An Integrated Chemical Environment to Support 21st Century Toxicology

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Traditional tests to evaluate chemicals for their potential impact on human and environmental health have been performed using animal models, with varying degrees of success in accurately identifying hazards. Advances in science and technology offer the potential for developing more effective approaches based on higher throughput testing methods and computational models. However, developing and evaluating these methods and models require high-quality curated data and appropriate tools. To address the need for these resources, NICEATM has developed the Integrated Chemical Environment (ICE). ICE has three components to assist researchers and regulators in evaluating chemical effects: a data integrator, computational models and workflows, and educational tutorials exploring these tools and on designing alternative approaches for scientific and regulatory needs. The data integrator brings together curated in vivo test data, reference chemical information, in vitro assay data (including data from high throughput screening programs), and in silico predictions. The ICE interface integrates these data in a meaningful and transparent format to facilitate hypothesis generation and testing. Users can query these data collections focusing on endpoints of interest, such as acute systemic toxicity or skin sensitization. Open-source computational software and workflows available via the resource use data obtained either from the ICE integrator or provided by the user to perform in silico predictions (e.g. IVIVE/PBPK modeling, structure-based property values, or toxicity pathway signatures). The ICE educational resources allow users to explore the computational methods and learn more about their capabilities and limitations as well as the needs and challenges associated with developing new chemical evaluation methods. Our ultimate goal is for ICE to support the growing community of novel test method developers and users as part of a strategy for implementing 21st century toxicity testing approaches. *This project was funded in whole or in part with Federal funds from the NIEHS, NIH under Contract No. HHSN273201500010C.*

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