Electronic Supplementary Material (ESI) for Metallomics.

Electronic Supplementary Information

For the Article Titled

"Kinetics of competitive Cd^{2+} binding pathways: The realistic structure of intrinsically disordered, partially metallated metallothioneins"

Daisy L. Wong, Natalie C. Korkola, Martin J. Stillman

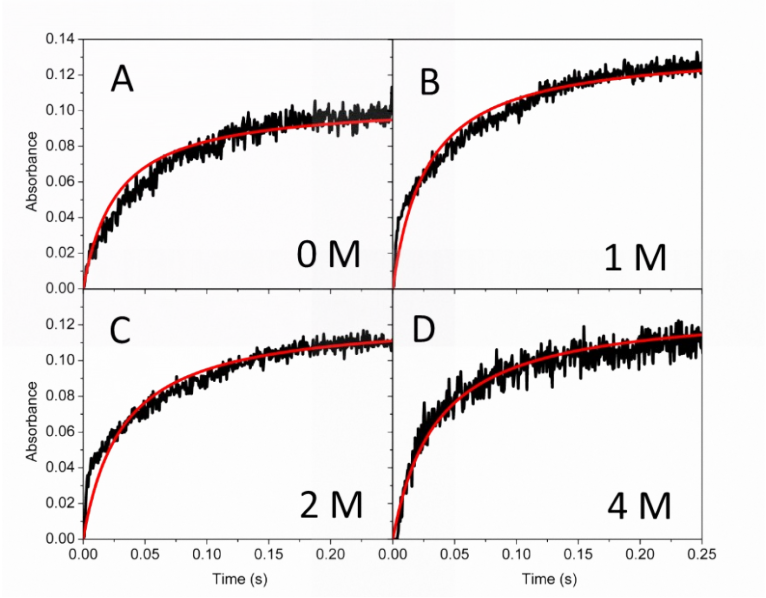

Figure S1. The kinetics traces of the binding of 2.5 eq of Cd to apoMT at pH 5 in the presence of increasing amounts of GdmCl at concentrations of A) 0 M, B) 1 M, C) 2 M, and D) 4 M.

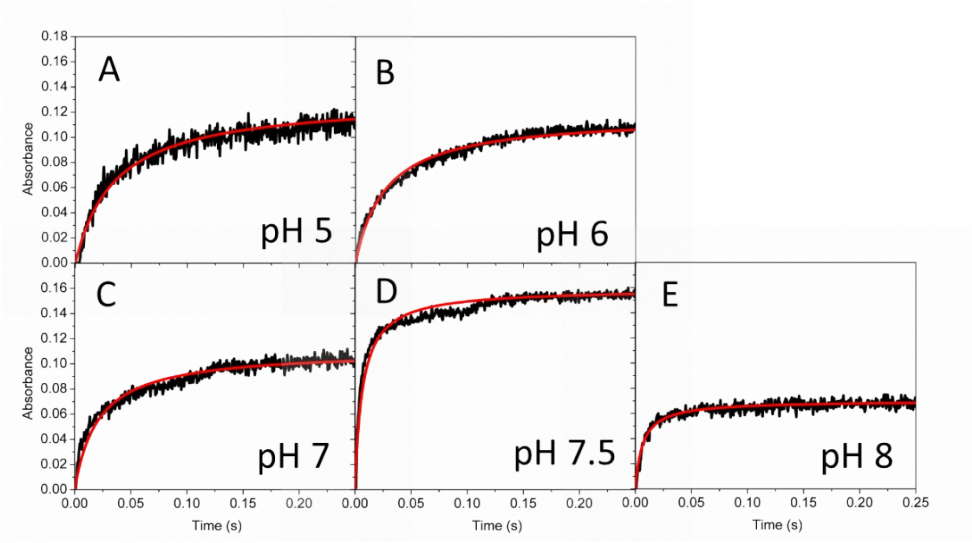

Figure S2. The kinetics traces of the binding of 2.5 eq of Cd to apoMT in the presence of 4 M GdmCl at pH A) 5, B) 6, C) 7, D) 7.5, and E) 8.

