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Session Title: **The Growing Impact of Public Domain Chemistry Resources**

**DSSTox ToxCast and Tox21 Chemical Inventories: Laying the Foundation for the U.S. EPA's Computational Toxicology Research Programs**

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High quality chemical structure inventories provide the foundation of the U.S. EPA's ToxCast and Tox21 projects, which are employing high-throughput technologies to screen thousands of chemicals in hundreds of biochemical and cell-based assays, probing a wide diversity of targets, pathways and mechanisms related to toxicity. The ToxCast chemical library consists of approximately 1800 compounds and is incorporated into the more diverse Tox21 chemical library (more than 8000 unique substances). These chemical libraries are unprecedented in their scope, structural diversity, multiple use-scenarios (pesticides, industrial, food-use, drugs, etc.), and chemical feature characteristics in relation to toxicology. Public chemical databases built to support these efforts consist of high quality DSSTox chemical structures and substance descriptions linked to curated test sample information. Cheminformatics, feature and property profiling of these libraries in relation to biological activity serve as essential components of toxicity prediction strategies. Abstract does not represent EPA policy.

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