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Deep learning model that predicts the mechanism of action and therapeutic utility of uncharacterized chemical compounds, relevant pharmaceutical implications for drug re-purposing

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Inventors

E. Brown

S. French

A. Bing Ya Guo

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Contact

Amy Hector –

Business Development Officer

905-525-9140 ext. 28642

hectoraj@mcmaster.ca

<http://milo.mcmaster.ca>

Abstract

In small molecule drug discovery pipelines, identification of mechanism of action and therapeutic potential of compounds with known bioactivity is a time-intensive process, often taking years to arrive at a conclusion. Current methods focus on a single therapeutic indication (i.e. antibacterial, non-steroidal anti-inflammatory, anticancer) which are typically hypothesis-driven, intuitive, and slow. Therefore, there is a need for improved predictive tools in identifying possible mechanisms of action and therapeutic utilities.

Gene expression studies of a wide variety of cell types have revealed that various cell systems have complex unique fingerprint responses to chemical perturbants. Researchers at McMaster have developed a deep learning model which predicts the mechanism of action of chemical compounds based on such microbial fingerprint responses. This densely connected network uses unique microbial responses to chemical inputs to map unknown (test set) compounds to a well-annotated database (training set) of compounds. By utilizing a sensitive microorganism reporter, the biological activity inherent in any drug may be detected, even if it is not an antibiotic.

Applications

Predict the mechanism of action and therapeutic utility of uncharacterized chemical compounds with potential applications in drug repurposing (beyond antimicrobials) and the development of novel therapies.

Advantages

- Reports on the ability of microorganisms to elicit unique stress response fingerprints based on the chemical structure of compounds they are exposed to. This includes (but is not limited to) anticancer drugs, psychoactive drugs, antibiotics, and non-steroidal anti-inflammatory drugs.
- Can be used in any organism with some genetic manipulation, and any growth media/environment.
- Model accuracy >98% with a 20/80 (test/training) split of our existing data with antimicrobials.