United States Environmental Protection Agency

ISEA Presentation, Durham, NC, 15 October 2007

TOXICO-CHEMINFORMATICS:
NEW AND EXPANDING PUBLIC RESOURCES TO SUPPORT CHEMICAL TOXICITY ASSESSMENTS

Ann Richard richard.ann@epa.gov

Office of Research and Development
National Center for Computational Toxicology

Part I.

The Problem

Chemical Research in Toxicology

JULY 2007
VOLUME 20, NUMBER 7

Editorial

The Future of Toxicology—Wrap Up

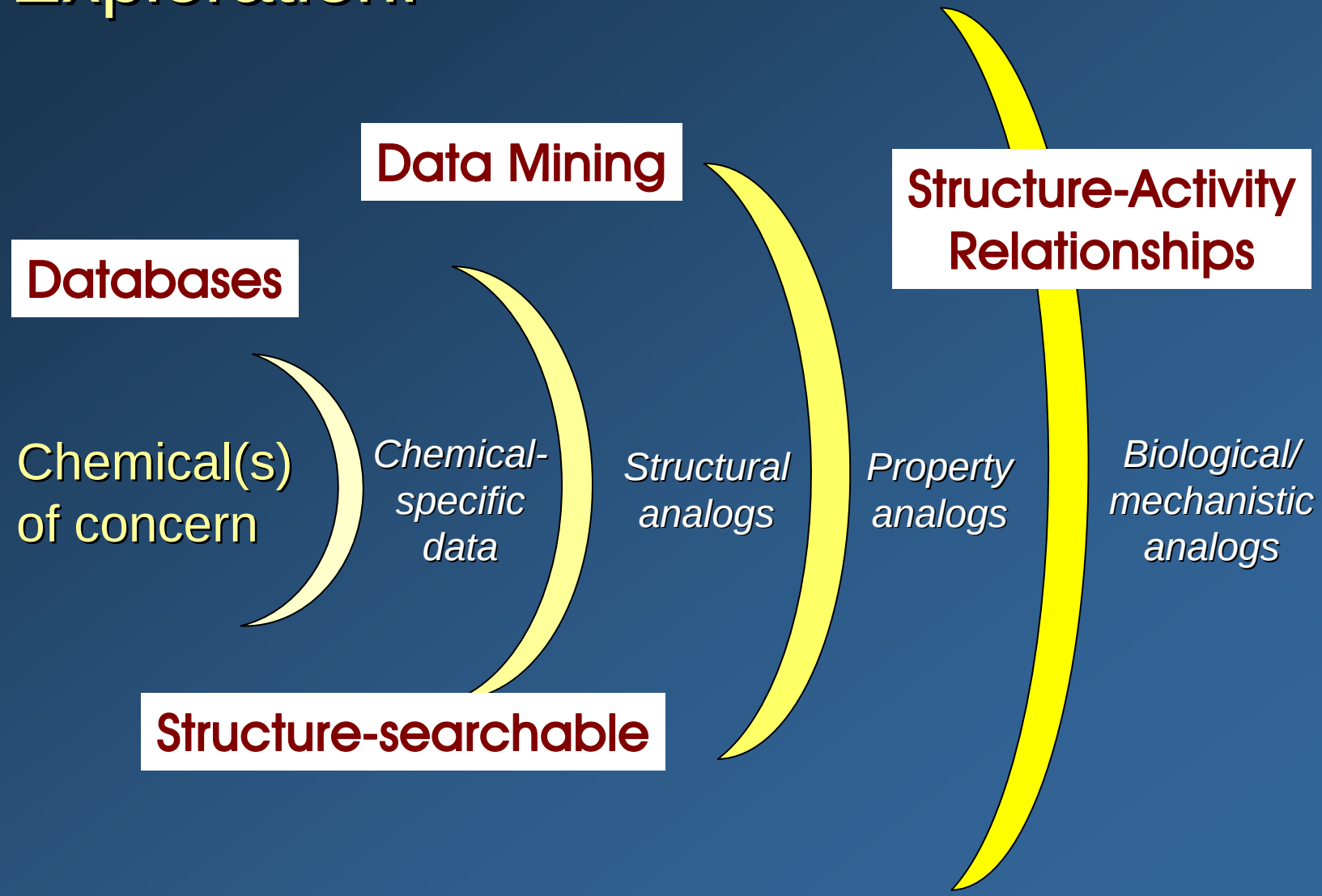
Aaron T. Jacobs and Lawrence J. Marnett*

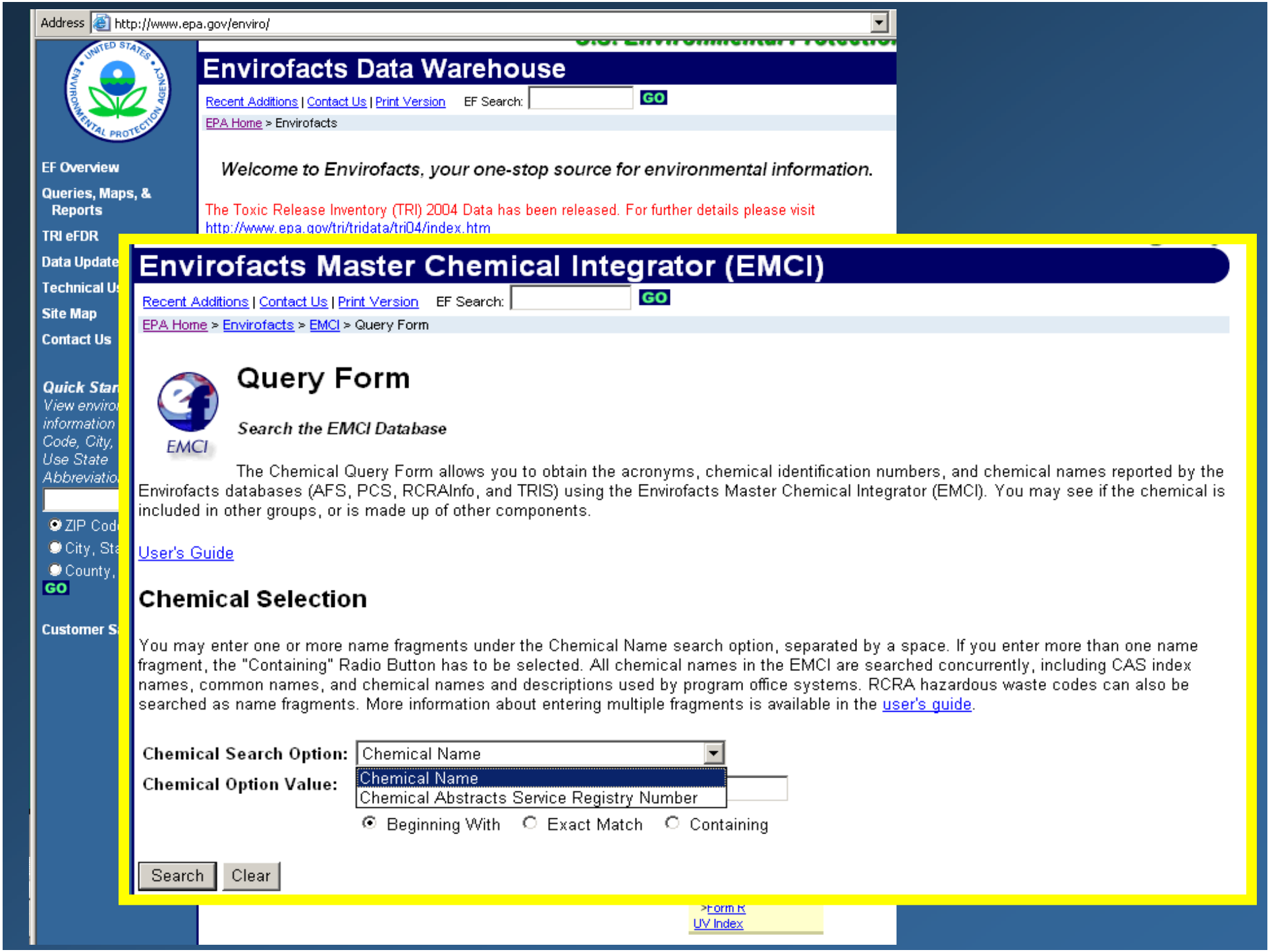
A.B. Hancock Jr. Memorial Laboratory for Cancer Research
Departments of Biochemistry, Chemistry, and Pharmacology
Vanderbilt Institute of Chemical Biology
Center in Molecular Toxicology
Vanderbilt-Ingram Cancer Center
Vanderbilt University School of Medicine
Nashville, Tennessee 37232

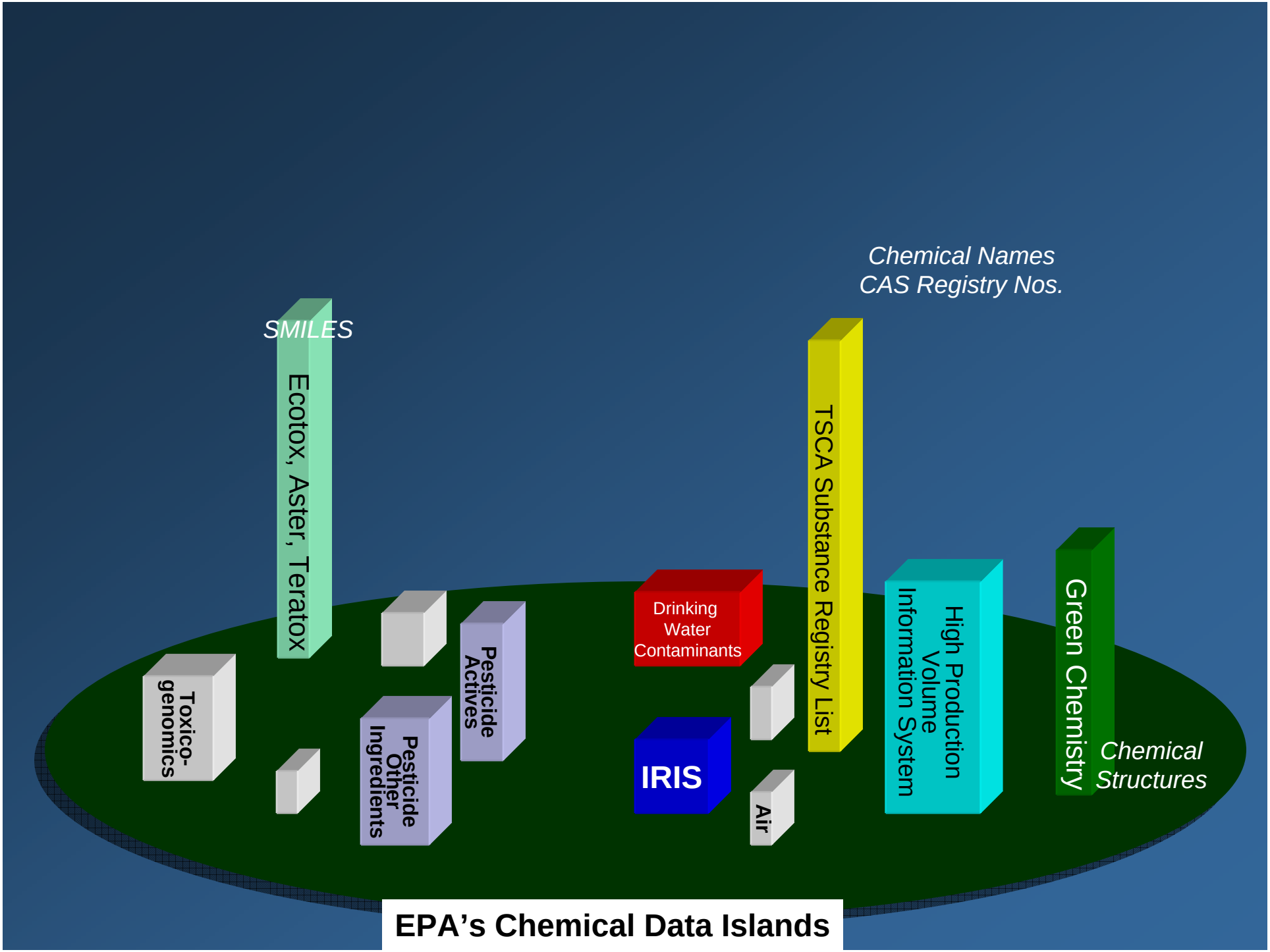
Wither toxicology? We have enjoyed a series of informative, occasionally provocative, commentaries on this subject from a paucity of compelling problems to work on that would generate a broad mandate for large-scale investment in toxicol-

"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."

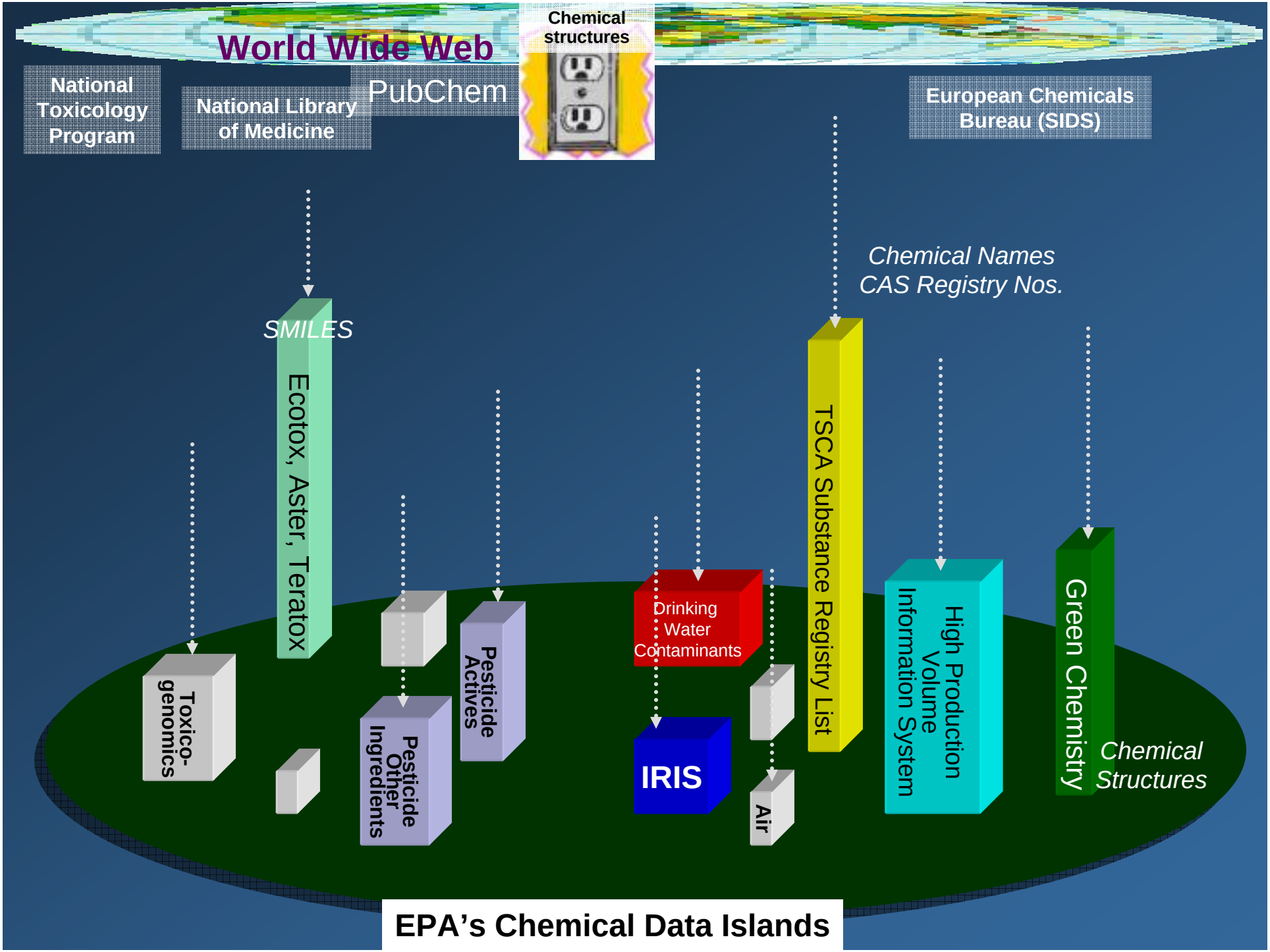
Chemistry-based Data Mining & Exploration:

