



ACToR: Aggregated Computational Toxicology Resource

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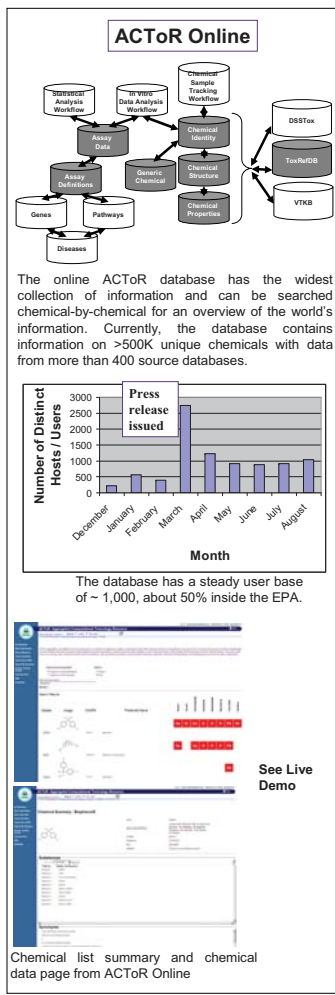
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Science Question

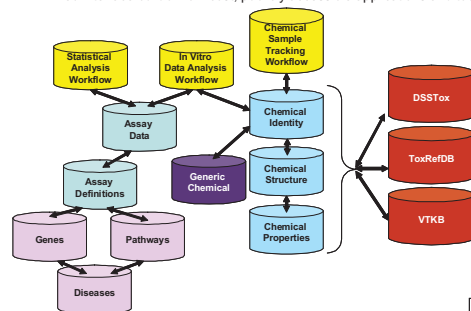
- ACToR was developed to address several needs of the NCCT, the EPA and the broader community of researchers on environmental chemicals:
1. What is the collection of chemicals of most concern to the EPA?
 2. What toxicology, exposure, use, *in vitro* and regulatory information is known for these chemicals?
 3. Can this information be collected in one place to allow easy access by researchers around the world?
 4. Can information on the structure, properties and activity of chemicals be tabulated for use in computational modeling efforts?

Research Goals

ACToR aims to provide a unified, centralized resource of data on environmental chemicals including toxicology, *in vitro* assay data, and chemical structure information. By gathering information on the type and location of toxicity or exposure data associated with environmental chemicals into a single, searchable, publicly accessible web-site, ACToR is providing the basis for chemical selection and screening within NCCT projects, such as ToxCastTM and Tox21. ACToR is also coordinating with the DSSTox project to incorporate quality chemical review and structure-annotation for the chemical data sets of highest interest to the various NCCT projects. In addition to its use in supporting various NCCT and EPA projects, ACToR is a publicly available EPA resource that enables other government agencies, industry, and academic researchers to quickly search and collate toxicity-related information on chemicals of interest. As such, it will promote and encourage other entities to adopt standards for chemical representation and broadly survey chemical information pertaining to toxicology resources on the Internet.

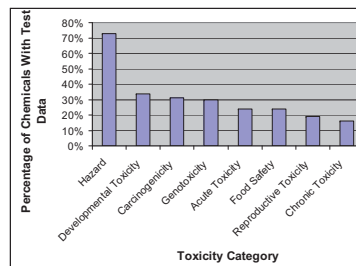


ACToR is a web-based informatics platform, organized at the top level by chemical and chemical structure that is indexing, collecting, and organizing many types of data on environmental chemicals. Environmental chemicals are defined as those likely to be in the environment, including all chemicals regulated or tracked by the EPA, as well as related chemicals, such as pharmaceuticals that find their way into water sources. ACToR is indexing and linking to data from hundreds of sources, including the EPA, FDA, CDC, NIH, academic groups, other governmental agencies (state and national), *in vitro* bioassay data, use levels, exposure information, chemical structure, regulatory information and other descriptive data. Planning for the project began in mid-FY07; beta versions were available inside the EPA since early FY08, and a public version became available in December 2008. ACToR consists of a back-end database and a front-end web interface built on low-cost, publicly accessible applications and tools.

