Utilizing BASIL Consortium Modules to Characterize Putative Kinases of Unknown Function

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First published: 18 April 2020
https://doi-org.ezproxy.rit.edu/10.1096/fasebj.2020.34.s1.06881

Abstract

The Protein Data Bank (PDB) contains 157,712 solved protein structures, with 4,465 of these listed as having an unknown function. We are interested in identifying novel kinases, and screened for them using modules from the BASIL Consortium's curriculum. BLASTp was initially used to analyze almost 1,500 protein structures of unknown function, narrowing the list to 12 putative kinases. Next, *in silico* tools including Pfam, DALI, PANNZER, SANS, and ProMOL (a PyMOL plug-in) were used to further characterize these putative kinases. Two structures were identified as likely kinases: 1ZBS and 3DNU. The 1ZBS protein is predicted to be an N-acetyl-glucosamine (NAG) kinase. The 3DNU protein appears to be a toxin-antitoxin type 2 protein that functions as a serine-threonine kinase. To further confirm these assignments, docking simulations were performed with the PyRx plug-in for PyMOL. NAG plus ATP could be docked into the 1ZBS protein with a good calculated binding affinity, supporting its function as a NAG kinase. Similarly, ATP and the tri-peptide RTV were stably docked with the 3DNU protein. *In vitro* confirmation of these *in silico* results is now underway for both 1ZBS and 3DNU. Protein over-expression and purification are being optimized, and the purified proteins will be used to confirm the identification of NAG/ATP and RTV/ATP respectively as viable substrates for these enzymes.

Support or Funding Information

This project is supported by NSF IUSE 1709170