Modelling of interactions of proteins and peptides with metal ions

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Abstract: An approach for *in silico* prediction and estimation of selectivity properties of metal-binding peptides is suggested. An in-depth analysis is performed to disclose the justifiability and limitations of this approach. The study is divided into three parts. First part investigates the soundness of two quantum chemical methods (MP2 and DFT) for their use in the set-up quest. The testing includes comparison with CCSD(T), effect of basis selection, performance of the two methods in geometry optimizations and effect of implicit solvent model.

Second part foreshadows the approach of searching for a metal selective peptide by thoroughly investigating the ability of simple representative systems, derived from their metalloprotein templates, to retain the property of interest.

Final part describes the initial step of extensive combinatorial approach towards examination of vast number of simple systems that represent metal-binding sites, and which are to be used for prediction of metal-selectivity through exploitation of the described approach and, ultimately, to the *de novo* design of metalloproteins with desired properties.