
De Novo Design of Ligands for Metal Separation

Project ID: 55223

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Research Objective

This application focuses on the development of appropriate computation tools and parameters for the de novo design of selective metal ligands.

Research Progress and Implications

We have developed a successful suite of tools for computer-aided design of ligands for receptors of known three-dimensional structure (structure-based design), including the prediction of affinity. Adaptation of the algorithms to place donor atoms at appropriate geometrical locations surrounding the metal of interest, rather than filling up a cavity with donor/acceptor atoms placed optimally to interact with a protein active site, is straightforward. Appropriate geometrical parameters for metals can be derived from crystal structures and force constants adapted from recent advances in theories of metal-ligand interactions. The practical goal is computer-aided design of ligands which would be selective for one metal over another with a predicted selectivity ratio and affinity.