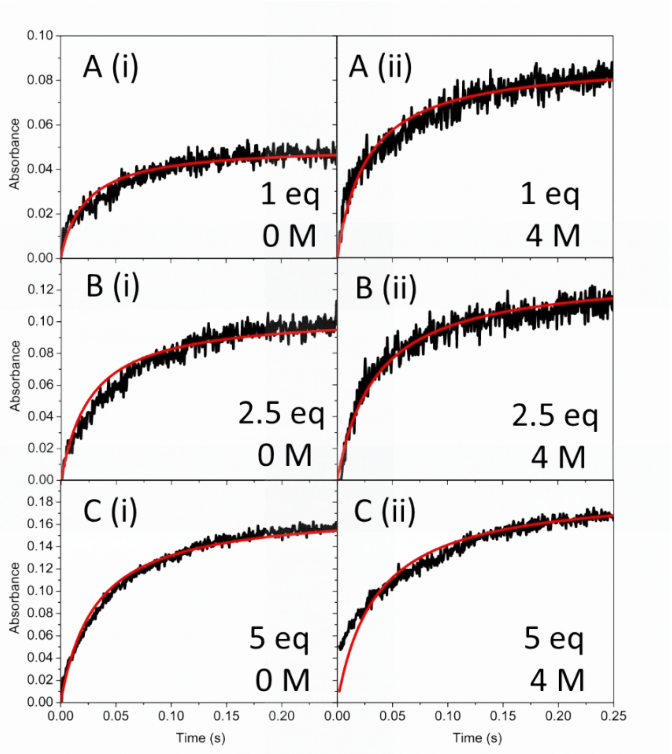

Figure S3. The kinetics traces of the binding of apoMT to A) 1, B) 2.5, and C) 5 equivalents of cadmium at pH 5 and in the presence of (i) 0 M and (ii) 4 M of GdmCl.

