AI/ML AND VIRTUAL HUMAN PLATFORMS FOR THREAT AGENT HAZARD ASSESSMENT AND MEDICAL COUNTERMEASURE DISCOVERY AND DRUG DEVELOPMENT

Machine Learning And Ai Applications For Assessing 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: Use artificial intelligence (AI) techniques based on systems toxicology approaches combined with multi-tasking and transfer learning concepts to efficiently train deep neural networks when a limited amount of training data are available.

Results: We developed multiple in silico models and tools for pre-clinical evaluation of drugs and countermeasures, such as in assessing Ames mutagenicity, hERG for cardiac toxicities, drug efflux via P-glycoproteins, and drug metabolism via cytochrome P450 enzymes. These models can predict properties for over 80% of all compounds with an average prediction accuracy of 85%, rivaling inter-laboratory assay reproducibility.

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.