



EUROPEAN
COMMISSION

Community Research



RISKCYCLE (#226552)

Deliverable 4.2. – List of databases and meta-databases

Deliverable of WP4

D.4.2: List of databases and meta-databases

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Grant Agreement number: 226552

Project Acronym: RISKCYCLE

Project title: Risk-based management of chemicals and products in a circular economy at a global scale

Funding Scheme: 7th Framework Program (FP7)

Project starting date: 01 September 2009

Project duration: 36 months

Name of the scientific representative of the project's coordinator and organisation: Prof. Dr.-Ing. habil. Dr. h.c. Bernd Bilitewski

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1 Description of the list

Partners IRFMN and URV have identified a list of 23 databases of physico-chemical properties, toxicological and ecotoxicological characterization and data from *in vivo* and *in vitro* assay.

The suggested data collections will be used to obtain information on previously selected additives and results will be compared.

2 Ecotoxicological databases

The list below contains databases for ecotoxicological properties like aquatic and terrestrial toxicity, both acute then chronic data.

2.1 Acute Toxicity Test Database Query (from CERC)

Name Acute Toxicity Test Database Query (from CERC)

URL <http://www.cerc.usgs.gov/data/acute/multiselect.asp>

Instructions:

- 1) Select search terms from **either one or both lists** on the right. Use the "CTRL" key to select multiple search terms.
- 2) Select the sort order by using the list below.
- 3) Push the "Run Query" button.
- 4) If you've selected a large dataset the results could take some time to load.
- 5) Refine your search by using the lists provided on the results page.
- 6) Download a text file with your results or start a new query at any time by following the links on the results page.

Chemicals List:

- 2,3,4,6-TETRACHLOROPHENOL
- 2,3,5-TRIMETHYL NAPHTHALENE
- 2,3,6-TRICHLORO BENZOIC ACID
- 2,3,6-TRIMETHYL NAPHTHALENE
- 2,4,5-T BUTOXYETHANOL ESTER
- 2,4,5-T TRIETHYLAMINE SALT
- 2,4-D
- 2,4-D BUTOXYETHANOL ESTER
- 2,4-D BUTYL ESTER
- 2,4-D DIMETHYLAMINE SALT
- 2,4-D DODECYL/TETRADODECYL AMINE SALT
- 2,4-D ISOOCTYL ESTER
- 2,4-D OLEYLPROPYLENEDIAMINE SALT
- 2,4-D PROPYLENE GLYCOL BUTYL ETHER ESTER
- 2,4-D/2,4,5-T 18%/9%
- 2,4-D/2,4,5-T 24%/28%
- 2,4-D/2,4,5-T 30%/28%
- 2,4-D/2,4,5-T 34%/17%
- 2,4-DB
- 2,6-DICHLOROBENZOIC ACID
- 2,6-DIOCTADECYL-P-CRESOL
- 2-ETHYLHEXANOL
- 2-HYDROXY-2',4,4'-TRICHLORODIPHENYL ETHER
- 2-HYDROXY-4,4'-DICHLORODIPHENYL ETHER
- 6-CHLORO-2-PICOLINIC ACID
- ACEPHATE
- ACETONE
- AERO XANTHATE 343
- AEROFROTH 71
- AKTON
- ALACHLOR
- ALDICARB
- ALDRIN
- ALL ETHRIN

Species List:

- ACRONEURIA SP.
- APPLE SNAIL
- APELLUS BREVICAUDUS
- ATHERIX VARIEGATA
- ATLANTIC SALMON
- BAETIS SP
- BLACK BULLHEAD
- BLACK CRAPPIE
- BLUEGILL
- BROOK TROUT
- BROWN TROUT
- CARP
- CHANNEL CATFISH
- CHAOBORUS SP.
- CHINOOK SALMON
- CHIRONOMUS PLUMOSUS
- CLAASSENIA SABULOSA
- COHO SALMON
- CUTTTHROAT TROUT
- CYPRIDOPSIS VIDUA
- DAPHNIA MAGNA
- DAPHNIA PULEX
- EPHEMERELLA SP.
- FATHEAD MINNOW
- FOWLERS TOAD
- GAMMARUS FASCIATUS
- GAMMARUS LACUSTRIS
- GAMMARUS PSEUDOLIMNAEUS
- GOLDFISH
- GREEN SUNFISH
- HEXAGENIA BILINEATA
- HYDROPSYCHE SP.
- ISCHNURA VERTICALIS
- ISOPHEMUS SP.

SHORT DESCRIPTION The database summarizes the results from aquatic acute toxicity tests conducted by the Columbia Environmental Research Center

Nr of ENDPOINTS/TESTS 66

Nr of CHEMICALS 410

QUALITY CONTROL

Deliverable 4.2: List of databases.

2.2 PAN

Name PAN Pesticides
URL <http://www.pesticideinfo.org/>

The screenshot shows the homepage of the PAN Pesticide Database. At the top, there is a blue header with the text "PAN Pesticide Database" and a "JOIN PAN >>" button. Below the header, there is a "Home" link and a "Help | Feedback" link. The main content area features a paragraph describing the database as a one-stop location for toxicity and regulatory information. It includes a "Search" section with links to "Chemicals or Alphabetized Chemical List", "Products", "International Pesticide Registration", "Poisoning Diagnostics", and "Aquatic Ecotoxicity". There is also a "California Data" section with links to "Pesticide Use Reports" and "Pesticides and Air", and a "Help and Other Resources" section with links to "Help Getting Started", "Pesticide Tutorial and Reference", "Least/Non-Toxic Alternatives", "Links to Other Resources", and "Get Active!". A "NOTE" section at the bottom provides information about the accuracy of the data and the responsibility of the Pesticide Action Network. The footer contains a citation and a copyright notice.

