United States Environmental Protection Agency

Exposure CoP Meeting, 12 August 2008

TOXICO-CHEMINFORMATICS:

DSSTox and Chemical Structure Annotation for improved data access

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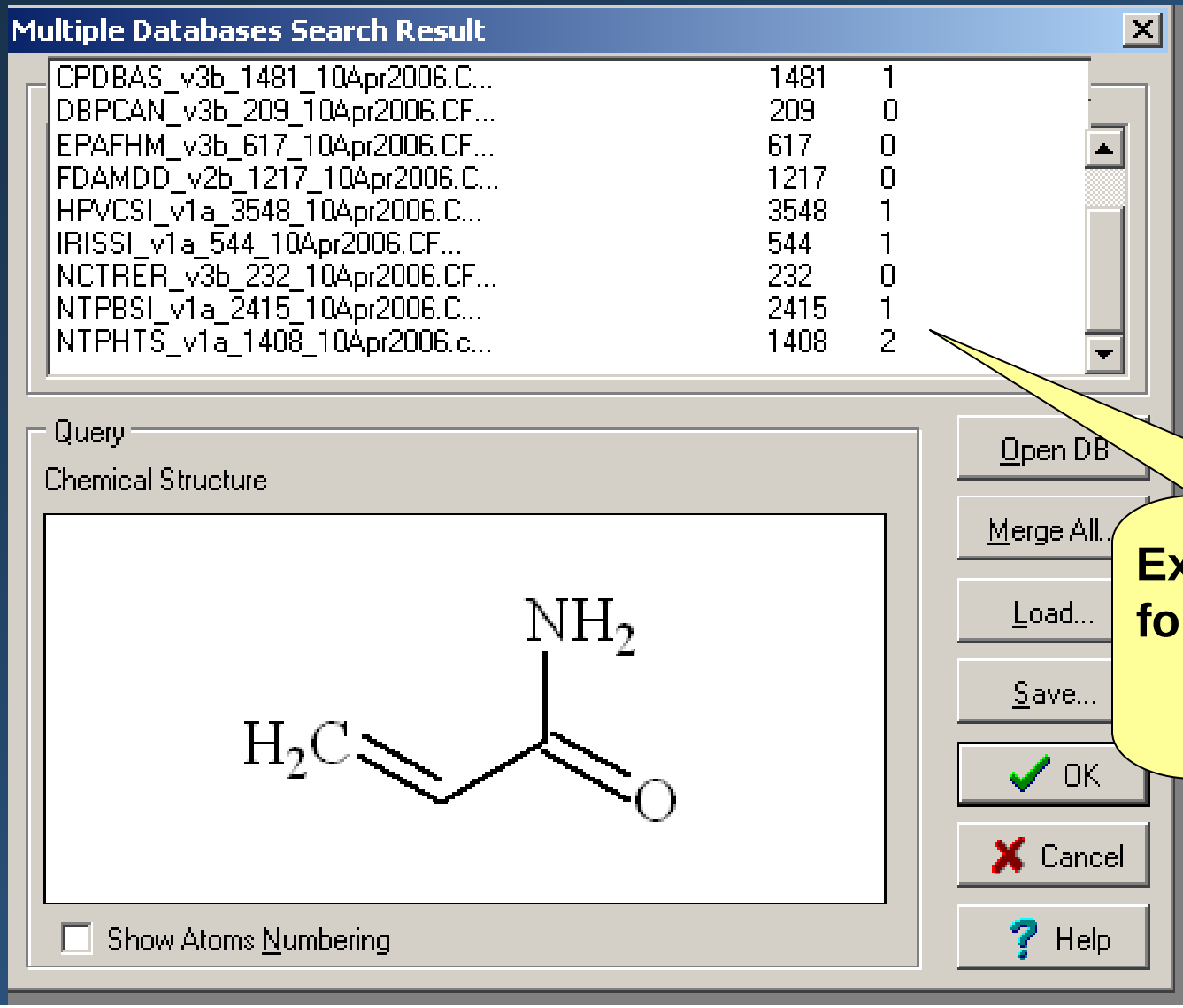
Office of Research and Development
National Center for Computational Toxicology

Part I.

Relational Structure-Analog Searching

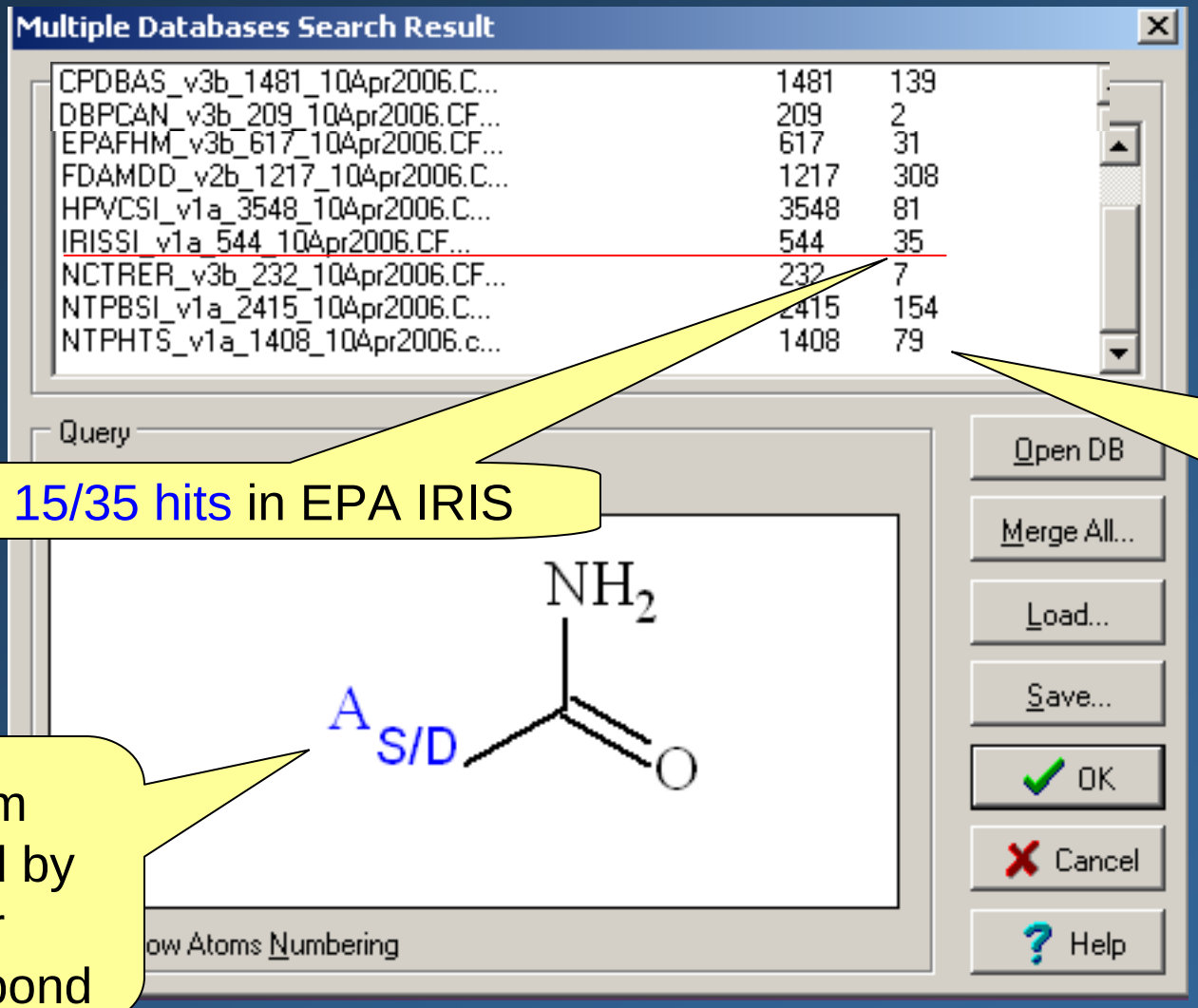
Structure Searching Across 9 Diverse Toxicity Databases:



Exact match search for Acrylamide:

Result: 6 hits

Generalized Sub-Structure Searching Across 9 Diverse Toxicity Databases:



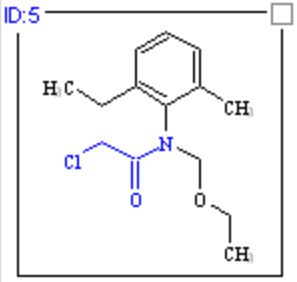
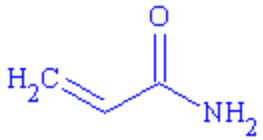
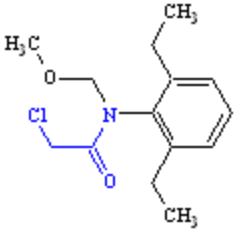
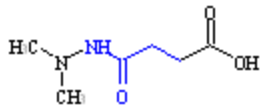
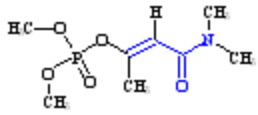
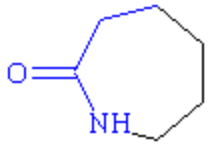
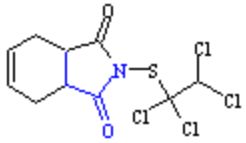
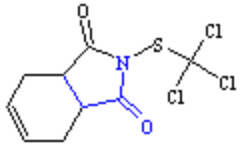
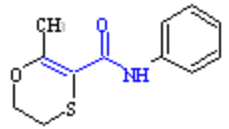
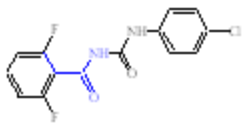
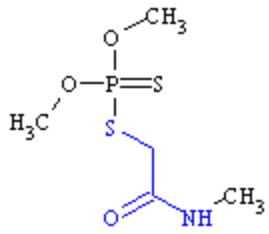
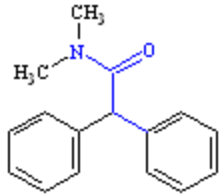
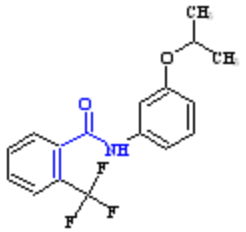
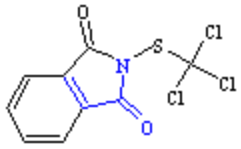
View 15/35 hits in EPA IRIS

Result: 836 hits

Any atom attached by single or double bond

Generalized Sub-Structure Searching Across 9 Diverse Toxicity Databases:

15/35 Hits in IRIS containing acrylamide-like moiety

ID:5 	ID:12 	ID:16 	ID:17 	ID:58 
Acetochlor 34256-82-1	Acrylamide 79-06-1	Alachlor 15972-60-8	Daminozide 1596-84-5	Bentazon 25057-89-0
ID:71 	ID:99 	ID:100 	ID:101 	ID:108 
Bidrin 141-66-2	Caprolactam 105-60-2	Captafol 2425-06-1	Captan 133-06-2	Carboxin 5234-68-4
ID:206 	ID:210 	ID:229 	ID:266 	ID:268 
Diflubenzuron 35367-38-5	Dimethoate 60-51-5	Diphenamid 957-51-7	Flutolanil 66332-96-5	N-(Trichloromethylthio)phthali 133-07-3

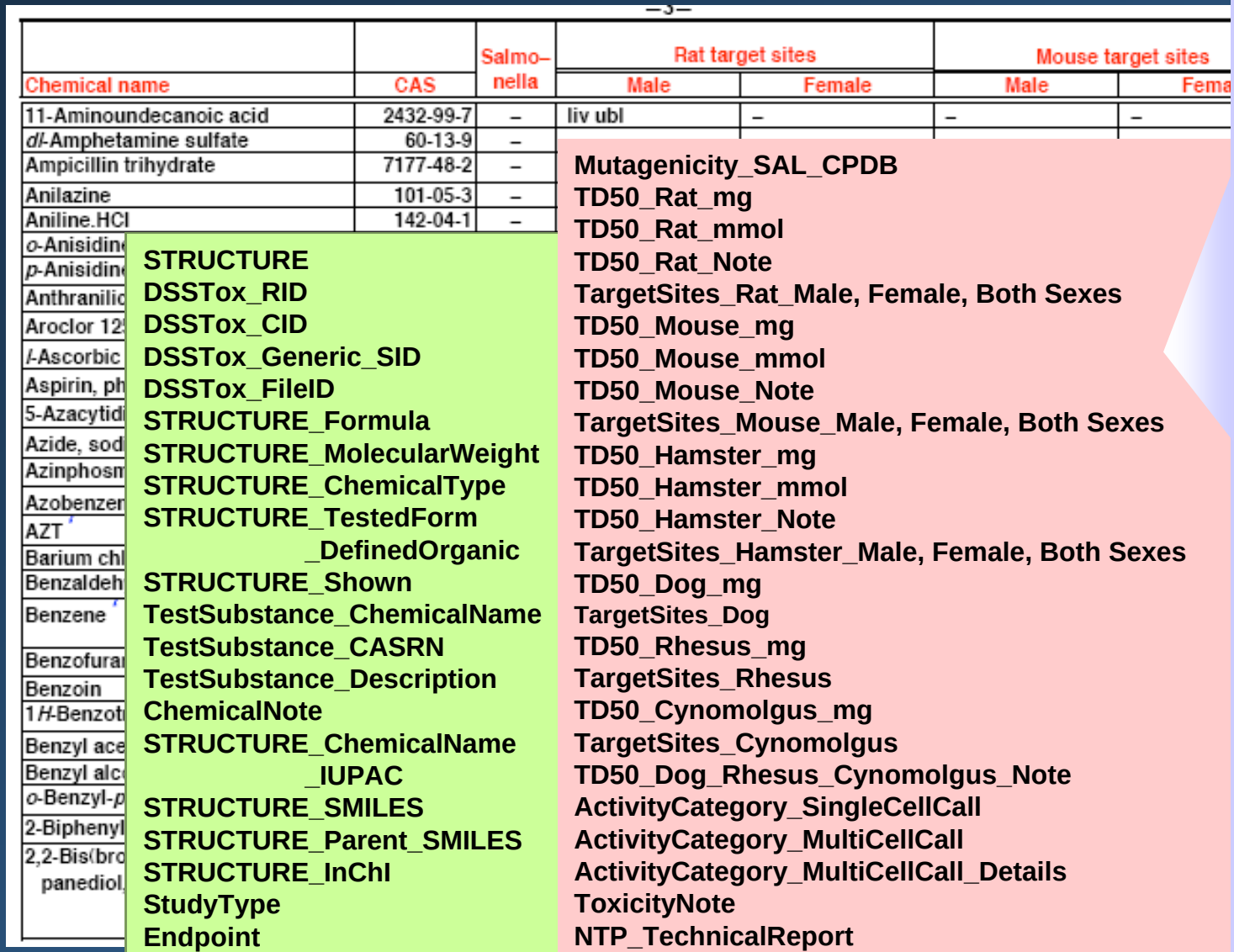
Relational Biological Content Searching: Carcinogenic Potency Database – All Species (CPDBAS_1547)

Chemical name	CAS	Salmo–nella	Rat target sites		Mouse target sites	
			Male	Female	Male	Female
11-Aminoundecanoic acid	2432-99-7	–	liv ubl	–	–	–
dl-Amphetamine sulfate	60-13-9	–	–	–	–	–
Ampicillin trihydrate	7177-48-2	–	_[e]	–	–	–
Anilazine	101-05-3	–	–	–	–	–
Aniline.HCl	142-04-1	–	per spl vsc	per	–	–
o-Anisidine.HCl	134-29-2	+	kid thy ubl	ubl	ubl	ubl
p-Anisidine.HCl	20265-97-8	+	_[a]	–	–	–
Anthranilic acid	118-92-3	–	–	–	–	–
Aroclor 1254	11097-69-1	–	_[a]	_[a]	.	.
l-Ascorbic acid	50-81-7	–	–	–		
Aspirin, phenacetin, and caffeine	8003-03-0	–	–			
5-Azacytidine	320-67-2	+	l			
Azide, sodium	26628-22-8	+	–	–		
Azinphosmethyl	86-50-0	+	_[a]	–		
Azobenzene	103-33-3	+	spl vsc	spl		
AZT	30516-87-1	+	.	.		
Barium chloride dihydrate	10326-27-9	–	–	–		
Benzaldehyde	100-52-7	–	–	–		
Benzene	71-43-2	–	ezy orc ski	ezy orc s		
Benzofuran	271-89-6	–	–	kid[5]		
Benzoin	119-53-9	–	–	–		
1*H*-Benzotriazole	95-14-7	+	_[a]	_[a]		
Benzyl acetate	140-11-4	–	_[e]	–		
Benzyl alcohol	100-51-6	–	–	–		
o-Benzyl-*p*-chlorophenol	120-32-1	–	–	_[e]	kid	–
2-Biphenylamine.HCl	2185-92-4	+	–	–	_[a]	vsc
2,2-Bis(bromomethyl)-1,3-propanediol, technical grade	3296-90-0	+	eso ezy hmo lgi lun mgl orc per ski smi sto sub tes thy ubl	eso mgl orc thy	hag kid lun	hag lun ski sub

Convert tabular data to structured data model:

- Pure text & numeric fields
- No abbreviations
- Chemical-structures
- Activity-related fields
- Standardized entries

Relational Biological Content Searching: Carcinogenic Potency Database – All Species (CPDBAS_1547)



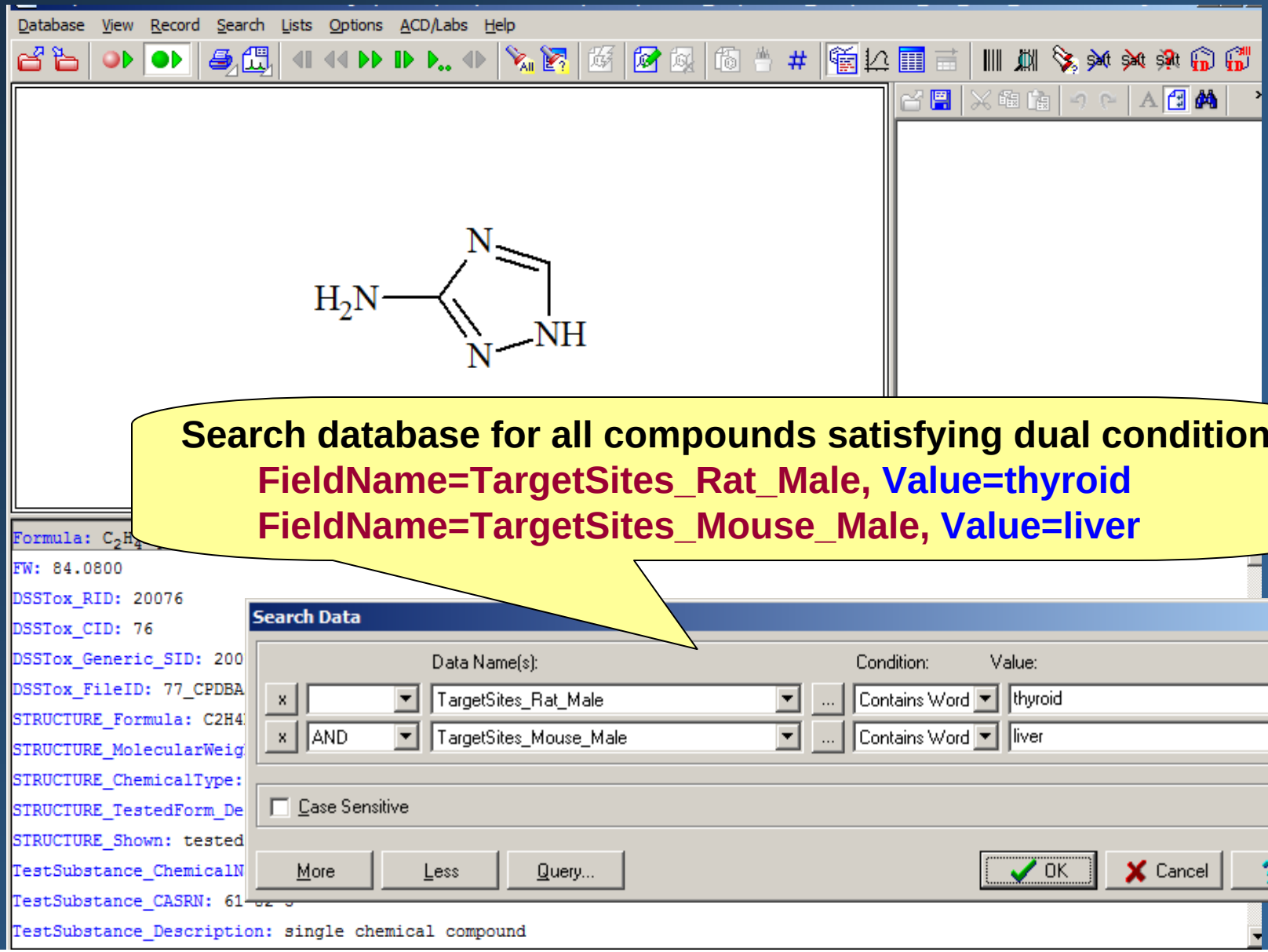
Chemical name	CAS	Salmo-nella	Rat target sites: Male	Rat target sites: Female	Mouse target sites: Male	Mouse target sites: Fema
11-Aminoundecanoic acid	2432-99-7	–	liv ubl	–	–	–
dl-Amphetamine sulfate	60-13-9	–				
Ampicillin trihydrate	7177-48-2	–				
Anilazine	101-05-3	–				
Aniline.HCl	142-04-1	–				
o-Anisidine						
p-Anisidine						
Anthranilic						
Aroclor 12						
l-Ascorbic						
Aspirin, ph						
5-Azacytidi						
Azide, sod						
Azinphosm						
Azobenzer						
AZT						
Barium chl						
Benzaldeh						
Benzene						
Benzofura						
Benzoin						
1*H*-Benzot						
Benzyl ace						
Benzyl alc						
o-Benzyl-*p*						
2-Biphenyl						
2,2-Bis(bro panediol						

STRUCTURE
DSSTox_RID
DSSTox_CID
DSSTox_Generic_SID
DSSTox_FileID
STRUCTURE_Formula
STRUCTURE_MolecularWeight
STRUCTURE_ChemicalType
STRUCTURE_TestedForm
_DefinedOrganic
STRUCTURE_Shown
TestSubstance_ChemicalName
TestSubstance_CASRN
TestSubstance_Description
ChemicalNote
STRUCTURE_ChemicalName
_IUPAC
STRUCTURE_SMILES
STRUCTURE_Parent_SMILES
STRUCTURE_InChI
StudyType
Endpoint
Species

Mutagenicity_SAL_CPDB
TD50_Rat_mg
TD50_Rat_mmol
TD50_Rat_Note
TargetSites_Rat_Male, Female, Both Sexes
TD50_Mouse_mg
TD50_Mouse_mmol
TD50_Mouse_Note
TargetSites_Mouse_Male, Female, Both Sexes
TD50_Hamster_mg
TD50_Hamster_mmol
TD50_Hamster_Note
TargetSites_Hamster_Male, Female, Both Sexes
TD50_Dog_mg
TargetSites_Dog
TD50_Rhesus_mg
TargetSites_Rhesus
TD50_Cynomolgus_mg
TargetSites_Cynomolgus
TD50_Dog_Rhesus_Cynomolgus_Note
ActivityCategory_SingleCellCall
ActivityCategory_MultiCellCall
ActivityCategory_MultiCellCall_Details
ToxicityNote
NTP_TechnicalReport
Website_URL

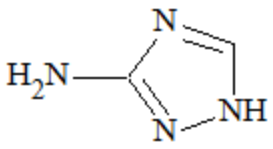
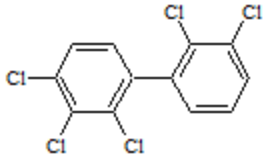
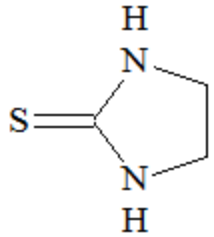
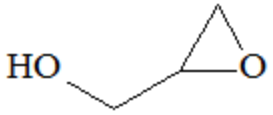
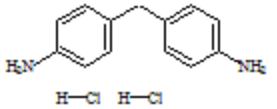
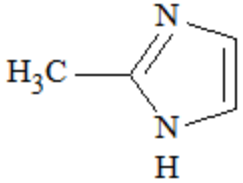
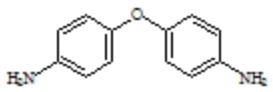
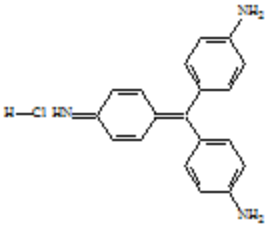
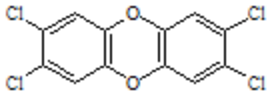
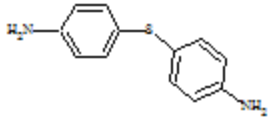
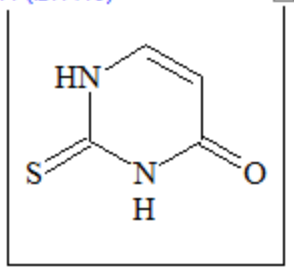
adrenal gland;
bone;
clitoral gland;
esophagus;
ear/Zymbal's gland;
gall bladder;
harderian gland;
hematopoietic system;
kidney;
large intestine;
liver;
lung;
mesovarium;
mammary gland;
mixture;
myocardium;
nasal cavity
nervous system;
oral cavity
ovary;
pancreas;
peritoneal cavity;
pituitary gland;
preputial gland;
prostate;
skin;
small intestine;
spleen;
stomach;
subcutaneous tissue;
all tumor bearing animals;
testes;
thyroid gland;
urinary bladder;
uterus;
vagina;
vascular system.

