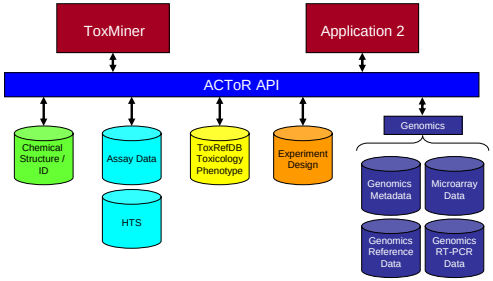
ACToR – Aggregated Computational Toxicology Resource

Richard Judson[1], Ann Richard[1], Matt Martin[1], David Dix[1], Keith Houck[1], Maritja Wolf[2], Tommy Cathey[2] (1) National Center for Computational Toxicology, U.S. EPA (2) Lockheed Martin

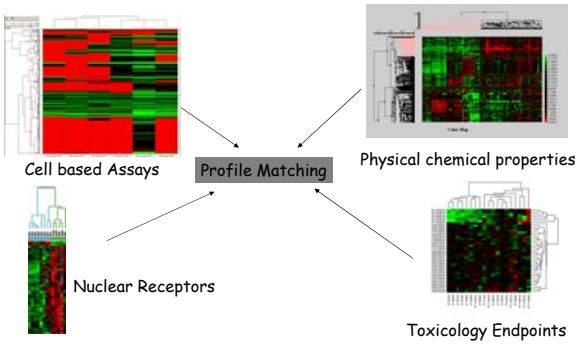
Abstract: One goal of the field of Computational Toxicology is to predict chemical toxicity by combining computer models with biological and toxicological data. To achieve this goal, there is a need for large amounts of diverse, high quality, curated data that is easily accessible by modelers. We are developing the ACToR system (Aggregated Computational Toxicology Resource) to serve as a repository for a variety of types of chemical, biological and toxicological data that can be used for predictive modeling of chemical toxicology. ACToR is comprised of several independent databases, tied together through links to a common database of chemical structures and properties. The main databases cover biochemical (HTS) and cell-based assays, detailed *in vivo* toxicology data (ToxRefDB) , experimental design information, genomics (mainly microarray) data, and reference information on genes and pathways. The system is collecting information from multiple sources both within and external to the EPA. Users will be able to access data through the web, initially on the EPA Intranet. The first use of ACToR will be to provide a repository and context for data from the ToxCast program, whose goal is to use in vitro biochemical and genomics assays to prioritize environmental chemicals for further testing.

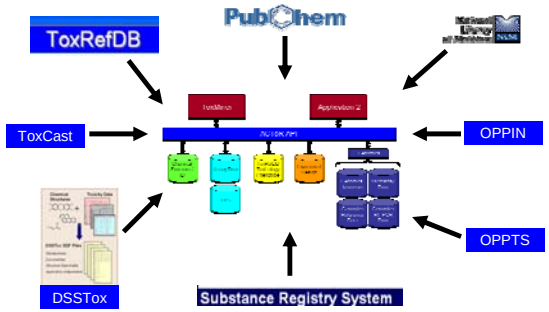


ACToR Goals

- Compile sources of quantitative toxicology data on chemicals of interest to EPA
- Link diverse data sets together based on chemical ID and structure
- Support ToxCast and other research programs at EPA
- Provide easy assess to users of quantitative toxicology data

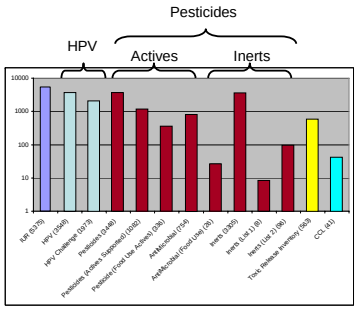
ToxCast Chemical Prioritization Using HTS and Genomics





Example Data Collections in ACToR

- PUBCHEM - PubChem provides information on the biological activities of small molecules.DSSTOX Distributed Structure Searchable Toxicity
  - •CPDBAS -Cancer Potency Database
  - •EPAFHM - EPA Fat Head Minnow Data
  - •FDAMDD - FDA Minimum Daily Dose
  - •IRIS - EPA Integrated Risk Information System
- SRS – EPA Substance registry System
  - •CERCLA - Comprehensive Environmental Response, Compensation, And Liability Act Hazardous Substances
  - •HDDs / HDFs - Dibenzo-para-dioxins/dibenzofurans
  - •IARC - International Agency for Research on Cancer
  - •NTP Chemicals - National Toxicology Program Chemical Health and Safety Data (Other Source)
  - •SIDS - Screening Information Data Set-High Production Volume Chemicals (Other Source)
- California EPA - California EPA list of substances of concern for cancer and developmental defects
- Scorecard - California EPA list of substances of concern for cancer and developmental defects
- KIDB - KI DB - database of Ki values from UNC (PDSP)
- HPV Challenge - The U.S. high production volume (HPV) challenge chemicals
- OPPIN Active - Active pesticide ingredients
- OPPIN Antimicrobials - Active antimicrobial ingredients
- OPPIN Inerts - OPPIN Inert Pesticide Ingredients
- TRI - Tox Release Inventory List



ToxCast Target Chemicals ~11,000