SHORT DESCRIPTION The Pesticide Action Network (PAN) Pesticide Database lists toxicity data and regulatory information for pesticides.

Nr of ENDPOINTS/TESTS Whatever available

Nr of CHEMICALS 6400

QUALITY CONTROL YES

2.3 TOXNET

Name TOXNET

URL <http://toxnet.nlm.nih.gov/>

United States National Library of Medicine

TOXNET
Toxicology Data Network

TOXNET PDA Access | SIS Home | About Us | Site Map & Search | Contact Us

▶ Env. Health & Toxicology ▶ TOXNET

TOXNET - Databases on toxicology, hazardous chemicals, environmental health, and toxic releases.

Select Database

- ChemIDplus
- HSDB
- TOXLINE
- CCRIS
- DART
- GENETOX
- IRIS
- ITER
- LactMed
- Multi-Database
- TRI
- Haz-Map
- Household Products
- TOXMAP

Search All Databases

Enter term(s) to search all databases.

(e.g. asthma air pollution, ibuprofen fever, vinyl chloride)

Search Clear Help

TOXNET Search Options

- Search all databases: Enter term(s) in box above
- Search a specific database: Click database at left
- Database description: Click on the ?

Env. Health & Toxicology

Portal to environmental health and toxicology resources

VISIT SITE

Support Pages

- ▶ Help
- ▶ TOXNET FAQ
- ▶ TOXNET Update Status
- ▶ Fact Sheet
- ▶ Database Description
- ▶ Training Manual & Schedule
- ▶ News

Additional Resource

- CPDB

Copyright, Privacy, Accessibility
U.S. National Library of Medicine, 8600 Rockville Pike, Bethesda, MD 20894
National Institutes of Health, Health & Human Services

SHORT DESCRIPTION Databases on toxicology, hazardous chemicals, environmental health, and toxic releases

Nr of ENDPOINTS/TESTS Toxicity 5-7 endpoints,
physicochemical properties 7 endpoints

Nr of CHEMICALS >295000

QUALITY CONTROL very probably yes

Deliverable 4.2: List of databases.

2.4 ECOTOX

Name ECOTOX

URL http://cfpub.epa.gov/ecotox/ecotox_home.cfm

The screenshot shows the ECOTOX Database homepage. At the top, there is a navigation bar with the EPA logo on the left and the text 'U.S. ENVIRONMENTAL PROTECTION AGENCY' on the right. Below the navigation bar, the title 'ECOTOX Database' is displayed. A search bar is present with options for 'All EPA' and 'This Area'. A sidebar on the left contains a list of links: Home, About ECOTOX, Limitations, Help Center, Frequent Questions, Quick Database Query, Advanced Database Query, Data Downloads, Browse Chemicals, Browse Effects, Browse Species, and Send Comments. The main content area features two large icons for 'Quick Database Query' and 'Advanced Database Query'. Below these icons, a welcome message states: 'Welcome to ECOTOX Release 4.0. The ECOTOX (ECOTOxicology) database provides single chemical toxicity information for aquatic and terrestrial life.' It also provides information on the latest data releases, a link to 'Recent Additions', and a link to the 'Quick User Guide' (PDF, 2 p., 244 KB). A note indicates that users need to turn off pop-up blockers. A footer section contains links to 'Office of Research and Development', 'National Health and Environmental Effects Research Laboratory', and 'Mid-Continent Ecology Division'. At the bottom, there are links for 'EPA Home', 'Privacy and Security Notice', and 'Contact Us', along with the URL 'http://cfpub.epa.gov/ecotox/ecotox_home.cfm' and the date 'Last updated on lunedì 26 luglio 2010'.

SHORT DESCRIPTION

USEPA database on ecotoxicological properties toxicity data from the peer-reviewed literature for aquatic life, terrestrial plants and terrestrial wildlife

Nr of ENDPOINTS/TESTS

Whatever available

Nr of CHEMICALS

715.000

QUALITY CONTROL

updated

2.5 Danish (Q)SAR database

Name Danish (Q)SAR Database
URL <http://130.226.165.14/index.html>



Danish (Q)SAR Database

with financial support from the [European Chemicals Bureau](#) and in cooperation with
[Laboratory of Mathematical Chemistry](#), Bourgas, Bulgaria

[Terms of use](#)

SHORT DESCRIPTION Databases on toxicological and ecotoxicological parameters. All values included in the model are estimated with different models. Ecotoxicological models have been developed with Multicase by multilinear regression based on chemical molecule fragments and experimental data. The estimated toxicological and ecotoxicological properties are directed towards regulatory purposes.