Relational Biological Content Searching: Carcinogenic Potency Database – All Species (CPDBAS_1547)



ACD/ChemFolder: Database Window - [C:\USERS\ANN\DOCUMENTS\DS...D\CPDBAS_V5\CPDBAS_V5B\CPDBAS_V5B_1547_10FEB2008.CFD]

Database View Record Search Lists Options ACD/Labs Help

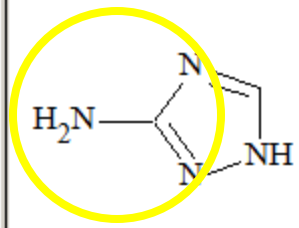
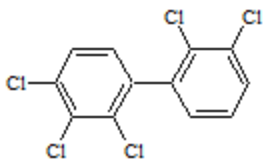
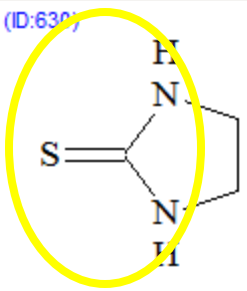
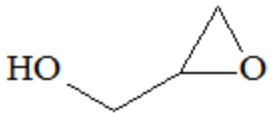
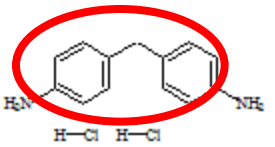
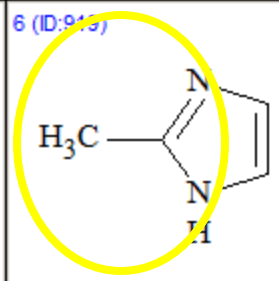
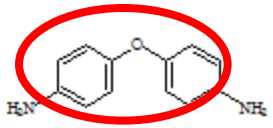
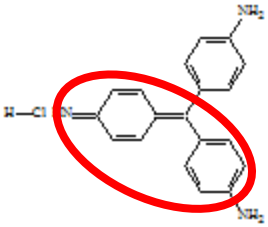
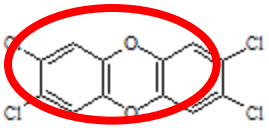
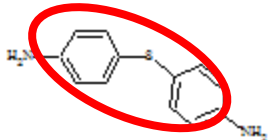
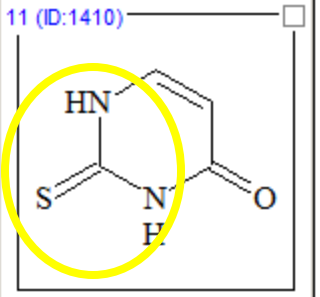
1 (ID:77)	2 (ID:103)	3 (ID:630)	4 (ID:697)	5 (ID:911)	6 (ID:919)
					
3-Aminotriazole thyroid gland liver inactive	Aroclor 1254 thyroid gland liver inactive	Ethylene thiourea thyroid gland liver; pituitary gland; thyroid gla active	Glycidol ear Zymbals gland; large intesti harderian gland; liver; lung; ski active	4,4'-Methylenedianiline.2HCl liver; thyroid gland adrenal gland; liver; thyroid gla active	2-Methylimidazole thyroid gland liver; thyroid gland inactive
7 (ID:1144)	**8 (ID:1307)**	**9 (ID:1378)**	**10 (ID:1407)**	**11 (ID:1410)**	
					
4,4'-Oxydianiline liver; thyroid gland harderian gland; liver active	p-Rosaniline.HCl ear Zymbals gland; liver; skin; liver active	2,3,7,8-Tetrachlorodibenzo-p-d oral cavity; thyroid gland liver inactive	4,4'-Thiodianiline ear Zymbals gland; large intesti liver; thyroid gland active	Thiouracil thyroid gland liver	

TestSubstance_ChemicalNam
e
TargetSites_Rat_Male
TargetSites_Mouse_Male
Salmonella Mutagenicity

Search Results: 9 hits / 1547 total
TargetSites_Rat_Male = thyroid
& TargetSites_Mouse_Male = liver

ACD/ChemFolder: Database Window - [C:\USERS\ANN\DOCUMENTS\DS...D\CPDBAS_V5\CPDBAS_V5B\CPDBAS_V5B_1547_10FEB2008.CFD]

Database View Record Search Lists Options ACD/Labs Help

1 (ID:77) 	2 (ID:103) 	3 (ID:630) 	4 (ID:697) 	5 (ID:911) 	6 (ID:919) 
3-Aminotriazole thyroid gland liver inactive	Aroclor 1254 thyroid gland liver inactive	Ethylene thiourea thyroid gland liver; pituitary gland; thyroid gla active	Glycidol ear Zymbals gland; large intesti harderian gland; liver; lung; ski active	4,4'-Methylenedianiline.2HCl liver; thyroid gland adrenal gland; liver; thyroid gla active	2-Methylimidazole thyroid gland liver; thyroid gland inactive
7 (ID:1144) 	8 (ID:1307) 	9 (ID:1378) 	10 (ID:1407) 	11 (ID:1410) 	
4,4'-Oxydianiline liver; thyroid gland harderian gland; liver active	p-Rosaniline.HCl ear Zymbals gland; liver; skin; liver active	2,3,7,8-Tetrachlorodibenzo-p-d oral cavity; thyroid gland liver inactive	4,4'-Thiodianiline ear Zymbals gland; large intesti liver; thyroid gland active	Thiouracil thyroid gland liver	

TestSubstance_ChemicalNam
e
TargetSites_Rat_Male
TargetSites_Mouse_Male
Salmonella Mutagenicity

Search Results: 9 hits / 1547 total
TargetSites_Rat_Male = thyroid
& TargetSites_Mouse_Male = liver

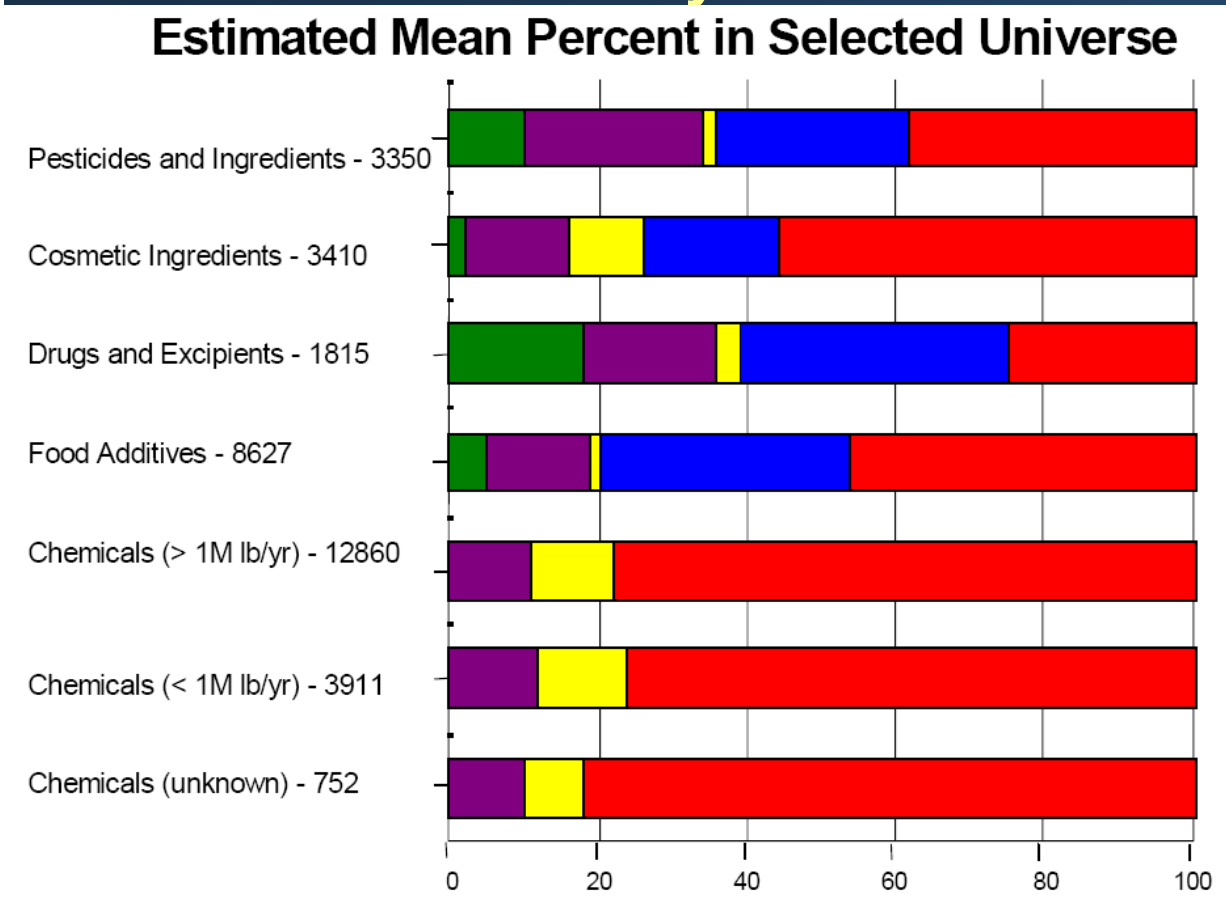
Relational & Structure-Analog Searching Requirements:

- Standardization
- Chemical Structure Indexing
- Internet Linkages

Part II.

The Problem

Environmental Chemicals:
Toxicity Assessment Data Gaps



Complete Hazard Assessment Possible
Minimal Information Available
No Toxicity Information Available
Partial Hazard Assessment Possible
Some Toxicity Information Available

Strategies for Closing the Chemical Data Gap

by John S. Applegate and Katherine Baer

A Center for Progressive Reform Publication *April 2006*

Chemical Research in Toxicology

JULY 2007
VOLUME 20, NUMBER 7

Editorial

Aaron T. Jacobs and Lawrence J. Marnett*

A.B. Hancock Jr. Memorial Laboratory for Cancer Research
Departments of Biochemistry, Chemistry, and Pharmacology
Vanderbilt Institute of Chemical Biology
Center in Molecular Toxicology
Vanderbilt-Ingram Cancer Center
Vanderbilt University School of Medicine
Nashville, Tennessee 37232

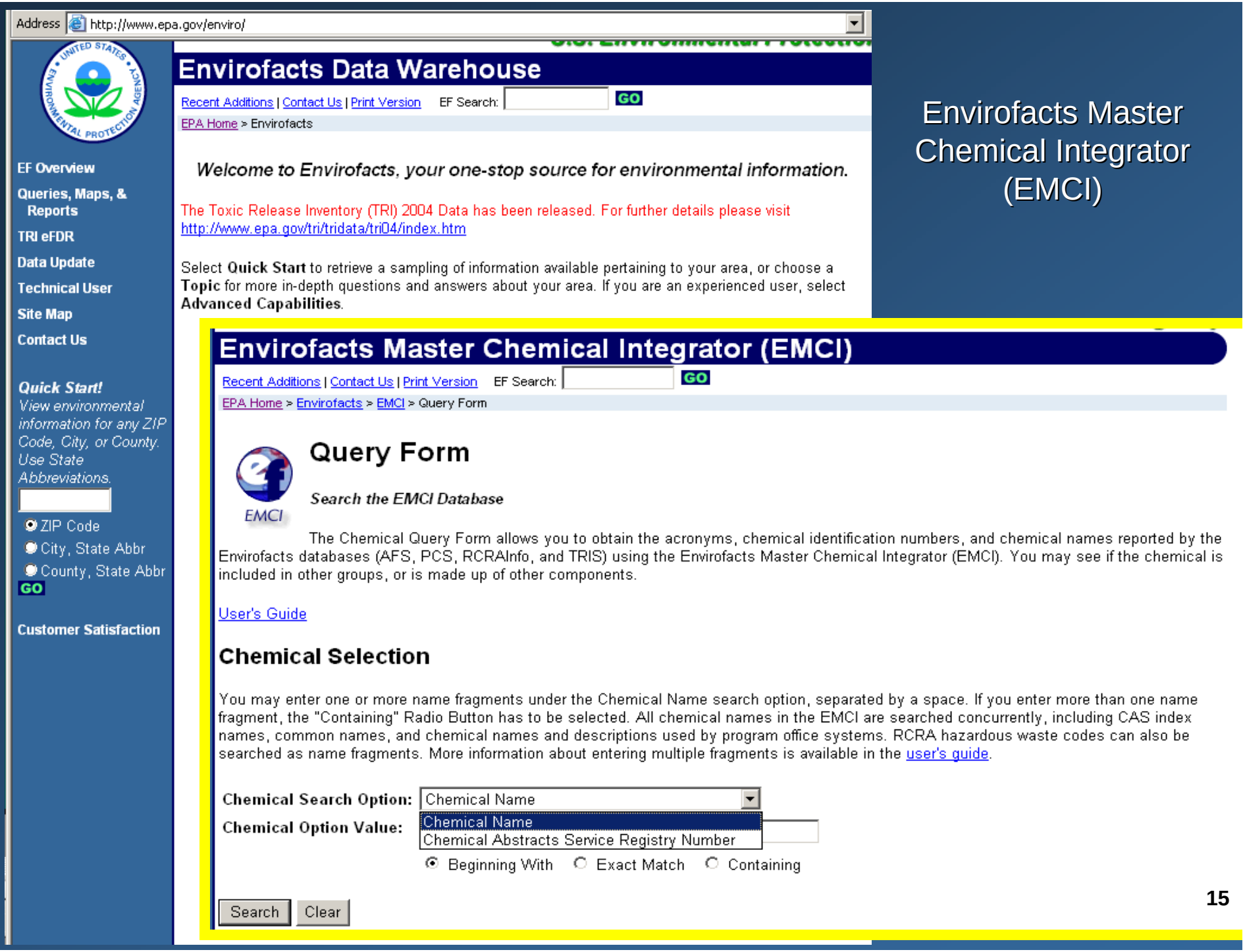
TX7001564

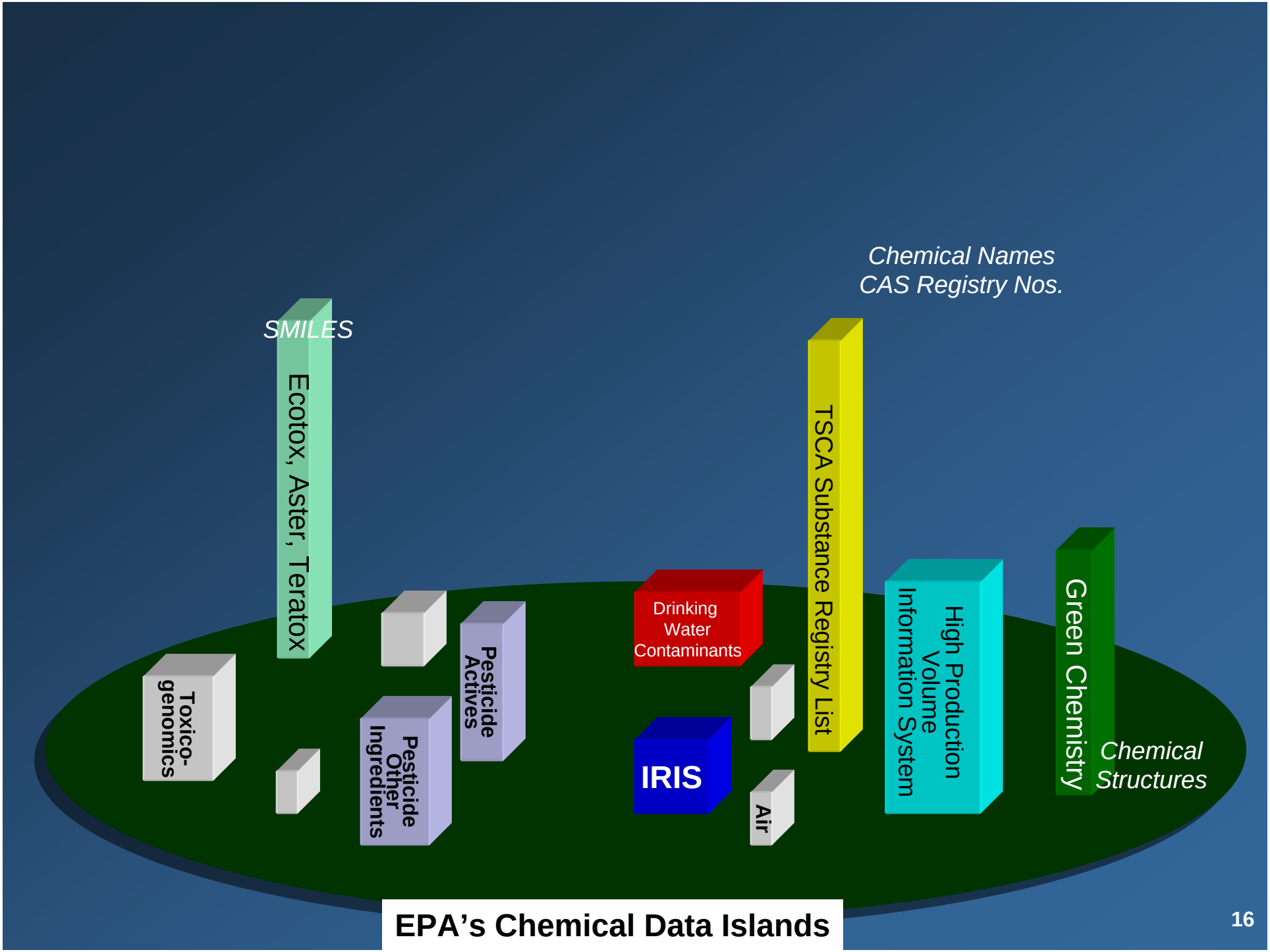
The Future of Toxicology—Wrap Up

Wither toxicology? We have enjoyed a series of informative, occasionally provocative, commentaries on this subject from a paucity of compelling problems to work on that would generate a broad mandate for large-scale investment in toxicol-

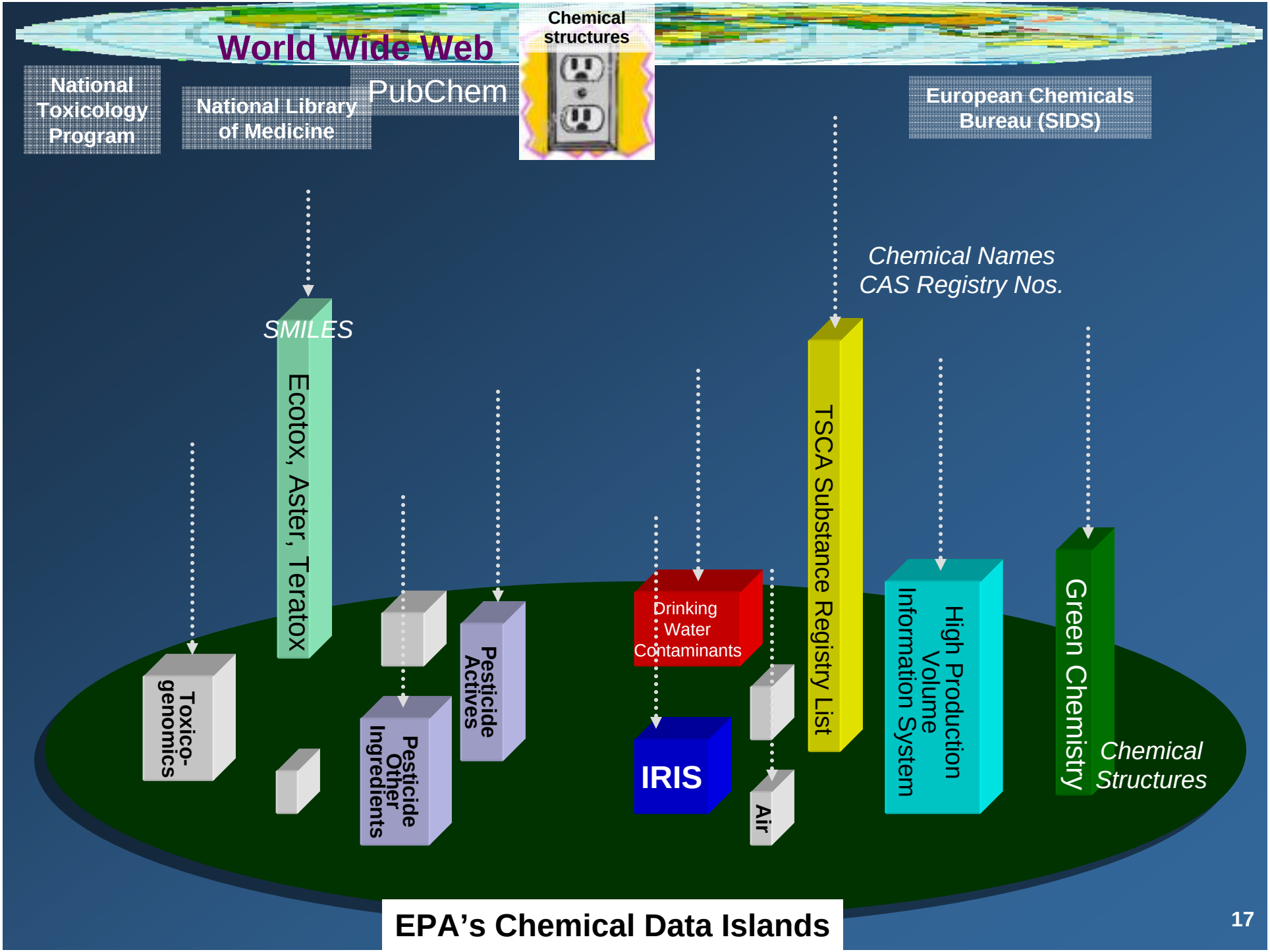
"A major focus for the future of computational toxicology will be integration and analysis of large data sets. The current state of toxicity databases is something of a mess. There are a number of databases, each with differing content, architecture, and searchability, that makes the task of integration extremely difficult."

