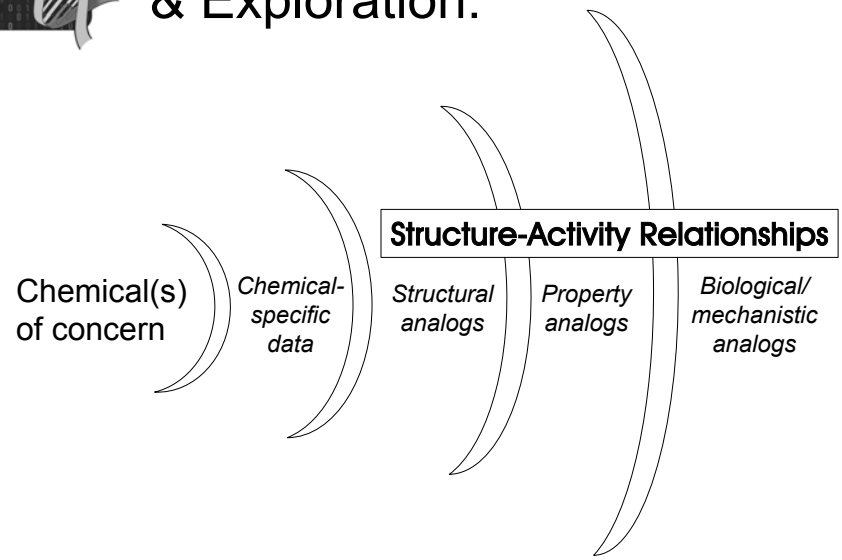
DSSTox Public Toxicity Database Network:

Progress Report and New Initiatives to Expand Chemoinformatic Capabilities

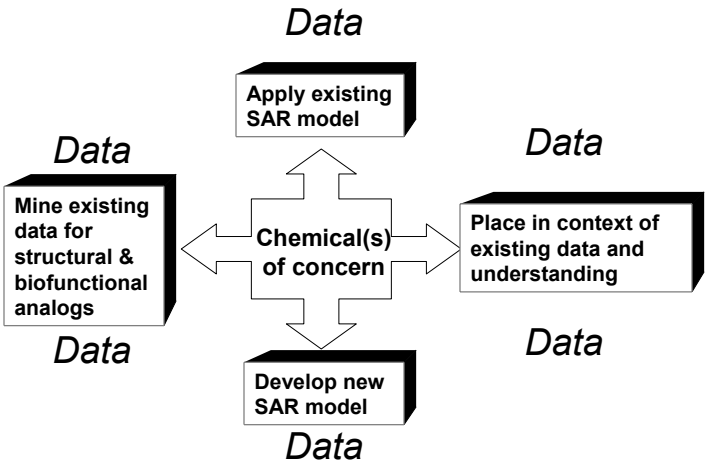
Ann Richard

Environmental Carcinogenesis Division
National Health & Environmental Effects Research Lab
US Environmental Protection Agency

Chemistry-based Data Mining & Exploration:

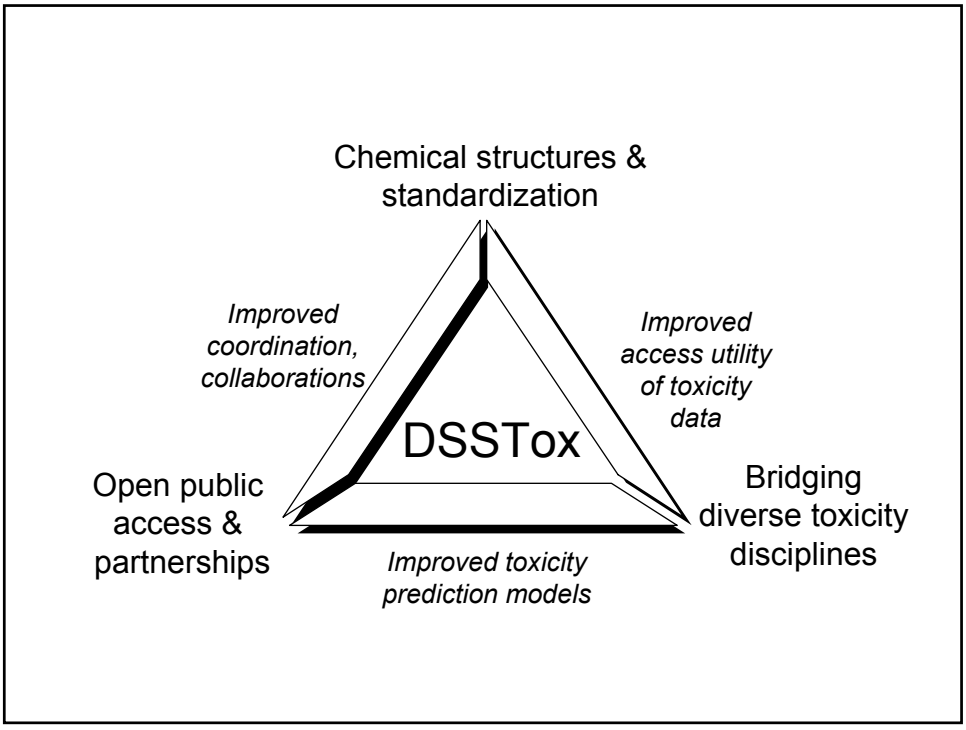


Structure-based Screening & Prioritization:



Limitations of Public Toxicity Data for Use in SAR:

- Scattered sources
- Non-standard formats
- Diverse information content
- Lack of chemical structure annotation
- Cannot access full database



http://www.epa.gov/nheerl/dsstox

U.S. Environmental Protection Agency

Distributed Structure-Searchable Toxicity (DSSTox) Public Database Network

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- Work in Progress
- Frequent Questions
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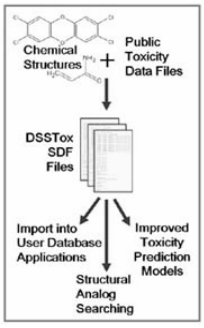
- Central Field Definition Table
- Apps, Tools & More
- DSSTox Community
- Site Map
- Glossary of Terms
- Help

The Distributed Structure-Searchable Toxicity (DSSTox) Database Network provides a community forum for publishing standard format, structure-annotated chemical toxicity data files for open public access. Project goals are to:

- Encourage use of DSSTox Standard Chemical Structure Fields and SDF standard format files for publishing chemical toxicity databases;
- Coordinate with outside public efforts to encourage chemical structure annotation, data standardization, and open public access to toxicity databases;
- Involve the user community in the effort to migrate more public toxicity data into the DSSTox standardized format for publishing;
- Provide full, open access to toxicity data files for structure-analog searching and for facilitating development of improved models for predicting toxicity based on chemical structure.

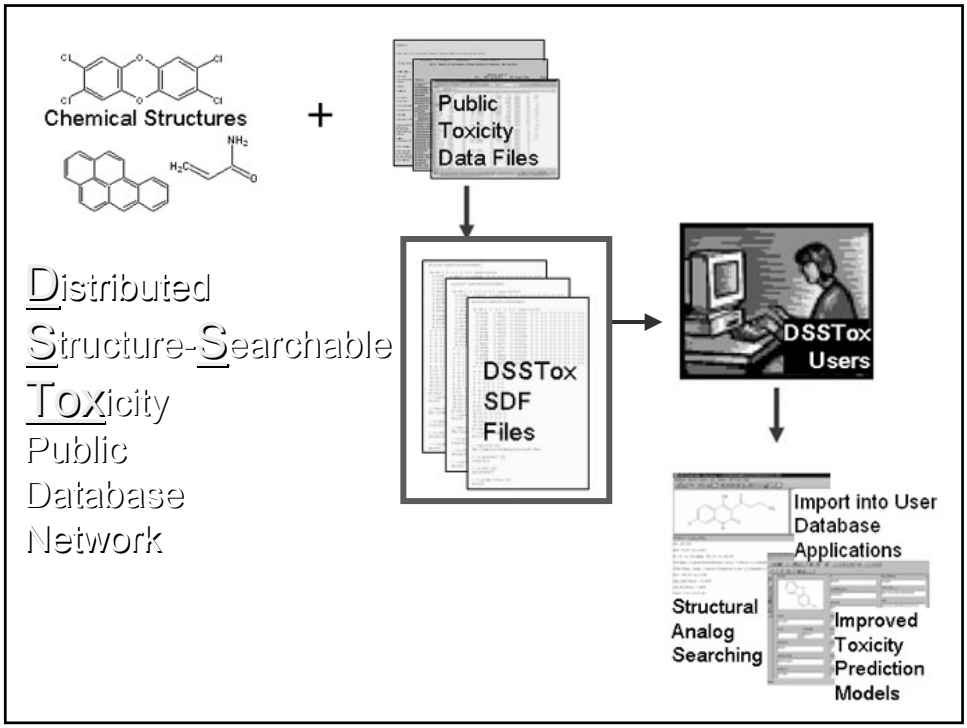
Distributed: Decentralized set of standardized, field-delimited databases, each separately authored and maintained, that are able to accommodate diverse chemical toxicity data content;
Structure-Searchable: Standard format (SDF) structure-data files that can be readily imported into available Chemical Relational Databases and structure-searched;
Tox: Toxicity data as it exists in widely disparate forms in current public databases, spanning diverse toxicity endpoints, test systems, levels of biological content, degrees of summarization, and information content.

