Supporting Information

The Importance of Stereochemically Active Lone Pairs For Influencing Pb(II) and As(III) Protein Binding

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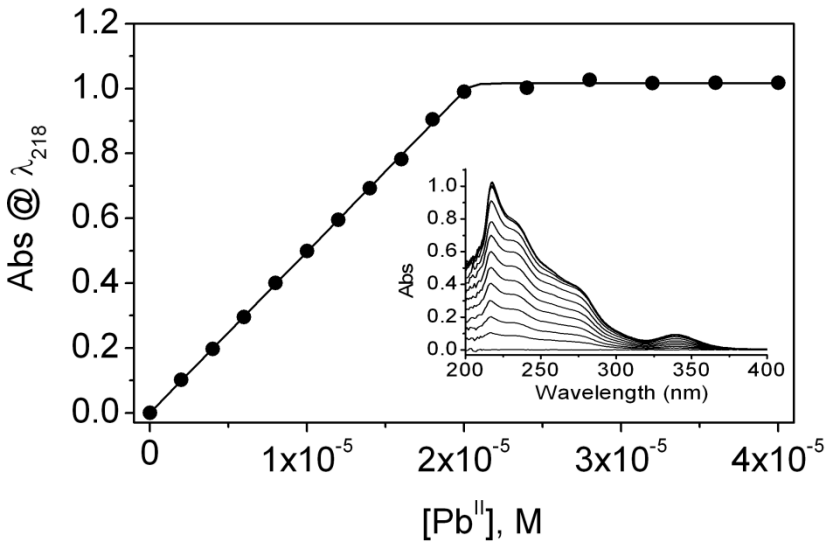

Figure S1**.** UV/Vis titration of $Pb(NO_3)_2$ into **TRI**L12AL16C (60 uM, 100 mM TrisHCl buffer, pH 8.0). The spectral change at 218 nm was plotted as a function of $Pb(NO_3)_2$ concentration and the plot showed that 1 equivalent of Pb(II) bind per peptide trimer. The solid line represents a nonlinear, least square fitting curve generated using 1:1 binding model by ORIGIN with K_a = 5.6(±1)×10^8 M^{-1}. The inset depicts the UV/Vis spectral change from each addition of 0.1 equivalent of Pb(II).

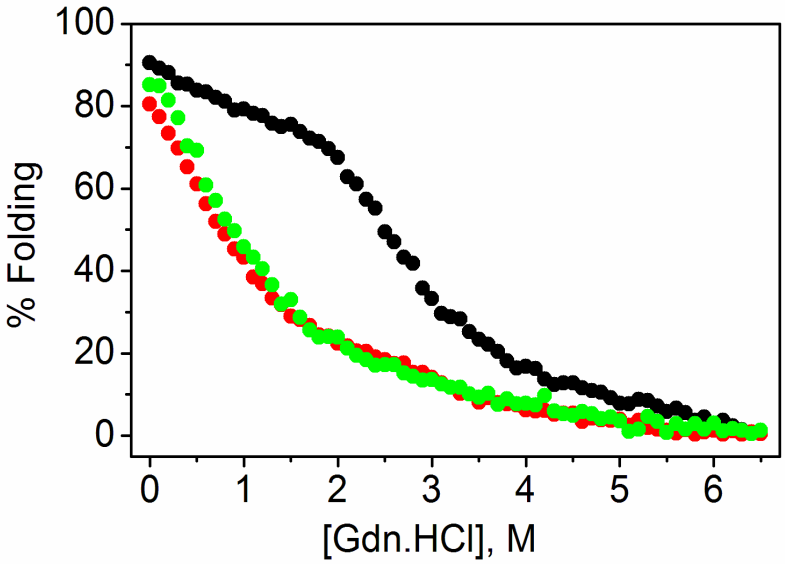

Figure S2**.** Guanidinium hydrochloride (Gdn.HCl) denaturation curves showing the stability of apopeptide: **TRI**L2WL16C (black), **TRI**L12AL16C (red), and **TRI**L2WL12AL16C (green). The data were collected at 10 μM peptide monomer in TrisHCl buffer at pH 8.0. $[\theta]_{222}$ is converted into % folded and plotted against Gdn.HCl concentration.

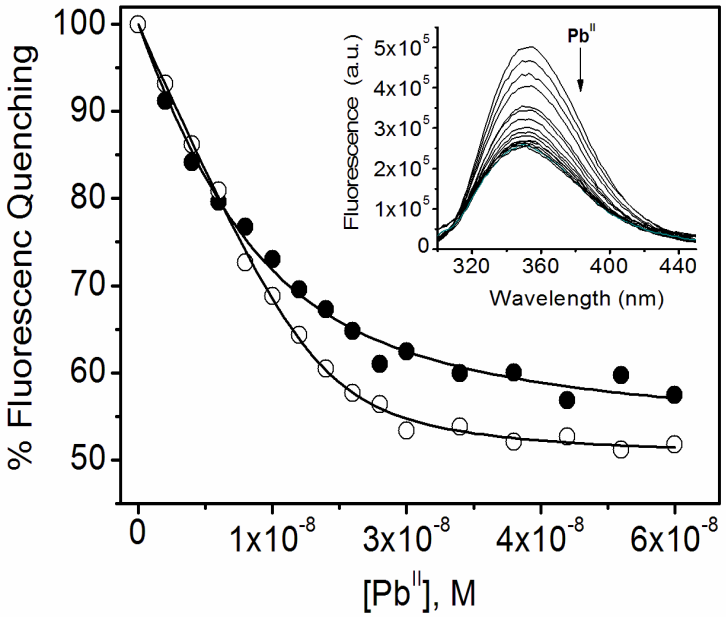

Figure S3. Change in fluorescence intensity upon binding of Pb(II) to the peptide **TRI**L2WL16C (filled circle) and **TRI**L2WL12AL16C (open circle) (30 nM trimer). The Trp was excited at 280 nm and the fluorescence quenching was traced at 354 nm. The curves represent the best fit to Equation 1 by non linear least squares analysis using ORIGIN software. In inset fluorescence quenching spectra were shown for the addition of Pb(II) to **TRI**L2WL12AL16C.