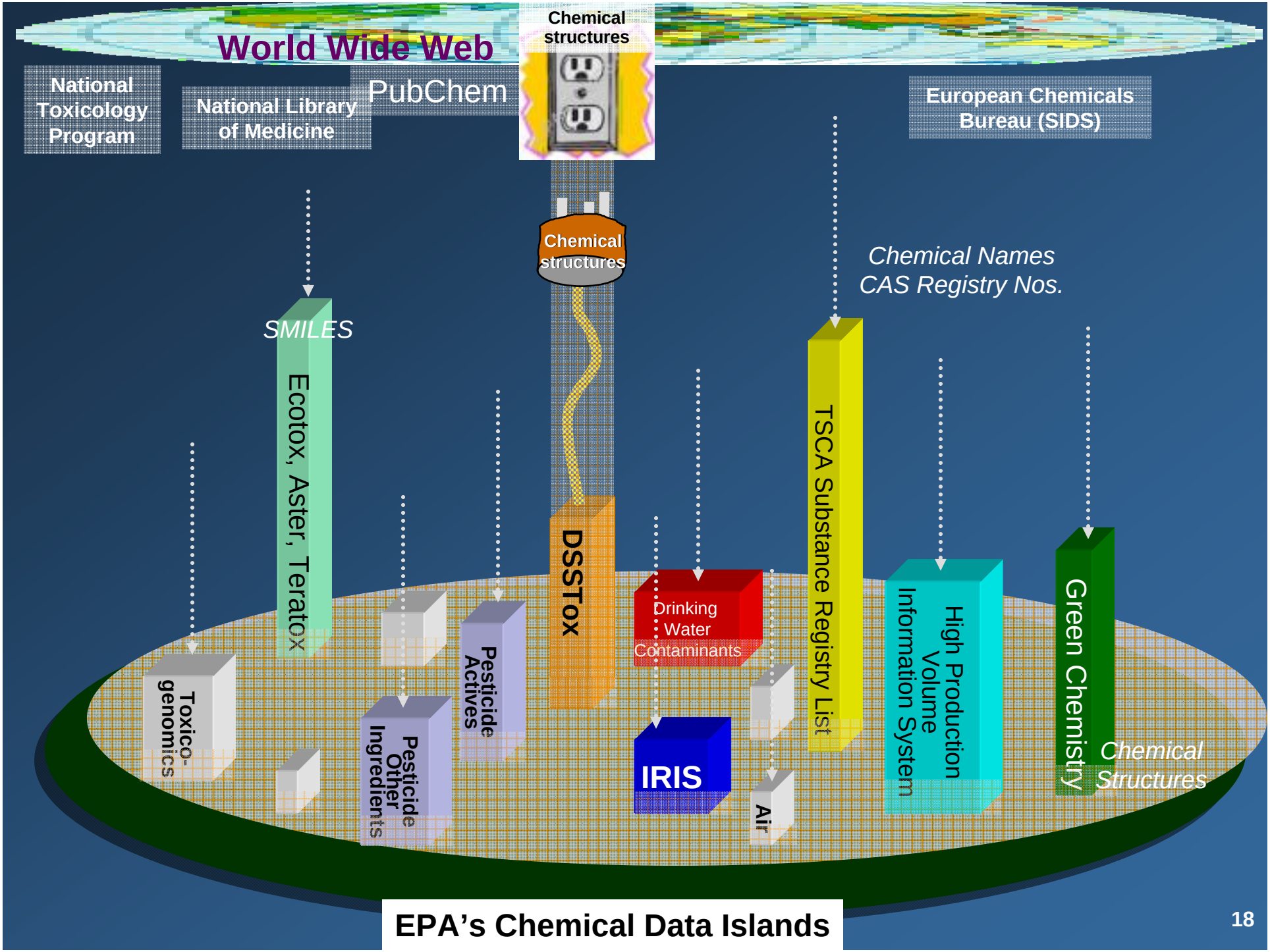
Envirofacts Master Chemical Integrator (EMCI)





EPA's Chemical Data Islands


World Wide Web
Chemical structures
National Toxicology Program
National Library of Medicine
PubChem
European Chemicals Bureau (SIDS)
Chemical Names
CAS Registry Nos.
SMILES
Ecotox, Aster, Teratox
TSCA Substance Registry List
High Production Volume Information System
Green Chemistry
Chemical Structures
Toxico-genomics
Pesticide Actives
Pesticide Other Ingredients
Drinking Water Contaminants
IRIS
Air
EPA's Chemical Data Islands



EPA's Chemical Data Islands

Part III.

Chemical Structure-Indexing

U.S. Environmental Protection Agency

Distributed Structure-Searchable Toxicity (DSSTox) Public Database Network

Recent Additions | Contact Us

You are here: EPA Home » Com
Database Network

Chemical structure-annotation Data standards & integration

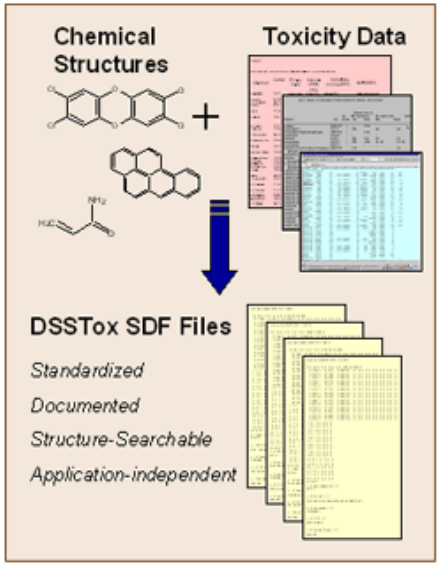
- About DSSTox
- Work in Progress
- Frequent Questions
- Structure Data Files
- Central Field Definition Table
- Apps, Tools & More
- DSSTox Community
- Site Map
- Glossary of Terms
- Help

DSSTox

Distributed Structure-Searchable Toxicity (DSSTox) Database Network is a project of EPA's Computational Toxicology Program, helping to build a public data foundation for improved structure-activity and predictive toxicology capabilities. The DSSTox website provides a public forum for publishing downloadable, structure-searchable, standardized chemical structure files associated with toxicity data. More>

EPA DSSTox Structure-Browser v1.0 GO

DSSTox Structure-Browser information Page



- DSSTox Graphic Flowchart
- DSSTox Project Goals
- DSSTox Publications

Recent Additions: 27 September 2007

- TOXCST: Research Chemical Inventory for EPA's ToxCast Program - Updated to v2a

Recent Additions: 28 August 2007

***Launch of DSSTox Structure-Browser v1.0:**

- A new structure-search capability for published DSSTox Data Files, allows users to search by DSSTox Standard Chemical Fields and includes options for:
  - **Text Search:** Chemical Name, CAS RN, InChI, Formula
  - **Structure Search (*Exact, Substructure, Similarity*):** SMILES or Structure Drawing Tool entry

***Revised Standard ID Fields for all DSSTox files:**

- Modified Record, File, Chemical, and Substance ID fields to index all unique DSSTox structures and substances, also with respect to file record and version

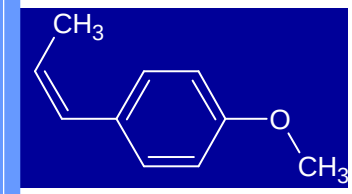
DSSTox Data Files: Details>

CPDBAS_v4a_1481_15Jun2007 **New content*
DBPCAN_v4a_209_15Jun2007
EPAFHM_v4a_617_15Jun2007
FDAMDD_v3a_1216_25Jul2007
HPVCSI_v2a_3548_15Aug2007**New content*
IRISTR_v1a_544_28Jul2007 **New file*
NCTRER_v4a_232_15Jun2007
NTPBSI_v2a_2293_24Aug2007 **Updated content*
NTPHTS_v1a_1408_25Jul2007
TOXCST_v2a_320_25Sep2007 **Updated*

More on Data File Types

DSSTox Standard Chemical Fields:

STRUCTURE ↔ **STRUCTURE_Shown** ↔ **DSSTox_Generic_SID**



- tested chemical,
- general form of chemical,
- active ingredient of formulation,
- representative isomer in mixture,
- representative component in mixture,
- monomer of polymer

, simplified to parent

TestSubstance_ChemicalName

TestSubstance_CASRN

TestSubstance_Description

- single chemical compound
- macromolecule
- mixture or formulation
- unspecified or multiple forms

DSSTox_CID

STRUCTURE_Formula

STRUCTURE_MolecularWeight

STRUCTURE_ChemicalType

- defined organic
- inorganic
- organometallic

ChemicalNote

- description of mixture
- nature & CAS of components
- tautomers
- stereochemistry

STRUCTURE_TestedForm_DefinedOrganic

- parent,
- salt Na, Cl, etc
- complex HCl, H2O, mesylate, etc

STRUCTURE_ChemicalName_IUPAC

STRUCTURE_SMILES

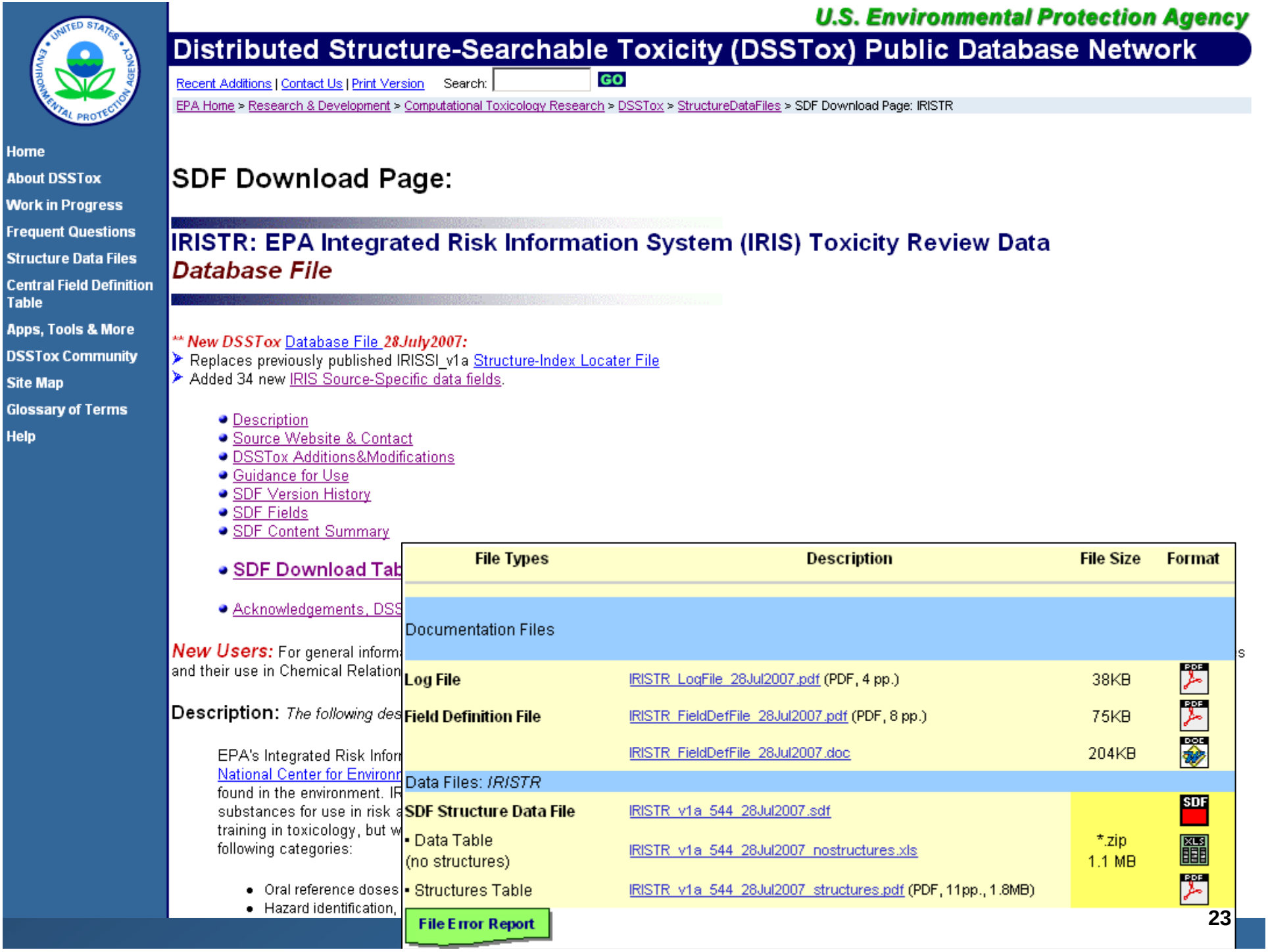
STRUCTURE_Parent_SMILES

STRUCTURE_InChI

DSSTox_RID

DSSTox_FileID

NAMEID	version #records date	Expanded DSSTox Data File Title & Description
CPDBAS	v5b 1547 10Feb2008	**Carcinogenic Potency Database Summary Tables - All Species:** Tumor target site incidence, TD50 potencies, summary activity calls for rat, mouse, hamster, dog, and/or non-human primate; data reviewed and compiled from literature and NTP studies.
DBPCAN	v4b 209 15Feb2008	**EPA Water Disinfection By-Products with Carcinogenicity Estimates Database:** Carcinogenicity estimates (high, moderate, low concern) by EPA experts using a mechanism-based analog SAR approach on a set of 209 water disinfection by-products, mostly small halogenated organics.
EPAFHM	v4b 617 15Feb2008	**EPA Fathead Minnow Acute Toxicity Database:** Acute toxicities of 617 chemicals tested in common assay, with mode-of-action assessments and confirmatory measures.
FDAMDD	v3b 1216 15Feb2008	**FDA Center for Drug Evaluation & Research - Maximum (Recommended) Daily Dose Database:** Maximum (recommended) daily dose (MRDD) values for 1216 pharmaceuticals in mg/kg-body weight (bw)/day, converted to mmol and normalized to dataset; MRDD values extracted from public literature sources.
HPVCSI	v2c 3548 15Feb2008	**EPA High Production Volume Challenge Program** Structure-Index File: Compiled structures for three chemical lists provided on EPA HPV Challenge Program website; each record includes reference index to dated list.
HPVISD	v1b 1006 15Feb2008	**EPA High Production Volume Information System (HPV-IS) Data** Structure-Index Locator File: Compiled structures for the chemical inventory of the on-line EPA HPV-IS with chemical-specific URLs linking to HPV-IS data pages containing chemical properties, fate properties and toxicity data.
IRISTR	v1b 544 15Feb2008	**EPA Integrated Risk Information System (IRIS) Toxicity Review Data File:** Compiled structures for EPA IRIS website with chemical-specific URLs linking to risk assessment summary data pages for 544 chemical substances.
NCTRER	v4b 232 15Feb2008	**FDA National Center for Toxicological Research (NCTR) - Estrogen Receptor Binding Database:** Estrogen receptor relative binding affinities tested in a common in vitro assay for 232 chemicals, listed with chemical class-based structure-activity features.
NTPBSI	v2b 2293 15Feb2008	**National Toxicology Program (NTP) On-line Chemical Bioassay Database** Structure-Index Locator File: Compiled structures for the NTP On-line Database with chemical-specific URLs linking to NTP study summary pages; file includes fields for each of 4 main bioassay study areas with indicator values specifying presence or absence of study data for the chemical substance record.
NTPHTS	v2b 1408 15Feb2008	**National Toxicology Program (NTP) High-Throughput Screening Project** Structure-Index File: Compiled structures for set of 1408 NTP chemical substances provided to the NIH Chemical Genomics Center for HTS bioassay testing and to PubChem (PubChem_CIDs and PubChem_SIDs included in NTPHTS_v2a file); NCGC HTS bioassay data are being deposited into PubChem and can be retrieved with these PubChem chemical CID and SID record listings.
TOXCST	v2b 320 08Feb2008	**Research Chemical Inventory for EPA's ToxCast™ Program** Structure-Index File: Compiled structures for 320 chemical substances that are candidates for Phase I High-Throughput screening (HTS) within the EPA ToxCast™ program. File will be updated with links to PubChem CIDs and SIDs for retrieving assay data, and with updates to chemical inventory as Program moves to Phase II and beyond.



U.S. Environmental Protection Agency

Distributed Structure-Searchable Toxicity (DSSTox) Public Database Network

Recent Additions | Contact Us | Print Version Search: GO

EPA Home > Research & Development > Computational Toxicology Research > DSSTox > StructureDataFiles > SDF Download Page: IRISTR

Home
About DSSTox
Work in Progress
Frequent Questions
Structure Data Files
Central Field Definition Table
Apps, Tools & More
DSSTox Community
Site Map
Glossary of Terms
Help

SDF Download Page:

IRISTR: EPA Integrated Risk Information System (IRIS) Toxicity Review Data *Database File*

** *New DSSTox* Database File *28July2007:*
- Replaces previously published IRISSI_v1a Structure-Index Locater File
- Added 34 new IRIS Source-Specific data fields.

- Description
- Source Website & Contact
- DSSTox Additions&Modifications
- Guidance for Use
- SDF Version History
- SDF Fields
- SDF Content Summary

- SDF Download Tab

- Acknowledgements, DSS

New Users: For general inform and their use in Chemical Relation s

Description: *The following des*

EPA's Integrated Risk Infor National Center for Environr found in the environment. IR substances for use in risk a training in toxicology, but w following categories:

- Oral reference doses
- Hazard identification,

File Types	Description	File Size	Format
Documentation Files			
Log File	IRISTR_LogFile_28Jul2007.pdf (PDF, 4 pp.)	38KB	PDF
Field Definition File	IRISTR_FieldDefFile_28Jul2007.pdf (PDF, 8 pp.)	75KB	PDF
	IRISTR_FieldDefFile_28Jul2007.doc	204KB	DOC
Data Files: *IRISTR*			
SDF Structure Data File	IRISTR_v1a_544_28Jul2007.sdf	*.zip 1.1 MB	SDF
• Data Table (no structures)	IRISTR_v1a_544_28Jul2007_nostructures.xls		XLS
• Structures Table	IRISTR_v1a_544_28Jul2007_structures.pdf (PDF, 11pp., 1.8MB)		PDF

File Error Report

U.S. Environmental Protection Agency

Integrated Risk Information System

Recent Additions | Contact Us | Print Version Search: GO

EPA Home > Browse EPA Topics > Human Health > Health Effects > IRIS Home > IRIS Search

- Recent Additions
- Newsroom
- Search IRIS
- Multiple Substance Reports
- What is IRIS?
- IRIS Guidance Documents
- Related L
- Downloac
- IRIS Traci
- Help

Search IRIS

The Search IRIS page enables users to find IRIS files, identify substances with similar toxicological properties, and conduct other comparative analyses of IRIS data. The CASRN and Keyword Search options enable users to determine whether a substance not included on the List of IRIS Substances is listed under a synonym or addressed in IRIS as part of a broader substance category (e.g., Lead and compounds, PCBs). The Keyword Search can also be used to locate information on general topics either within the IRIS summaries and Toxicological Reviews

Search IRIS by Keyword go

List of IRIS Substances

- (•) Full IRIS Summaries/Toxicological Reviews
- ( ) Entire IRIS Website

U.S. Environmental Protection Agency

Integrated Risk Information System

Recent Additions | Contact Us | Print Version Search: GO

EPA Home > Browse EPA Topics > Human Health > Health Effects > IRIS Home > IRIS Summaries

IRIS Substance List

The substances are listed in alphabetical order. You can click on the first letter of the substance you want which will bring you to the section that the substance is in, or use your browser's Find command to search for a substance name or Chemical Abstracts Service Registry Number typically about 15K to 40K in size, within a range from less

he Search page)

Search IRIS by Keyword go

List of IRIS Substances

- (•) Full IRIS Summaries/Toxicological Reviews
- ( ) Entire IRIS Website

Search by:
Chemical Name
CAS Registry #

A B C D E F G H I J K L M N O P Q R S T U V W X Y Z

Substance Name	Chemical Abstracts Service Registry Number (CASRN)	Last Significant Revision**
Acenaphthene • QuickView	CASRN 83-32-9	11/01/1990
Acenaphthylene • QuickView	CASRN 208-96-8	01/01/1991
Acephate • QuickView	CASRN 30560-19-1	05/01/1989
Acetaldehyde • QuickView	CASRN 75-07-0	10/01/1991

U.S. Environmental Protection Agency

Integrated Risk Information System

Recent Additions | Contact Us Search: All EPA IRIS Go

You are here: EPA Home » Human Health » IRIS » IRIS Summaries » IRIS Quickviews

Aniline Quickview (CASRN 62-53-3)

Quickview Navigation

- view Anilin

Health assessm
comprehensive
Regional Offices

Disclaimer: Thi
the Full IRIS Su

For definitions

Status of

File First On-Lin
Last Significant

Category (sec
Oral RfD Assess
Inhalation RfC As
Carcinogenicity As

Chronic Health Hazard Assessments for Noncarcinogenic Effects

Carcinogenicity Assessment for Lifetime Exposure

Weight of Evi

Weight of Evider

B2 (Probable hum

Weight of Evider

Induction of tumo
genetic toxicologi

This may be a syn

Principal and

- 20-26

Confidence in

- Study
- Databa
- RfC --

Quantitative Estimate of Carcinogenic Risk from Oral Exposure

Oral Slope Factor(s)	Extrapolation Method
5.7 x10^{-3} per mg/kg-day	Linearized multistage procedure, extra risk

Drinking Water Unit Risks
1.6x10^{-7} per ug/L

Risk Level	Concentration
E-4 (1 in 10,000)	6x10^{2} ug/L
E-5 (1 in 100,000)	6x10^{1} ug/L
E-6 (1 in 1,000,000)	6 ug/L

Dose-Response Data (Carcinogenicity, Oral Exposure)

Tumor Type: Spleen, combined fibrosarcoma, stromal sarcoma, capsular sarcoma and hemangiosarcoma
Test Species: Rat/CD-F, male
Route: Oral, Diet
Reference: CIIT, 1982

IRISTR SDF Fields (55 total)

DSSTox Standard Chemical Fields (18)

DSSTox Standard Toxicity Fields (3)

Oral_RfD_Assessed
Oral_RfD_CriticalEffects
Oral_RfD_mg_per_kg_day
Oral_RfD_mmol_per_kg_day
Oral_RfD_Notes
Oral_RfD_Confidence

Inhalation_RfC_Assessed
Inhalation_RfC_CriticalEffects
Inhalation_RfC_mg_per_m3
Inhalation_RfC_mmol_per_m3
Inhalation_RfC_Notes
Inhalation_RfC_Confidence

WtOfEvidence_Cancer_Assessed
WtOfEvidence_Cancer_Concern
WtOfEvidence_1986GuidelineCategories
WtOfEvidence_UpdatedGuidelineUsed
WtOfEvidence_Cancer_Narrative

DrinkingWater_OralSlope_Assessed
DrinkingWater_PrecursorEffect_TumorType
DrinkingWater_OralSlopeFactor_mg_per_kg_day
DrinkingWater_OralSlopeFactor_mmol_per_kg_day
DrinkingWater_ExtrapolationMethod_Notes
DrinkingWater_UnitRisk_microg_per_L
DrinkingWater_UnitRisk_micromol_per_L
DrinkingWater_StudyRoute

Inhalation_UnitRisk_Assessed
Inhalation_PrecursorEffect_TumorType
Inhalation_UnitRisk_microg_per_m3
Inhalation_UnitRisk_micromol_per_m3
Inhalation_StudyRoute
Inhalation_ExtrapolationMethod_Notes

TotalAssessments
Note_IRISTR
Website_URL (field contains chemical-specific links to IRIS "Quick View

IRISTR Toxicity Review Areas	Totals_v1a*
Oral RfDs	357
Inhalation RfCs	70
Weight of Evidence Characterizations	243
Oral Slope Factors/Drinking Water Unit Risks	76
Air Unit Risks	54
Total Assessments	800

Number of IRISTR Toxicity Review Assessments per Chemical	Totals_v1a**
0	(39)
1	323
2	101
3	54
4	22
5	5
Total Assessments	800

Part IV.