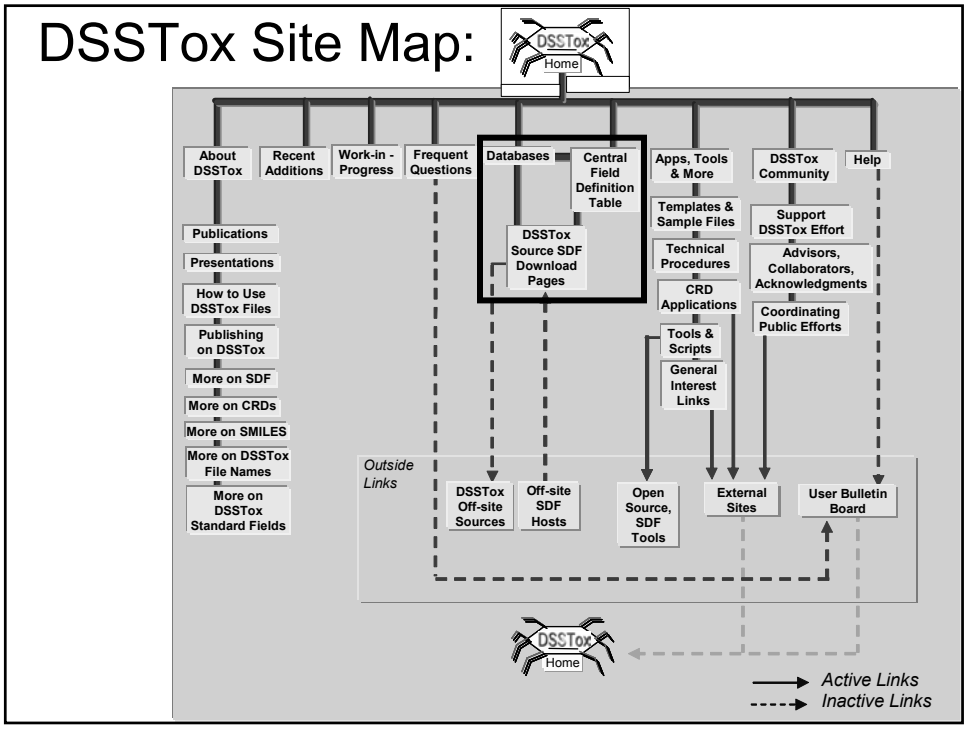


DSSTox Graphic Flowchart

Current Database Offerings:
CPDBRM,CPDBHA,CPDBDG,CPDBPR*
DBPCAN
EPAFHM
NCTRER

* CPDBPR last updated 29Mar04


Chemical Structures
+
Public
Toxicity
Data Files
Distributed
Structure-Searchable
Toxicity
Public
Database
Network
DSSTox
SDF
Files
DSSTox
Users
Import into User
Database
Applications
Structural
Analog
Searching
Improved
Toxicity
Prediction
Models


DSSTox Site Map:
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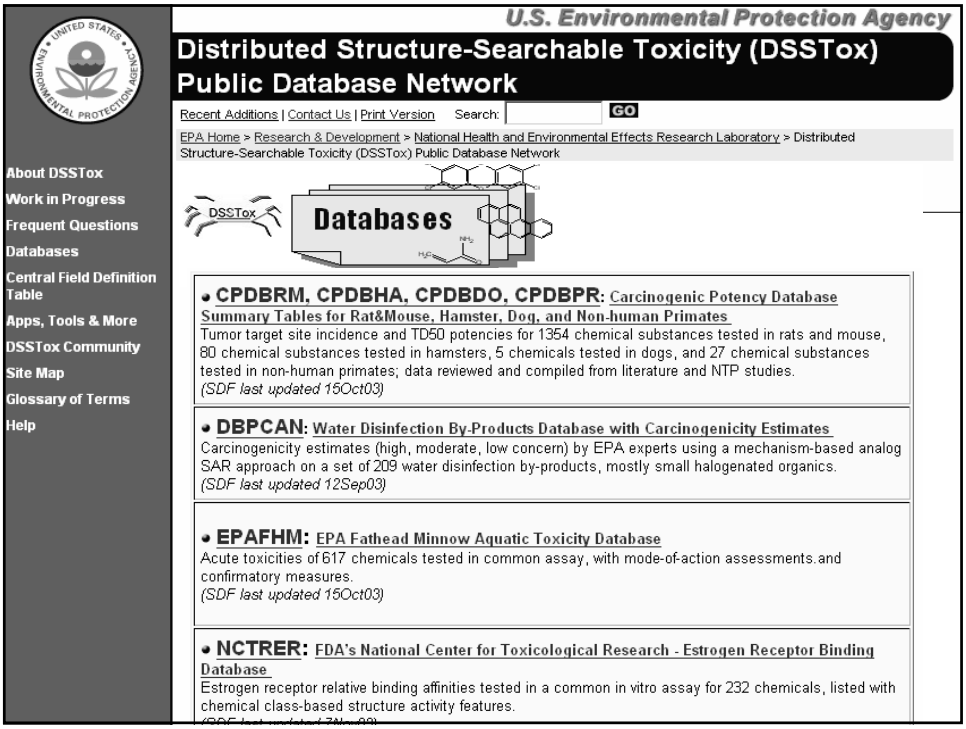
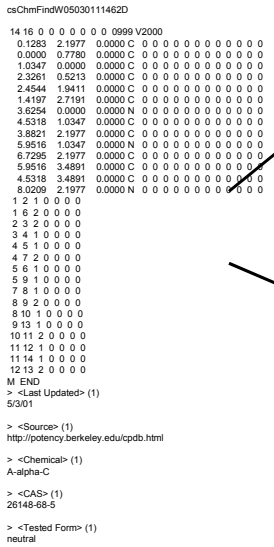
More on SDF
More on CRDs
More on SMILES
More on DSSTox File Names
More on DSSTox Standard Fields
DSSTox Source SDF Download Pages
Templates & Sample Files
Technical Procedures
CRD Applications
Tools & Scripts
General Interest Links
Support DSSTox Effort
Advisors, Collaborators, Acknowledgments
Coordinating Public Efforts
Outside Links
DSSTox Off-site Sources
Off-site SDF Hosts
Open Source, SDF Tools
External Sites
User Bulletin Board
DSSTox
Home
Active Links
Inactive Links



DSSTox Toxicity Database Standards:

- Data file format (SDF)
- File naming convention
- Chemical structure information fields
- Documentation requirements
- Publishing requirements

DSSTox SDF files



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   0.0000   0.7780   0.0000 C  0  0  0  0  0  0  0  0  0  0  0  0
   1.0347   0.0000   0.0000 C  0  0  0  0  0  0  0  0  0  0  0  0
   2.3261   0.5213   0.0000 C  0  0  0  0  0  0  0  0  0  0  0  0
   2.4544   1.9411   0.0000 C  0  0  0  0  0  0  0  0  0  0  0  0
   1.4197   2.7191   0.0000 C  0  0  0  0  0  0  0  0  0  0  0  0
   3.6254   0.0000   0.0000 N  0  0  0  0  0  0  0  0  0  0  0  0
   4.5318   1.0347   0.0000 C  0  0  0  0  0  0  0  0  0  0  0  0
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   5.9516   1.0347   0.0000 N  0  0  0  0  0  0  0  0  0  0  0  0
   6.7295   2.1977   0.0000 C  0  0  0  0  0  0  0  0  0  0  0  0
   5.9516   3.4891   0.0000 C  0  0  0  0  0  0  0  0  0  0  0  0
   4.5318   3.4891   0.0000 C  0  0  0  0  0  0  0  0  0  0  0  0
   8.0209   2.1977   0.0000 N  0  0  0  0  0  0  0  0  0  0  0  0
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  1  6  2  0  0  0  0
  2  3  2  0  0  0  0
  3  4  1  0  0  0  0
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  4  7  2  0  0  0  0
  5  6  1  0  0  0  0
  5  9  1  0  0  0  0
  7  8  1  0  0  0  0
  8  9  2  0  0  0  0
  8 10  1  0  0  0  0
  9 13  1  0  0  0  0
 10 11  2  0  0  0  0
 11 12  1  0  0  0  0
 11 14  1  0  0  0  0
 12 13  2  0  0  0  0
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5/3/01

>  <Source> (1)
http://potency.berkeley.edu/cpdb.html

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>  <CAS> (1)
26148-68-5

>  <Tested Form> (1)
neutral
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SAR Model Development "Training Sets"

- improved predictive tox models
- more comparable models
- dramatically lowered barriers to use

Chemical Relational Database:

sub-structure, text, property searching

- analog searches
- search across diverse toxicity endpoints
- search across chemical and toxicity fields

DSSTox File Naming Standard:

EPAFHM_v1a_617_15Oct03.sdf (.xls)

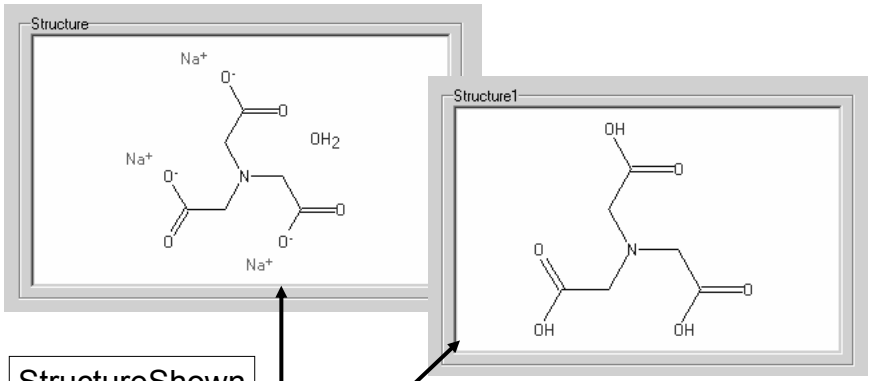
- *6 letter NAMEID*
- *Number of records*
- *Date of last modification*
- *File type*

version 1: major modifications or data additions

revision a: error corrections, minor additions

DSSTox Standard Chemical Fields:

