Modeling Metal Protein Complexes from Experimental Extended X-ray Absorption Fine-Structure using Genetic Algorithms

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Abstract

Experimental Extended X-ray Absorption Fine-Structure(EXAFS) spectra carry information about the chemical structure of metal protein complexes. However, predicting the structure of such complexes from EXAFS spectra is not an easy task. To solve this problem we will generate a number of model structures and compare their EXAFS spectra to the experimental EXAFS. Since many generated structures will share similar EXAFS spectra we will be attempting to use genetic algorithms to generate a population of possible structure candidates.