

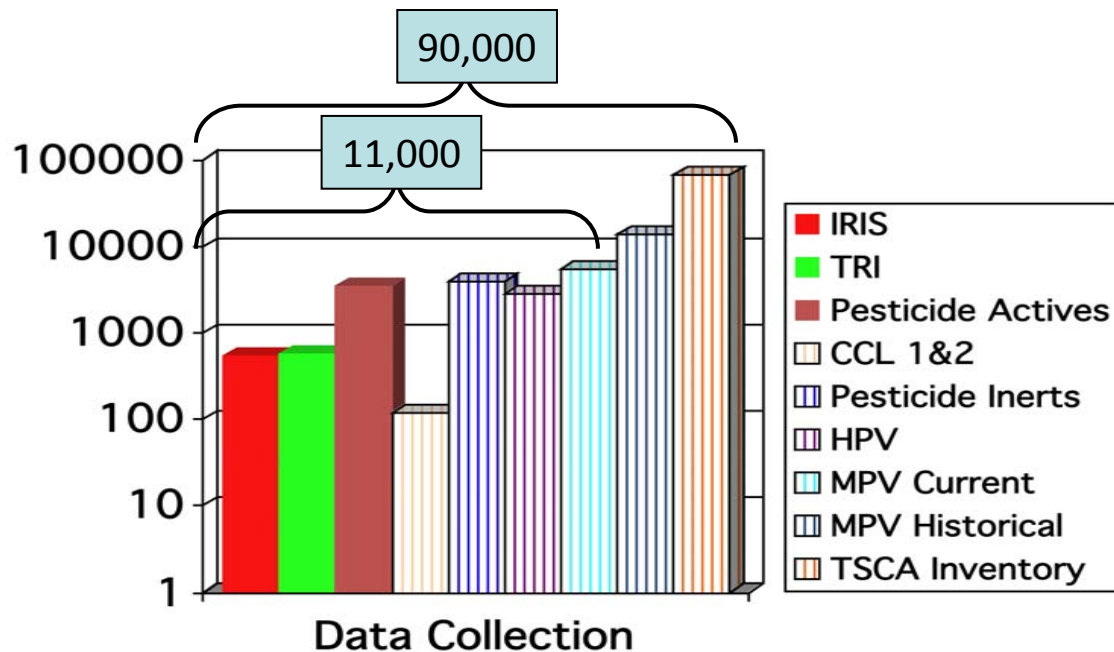
ACToR Aggregated Computational Toxicology Resource