- Structure — *2D chemical structure*
- StructureShown — *Description of displayed 2D structure*
  - ***tested form, simplified to parent, predicted form, active ingredient of formulation, general form***
- Formula — *Empirical molecular formula*
- MolWeight — *Molecular weight in atomic units*
- CAS — *Chem Abstracts Service No. for StructureShown*
- SMILES — *Linear text notation for 2D StructureShown*
- DSSTox_ID — *Counter allows unique identification of record*
- DSSTox_FileName — *Name of file included in each record*
- ChemName — *Chemical name from original data base*
- SubstanceType — *Broad substance classification*
  - ***defined organic, inorganic, organometallic, polymer, mixture or unknown***
- TestedForm — *Tested form of chemical*
  - ***parent, salt, complex, unknown or multiple forms***
- AddToParent — *Salt counterions or complexed moieties*
- CAS_TestedForm — *CAS No. for tested form of chemical*
- SMILES_TestedForm — *SMILES code for the tested form of the chemical*
- ChemNote — *Additional qualifier info for chemical fields*
  - ***defined mixture characteristics, uncertainty in structure or CAS, stereochem, replicate, etc.***
- ChemCount — *Counter for structure or CAS duplications in db*

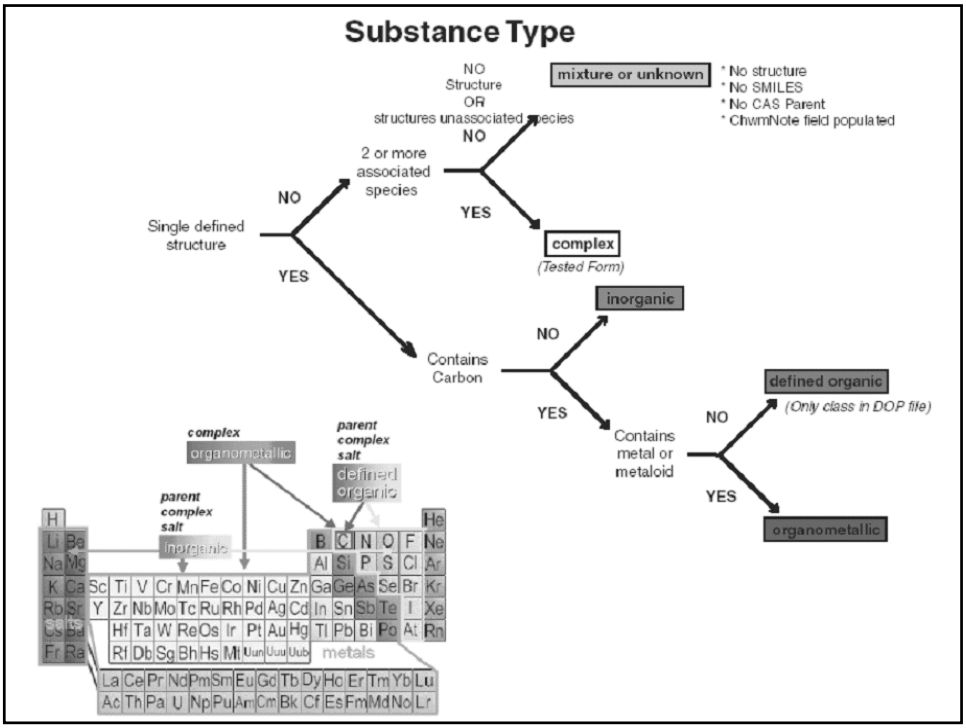


StructureShown

Tested form
Simplified to parent
General form
Active ingredient of formulation
Monomer of polymeric form

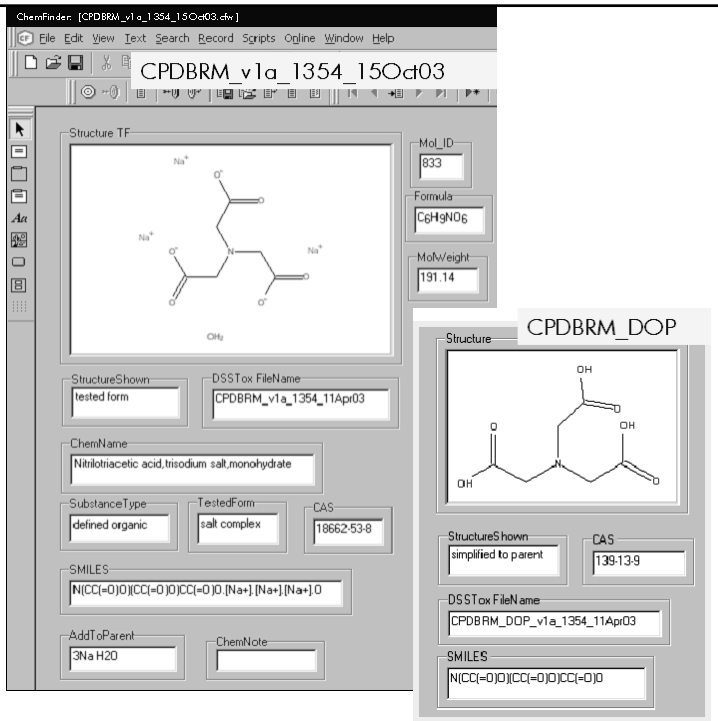
Linked-content fields

CAS
SMILES
Formula
MolWt



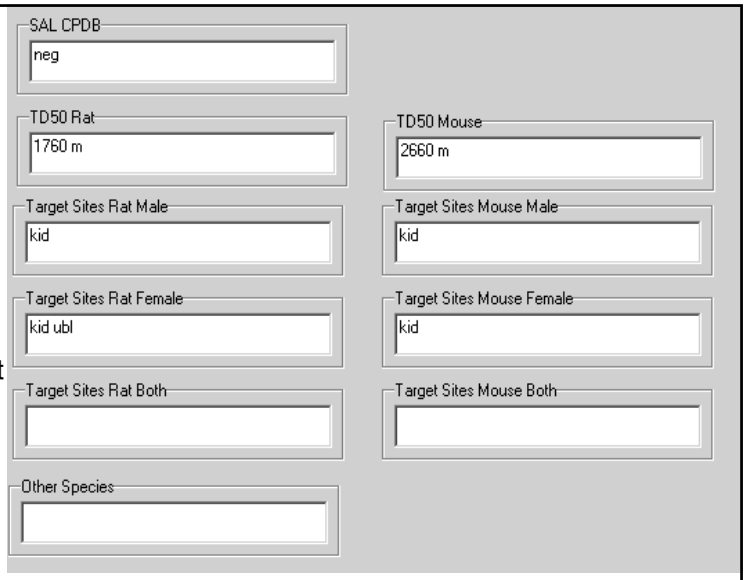
DSSTox Standard Chemical Fields:

CambridgeSoft ChemFinder Application view after SDF import



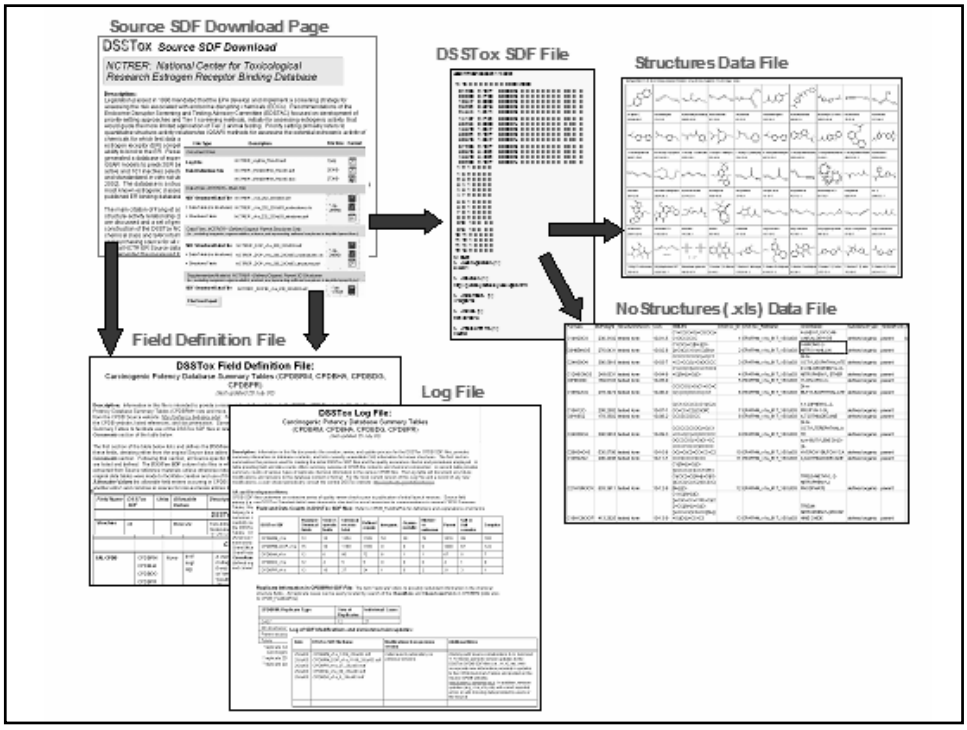
DSSTox Source-Specific Fields:

