Supplemental Materials

Modeling Structural Coordination and Ligand Binding in Zinc Proteins with a Polarizable Potential

Zhang, Jiajing; Yang, Wei; Piquemal, Jean-Philip; Ren, Pengyu

Table S1. Heterodimer binding energy and energy components (kcal/mol) computed by AMOEBA for configurations shown in Figure 1 and Table 3.

Configuration	AMOEBA		AMOEBA Decomposition		
	Distance	E_{int}	E_{vdW}	E_{perm}	E_{pol}
Conf. A: $CH3COO^-$ - water (External)	1.74 (O…H)	-17.81	6.40	-16.70	-7.52
Conf. B: $CH3COO^-$ - water (Bridge)	3.18 (C…O) 1.96(O1…H1) 1.96(O2…H2)	-22.93	6.52	-22.47	-6.97
Conf. C: $CH3COO^-$ - Zn^{2+} (External)	1.72(O…Zn)	-356.59	75.73	-320.63	-111.69
Conf. D: $CH3COO^-$ - Zn^{2+} (Bridge) [a]	2.10 (C…Zn) 1.81(O…Zn)	-442.30	81.80	-396.45	-127.65
Conf. E: $CH3S^-$ - water	2.14 (S…H)	-21.30	6.62	-20.04	-7.88
Conf. F: $CH3S^-$ - Zn^{2+}	2.06 (S…Zn)	-391.76	58.87	-353.70	-96.93

Conf. G: Imidazole - water	2.11 (N…H)	-8.10	2.22	-8.19	-2.13
Conf. H: Imidazole – Zn^{2+}	1.75 (N…Zn)	-172.25	62.13	-117.44	-116.93

[a] with C-O-Zn angle at 150º.