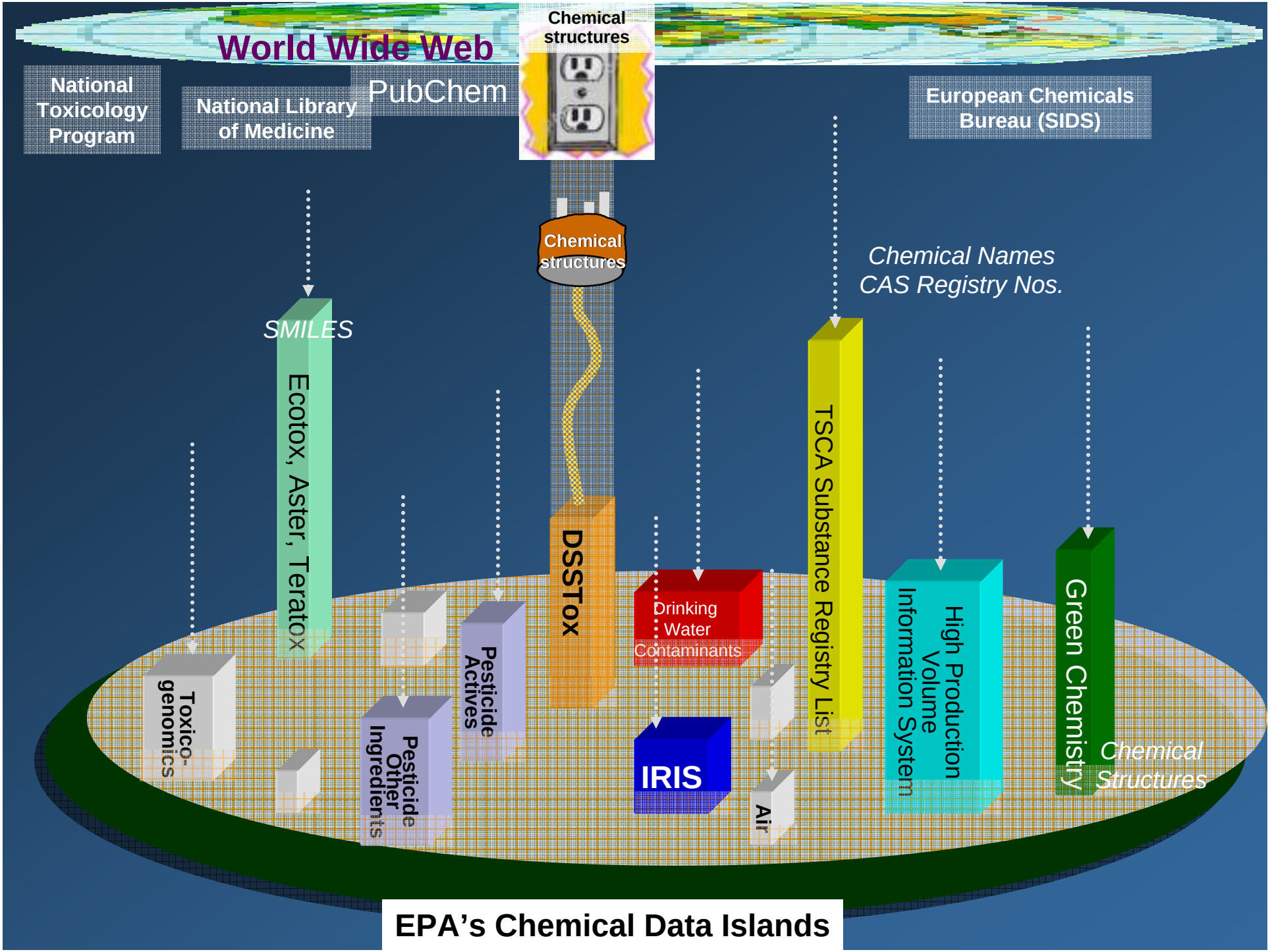



Address http://www.epa.gov/enviro/
Envirofacts Data Warehouse
Recent Additions | Contact Us | Print Version EF Search: GO
EPA Home > Envirofacts
Welcome to Envirofacts, your one-stop source for environmental information.
The Toxic Release Inventory (TRI) 2004 Data has been released. For further details please visit
http://www.epa.gov/tri/tridata/tri04/index.htm
EF Overview
Queries, Maps, & Reports
TRI eFDR
Data Update
Technical U
Site Map
Contact Us
Quick Star
View enviro
information
Code, City,
Use State
Abbreviatio
ZIP Cod
City, Sta
County,
GO
Customer S
Envirofacts Master Chemical Integrator (EMCI)
Recent Additions | Contact Us | Print Version EF Search: GO
EPA Home > Envirofacts > EMCI > Query Form
EMCI
Query Form
Search the EMCI Database
The Chemical Query Form allows you to obtain the acronyms, chemical identification numbers, and chemical names reported by the Envirofacts databases (AFS, PCS, RCRAInfo, and TRIS) using the Envirofacts Master Chemical Integrator (EMCI). You may see if the chemical is included in other groups, or is made up of other components.
User's Guide
Chemical Selection
You may enter one or more name fragments under the Chemical Name search option, separated by a space. If you enter more than one name fragment, the "Containing" Radio Button has to be selected. All chemical names in the EMCI are searched concurrently, including CAS index names, common names, and chemical names and descriptions used by program office systems. RCRA hazardous waste codes can also be searched as name fragments. More information about entering multiple fragments is available in the user's guide.
Chemical Search Option: Chemical Name
Chemical Option Value:
Chemical Name
Chemical Abstracts Service Registry Number
Beginning With Exact Match Containing
Search Clear
>Form R
UV Index



EPA's Chemical Data Islands

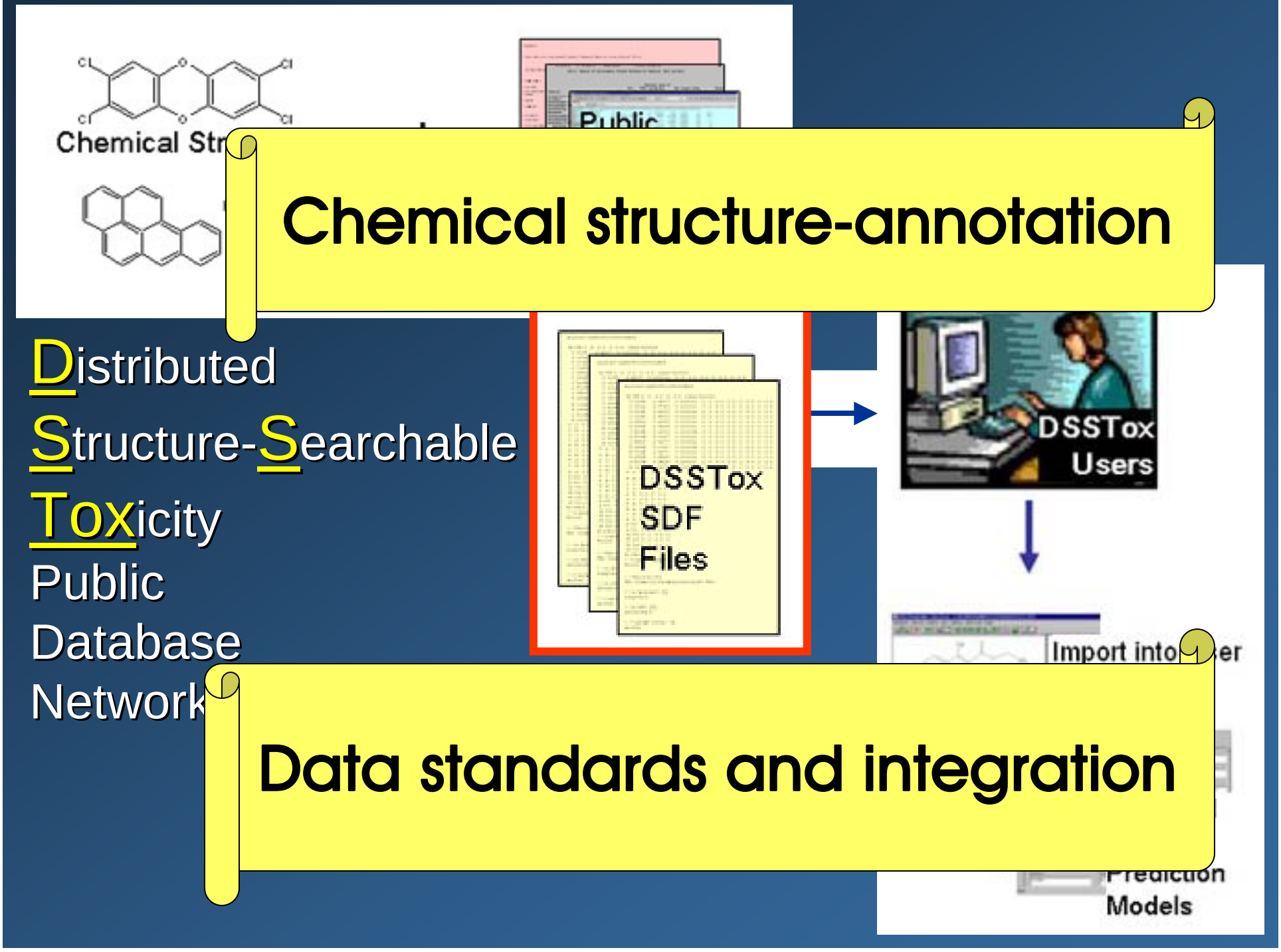

World Wide Web
Chemical structures
National Toxicology Program
National Library of Medicine
PubChem
European Chemicals Bureau (SIDS)
Chemical Names
CAS Registry Nos.
SMILES
Ecotox, Aster, Teratox
TSCA Substance Registry List
High Production Volume Information System
Green Chemistry
Chemical Structures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



EPA's Chemical Data Islands

Part II.

Data Linkages


Chemical Str
Public
Chemical structure-annotation
Distributed
Structure-Searchable
Toxicity
Public
Database
Network
DSSTox
SDF
Files
DSSTox
Users
Import into
Prediction
Models
Data standards and integration

U.S. Environmental Protection Agency

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

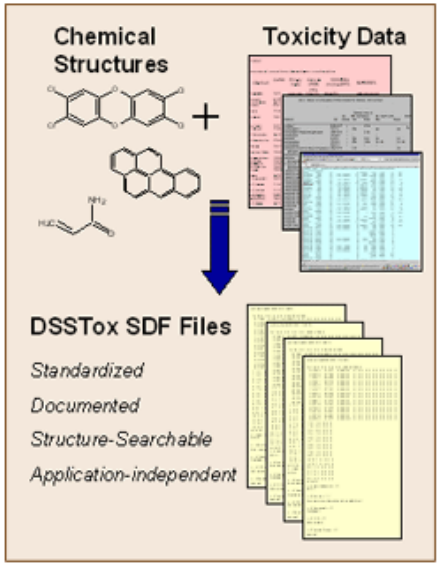
DSSTox

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

Distributed Structure-Searchable Toxicity (DSSTox) Database Network is a project of EPA's 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

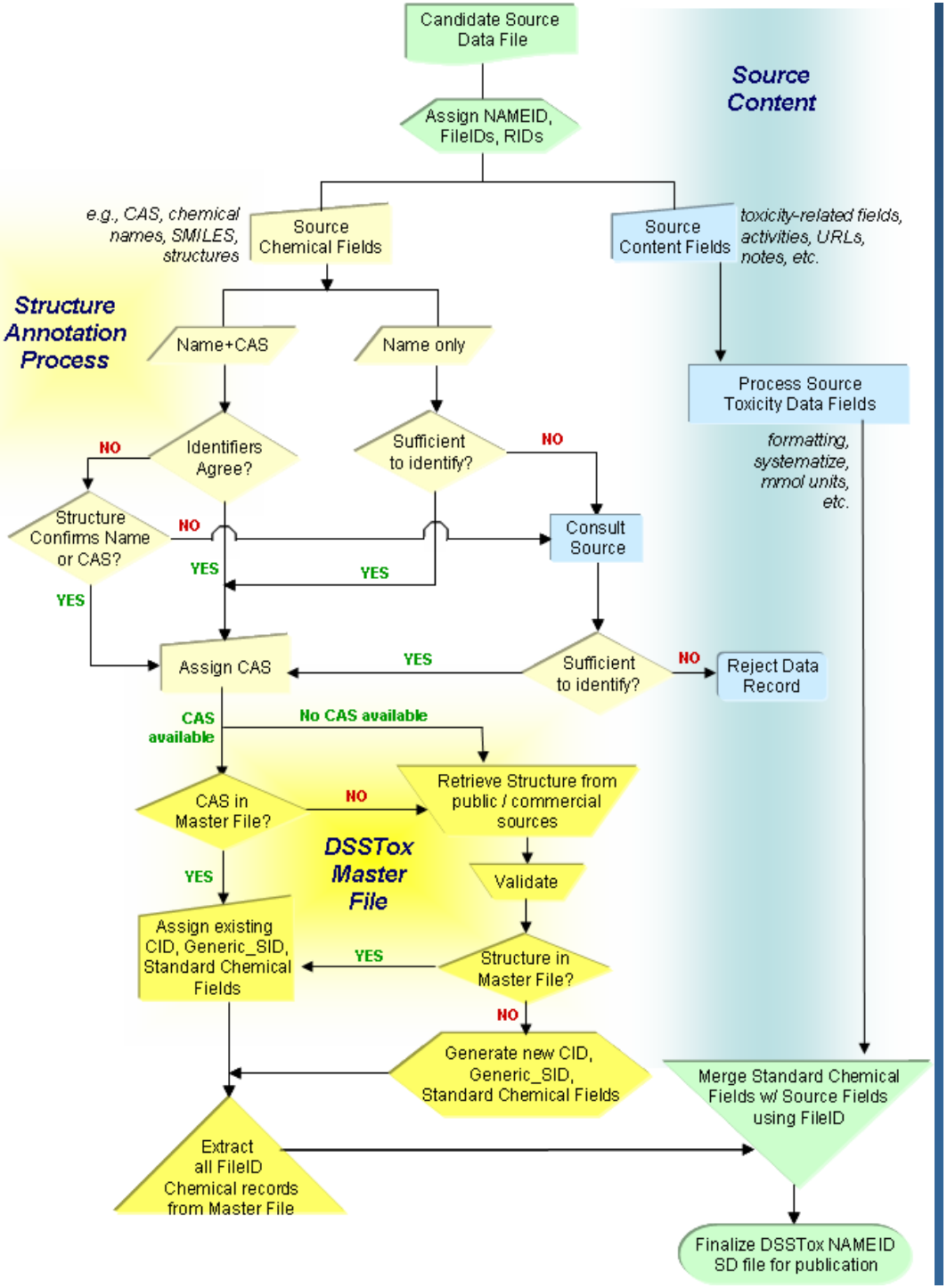
STRUCTURE_InChI

DSSTox_RID

DSSTox_FileID

DSSTox Chemical Quality Assurance Procedures:

- Chemical identification
- Structure annotation
- Internal consistency
- Quality review



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

NAMEID	version #records date	Expanded DSSTox Data File Title & Description	Status
CPDBAS	v4a 1481 15Jun2007	**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.	*Updated*
DBPCAN	v4a 209 15Jun2007	**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.	*Updated*
EPAFHM	v4a 617 15Jun2007	**EPA Fathead Minnow Acute Toxicity Database:** Acute toxicities of 617 chemicals tested in common assay, with mode-of-action assessments and confirmatory measures.	*Updated*
FDAMDD	v3a 1216 25Jul2007	**FDA Center for Drug Evaluation & Research - Maximum (Recommended) Daily Dose Database:** Maximum (recommended) daily dose (MRDD) values for 1217 pharmaceuticals in mg/kg-body weight (bw)/day, converted to mmol and normalized to dataset; MRDD values extracted from public literature sources.	*Updated*
HPVCSI	v2a 3548 15Aug2007	**EPA High Production Volume Challenge Program Structure-Index Locator File:** Compiled structures for three chemical lists provided on EPA HPV Challenge Program website; each record includes reference index to dated list.	*Updated*
IRISTR	v1a 544 15Aug2007	**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.	***New*
NCTRER	v4a 232 15Jun2007	**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.	*Updated*
NTPBSI	v2a 2293 24Aug2007	**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.	*Updated*
NTPHTS	v2a 1408 25Jul2007	**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.	*Updated*
TOXCST	v2a 320 25Sep2007	**Research Chemical Inventory for EPA's ToxCast ™ Program Structure-Index File:** Compiled structures for set of 340 chemical substances that are candidates for Phase I High-throughput screening (HTS) testing 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.	*Updated*

CPDBAS_v4a_1481

STRUCTURE
DSSTox_CID
DSSTox_SID
DSSTox_ID_FileName
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

SAL_CPDB
TD50_Rat_mg/kg/day
TD50_Rat_mmol/kg/day
TargetSites_Rat_Male, Female, Both Sexes
TD50_Mouse_mg/kg/day
TD50_Mouse_mmol/kg/day
TargetSites_Mouse_Male, Female, Both Sexes
TD50_Hamster_mg/kg/day
TD50_Hamster_mmol/kg/day
TargetSites_Hamster_Male, Female, Both Sexes
TD50_Dog_mg/kg/day
TargetSites_Dog
TD50_Rhesus_mg/kg/day
TargetSites_Rhesus
TD50_Cynomolgus_mg/kg/day
TargetSites_Cynomolgus
ActivityCategory_SingleCellCall
ActivityCategory_MultiCellCall
ToxicityNote
NTP_TechnicalReport
Website_URL

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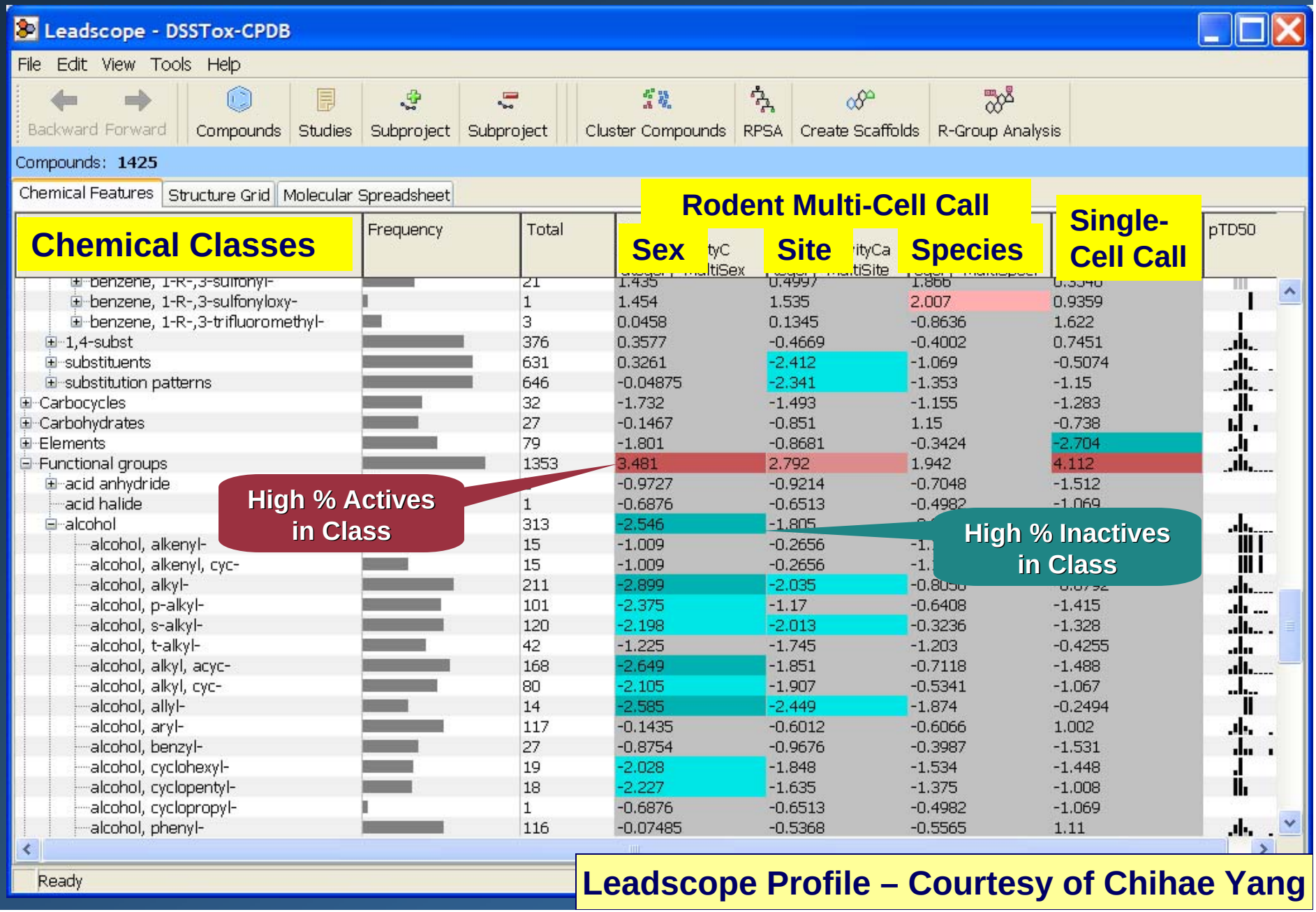
1

multisite
multisex
multispecies

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.

Chemical-Biological Profiling of CPDBAS Activities



Leadscope Profile – Courtesy of Chihae Yang

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Distributed Structure-Searchable Toxicity (DSSTox) Public Database Network

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

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- Frequent Questions
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- Central Field Definition Table
- Apps, Tools & More
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- Glossary of Terms
- Help

SDF Download Page:

TOXCST: Research Chemical Inventory for EP
Structure-Index File

** *New DSSTox* Structure-Index File *03August2007*

➢ *File corresponds to the Phase I candidate chemical list for EPA's ToxCast re*

Quick & Easy File Downloads: FTP Download Instructions

- Description
- Source Website & Contact
- SDF Fields
- SDF Content Summary
- SDF Version History

- **SDF Download Table** Download

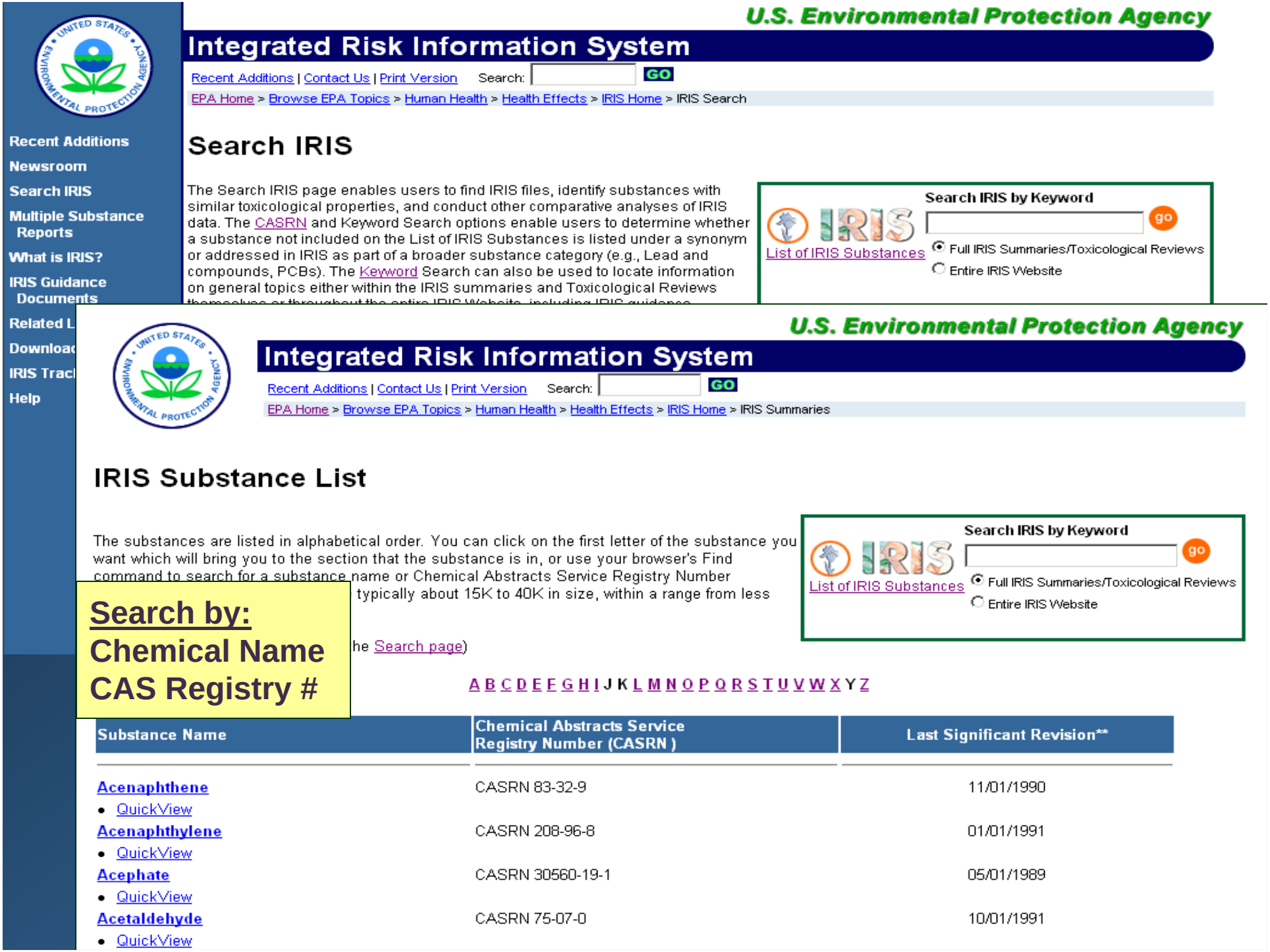
- Acknowledgements, DSSTox Citation & Disclaimer

TOXCST SDF Content Summary - *25 September 2007*

TOXCST SDF Content	Totals_v1a	Totals_v2a*
# Records	340	320
DSSTox Standard Chemical Fields	18	18
TOXCST Source Fields	3	3
Total # Fields	21	21
Chemical Content	**Counts_v1a**	**Counts_v2a**
STRUCTURE_ChemicalType:		
defined organic	331	313
inorganic	1	1
organometallic	8	6
no structure	0	0
STRUCTURE_TestedForm_DefinedOrganic:		

Documentation Files: *TOXCST*			
Log File	TOXCST_LogFile_25Sep2007.pdf	35KB	PDF
Data Files: *TOXCST*			
SDF Structure Data File	TOXCST_v2a_320_25Sep2007.sdf	911KB	SDF
▪ Data Table (no structures)	TOXCST_v2a_320_25Sep2007_nostructures.xls	186KB	XLS
▪ Structures Table	TOXCST_v2a_320_25Sep2007_structures.pdf (7 pp.)	1.4 MB	PDF

File Error Report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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
Download
IRIS Trac
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
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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
CASRN 83-32-9
11/01/1990
QuickView
Acenaphthylene
CASRN 208-96-8
01/01/1991
QuickView
Acephate
CASRN 30560-19-1
05/01/1989
QuickView
Acetaldehyde
CASRN 75-07-0
10/01/1991
QuickView

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
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Regional Offices

Disclaimer: Thi
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For definitions

Status of

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Oral RfD Assess
Inhalation RfC As
Carcinogenicity As

Chronic Health Hazard Assessments for Noncarcinogenic Effects

Carcinogenicity Assessment for Lifetime Exposure

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- Databa
- RfC --

Quantitative Estimate of Carcinogenic Risk from Oral Exposure

Oral Slope Factor(s)	Extrapolation Method
5.7×10^{-3} per mg/kg-day	Linearized multistage procedure, extra risk

Drinking Water Unit Risks
1.6×10^{-7} per ug/L

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

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SDF Download Page:

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

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.