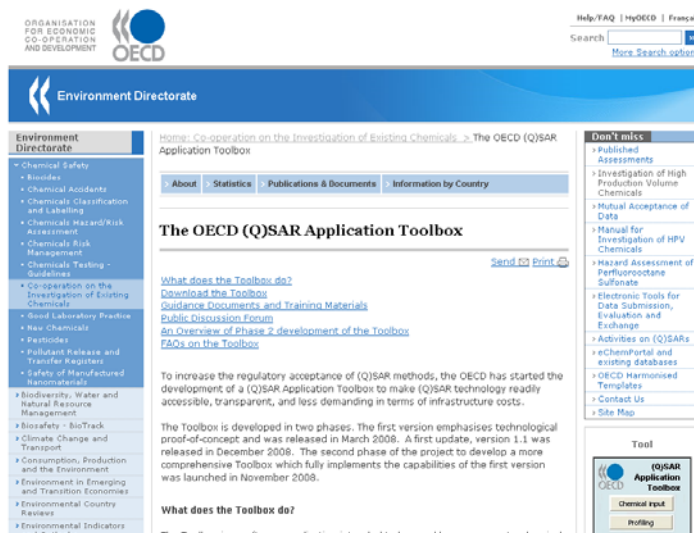
Nr of ENDPOINTS/TESTS	Standard test parameters
Nr of CHEMICALS	166,000 organic chemicals
QUALITY CONTROL	Model domain info is given

2.6 OECD QSAR tool box

Name OECD QSAR tool box

URL

http://www.oecd.org/document/54/0,3343,en_2649_34379_42923638_1_1_1_1,00.html



SHORT DESCRIPTION

The Toolbox is a software application intended to be used by governments, chemical industry and other stakeholders in filling gaps in (eco)toxicity data needed for assessing the hazards of chemicals. The Toolbox incorporates information and tools from various sources into a logical workflow. Crucial to this workflow is grouping chemicals into chemical categories. It contains EPISUITE v3.20, MultiCase, Super-Frag and ToxTree v1.5. Read-across, trend analysis and QSAR models can be used to estimate missing values.

Nr of ENDPOINTS/TESTS

Whatever available

Nr of CHEMICALS

QUALITY CONTROL

The Toolbox provides information on the quality assurance process performed by the donator, as well as full references of experimental results published in the open literature. This should allow the user to decide whether the data is adequate for their purposes.

2.7 DSSTox - Distributed Structure-Searchable Toxicity

Name DSSTox - Distributed Structure-Searchable Toxicity

URL http://www.epa.gov/dsstox_structurebrowser/

The screenshot shows the EPA DSSTox Structure Browser v2.0 search interface. It features a search bar with a dropdown menu set to 'Auto-detect' and a 'Search' button. Below this is a section for 'DSSTox Chemical Structure Search' with a text input for 'Enter SMILES string' and a 'Search Options' dropdown. A 'Data Files to Search' panel on the right allows selecting between 'All DSSTox Files' and 'Selected DSSTox Files'. At the bottom, there are 'Clear', 'Search', and 'Report Difficulties' buttons.

SHORT DESCRIPTION easy-to-use structure-searching capability through the chemical inventory of published DSSTox Data Files

Nr of ENDPOINTS/TESTS Whatever available

Nr of CHEMICALS 9300

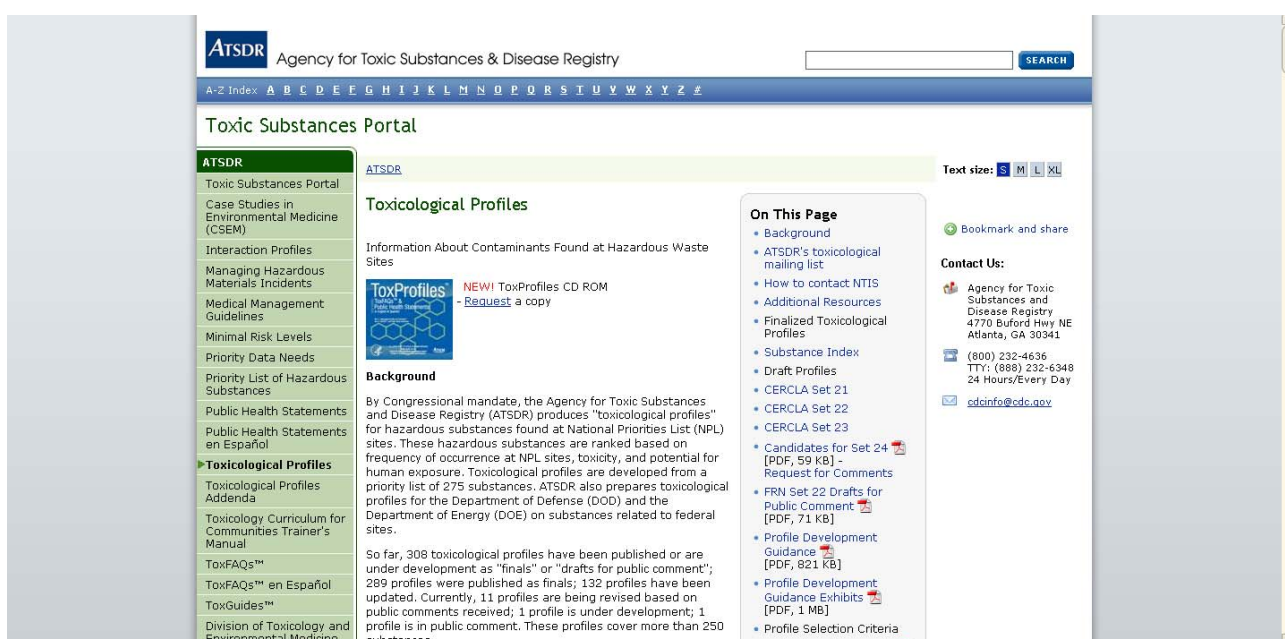
QUALITY CONTROL Quality Review of New Data

3 Toxicological database

The suggest list includes databases for human toxicological parameters like reference doses, slope factors, cancerogenic potency and mutagenicity.

