

Supplementary material

The use of permeation liquid membranes for free zinc measurements in aqueous solution

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Table S1. Zn and ligand concentrations used for PLM measurements shown in Fig. 5

Background solutions always contained: 400 μM $\text{Ca}(\text{NO}_3)_2$, 500 μM KNO_3 , 2.5 mM MOPS, pH 7.2 (adjusted with 1 M NaOH)

EDTA											
Total ligand (μM)	0.1-M lauric acid			Total ligand (μM)	0.05-M lauric acid			Total ligand (μM)	0.025-M lauric acid		
	$[\text{Zn}]_{\text{tot}}$ (μM)	$[\text{Zn}^{2+}]_{\text{MINEQL}}$ (nM)	$[\text{Zn}^{2+}]_{\text{PLM}}$ (nM)		$[\text{Zn}]_{\text{tot}}$ (μM)	$[\text{Zn}^{2+}]_{\text{MINEQL}}$ (nM)	$[\text{Zn}^{2+}]_{\text{PLM}}$ (nM)		$[\text{Zn}]_{\text{tot}}$ (μM)	$[\text{Zn}^{2+}]_{\text{MINEQL}}$ (nM)	$[\text{Zn}^{2+}]_{\text{PLM}}$ (nM)
20.8	20	13.2	25	2	2	32	54	2	2	32	15
20.65	20	17.3	14	2	2	32	71	2	2	32	71
20.37	20	25.2	97	2	2	32	59	1.9	2	107	214
19.5	20	509	867	1.75	2	249	251	1.9	2	107	153
19.25	20	699	869	1.75	2	249	242	1.8	2	201	246
				1.5	2	492	494	1.8	2	201	264
				1	2	981	898	1.75	2	249	477
				3.5	4	490	447	1.75	2	249	472
				3.5	4	490	442	1.5	2	492	643
				3	4	982	836	1.5	2	492	797
				3	4	982	913	1.25	2	736	957
				2	4	1960	1740	1.25	2	736	1060
				2	4	1960	1805	1	2	981	1054
								1	2	981	1239
Citrate											
Total ligand (μM)	0.1-M lauric acid			Total ligand (μM)	0.05-M lauric acid			Total ligand (μM)	0.025-M lauric acid		
	$[\text{Zn}]_{\text{tot}}$ (μM)	$[\text{Zn}^{2+}]_{\text{MINEQL}}$ (nM)	$[\text{Zn}^{2+}]_{\text{PLM}}$ (nM)		$[\text{Zn}]_{\text{tot}}$ (μM)	$[\text{Zn}^{2+}]_{\text{MINEQL}}$ (nM)	$[\text{Zn}^{2+}]_{\text{PLM}}$ (nM)		$[\text{Zn}]_{\text{tot}}$ (μM)	$[\text{Zn}^{2+}]_{\text{MINEQL}}$ (nM)	$[\text{Zn}^{2+}]_{\text{PLM}}$ (nM)
2500	20	33.5	80	1450	20	50	79	1450	20	50	112
1450	20	50	130	1450	20	50	70	1450	20	50	123
1200	20	62	164	1450	20	50	70	1450	20	50	110
500	20	237	635	1000	20	76	106	1000	20	76	127
300	20	705	1437	1000	20	76	97	1000	20	76	160
				500	20	237	317	500	20	237	319
				500	20	237	321	500	20	237	358
				350	20	515	719	350	20	515	652
				350	20	515	554	350	20	515	623
				250	20	989	913	250	20	989	1349
				250	20	989	954	250	20	989	1177

Table S1. (Cont.)

Total ligand (μM)	0.1-M lauric acid			L-Histidine 0.05-M lauric acid			0.025-M lauric acid				
	$[\text{Zn}]_{\text{tot}}$ (μM)	$[\text{Zn}^{2+}]_{\text{MINEQL}}$ (nM)	$[\text{Zn}^{2+}]_{\text{PLM}}$ (nM)	$[\text{Zn}]_{\text{tot}}$ (μM)	$[\text{Zn}^{2+}]_{\text{MINEQL}}$ (nM)	$[\text{Zn}^{2+}]_{\text{PLM}}$ (nM)	$[\text{Zn}]_{\text{tot}}$ (μM)	$[\text{Zn}^{2+}]_{\text{MINEQL}}$ (nM)	$[\text{Zn}^{2+}]_{\text{PLM}}$ (nM)		
1500	20	39	255	1300	20	50	163	1300	20	50	158
1400	20	44	281	1300	20	50	178	1300	20	50	159
1250	20	55	342	1300	20	50	171	800	20	124	500
850	20	111	641	800	20	124	333	800	20	124	645
300	20	664	1236	800	20	124	356	500	20	285	1063
				500	20	285	757	500	20	285	1010
				500	20	285	693	300	20	664	1937
				300	20	664	950	300	20	664	1891
				300	20	664	1248	200	20	1230	3362
				200	20	1230	1816	200	20	1230	3451
				200	20	1230	1767				

Table S2. Deprotonation and stability constants used for Zn speciation calculations using MINEQL were taken from NIST database^[30]

For other inorganic Zn complexes default values from MINEQL version 4.6 were used

Ligands and species	Logarithm of deprotonation and stability constants used for calculation with MINEQL at I = 0, 25 °C
EDTA	
HEDTA	11.09
H ₂ EDTA	17.90
H ₃ EDTA	21.04
H ₄ EDTA	23.27
H ₅ EDTA	24.77
H ₆ EDTA	24.54
ZnEDTA	18.30
ZnHEDTA	21.76
ZnH ₂ EDTA	23.18
Citrate	
HCIT	6.33
H ₂ CIT	11.13
H ₃ CIT	14.25
ZnCIT	6.12
Zn(CIT) ₂	7.48
ZnHCIT	10.20
L-Histidine	
HHIS	9.33
H ₂ HIS	15.38
H ₃ HIS	16.85
ZnHIS	6.95
ZnHIS ₂	12.72
ZnHHIS	11.59
ZnHHIS ₂	18.52
Zn(HHIS) ₂	23.96