

Microsymposium

MS39.O05

ProMOL: Improved approaches to identification of the function of proteins

H. Bernstein¹, P. Craig², A. Bangura², A. Grier², M. Osipovitch², V. Kovuri², T. McKay², K. Hart², W. Tedla-Boyd², G. Dodge², A. Hartung²

¹*Dowling College, Dept. Mathematics and Computer Science, Shirley, NY, USA,* ²*Rochester Institute of Technology, School of Chemistry and Materials Science, Rochester NY, USA*

The goal of this project is to improve and extend best practices in the algorithmic and biochemical identification of the function of proteins, and to make these resources available to the life science education and research communities. In the earlier phases of this project we developed the ProMOL plugin for PyMOL, a tool used to explore the catalytic site structural homologies between proteins of known function and those for which functions are not yet known, and we have applied it to examine more than 3000 structures in the Protein Data Bank for which functions are not yet known. Although catalytic site structural homology alone is not sufficient to define the function of a protein, it provides one mechanism which, when combined with other structural and sequence motifs, can suggest candidates for experimental verification. In addition, similar, non-catalytic structural motifs can be indicative of non-catalytic functions. The motif library is being extended to include NMR structures, metal ions, and non-catalytic motifs. A database of results has been established. The combination of in-silico characterization and wet-lab characterization has proven to be a suitable task for undergraduate biochemistry students and partnerships to embed this work in undergraduate curricula are being established.

Keywords: Protein Function, Structural Motif, ProMOL