3.1 ATSDR

Name ATSDR – Toxic substances profile
 URL <http://www.atsdr.cdc.gov/toxprofiles/index.asp>



SHORT DESCRIPTION The Agency for Toxic Substances and Disease Registry (ATSDR) produces "toxicological profiles" for hazardous substances found at National Priorities List (NPL) sites. These hazardous substances are ranked based on frequency of occurrence at NPL sites, toxicity, and potential for human exposure. toxicity tests conducted by the Columbia Environmental Research Center

Nr of ENDPOINTS/TESTS Whatever available

Nr of CHEMICALS 275

QUALITY CONTROL Very probably yes

Deliverable 4.2: List of databases.

3.2 IRIS

Name IRIS – Integrated risk information system

URL <http://www.epa.gov/ncea/iris/>

The screenshot shows the IRIS website interface. At the top, it says 'U.S. ENVIRONMENTAL PROTECTION AGENCY' and 'Integrated Risk Information System (IRIS)'. A search bar is present with 'All EPA' and 'IRIS' selected. Below the search bar, there's a breadcrumb trail: 'You are here: EPA Home » Research & Development » NCEA » Integrated Risk Information System (IRIS)'. The main content area includes a description of IRIS, a 'Getting Started with IRIS' section with links like 'An overview of the web site', 'What is IRIS?', and 'How does EPA decide which substances to add or update?'. There's also a 'Using the IRIS Database' section with links for 'IRIS Process (2009 Update)', 'Advanced Search in IRIS', 'Compare IRIS Values', and 'Download IRIS'. A 'New Assessments and Reviews' section contains a table of recent documents.

Substance	Milestone	Meeting/Release date
Formaldehyde-Inhalation Assessment	External Peer-Review Draft Interagency Science Consultation Draft Listening Session	06/02/2010 06/02/2010 07/27/2010
Dioxin Reanalysis	External Peer-Review Draft Interagency Science Consultation Draft Listening Session	05/21/2010 05/21/2010 07/09/2010
Hexachloroethane	External Peer-Review Draft Interagency Science Consultation Draft Listening Session	05/13/2010 05/13/2010 06/16/2010
Dichloromethane (Methylene Chloride)	External Peer-Review Draft	03/31/2010

SHORT DESCRIPTION The toxicological reviews & support documents are listed in alphabetical order by substance name. At this time, toxicological reviews and support documents are available only for the new or re-assessed substance summaries added to the IRIS Web site since 1997. The toxicological review/support documents listed below are available online by clicking on the document titles.

Nr of ENDPOINTS/TESTS What is available

Nr of CHEMICALS >1000

QUALITY CONTROL Accuracy and Quality by EPA's National Center for Environmental Assessment (NCEA) within the Office of Research and Development (ORD).

