

Analyzing and predicting metal binding sites in proteins

BBSRC PhD project proposal

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Collaborating PI: Prof Steve Perkins (Structural & Molecular Biology)

PhD Project Description:

Metal binding is critical to the structural integrity and/or function of many proteins including key enzymes. Understanding metal binding will allow engineering of metal binding sites and prediction is key for low resolution structures (such as from structural genomics) where binding sites may not be resolved.

This project will build on our previous work on predicting metal binding sites. We will create an automatically maintained database of metal binding sites in the PDB and, through analysis and machine learning, will implement novel prediction methods. In collaboration with Steve Perkins, who has identified a zinc binding site at an interface in Factor H, a particular focus will be on binding sites at chain interfaces, especially important where the complex is unsolved.

The First Rotation:

The student will become familiar with the existing tools and analyses and extend that work to predict metal binding sites in Factor H.

The Second Rotation:

The student will test the results of the prediction work using site-directed mutagenesis and analytical ultracentrifugation on Factor H