AI-POWERED DIAGNOSTICS

Finch: An AI-powered Toolbox For The Prediction Of Chemical Mixture's Physiological Function And Hazard Profiles.

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The need to holistically view human interactions with chemical mixtures is driving a paradigm shift in the chemical risk assessment field that necessitates product/mixture over single compound testing, elimination of animal testing, and new modeling approaches to understand mixture activity profiles. Unfortunately, most computational models primarily focus on the analysis and estimation of single chemical species with very few viable mixture models that go beyond conventional modeling approaches. Conventional mixture modeling approaches, such as concentration addition (CA) and independent action (IA), are limited by their ability to handle multiple Modes of Action (MoA), and often overlook synergistic/antagonistic effects. Therefore, a fast and efficient model for mixture prediction that goes beyond conventional approaches would be an asset to regulatory entities, as well as warfighters that are concerned with safety profiles.

Finch is a novel workflow that addresses these challenges by leveraging deep Learning (DL) embeddings and multi-task quantitative structure-activity relationship (QSAR) models for enhanced chemical exposure prediction. The use of DL embeddings maximizes information in the latent space from a vast number of inputs, including molecular descriptors, physiochemical properties, and structural fingerprints derived from a SMILES input. The extensive base of inputs will ensure the chemical structure of each ingredient is sufficiently represented. DL embeddings are employed to distill critical features and preserve information into a latent space, enhancing the predictive capability of subsequent machine learning models. The multi-task learning aspect of Finch is particularly advantageous as it allows for the simultaneous optimization of multiple loss functions. This approach is beneficial as it uses all the available data across the different tasks to learn generalized representations, which can aid in effectively capturing complex ingredient interactions within mixtures (e.g., antagonistic, or synergistic).

To both validate and enhance the predictive capability of Finch, we are conducting high-throughput experiments on A549 and THLE-2 cell lines in a 96-well plate platform to assess cell cytotoxicity in response to chemical mixtures. The data derived from these experiments serve as a robust foundation for training our DL-embedded QSAR models. The integration of empirical data and DL embeddings ensures that the models are robust, enhancing their relevance and utility for stakeholders in chemical safety evaluation.

The DL embedded multi-task QSAR models developed in Finch is poised to benefit the customer by providing a fast and accurate prediction of both the function and the hazard profiles of a chemical mixture. This will reduce the time and cost required for mixture characterization, allowing for the efficient prioritization of mixtures that warrant further experimental testing. Through these models, many mixtures can be evaluated and only the most toxic mixtures will be sent to experimental testing. This computational-experimental synergy has the potential to greatly enhance the throughput and cost-effectiveness of safety assessments in various applications, making it an invaluable tool for stakeholders in the domain of chemical risk assessment.

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