3.3 ISS/ISPEsL database

Name ISS/ISPEsL Database

URL http://www.apat.gov.it/site/it-IT/Temi/Siti_contaminati/Analisi_di_rischio

	A	B	C	D	E	F	G	H	I	J	K	L	N	O	P	Q	R
		Numero CAS	Cat. Carc. UE	Classe Cancer. EPA	SF Ing. [mg/kg-giorno] ¹	Rif.	SF Inal. [mg/kg-giorno]	Rif.	RfD Ing. (mg/kg-d)	Rif.	RfD Inal. (mg/kg-d)	Rif.	Fattore di assorbimento dermico con suolo [adim.]	Rif	Coefficiente di permeabilità [cm/ora]	Rif	
30	Benzene	71-43-2	1	A	5.50E-02	I	2.73E-02	I	4.00E-03	I	8.55E-03	I	0.1		2.10E-02		
31	Etilbenzene	100-41-4	-	D	-	-	-	-	1.00E-01	I	2.85E-01	I	0.1		7.40E-02		
32	Stirene	100-42-5	-	D	-	-	-	-	2.00E-01	I	2.85E-01	I	0.1		5.50E-02		
33	Toluene	108-88-3	3	D	-	-	-	-	8.00E-02	I	1.43E+00	I	0.1		4.50E-02		
34	m-Xilene	108-32-3	-	D	-	-	-	-	2.00E-01	I	2.00E-01	I	0.1		8.00E-02		
35	o-Xilene	95-47-6	-	D	-	-	-	-	2.00E-01	I	2.00E-01	I	0.1		8.00E-02		
36	p-Xilene	106-42-3	-	D	-	-	-	-	2.00E-01	I	2.00E-01	I	0.1		8.00E-02		
37	Xilene	1330-20-7	-	D	-	-	-	-	2.00E-01	I	2.00E-01	I	0.1		8.00E-02		
38	Aromatici policiclici																
	Benzo(a)antracene	56-55-3	2	B2	7.30E-01	E	6.00E-01	E	-	-	2.85E-01	TX	0.13	30	8.10E-01		
39	Benzo(a)pirene	50-32-8	2	B2	7.30E+00	I	7.32E+00	PS	-	-	3.14E+00	TX	0.13		1.20E+00		
40	Benzo(b)fluorantene	205-99-2	2	B2	7.30E-01	E	6.00E-01	E	-	-	2.85E-01	TX	0.13		1.20E+00		
41	Benzo(g,h,i)perilene	191-24-2	-	D	-	-	-	-	3.00E-02	B	3.00E-02	B	0.13		1.66E+00		
42	Benzo(k)fluorantene	207-08-9	2	B2	7.30E-02	N	3.10E-02	E	-	-	2.85E-02	TX	0.13		1.20E+00		
43	Crisene	218-01-9	2	B2	7.00E-03	TX	6.10E-03	TX	3.00E-02	B	3.00E-02	R	0.13		8.10E-01		
44	Dibenzo(a,e)pirene	192-65-4	-	-	7.30E+00	26	-	-	-	-	-	-	0.13		-		
45	Dibenzo(a,h)pirene	189-64-0	-	-	7.30E+01	26	-	-	-	-	-	-	0.13		-		
46	Dibenzo(a,i)pirene	189-55-9	-	-	7.30E+01	26	-	-	-	-	-	0.13	-		-		
47	Dibenzo(a,j)pirene	191-30-0	-	-	7.30E+02	31	-	-	-	-	-	0.13	-		-		
48	Dibenzopireni	-	-	-	-	-	-	-	-	-	-	0.13	-		-		
49	Dibenzo(a,h)antracene	53-70-3	2	B2	7.30E+00	N	7.30E+00	E	-	-	-	-	0.13		2.70E+00		
50	Indenopirene	193-39-5	-	B2	7.30E-01	E	3.10E-01	N	3.00E-02	B	3.14E+00	TX	0.13		1.90E+00		
51	Pirene	129-00-0	-	D	-	-	-	-	3.00E-02	I	3.00E-02	I	0.13	3.24E-01			
52	Alifatici clorurati cancerogeni																
53	1,1,2,2-Tetracloroetano	79-34-5	-	C	2.00E-01	I	2.00E-01	I	6.00E-02	I	2.00E-01	TX	0.1	9.00E-03			
54	1,1,2-Tricloroetano	79-00-5	3	C	5.70E-02	I	5.60E-02	I	4.00E-03	I	5.70E-02	TX	0.1	8.40E-03			
55	1,1-Dicloroetilene	75-35-4	3	C	6.00E-01	I	1.75E-01	I	8.00E-02	I	8.74E-02	I	0.1	1.60E-02			
56	1,2,3-Tricloropropano	96-18-4	2	C	7.00E+00	H	7.00E+00	R	6.00E-03	I	6.00E-03	R	0.1	-			

SHORT DESCRIPTION

Database on Human toxicological and physico-chemical properties used for risk assessment of polluted site, Human reference doses and slope factors, dermal absorption factors

Nr of ENDPOINTS/TESTS

5 :oral Rfd, oral SF, inhalation RfD, inhalation SF, dermal absorption factors.

Nr of CHEMICALS

150

QUALITY CONTROL

updated

3.4 HSDB

Name HSDB - Hazardous Substances Data Bank
 URL <http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB>

Hazardous Substances Data Bank (HSDB) - Comprehensive, peer-reviewed toxicology data for about 5,000 chemicals.

Select Database

- ChemIDplus
- **HSDB**
- TOXLINE
- CCRIS
- DART
- GENETOX
- IRIS
- ITER
- LactMed
- Multi-Database
- TRI
- Haz-Map
- Household Products
- TOXMAP
- TOXNET Home

Search HSDB

(e.g. antifreeze kidney failure, chromium compounds, 7718-54-9)

Search Clear Help

For chemicals, add synonyms and CAS numbers to search:
 Yes No

Limits Browse the Index

Env. Health & Toxicology

Portal to environmental health and toxicology resources

Support Pages

- ▶ Help
- ▶ Fact Sheet
- ▶ Sample Record
- ▶ HSDB Scientific Review Panel
- ▶ TOXNET FAQ

Additional Resource

- CPDB

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 U.S. National Library of Medicine, 8600 Rockville Pike, Bethesda, MD 20894
 National Institutes of Health, Health & Human Services

SHORT DESCRIPTION

It focuses on the toxicology of potentially hazardous chemicals. It is enhanced with information on human exposure, industrial hygiene, emergency handling procedures, environmental fate, regulatory requirements, nanomaterials, and related areas. All data are referenced and derived from a core set of books, government documents, technical reports and selected primary journal literature.

