



DSSTox & Chemical Information Technologies in Support of Toxicity Prediction

Ann Richard¹, Maritja Wolf², Matthew Martin¹, David Reif¹, Richard Judson¹

research&development

¹U.S EPA, ORD, Computational Toxicology Research Program; ²Lockheed Martin – Contractor to the US EPA

Science Question

Accurate chemical structure annotation, and the integrity and comparability of chemical information associated with bioassay and toxicity data, are essential for building cheminformatics capabilities in support of improved toxicity prediction models. The information takes two substantially different forms:

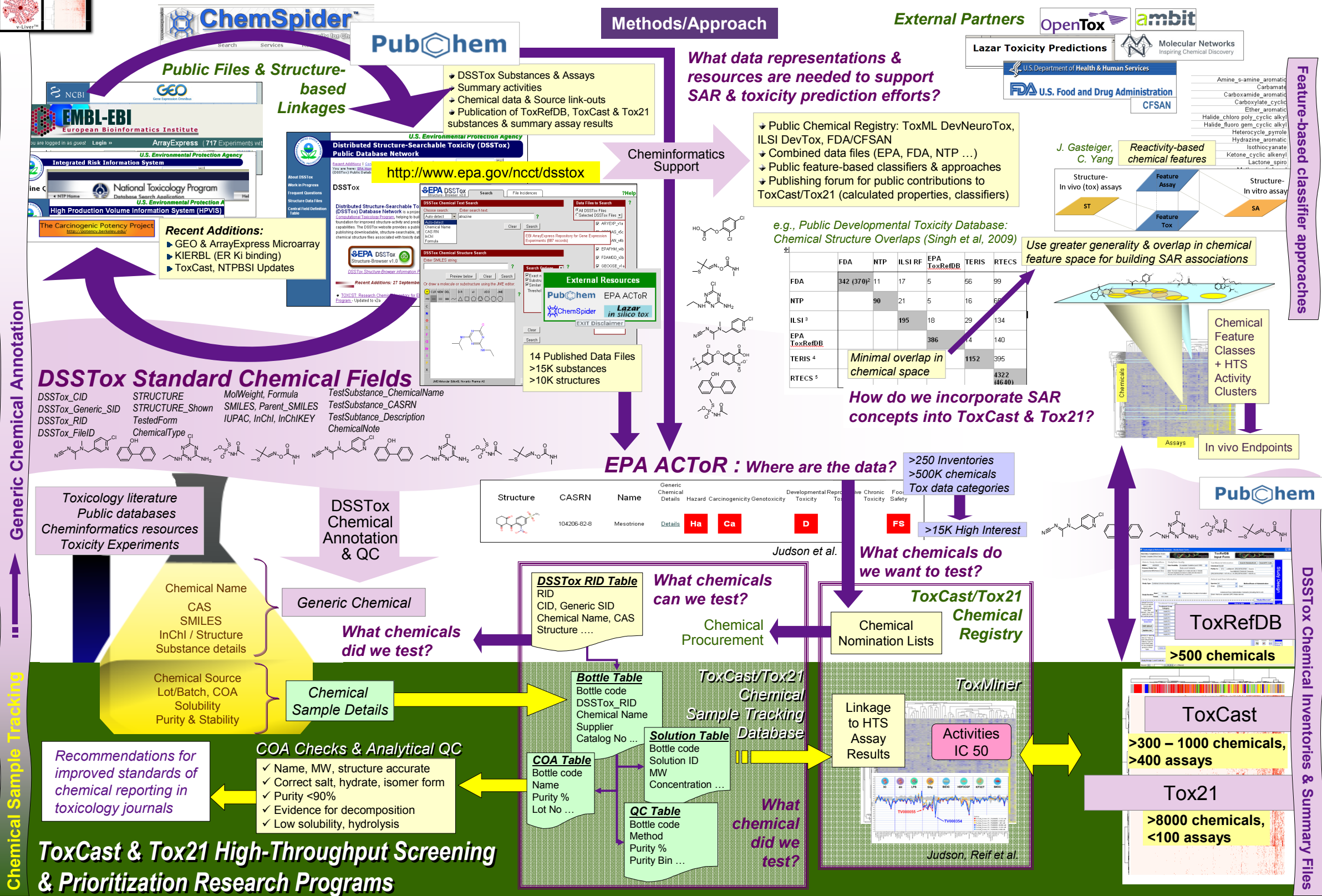
- Generic chemical annotation
- Chemical sample tracking

The DSSTox project is creating a high quality, computable, public toxico-cheminformatics foundation for use in building structure-activity and data mining capabilities. Within NCCT, DSSTox provides primary support of ToxCast and Tox21 test programs through chemical sample tracking and QC, linked to generic chemical inventories. In addition, publicly available, extensible feature-based classifiers are being developed for use in model development. These activities are in support of the broad questions:

- What are key requirements for building a public toxico-cheminformatics capability?
- What are chemical structure-based determinants of toxicological activity?

Research Goals

- To create a high quality public toxico-cheminformatics foundation to facilitate exploration of the structural basis for toxicological activity outcomes.
- To build structure-based linkages of toxicological inventories to and from EPA and external Internet data/application resources.
- To set high standards for chemical reporting and representation in association with new testing programs, ToxCast and Tox21.
- To encourage use of reactivity and feature-based chemical classifier representations, in conjunction with HTS assay data, to build new capabilities for predictive toxicology.



ToxCast & Tox21 High-Throughput Screening & Prioritization Research Programs

UNITED STATES ENVIRONMENTAL PROTECTION AGENCY



COMPUTATIONAL TOXICOLOGY

This poster does not necessarily reflect EPA policy. Mention of trade names or commercial products does not constitute endorsement or recommendation for use.