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The SECSG Protein-to-Structure Pipeline: Potential and Limitations. J. Rose¹, Z.-J. Liu¹, D. Lin¹, W. Tempel¹, L.R. Chen¹, A. Shah¹, J. Richardson², D. Richardson², G. Newton¹, J. Ng³, B.C. Wang¹, Southeast Collaboratory for Structural Genomics, ¹Dept. of Biochemistry & Molecular Biology, Univ. of Georgia, Athens, GA 30602, ²Dept. of Biochemistry, Duke Univ. Medical Center, Durham, NC 27710, ³Laboratory for Structural Biology, Univ. of Alabama, Huntsville, 35889 USA.

A high-throughput pipeline that encompasses all aspects of structure determination will be reported. It includes three components: crystallization/crystal salvaging, data collection/structure solution and structure refinement/validation. It is capable of screening/optimizing and diffraction characterization of 35 new proteins and producing 4 plus crystal structures per week, although a full operation is currently limited by protein supply.

High throughput is achieved by novel methodologies, home and synchrotron X-rays, robotics and data management. A crystal salvaging pathway is provided for those proteins that either fail to crystallize or produce crystals of limited diffraction quality. A novel cluster based structure determination engine that automatically samples parameter space combined with high quality SAS data maximizes success of the structure determination. MolProbity validation integrated into the refinement ensures high quality results.

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