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**High-throughput Structural Prediction and Functional Annotation of Proteomic Sequences.** Dana Haley-Vicente, Life Science, Accelrys Inc., 10188 Telesis Court, Suite 100, San Diego, CA 92121 USA.

Targets in structural genomics initiatives are often selected because they represent a family of proteins for which no three dimensional structure or fold is known. Such 3D information is crucial for rational drug design, diagnosis and treatment of disease, and advancing our understanding of basic biology. Once a representative structure for the family has been determined structures, for the other family members which are similar in sequence can be inferred by comparative modeling techniques. Here we introduce a high-throughput in-silico strategy to obtaining protein structures of similar and distantly related proteins within a family based on sequence and fold comparisons. Using Discovery Studio GeneAtlas<sup>®</sup>, an automated, high-throughput structure prediction and functional annotation pipeline, we are able to rapidly functionally annotate sequences and calculate homology models for thousands of proteins. Experimental templates for the model generation are identified using the combination of sequence comparison using PSI-BLAST and fold recognition using SeqFold. As an example, we will show functional annotation and comparative models of the SARS and West Nile virus proteomes. Recent experimental structure data have validated the accuracy of the 3D models created. This data has allowed us to perform structure-based drug design studies to generate new lead candidates to fight the diseases that are caused by these deadly viruses.