Network-based algorithm for identifying a drug's mechanism of action

Identifying the mechanism of action (MoA) of compounds is critical for drug discovery and development. However, current approaches to identifying these pathways are expensive and time-consuming, and often result in the development of drugs with limited potency and safety. This technology utilizes a computational approach to identify changes in gene expression that produce a compound’s pharmacological effects. By accurately and robustly identifying a drug’s biochemical interactions, this technology may improve drug discovery and development, and could serve as a tool for studying drug-associated side effects and toxicity.

Detecting Mechanism of Action using Network Dysregulation (DeMAND) can more accurately predict drug toxicity and efficacy

DeMAND is a network-based algorithm capable of reliably identifying perturbations in gene expression linked to the pharmacological effects of a compound. Specifically, this computational method works by comparing gene expression profiles following drug treatment with untreated control samples. By monitoring and identifying changes in expression of an entire profile of genes, this method eliminates the need for a priori information regarding the genetic pathway affected by a drug of interest. This technology has the potential to improve the success rate of drug discovery, development, and repositioning by more accurately predicting both drug toxicity and efficacy.

This method has been demonstrated to successfully predict the mechanism of action for multiple anticancer compounds, including identification of a novel MoA for the drug Altretamine.

Lead Inventor:
Andrea Califano, Ph.D.

Applications:
- Algorithm for determining the mechanism of action of a compound of interest
- Means of predicting drug interactions prior to clinical trials
• Drug discovery and development
• Drug repositioning
• Studies on drug side effects

Advantages:
• Network-based algorithm detects gene expression changes not only for a target gene, but also surrounding and downstream genetic changes
• Avoids limitations associated with experimental approaches
• Does not require prior knowledge of relevant genetic sub-networks to identify a drug’s mechanism of action

Patent Information:
Patent Pending
Tech Ventures Reference: IR CU14294

Related Publications:

Inventors

Andrea Califano Ph.D.