

Annotating High-Throughput Screening Assays: Facilitating Interpretation and Data Use

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Publicly available high-throughput screening (HTS) data have the potential to facilitate the development of computational approaches for chemical assessments and provide mechanistic insight on chemical effects and hazard. However, linking HTS data to toxicologically relevant mechanistic pathways or regulatory endpoints remains a challenge and requires detailed information about both assay technology and the assay's biological context. In this project, we annotated thousands of assay endpoints from the U.S. Environmental Protection Agency's ToxCast program, including results from the Tox21 HTS program, using existing controlled assay ontologies. Use of these ontologies facilitates stakeholder understanding, provides terminology that offers additional context, and informs upon the biological relevance of heterogeneous *in vitro* HTS assay readouts. Assay annotations are leveraged to complete a standardized data reporting template: OECD Harmonized Template (OHT) 201. OHT201 is an internationally recognized template used to report chemical test result summaries for intermediate effects. It captures assay technology information as well as mechanistic outcomes and interpretation obtained from *in vitro*, *ex vivo*, or *in silico* methods. We used a KNIME workflow applied via the IUCLID portal to populate the OHT201 form based on expert curation of existing annotations associated with fields in the form. These activities are expected to increase accessibility to annotated HTS data and provide context to facilitate the identification of data gaps, characterization of mechanistic plausibility, and further investigation into regulatory-relevant endpoints such as endocrine disruption, carcinogenicity, developmental toxicity, etc. This abstract was funded by NIEHS under Contract No. HHSN273201500010C.