Characterization of Putative Kinases with a Solved Structure but Unknown Function from the Protein Data Bank

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Abstract

The protein databank (PDB) contains 146,000 structures, with approximately 4300 of those currently classified as having “unknown function”. Of those, about 2500 are expected to be enzymes, based on structures with known function(s) in the PDB. The Biochemistry Authentic Scientific Inquiry Lab (BASIL) project has defined a series of in silico and in vitro modules that allow prediction and confirmation of function(s) for these proteins. To date, BASIL has focused primarily on putative hydrolases, especially the NUDIX hydrolases. We are adapting the BASIL modules for use with a novel category of proteins, putative kinases (EC 2.7.X.X). Kinases were selected because of their abundance in humans (over 500 members of the kinase superfamily) and their involvement in almost every aspect of cellular function. Utilizing ProMol and the Mechanism and Catalytic Site Atlas (M-CSA), we are defining units and test motifs for identification of putative kinases with unknown function within the PDB. These putative kinases are being further characterized utilizing a variety of in silico tools, including BLAST, Pfam, and Dali. In parallel, we are optimizing bacterial protein overexpression of the kinase(s), affinity chromatography purification of the protein(s), and the in vitro kinase assays. This should allow experimental confirmation of the kinase function(s) identified computationally. To support expansion of these modules to concurrent analyses by multiple students, we are designing reliable controls and a consistent workflow for the computational and in vitro analyses of kinase function. Overall, adaptation of the BASIL modules is allowing us to design a method for student characterization of multiple putative kinases simultaneously.

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