NICEATM Computational Tools and Data Resources

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Implementing new approach methodologies (NAMs) for chemical safety assessment requires resources that can support both development and evaluation of NAMs. The National Toxicology Program Interagency Center for the Evaluation of Alternative Toxicological Methods (NICEATM) works with a wide range of stakeholders to advance NAMs that reduce or replace animal use while protecting human health and the environment. In partnership with stakeholders from government, industry, and academia, NICEATM has developed a set of computational tools and data resources. These resources give developers and users of NAMs direct access to curated, computationally accessible in vitro, in chemico, and in vivo data as well as chemical information. NICEATM also provides in silico tools for comparing chemical lists based on their physicochemical properties and for estimating in vivo equivalent doses based on in vitro bioactivity. This presentation describes NICEATM's approaches for data acquisition and curation, including how we facilitate these labor-intensive processes and how users can access our compiled datasets. We provide an overview of our annotation of assay data, which supports Findable, Accessible, Interoperable, and Reusable (FAIR; https://www.go-fair.org/fair-principles/) principles to achieve optimal value and enhance data reusability. We also summarize the development and application of computational tools, including quantitative structure-activity relationship models included in the Open Structure-activity/property Relationship App (OPERA) and physiologically based pharmacokinetic models that facilitate in vitro to in vivo extrapolation accessible through the Integrated Chemical Environment (ICE; https://ice.ntp.niehs.nih.gov/). This project was funded in whole or in part with federal funds from the NIEHS, NIH under Contract No. HHSN273201500010C.