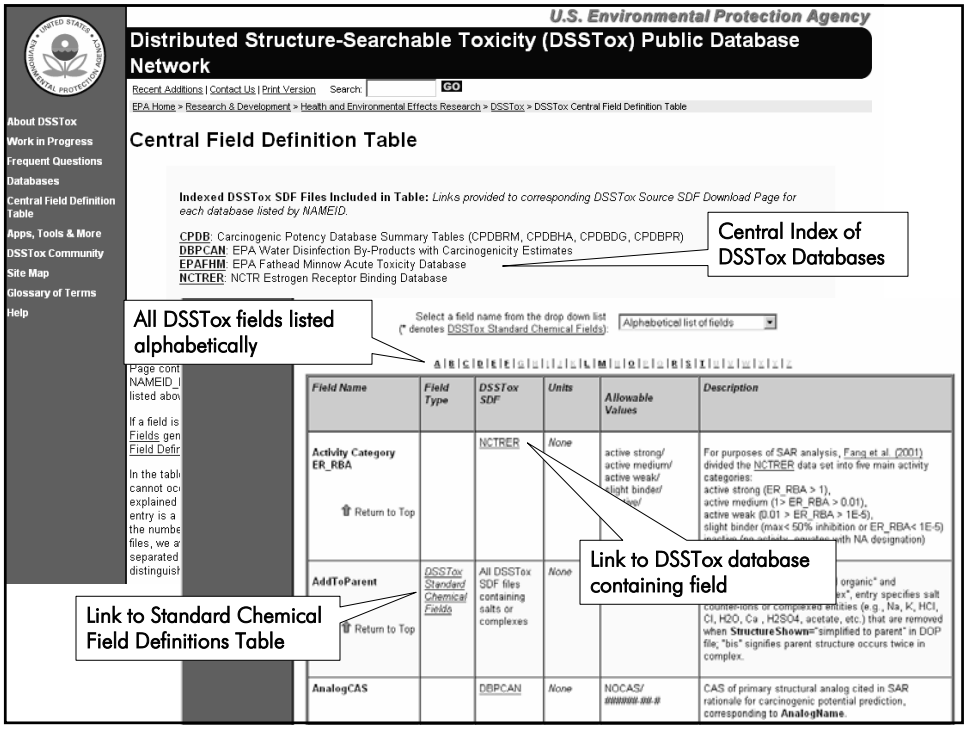
CambridgeSoft ChemFinder Application view after SDF import



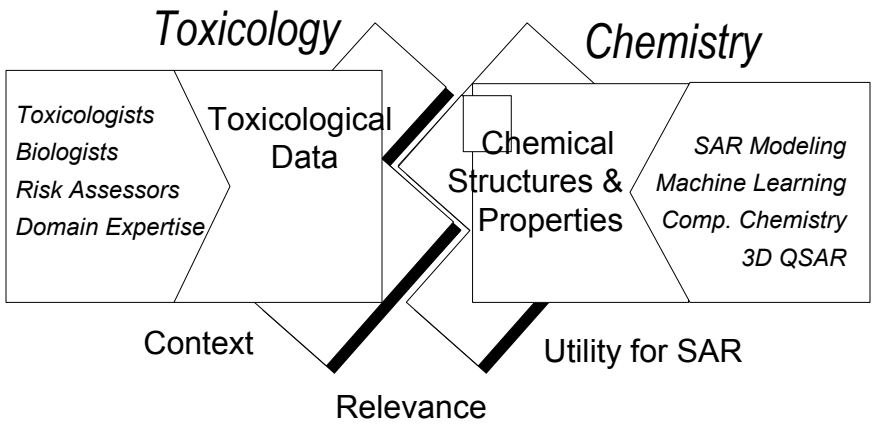
CPDBRM_v1a_1354_15Oct03

CPDBRM_DOP_v1a_1354_15Oct03





DSSTox Database Design:



Integrating Diverse Databases from a Chemical Structure Perspective:

CPDB DBPCAN EPAFHM NCTRER ….

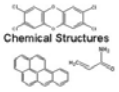
Standard Chemical Fields

Standard Tox Fields: *species, sex, strain, assay, dose*

CPDB	DBPCAN	EPAFHM	NCTRER
SAL CPDB	ChemClass DBP	ChemClass FHM	NCTRlogRBA
TD50 Rat	Concern Level	MOA	ER RBA
TD50Mouse	Rationale	MOACONF	ChemClass ERB
Target Sites Rat Male	Rational Source	CLOGP	Activity Group ERB
Target Sites Rat Female	Analog ChemName	LC50	Rationale ChemClass ERB
Target Sites Mouse Male	AnalogCAS	LC50NOTE	MeanChem Class ERB RBA
….	AnalogSMILES	LC50RATIO	LogP
Other Species		MIXMOA	F1, F2, …F6
		TOXINDEX	
		FATS	
		BEHAVIOR	

DSSTox Project Feasibility:

Direct Benefits to Data Source Collaborators



Chemical structure annotation
Construct standardized DSSTox data file

\+ Source Tox DB_i

Main-author of DSSTox "publication"
Reach audience of potential users/collaborators
Control presentation of data

DSSTox Toxicity Data Files

DSSTox DBs

DB_i DB1 DB2 DB3 DB4 DB5 DB6 DB7

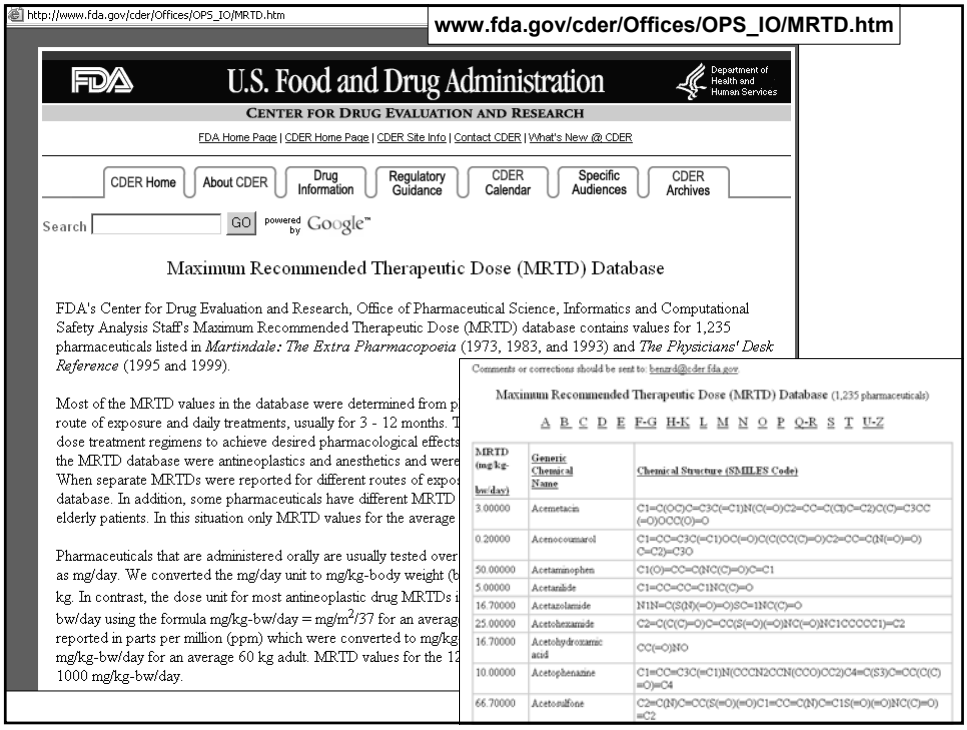
DSSTox Standard Chemical Fields

Source DB can now be linked with DSSTox DB library and structure searched.

Migrate More Public Toxicity Data into DSSTox Standard Format: Phase II, III, …

- FDA Max Recommended Therapeutic Dose - Pharmaceuticals
- NCTR Androgen, Thyroid, and Endocrine Disruption Databases
- NTP Immunotox battery tests

- NTP Rodent carcinogenicity bioassays, subchronic bioassays, developmental, repro, immuno, etc.
- UniLever Skin Sensitization database
- DNA Intercalators Database
- EPA's High Production Volume (HPV) chemicals structure index file
- EPA's Integrated Risk Information System (IRIS) structure index file
- ICVAM databases on LD50, skin sensitization, local lymph node assay, skin corrosivity, endocrine disruption, etc
- EPA pesticide ecotoxicity database
- Developmental toxicity database (literature – FDA,TOPKAT)

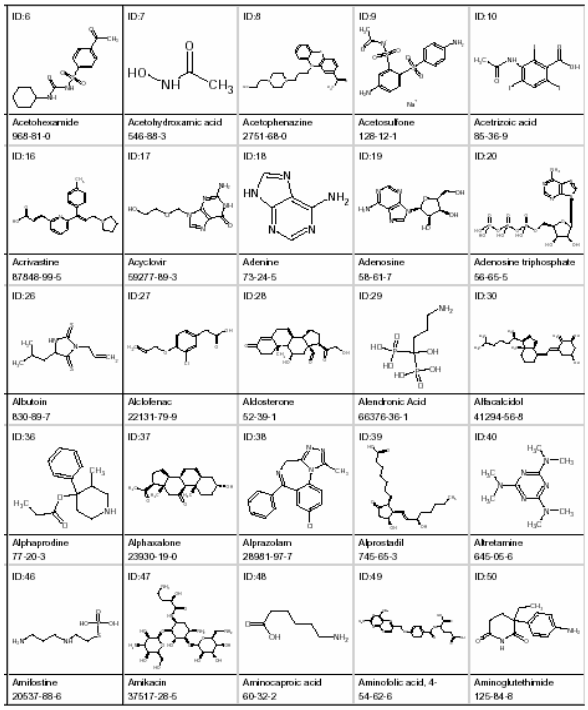


FDAMDD:

