Supporting Information

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The Importance of Stereochemically Active Lone Pairs For Influencing Pb\textsuperscript{II} and As\textsuperscript{III} Protein Binding

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Figure S1. UV/Vis titration of Pb(NO$_3$)$_2$ into TRIL12AL16C (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 $K_a = 5.6(\pm 1) \times 10^8$ 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: TRIL2WL16C (black), TRIL12AL16C (red), and TRIL2WL12AL16C (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 **TRIL2WL16C** (filled circle) and **TRIL2WL12AL16C** (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 **TRIL2WL12AL16C**.

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.