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

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

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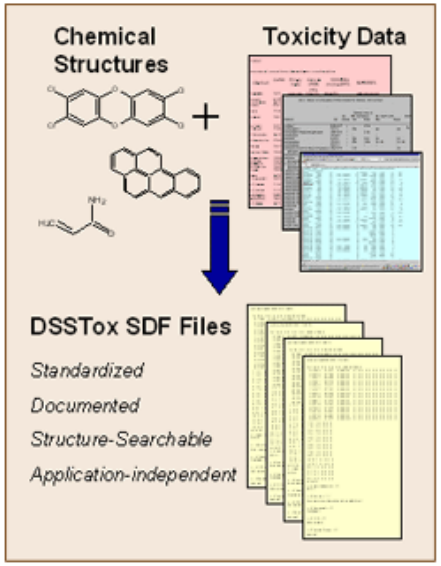
EPA DSSTox Structure-Browser v1.0 GO

DSSTox Structure-Browser information Page



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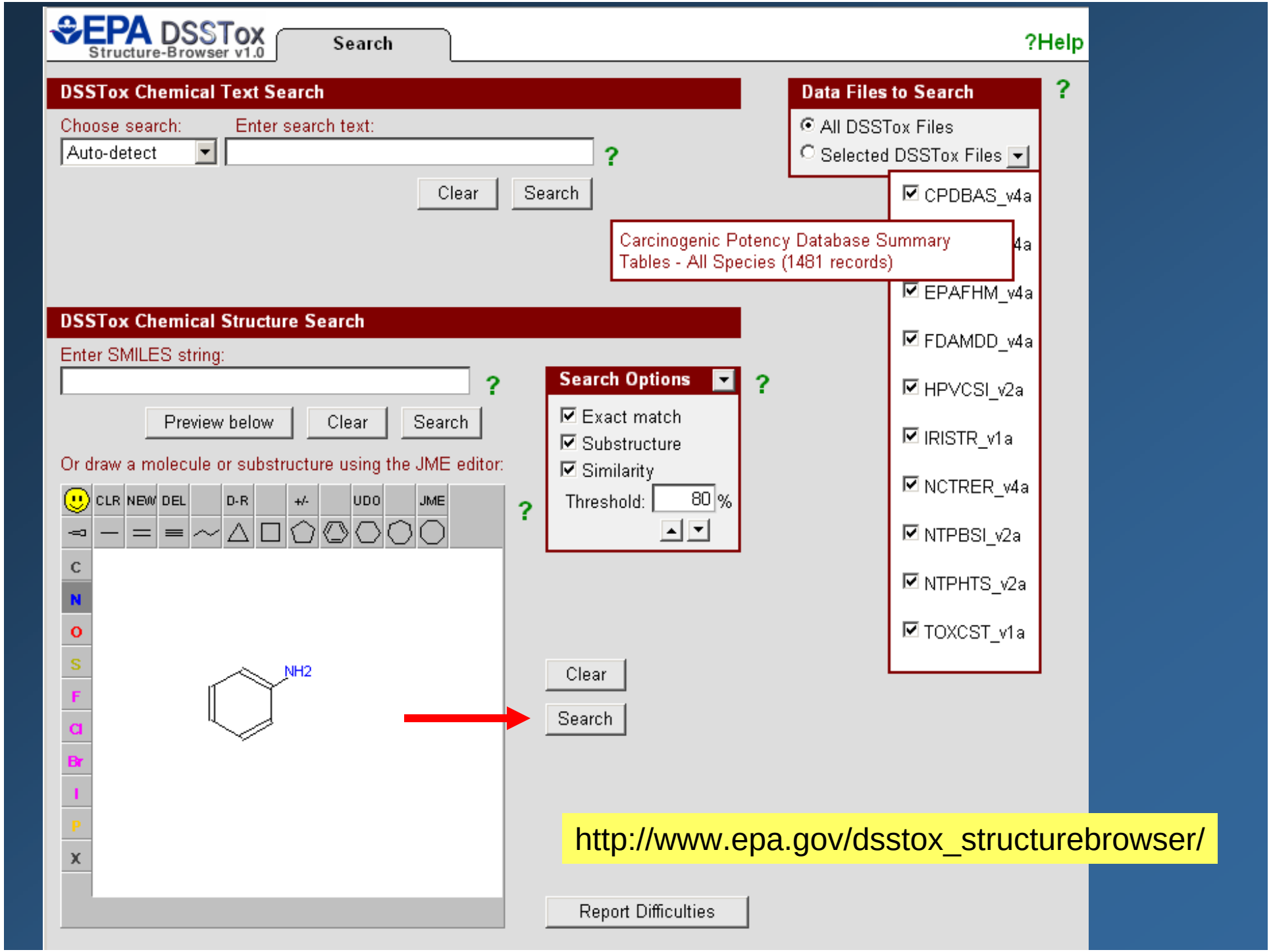
DBPCAN_v4a_209_15Jun2007
EPAFHM_v4a_617_15Jun2007
FDAMDD_v3a_1216_25Jul2007
HPVCSI_v2a_3548_15Aug2007***New content*
IRISTR_v1a_544_28Jul2007 ***New file*
NCTRER_v4a_232_15Jun2007
NTPBSI_v2a_2293_24Aug2007 ***Updated content*
NTPHTS_v1a_1408_25Jul2007
TOXCST_v2a_320_25Sep2007 ***Updated*

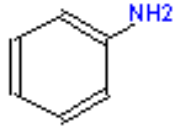
More on Data File Types


EPA DSSTox
Structure-Browser v1.0
Search
?Help
DSSTox Chemical Text Search
Choose search:
Auto-detect
Enter search text:
Clear
Search
Data Files to Search
All DSSTox Files
Selected DSSTox Files
CPDBAS_v4a
Carcinogenic Potency Database Summary Tables - All Species (1481 records)
EPAFHM_v4a
FDAMDD_v4a
HPVCSI_v2a
IRISTR_v1a
NCTRER_v4a
NTPBSI_v2a
NTPHTS_v2a
TOXCST_v1a
DSSTox Chemical Structure Search
Enter SMILES string:
Preview below
Clear
Search
Search Options
Exact match
Substructure
Similarity
Threshold: 80 %
Or draw a molecule or substructure using the JME editor:
CLR NEW DEL D-R +/- UDO JME
C N O S F Cl Br I P X
NH2
Clear
Search
Report Difficulties
http://www.epa.gov/dsstox_structurebrowser/

EPA DSSTox Structure-Browser v1.0

Search | File Incidences | ?Help

Search Results Summary for DSSTox Substances - File Breakdown Incidences

Query	Results Type	Hits	Display
Structure: 	Exact matches	1	Details
	Substructures	1130	Details
	Similarity > 80%	8	Details

?

DSSTox File ?	Total#Records	Exact matches	Substructures	Similarity > 80%
CPDBAS_v4a	1481	1	309	7
DBPCAN_v4a	209	-	1	-
EPAFHM_v4a	617	1	102	1
FDAMDD_v4a	1216	-	261	-
HPVCSI_v2a	3548	1	216	4
IRISTR_v1a	544	1	68	2
NCTRER_v4a	232	-	10	-
NTPBSI_v2a	2293	1	494	5
NTPHTS_v2a	1408	1	313	3
TOXCST_v1a	340	-	80	-
Total Unique Substance Hits		**1**	**1130**	**8**
Total Substance Hits - All Files		**6**	**1854**	**22**

?

EPA DSSTox Structure-Browser v1.0

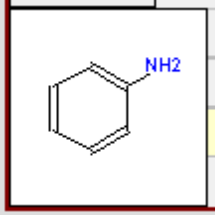
Search | File Incidences | **Search Details** | ?Help

Details

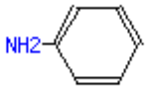
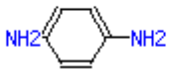
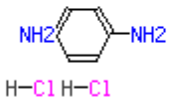
Output Options

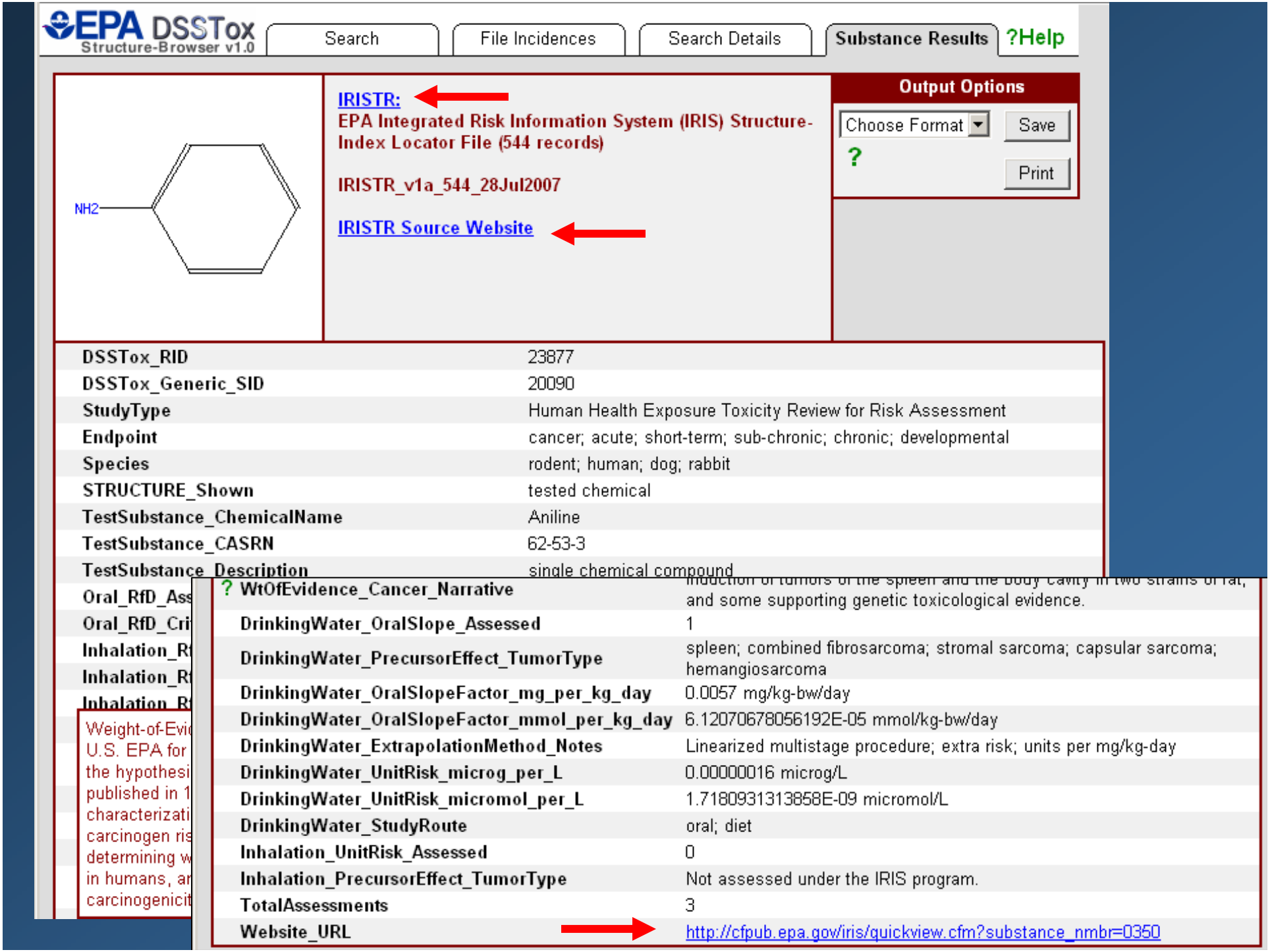
Choose Format | Save | Print

?

Query	Results Type	Hits	Display
Structure: 	Exact matches	1	Details
	Substructures	1130	Details
	Similarity > 80%	8	Details

?

? DSSTox Substance ID	? Similarity Score%	Structure Match	Substance Name	CASRN	Substance Description	Details (Data Files)
20090	100		Aniline	62-53-3	single chemical compound	CPDBAS EPAFHM HPVCSI IRISTR NTPBSI NTPHTS
20091	94.1		Aniline.HCl	142-04-1	single chemical compound	CPDBAS NTPBSI
21138	94.1		p-Phenylenediamine	106-50-3	single chemical compound	CPDBAS HPVCSI
21141	88.8		p-Phenylenediamine.2HCl	624-18-0	single chemical compound	CPDBAS NTPBSI


EPA DSSTox
Structure-Browser v1.0
Search
File Incidences
Search Details
Substance Results
?Help
NH2
IRISTR:
EPA Integrated Risk Information System (IRIS) Structure-Index Locator File (544 records)
IRISTR_v1a_544_28Jul2007
IRISTR Source Website
Output Options
Choose Format
Save
Print
DSSTox_RID 23877
DSSTox_Generic_SID 20090
StudyType Human Health Exposure Toxicity Review for Risk Assessment
Endpoint cancer; acute; short-term; sub-chronic; chronic; developmental
Species rodent; human; dog; rabbit
STRUCTURE_Shown tested chemical
TestSubstance_ChemicalName Aniline
TestSubstance_CASRN 62-53-3
TestSubstance_Description single chemical compound
? WtOfEvidence_Cancer_Narrative
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
Website_URL http://cfpub.epa.gov/iris/quickview.cfm?substance_nmbr=0350

Aniline Quickview (CASRN 62-53-3)

Quickview Navigation
+ Expand navigation:

- view Aniline Summary

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 Full IRIS Summary to put this information into complete context.

For definitions of terms in the IRIS Web site, refer to the IRIS Glossary.

