Computational Polypharmacology: Combining simulations, big data, and machine learning

DATE
Wednesday, October 10, 2018

LOCATION
UHS 130
(Beside Employee Health)

TIME
12:00—1:00 pm
Pizza will be served beginning at 11:50 a.m.

Using machine learning to score potential drug candidates may offer an advantage over traditional imprecise scoring functions because the parameters and model structure can be learned from the data. However, models may lack interpretability, are often overfit to the data, and are not generalizable to drug targets and chemotypes not in the training data. Benchmark datasets are prone to artificial enrichment and analogue bias due to the overrepresentation of certain scaffolds in experimentally determined active sets. Datasets can be evaluated using spatial statistics to quantify the dataset topology and better understand potential biases. Dataset clumping comprises a combination of self-similarity of actives and separation from decoys in chemical space and is associated with overoptimistic virtual screening results. This talk explores data, methods, and potential data biases relevant to computational drug binding predictions.

Presented by:
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REGISTRATION REQUIRED
To reserve your place, please email CCTS at CCTS@UKY.EDU by Monday, October 8, 2018. If you require special physical arrangements to attend this program, please call 323-8545.

CCTS Biomedical Informatics (BMI) Core
The Biomedical Informatics (BMI) Core provides access to biomedical informatics expertise, technologies, and data management platforms to CCTS and their investigators. The CCTS BMI team integrates the CCTS BMI Core, Institute for Biomedical Informatics (IBI) and the Institute for Pharmaceutical Outcomes and Policy (IPOP) housed in the College of Pharmacy.

The Institute for Biomedical Informatics (IBI) translates data to knowledge to improve human health and effectively use the latest technology and tools for the advancement of biological sciences. The IBI promotes translational team science and engages the entire campus to develop and grow informatics and data science training programs; share research and data infrastructure; and enable technology innovation.