

Providing Insight into Chemical Activity Through Data Curation and Assay Annotation

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The development of new approach methodologies that do not use animals for toxicity testing relies on access to data sets that are maintained, easily accessed, and curated. Resources providing data should consider the needs of users with diverse backgrounds to support widespread utility. For example, data resources in which assays are annotated with biological function or process information can facilitate interpretation of in vitro data by providing context for individual assays and relationships with regulatory endpoints. The National Toxicology Program's Integrated Chemical Environment (ICE) (<https://ice.ntp.niehs.nih.gov/>) is a free public resource supporting development, evaluation, and application of alternative test methods. ICE contains data from sources such as method validation studies, systematic literature reviews, Tox21, and U.S. Environmental Protection Agency pesticide registrations. To enhance the usefulness of data in ICE, we have annotated assays to associate them with mechanistic targets for both in vitro high-throughput screening and in vivo guideline-like toxicity studies. Data download options support detailed user exploration of chemical bioactivity. A major goal for ICE is to provide 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. The presentation will describe our curation processes and case studies using ICE data.

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