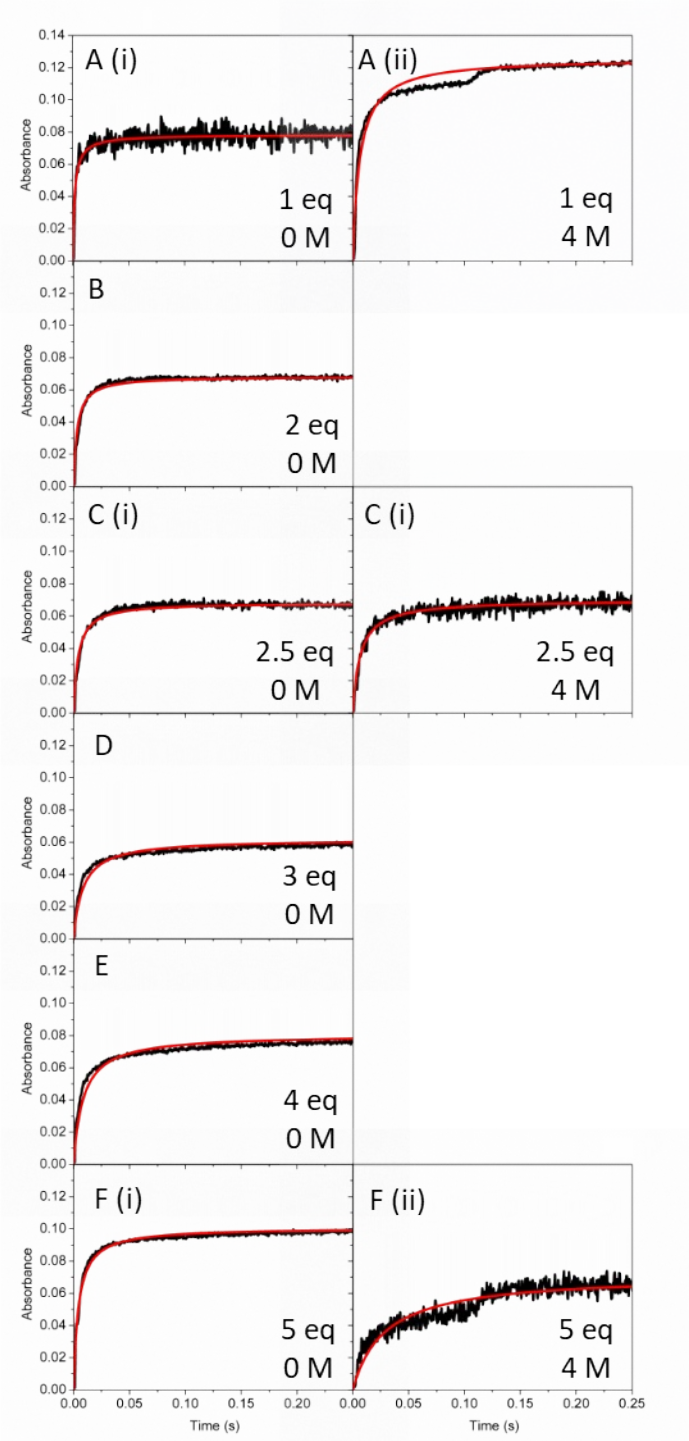

Figure S4. The kinetics traces of the binding of apoMT to A) 1, B) 2, C) 2.5, D) 3, E) 4, and F) 5 equivalents of cadmium at pH 8 and in the presence of (i) 0 M and (ii) 4 M of GdmCl.

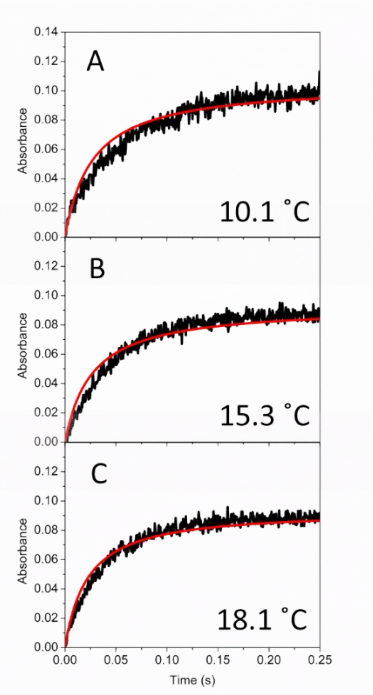

Figure S5. The kinetics traces of the binding of 2.5 eq of Cd to apoMT at pH 5 and with no denaturant at temperatures of A) 10.1 ˚C, B) 15.3 ˚C, and C) 18.1 ˚C.

Chart of all Observed Rate Constants

Figure	Constant Conditions	Variable Conditions	K_{obs} ($10^6 s^{-1}$)	Standard Deviation
pH Titration	4 M GdmCl 2.5 eq Cd (II) 10 ˚C	pH 5	215.48	3.127 (1.45%)
		pH 6	317.95	2.842 (0.89%)
		pH 7	422.40	5.084 (1.20%)
		pH 7.5	918.93	8.412 (0.92%)
		pH 8	2150.00	41.75 (1.94%)
Cd Titration	pH 5 0 M GdmCl 10 ˚C	1 eq	830.89	21.57 (2.60%)
		2.5 eq	353.97	3.797 (1.07%)
		5 eq	182.60	1.252 (0.69%)
	pH 5 4 M GdmCl 10 ˚C	1 eq	404.28	7.262 (1.80%)
		2.5 eq	215.48	3.127 (1.45%)
		5 eq	147.17	1.313 (0.89%)
	pH 8 0 M GdmCl 10 ˚C	1 eq	7198.20	265.4 (3.69%)
		2 eq	4690.10	72.29 (1.54%)
		2.5 eq	3633.30	78.59 (2.16%)
		3 eq	1953.90	19.02 (0.97%)
		4 eq	1459.70	10.27 (0.70%)
		5 eq	2318.80	11.29 (0.49%)
	pH 8 4 M GdmCl 10 ˚C	1 eq	1238.10	9.705 (0.78%)
		2.5 eq	2150.00	41.75 (1.94%)
		5 eq	878.86	14.15 (1.61%)
GdmCl Titration	pH 5 2.5 eq Cd (II) 10 ˚C	0 M	353.97	3.797 (1.07%)
		1 M	265.67	1.827 (0.69%)
		2 M	252.91	1.58 (0.62%)
		4 M	215.48	3.127 (1.45%)
Temperature Dependence	pH 5 0 M GdmCl 2.5 eq Cd (II)	10.1 ˚C	353.97	3.797 (1.07%)
		15.3 ˚C	407.14	4.142 (1.02%)
		18.1 ˚C	468.10	7.597 (1.62%)