UNITED STATES ENVIRONMENTAL PROTECTION AGENCY

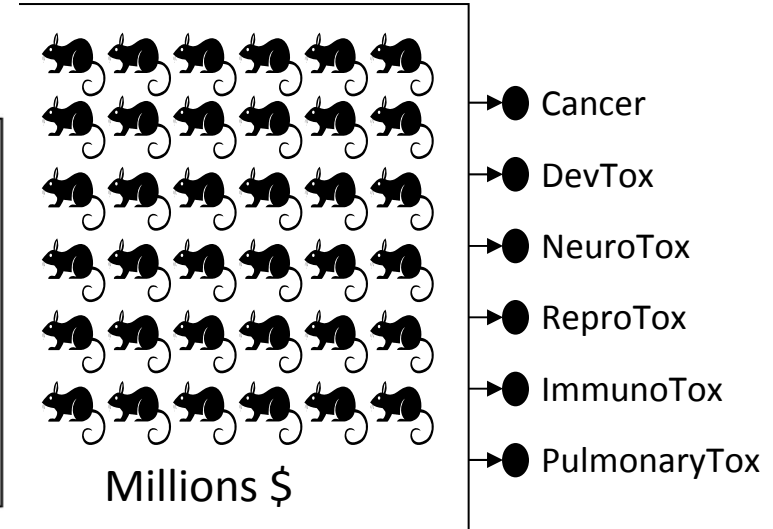


Change Needed Because

Too Many Chemicals

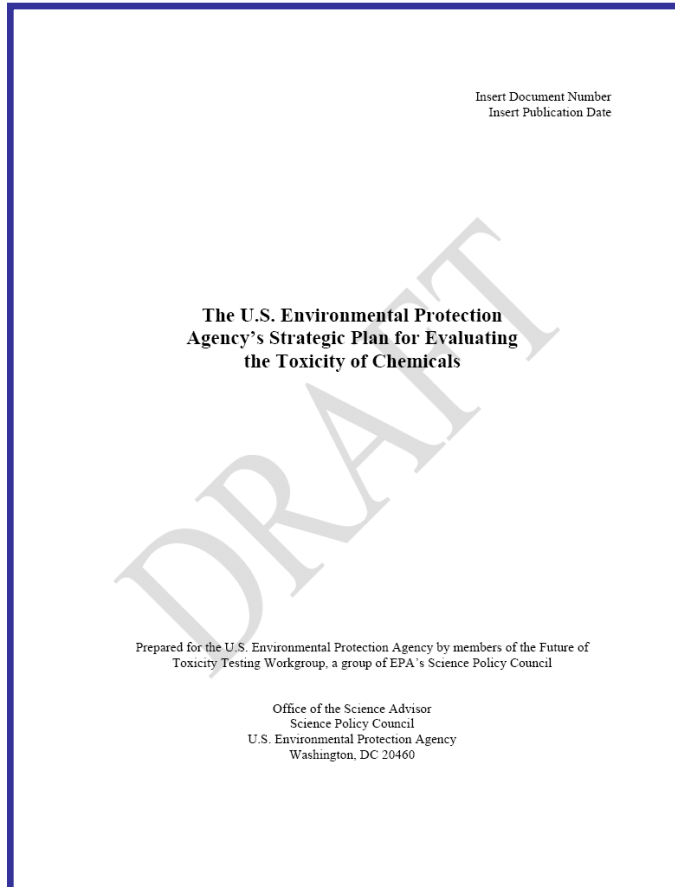


Too High a Cost



...and not enough data.

EPA Reacts to Challenge of the NRC on the Future of Toxicity Testing



Strategic Goals

- Toxicity Pathway ID and Screening
- Toxicity Based Risk Assessment
- Institutional Transition

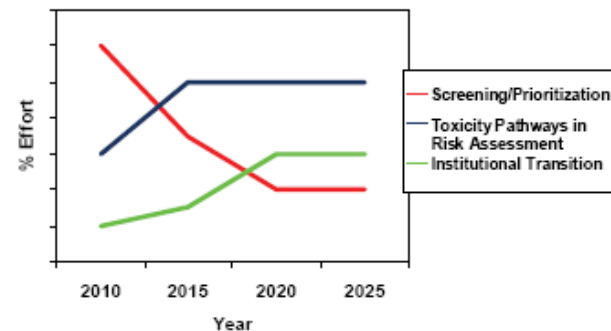


Figure 6. Relative (%) emphasis of the three main components of this strategic plan over its expected 20-year duration.

The Chemical Landscape Project

- What is the unique set of chemicals EPA is most concerned with?
- Targets for the overall ToxCast Program
- How much is known about these chemicals?
- Where are the data gaps?
- Collaboration across EPA
 - ORD, OPP, OPPT, OW, GLNPO, EDSP
- Running this study required building a database
 - Origin of the ACToR project

Summary of Chemical Landscape Analysis

- Total Count: 9,912
- Fraction of chemicals evaluated for specific classes of toxicity:
 - General Hazard (usually acute data) 59%
 - Carcinogenicity 26%
 - Genotoxicity 28%
 - Developmental Toxicity 29%
 - Reproductive Toxicity 11%

EHP Electronic Publication, December 2008

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Data Collection: EPA CCL3

Name: [EPA CCL3 List.pdf](#)

Description: EPA has drinking water regulations for more than 90 contaminants. The Safe Drinking Water Act (SDWA) includes a process that we must follow to identify and list unregulated contaminants which may require a national drinking water regulation in the future. EPA must periodically publish this list of contaminants (called the Contaminant Candidate List or CCL). In February 2008 we announced the draft CCL 3.