Data Linkages

U.S. ENVIRONMENTAL PROTECTION AGENCY

Distributed Structure-Searchable Toxicity (DSSTox) Public Database Network

Bookmark

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You are here: EPA Home » Computational Toxicology Research » Distributed Structure-Searchable Toxicity (DSSTox) Public Database Network

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

DSSTox

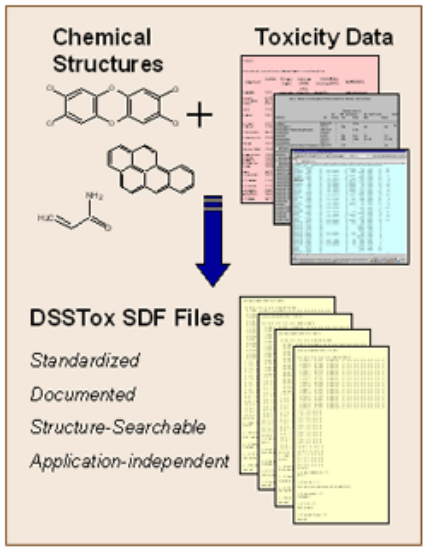
http://www.epa.gov/ncct/dsstox/

Distributed Structure-Searchable Toxicity (DSSTox) Database Network is a project of EPA's National Center for Computational Toxicology, helping to build a public data foundation for improved structure-activity and predictive toxicology capabilities. The DSSTox website provides a public forum for publishing downloadable, structure-searchable, standardized chemical structure files associated with toxicity data. More>

EPA DSSTox Structure-Browser GO

Click

DSSTox Structure-Browser information Page



- DSSTox Graphic Flowchart
- DSSTox Project Goals
- DSSTox Publications

29 April 2008

- Minor QA revisions to TOXCST and CPDBAS.

24 April 2008

- NTPBSI: National Toxicology Program Bioassay On-line Database Structure-Index Locator File ** *Updated to v3a*

- All current DSSTox Data File substance inventories are now available in PubChem, with explicit DSSTox bioassay summary data provided for main data files (see listing below).

Note: Updated instructions and PubChem_SID txt files for use in searching and retrieving PubChem data for DSSTox substances will soon be posted on this website (*est. May 2008*).

25 February 2008

***File Updates and Enhancements:**

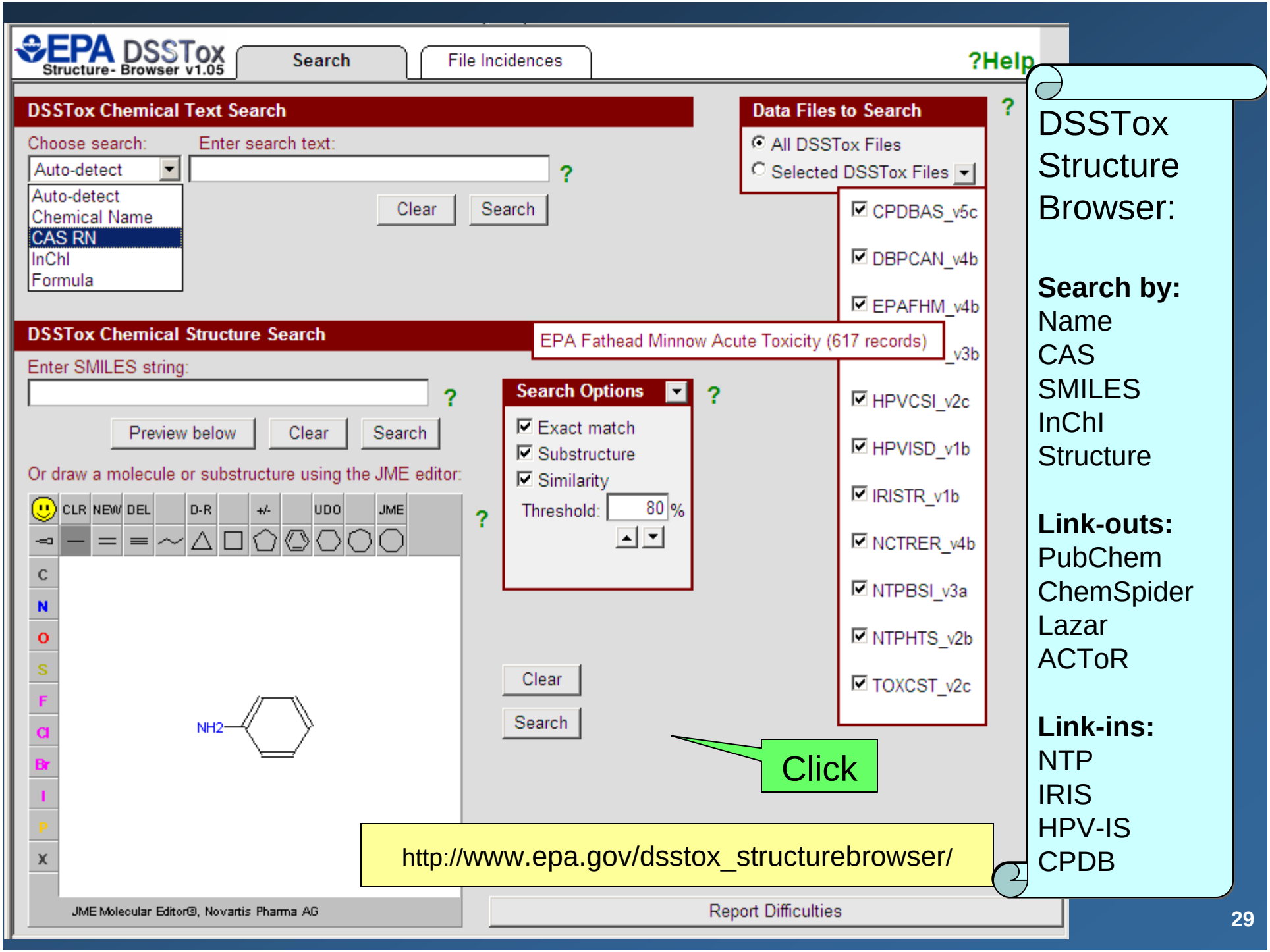
- Addition of new DSSTox Standard Chemical Field to all files: STRUCTURE_InChIKey

- Additional QA review, structure/CAS modifications, elimination of abbreviations in field entries, etc.

DSSTox Data Files: Details>

CPDBAS_v5c_1547_29Apr2008 *revise
DBPCAN_v4b_209_15Feb2008
EPAFHM_v4b_617_15Feb2008
FDAMDD_v3b_1216_15Feb2008
HPVCSI_v2c_3548_15Feb2008
HPVISD_v1b_1006_15Feb2008
IRISTR_v1b_544_15Feb2008
NCTRER_v4b_232_15Feb2008
NTPBSI_v3a_2303_24Apr2008 *update
NTPHTS_v1b_1408_15Jul2008
TOXCST_v2c_320_29Apr2008 *revise

>Other (non-DSSTox) Data Files



DSSTox Structure Browser:

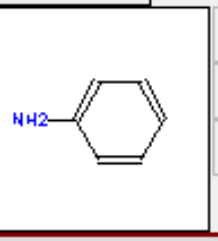
Search by:
Name
CAS
SMILES
InChI
Structure

Link-outs:
PubChem
ChemSpider
Lazar
ACToR

Link-ins:
NTP
IRIS
HPV-IS
CPDB

EPA DSSTox Structure- Browser v1.05 | Search | File Incidences | ?Help

Search Results Summary for DSSTox Substances - File Breakdown Incidences

Query	Results Type	Hits	Display
Structure: 	Exact matches	1	Details
	Substructures	1129	Details
	Similarity ≥ 76.1%	11	Details

Click

?

External Resources: PubChem | EPA ACToR | ChemSpider | Lazar in silico tox

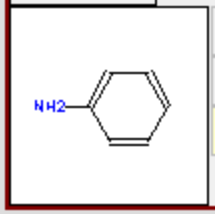
DSSTox File ?	Total#Records	Exact matches	Substructures	Similarity ≥ 76.1%
CPDBAS_v5c	1547	1	315	9
DBPCAN_v4b	209	-	1	-
EPAFHM_v4b	617	1	102	1
FDAMDD_v3b	1216	-	261	-
HPVCSI_v2c	3548	1	219	4
HPVISD_v1b	1006	-	48	-
IRISTR_v1b	544	1	68	2
NCTRER_v4b	232	-	10	-
NTPBSI_v3a	2303	1	496	8
NTPHTS_v2b	1408	1	313	6
TOXCST_v2c	320	-	72	-
Total Unique Substance Hits		**1**	**1129**	**11**
Total Substance Hits - All Files		**6**	**1905**	**30**

?

EPA DSSTox Structure- Browser v1.05

Search | File Incidences | Search Details | ?Help

Details

Query	Results Type	Hits	Display
Structure: 	Exact matches	1	Details
	Substructures	1129	Details
	Similarity ≥ 76.1%	11	Details

?

Output Options

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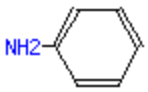
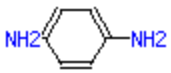
?

External Resources

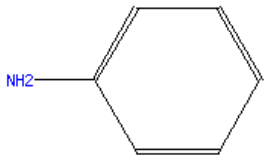
PubChem | EPA ACToR | ChemSpider | Lazar in silico tox

? DSSTox Substance ID | ? Similarity Score% | Structure Match | Substance Name | CASRN | Substance Description | Details (Data Files)

Click SS to submit displayed structure for structure search.

DSSTox Substance ID	Similarity Score%	Structure Match	Substance Name	CASRN	Substance Description	Details (Data Files)
20090	100	 SS	Aniline	62-53-3	single chemical compound	CPDBAS EPAFHM HPVCSI IRISTR NTPBSI NTPHTS
20091	94.1	 SS	Aniline.HCl	142-04-1	single chemical compound	CPDBAS NTPBSI
21138	94.1	 SS	p-Phenylenediamine	106-50-3	single chemical compound	CPDBAS HPVCSI

Click



IRISTR:
EPA Integrated Risk Information System (IRIS) Structure-Index Locator File (544 records)

IRISTR_v1b_544_15Feb2008

IRISTR Source Website

View IRIS Chemical Substance Data Page

Click

Output Options

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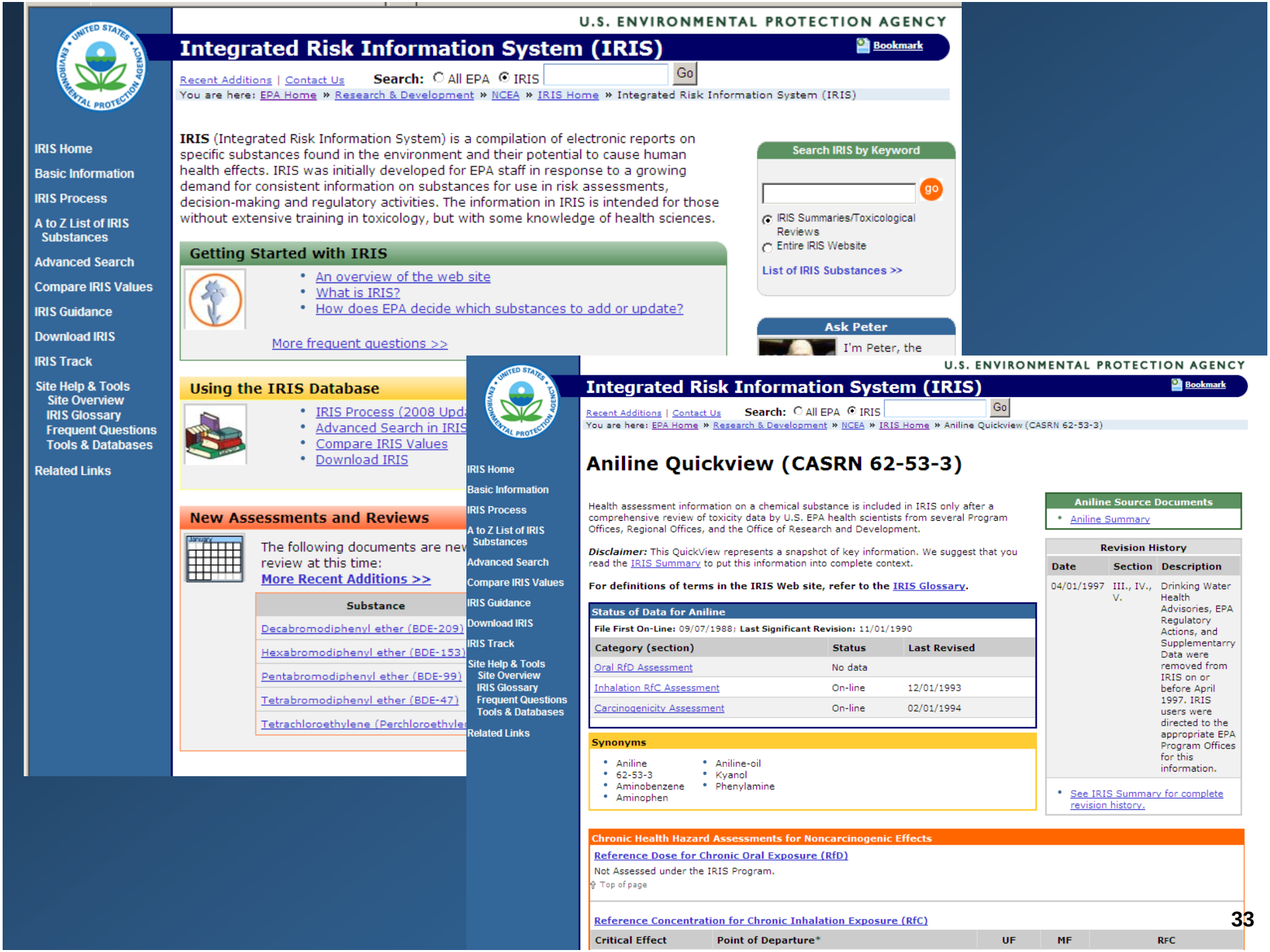
External Resources

PubChem | EPA ACToR | ChemSpider | Lazar in silico tox

DSSTox_RID	23877
DSSTox_Generic_SID	20090
TestSubstance_ChemicalName	Aniline
TestSubstance_CASRN	62-53-3
TestSubstance_Description	single chemical compound
STRUCTURE_Shown	tested chemical
StudyType	Human Health Exposure Toxicity Review for Risk Assessment
Endpoint	cancer; acute; short-term; sub-chronic; chronic; developmental
Species	rodent; human; dog; rabbit
Oral_RfD_Assessed	0
Oral_RfD_CriticalEffects	Not assessed under the IRIS program.
Inhalation_RfC_Assessed	1
Inhalation_RfC_CriticalEffects	mild spleen toxicity
Inhalation_RfC_mg_per_m3	0.001 mg/m3
Inhalation_RfC_mmol_per_m3	1.07380820711613E-05 mmol/m3
Inhalation_RfC_Notes	NOAEL (No observed adverse effect level) HEC (Human Equivalent Concentration): 3.4 mg/m3
Inhalation_RfC_Confidence	Low
WtOfEvidence_Cancer_Assessed	1
WtOfEvidence_Cancer_Concern	Medium
WtOfEvidence_1986GuidelineCategories	B2; Probable human carcinogen - based on sufficient evidence of carcinogenicity in animals
WtOfEvidence_Cancer_Narrative	Induction of tumors of the spleen and the body cavity in two strains of rat; and some supporting genetic toxicological evidence.
DrinkingWater_OralSlope_Assessed	1
DrinkingWater_PrecursorEffect_TumorType	spleen; combined fibrosarcoma; stromal sarcoma; capsular sarcoma; hemangiosarcoma
DrinkingWater_OralSlopeFactor_mg_per_kg_day	0.0057 mg/kg-bw/day
DrinkingWater_OralSlopeFactor_mmol_per_kg_day	6.12070678056192E-05 mmol/kg-bw/day
DrinkingWater_ExtrapolationMethod_Notes	Linearized multistage procedure; extra risk; units per mg/kg-day
DrinkingWater_UnitRisk_microg_per_L	0.00000016 microg/L
DrinkingWater_UnitRisk_micromol_per_L	1.7180931313858E-09 micromol/L
DrinkingWater_StudyRoute	oral; diet
Inhalation_UnitRisk_Assessed	0
Inhalation_PrecursorEffect_TumorType	Not assessed under the IRIS program.
TotalAssessments	3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IRIS (Integrated Risk Information System) is a compilation of electronic reports on specific substances found in the environment and their potential to cause human health effects. IRIS was initially developed for EPA staff in response to a growing demand for consistent information on substances for use in risk assessments, decision-making and regulatory activities. The information in IRIS is intended for those without extensive training in toxicology, but with some knowledge of health sciences.
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The following documents are nev
review at this time:
More Recent Additions >>
Substance
Decabromodiphenyl ether (BDE-209)
Hexabromodiphenyl ether (BDE-153)
Pentabromodiphenyl ether (BDE-99)
Tetrabromodiphenyl ether (BDE-47)
Tetrachloroethylene (Perchloroethyle
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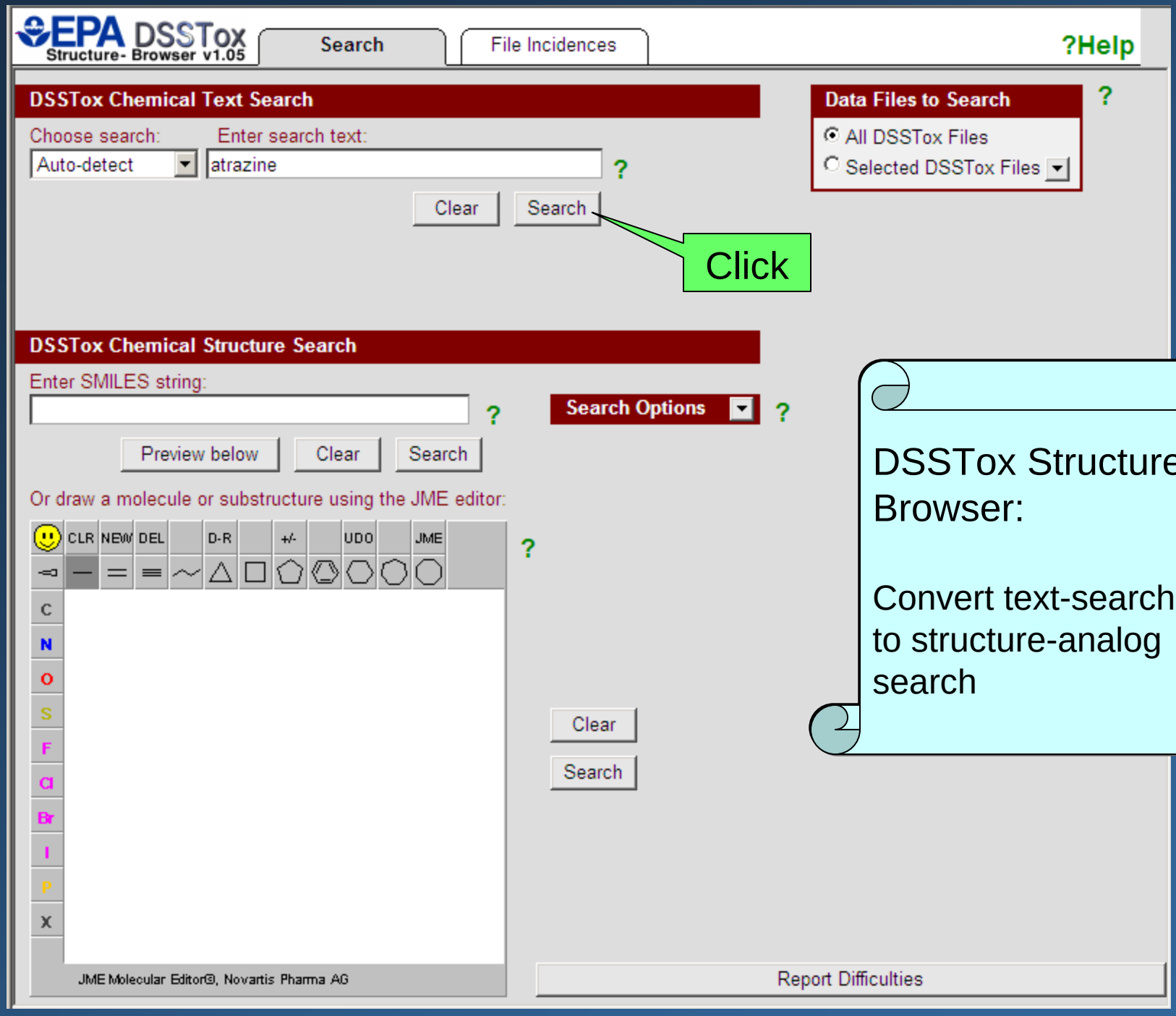
You are here: EPA Home » Research & Development » NCEA » IRIS Home » Aniline Quickview (CASRN 62-53-3)
Aniline Quickview (CASRN 62-53-3)
Health assessment information on a chemical substance is included in IRIS only after a comprehensive review of toxicity data by U.S. EPA health scientists from several Program Offices, Regional Offices, and the Office of Research and Development.
Disclaimer: This QuickView represents a snapshot of key information. We suggest that you read the IRIS Summary to put this information into complete context.
For definitions of terms in the IRIS Web site, refer to the IRIS Glossary.
Aniline Source Documents
Aniline Summary
Revision History
Date | Section | Description
04/01/1997 | III., IV., V. | Drinking Water Health Advisories, EPA Regulatory Actions, and Supplementarry Data were removed from IRIS on or before April 1997. IRIS users were directed to the appropriate EPA Program Offices for this information.
See IRIS Summary for complete revision history.
Status of Data for Aniline
File First On-Line: 09/07/1988; Last Significant Revision: 11/01/1990
Category (section) | Status | Last Revised
Oral RfD Assessment | No data
Inhalation RfC Assessment | On-line | 12/01/1993
Carcinogenicity Assessment | On-line | 02/01/1994
Synonyms
Aniline
62-53-3
Aminobenzene
Aminophen
Aniline-oil
Kyanol
Phenylamine
Chronic Health Hazard Assessments for Noncarcinogenic Effects
Reference Dose for Chronic Oral Exposure (RfD)
Not Assessed under the IRIS Program.
Top of page
Reference Concentration for Chronic Inhalation Exposure (RfC)
Critical Effect | Point of Departure* | UF | MF | RfC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Structure- Browser v1.05
Search
File Incidences
?Help
DSSTox Chemical Text Search
Choose search:
Enter search text:
Auto-detect
atrazine
Clear
Search
Click
Data Files to Search
All DSSTox Files
Selected DSSTox Files
DSSTox Chemical Structure Search
Enter SMILES string:
Search Options
Preview below
Clear
Search
Or draw a molecule or substructure using the JME editor:
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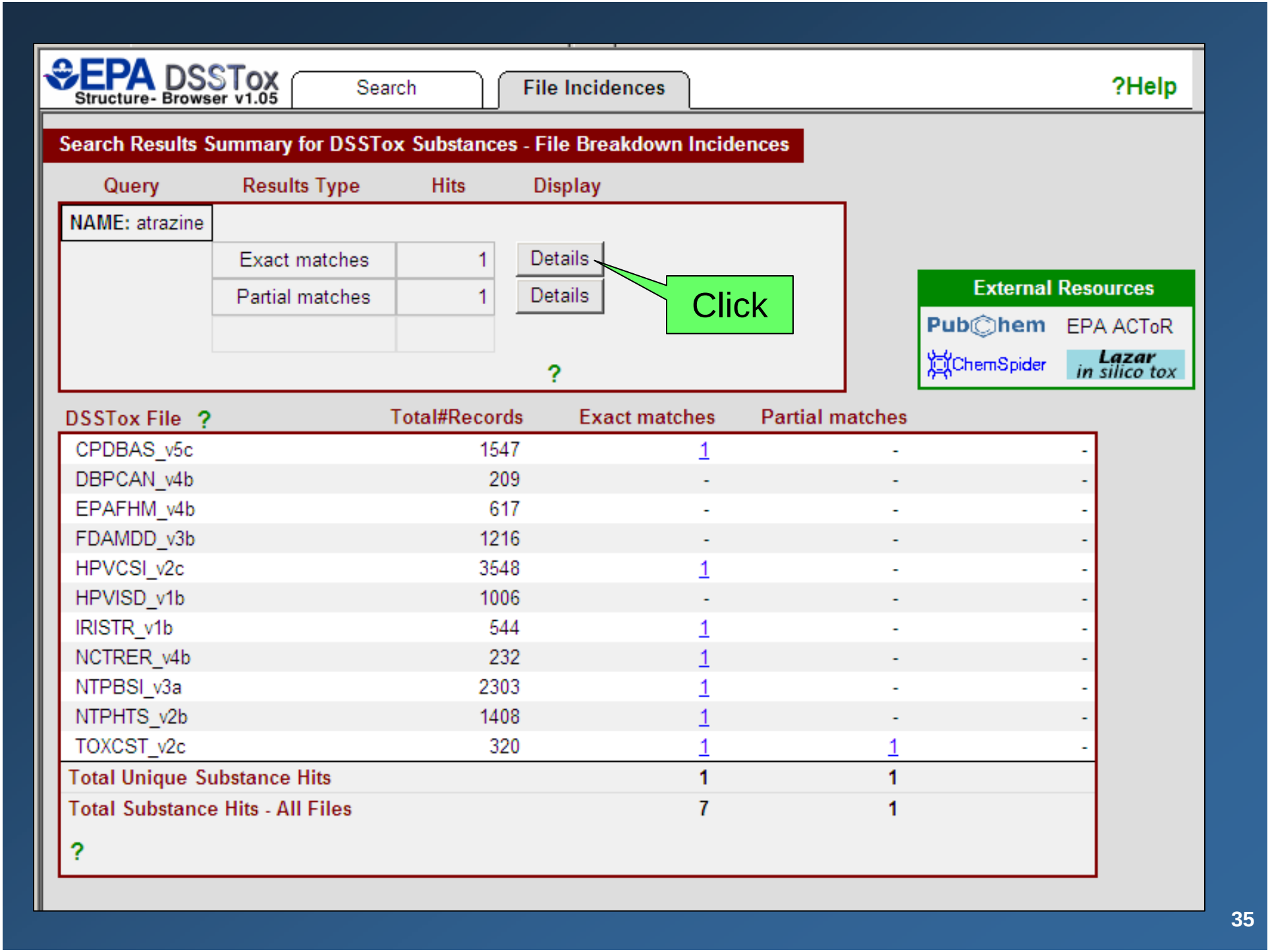
NEW
DEL
D-R
+/-
UDO
JME
C
N
O
S
F
Cl
Br
I
P
X
JME Molecular Editor©, Novartis Pharma AG
Clear
Search
Report Difficulties
DSSTox Structure Browser:
Convert text-search to structure-analog search


