



Sřredoevropský technologický institut, výzkumná skupina Chytré nanostroje
 Laboratoř metalomiky a nanotechnologií, Mendelova univerzita v Brně



Seminář/Seminar PRO25_4723

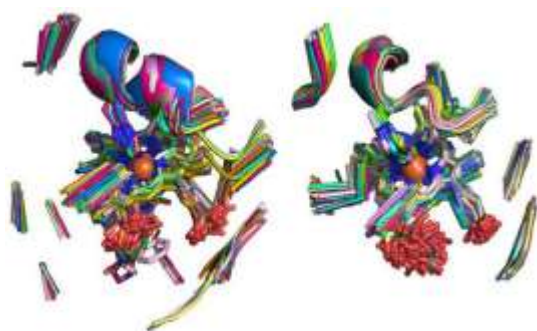
Vás zve na seminář:

Hidden relationships between metalloproteins unveiled by structural comparison of their metal sites- review

RNDr. Ondřej Zítka, Ph.D.

Abstrakt

Metalloproteins account for a substantial fraction of all proteins. They incorporate metal atoms, which are required for their structure and/or function. Here we describe a new computational protocol to systematically compare and classify metal-binding sites on the basis of their structural similarity. These sites are extracted from the MetalPDB database of minimal functional sites (MFSs) in metal-binding biological macromolecules. Structural similarity is measured by the scoring function of the available Metals² program. Hierarchical clustering was used to organize MFSs into clusters, for each of which a representative MFS was identified. The comparison of all representative MFSs provided a thorough structure-based classification of the sites analyzed. As examples, the application of the proposed computational protocol to all heme-binding proteins and zinc-binding proteins of known structure highlighted the existence of structural subtypes, validated known evolutionary links and shed new light on the occurrence of similar sites in systems at different evolutionary distances. The present approach thus makes available an innovative viewpoint on metalloproteins, where the functionally crucial metal sites effectively lead the discovery of structural and functional relationships in a largely protein-independent manner. doi:10.1038/srep09486



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