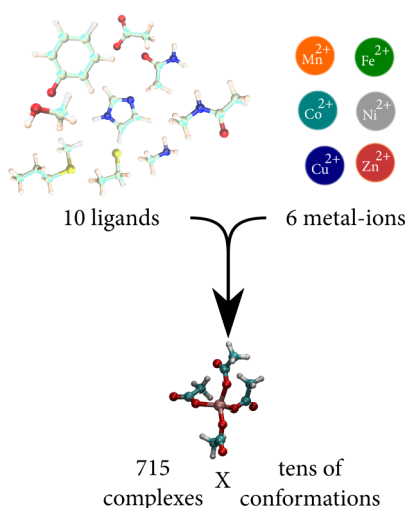


# Metal-ligand Complex Database as a Starting Point for Development of Metal-Protein Potentials

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Development of computationally accessible but sufficiently accurate potentials requires rich and consistent reference data. This work presents the construction of a database of metal-ligand complexes that serve as models for metal-protein interactions. The data is obtained using a DFT protocol combined with implicit solvation methods. The database combines several divalent metal-ions ( $\text{Mn}^{2+}$ ,  $\text{Fe}^{2+}$ ,  $\text{Co}^{2+}$ ,  $\text{Ni}^{2+}$ ,  $\text{Cu}^{2+}$ ,  $\text{Zn}^{2+}$ ) with ligands representing amino acid side-chains in fixed geometries. Emphasis is placed on exploring combinations of ligands and their mutual orientations.



*Figure 1: Target content of the database*

We hope that the database could serve as a starting point for development of metal-protein potentials, validation of force-field parameters, and identifying which degrees of freedom need to be sampled more thoroughly, in order to capture the complexity of metal-protein interactions.