Nr of ENDPOINTS/TESTS

What is available

Nr of CHEMICALS

5000

QUALITY CONTROL

peer-reviewed by the Scientific Review Panel

3.5 CCRIS

Name Chemical Carcinogenesis Research Information System (CCRIS)
 URL http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?CCRIS

The screenshot shows the TOXNET website interface. At the top left is the NLM logo and 'United States National Library of Medicine'. To the right is the 'TOXNET Toxicology Data Network' header. Below this is a navigation bar with links: 'TOXNET PDA Access', 'SIS Home', 'About Us', 'Site Map & Search', and 'Contact Us'. A breadcrumb trail shows 'Env. Health & Toxicology > TOXNET > CCRIS'. The main content area is titled 'Chemical Carcinogenesis Research Information System (CCRIS) - Carcinogenicity and mutagenicity test results for over 8,000 chemicals.' Below this are three main sections: 'Select Database' (a list of databases with 'CCRIS' selected), 'Search CCRIS' (a search form with a text input, 'Search', 'Clear', and 'Help' buttons, and radio buttons for 'Yes' and 'No'), and 'Env. Health & Toxicology' (a 'Portal to environmental health and toxicology resources' with a 'VISIT SITE' button). Below the search form is an 'Additional Resource' section with 'CPDB'. On the right side, there is a 'Support Pages' section with links to 'Help', 'Fact Sheet', 'Sample Record', and 'TOXNET FAQ'. At the bottom, there is a footer with 'Copyright, Privacy, Accessibility' and contact information for the U.S. National Library of Medicine.

SHORT DESCRIPTION

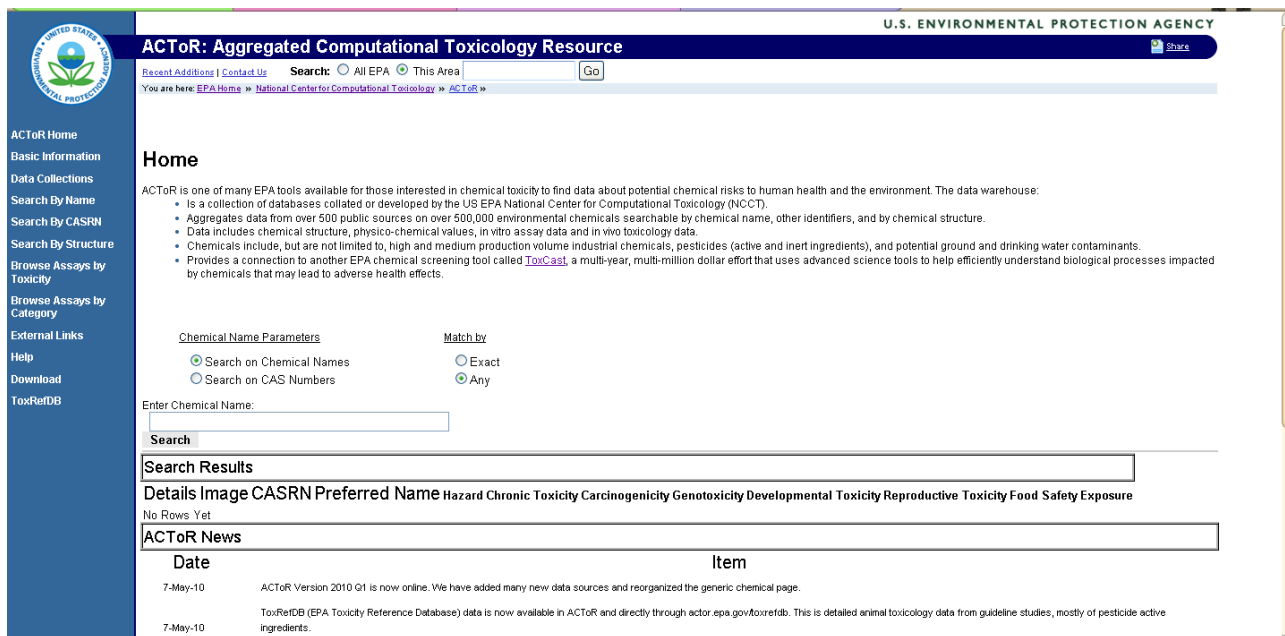
Nr of ENDPOINTS/TESTS Carcinogenicity, mutagenicity, tumor promotion, and tumor inhibition

Nr of CHEMICALS 9000

QUALITY CONTROL Test results have been reviewed by experts in carcinogenesis and mutagenesis

3.6 AcToR

Name ACToR (Aggregated Computational Toxicology Resource)
 URL <http://actor.epa.gov/actor/faces/ACToRHome.jsp>



SHORT DESCRIPTION a collection of databases collated or developed by the US EPA National Center for Computational Toxicology (NCCT) Chemical structure, physico-chemical values, *in vitro* assay data, and *in vivo* toxicology data

Nr of ENDPOINTS/TESTS Whatever available

Nr of CHEMICALS 500,000

QUALITY CONTROL updated

3.7 CPDB

Name The Carcinogenic Potency Database (CPDB)
URL <http://potency.berkeley.edu/chemnameindex.html>



The Carcinogenic Potency Project
<http://potency.berkeley.edu/>



All Results On Each Chemical in the Carcinogenic Potency Database (CPDB) <http://potency.berkeley.edu/>

To obtain the full results in the Carcinogenic Potency Database, click on any chemical name.

This list is searchable by chemical name or by Chemical Abstracts Registry Number (CAS) using the Find command in your web browser. If the name you are seeking is not in this list, click to see [Synonyms](#).

The Web page for each individual chemical provides both summary and detailed information. A summary table reports positivity, target sites and carcinogenic potency (TD₅₀) in each species tested: rats, mice, hamsters, dogs, or nonhuman primates. Detailed CPDB results of each experiment are given in a format suitable for screen viewing. Included are, for example, experimental protocol, tumor incidence, dose-response, TD₅₀ and its statistical significance, and citation. Pop-up windows define each code, for example, strain of animal, route of administration, tissue and tumor type. Chemical information is provided, including SMILES and InChI codes, and chemical structure.

