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Global Protein Surface Survey: A Comprehensive Survey of Protein Surface Features. T.A. Binkowski, A. Joachimiak, Structural Biology Center & Midwest Center for Structural Genomics, Argonne National Laboratory, Argonne, IL 60439, USA.

As structural genomics efforts continue to populate the protein fold space at rapid pace, an exponential growth in protein surface information follows suit. These surfaces contain a wealth of information about protein function. The Global Protein Surface Survey (GPSS) is the first effort to identify and organize surfaces from structures deposited in the Protein Data Bank. Surface libraries have been compiled that represent all geometrically defined solvent accessible cavities and interior voids as well as ligand, metal, DNA and peptide binding surfaces. Publicly available annotation is mapped onto surfaces. The role of surface analysis in understanding the biological roles of proteins is becoming an increasingly important part of the effort at the Midwest Center for Structural Genomics. Utilizing a novel search algorithm, hypothetical protein surfaces are queried against the GPSS libraries for function prediction. We present results utilizing surface comparisons from several newly solved structures. The GPSS is available at <http://gpss.mcsg.anl.gov>.

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