COMPUTATIONAL CHEMOGENOMICS: EXTRACTING KNOWLEDGE FROM BIOCHEMICAL DATA

Jordi Mestres

Chemogenomics Laboratory, Research Unit on Biomedical Informatics,
Municipal Institute of Medical Researh (IMIM), University Pompeu Fabra (UPF),
Barcelona (Catalonia), Spain
http://cgl.imim.es/

In recent years, the establishment of high-throughput screening technologies and recent advances in protein expression, production and X-ray crystallography have led to an explosion of both response data (e.g., potency, affinity, metabolism, toxicity) on the interaction between proteins and ligands, and structural data on proteins and protein-ligand complexes, respectively. The question now is, how should these data be organised and how could they be analysed so knowledge, in the form of some trends, rules, or models connecting both chemical and biological spaces, can be extracted from them? This talk will attempt addressing this question by presenting some of our recent efforts to, on one hand, identify and classify chemical and biological entities and, on the other hand, develop new biochemoinformatics tools to extract knowledge from chemical and biological data.