[A-α-C \(CAS 26148-68-5\)](#)
[Acesulfame-K \(CAS 55589-62-3\)](#)
[Acetaldehyde \(CAS 75-07-0\)](#)
[Acetaldehyde methylformylhydrazone \(CAS 16568-02-8\)](#)
[Acetaldoxime \(CAS 107-29-9\)](#)
[Acetamide \(CAS 60-35-5\)](#)
[Acetaminophen \(CAS 103-90-2\)](#)
[Acetohexamide \(CAS 968-81-0\)](#)
[Acetone\[4-\(5-nitro-2-furyl\)-2-thiazolyl\]hydrazone \(CAS 18523-69-8\)](#)
[Acetonitrile \(CAS 75-05-8\)](#)
[Acetoxime \(CAS 127-06-0\)](#)
[1'-Acetoxysafrole \(CAS 34627-78-6\)](#)
[N'-Acetyl-4-\(hydroxymethyl\)phenylhydrazine \(CAS 65734-38-5\)](#)
[1-Acetyl-2-isonicotinylhydrazine \(CAS 1078-38-2\)](#)

SHORT DESCRIPTION

The Carcinogenic Potency Database (CPDB) is a unique and widely used international resource of the results of 6540 chronic, long-term animal cancer tests on 1547 chemicals.

Nr of ENDPOINTS/TESTS TD50

Nr of CHEMICALS 1547

QUALITY CONTROL

4 PHYSICOCHEMICAL PROPERTIES

4.1 Chemical and Physical Properties Database

Name Chemical and Physical Properties Database
URL <http://www.dep.state.pa.us/physicalproperties/Default.htm>

The screenshot shows the homepage of the Pennsylvania Department of Environmental Protection's Chemical and Physical Properties Database. The header includes a search bar and the department's logo. The main content area features a navigation menu with links for 'Property Search', 'Search CAS Number', and 'Home'. A 'WELCOME' message follows, explaining the database's purpose and providing instructions on how to use it. At the bottom, there is a contact information section for Samuel Fang and a link to the Bureau of Land Recycling and Waste Management Homepage.

SHORT DESCRIPTION Database on physicochemical properties. Free access.

Nr of ENDPOINTS/TESTS 12: aqueous solubility, attenuation Lambda in Groundwater, boiling point, density, diffusivity in air, diffusivity in water, Henry's law constant, logP, Koc, melting point, molecular weight and vapour pressure

Nr of CHEMICALS

QUALITY CONTROL updated

4.2 EPISuite

Name	EPI SUITE v4.0
URL	http://www.epa.gov/oppt/exposure/pubs/episuitedl.htm
SHORT DESCRIPTION	The EPI (Estimation Programs Interface) Suite™ is a Windows®-based suite of physical/chemical property and environmental fate estimation programs developed by the EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC). EPI Suite™ uses a single input to run the following estimation programs: KOWWIN™, AOPWIN™, HENRYWIN™, MPBPWIN™, BIOWIN™, BioHCwin, KOCWIN™, WSKOWWIN™, WATERNT™, BCFBAF™, HYDROWIN™, KOAWIN and AEROWIN™, and the fate models WVOLWIN™, STPWIN™ and LEV3EPI™. ECOSAR™, which estimates ecotoxicity, is also included in EPI Suite™
Nr of ENDPOINTS/TESTS	
Nr of CHEMICALS	
QUALITY CONTROL	Information on validation varies with the program and includes detailed statistics for some. For others, where multiple independent studies have been done, brief summaries and references are provided

Deliverable 4.2: List of databases.

4.3 BSAF

Name BSAF (Biota-Sediment Accumulation Factor)
URL http://www.epa.gov/med/Prods_Pubs/bsaf.htm

The screenshot shows the EPA website page for BSAF. The header includes the EPA logo and the text 'U.S. ENVIRONMENTAL PROTECTION AGENCY'. The main heading is 'Mid-Continent Ecology Division'. Below this, there is a search bar with 'All EPA' selected and 'This Area' as an option. A breadcrumb trail reads: 'You are here: EPA Home » Research & Development » Health and Environmental Effects Research » Mid-Continent Ecology Division » Products & Publications » BSAF (Biota-Sediment Accumulation Factor)'. The main content area is titled 'BSAF (Biota-Sediment Accumulation Factor)'. The text describes the data set, its purpose, and provides contact information for the ECOTOX helpline. A footer section contains links to 'Research and Development Home', 'NHEERL Home', and 'Grosse Ile Home', along with 'EPA Home', 'Privacy and Security Notice', and 'Contact Us'. The URL 'http://www.epa.gov/med/Prods_Pubs/bsaf.htm' and a 'Print As-Is' link are also present. The page was last updated on 'martedì 10 febbraio 2009'.

SHORT DESCRIPTION biota-sediment accumulation factors for nonionic organic chemicals, e.g., PCBs, PCDDs, PCDFs, DDTs, PAHs, and pesticides

Nr of ENDPOINTS/TESTS

Nr of CHEMICALS 20000

QUALITY CONTROL

4.4 SPARC

Name SPARC
URL <http://ibmlc2.chem.uga.edu/sparc/>

September 2009 release v4.5.1529-p4.5.1529

SPARC PERFORMS AUTOMATED REASONING IN CHEMISTRY v4.5

WELCOME TO THE SPARC ON LINE CALCULATOR

Current type is not set
Press buttons above to choose type.