EPA DSSTox
Structure- Browser v1.05
Search
File Incidences
?Help
Search Results Summary for DSSTox Substances - File Breakdown Incidences
Query
Results Type
Hits
Display
NAME: atrazine
Exact matches
1
Details
Partial matches
1
Details
Click
?
External Resources
PubChem
EPA ACToR
ChemSpider
Lazar in silico tox
DSSTox File ?
Total#Records
Exact matches
Partial matches
CPDBAS_v5c 1547 1 - -
DBPCAN_v4b 209 - - -
EPAFHM_v4b 617 - - -
FDAMDD_v3b 1216 - - -
HPVCSI_v2c 3548 1 - -
HPVISD_v1b 1006 - - -
IRISTR_v1b 544 1 - -
NCTRER_v4b 232 1 - -
NTPBSI_v3a 2303 1 - -
NTPHTS_v2b 1408 1 - -
TOXCST_v2c 320 1 1 -
Total Unique Substance Hits 1 1
Total Substance Hits - All Files 7 1
?

EPA DSSTox Structure- Browser v1.05

Search | File Incidences | Search Details | ?Help

Details

Query	Results Type	Hits	Display
NAME: atrazine	Exact matches	1	Details
	Partial matches	1	Details

?

Output Options

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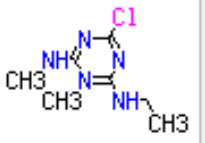
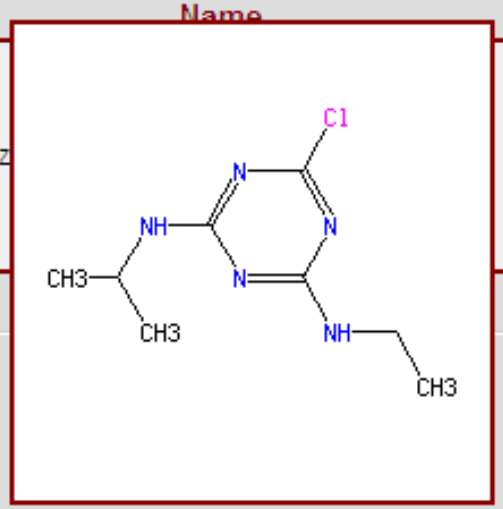
External Resources

PubChem | EPA ACToR | ChemSpider | Lazar in silico tox

? Click SS to submit displayed structure for structure search.

? DSSTox Substance ID	? Similarity Score%	Structure Match	Substance Name	CASRN	Substance Description	Details (Data Files)
20112	100	 SS	Atraz	1912-24-9	single chemical compound	CPDBAS IRISTR NTPBSI TOXCST HPVCSI NCTRER NTPHTS

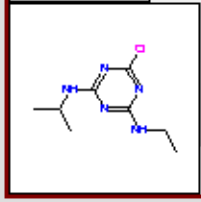


Click to submit for structure search

EPA DSSTox Structure- Browser v1.05

Search | File Incidences | Search Details | ?Help

Details

Query	Results Type	Hits	Display
Structure: 	Exact matches	1	Details
	Substructures	2	Details
	Similarity ≥ 51.2%	12	Details

?

Output Options

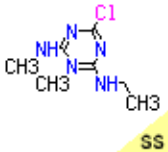
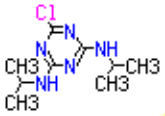
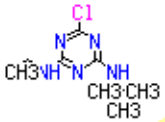
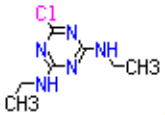
Choose Format | Save | Print

?

External Resources

PubChem | EPA ACToR | ChemSpider | Lazar in silico tox

Click SS to submit displayed structure for structure search.

? DSSTox Substance ID	? Similarity Score%	Structure Match	Substance Name	CASRN	Substance Description	Details (Data Files)
20112	100	 SS	Atrazine	1912-24-9	single chemical compound	CPDBAS HPVCSI IRISTR NCTRER NTPBSI NTPHTS TOXCST
21196	99	 SS	Propazine	139-40-2	single chemical compound	CPDBAS HPVCSI IRISTR TOXCST
27608	96.3	 SS	1,3,5-Triazine-2,4-diamine, 6-chloro-N-(1,1-dimethylethyl)-N'-ethyl-	5915-41-3	single chemical compound	HPVCSI
21268	96.2	 SS	Simazine	122-34-9	single chemical compound	CPDBAS HPVCSI IRISTR NCTRER TOXCST

EPA DSSTox Structure- Browser v1.05

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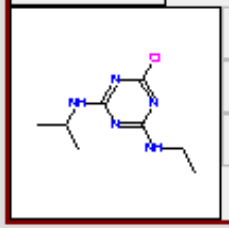
Search Results Summary for DSSTox Substances - File Breakdown Incidences

Query	Results Type	Hits	Display
Structure: 	Exact matches	1	Details
	Substructures	2	Details
	Similarity ≥ 51.2%	12	Details

?

Click

External Resources

PubChem | EPA ACToR | ChemSpider | Lazar in silico tox

DSSTox File ?	Total#Records	Exact matches	Substructures	Similarity ≥ 51.2%
CPDBAS_v5c	1547	1	2	4
DBPCAN_v4b	209	-	-	-
EPAFHM_v4b	617	-	-	-
FDAMDD_v3b	1216	-	-	1
HPVCSI_v2c	3548	1	2	4
HPVISD_v1b	1006	-	-	-
IRISTR_v1b	544	1	2	8
NCTRER_v4b	232	1	1	3
NTPBSI_v3a	2303	1	1	3
NTPHTS_v2b	1408	1	1	1
TOXCST_v2c	320	1	2	9
Total Unique Substance Hits		**1**	**2**	**12**
Total Substance Hits - All Files		**7**	**11**	**33**

?

NCBI PubChem Compound

PubChem Compound | GO

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PubChem » Compound Summary

atrazine - Compound Summary (CID: 2256)

A selective triazine herbicide. Inhalation hazard is low and there are no apparent skin manifestations or other toxicity in humans. Acutely poisoned sheep and cattle may show muscular spasms, fasciculations, stiff gait, increased respiratory rates, adrenal degeneration, and congestion of the lungs, liver, and kidneys. (From The Merck Index, 11th ed)

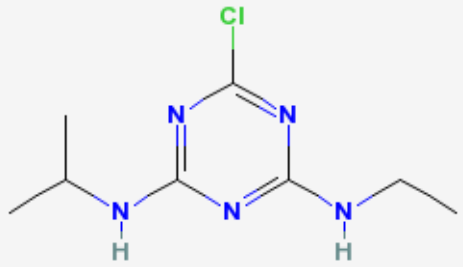

Table of Contents

- Drug and Chemical Info
- BioActivity Results
- Synonyms
- Properties
- Descriptors
- Compound Info
- Substance Info
  - Category
- Exports

Compound ID	**2256**
Molecular Weight	215.68326 [g/mol]
Molecular Formula	$C_8H_{14}ClN_5$
XLogP	1.7
H-Bond Donor	2
H-Bond Acceptor	5

Drug and Chemical Info from MeSH: (Total:1)

Atrazine

Pharmacological Action

Herbicides

Classification

Heterocyclic Compounds

Heterocyclic Compounds, 1-Ring

Triazines

Atrazine

Click

Links

Protein Structure (1)

NLM Toxicology Link

Chemical Structure Search

BioActivity Summary:

This Compound

with Similar Compounds

United States National Library of Medicine

ChemIDplus Advanced

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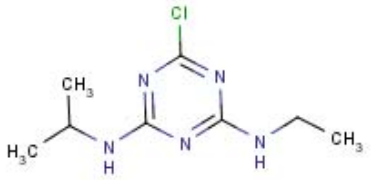
Env. Health & Toxicology | TOXNET | ChemIDplus Lite | Advanced

NAME: Atrazine [ANSI:BSI:ISO]
RN: 1912-24-9



MW: 215.687
Enlarge Structure

Basic Information

- Full Record
- Structure
- Names & Synonyms
- Formulas
- Classification Codes
- Registry Numbers
- Notes
- Toxicity
- Physical Properties

For more information about this substance, you may select from the the links below.

File Locator

CCRIS	NCI Chem Carcino Res Info Sys
DART	Developmental and Reprod.Tox.
EINECS	EU Inv of Exist. Comm. Chem Sub
EMIC	Env. Mutagen Info. Center
GENETOX	EPA GENetic TOXicology
HSDB	Hazardous Substances Data Bank
Haz-Map	Occ. Exposure to Haz. Agents
Household Products	Household Products Database
IRIS	EPA Integrated Risk Info. System
ITER	International Tox. Est. for Risk
MeSH	Medical Subject Headings File
MeSH Heading	Medical Subject Headings
PubChem	PubChem
PubMed	Biomedical Citations From PubMed
PubMed Cancer	Cancer Citations from PubMed
PubMed Toxicology	Toxicology Citations From PubMed
RTECS	Reg. of Toxic Eff. of Chem. Sub.
TOXLINE	NLM TOXLINE on TOXNET

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- Start New Query
- Modify Query
- Show Query
- Search History
- Structure Similarity Search
- Structure Salt/Parent Search
- Transfer Structure
- Basic ChemIDplus Search

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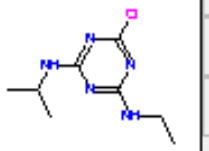
Search Results Summary for DSSTox Substances - File Breakdown Incidences

Query	Results Type	Hits	Display
Structure: 	Exact matches	1	Details
	Substructures	2	Details
	Similarity ≥ 51.2%	12	Details

?

Click

External Resources

PubChem EPA ACToR ChemSpider Lazar in silico tox

DSSTox File ?	Total#Records	Exact matches	Substructures	Similarity ≥ 51.2%
CPDBAS_v5c	1547	1	2	4
DBPCAN_v4b	209	-	-	-
EPAFHM_v4b	617	-	-	-
FDAMDD_v3b	1216	-	-	1
HPVCSI_v2c	3548	1	2	4
HPVISD_v1b	1006	-	-	-
IRISTR_v1b	544	1	2	8
NCTRER_v4b	232	1	1	3
NTPBSI_v3a	2303	1	1	3
NTPHTS_v2b	1408	1	1	1
TOXCST_v2c	320	1	2	9
Total Unique Substance Hits		**1**	**2**	**12**
Total Substance Hits - All Files		**7**	**11**	**33**

?

InChI=1/C8H14ClN5/c1-4-10-7-12-6(9)13-8(14-7)11-...

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Building a Structure Centric Community for Chemists

Search...

Home Search Services Resources About Login

Top
Inherent Properties
Predicted Properties
Focused Libraries
Data Sources
Synonyms
Database IDs
Miscellaneous
LASSO
Spectra
Images
CIFs
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Inherent Properties, Identifiers and References

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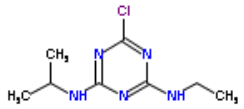

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Quick Links: Permalink Similar Isomers

ChemSpider ID:	2169
Empirical Formula:	$C_8H_{14}ClN_5$
Molecular Weight:	215.6833
Nominal Mass:	215 Da
Average Mass:	215.6833 Da
Monoisotopic Mass:	215.093773 Da

Systematic Name:	6-chloro-N'-ethyl-N-isopropyl-1,3,5-triazine-2,4-diamine
SMILES:	Clc1nc(nc(n1)NC(C)C)NCC
InChI:	InChI=1/C8H14ClN5/c1-4-10-7-12-6(9)13-8(14-7)11-5(2)3/h5H,4H2,1-3H3,(H2,10,11,12,13,14)
InChIKey:	MXWJVTOOROXGIU-UHFFFAOYAJ

Wikipedia Article(s)

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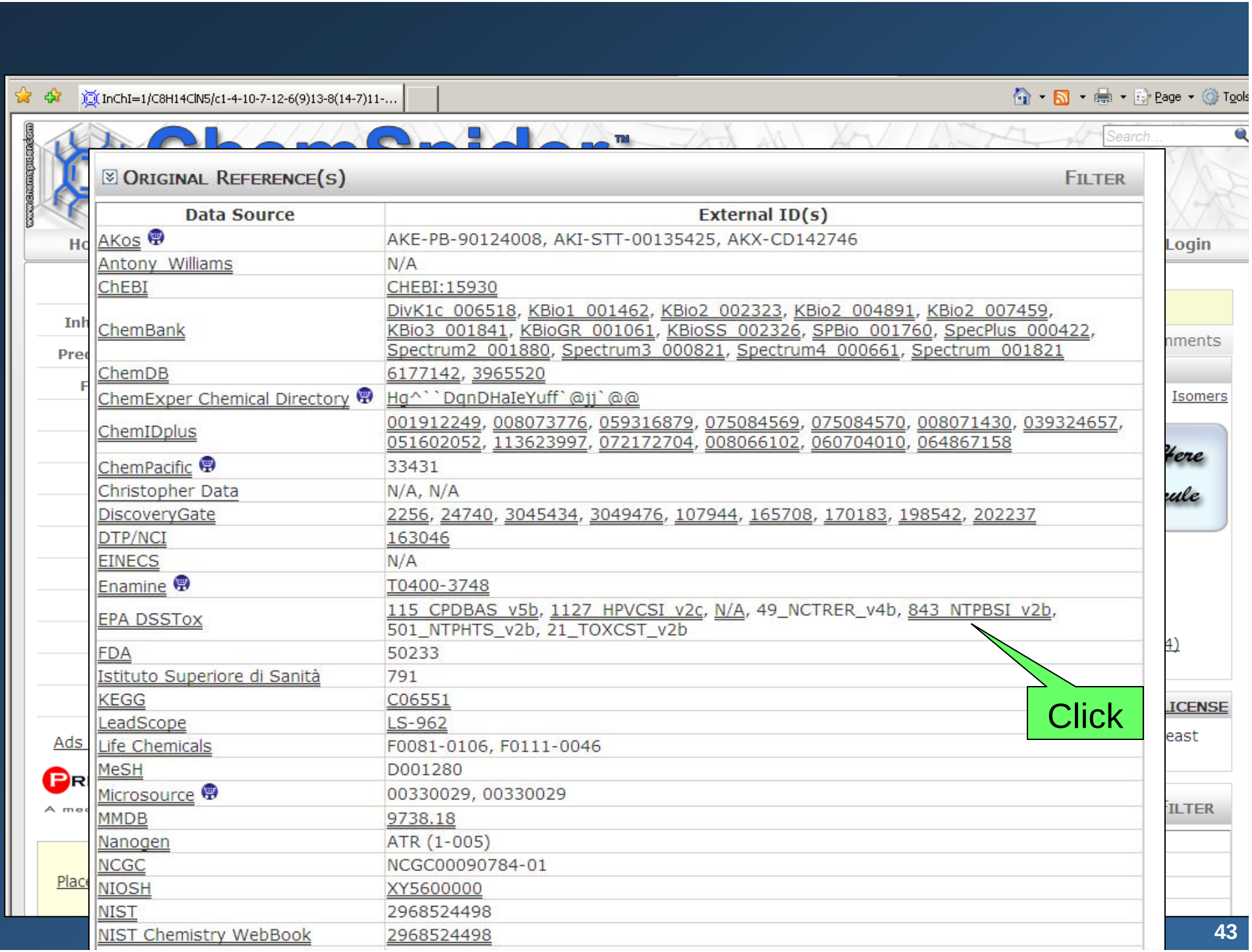
Candex is a dietary supplement manufactured by Pure Essence. It is marketed as an enzymatic remedy to treat the yeast infection CandidaPure Essence Labs., but is unapproved. Read more... or Edit at Wikipedia...