ID: 139

Institutional Source: EPA



Source Type: Chemicals

Number of Substances: 93

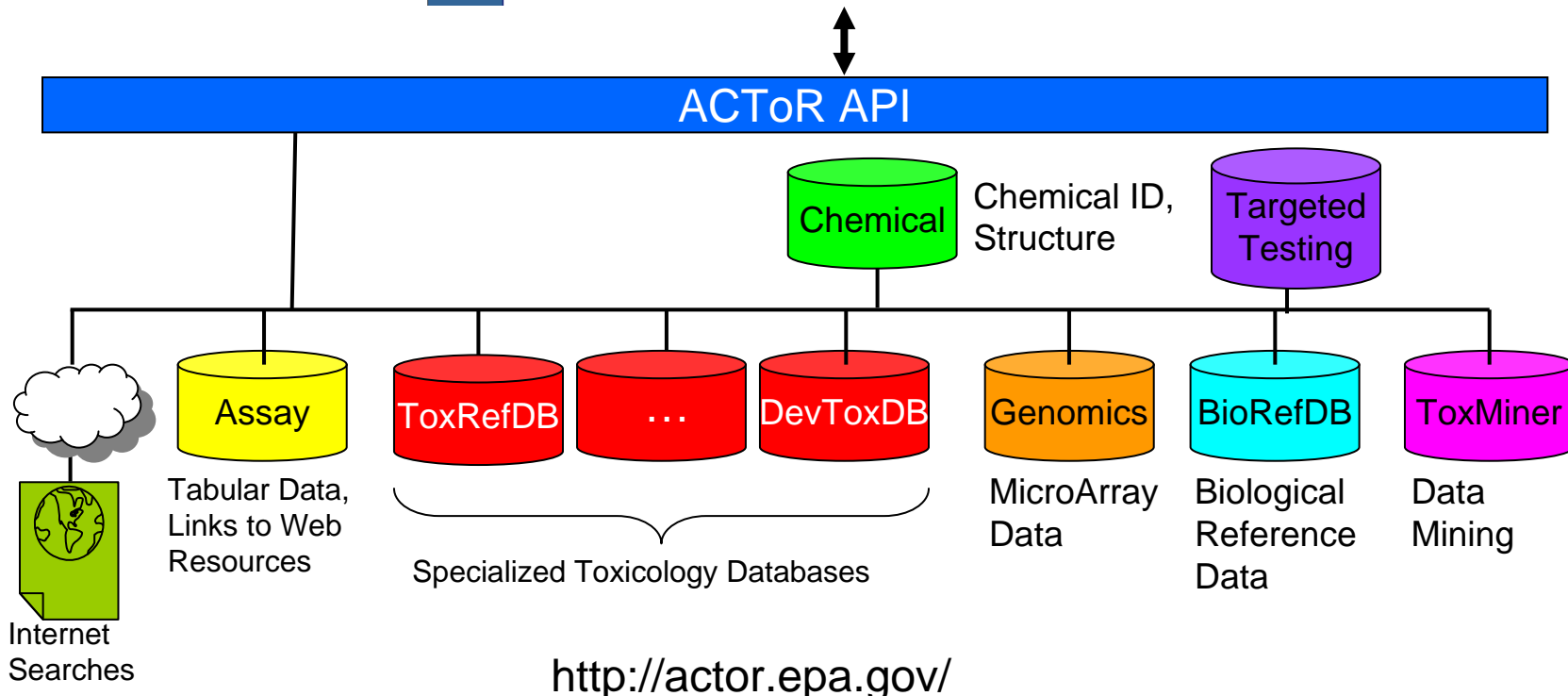
Number of Generic Chemicals: 92

Chemical Table

Page 1 of 2: [List](#)

Structure	Name	CASRN	Generic Chemical Details	Hazard	Genotoxicity	Developmental Toxicity	Reproductive Toxicity	Chronic Toxicity	Food Safety
	1,1,1,2-Tetrachloroethane	630-20-6	Details	Ha	Ca	G	D	R	Cr
	1,1-Dichloroethane	75-34-3	Details	Ha	Ca	G	D	R	Cr

ACToR Web
Browser



ACToR Definitions

- Substance
 - A chemical from one source
 - Name(s), CASRN
 - Source-specific unique ID
 - Assay Data
- Compound
 - Chemical structure from one source
 - Source-specific unique ID
- Generic Chemical
 - CASRN
 - Link to many substance (each with same CASRN)
 - Link to at most one compound
 - Links to all assay data from substances with same CASRN

ACToR Definitions

- Assay
 - A collection of data on one or more substances
 - Comes from one data source
 - Can have several types of data included
 - Looks like an Excel spreadsheet
- Assay Component
 - One column of an assay table
- Assay Result
 - A data value for one substance and one assay component

- Assay Phenotype
 - Type of disease associated with the assay
 - Carcinogenicity, GeneTox, ...
- Assay Category
 - Type of data: tabular, links to the web, human exposure
 - Allows assays to be grouped together
- Data Collection
 - A source of data
 - Substances
 - Compounds
 - Assays

Main Data Views

- Search by names, CASRN, Structure
- View lists of chemicals
- View lists of assays
- View list of assay collections
- View data associated with a generic chemical

Chemical List View

Data Collection | ACToR | US EPA - Windows Internet Explorer provided by EPA

http://actor.epa.gov/actor/faces/DataCollectionSummary.jsp

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Data Collection : NTP Nominations

Name: NTP Nominations
[EXIT Disclaimer](#) [Link Out](#)
 Description: Substances Nominated for testing from 2000 to current. Formal process for nomination and selection; most interest in chemicals of high concern or where data gaps exist.
 ID: 221
 Institutional Source: NTP
 Source Type: Chemicals+URLs
 Number of Substances: 150
 Number of Generic Chemicals: 145

[Hide Chemical Table](#)

