Predicting Mechanisms of Action, Human Toxicity and Optimizing Indication using Biology-driven AI

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My group has developed robust Artificial Intelligence approaches to address several of the difficult challenges encountered during drug discovery and development. This includes therapeutic target discovery using data integration, systems biology and machine learning, predicting the target(s) of small molecules without known mechanisms of action in order to inform clinical trial design, indication prediction for existing molecules, clinical trial outcome and adverse event prediction, and predicting effective combinations. In this talk I will describe how we used machine learning to predict toxicity of drug candidates ahead of human trials. I will also describe a computational approach called BANDIT that integrates multiple data types to predict mechanisms of action. BANDIT was used to uncover novel microtubule targeting agents and identified a novel and unexpected target for an investigational anticancer agents, thus allowing optimal clinical positioning and clinical trial design and ultimately clinical success.