Annotating and Visualizing In Vitro Data to Gain Context

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Availability of in vitro high-throughput screening (HTS) assay data is facilitating the development of computational approaches for chemical hazard assessment. Linking HTS data to regulatory endpoints remains a challenge and requires detailed information about assays as well as an understanding of biological context. For example, data from the U.S. Environmental Protection Agency's ToxCast HTS program are annotated by technology platform, assay design, and assay/gene target information, yet it remains a challenge to provide toxicological context for potential regulatory applications. Here we present a mapping approach for HTS assay endpoints that moves beyond technology-based assay annotations. Our mapping provides a robust assay grouping schema applicable beyond HTS datasets in a toxicological endpoint-based framework. This expert-led curation and annotation is available in the Integrated Chemical Environment (ICE). Annotations map assays to regulatory toxicological endpoints of interest through structured vocabularies allowing data to be searched, grouped, and visualized by regulatory endpoint. The annotations increase accessibility for those unfamiliar with individual assays by providing context for in vitro assays (and in vivo data or in silico predictions in ICE) to facilitate identification of data gaps, insight into mechanistic plausibility, and investigation into regulatory-relevant endpoints. Finally, we highlight that while single assay results are generally insufficient for regulatory application, this approach helps integrate results from multiple assays and provides data visualization to aid review of a chemical's potential activity for selected regulatory endpoints. This project was funded with federal funds from the NIEHS, NIH under Contract No. HHSN273201500010C.