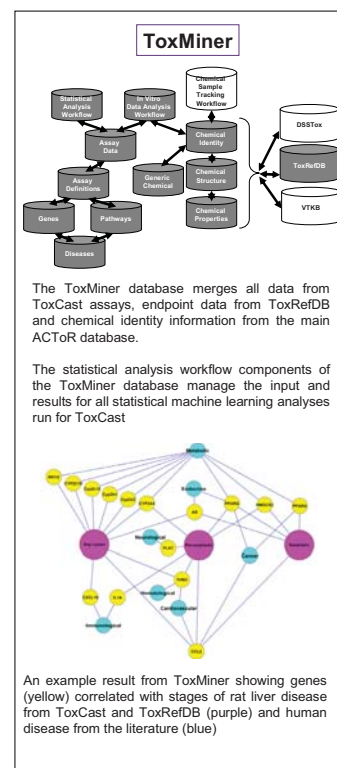
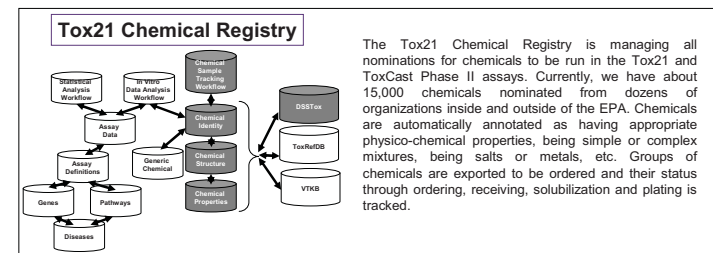


Data Sets currently in ACToR by Number of Chemicals

Chemical	Assay Data	Chemical Structure	Chemical Properties	Genes	Pathways	Diseases
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Summary of toxicity data coverage in ACToR for 17,414 chemicals nominated for the Tox21 program



Results/Conclusions

The ACToR databases have proven to be flexible and scalable enough to handle all of the types of data imported as part of the ACToR and ToxCast projects.

Impact and Outcomes

1. Statistical analysis of ToxCast Phase I has been greatly aided by the organization provided by ToxMiner.
2. ACToR Online is becoming widely used as a source of information on a variety of environmental chemicals.
3. The Tox21 workflow database has enabled us to manage nominations from dozens of organizations and to rationalize the process of selecting thousands of chemicals to push into the Tox21 and ToxCast Phase II assays.

Future Directions

- FY09**
- Initial public deployment.
 - Release of version 2, including refined chemical structure information.
 - Develop workflow for tabularization of data buried in text reports.
 - Integrate all ToxCast and ToxRefDB data.
 - Quarterly releases with new data.
- FY10**
- Quarterly releases with new data.
 - Implementation of a process to gather tabular data on priority chemicals from text reports.
 - Survey sources of chemical use and exposure data and import any remaining sources.
 - Develop flexible query interface and data download process.
 - Develop process to extract data from open literature.

- FY11 and FY12**
- Quarterly releases with new data

References

- R. Judson, A. Richard, D. Dix, K. Houck, F. Eltoumy, M. Martin, T. Cathey, T.R. Transue, R. Spencer, M. Wolf, "ACToR - Aggregated Computational Toxicology Resource", Toxicology and Applied Pharmacology, Vol. 233, 7-13 (2008).
- R. Judson, A. Richard, D.J. Dix, K. Houck, M. Martin, R. Kavlock, V. Dellarco, T. Henry, T. Holderman, P. Sayre, S. Tan, T. Carpenter, E. Smith, "The Toxicity Data Landscape for Environmental Chemicals", Environmental Health Perspectives, Vol. 117, 685 (2008)

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