Original Reference(s)

Filter

Data Source	External ID(s)
AKos	AKE-PB-90124008, AKI-STT-00135425, AKX-CD142746
Antony Williams	N/A
ChEBI	CHEBI:15930


InChI=1/C8H14ClN5/c1-4-10-7-12-6(9)13-8(14-7)11-...
Page
Tools
ChemSpider™
Search...
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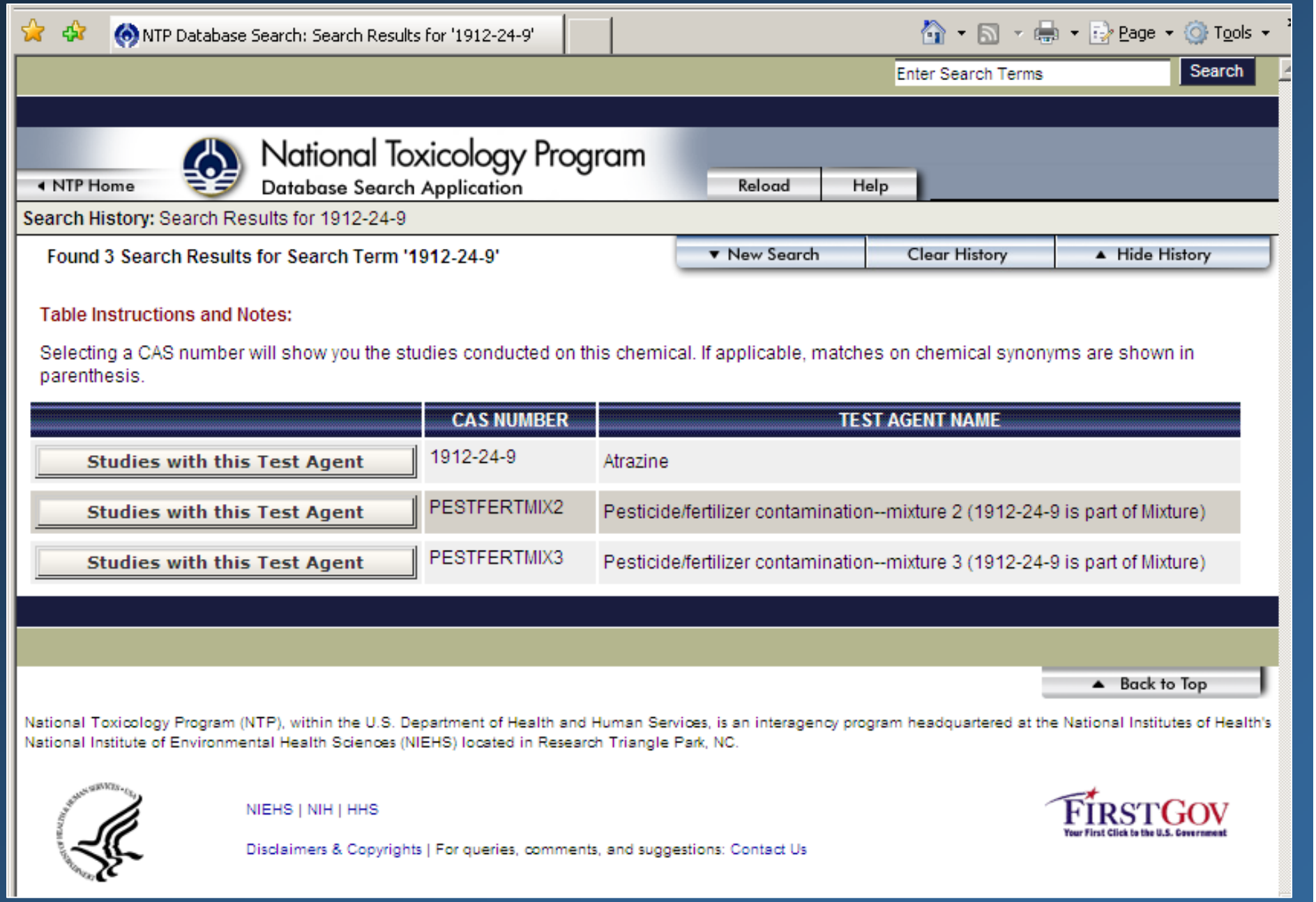
ORIGINAL REFERENCE(S)
FILTER
Data Source
External ID(s)
AKos
AKE-PB-90124008, AKI-STT-00135425, AKX-CD142746
Antony_Williams
N/A
ChEBI
CHEBI:15930
ChemBank
DivK1c_006518, KBio1_001462, KBio2_002323, KBio2_004891, KBio2_007459, KBio3_001841, KBioGR_001061, KBioSS_002326, SPBio_001760, SpecPlus_000422, Spectrum2_001880, Spectrum3_000821, Spectrum4_000661, Spectrum_001821
ChemDB
6177142, 3965520
ChemExper Chemical Directory
Hg^``DqnDHaIeYuff`@jj`@@
ChemIDplus
001912249, 008073776, 059316879, 075084569, 075084570, 008071430, 039324657, 051602052, 113623997, 072172704, 008066102, 060704010, 064867158
ChemPacific
33431
Christopher Data
N/A, N/A
DiscoveryGate
2256, 24740, 3045434, 3049476, 107944, 165708, 170183, 198542, 202237
DTP/NCI
163046
EINECS
N/A
Enamine
T0400-3748
EPA DSSTox
115_CPDBAS_v5b, 1127_HPVCSI_v2c, N/A, 49_NCTRER_v4b, 843_NTPBSI_v2b, 501_NTPHTS_v2b, 21_TOXCST_v2b
FDA
50233
Istituto Superiore di Sanità
791
KEGG
C06551
LeadScope
LS-962
Life Chemicals
F0081-0106, F0111-0046
MeSH
D001280
Microsource
00330029, 00330029
MMDB
9738.18
Nanogen
ATR (1-005)
NCGC
NCGC00090784-01
NIOSH
XY5600000
NIST
2968524498
NIST Chemistry WebBook
2968524498
Click


NTP Database Search: Search Results for '1912-24-9'
Page
Tools
Enter Search Terms
Search
National Toxicology Program
Database Search Application
NTP Home
Reload
Help
Search History: Search Results for 1912-24-9
Found 3 Search Results for Search Term '1912-24-9'
New Search
Clear History
Hide History
Table Instructions and Notes:
Selecting a CAS number will show you the studies conducted on this chemical. If applicable, matches on chemical synonyms are shown in parenthesis.
CAS NUMBER
TEST AGENT NAME
Studies with this Test Agent
1912-24-9
Atrazine
Studies with this Test Agent
PESTFERTMIX2
Pesticide/fertilizer contamination--mixture 2 (1912-24-9 is part of Mixture)
Studies with this Test Agent
PESTFERTMIX3
Pesticide/fertilizer contamination--mixture 3 (1912-24-9 is part of Mixture)
Back to Top
National Toxicology Program (NTP), within the U.S. Department of Health and Human Services, is an interagency program headquartered at the National Institutes of Health's National Institute of Environmental Health Sciences (NIEHS) located in Research Triangle Park, NC.
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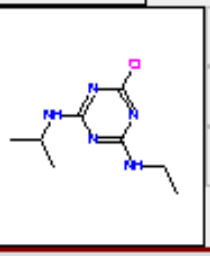
EPA DSSTox Structure- Browser v1.05

Search | File Incidences | ?Help

Search Results Summary for DSSTox Substances - File Breakdown Incidences

Query	Results Type	Hits	Display
Structure: 	Exact matches	1	Details
	Substructures	2	Details
	Similarity ≥ 51.2%	12	Details

?

External Resources

PubChem EPA ACToR

ChemSpider Lazar in silico tox

Click

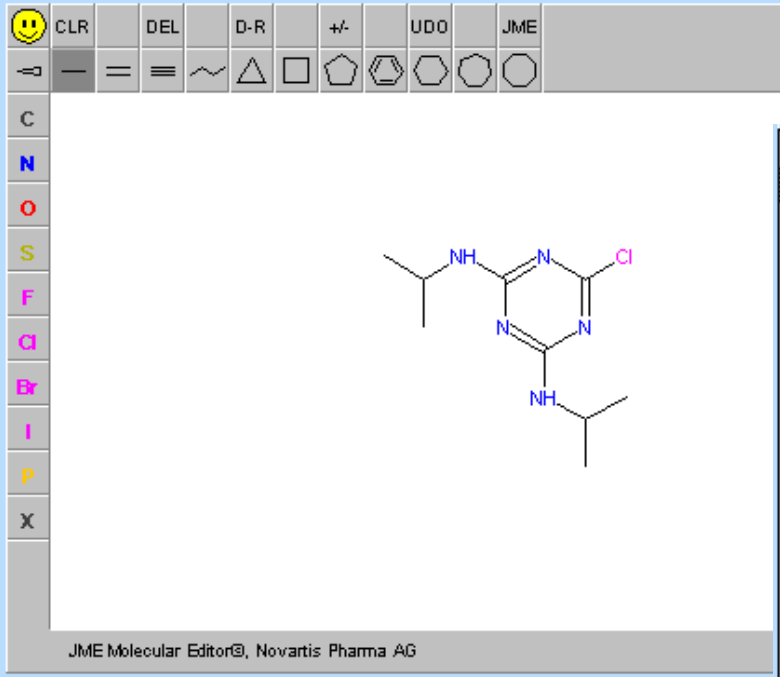
DSSTox File ?	Total#Records	Exact matches	Substructures	Similarity ≥ 51.2%
CPDBAS_v5c	1547	1	2	4
DBPCAN_v4b	209	-	-	
EPAFHM_v4b	617	-	-	
FDAMDD_v3b	1216	-	-	1
HPVCSI_v2c	3548	1	2	4
HPVISD_v1b	1006	-	-	-
IRISTR_v1b	544	1	2	8
NCTRER_v4b	232	1	1	3
NTPBSI_v3a	2303	1	1	3
NTPHTS_v2b	1408	1	1	1
TOXCST_v2c	320	1	2	9
Total Unique Substance Hits		1	2	12
Total Substance Hits - All Files		7	11	33

?

Lazar Toxicity Predictions

Input | Validation | Documentation

1. Draw a chemical structure (help)

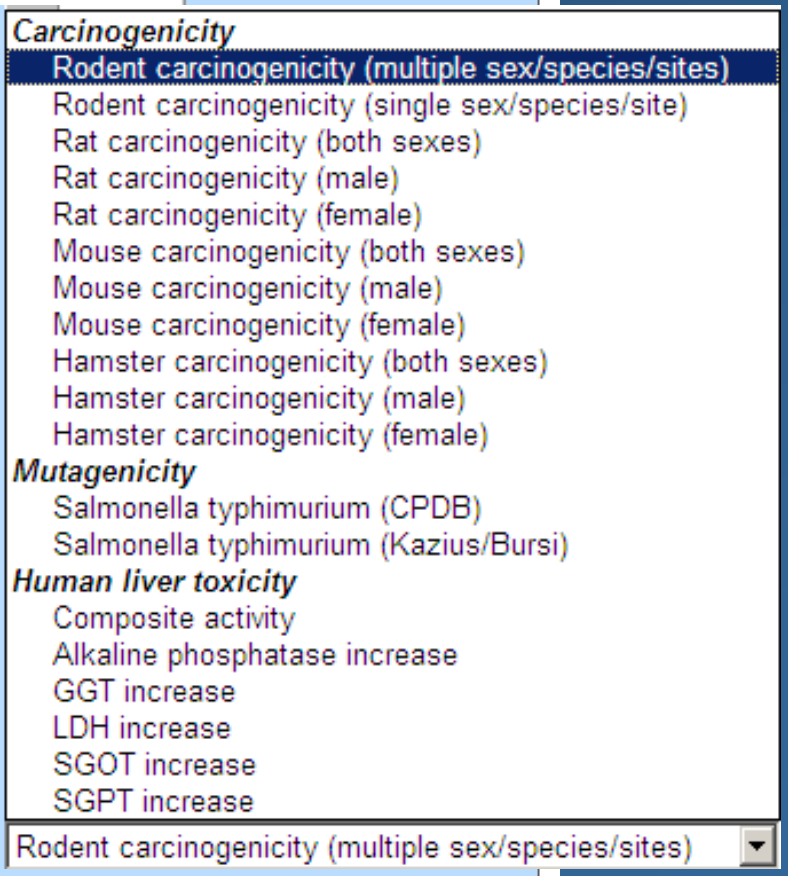


or enter the SMILES string

ClC1=NC(=NC(=N1)NC(C)C)NC(C)C

2. Select a toxic endpoint

Rodent carcinogenicity (multiple sex/species/sites)

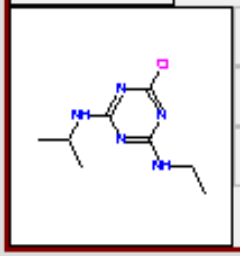


3. Predict

EPA DSSTox Structure- Browser v1.05

Search | File Incidences | ?Help

Search Results Summary for DSSTox Substances - File Breakdown Incidences

Query	Results Type	Hits	Display
Structure: 	Exact matches	1	Details
	Substructures	2	Details
	Similarity ≥ 51.2%	12	Details

?

External Resources

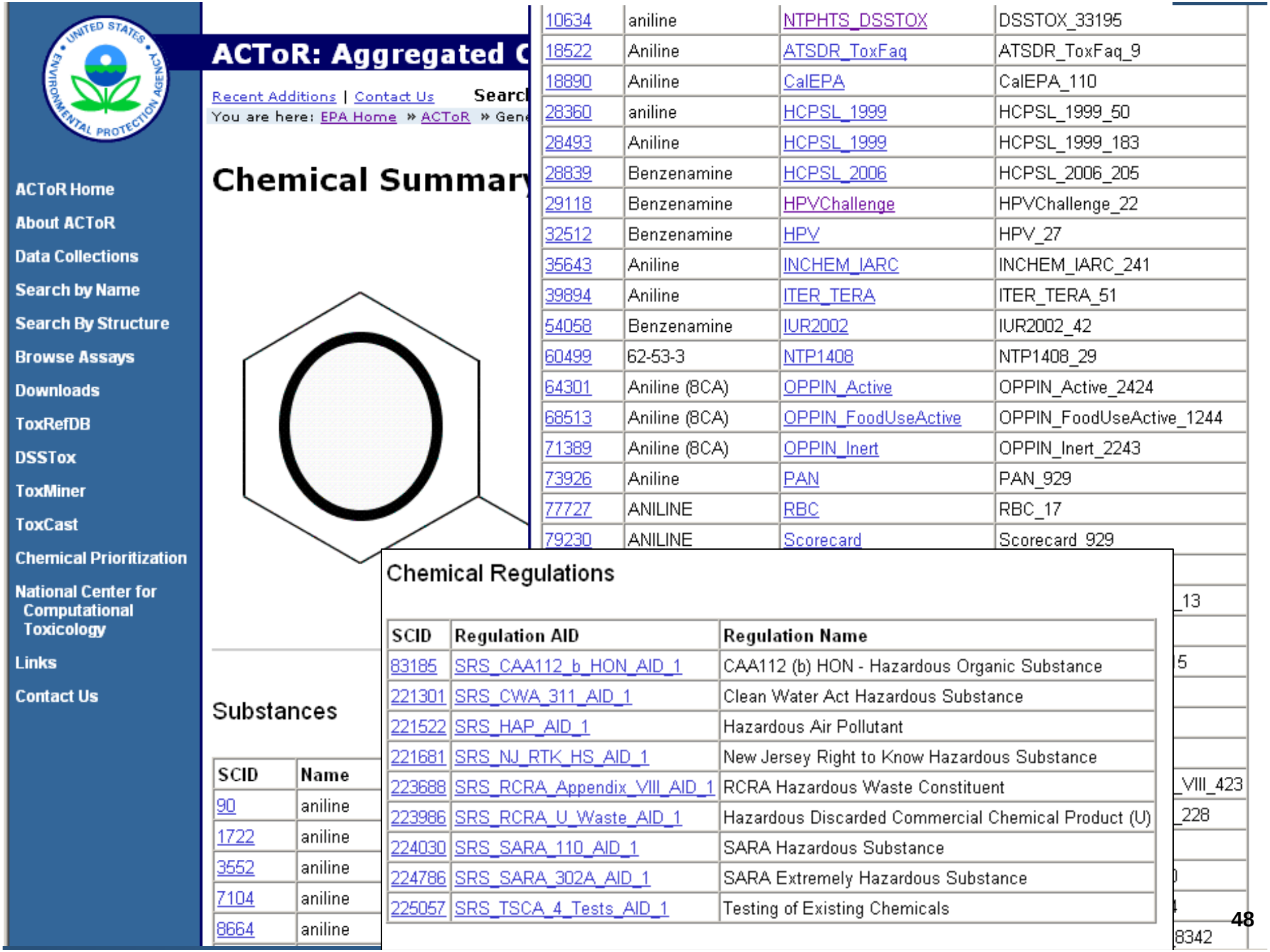
PubChem EPA ACToR

ChemSpider Lazar in silico tox

Click

DSSTox File ?	Total#Records	Exact matches	Substructures	Similarity ≥ 51.2
CPDBAS_v5c	1547	1	2	
DBPCAN_v4b	209	-	-	
EPAFHM_v4b	617	-	-	
FDAMDD_v3b	1216	-	-	1
HPVCSI_v2c	3548	1	2	4
HPVISD_v1b	1006	-	-	-
IRISTR_v1b	544	1	2	8
NCTRER_v4b	232	1	1	3
NTPBSI_v3a	2303	1	1	3
NTPHTS_v2b	1408	1	1	1
TOXCST_v2c	320	1	2	9
Total Unique Substance Hits		1	2	12
Total Substance Hits - All Files		7	11	33

?



ACToR: Aggregated C

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Chemical Summary

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10634	aniline	NTPHTS_DSSTOX	DSSTOX_33195
18522	Aniline	ATSDR_ToxFaq	ATSDR_ToxFaq_9
18890	Aniline	CalEPA	CalEPA_110
28360	aniline	HCPSL_1999	HCPSL_1999_50
28493	Aniline	HCPSL_1999	HCPSL_1999_183
28839	Benzenamine	HCPSL_2006	HCPSL_2006_205
29118	Benzenamine	HPVChallenge	HPVChallenge_22
32512	Benzenamine	HPV	HPV_27
35643	Aniline	INCHEM_IARC	INCHEM_IARC_241
39894	Aniline	ITER_TERA	ITER_TERA_51
54058	Benzenamine	IUR2002	IUR2002_42
60499	62-53-3	NTP1408	NTP1408_29
64301	Aniline (8CA)	OPPIN_Active	OPPIN_Active_2424
68513	Aniline (8CA)	OPPIN_FoodUseActive	OPPIN_FoodUseActive_1244
71389	Aniline (8CA)	OPPIN_Inert	OPPIN_Inert_2243
73926	Aniline	PAN	PAN_929
77727	ANILINE	RBC	RBC_17
79230	ANILINE	Scorecard	Scorecard_929

Chemical Regulations

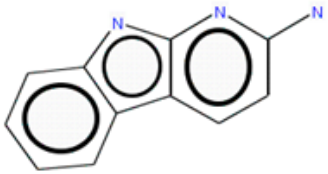
SCID	Regulation AID	Regulation Name
83185	SRS_CAA112_b_HON_AID_1	CAA112 (b) HON - Hazardous Organic Substance
221301	SRS_CWA_311_AID_1	Clean Water Act Hazardous Substance
221522	SRS_HAP_AID_1	Hazardous Air Pollutant
221681	SRS_NJ_RTK_HS_AID_1	New Jersey Right to Know Hazardous Substance
223688	SRS_RCRA_Appendix_VIII_AID_1	RCRA Hazardous Waste Constituent
223986	SRS_RCRA_U_Waste_AID_1	Hazardous Discarded Commercial Chemical Product (U)
224030	SRS_SARA_110_AID_1	SARA Hazardous Substance
224786	SRS_SARA_302A_AID_1	SARA Extremely Hazardous Substance
225057	SRS_TSCA_4_Tests_AID_1	Testing of Existing Chemicals

Substances

SCID	Name
90	aniline
1722	aniline
3552	aniline
7104	aniline
8664	aniline

Generic Chemical

Preferences: Refresh | Visibility | Table Size | Select Skin



GCID: 1
CASRN: 26148-68-5
CID: 11869
CCID: 11869
Formula: C11H9N3
MW: 183.212
SMILES: NC1C=CC2=C(N=1)NC3=CC=CC=C23
INCHI: InChI=1/C11H9N3/c12-10-6-5-8-7-3-1-2-4-9(7)13-11(8)
QC Status: QUEUED

Substances

Chemical Id	Data Collection	Name
1	CPDBAS_DSSTOX	A-alpha-C
18819	CalEPA	A-alpha-C (2-Amino-9H-pyrido[2,3-b]indole)
35633	INCHEM_IARC	A-alpha-C (2-Amino-9H-Pyrido[2,3-b]Indole)
78935	Scorecard	2-AMINO-9H-PYRIDO (2,3-B) INDOLE (A-ALPHA-C)
95724	SRS_CAS-9CI	2-Amino-9H-pyrido[2,3-b]indole
168920	SRS_ChemIDStd	2-Amino-9H-pyrido[2,3-b]indole
514465	ChemIDplus	1H-Pyrido(2,3-b)indol-2-amine
919306	EPA	26148-68-5
1413536	EPA_SRS_NTS	1H-Pyrido[2,3-b]indol-2-amine

Notes

Chemical Id	Data Collection	Note
1	CPDBAS_DSSTOX	blank
1413536	EPA_SRS_NTS	ACD/Name-to-Structure Batch v. 8.05

Synonyms

Name
.
1H-Pyrido(2,3-b)indol-2-amine
1H-Pyrido[2,3-b]indol-2-amine
2-AMINO-9H-PYRIDO (2,3-B) INDOLE (A-ALPHA-C)
2-AMINO-9H-PYRIDO(2,3-B)INDOLE
2-Amino-9H-pyrido[2,3-b]indole
2-Amino-alpha-carboline
26148-68-5
9H-Pyrido(2,3-b)indole, 2-amino-
9H-pyrido[2,3-b]indol-2-amine

Previous | 1-10 of 17 | Next 7

MSDS

MSDS Id

No rows yet.

Mesh

Mesh Name

PubMed via MeSH: 2-amino-9H

External Search

External Search

TOXNET CCRIS
TOXNET DART ETIC
TOXNET EMIC
TOXNET GENETOX
TOXNET HazMap
TOXNET Houshold Products
TOXNET HSDB
TOXNET MESH Headings
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U.S. ENVIRONMENTAL PROTECTION AGENC

ACToR: Aggregated Computational Toxicology Resource

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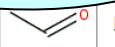
Data Collection

Name: IRISTR_DSSTOX

Description: EPA Integrated Risk Information System http://www.epa.gov/iris/. A structure index file with links to webpage for
Source Type: DSSTox Collection
Number of Substances: 544
Number of Generic Chemicals: 536
Compilation Date: 9/27/2007
Compilation Instructions: Download SD and excel files from DSSTox site. Preprocess according to ToxCast SOP 004

Fetch Size: 100 Offset: 0 Fetch

Generic Chemical	CASRN	Structure	Substance	Source SID	Name	Structure	PhysicoChemical	Biochemical	In vivo toxicology (tabular primary)	In vivo toxicology (study listing primary)	In vivo toxicology (tabular secondary)	In vivo toxicology (summary calls)	In vivo toxicology (summary report via URL)	Regulation	Chemical Use Level	Carcinogenicity	GeneTox	DevTox	ReproTox	EcoTox	FoodSafe
Details	83-32-9		Details	DSSTOX_1774	Acenaphthylene, 1,2-dihydro-	1687	10	7	1	1	4	3	5	5		5	6	3	3	1	
Details	208-96-8		Details	DSSTOX_3845	Acenaphthylene	5129					1	1	3	2		4	3	3	2	1	
				DSSTOX_3846	Acephate	5130	9			6	1	10	5	1		9	4	6	5	3	
Details	75-07-0		Details	DSSTOX_2	Acetaldehyde	2	9	40	3	1	4	16	8	9		14	9	5	3	2	1

Where are the data??

U.S. Environmental Protection Agency

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IRIS Substance List

The substances are listed in alphabetical order. You can click on the first letter of the substance you want which will bring you to the section that the substance is in, or use your browser's Find command to search for a substance name or Chemical Abstracts Service Registry Number (CASRN). These substance files are typically about 15K to 40K in size, within a range from less than 10K up to about 120K.

