

## Tox21 and ToxCast Chemical Landscapes: Laying the Foundation for 21st Century Toxicology

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The U.S. Environmental Protection Agency's ToxCast project and the related, multi-Agency Tox21 project are employing high-throughput technologies to screen hundreds to thousands of chemicals in hundreds of assays, probing a wide diversity of biological targets, pathways and mechanisms for use in predicting in vivo toxicity. The ToxCast chemical library consists of 960 unique chemicals (including Phase I and II) and was constructed to span a diverse range of chemical structures and use categories. This library is fully incorporated into EPA's approximately 4000 chemical contribution to the larger, more diverse Tox21 chemical library (totaling 10K). These chemical libraries represent central pillars of the ToxCast and Tox21 projects and are unprecedented in their scope, structural diversity, multiple use-scenarios (pesticides, industrial, food-use, drugs, etc.), and chemical feature characteristics in relation to toxicology. Chemical databases built to support these efforts consist of high quality DSSTox chemical structures and generic substance descriptions linked to curated test sample information (supplier, lot, batch, water content, analytical QC). Cheminformatics, feature and property profiling, and a priori and interactive categorization of these libraries in relation to biological activity will serve as essential components of toxicity prediction strategies. [Abstract does not represent EPA policy.]