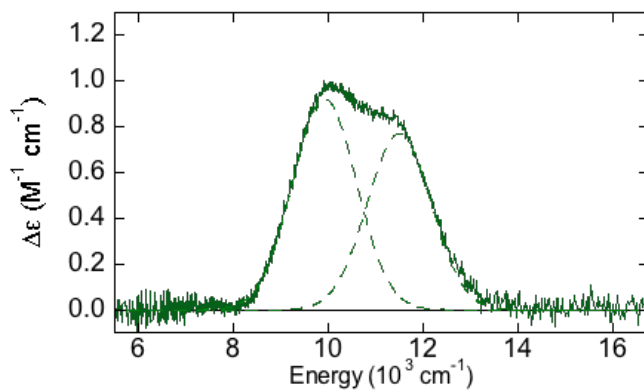
Figure S2. 5 K, 7 T NIR MCD spectra of $\Delta His_3Asp(H103A)/Ca(II)/Fe(II)$ in a saturated sucrose buffer solution. Gaussian fits are shown as dashed green lines.