(To search the IRIS database, go to the Search page)

List of IRIS Substances

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Full IRIS Summaries/Toxicological Reviews

Entire IRIS Website

Structure-search

EPA DSSTox Structure-Browser v1.0 GO

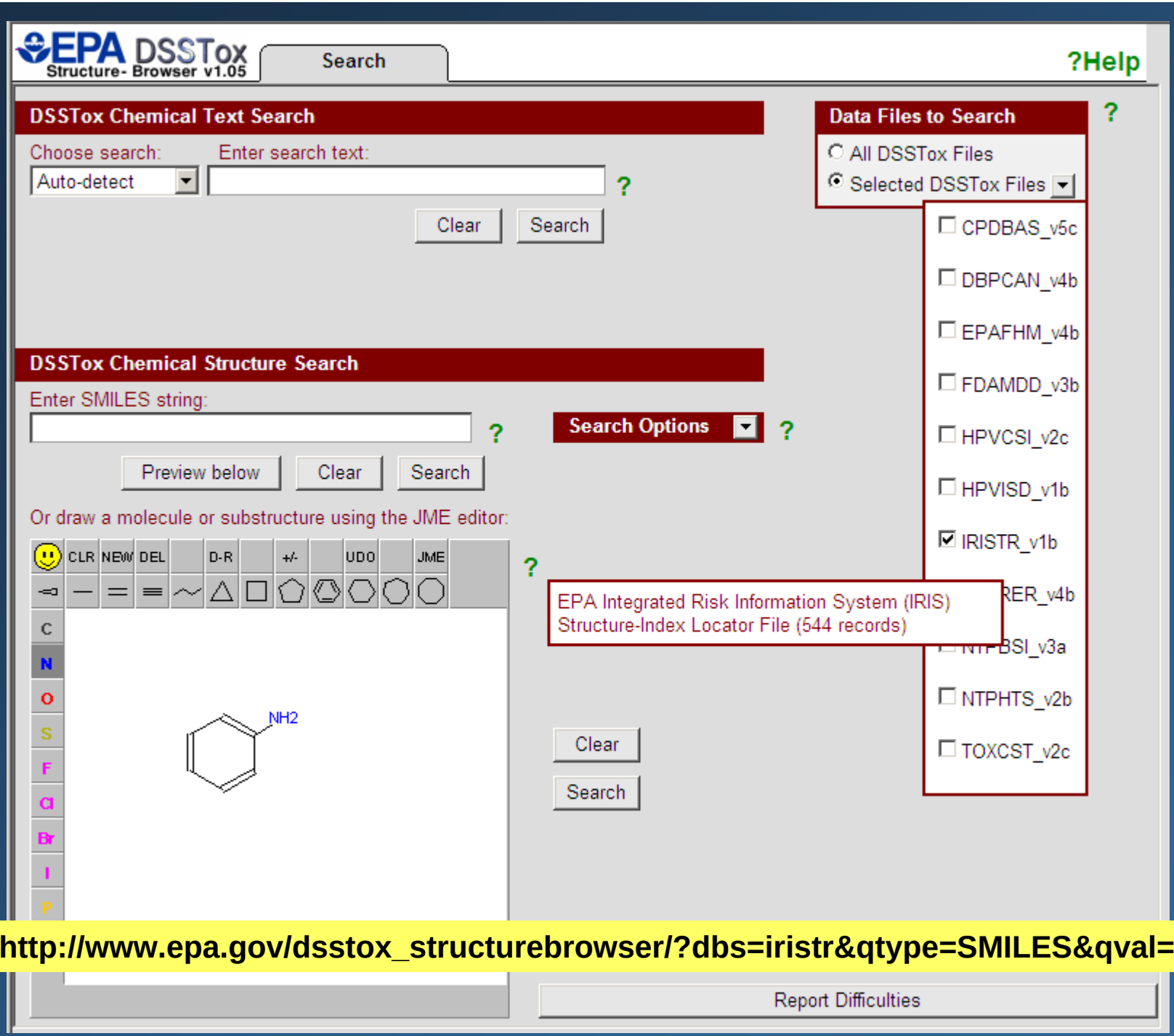
You will need Adobe Reader to view some of the files on this page. See EPA's PDF page to learn more.

A B C D E F G H I J K L M N O P Q R S T U V W X Y Z

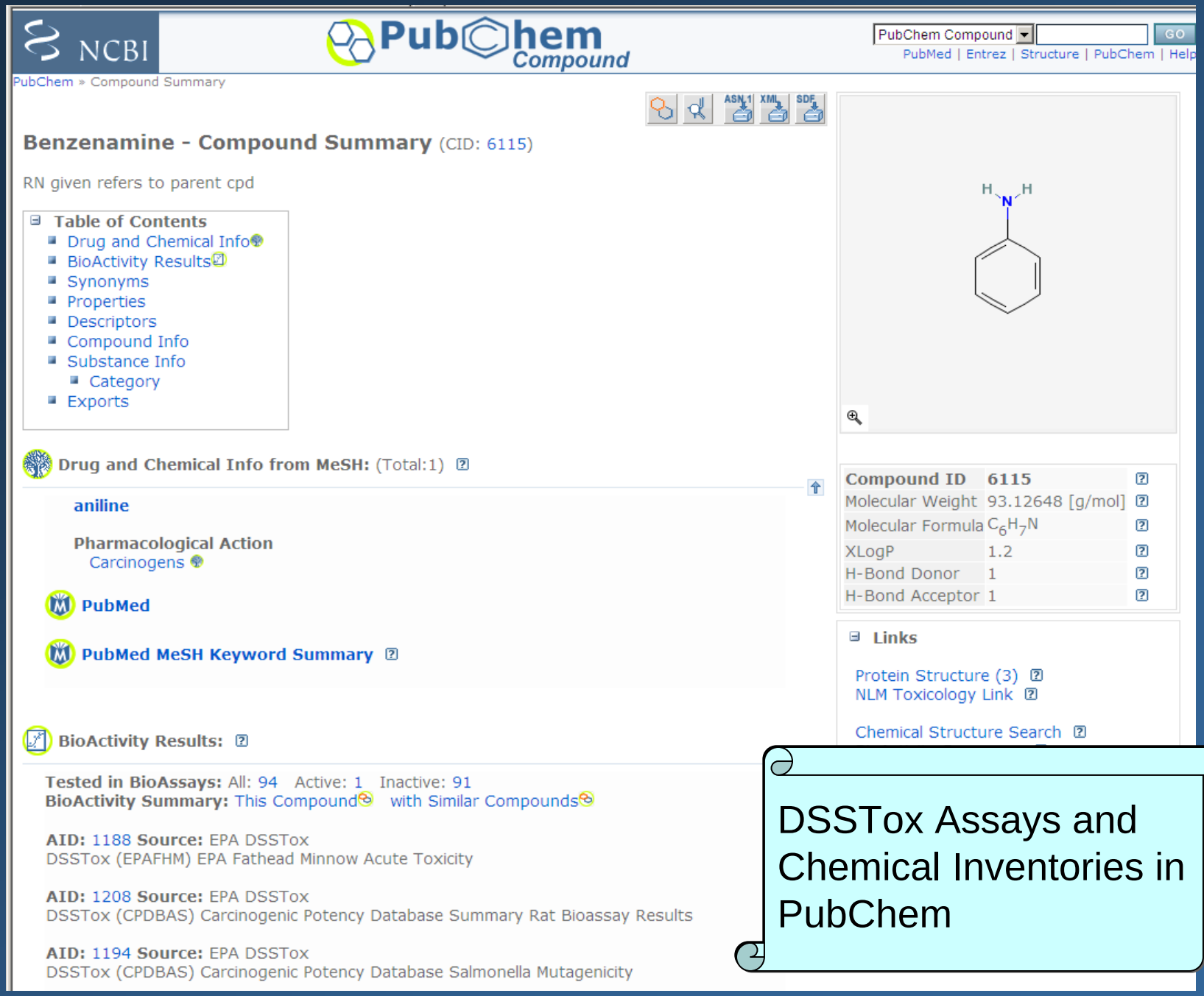
Substance Name	Chemical Abstracts Service Registry Number (CASRN)	Last Significant Revision*
Acenaphthene	CASRN 8	
• QuickView		
Acenaphthylene	CASRN 2	
• QuickView		
Acephate	CASRN 3	
• QuickView		
Acetaldehyde	CAS	
• QuickView		
Acetochlor	CASRN 34256-82-1	09/01/1993

DSSTox Structure Browser:

- External URL link-in
- Dedicated searching through indexed db



http://www.epa.gov/dsstox_structurebrowser/?dbs=iristr&qtype=SMILES&qval=c1ccccc1N



DSSTox Assays and Chemical Inventories in PubChem

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Structure Search

Database ID(s)

Predicted Properties

LogP:	ACD/LogP: 0.94 XLogP: 1.20 ALOGPS: 1.30	**# of Rule of 5 Violations:**	0
ACD/LogD (pH 5.5):	0.88	**ACD/LogD (pH 7.4):**	0.94
ACD/BCF (pH 5.5):	2.68	**ACD/BCF (pH 7.4):**	3.03
ACD/KOC (pH 5.5):	68.18	**ACD/KOC (pH 7.4):**	76.85
#H bond acceptors:	1	**#H bond donors:**	2
#Freely Rotating Bonds:	1	**Polar Surface Area:**	3.24 Å^2
Index of Refraction:	1.579	**Molar Refractivity:**	30.48 cm^3
Molar Vo			
Surface T			
Flash Poi			
Boiling P			

User Data

- **Experimental Physchem Properties**
  - **Melting Point:** -6
  - **Melting Point:** -6
  - **Melting Point:** -6 C
  - **Boiling Point:** 183-184
  - **Boiling Point:** 183-184
  - **Boiling Point:** 363F
  - **Boiling Point:** 184 C
  - **Flash Point:** 70(158F)
  - **Flash Point:** 70(158F)
  - **Flash Point:** 158F
  - **Flash Point:** 70 C
  - **Freezing Point:** 21F
  - **Specific Gravity:** 1.021
  - **Specific Gravity**
  - **Specific Gravity**
  - **Refraction Inde**
  - **Refraction Inde**
  - **LogP:** 0.90
  - **Solubility:** Solub
  - **Solubility:** 4%
  - **Ionization Pote**
  - **Vapor Pressure**
- **Miscellaneous**
  - **Appearance:** Co solid below 21F.]
  - **Appearance:** co
  - **Applications:** C
  - **Stability:** Stable zinc, aluminium.
  - **Toxicity:** ORL-R 254 mg kg-1 , O
  - **Safety:** WARNIN

EPI Summary

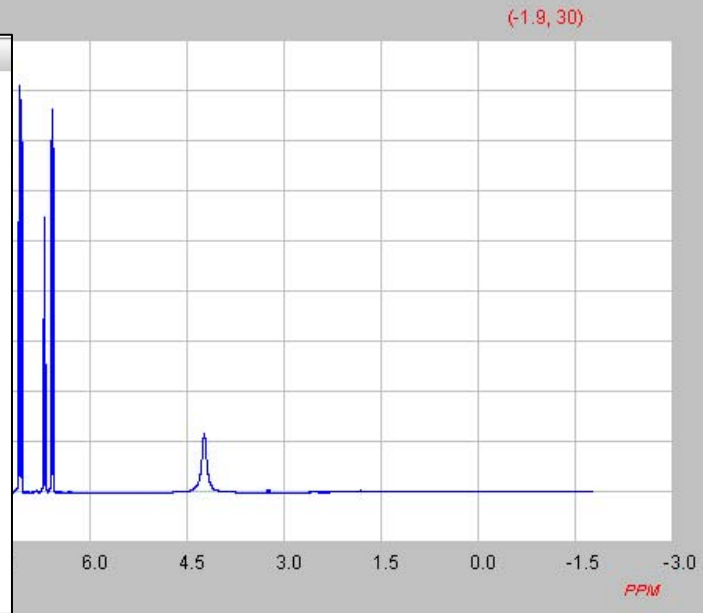
```
Log Octanol-Water Partition Coef (SRC):
   Log Kow (KOWWIN v1.67 estimate) =  1.08
   Log Kow (Exper. database match) =  0.90
      Exper. Ref:  Hansch,C et al. (1995)

Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1.42):
   Boiling Pt (deg C):  183.99  (Adapted Stein & Brown method)
   Melting Pt (deg C):  -6.16  (Mean or Weighted MP)
   VP(mm Hg,25 deg C):  0.791  (Mean VP of Antoine & Grain methods)
   MP  (exp database):  -6 deg C
   BP  (exp database):  184.1 deg C
   VP  (exp database):  4.90E-01 mm Hg at 25 deg C

Water Solubility Estimate from Log Kow (WSKOW v1.41):
   Water Solubility at 25 deg C (mg/L):  2.082e+004
      log Kow used: 0.90 (expkow database)
      no-melting pt equation used
    Water Sol (Exper. database match) =  3.6e+004 mg/L (25 deg C)
      Exper. Ref:  YALKOWSKY,SH & DANNENFELSER,RM (1992)

Water Sol Estimate from Fragments:
   Wat Sol (v1.01 est) =  18790 mg/L
   Wat Sol (Exper. database match) =  36000.00
```

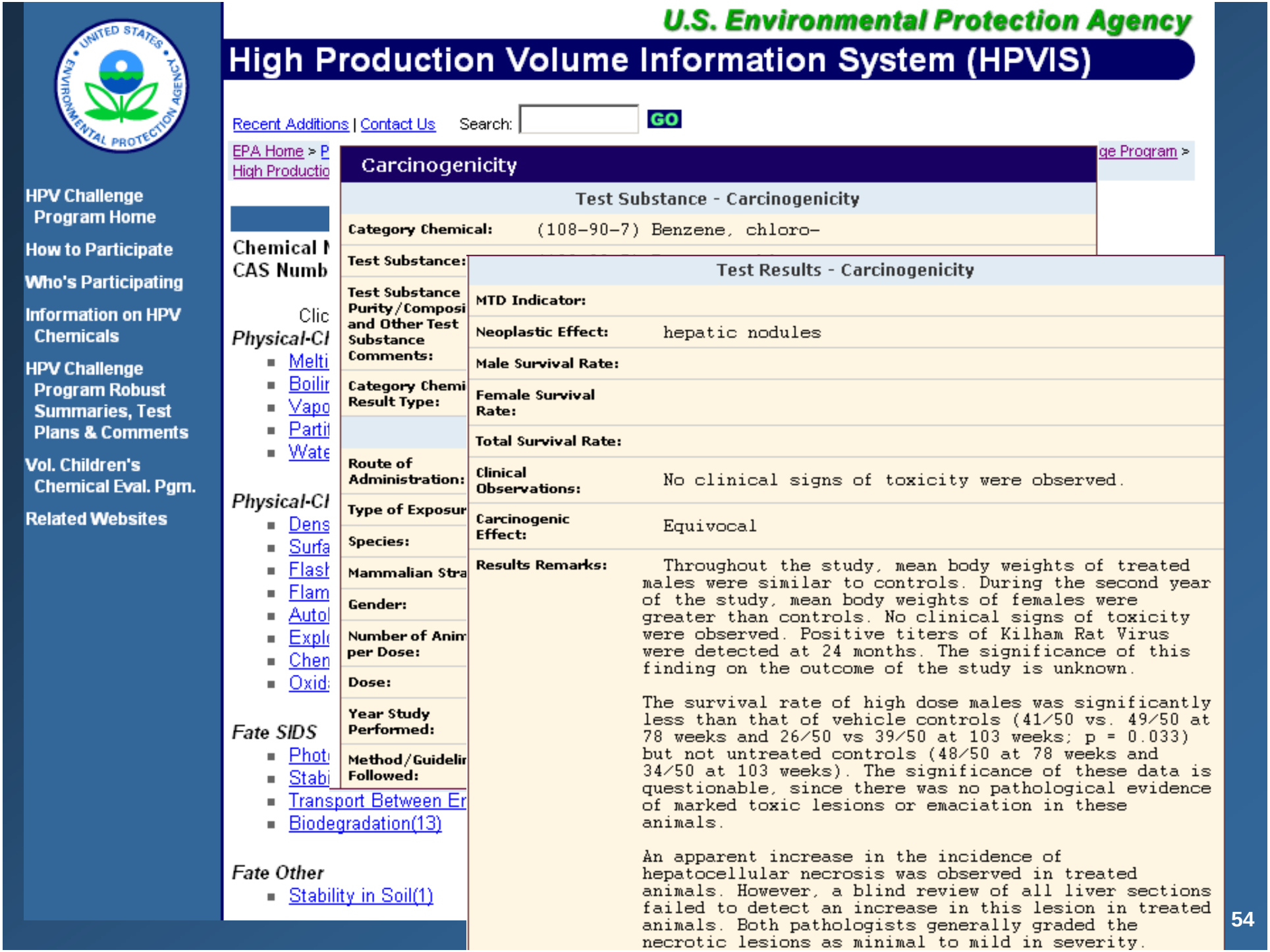
Spectra

Type: HNMR

Associated Hyperlink: usefulchem.wikispaces.com/Exp093

Comments: Dr. Jean-Claude Bradley's Lab at Drexel University Philadelphia PA

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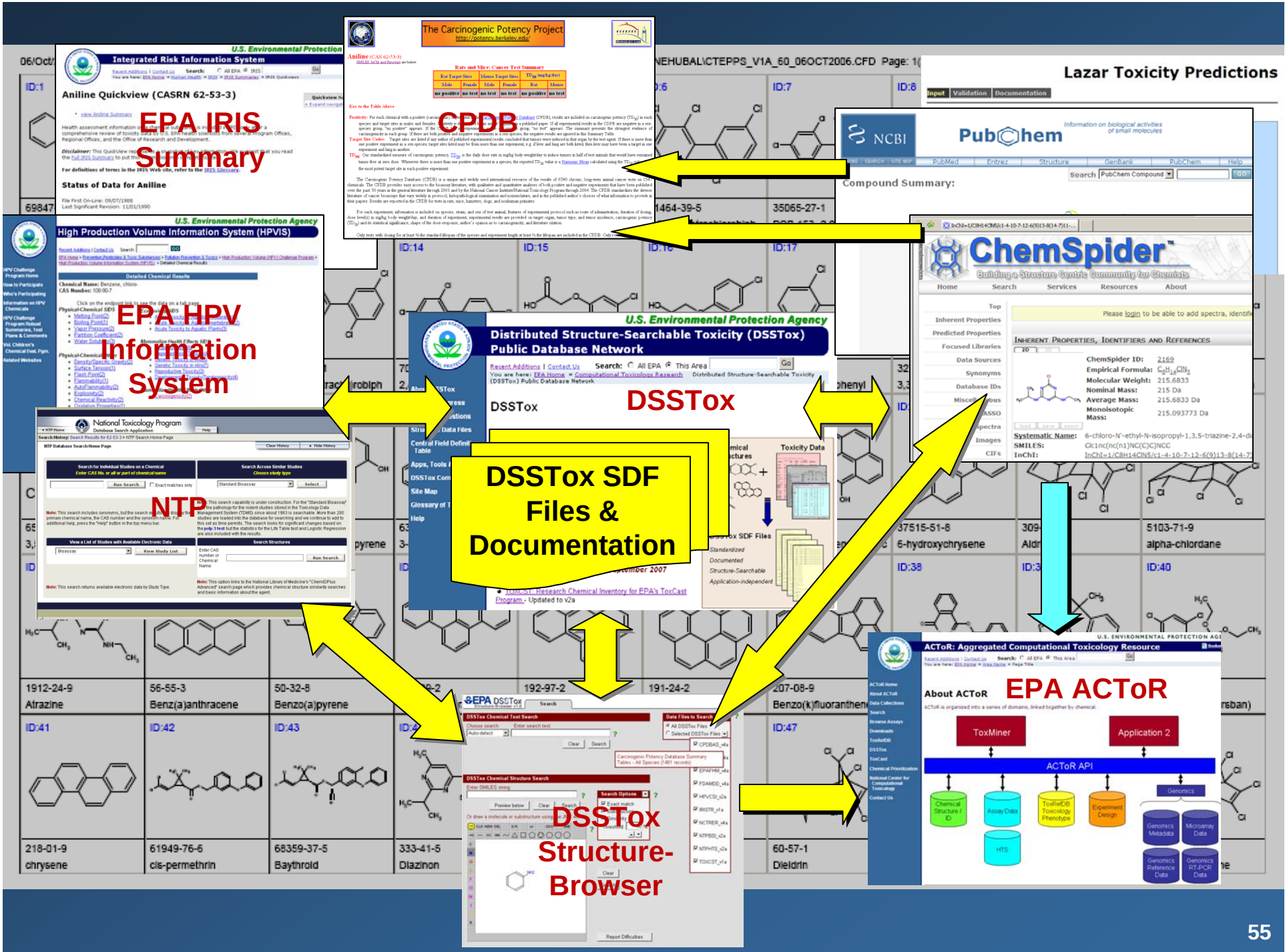
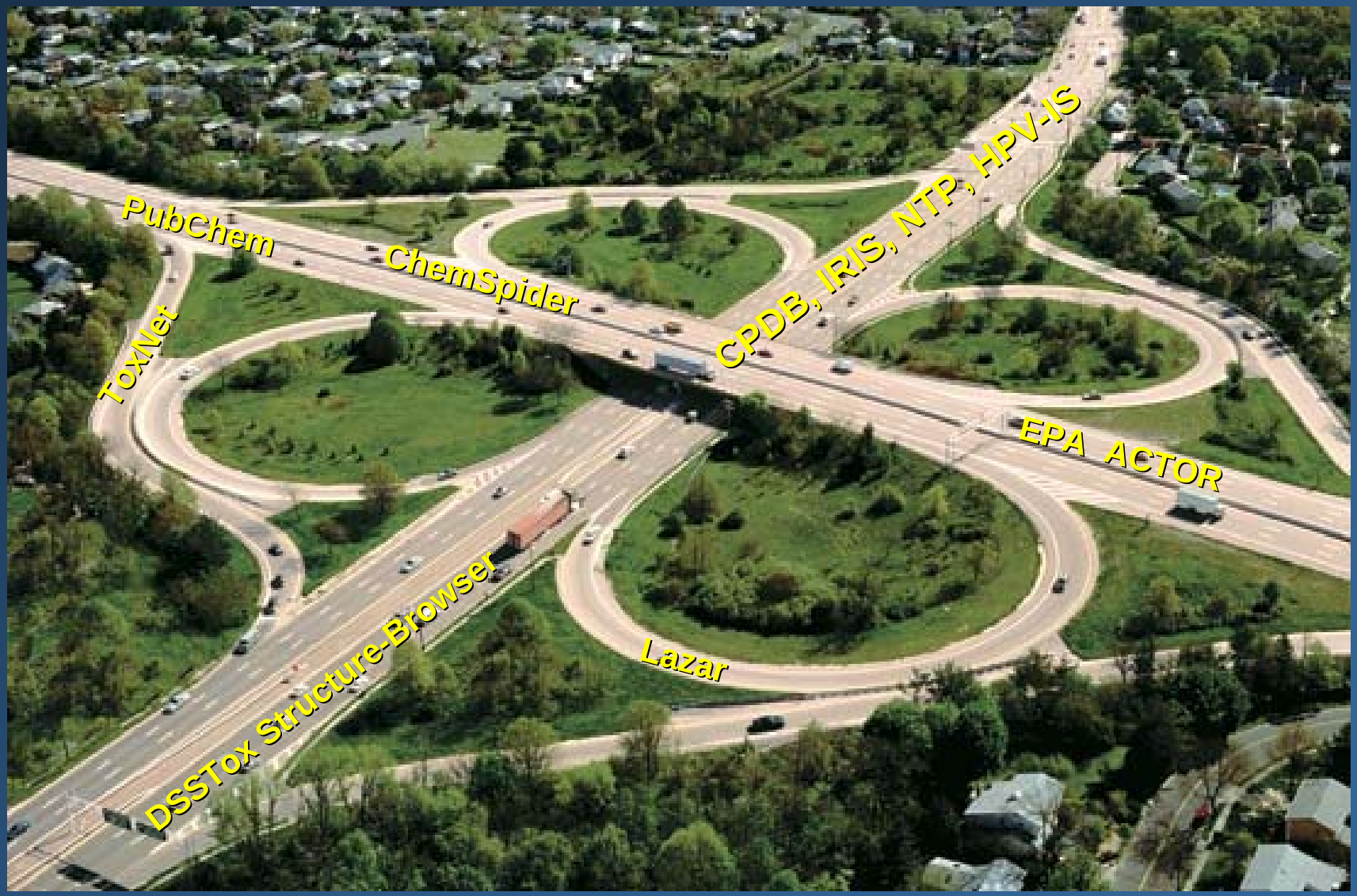
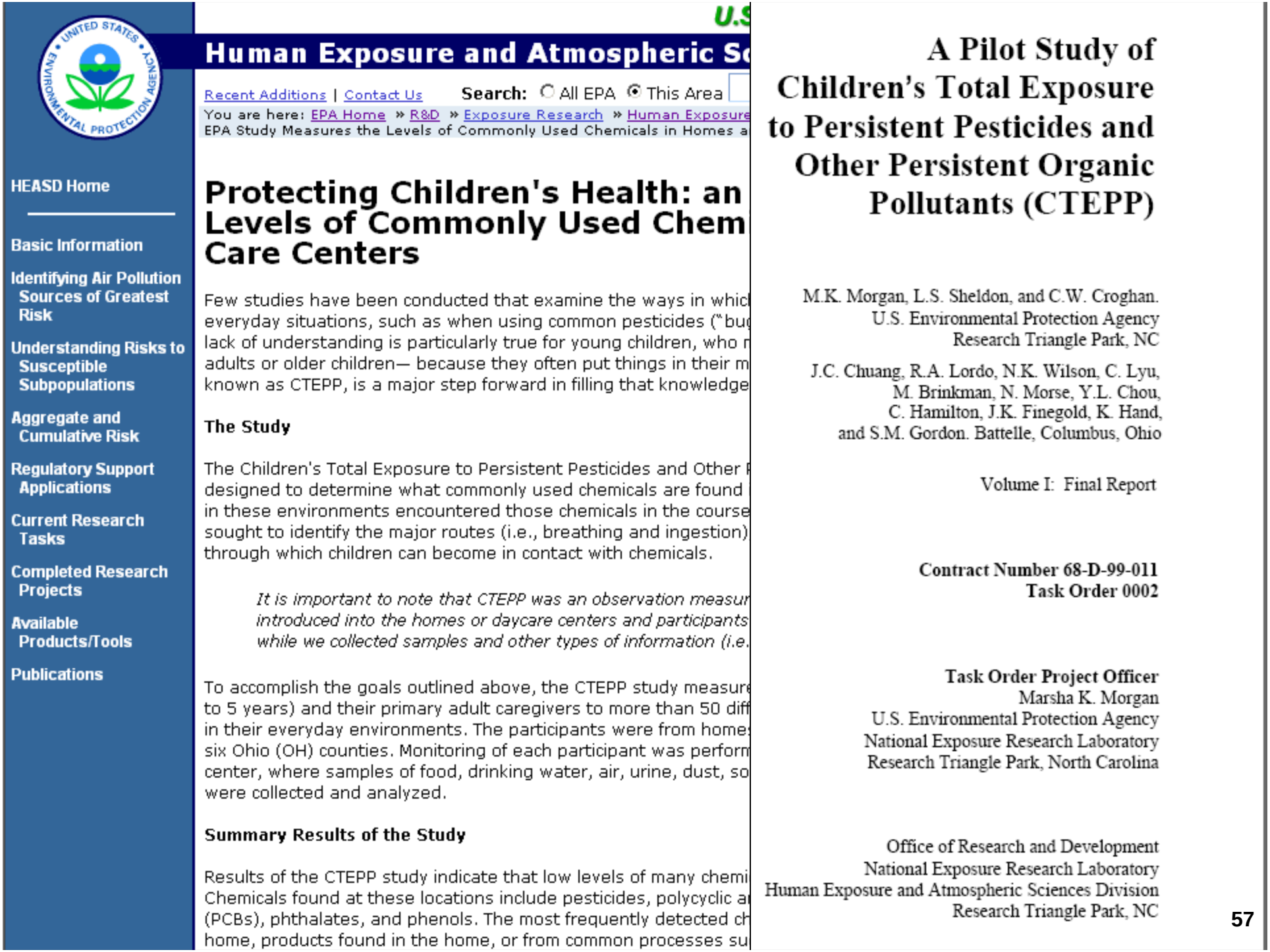
Information on HPV Chemicals
HPV Challenge Program Robust Summaries, Test Plans & Comments
Vol. Children's Chemical Eval. Pgm.
Related Websites
Carcinogenicity
Test Substance - Carcinogenicity
Category Chemical: (108-90-7) Benzene, chloro-
Test Substance:
Test Substance Purity/Composi and Other Test Substance Comments:
Category Chemi Result Type:
Route of Administration:
Type of Exposur
Species:
Mammalian Stra
Gender:
Number of Anim per Dose:
Dose:
Year Study Performed:
Method/Guideli Followed:
Test Results - Carcinogenicity
MTD Indicator:
Neoplastic Effect: hepatic nodules
Male Survival Rate:
Female Survival Rate:
Total Survival Rate:
Clinical Observations: No clinical signs of toxicity were observed.
Carcinogenic Effect: Equivocal
Results Remarks: Throughout the study, mean body weights of treated males were similar to controls. During the second year of the study, mean body weights of females were greater than controls. No clinical signs of toxicity were observed. Positive titers of Kilham Rat Virus were detected at 24 months. The significance of this finding on the outcome of the study is unknown.
The survival rate of high dose males was significantly less than that of vehicle controls (41/50 vs. 49/50 at 78 weeks and 26/50 vs 39/50 at 103 weeks; p = 0.033) but not untreated controls (48/50 at 78 weeks and 34/50 at 103 weeks). The significance of these data is questionable, since there was no pathological evidence of marked toxic lesions or emaciation in these animals.
An apparent increase in the incidence of hepatocellular necrosis was observed in treated animals. However, a blind review of all liver sections failed to detect an increase in this lesion in treated animals. Both pathologists generally graded the necrotic lesions as minimal to mild in severity.
Fate SIDS
Transport Between Er
Biodegradation(13)
Fate Other
Stability in Soil(1)