SHORT DESCRIPTION Databases and models to predict physicochemical properties. Free access.

Nr of ENDPOINTS/TESTS

Nr of CHEMICALS updated

QUALITY CONTROL

5 In vivo studies and bioassays

5.1 ToxRefDB

Name ToxRefDB (Toxicity Reference Database)

URL <http://actor.epa.gov/toxrefdb/faces/Home.jsp>

SHORT DESCRIPTION	captures thousands of in vivo animal toxicity studies on hundreds of chemicals
Nr of ENDPOINTS/TESTS	Whatever available
Nr of CHEMICALS	424 (?)
QUALITY CONTROL	updated

5.2 ToxCast

Name ToxCast

URL <http://epa.gov/ncct/toxcast/>

SHORT DESCRIPTION

Uses data from state-of-the-art high-throughput screening (HTS) bioassays.

Nr of ENDPOINTS/TESTS Whatever available

Nr of CHEMICALS 300

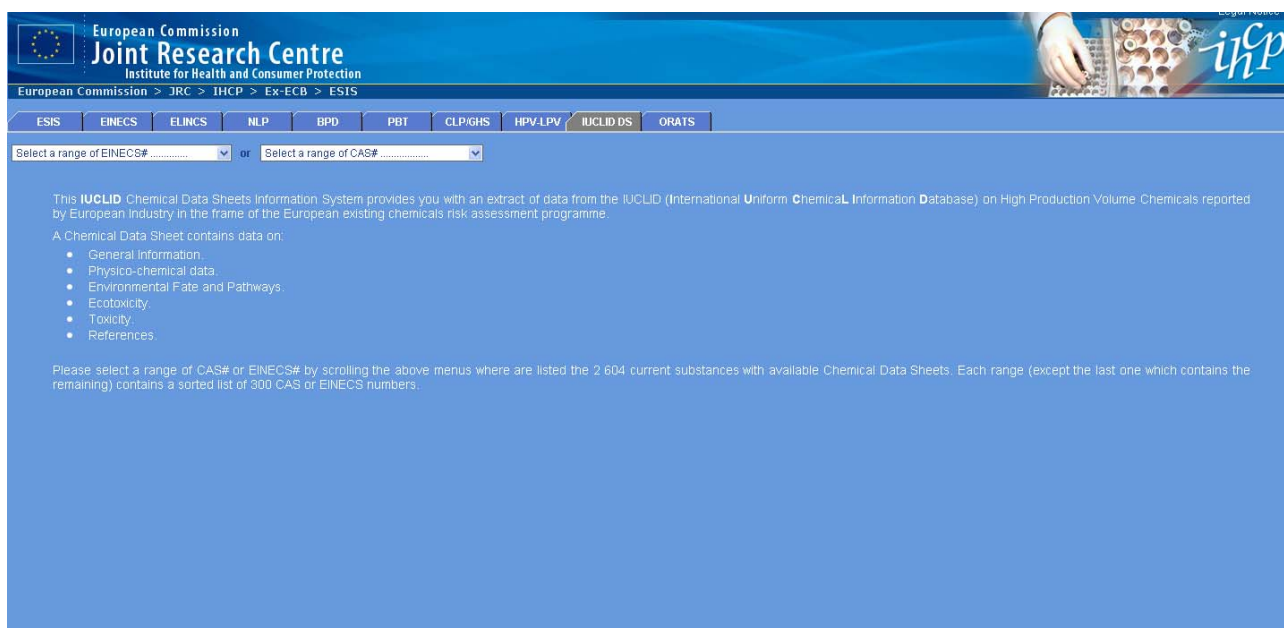
QUALITY CONTROL

6 Other databases

6.1 IUCLID

Name IUCLID

URL <http://ecb.jrc.ec.europa.eu/esis/index.php?PGM=dat>



SHORT DESCRIPTION

This IUCLID Chemical Data Sheets Information System provides you with an extract of data from the IUCLID (International Uniform Chemical Information Database) on High Production Volume Chemicals reported by European Industry in the frame of the European existing chemicals risk assessment programme.

Nr of ENDPOINTS/TESTS What is available

Nr of CHEMICALS 2604

QUALITY CONTROL

6.2 ChemSpider

Name ChemSpider
 URL www.chemspider.com

SHORT DESCRIPTION ChemSpider is a free-to-access collection of compound data from across the web

Nr of ENDPOINTS/TESTS Whatever available

Nr of CHEMICALS 25M

QUALITY CONTROL Automated chemistry checking of structures on loading
 Manual comment and correction tools offer crowd-sourced curation with expert review

6.3 CHIRP

Name CHIRP
 URL <http://www.safe.nite.go.jp/english/db.html>

SHORT DESCRIPTION Chemical Risk Information Platform developed by Data Analysis Division,

Chemical Management Center of National Institute of Technology and Evaluation (Japan). It contains many data of environmental interest. Free access

Nr of ENDPOINTS/TESTS Whatever available

Nr of CHEMICALS

QUALITY CONTROL updated