17th Annual LBRN Meeting - 2019

Keynote Talk - January 19th, 2019 - 8:15 to 9:00 AM

Comprehensive Solution to Characterize and Treat Disease

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Abstract: Discovery and development of small molecule compounds into therapeutics is time and resource intensive, a process that can be made more efficient by computational drug repurposing. We have developed the Computational Analysis of Novel Drug Opportunities (CANDO) platform for shotgun drug repurposing, i.e., screen and rank every existing human use drug or compound for every disease/indication. The modeling pipeline in CANDO predicts interactions between every compound and every protein structure present in corresponding curated libraries to generate compound-proteome interaction signatures that are then analysed and compared to identify similar drug behavior. For each drug, CANDO produces a ranked list relative to every other compound based on the similarity of their interaction signatures. The performance of CANDO is evaluated based on its ability to recover drugs approved for each indication within a particular cutoff of the corresponding ranked compound similarity lists; top ranked compounds other than the known approved drugs are hypothesized to be novel putative therapeutics for that indication. We have added new ligand-based virtual screening, data fusion, and decision tree pipelines, as well as made improvements to existing pipelines, to better understand drug behavior and improve benchmarking performance. The presentation will address the latest improvements to the CANDO platform and its potential to substantially increase drug recovery accuracy via the integration of multiple pipelines to determine similarity of compound behavior, thereby increasing our confidence in generating putative therapeutic repurposing candidates.

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