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Exploring Protein Surface Analysis in Structural Genomics. T.A. Binkowski, A. Joachimiak, Structural Biology Center & Midwest Center for Structural Genomics, Argonne National Laboratory, Argonne, IL 60439.

Protein surface analysis has become a powerful method for discovering novel functional relationships in proteins, for functional annotation of structures with unknown biological roles, and for inquires on evolutionary origins of structural elements important for protein function. It has proven especially useful in expanding the high-throughput structural genomics pipeline, where newly determined protein structures are, by design, unrelated to other known proteins which challenge the limits of current methods of functional inference based on primary sequence and backbone structure. We present results utilizing surface comparisons from several structural genomics proteins solved at the Midwest Center for Structural Genomics, including proteins from *E. coli*, *P. aeruginosa*, *V. cholerae*, *T. acidophilum*, and *N. meningitidis*. The identification of similar protein surfaces has proven useful to identify and classify active sites, infer information about biochemical activities, drive ligand binding studies and to prevent functional misclassification despite overall structural similarity.

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