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

Chronic Health Hazard Assessments for Noncarcinogenic Effects

Reference Dose for Chronic Oral Exposure (RfD)

Not Assessed under the IRIS Program

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Multiple Substance Reports
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IRIS Guidance Documents
Related Links
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Help

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

Search IRIS by Keyword go

Full IRIS Summaries/Toxicological Reviews

Entire IRIS Website

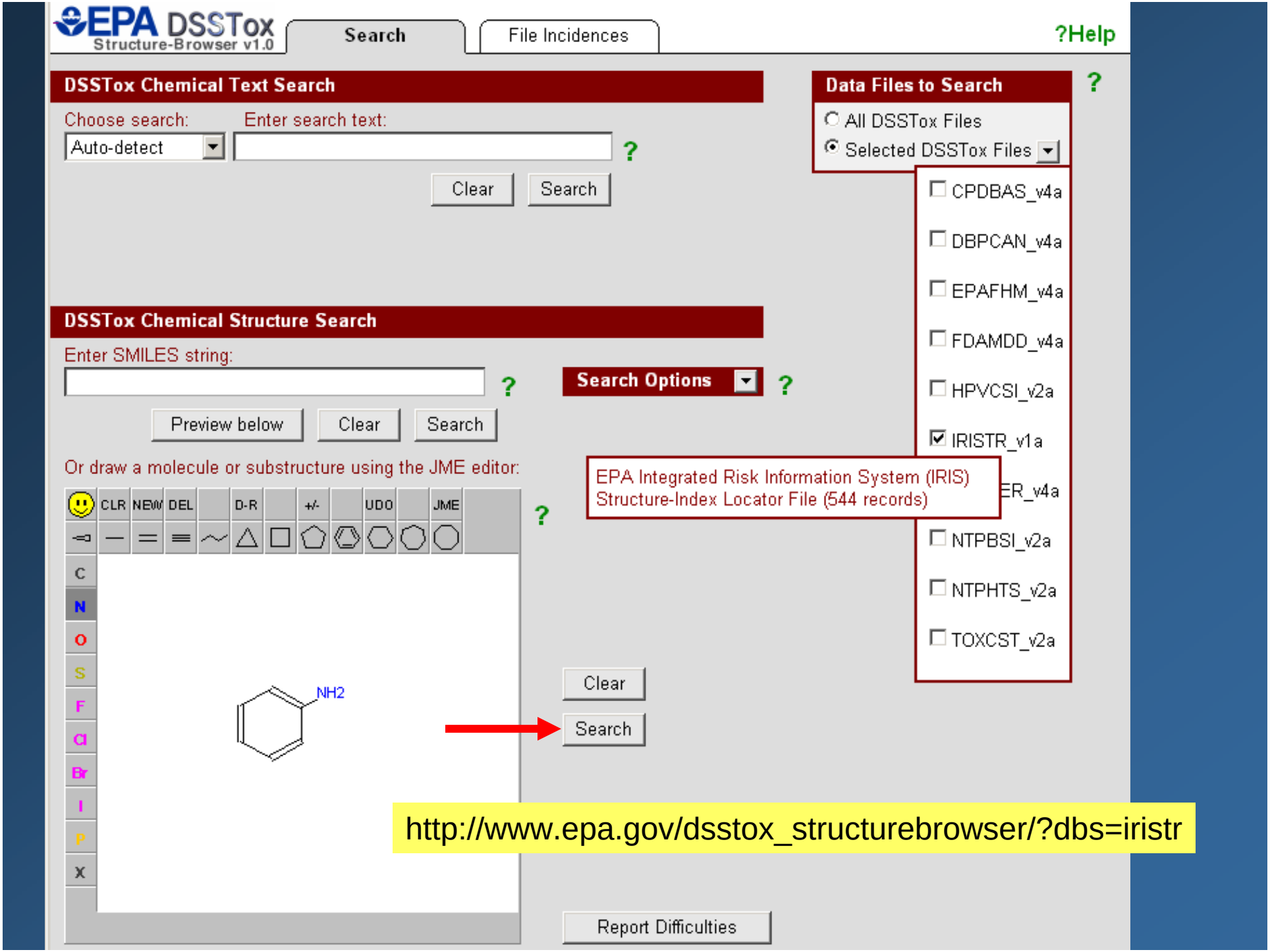
Structure-search

EPA DSSTox GO Structure-Browser v1.0

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

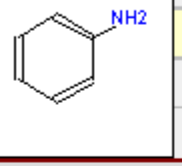
Substance Name	Chemical Abstracts Service Registry Number (CASRN)	Last Significant Revision*
Acenaphthene	CASRN 83-32-9	11/01/1990
• QuickView		
Acenaphthylene	CASRN 208-96-8	01/01/1991
• QuickView		
Acephate	CASRN 30560-19-1	05/01/1989
• QuickView		
Acetaldehyde	CASRN 75-07-0	10/01/1991
• QuickView		
Acetochlor	CASRN 34256-82-1	09/01/1993


EPA DSSTox
Structure-Browser v1.0
Search
File Incidences
?Help
DSSTox Chemical Text Search
Choose search:
Auto-detect
Enter search text:
Clear
Search
Data Files to Search
All DSSTox Files
Selected DSSTox Files
CPDBAS_v4a
DBPCAN_v4a
EPAFHM_v4a
FDAMDD_v4a
HPVCSI_v2a
IRISTR_v1a
NTPBSI_v2a
NTPHTS_v2a
TOXCST_v2a
DSSTox Chemical Structure Search
Enter SMILES string:
Search Options
Preview below
Clear
Search
Or draw a molecule or substructure using the JME editor:
CLR
NEW
DEL
D-R
+/-
UDO
JME
NH2
EPA Integrated Risk Information System (IRIS)
Structure-Index Locator File (544 records)
Clear
Search
Report Difficulties
http://www.epa.gov/dsstox_structurebrowser/?dbs=iristr

EPA DSSTox Structure-Browser v1.0

Search | File Incidences | Search Details | ?Help

Details

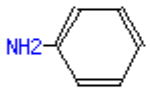
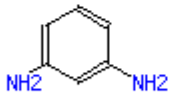
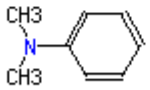
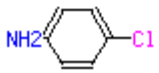
Query	Results Type	Hits	Display
Structure: 	Exact matches	1	Details
	Substructures	68	Details
	Similarity > 80%	2	Details

?

Output Options

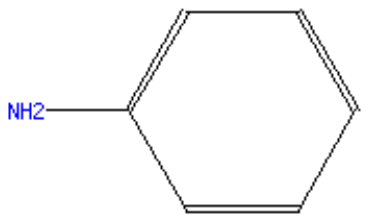
Choose Format | Save | Print

?

DSSTox Substance ID	Similarity Score%	Structure Match	Substance Name	CASRN	Substance Description	Details (Data Files)
20090	100		Aniline	62-53-3	single chemical compound	IRISTR
21137	88.8		m-Phenylenediamine	108-45-2	single chemical compound	IRISTR
20507	69.5		N,N-Dimethylaniline	121-69-7	single chemical compound	IRISTR
20295	61.5		p-Chloroaniline	106-47-8	single chemical compound	IRISTR

EPA DSSTox Structure-Browser v1.0

Search | File Incidences | Search Details | **Substance Results** | ?Help



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

IRISTR_v1a_544_28Jul2007

IRISTR Source Website

Output Options

Choose Format | Save | ? | Print

PubChem

Links directly to chemical data page for Aniline in PubChem

DSSTox_RID	23877
DSSTox_Generic_SID	20090
StudyType	Human Health Exposure Toxicity Review for Risk Assessment
Endpoint	cancer; acute; short-term; sub-chronic; chronic; developmental
Species	rodent; human; dog; rabbit
STRUCTURE_Shown	tested chemical
TestSubstance_ChemicalName	Aniline
TestSubstance_CASRN	62-53-3
TestSubstance_Description	single chemical compound
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

Weight-of-Evidence (WOE) for Carcinogenicity is a system used by the U.S. EPA for characterizing the extent to which the available data support the hypothesis that an agent causes cancer in humans. Revised guidelines published in 1996, 1999, and 2005 have modified these cancer risk characterizations. The approach outlined in EPA"s guidelines for carcinogen risk assessment (2005) considers all scientific information in determining whether and under what conditions an agent may cause cancer in humans, and provides a narrative approach to characterize carcinogenicity rather than categories. Click the ? for more details.

E-05 mmol/m3

ed adverse effect level) HEC (Human Equivalent

mg/m3

n carcinogen - based on sufficient evidence of

nimals

NCBI

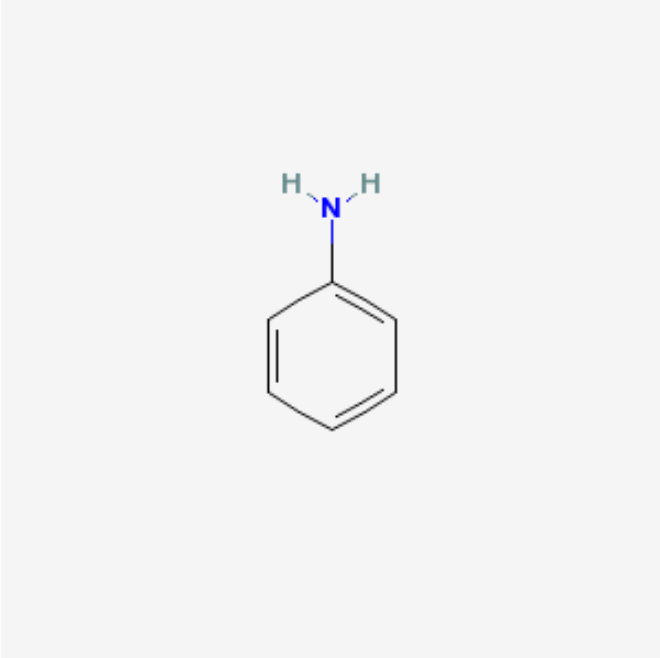
PubChem

Information on biological activities of small molecules

HOME | SEARCH | SITE MAP | PubMed | Entrez | Structure | GenBank | PubChem | Help

Search PubChem Compound GO

Compound Summary:



CID: 6115

BioActivity: Summary

All: 53 Links
Active: 6 Links
Inactive: 45 Links
Inconclusive: 1 Link

Protein Structures: 3 Links

Protein Sequences: 15 Links

NLM Toxicology: Link

Substances:

All: 270 Links
Same: 28 Links
Mixture: 242 Links

Related Compounds:

Same, Connectivity: 13 Links

Similar Compounds: 164 Links

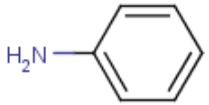
Structure Search

MeSH | Synonyms | Properties | Descriptors | Category | Exports

United States National Library of Medicine

ChemIDplus Advanced

NAME: Aniline
RN: 62-53-3



Basic Information

Full Record

Structure

Names & Synonyms

Formulas

Classification Codes

Registry Numbers

Toxicity

Physical Properties

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

File Locator

AIDSLINE	AIDS Citations from MEDLINE
CANCERLIT	CANCER LITerature from Medline
CCRIS	NCI Chem Carcino Res Info Sys
DART/ETIC	Developmental and Reprod.Tox.
DSL	Domestic Sub. List of Canada
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
IRIS	EPA Integrated Risk Info. System
ITER	International Tox. Est. for Risk
MEDLINE	MEDical literature onLINE
MeSH	Medical Subject Headings File
PubChem	PubChem
RTECS	Reg. of Toxic Eff. of Chem. Sub.
TOXLINE Core	NLM TOXLINE Core from MEDLINE
TOXLINE Special	NLM TOXLINE Special on TOXNET
TOXMAP	NLM Enviro. Health e-Maps
TRI2000	EPA Toxics Release Inv. 2000

Search Navigation

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Structure Similarity Search

Structure Salt/Parent Search

Transfer Structure

Basic ChemIDplus Search

NCBI

PubChem

Information on biological activities of small molecules

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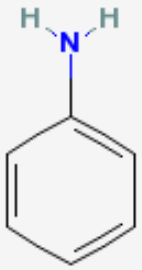
Search PubChem Compound GO

Compound Summary:



CID: 6115

BioActivity: Summary

All: 53 Links
Active: 6 Links
Inactive: 45 Links
Inconclusive: 1 Link

Protein Structures: 3 Links

Protein Sequences: 15 Links

NLM Toxicology: Link

Substances:

All: 270 Links
Same: 28 Links
Mixture: 242 Links

Related Compounds:

Same, Connectivity: 13 Links

Similar Compounds: 164 Links

Structure Search

MeSH | Synonyms | Properties | Descriptors | Category | Exports

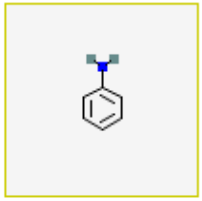
NCBI

PubChem

Information on biological activities of small molecules

HOME | SEARCH | SITE MAP | PubMed | Entrez | Structure | GenBank | PubChem | Help

BioActivity Summary: -- Original CID: 6115



Total BioAssay Count: 47

Total Substance Count: 4

Total Compound Count: 1

Tested: 1
Active: 1
Inactive: 1

Revise Substance Selection:

Select Active
Add Active
Add Tested
Add Similar Substances

Revise BioAssay Selection:

Select Active
Add Active

Structure Activity Analysis

BioAssay Data Table

		AID						
42	☐	426		1		1	Confirmatory	Cell Viability - Jurkat
43	☐	421		1		1	Confirmatory	Cell Viability - BJ
44	☐	356				1	Confirmatory	EPA Fathead Minnow Acute Toxicity database (EPAFHM)
45	☐	352		1		1	Other	Carcinogenic Potency Database (CPDBAS)
46	☐	256		1		1		NCI In Vivo Anticancer Drug Screen. Data for tumor model L1210 Leukemia
47	☐	248		1		1		

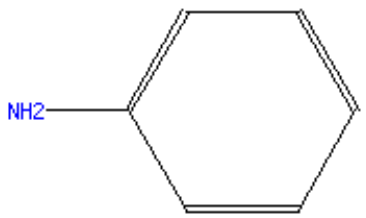
Tot

#		AID	Active	Inactive	Discrepant	Tested	Outcome Method	
1	☐	175	1	1	1	1		NCI Yea
2	☐	167	1	1	1	1		NCI Yeast Anticancer Drug Screen. Data for the bub3 strain

Current DSSTox files will be deposited in PubChem, providing links to DSSTox files (e.g., IRISTR) and Source web pages (EPA IRIS)

EPA DSSTox Structure-Browser v1.0

Search | File Incidences | Search Details | **Substance Results** | ?Help



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

IRISTR_v1a_544_28Jul2007

IRISTR Source Website

Output Options

Choose Format | Save | ? | Print

PubChem

EPA ACToR

Links directly to chemical data page for Aniline in EPA ACToR

DSSTox_RID	23877
DSSTox_Generic_SID	20090
StudyType	Human He
Endpoint	cancer; ac
Species	rodent; hu
STRUCTURE_Shown	tested chemical
TestSubstance_ChemicalName	Aniline
TestSubstance_CASRN	62-53-3
TestSubstance_Description	single chemical compound
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

Weight-of-Evidence (WOE) for Carcinogenicity is a system used by the U.S. EPA for characterizing the extent to which the available data support the hypothesis that an agent causes cancer in humans. Revised guidelines published in 1996, 1999, and 2005 have modified these cancer risk characterizations. The approach outlined in EPA"s guidelines for carcinogen risk assessment (2005) considers all scientific information in determining whether and under what conditions an agent may cause cancer in humans, and provides a narrative approach to characterize carcinogenicity rather than categories. Click the ? for more details.

