REVOLUTIONIZING BIOMEDICAL RESEARCH: INTEGRATING CUTTING-EDGE AI/ML TO UNLEASH INNOVATION IN DRUG DISCOVERY AND THERAPEUTICS DEVELOPMENT

Toxidrome Screening: AI-based Safety Assessment Of Chemicals

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Background: Toxidromes constitute patterns of symptoms and signs caused by specific toxic effects that guide emergency treatments. Computational identification of chemicals that cause different toxidromes allows us to rapidly screen novel compounds and compound classes as to their potential toxicity.

Objective: Create a computational toolset that can map chemicals to their potential toxidromes.

Methods: We used a communicative message passing neural network (CMPNN) in combination with multi-task training and ensemble models to develop reliable prediction models. For toxidromes that do not have well-defined molecular mechanisms or sufficient data to train deep learning models, we used the similarity ensemble approach instead of the common Tanimoto similarity approach to develop computational tools for rapid identification of chemicals with potential to cause these toxidromes.

Results: We created accurate prediction models for nine toxidromes: the Opioid, Convulsant, Cholinergic, Anticholinergic, Sympathomimetic, Anticoagulant, Acute exposure, Irritant/Corrosive, and Knockdown toxidromes. These prediction models, which solely use chemical structures as input to create the predictions, are available at the publicly accessible toxidrome profiler website (https://toxidrome.bhsai.org/).

Conclusion: The developed toxidrome profiling tool provides a rapid means to screen for toxicity of environmental chemicals and map out potential adverse health effects of drugs or drug candidates. Rapid identification of adverse health effects using AI-based prediction models allows for identifying and classifying the harmful effects of novels compounds.

Liu R, AbdulHameed MDM, Xu Z, Clancy B, Desai V, Wallqvist A. Rapid screening of chemicals for their potential to cause specific toxidromes. Frontiers in Drug Discovery 4: 1324564 (2024).