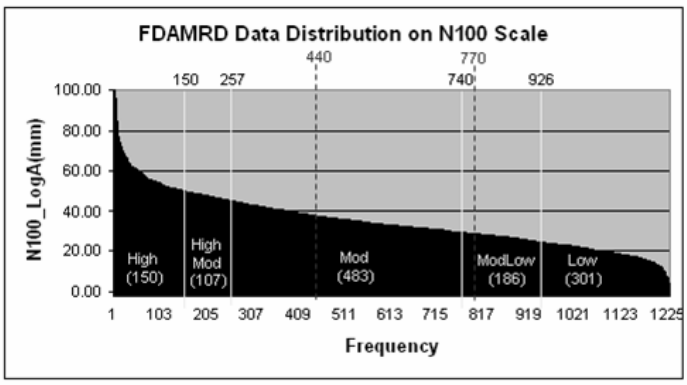
FDA's Maximum Daily (recommended therapeutic) Dose Database

✓*1227 chemicals*
✓ *2173 CAS identified*

- CAS_Other
- SMILES_nostereo
- SMILES_stereo
- StudyType
- Species
- Endpoint
- Therap_Cat
- Dose_MRDD_mg
- Dose_MRDD_mm
- LOG10_MRDD_mm
- N100_MRDD_mm
- Activity_Category



FDAMDD:
Distribution of N100_MRDD_mm values and Activity_Category cutoffs for 1227 chemicals

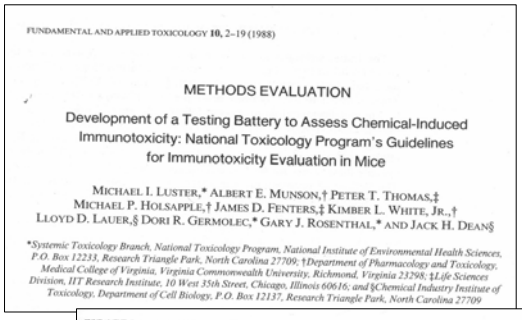


N100 Scale:
High (100-50)
HighMod (50-45)
Mod (45-30)
ModLow (30-25)
Low (25-0)

MCASE (approx):
High (100-37.8)
Mod (37.8-29.3)
Low (29.3-0)

NTPIMT: National Toxicology Program Immunotox Battery

- 50 chemicals
- 12 immunotox measures
- comparison to rodent carcinogenicity response



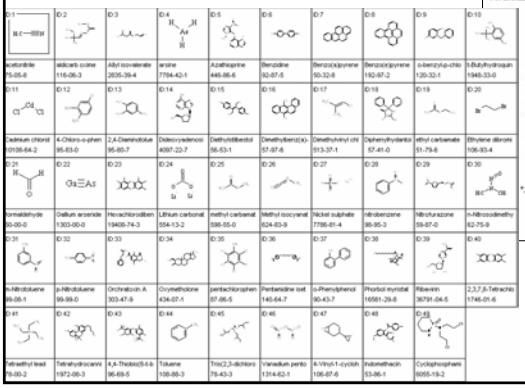
FUNDAMENTAL AND APPLIED TOXICOLOGY **10**, 2–19 (1988)

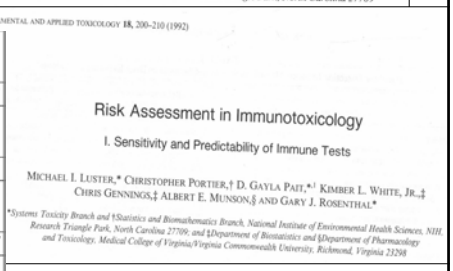
METHODS EVALUATION

Development of a Testing Battery to Assess Chemical-Induced Immunotoxicity: National Toxicology Program's Guidelines for Immunotoxicity Evaluation in Mice

MICHAEL I. LUSTER,* ALBERT E. MUNSON,† PETER T. THOMAS,‡ MICHAEL P. HOLSAPPLE,† JAMES D. FENTERS,‡ KIMBER L. WHITE, JR.,† LLOYD D. LAUER,§ DORI R. GERMOLEC,* GARY J. ROSENTHAL,* AND JACK H. DEAN§

*Systemic Toxicology Branch, National Toxicology Program, National Institute of Environmental Health Sciences, P.O. Box 12233, Research Triangle Park, North Carolina 27709; †Department of Pharmacology and Toxicology, Medical College of Virginia, Virginia Commonwealth University, Richmond, Virginia 23298; ‡Life Sciences Division, IIT Research Institute, 10 West 35th Street, Chicago, Illinois 60616; and §Chemical Industry Institute of Toxicology, Department of Cell Biology, P.O. Box 12137, Research Triangle Park, North Carolina 27709





FUNDAMENTAL AND APPLIED TOXICOLOGY **18**, 200–210 (1992)

Risk Assessment in Immunotoxicology

I. Sensitivity and Predictability of Immune Tests

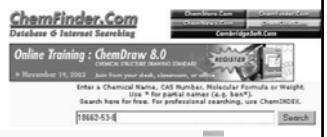
MICHAEL I. LUSTER,* CHRISTOPHER PORTIER,† D. GAYLA PAIT,*,‡ KIMBER L. WHITE, JR.,‡ CHRIS GENNINGS,‡ ALBERT E. MUNSON,§ AND GARY J. ROSENTHAL*

*Systems Toxicity Branch and †Statistics and Biomathematics Branch, National Institute of Environmental Health Sciences, NIH, Research Triangle Park, North Carolina 27709; and ‡Department of Biostatistics and §Department of Pharmacology and Toxicology, Medical College of Virginia/Virginia Commonwealth University, Richmond, Virginia 23298

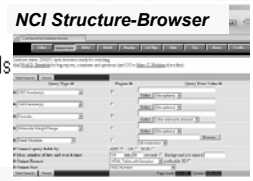
Coordinating Public Efforts:

DSSTox COMMUNITY

- ACD/Labs (Advanced Chemistry Development) ChemFolder Public Databases
- Cambridge-Soft's ChemFinder.Com Chemical Search Website
- FDA (Food & Drug Administration) Center for Drug Evaluation & Research
- ILSI (International Life Sciences Institute) SAR Toxicity Database Project, in collaboration with LHASA, Lmt.LIST (LeadScope In Silico Tox) Focus Group
- LIST (LeadScope In Silico Tox) Focus Group
- MGED: MIAMI-Tox
- NCI (National Cancer Institute) Public Data Outreach – Structure Web Browser
- NIEHS's National Center for Toxicogenomics
- NLM (National Library of Medicine) TOXNET
- NTP (National Toxicology Program) On-line Public Databases
- SRC (Syracuse Research Corporation) PBT-Profiler and Analog Search Tools



