

Integrated approaches for chemical safety assessment and drug discovery

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Toxicology is going through profound changes as the focus of investigation is shifting from the observation of apical phenomena to mechanistic aspects of the exposure. Toxicogenomics aims at clarifying the mechanism of action (MOA) of chemicals by using omics assays. The Adverse Outcome Pathways (AOP) concept is also emerging to contextualise toxicogenomics-derived MOA. At the Finnish Hub for Development and Validation of Integrated Approaches (FHAIVE) of Tampere University, we use advanced modelling of large amounts of data to anchor molecular assays to AOPs. We also combine big data science, artificial intelligence (AI), network science, toxicogenomics, molecular assays and cell technology to analyse a comprehensive knowledge graph comprising tens of millions of data points with the aim to develop AOP-derived New Methodology Approaches (NAMs). In this talk, I will discuss how integrated data-driven approaches can be used to unify the currently fragmented comprehension of the chemical-biological interactions, while guiding the development of safe and sustainable by design (SSbD) and effective by design (EbD) chemicals, drugs, and materials.