E-05 mmol/m3

ed adverse effect level) HEC (Human Equivalent

mg/m3

n carcinogen - based on sufficient evidence of

nimals

ACToR Home
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Data Collections
Search by Name
Search By Structure
Browse Assays
Downloads
ToxRefDB
DSSTox
ToxMiner
ToxCast
Chemical Prioritization
National Center for Computational Toxicology
Links
Contact Us

Search Results

Search Term: NAMES : EXACT : aniline

GCID	CASRN	Name	Structure	Bioassay	Literature	MESH	MSDS	Genomics	Hazard	Carcinogenicity	GeneTox	DevTox	ReproTox	DevNeuroTox	NeuroTox	ImmunoTox	ChronicTox	SubchronicTox	DermalTox	RespiratoryTox	AcuteTox	OtherTox	EcoTox	Regulation
88	62-53-3	Aniline	S	B		M	M		H	C	M	D	R		N	I	C		D		A	T	E	R
89	142-04-1	Aniline.HCl	S	B		M	M			C	M	D	R		N	I	C					T		R
131913	45497-73-2	142-04-1	S	B		M																		

Chemical Summary

ACToR Home
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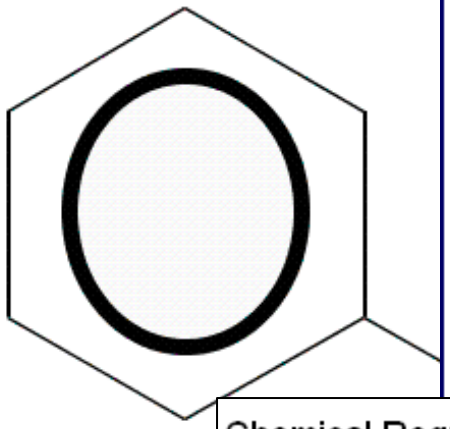
Data Collections
Search by Name
Search By Structure
Browse Assays
Downloads
ToxRefDB
DSSTox
ToxMiner
ToxCast
Chemical Prioritization
National Center for Computational Toxicology
Links
Contact Us



Substances

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

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

Data Collection: IRISTR_DSSTOX

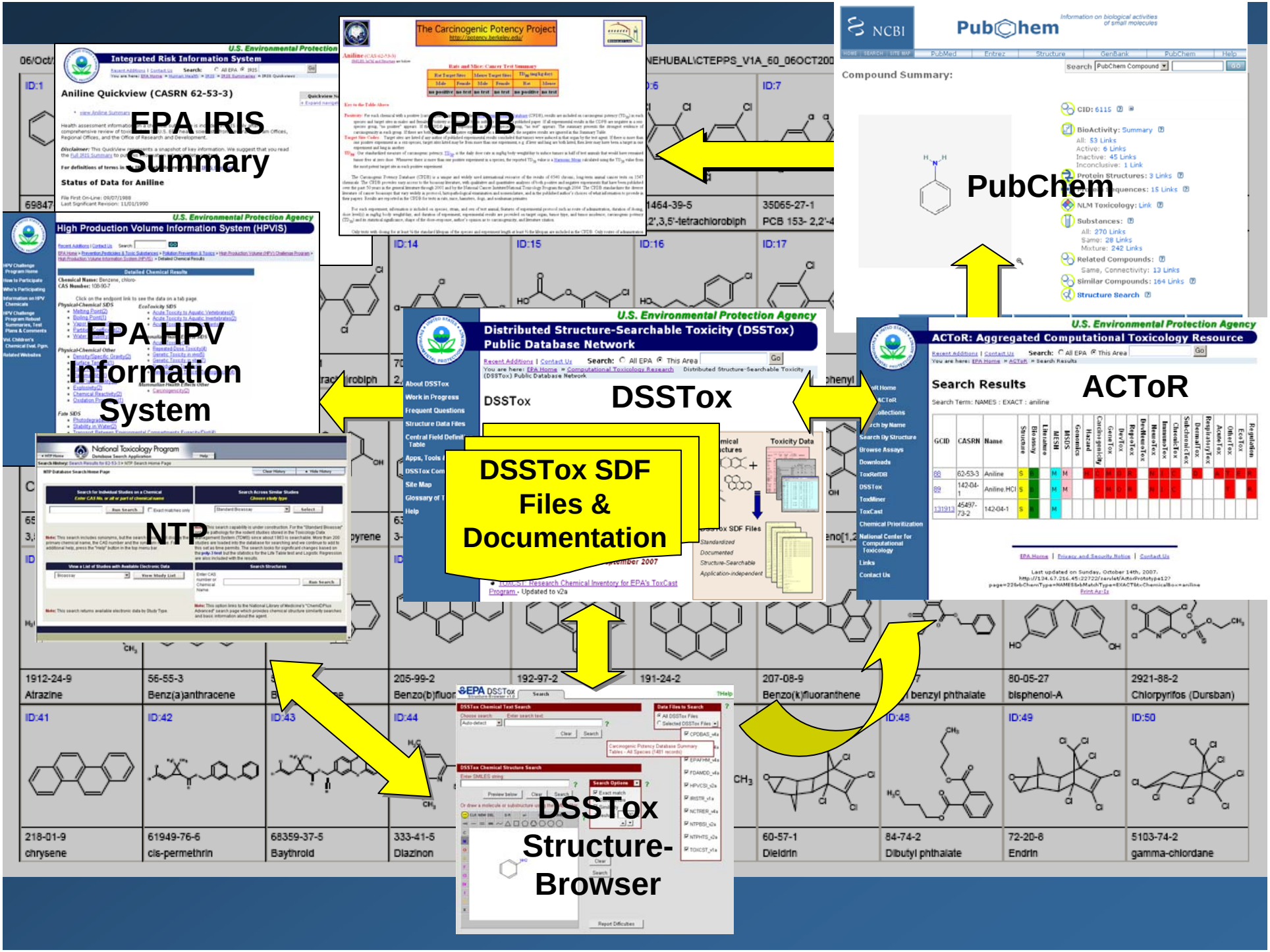
Name:	IRISTR_DSSTOX
Description	EPA Integrated Risk Information System http://www.epa.gov/iris/. A structure index file with links to webpage for each chemical (DSSTOX)
ID	7
Source Type	DSSTox Collection
Number of Substances	544
Number of Generic Chemicals	555

Show Assay Data

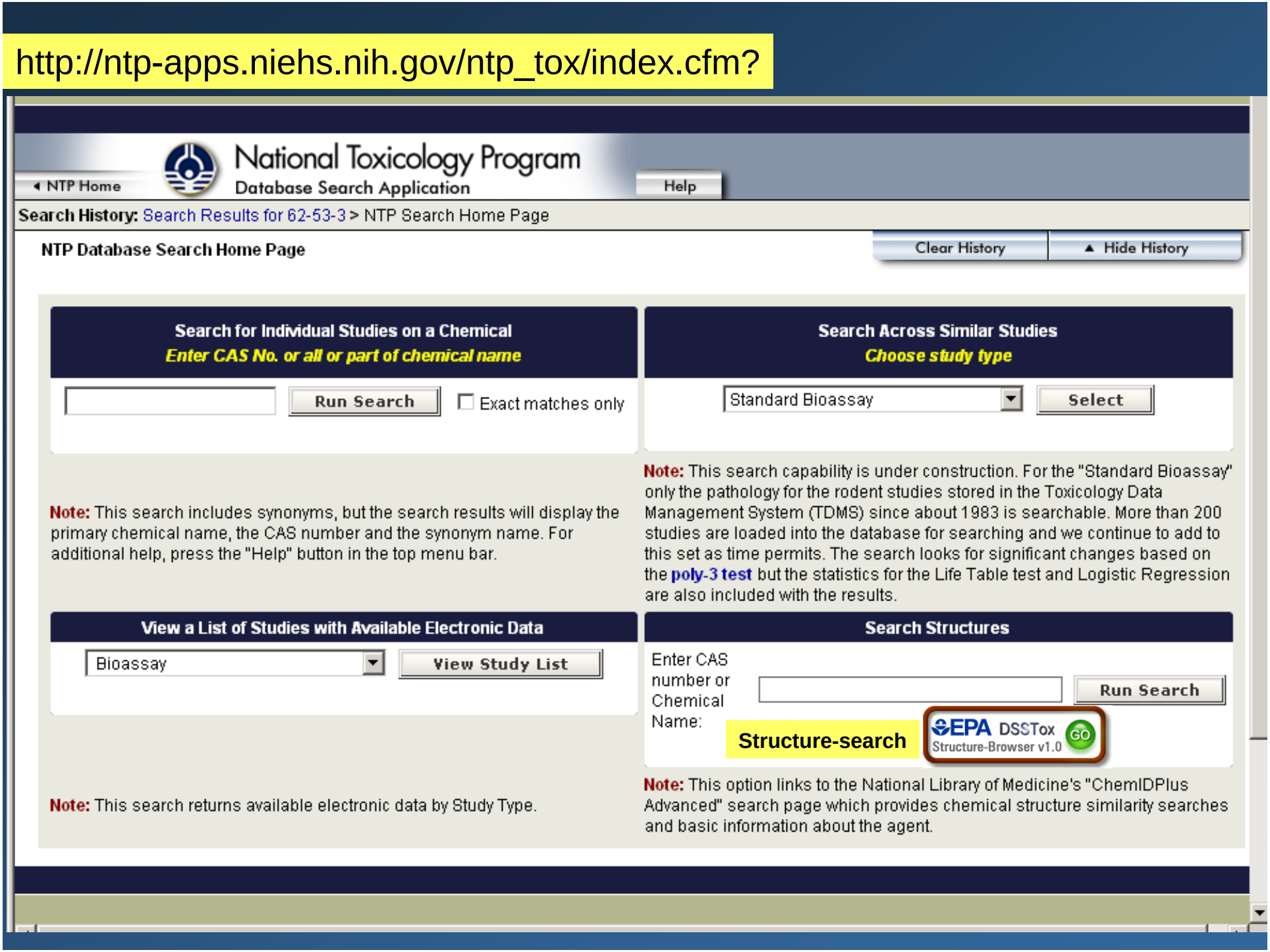
Page 1 of 6 : Next

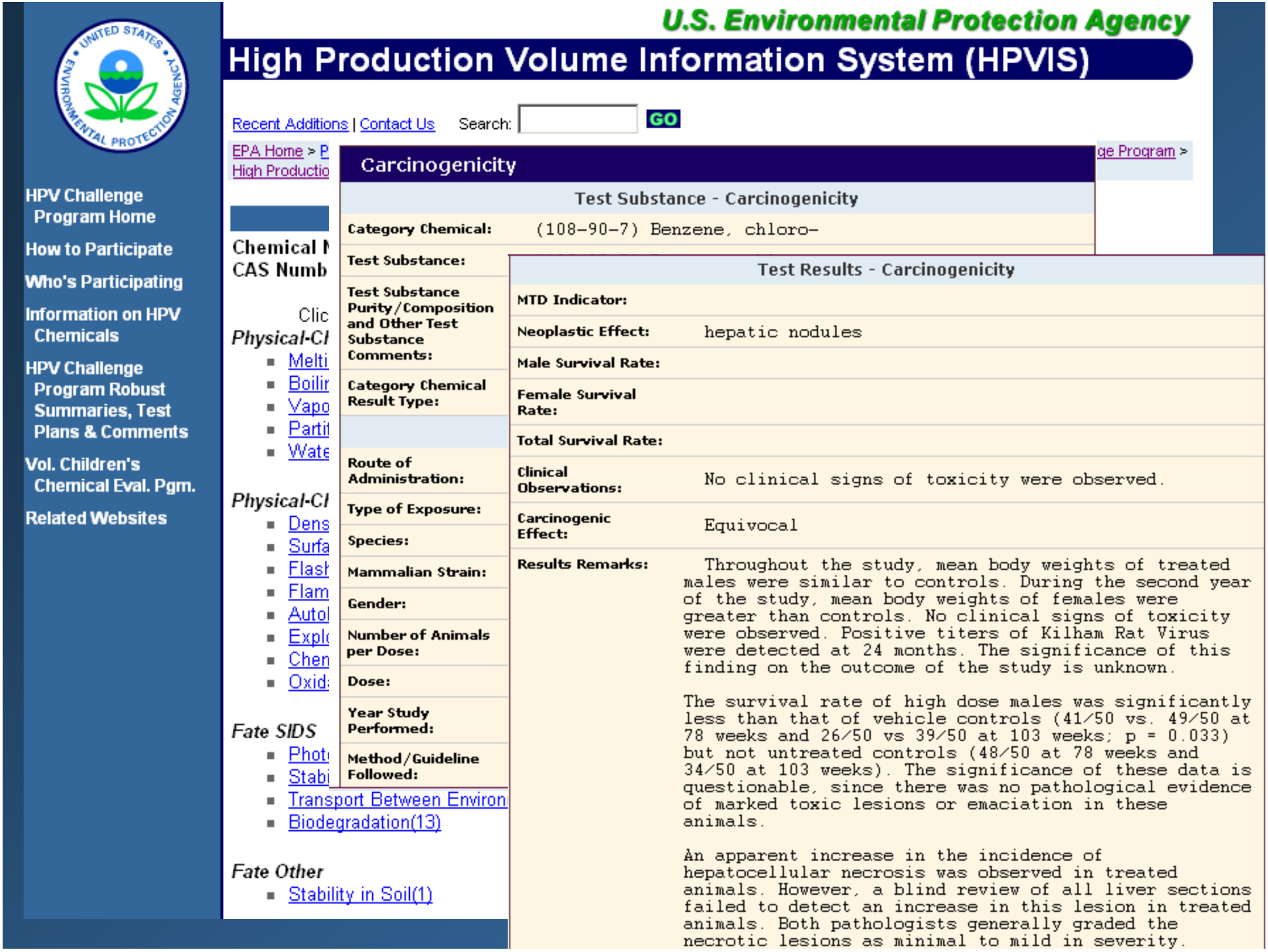
1 2 3 4 5 6

SCID	GCID	Source SID	CASRN	Name	Structure	Bioassay	Literature	MESH	MSDS	Genomics	Hazard	Carcinogenicity	GeneTox	DevTox	ReproTox	DevNeuroTox	NeuroTox	ImmunoTox	ChronicTox	SubchronicTox	DermalTox	RespiratoryTox	Acute Tox	OtherTox	EcoTox	Regulation	Description	Category	FoodSafe
7072	1670	DSSTOX_23845	83-32-9	1,2-dihydroacenaphthylene	S	B		M	M		H	C	M	D	R		N	I	C				A	T	E	R			
7073	6292	DSSTOX_23846	208-96-8	acenaphthylene	S			M			H	C	M	D	R		N	I	C		D		A	T	E	R			
7074	6293	DSSTOX_23847	30560-19-1	O,S-dimethyl acetylamidothiophosphate	S			M	M		H	C	M	D	R		N	I	C		D		A	T	E	R			
7075	2	DSSTOX_23848	75-07-0	acetaldehyde	S	B		M	M		H	C	M	D	R		N	I	C		D		A	T	E	R			F
7076	6294	DSSTOX_23849	34256-82-1	2-chloro-N-(ethoxymethyl)-N-(2-ethyl-6-methylphenyl)acetamide	S	B		M			H	C	M	D	R		N	I	C				A	T	E				
7077	1446	DSSTOX_23850	67-64-1	acetone	S	B		M	M		H	C	M	D	R		N	I	C		D		A	T	E	R			F
7078	9	DSSTOX_23851	75-05-8	acetonitrile	S	B		M	M		H	C	M	D	R		N	I	C		D		A	T	E	R			


EPA IRIS Summary
CPDB
PubChem
EPA HPV Information System
DSSTox
ACToR
DSSTox SDF Files & Documentation
NTP
DSSTox Structure-Browser

http://ntp-apps.niehs.nih.gov/ntp_tox/index.cfm?