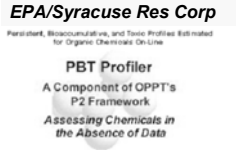
NCI Structure-Browser

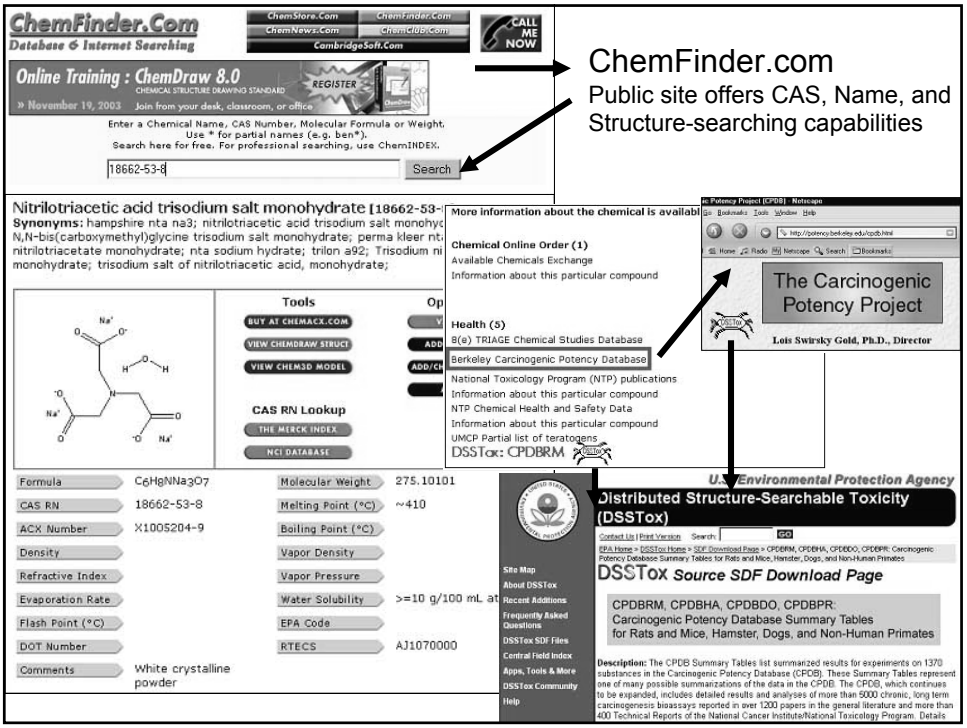


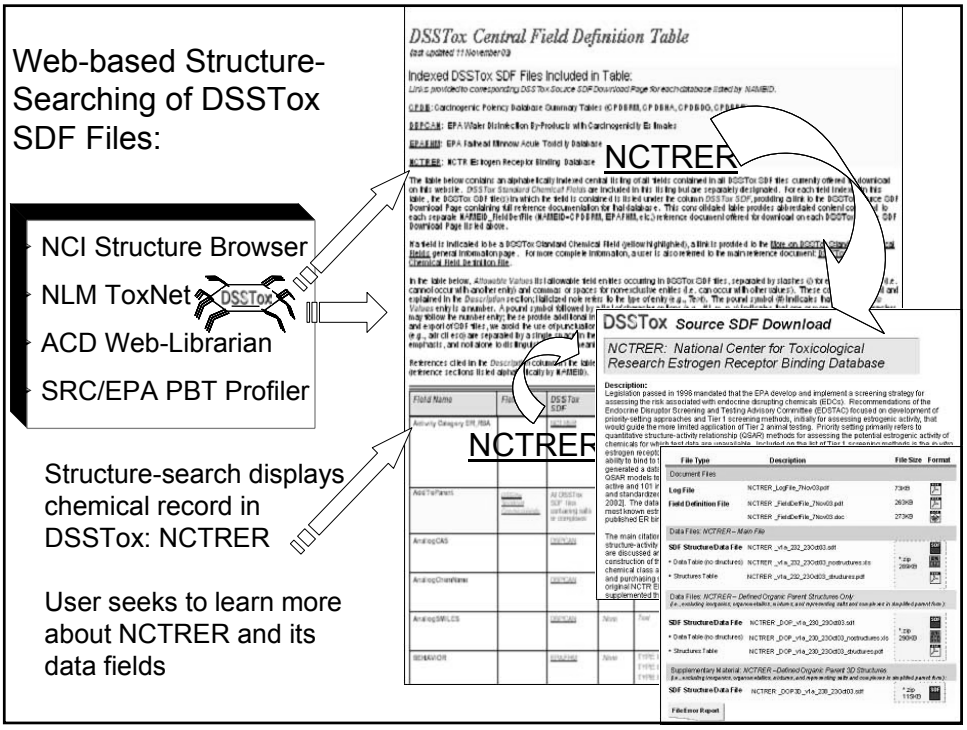
Advanced Chemistry Development

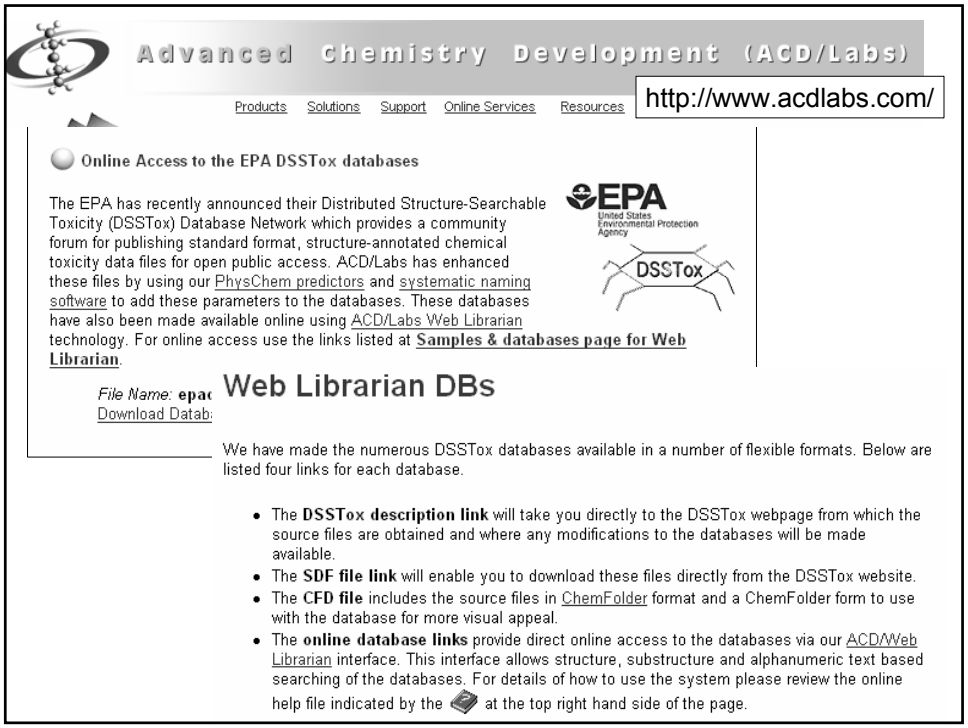
ISSCentral – Freeware CRD

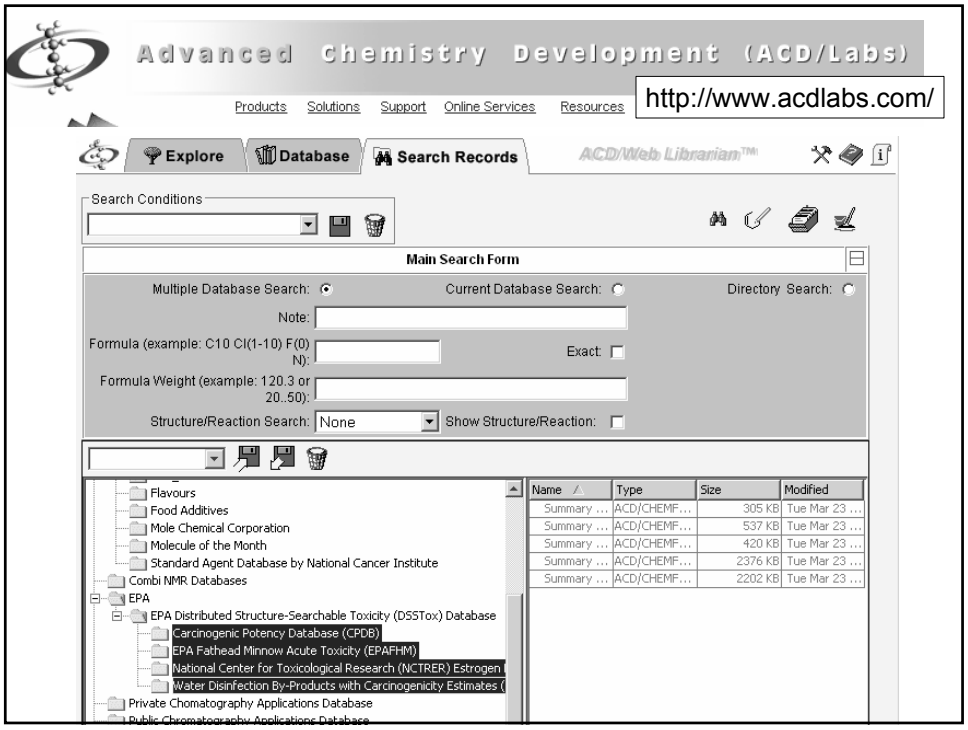
EPA/Syracuse Res Corp




ChemFinder.Com
Database & Internet Searching
Online Training : ChemDraw 8.0
Enter a Chemical Name, CAS Number, Molecular Formula or Weight.
Search here for free. For professional searching, use ChemINDEX.
18662-53-8
Search
ChemFinder.com
Public site offers CAS, Name, and Structure-searching capabilities
Nitrilotriacetic acid trisodium salt monohydrate [18662-53-
Synonyms: hampshire nta na3; nitrilotriacetic acid trisodium salt monohyc
N,N-bis(carboxymethyl)glycine trisodium salt monohydrate; perma kleer nt
nitrilotriacetate monohydrate; nta sodium hydrate; trilon a92; Trisodium ni
monohydrate; trisodium salt of nitrilotriacetic acid, monohydrate;
Tools
BUY AT CHEMACX.COM
VIEW CHEMDRAW STRUCT
VIEW CHEM3D MODEL
CAS RN Lookup
THE MERCK INDEX
NCI DATABASE
More information about the chemical is availabl
Chemical Online Order (1)
Available Chemicals Exchange
Information about this particular compound
Health (5)
B(e) TRIAGE Chemical Studies Database
Berkeley Carcinogenic Potency Database
National Toxicology Program (NTP) publications
Information about this particular compound
NTP Chemical Health and Safety Data
Information about this particular compound
UMCP Partial list of teratogens
DSSTox: CPDBRM
The Carcinogenic Potency Project
Lois Swirsky Gold, Ph.D., Director
Formula C6H8NNa3O7
CAS RN 18662-53-8
ACX Number X1005204-9
Density
Refractive Index
Evaporation Rate
Flash Point (°C)
DOT Number
Comments White crystalline powder
Molecular Weight 275.10101
Melting Point (°C) ~410
Boiling Point (°C)
Vapor Density
Vapor Pressure
Water Solubility >=10 g/100 mL at
EPA Code
RTECS AJ1070000
U.S. Environmental Protection Agency
Distributed Structure-Searchable Toxicity (DSSTox)
DSSTox Source SDF Download Page
CPDBRM, CPDBHA, CPDBDO, CPDBPR:
Carcinogenic Potency Database Summary Tables
for Rats and Mice, Hamster, Dogs, and Non-Human Primates
Description: The CPDB Summary Tables list summarized results for experiments on 1370 substances in the Carcinogenic Potency Database (CPDB). These Summary Tables represent one of many possible summarizations of the data in the CPDB. The CPDB, which continues to be expanded, includes detailed results and analyses of more than 5000 chronic, long term carcinogenesis bioassays reported in over 1200 papers in the general literature and more than 400 Technical Reports of the National Cancer Institute/National Toxicology Program. Details


Web-based Structure-Searching of DSSTox SDF Files:
NCI Structure Browser
NLM ToxNet
DSSTox
ACD Web-Librarian
SRC/EPA PBT Profiler
Structure-search displays chemical record in DSSTox: NCTRER
User seeks to learn more about NCTRER and its data fields
DSSTox Central Field Definition Table
Indexed DSSTox SDF Files Included in Table:
NCTRER
DSSTox Source SDF Download
NCTRER: National Center for Toxicological Research Estrogen Receptor Binding Database
NCTRER


Advanced Chemistry Development (ACD/Labs)
Products Solutions Support Online Services Resources
http://www.acdlabs.com/
Online Access to the EPA DSSTox databases
The EPA has recently announced their Distributed Structure-Searchable Toxicity (DSSTox) Database Network which provides a community forum for publishing standard format, structure-annotated chemical toxicity data files for open public access. ACD/Labs has enhanced these files by using our PhysChem predictors and systematic naming software to add these parameters to the databases. These databases have also been made available online using ACD/Labs Web Librarian technology. For online access use the links listed at Samples & databases page for Web Librarian.
EPA
United States Environmental Protection Agency
DSSTox
File Name: epa
Download Datab
Web Librarian DBs
We have made the numerous DSSTox databases available in a number of flexible formats. Below are listed four links for each database.
The DSSTox description link will take you directly to the DSSTox webpage from which the source files are obtained and where any modifications to the databases will be made available.
The SDF file link will enable you to download these files directly from the DSSTox website.
The CFD file includes the source files in ChemFolder format and a ChemFolder form to use with the database for more visual appeal.
The online database links provide direct online access to the databases via our ACD/Web Librarian interface. This interface allows structure, substructure and alphanumeric text based searching of the databases. For details of how to use the system please review the online help file indicated by the at the top right hand side of the page.


