



Spring 2012 Colloquium

Temple University
Computer and Information Sciences

Computational Approaches for Drug Repositioning

Lun Yang

GlaxoSmithKline

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Abstract:

Drug repositioning helps fully explore indications for marketed drugs and clinical candidates. Here I introduce several computational approaches that could be used in predicting new indications.

1) Chemical-protein Interactome (CPI), which mimics the interaction profile of drug across the human proteome, helps to conduct multi-dimensional analysis of drugs' perturbation towards the biological system. Both the off-targets and the associated off-systems could be identified to explore the molecular basis of drug's off-effects, which could be used to predict the new indications.

2) Clinical side-effects (SEs) provide a human phenotypic profile for the drug, which can suggest additional disease indications. Here I introduce a methodology named "Systematic Drug Repositioning Based on Clinical Side-Effects (DRoSEf)", which utilizes the SE information extracted from drug label and the 2D structure information of the compounds to suggest new indication for drug candidates in clinical pipeline.

Bio:

Dr. Lun Yang's research focuses on molecular modeling and data integration for drug repositioning and personalized medicine. He has authored about 20 articles in bioinformatics journals, 10 of which list him as the first author or corresponding author, including Bioinformatics, PLoS Computational Biology and Nucleic Acids Research. He also shares the authorships in top journals such as Nature Biotechnology and Briefings in Bioinformatics.

He serves as the principal investigator in the computational biology group at GlaxoSmithKline and focuses on developing innovative methodologies for drug repositioning. Before his appointment at GlaxoSmithKline, he is the investigator at U.S. Food and Drug Administration, developing computational methodologies for personalized medicine.