Structure	CASRN	Name	Generic	Hazard	Carcinogenicity	Genotoxicity	Developmental	Reproductive	Chronic	Food Safety
	6425-39-4	Morpholine, 4,4'-[oxydi(2,1-ethanediyl)]bis-	Details	Ha						
	5466-77-3	2-Ethylhexyl p-methoxycinnamate	Details	Ha	Ca	G				
	4246-51-9	1-Propanamine, 3,3'-[oxybis(2,1-ethanediyl)oxy]bis-	Details	Ha						
	504-29-0	2-Aminopyridine	Details	Ha	Ca	G			R	

Previous 1-10 of 149 Next 10

Red box indicates that data is available for that phenotype, not that chemical causes that phenotype

Statistics

Category	Count
Data Collections	261
Substances	1,578,922
Compounds	955,016
Generic Chemicals	531,517
Generic Chemicals with Structure	418,191
Assays	1,357
Assay Components	3,910
Assay Results	3,553,507

What's Next?

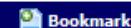
- More Data Collections
 - Development version >400
 - Current Focus on exposure / biomonitoring / food residues
- ToxRefDB
 - Compiling tabular information from guideline studies
 - EPA
 - NTP
 - Literature
- Cleanup of chemical structures
- Enhance generic chemical page

ToxRefDB

- Relational phenotypic/toxicity database
- Provides in vivo anchor for ToxCast predictions
- Three study types
 - Chronic/Cancer rat and mouse (Martin, et al, EHP 2008)
 - Rat multigenerational Reproduction (Martin, et al, submitted)
 - Rat & Rabbit developmental (Knudsen, et al, internal review)
- Two types of synthesis
 - Supervised (common individual phenotypes)
 - Unsupervised (machine based clustering of phenotype patterns)



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ToxRefDB Program Toxicology Reference Database

ToxRefDB was developed by the National Center for Computational Toxicology (NCCT) in partnership with EPA's Office of Pesticide Programs (OPP), to store data from in vivo animal toxicity studies. The initial focus was populating ToxRefDB with pesticide registration toxicity data that has been historically stored as hard-copy and scanned documents by OPP. A significant portion of these data have now been processed into ToxRefDB in a standardized and structured format. ToxRefDB currently includes chronic, cancer, sub-chronic, developmental, and reproductive studies on hundreds of chemicals, many of which are pesticide active ingredients. These data are now accessible and computable within ToxRefDB, and are serving as reference toxicity data for ORD research and OPP retrospective analyses. The primary research application of ToxRefDB is to provide toxicity endpoints for the development of ToxCast™ predictive signatures.

Data Set	Description	Download	Publication
Data Entry Tool & Controlled Vocabulary	The Data Entry Tool provided the user interface for all initial data input into ToxRefDB. The controlled vocabulary standardized the capturing of regulatory animal toxicity studies performed across various study types.	Download (15.5 MB, ZIP)	Martin et al. (2008) " Profiling Chemicals Based on Chronic Toxicity Results from the U.S. EPA ToxRef Database " Environmental Health Perspectives doi:10.1289/ehp.0800074
Chronic & Cancer Endpoints	Based on incidence, severity and potency, 26 primarily tissue-specific pathology endpoints were selected to uniformly classify 310 chemicals included in the manuscript's analysis. The 310 chemicals in this analysis largely overlap with the 320 ToxCast Phase I chemicals.	Download (2.7 MB, XLS)	Martin et al. (2008) " Profiling Chemicals Based on Chronic Toxicity Results from the U.S. EPA ToxRef Database " Environmental Health Perspectives doi:10.1289/ehp.0800074

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Last updated on Tuesday, October 21st, 2008.
<http://www.epa.gov/ncct/toxrefdb/>
[Print As-Is](#)

ToxRefDB website: <http://www.epa.gov/ncct/toxrefdb/>

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http://actor.epa.gov/actor/faces/ACToRHome.jsp

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ACToR (Aggregated Computational Toxicology Resource) is a collection of databases collated or developed by the US EPA National Center for Computational Toxicology (NCCT). More than 200 sources of publicly available data on environmental chemicals have been brought together and made searchable by chemical name and other identifiers, and by chemical structure. Data includes chemical structure, physico-chemical values, in vitro assay data and in vivo toxicology data. Chemicals include, but are not limited to, high and medium production volume industrial chemicals, pesticides (active and inert ingredients), and potential ground and drinking water contaminants.

Chemical Name Parameters Match by:

☒ Search on Chemical Names ☐ Exact

☐ Search on CAS Numbers ☒ Any

Enter Chemical Name:

Search

Structure CASRN Name

No Rows Yet

ACToR News

Date	Item
December 1, 2009	ACToR is ready for initial release
December 1, 2009	New data released from ToxRefDB: http://www.epa.gov/ncct/toxrefdb

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Last updated on Wednesday, April 1st, 2009
http://actor.epa.gov/actor/faces/ACToRHome.jsp
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