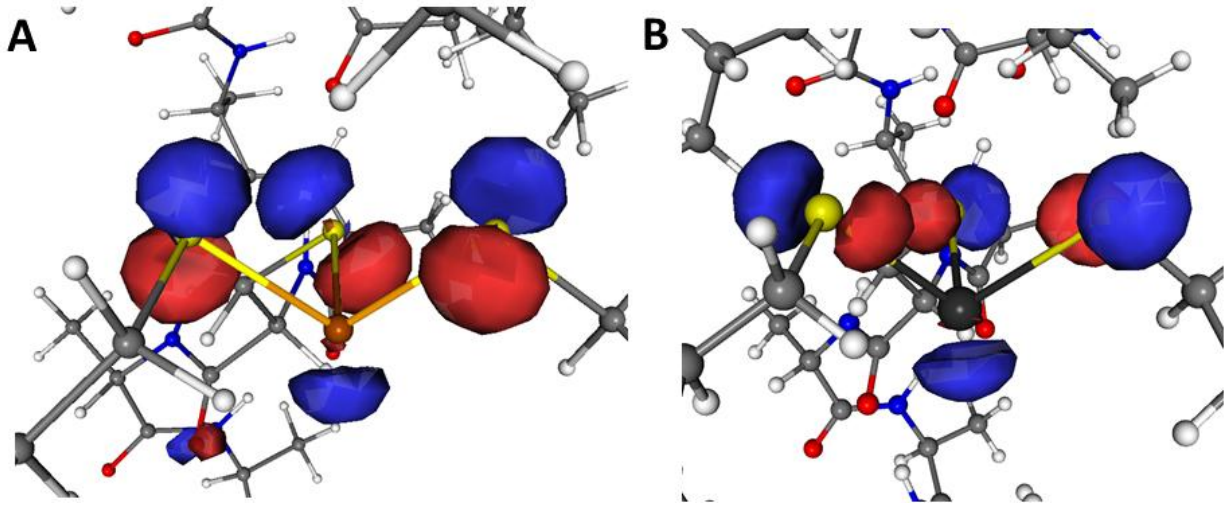

Figure S4. Mapping of isoenergy surfaces associated with the appropriate s and p orbitals for A) $As(ACA)_3$ and B) $Pb(ACA)_3$. The eigenvalue of the displayed orbital is -0.205285 Hartree for the As system, while in the case of the Pb system the associated eigenvalue is -0.09665 Hartree.

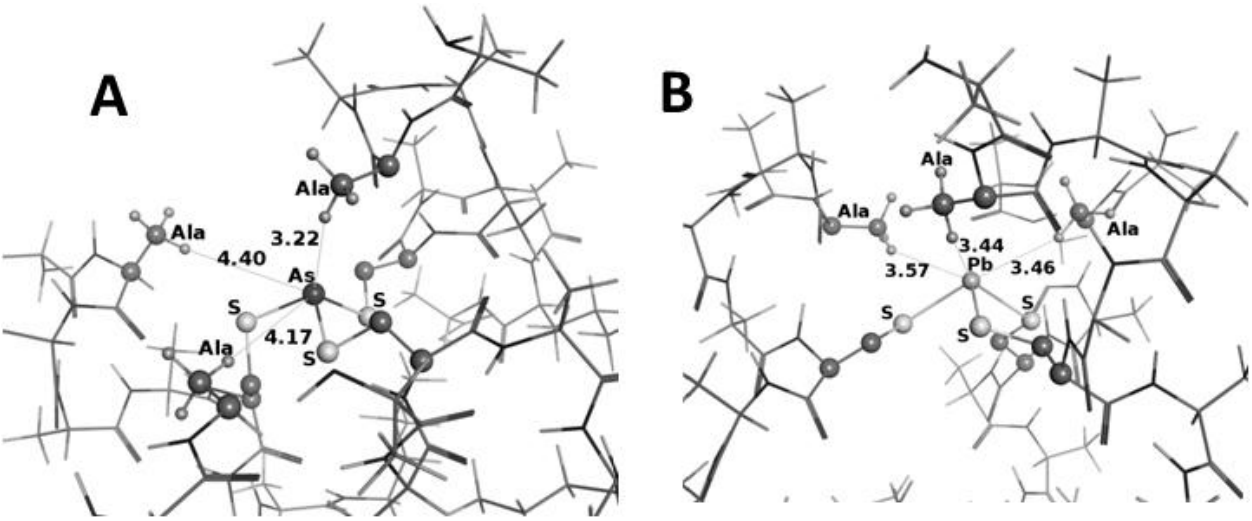

Figure S5. Closest H atom to M ion distances given in Angstrom. A) $As(III)(ACA)_3$ and B) $Pb(II)(ACA)_3$.