Supplementary Materials: Nickel Metalloregulators and Chaperones

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Table S1. The metal binding properties of the Ni(II)-responsive metalloregulators.

Protein	Organism	Number of Metal Ions per Functional Unit	K_d	pH [d]	CN #	Metal Site Structure	References
NikR	*E. coli*	4 Ni/tetramer	HA site: 6.8 pM [a]	7.5	4	$NiS(N_{Im})_3$	[1–3]
			HA site: 0.93 pM [a]	7.6			[4]
			HA site: 25 nM, 400 nM [b]	8.0			[5]
		2 Ni/tetramer	LA site: 29 nM [c]	7.5	6	$Ni(O)_6$ or $Ni(N/O)_4(N_{Im})_2$	[2,3,6]
		4 Ni/tetramer	LA site: 700 nM [b]	8.0	ND	ND	[5]
	H. pylori	4 Ni/tetramer	HA site: 12 nM, 125 nM [b]	7.0	4	$NiS(N_{Im})_3$	[7,8]
		10 Ni/tetramer	LA site: 0.5 μM [b]	7.0	ND	ND	[8]
Nur	*S. coelicolor*	4 Ni/tetramer	10 nM, 280 nM [b]	8.0	-	-	[5,9]
RcnR	*E. coli*	4 Ni/tetramer	<25 nM [a]	7.0	6	$NiSNH_2ON_{Im}(N/O)_2$	[10–13]
			17nM, 300 nM [b]	7.0			[5]
		4 Co/tetramer	5 nM [a]	7.0	6	$CoSNH_2(N_{Im})_2(O)_2$	[10–13]
InrS	*Synechocystis*	4 Ni/tetramer	0.02 pM [a]	7.8	4	$Ni(N_{Im})_2(S)_2$	[14,15]
			70 nM, 4.5 μM [b]	7.8			[5]
NmtR	*M. tuberculosis*	2 Ni/dimer	87 pM, 0.14 nM [a]	7.0	6	$NiNH_2(N_{Im})_4O$	[16,17]

The imidazole ligand from histidine is abbreviated as N_{Im}. [a] K_d determined using competition studies. [b] K_d determined by ITC. [c] K_d determined by direct metal titrations. [d] The pH of the buffer used in the metal binding studies. - There is some ambiguity.

Table S2. The metal binding properties of the Ni(II) chaperones.

Protein	Organism	Number of Metal Ions per Functional Unit	K_d	pH [e]	CN #	Metal Site Structure	References
HypA	*E. coli*	1 Ni/dimer	61 μM [c]	7.5	ND	ND	[18]
			75 nM [a]	7.5			[19]
		1 Zn/monomer	0.9 nM [a]	7.5	4	$Zn(S)_4$	[18]
	H. pylori	1 Ni/monomer	~1 μM [b]	7.2	6	$NiNH_2(N)_2O_2N_{Im}$	[20–23]
			58 μM, 1.3 μM [d]	8.25	ND	ND	[24]
		0.5 Ni/monomer	17 μM [b]	6.3	6	-	[21]
		1 Zn/monomer	ND	7.2	4	$Zn(S)_4$	[21]
			ND	6.3	4	$Zn(S)_3N_{Im}$	[21]
HypB	*E. coli*	2 Ni/dimer	HA site: 0.13 pM [a]	7.6	4	$NiNH_2(S)_3$	[25–27]
		2 Ni/dimer	LA site: 12 μM [c]	7.6	6	$NiS(N/O)_4N_{Im}$	[25,26]
		2 Zn/dimer	LA site: 1 μM [c]	7.6	4	$Zn(S)_{2.5}N/OZn(N_{Im})_{0.5}$	[25,26]
	H. pylori	2 Ni/dimer	1.7 μM [c], 0.21 μM [a]	7.4	4	NiS_4 [f]	[28,29]
			150 nM [a],	7.6			[30]
		2 Zn/dimer	1.2 nM [a]	7.6	ND	ND	[30]
	B. japonicum	18 Ni/dimer	2.3 μM [d]	8.3	ND	ND	[31]
SlyD	*E. coli*	7 Ni/monomer	<1.8 μM [a]	7.5	ND	ND	[32]
	H. pylori	2.4 Ni/monomer	2.74 μM [d]	7.6	ND	ND	[33]
		3.3 Zn/monomer	3.79 μM [d]	7.6	ND	ND	[33]
SlyD 155	*E. coli*	1 Ni/Monomer	65 nM [b]	7.5	6	$Ni(N/O)_{3-4}(N_{Im})_{2-3}$	[34]
UreE	*K. aerogenes*	6 Ni/dimer	9.6 μM [d]	7.2	6	$Ni(N/O)_{1-3}(N_{Im})_{3-5}$	[35]
	H. pylori	1 Ni/dimer	0.15 μM [b]	7.0	6	$Ni(N/O)_2(N_{Im})_4$	[36,37]

		1 Zn/dimer	0.49 μM [b]	7.0	5	$Zn(N/O)_2(N_{Im})_2Br$	[36,37]
	S. pasteurii	2 Ni/dimer	35 μM [c]	7.5	6	$Ni(N/O)(N_{Im})_2$	[38,39]
H144* UreE	*K. aerogenes*	2Ni/dimer	47 μM, 1.5 μM [d]	7.5	6	$Ni(N/O)_2(N_{Im})_4$ and $Ni(N/O)_4(N_{Im})_2$	[40]
			1.6 nM [b]				[41]

The imidazole ligand from histidine is abbreviated as N_{Im}. [a] K_d determined using competition studies. [b] K_d determined by ITC. [c] K_d determined by direct metal titrations. [d] Kd determined by equilibrium dialysis. [e] The pH of the buffer used in the metal binding studies. [f] The nickel site when GDP is bound. - There is some ambiguity.

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