EUROPEAN COMMISSION

Community Research

SEVENTH FRAMEWORK PROGRAMME

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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1 Descriprion 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.

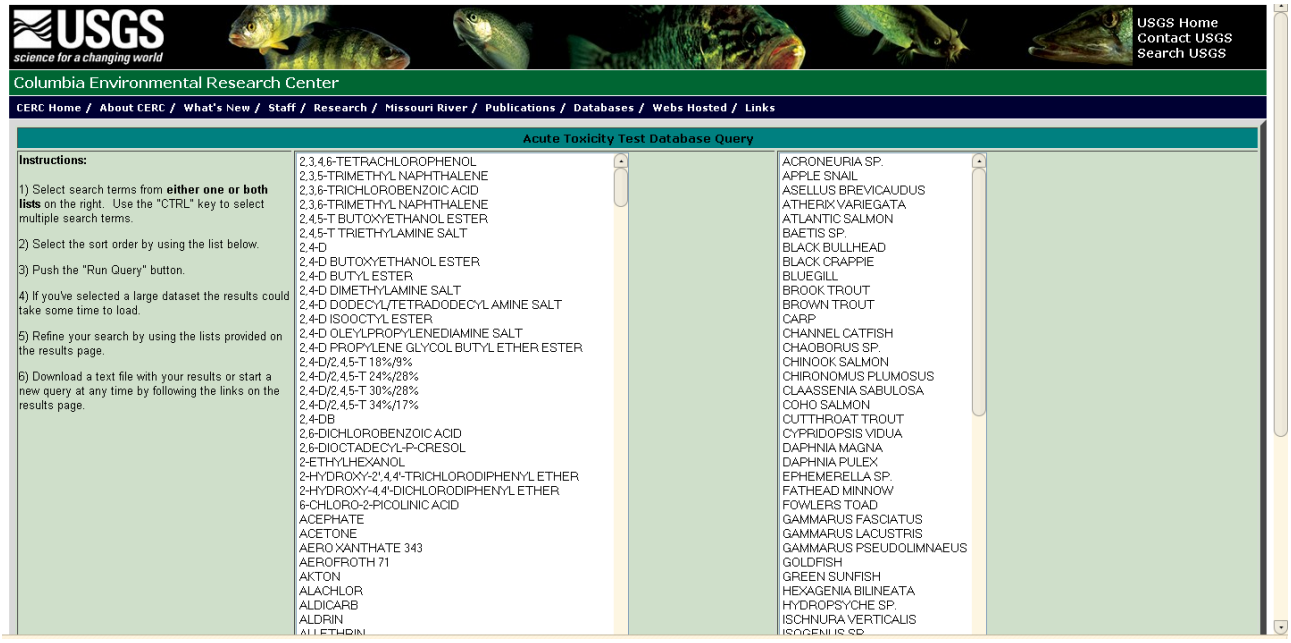
2 *Ecotoxicological databases*

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



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