Advanced Chemistry Development (ACD/Labs)
Products Solutions Support Online Services Resources
http://www.acdlabs.com/
Explore
Database
Search Records
ACD/Web Librarian™
Search Conditions
Main Search Form
Multiple Database Search:
Current Database Search:
Directory Search:
Note:
Formula (example: C10 Cl(1-10) F(0) N):
Exact:
Formula Weight (example: 120.3 or 20..50):
Structure/Reaction Search:
None
Show Structure/Reaction:
Flavours
Food Additives
Mole Chemical Corporation
Molecule of the Month
Standard Agent Database by National Cancer Institute
Combi NMR Databases
EPA
EPA Distributed Structure-Searchable Toxicity (DSSTox) Database
Carcinogenic Potency Database (CPDB)
EPA Fathead Minnow Acute Toxicity (EPAFHM)
National Center for Toxicological Research (NCTRER) Estrogen
Water Disinfection By-Products with Carcinogenicity Estimates
Private Chomatography Applications Database
Public Chromatography Applications Database
Name
Type
Size
Modified
Summary ... ACD/CHEMF... 305 KB Tue Mar 23 ...
Summary ... ACD/CHEMF... 537 KB Tue Mar 23 ...
Summary ... ACD/CHEMF... 420 KB Tue Mar 23 ...
Summary ... ACD/CHEMF... 2376 KB Tue Mar 23 ...
Summary ... ACD/CHEMF... 2202 KB Tue Mar 23 ...

Analog Search Component to Toxicity Estimation

Using the PBT Profiler

Information needed
Examples
Interpreting Results
What's new?

Related Links

About PBTs
PBT Strategy
TRI PBT Project
P2 Framework
Links & Contacts

Comments

Persistent, Bioaccumulative, and Toxic Profiles Estimated for Organic Chemicals On-Line

PBT Profiler

A Component of OPPT's P2 Framework

Assessing Chemicals in the Absence of Data

About
Methodology
Criteria
Anonymity & Security
Definitions
Terms of Use
Chemicals That Can't be Profiled

The PBT Profiler was developed as a voluntary screening tool to identify Pollution Prevention opportunities for chemicals without experimental data.

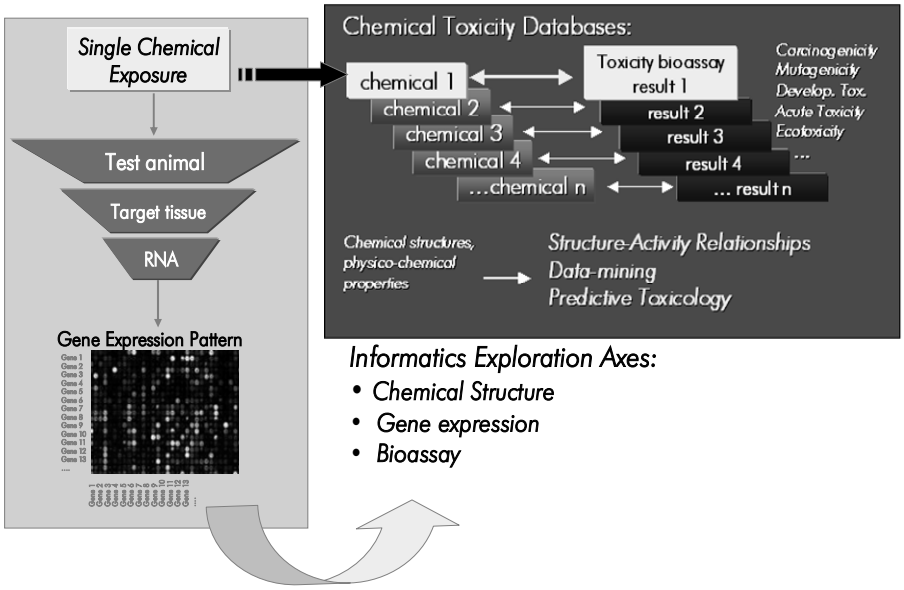
Users of the PBT Profiler acknowledge that they have read and accept the Terms of Use

Start the PBT Profiler

Developed by the Environmental Science Center under contract to the Office of Pollution Prevention and Toxics , U.S. Environmental Protection Agency

Computer Resources Donated by Syracuse Research Corporation *Ver 1.203* *Last Updated May 20, 2003*

Bioinformatics ….. meets Chemoinformatics



Informatics Exploration Axes:

- *Chemical Structure*
- *Gene expression*
- *Bioassay*

Chemical Effects in Biological System Knowledge-Base (CEBS)

Gene expression

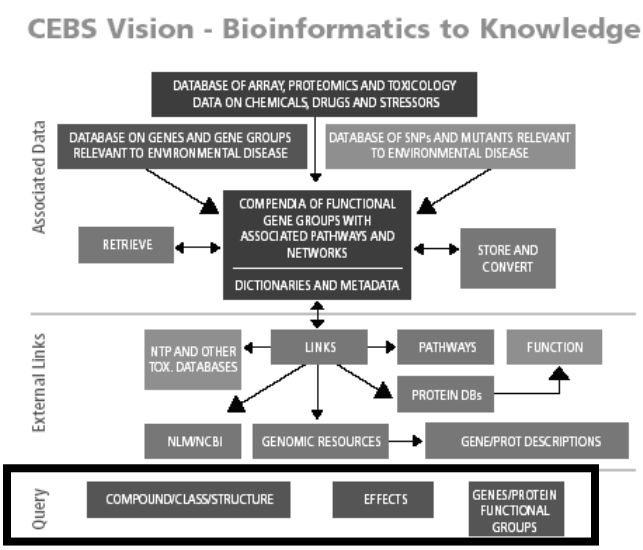
Gene Pathways

Gene Function

Proteomics

Metabonomics

Historical NTP Toxicity data



DSSTox / CEBS Collaboration:

Part 1 – DSSTox Annotation of CEB

Part 2 – Link CEBS to DSSTox Database Network

Part 3 – Add structural searchability to CEBS

DSSTox Database Network +

Gene expression

Gene Pathways

Gene Function

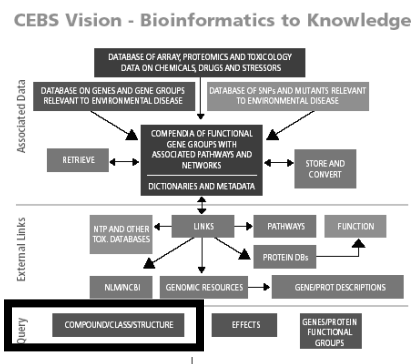
Proteomics

Metabonomics

DSSTox Toxicity Data Files

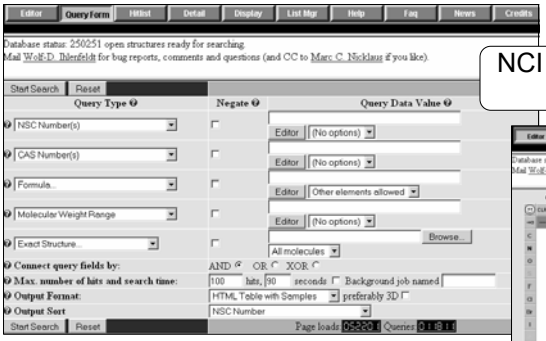
Historical NTP Toxicity data

DB1 DB2 DB3 DB4 DB5 DB6 DB7

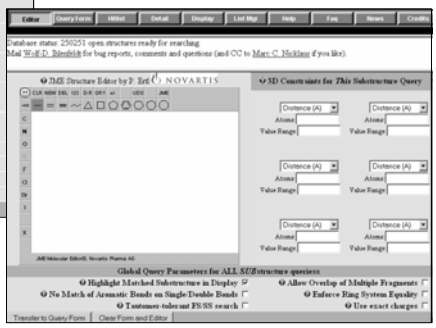


DSSTox Standard Chemical Fields

Chemical Relational Searching Capability:



NCI CACTVS Structure Browser:
http://cactus.nci.nih.gov/



Create a Public Domain Browser for CEBS:

