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

AI Applications For Assessing Safety Profiles Of Chemicals And Drugs

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Background: In evaluating chemicals and drugs, pharmacokinetic and toxic properties are important components for efficacy and safety assessments. Considerable progress has been made in the development of machine learning models to estimate such properties, yet important questions remain about their reliability and the limited availability of data to train such models.

Objective: Develop a prediction framework to accurately and rapidly forecast in vitro and in vivo chemical assay results with accuracies that are on par with experimental inter-laboratory reproducibility.

Methods: We used artificial intelligence (AI) techniques based on systems toxicology approaches combined with multi-tasking and transfer learning concepts to efficiently train deep neural networks with a limited amount of training data available.

Results: We developed multiple machine learning, deep neural network models, databases, and tools for evaluating potential adverse effects of chemicals and drugs, including toxicity profiling for endocrine disruptors, bile salt transporters, toxidrome effects, and transport proteins in the liver, kidney, and brain. These models and their aggregated prediction capabilities represent an unprecedented capability to accurately and rapidly predict the properties of a chemical compound or sets of compounds.

Conclusion: We successfully applied AI techniques to predict multiple important pharmacological endpoints, ranging from acute toxicity to specific liver and kidney damage, paving the way for including these capabilities in both drug development and threat assessments.