Nr of ENDPOINTS/TESTS 66

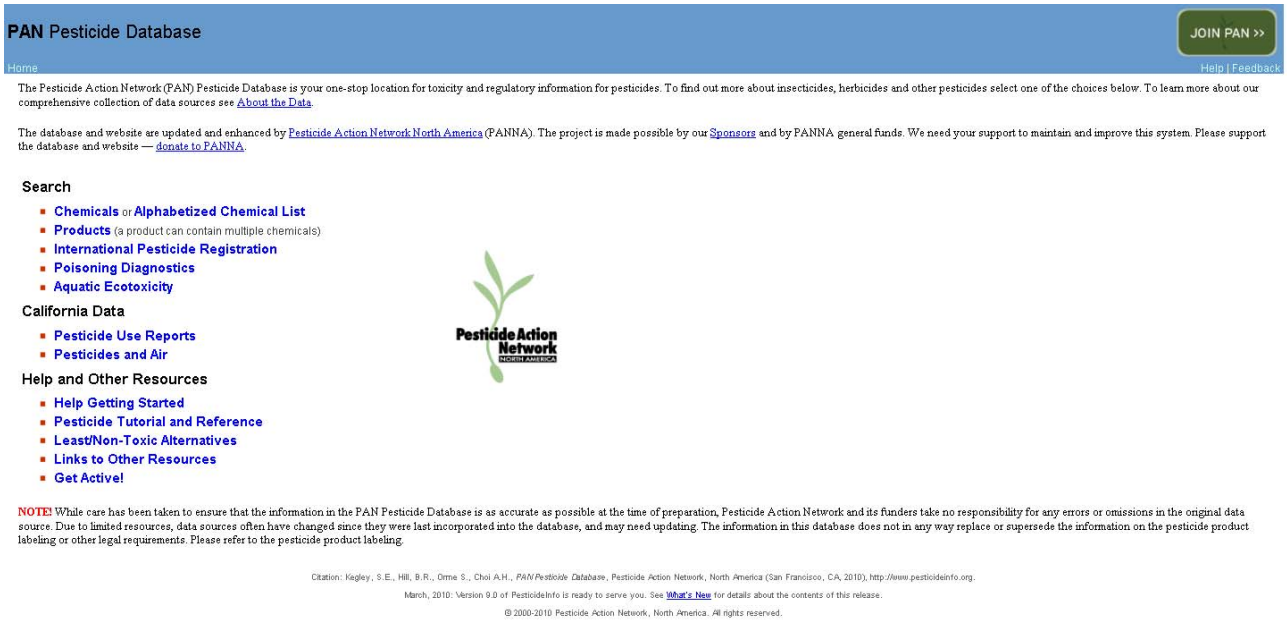
Nr of CHEMICALS 410

QUALITY CONTROL

2.2 PAN

Name PAN Pesticides

URL http://www.pesticideinfo.org/

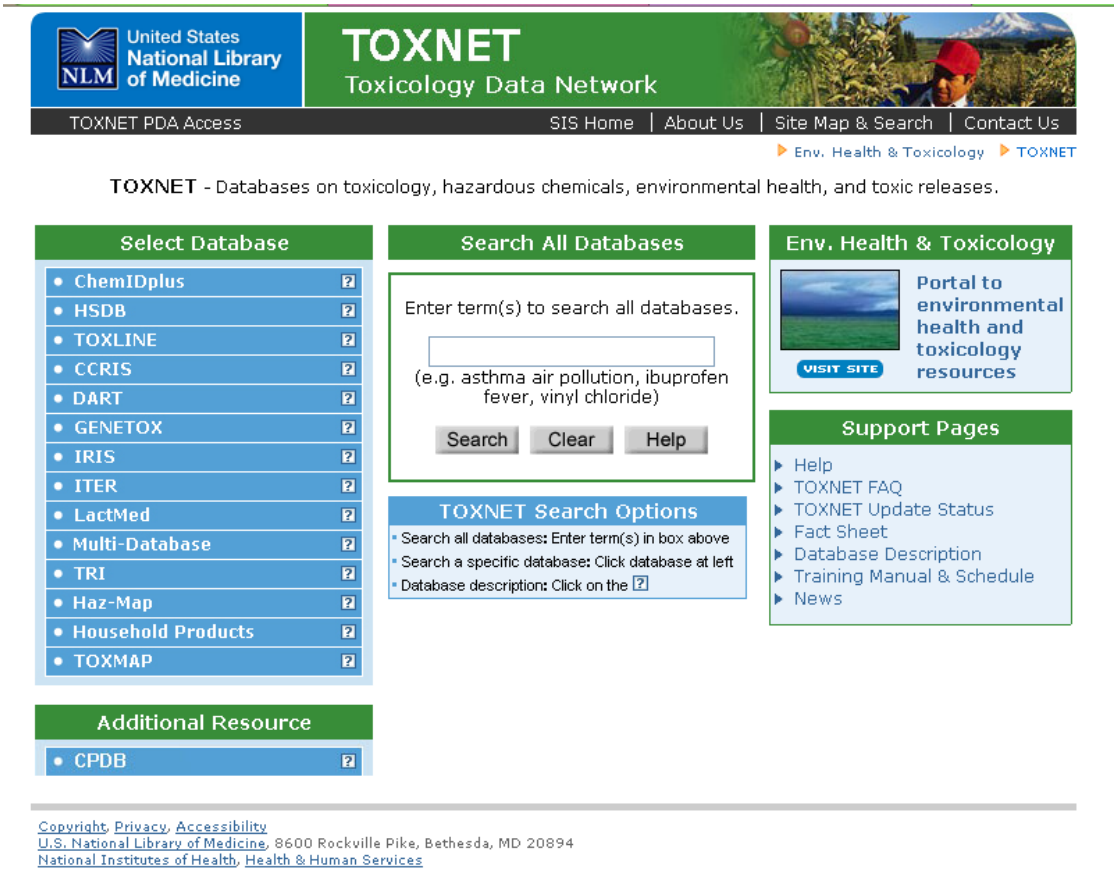


SHORT DESCRIPTION	The Pesticide Action Network (PAN) Pesticide Database lists toxicity data and regulatory information for pesticides.
Nr of ENDPOINTS/TESTS	Whatever available
Nr of CHEMICALS	6400
QUALITY CONTROL	YES