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Fate SIDS
- Photo
- Stabi
- Transport Between Environ
- Biodegradation(13)

Fate Other
- Stability in Soil(1)

Carcinogenicity

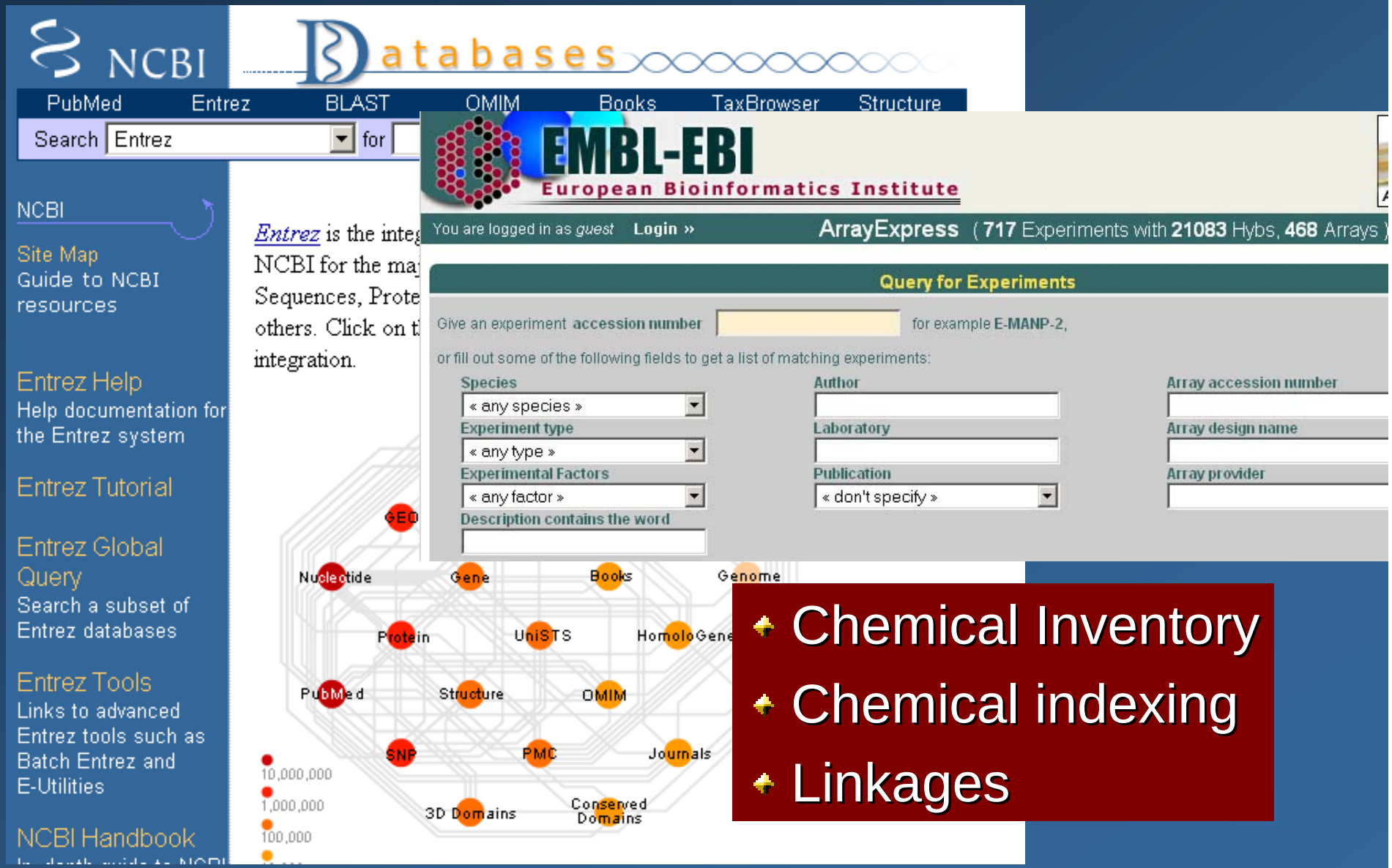
Test Substance - Carcinogenicity

Category Chemical:	(108-90-7) Benzene, chloro-
Test Substance:	
Test Substance Purity/Composition and Other Test Substance Comments:	
Category Chemical Result Type:	
Route of Administration:	
Type of Exposure:	
Species:	
Mammalian Strain:	
Gender:	
Number of Animals per Dose:	
Dose:	
Year Study Performed:	
Method/Guideline 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.

Public Genomic Databases

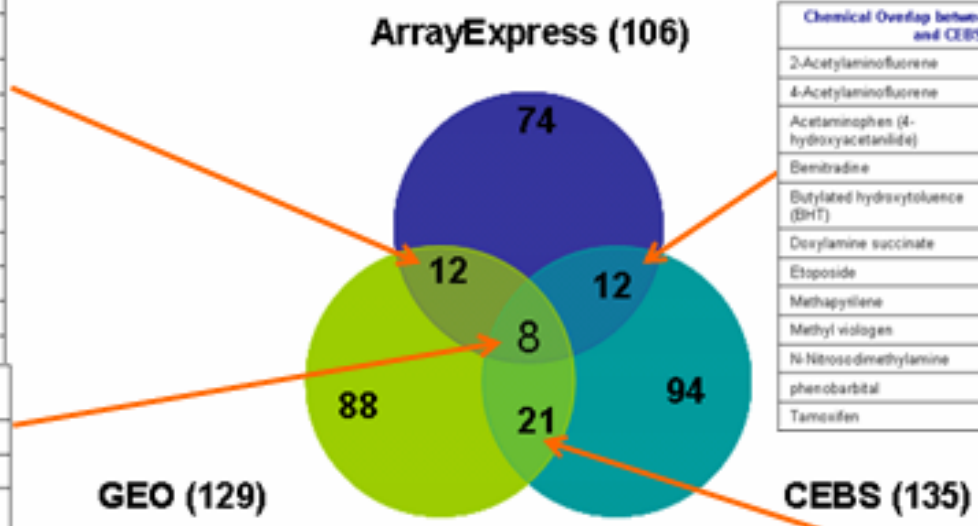


- Chemical Inventory
- Chemical indexing
- Linkages

Chemical Overlap Between ArrayExpress and GEO	
17beta-Estradiol	50-28-2
Genistein	446-72-0
Dexamethazone	50-02-2
Cycloheximide	66-81-9
Retinoic Acid	302-79-4
Hydrogen peroxide	7722-84-1
Terephthalic acid,TPA	100-21-0
Fenpropimorph	67306-03-0
5-Fluorouracil	51-21-8
Liothyronine;	6893-02-3
Mitomycin C	50-07-7
Paclitaxel	33069-62-4

Chemical Overlap between ArrayExpress, GEO, and CEBS	
cis-Dichlorodiamine platinum	15663-27-1
Clofibrate	637-07-0
Clotrimazole	23593-75-1
Ethanol	64-17-5
Ethinyl estradiol	57-63-6
Lipopolysaccharide (LPS)	NOCAS
Miconazole	22916-47-8
Valproic acid	99-66-1

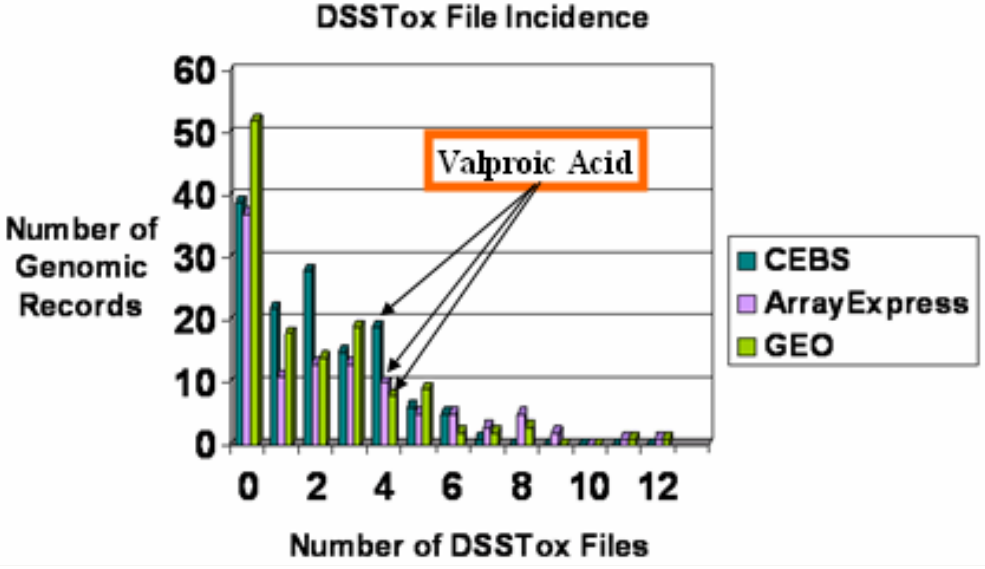
Overlap between Genomic Repository Chemical Space

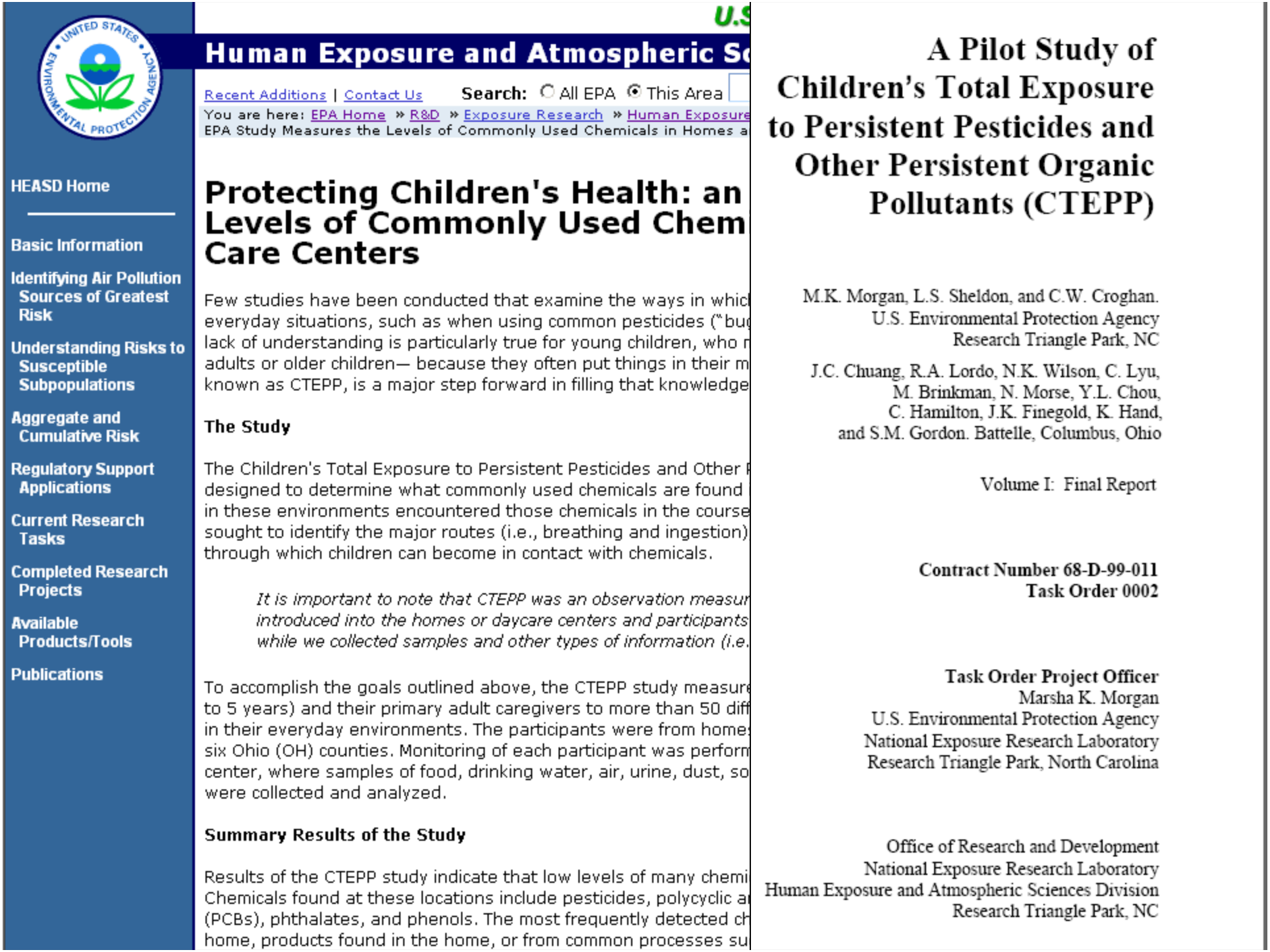


Chemical Overlap between ArrayExpress and CEBS	
2-Acetylaminofluorene	53-96-3
4-Acetylaminofluorene	28322-02-3
Acetaminophen (4-hydroxyacetanilide)	103-90-2
Benitradine	88133-11-3
Butylated hydroxytoluence (BHT)	128-37-0
Doxylamine succinate	562-10-7
Etoposide	33419-42-0
Methapyrilene	91-80-5
Methyl viologen	1910-42-5
N-Nitrosodimethylamine	62-75-9
phenobarbital	50-06-6
Tamoxifen	10540-29-1

Chemical Overlap between GEO and CEBS	
1,3-Bis(chloroethyl)-1-nitrosourea	154-93-8
Adriamycin, hydrochloride	25316-40-9
Allyl alcohol	107-18-6
alpha-Naphthyl isothiocyanate	551-06-4
Atorvastatin	134523-00-5
Bezafibrate	41859-67-0
Carbon tetrachloride	56-23-5
Dimethylformamide	68-12-2
Econazole	27220-47-9
Fenofibrate	49562-28-9
Fluconazole	86386-73-4
Fluvastatin	93957-54-1
Gemfibrozil	25812-30-0
Itraconazole	84625-61-6
Lovastatin	75330-75-5
Methotrexate	59-05-2
N-Nitrosodiethylamine	55-18-5
Rifampicin	13292-46-1
SIMVASTATIN	79902-63-9
Sodium arsenite	7784-46-5
Troglitazone	97322-87-7

Overlap between Genomic Chemical Space and DSSTox Chemical Space





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

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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 P
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 Estimated Ratios Between Selected Strata of Geometric Mean Potential Exposure and Potential Absorbed Dose Estimates in Participating NC and OH Children, When These Ratios Were Significantly Different from One at the 0.05 Level[a] (cont.)

