NICEATM Computational Tools and Resources Supporting Alternative Test Method Development and Evaluation

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Adoption of new approach methodologies (NAMs) for chemical safety assessment requires resources that can support both the development and evaluation of such approaches. To support widespread utility, resources must consider the needs of users with diverse backgrounds. For example, interpretation is facilitated by annotating the biological function an in vitro assay target. This annotation provides context and a possible linkage with regulatory toxicological endpoints. The National Toxicology Program Interagency Center for the Evaluation of Alternative Toxicological Methods (NICEATM) promotes the development and implementation of NAMs that reduce or replace animal use while still protecting human health and the environment. A major goal for NICEATM is to provide stakeholders with data that are Findable, Accessible, Interoperable, and Reusable (FAIR) to the greatest extent possible. The assay annotation is a step toward the goal of implementing FAIR Principles (https://www.go-fair.org/fair-principles/) to give data greater value and enhance their reusability. To support these activities, NICEATM, in partnership with stakeholders from government, industry, and academia, has developed a set of computational tools and resources. These resources give developers and users of NAMs direct access to curated, computationally accessible data along with in silico tools for calculating chemical-specific parameters and for predicting chemical-mediated bioactivity. This presentation describes NICEATM's approaches for data acquisition and curation, including a summary of tools that facilitate these labor-intensive processes, and a description of how to access our compiled datasets. We summarize our work in the development and use of computational tools including QSAR models available through the Open Structure-activity/property Relationship App (OPERA) and physiologically based pharmacokinetic models that facilitate in vitro to in vivo extrapolation. This project was funded in whole or in part with federal funds from the NIEHS, NIH under Contract No. HHSN273201500010C.