EPA IRIS Summary
CPDB
EPA HPV Information System
DSSTox
DSSTox SDF Files & Documentation
NTP
EPA ACToR
DSSTox Structure-Browser
Integrated Risk Information System
Aniline Quickview (CASRN 62-53-3)
The Carcinogenic Potency Project
High Production Volume Information System (HPVIS)
Distributed Structure-Searchable Toxicity (DSSTox) Public Database Network
National Toxicology Program
ACToR: Aggregated Computational Toxicology Resource
Lazar Toxicity Predictions
PubChem
ChemSpider
1912-24-9 Atrazine
56-55-3 Benz(a)anthracene
50-32-8 Benzo(a)pyrene
192-97-2
191-24-2
37515-51-8 6-hydroxychrysene
5103-71-9 alpha-chlordane
218-01-9 chrysene
61949-76-6 cis-permethrin
68359-37-5 Baythroid
333-41-5 Diazinon
60-57-1 Dieldrin


PubChem
ChemSpider
CPDB, IRIS, NTP, HPV-IS
ToxNet
EPA ACTOR
DSSTox Structure-Browser
Lazar



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Human Exposure and Atmospheric Sc

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EPA Study Measures the Levels of Commonly Used Chemicals in Homes a

HEASD Home

Basic Information

Identifying Air Pollution Sources of Greatest Risk

Understanding Risks to Susceptible Subpopulations

Aggregate and Cumulative Risk

Regulatory Support Applications

Current Research Tasks

Completed Research Projects

Available Products/Tools

Publications

Protecting Children's Health: an
Levels of Commonly Used Chem
Care Centers

Few studies have been conducted that examine the ways in whic
everyday situations, such as when using common pesticides ("bu
lack of understanding is particularly true for young children, who r
adults or older children— because they often put things in their m
known as CTEPP, is a major step forward in filling that knowledge

The Study

The Children's Total Exposure to Persistent Pesticides and Other
designed to determine what commonly used chemicals are found
in these environments encountered those chemicals in the course
sought to identify the major routes (i.e., breathing and ingestion)
through which children can become in contact with chemicals.

*It is important to note that CTEPP was an observation measur
introduced into the homes or daycare centers and participants
while we collected samples and other types of information (i.e.*

To accomplish the goals outlined above, the CTEPP study measure
to 5 years) and their primary adult caregivers to more than 50 diff
in their everyday environments. The participants were from homes
six Ohio (OH) counties. Monitoring of each participant was perform
center, where samples of food, drinking water, air, urine, dust, so
were collected and analyzed.

Summary Results of the Study

Results of the CTEPP study indicate that low levels of many chemi
Chemicals found at these locations include pesticides, polycyclic a
(PCBs), phthalates, and phenols. The most frequently detected ch
home, products found in the home, or from common processes su

A Pilot Study of Children's Total Exposure to Persistent Pesticides and Other Persistent Organic Pollutants (CTEPP)

M.K. Morgan, L.S. Sheldon, and C.W. Croghan.
U.S. Environmental Protection Agency
Research Triangle Park, NC

J.C. Chuang, R.A. Lordo, N.K. Wilson, C. Lyu,
M. Brinkman, N. Morse, Y.L. Chou,
C. Hamilton, J.K. Finegold, K. Hand,
and S.M. Gordon. Battelle, Columbus, Ohio

Volume I: Final Report

Contract Number 68-D-99-011
Task Order 0002

Task Order Project Officer
Marsha K. Morgan
U.S. Environmental Protection Agency
National Exposure Research Laboratory
Research Triangle Park, North Carolina

Office of Research and Development
National Exposure Research Laboratory
Human Exposure and Atmospheric Sciences Division
Research Triangle Park, NC

Table 9.3.3 Median Levels of 26 Target Pollutants in OH Multimedia Samples Collected from Home Environments[a]

Pollutant/Meta
Chlorpyrifos
Diazinon
3,5,6-TCP
alpha-Chlordane
gamma-Chlordane
p,p'-DDE
Cyfluthrin
cis-Permethrin
trans-Permethrin
2,4-D
Benz[*a*]anthracen
Benzo[b]fluoranth
Benzo[*k*]fluoranth
Benzo[*ghi*]peryle
Benzo[*a*]pyrene
Benzo[*e*]pyrene
Chrysene
Dibenz[*a,h*]anthra
Indeno[1,2,3-*cd*]p
Benzylbutylphtha
Di-*n*-butylphthala
Bisphenol-A
Pentachlorophenol
PCB 52
PCB 95
PCB 101

[a] For urine, the me
[b] "<" indicates tha
[c] Dashes indicate t

Table 9.3.5. Environmental and Food Samples: Estimated Ratios of Geometric Mean Pollutant Levels Between Urban and Rural, Low-Income and Middle/High-Income, and Home and Day Care Environments, When These Ratios Were Significantly Different from One at the 0.05 Level[a]

Pollutant/Metab
Chlorpyrifos
Diazinon
IMP
3,5,6-TCP
alpha-Chlordar
gamma-Chlorda
Cyfluthrin

Table 9.5.1 Median Values of Estimated Potential Exposure and Potential Absorbed Dose for Target Pollutants in Participating NC Preschool Children, by Exposure Route

Pollutant/Metab
Chlorpyrifos
Diazinon
3,5,6-TCP
alpha-Chlordane
gamma-Chlordane
p,p'-DDE
Heptachlor
Cyfluthrin
cis-Permethrin
trans-Permethrin
2,4-D
Benz[*a*]anthracene
Benzo[*b*]fluoranth
Benzo[*k*]fluoranth
Benzo[*ghi*]perylen
Benzo[*a*]pyrene
Benzo[*e*]pyrene
Chrysene
Dibenz[*a,h*]anthra
Indeno[1,2,3-*cd*]py
Benzylbutylphthal
Di-*n*-butylphthalat
Bisphenol-A
Pentachlorophenol

Table 9.5.5 Summary of Aggregate Potential Exposure and Aggregate Potential Absorbed Dose Estimates for Eight Pollutants in NC Study Participants[a]

Pollutant/ Metabolite	Type of Measure	N	% Detected	Arith. Mean	S.D.	Geom. Mean	Percentiles 25th	50th	75th	95th	Max.
OP Pesticides and Metabolite											
Chlorpyrifos	Children -- Aggregate Exposure[a]	109	100	359	801	174	78.9	152	295	1,180	7,630
Diazinon											
3,5,6-TCP											
cis-Permethrin											
trans-Permethrin											
2,4-D											

Table 9.5.9 [illegible]mated Ratios [illegible] and [illegible] OH [illegible] the 0.0[illegible]

Pollutant/ Metabolite	Exposure/Dos and Pa						
trans-Permethrin	Exposure/Inhal						
	Exposure/Dieta						
	Dose/Inhalation						
	Dose/Dietary In						
2,4-D	Exposure/Inhalatio						
	Exposure/Dietary Ingestion						
	Exposure/Indirect Ingestion	3.39**	0.27**	0.54*	2.80*	0.29**	
	Dose/Inhalation			1.94*			
	Dose/Indirect Ingestion	3.68**	0.25**	0.47*	2.84*	0.29**	
PAHs							
Benz[*a*]anthracene	Exposure/Indirect Ingestion				3.69**	0.43**	3.29**
	Dose/Indirect Ingestion				3.65**	0.43**	3.08**

Convert tabular data to structured data model:

- Pure text & numeric fields
- No abbreviations
- Chemical-structures
- Activity-related fields
- Standardized entries

CTEPPS_v1a_60

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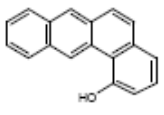	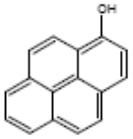	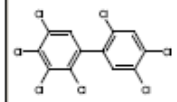	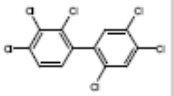	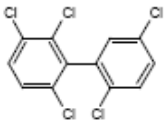	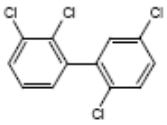	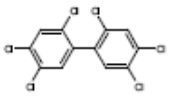	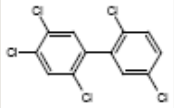	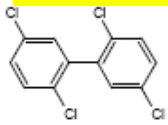	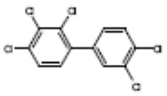
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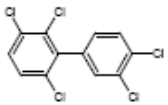	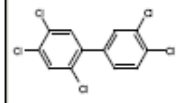	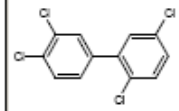	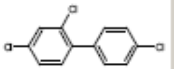	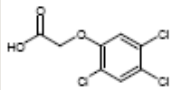	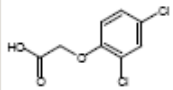	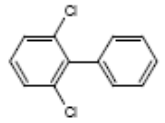	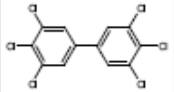	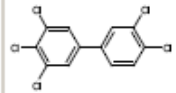	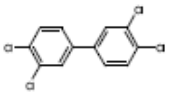
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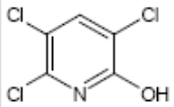	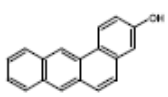	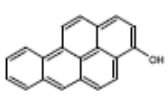	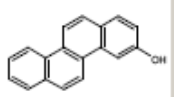	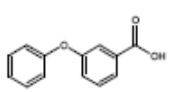	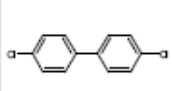	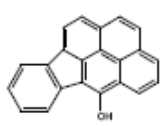	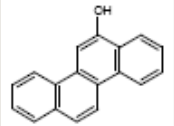	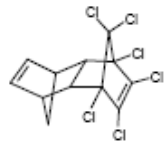	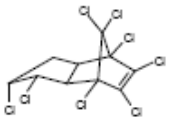
6515-38-4 3,5,6-TCP (3,5,6-trichlor	4834-35-9 3-hydroxybenz[a]anthrac	13345-21-6 3-hydroxybenz[a]pyrene	63019-39-6 3-hydroxychrysene	3739-38-6 3-phenoxybenzoic acid	2050-68-2 4,4'-dichlorobiphenyl	99520-67-9 6-hydroxy Indeno[1,2,3-c	37515-51-8 6-hydroxychrysene	309-00-2 Aldrin	5103-71-9 alpha-chlordane
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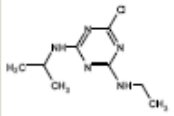
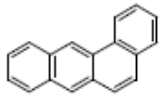
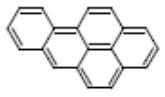
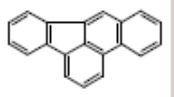
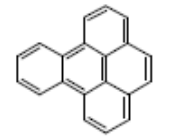
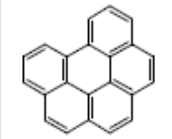
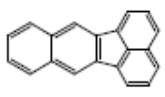
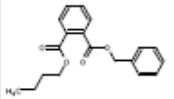
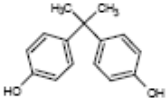
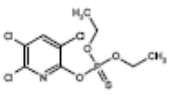
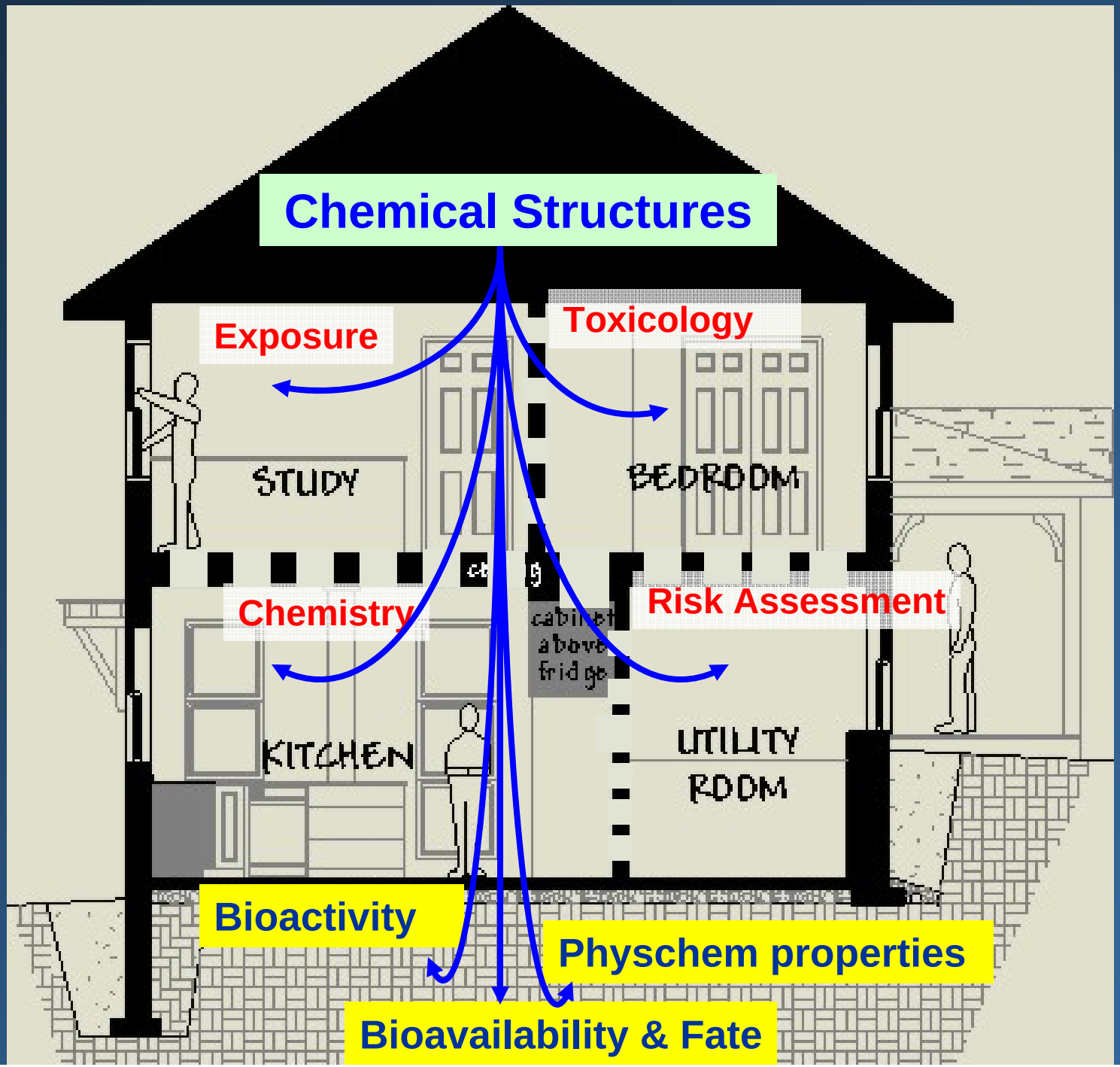
									
1912-24-9 Atrazine	56-55-3 Benz(a)anthracene	50-32-8 Benzo(a)pyrene	205-99-2 Benzo(b)fluoranthene	192-97-2 Benzo(e)pyrene	191-24-2 Benzo[g,h,i]perylene	207-08-9 Benzo(k)fluoranthene	85-68-7 Butyl benzyl phthalate	80-05-27 bisphenol-A	2921-88-2 Chlorpyrifos (Dursban)
ID:41	ID:42	ID:43	ID:44	ID:45	ID:46	ID:47	ID:48	ID:49	ID:50
218-01-9 chrysene	61949-76-6 cis-permethrin	68359-37-5 Baythroid	333-41-5 Diazinon	53-70-3 Dibenz(a,h)anthracene	1918-00-9 Dicamba	60-57-1 Dieldrin	84-74-2 Dibutyl phthalate	72-20-8 Endrin	5103-74-2 gamma-chlordane

ID:51	ID:52	ID:53	ID:54	ID:55	ID:56	ID:57	ID:58	ID:59	ID:60
76-44-8 Heptachlor	2814-20-2 4(1H)-Pyrimidinone, 6-m	193-39-5 Indeno[1,2,3-cd]pyrene	58-89-9 Lindane	104-40-5 nonylphenol (mixed)	72-55-9 p,p'-Dichlorodiphenyl dic	50-29-3 Dichlorodiphenyltrichlor	82-68-8 Pentachloronitrobenzen	87-86-5 Pentachlorophenol, purif	61949-77-7 trans-permethrin

Next steps:

- What data standards already exist in the exposure community?
- What modifications to existing exposure-related resources are required to build relational capability?
- What exposure-related resources can be indexed by chemical structure?
- What would the world of Exposure-informatics look like?


Chemical Structures
Exposure
Toxicology
STUDY
BEDROOM
Chemistry
Risk Assessment
cabinet above fridge
KITCHEN
UTILITY ROOM
Bioactivity
Physchem properties
Bioavailability & Fate

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