Pollutant/ Metabolite	Exposure/Dose Parameter and Pathway	Estimated Ratio of Geometric Means (When Significantly Different from 1 at the 0.05 Level)					
		North Carolina			Ohio		
		Urban vs. Rural	Low- vs. Mid/High-Income	Day Care vs. Home	Urban vs. Rural	Low- vs. Mid/High-Income	Day Care vs. Home
trans-Permethrin	Exposure/Inhalation		2.45**				
	Exposure/Dietary Ingestion						2.92**
	Dose/Inhalation		2.31**				
	Dose/Dietary Ingestion						2.72*
Acid Herbicides							
2,4-D	Exposure/Inhalation			2.23**			
	Exposure/Dietary Ingestion			1.59*			
	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**

CTEPPS_v1a_60

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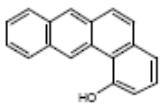	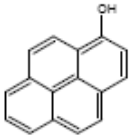	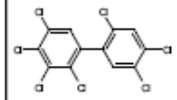	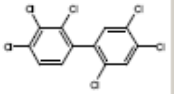	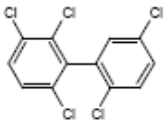	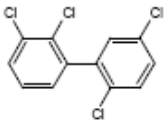	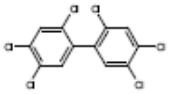	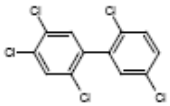	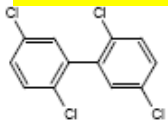	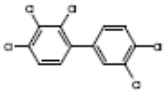
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1-hydroxybenz[a]anthrac	1-hydroxypyrene	2,2',3,4,4',5,5'-heptachlo	2,2',3,4,4',5'-hexachloro	2,2',3,5',6-pentachlorobi	2,2',3,5'-tetrachlorobiph	PCB 153- 2,2'-4,4',5,5'-h	2,2',4,5,5'-pentachlorobi	2,2',5,5'-tetrachlorobiph	2,3,3',4,4'-pentachlorobi
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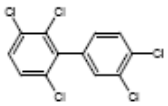	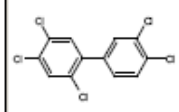	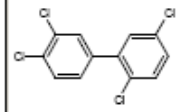	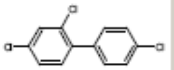	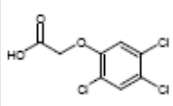	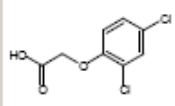	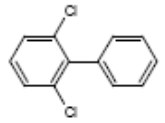	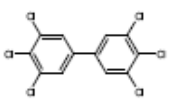	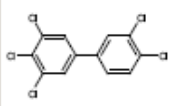	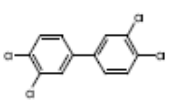
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2,3,3',4',6-pentachlorobi	PCB 118 (TEF evaluatio	2,3',4',5-tetrachlorobiph	2,4,4'-trichlorobiphenyl	2,4,5-Trichlorophenoxya	2,4-Dichlorophenoxyace	2,6-dichlorobiphenyl	3,3',4,4',5,5'-hexachloro	PCB 126- 3,3',4,4',5-pen	3,3',4,4'-tetrachlorobiph
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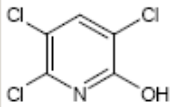	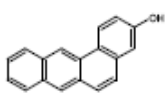	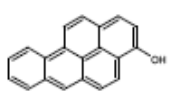	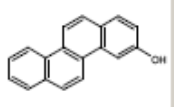	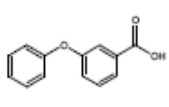	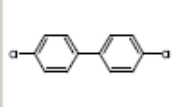	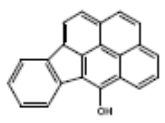	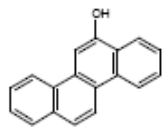	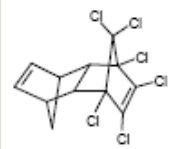	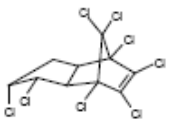
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3,5,6-TCP (3,5,6-trichlor	3-hydroxybenz[a]anthrac	3-hydroxybenz[a]pyrene	3-hydroxychrysene	3-phenoxybenzoic acid	4,4'-dichlorobiphenyl	6-hydroxy Indeno[1,2,3-c	6-hydroxychrysene	Aldrin	alpha-chlordane
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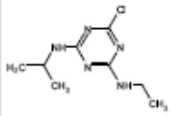	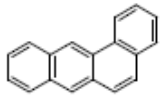	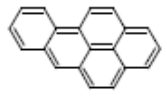	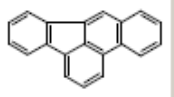	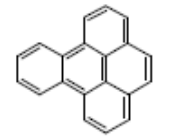	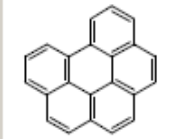	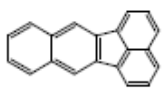	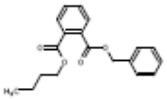	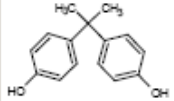	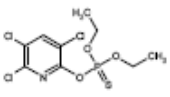
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Atrazine	Benz(a)anthracene	Benzo(a)pyrene	Benzo(b)fluoranthene	Benzo(e)pyrene	Benzo[g,h,i]perylene	Benzo(k)fluoranthene	Butyl benzyl phthalate	bisphenol-A	Chlorpyrifos (Dursban)
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218-01-9	61949-76-6	68359-37-5	333-41-5	53-70-3	1918-00-9	60-57-1	84-74-2	72-20-8	5103-74-2
chrysene	cis-permethrin	Baythroid	Diazinon	Dibenz(a,h)anthracene	Dicamba	Dieldrin	Dibutyl phthalate	Endrin	gamma-chlordane

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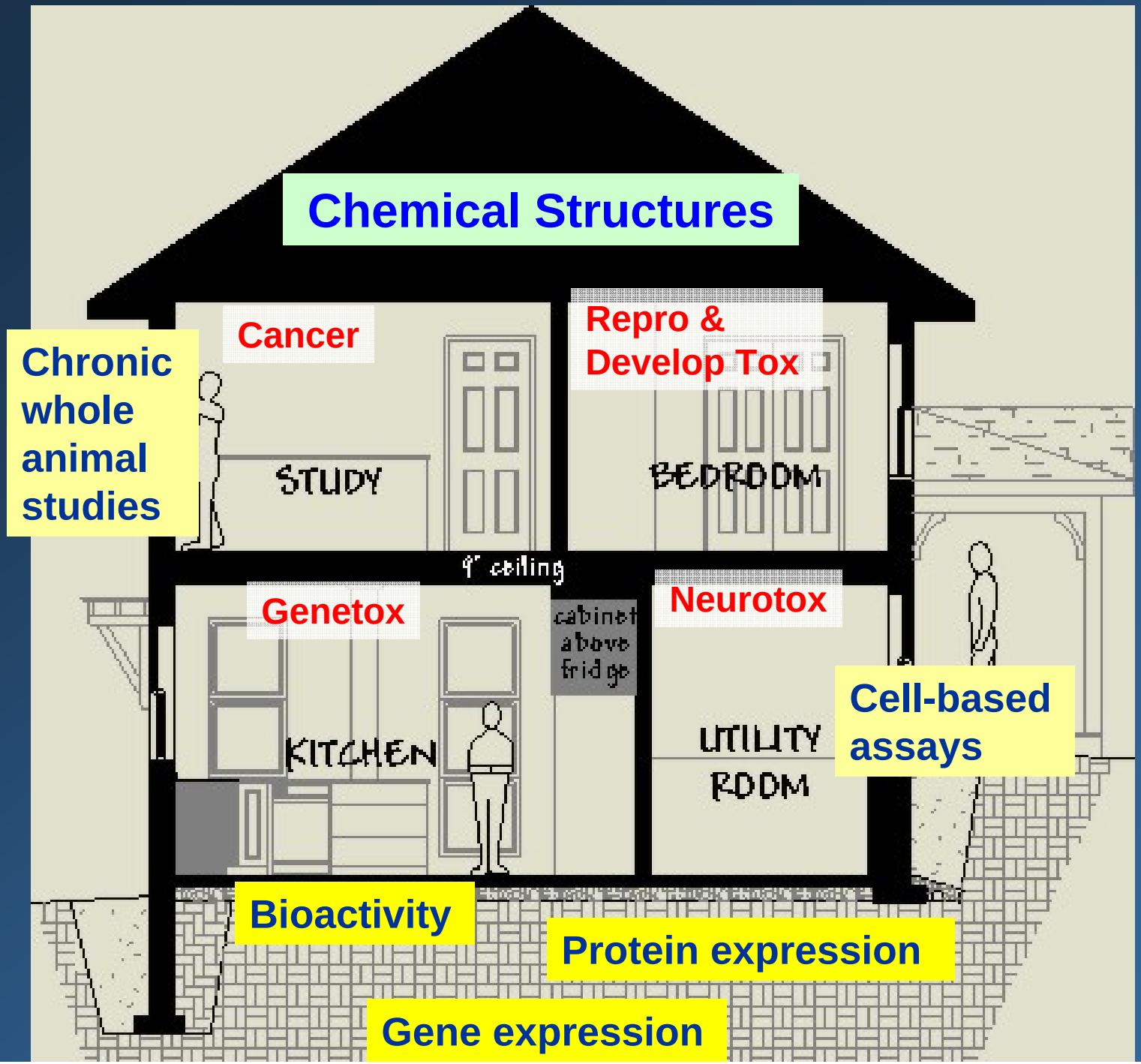
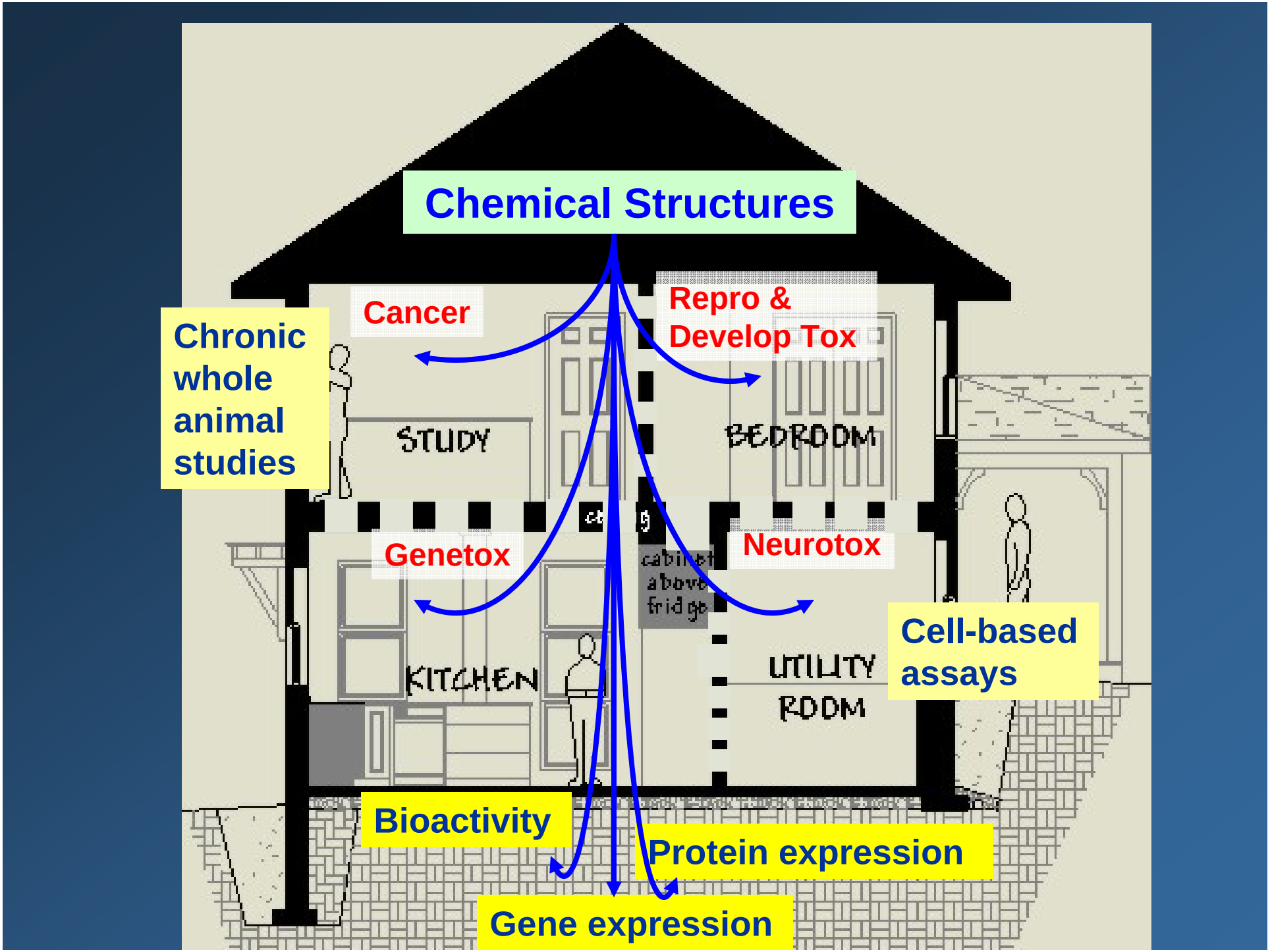
76-44-8	2814-20-2	193-39-5	58-89-9	104-40-5	72-55-9	50-29-3	82-68-8	87-86-5	61949-77-7
Heptachlor	4(1H)-Pyrimidinone, 6-m	Indeno[1,2,3-cd]pyrene	Lindane	nonylphenol (mixed)	p,p'-Dichlorodiphenyl dic	Dichlorodiphenyltrichlor	Pentachloronitrobenzen	Pentachlorophenol, purif	trans-permethrin

Next steps:

Begin to think about indexing of exposure-related information by chemical structure:

- What exposure-related information and resources can be linked to chemical structure?
- What modifications to existing exposure-related database resources are required?
- How can exposure-related content be systematized into a relational database environment?
- What would the world of Exposure-informatics look like?


Chemical Structures
Chronic whole animal studies
Cancer
Repro & Develop Tox
STUDY
BEDROOM
9' ceiling
Genetox
cabinet above fridge
Neurotox
Cell-based assays
KITCHEN
UTILITY ROOM
Bioactivity
Protein expression
Gene expression


Chemical Structures
Chronic whole animal studies
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STUDY
BEDROOM
Genetox
Neurotox
cabinet above fridge
KITCHEN
UTILITY ROOM
Cell-based assays
Bioactivity
Protein expression
Gene expression

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  Keith Houck

  Matt Martin

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  Rocky Goldsmith

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