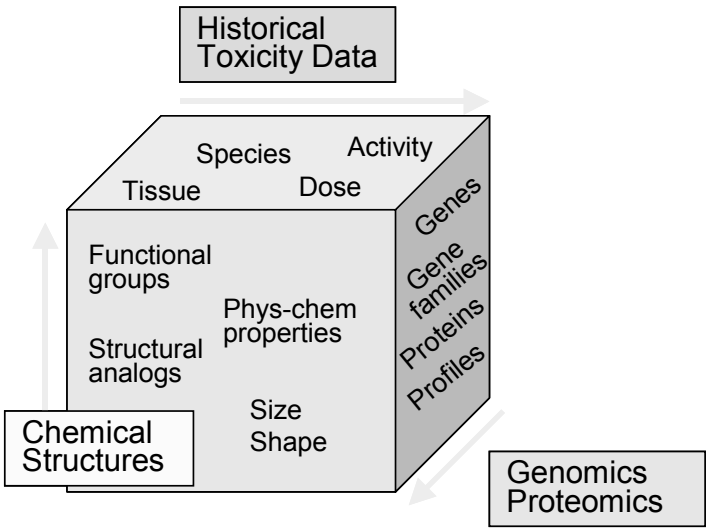
- NIH/NCI CACTVS Structure Browser
- JChem/Marvin
- LHASA VITIC

Chemistry Standards:

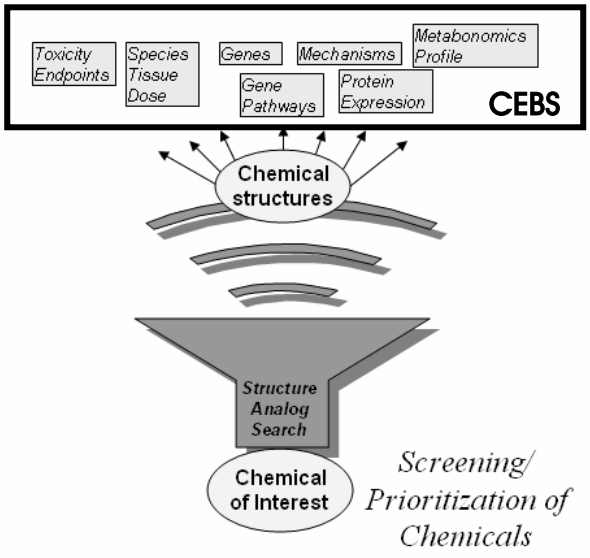
- INChI chemical codes
- IUPAC Names

CEBS Chemo-bioinformatics:

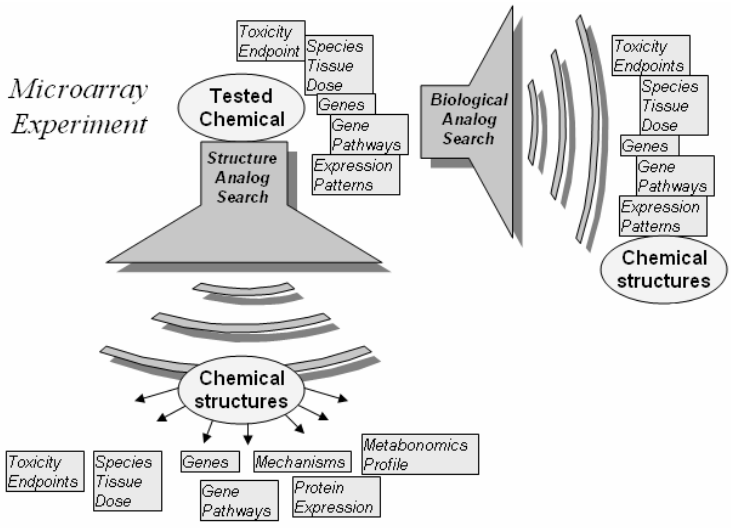
Expanded Relational Search Domains



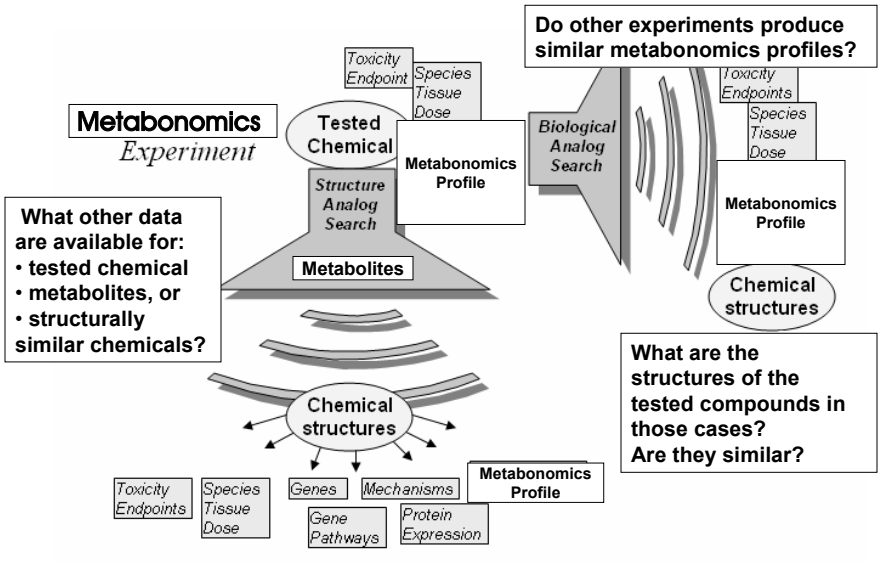
Gathering Data on Chemical Analogues



Exploring Broader Associations from Single Microarray Experiment



Exploring Broader Associations from Single Metabonomics Experiment



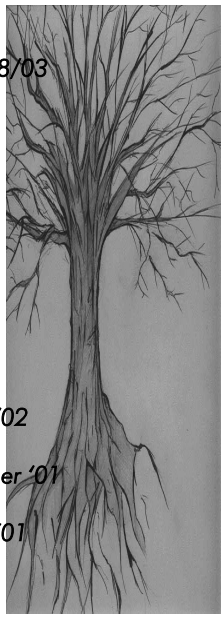
DSSTox Status & Future Directions:

- ✓ Outside Coordination:
  - *Tox standards efforts (ToxML, MIAMI-Tox)*
  - *Chemistry standards efforts (InCHI, IUPAC names)*
  - *Other public efforts (NCI, TOXNET, PBT, etc)*
- ✓ LHASA UK Tox DB – DSSTox public data distributor
- ✓ FDA, EPA, EU – assist in publishing non-proprietary toxicity data from internal databases
- ✓ EPA CompTox Augmented Funding Award – 1 yr: *Expand DSSTox public database offerings*
- ✓ EPA CompTox New Start Proposal – CEBS collaboration: *Undergoing review*

DSSTox Collaborators/Advisors/Acknowledgements:

• Cancer Potency Data Base - rodent carcinogenicity……	Lois Swirsky Gold, Thomas Slone
• EPA - Ecotoxicity (fathead minnow, Teratox)……	Chris Russom
• EPA/OPPT,OW – DBP cancer assessment……	Yin-tak Woo, Mary Manibusan
• FDA/NCTR - Estrogen receptor binding data base……	Weida Tong, Hong Fang
• FDA/CDER – Maximum recommended dose drugs ……	Dan Benz, Ed Matthews, Joe Contrera
• EPA/OPP, Ecotox – pesticides ……	Brian Montague, Pauline Wagner
• NTP Gene-tox data; IRIS ……	Errol Zeiger, Zeiger Consulting
• Nat Ctr Toxicogenomics: CEBS ……	Mike Waters, Ray Tennant
• GlaxoSK - GeneTox/NTP Salmonella database……	Neal Cariello, Vijay Gombar
• NIEHS/NTP Rodent carcinogenicity, etc ……	Skip Eastin, Doug Bristol
• Developmental toxicity ……	Vijay Gombar (GlaxoSK), Orest Macina
• ICVAM Toxicity databases ……	Ray Tice, Marc Jackson, ILS
• Unilever Skin Sensitization Database……	Martin Barrett, Marlin Consulting
• ZEBET Acute Toxicity Database ……	Julie Penzotti, Rational Discovery
• Tulane/Xavier Univ – Endocrine Disruption ……	Tom Wiese
• NCI – SDF tools, CACTVS structure browser……	Marc Nicklaus
• LeadScope – SDF/XML converter, FDA carcinogens ……	Chihae Yang
• SDF Viewer application ……	Thomas Harrocks, Intuitive Software Solutions
• ACD – ChemFolder, WebBase ……	Antony Williams, M Hachey, G Shear
• CambridgeSoft – ChemFinder application ……	Rich Talbot
• EPA scientific advisors ……	Stephen Nesnow, Adam Swank
• EPA/CSC – web development, IT ……	Brian Garges/ D Kanipe, D Marshall

DSSTox Development Team:



- ClarLynda Williams – Coordinator, Lead Project Technician
  - *NCCU/EPA COOP Student Trainee 12/00-12/02; EPA 12/02-8/03*
- Jamie Burch
  - *NCCU/EPA COOP Student Trainee 11/02-2/04*
- Brian Rogers
  - *NCCU/EPA COOP Student Trainee 1/04-present*
- Marty Wolf
  - *EPA Senior Environmental Employment Program 8/04-present*
- Audrey Evans
  - *ECO/EPA Summer Student Trainee, Summer '03*
- Todd Stewart
  - *EPA-UNC Student COOP, Spring/Summer 02*
- Nina Fields
  - *Shaw Univ. High School Minority Mentoring Program, Summer '02*
- James Beidler
  - *EPA Summer Student Employee, Warren-Wilson College, Summer '01*
- Daniel Ohuoba
  - *Shaw Univ. High School Minority Mentoring Program, Summer '01*
- Adam Swank
  - *ECD, EPA*

Optional DSSTox Website Tour

http://www.epa.gov/nheerl/dsstox/