2.3 TOXNET

Name TOXNET

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



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

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

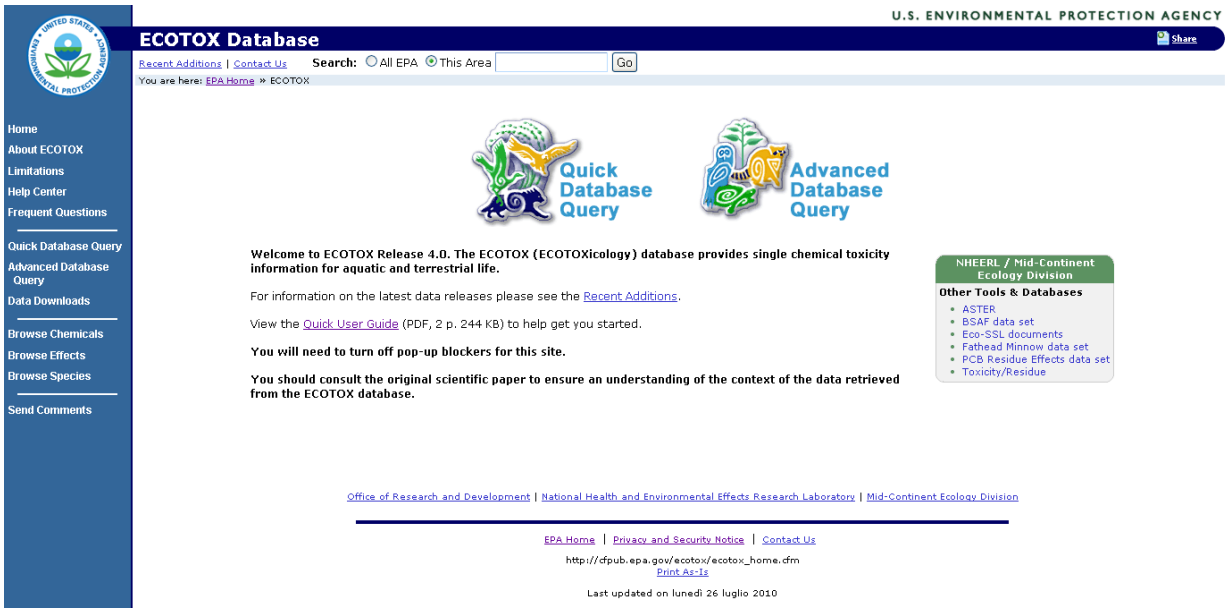
Nr of CHEMICALS >295000

QUALITY CONTROL very probably yes

2.4 ECOTOX

Name ECOTOX

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



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

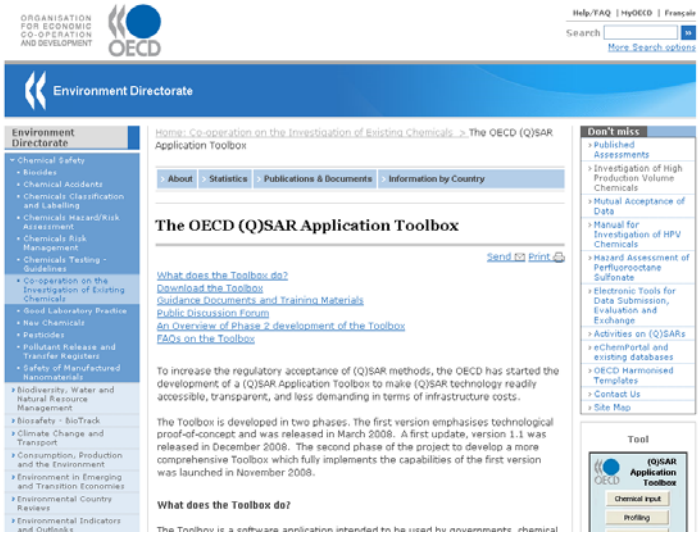
SHORT DESCRIPTION	Databases on toxicological and ecotoxicological parameters.All values included in the model are estimated with different models. Ecotoxicological models have been developed with Multicase by multilinear regression based on chemical molecule fragments and experimental data. The estimated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

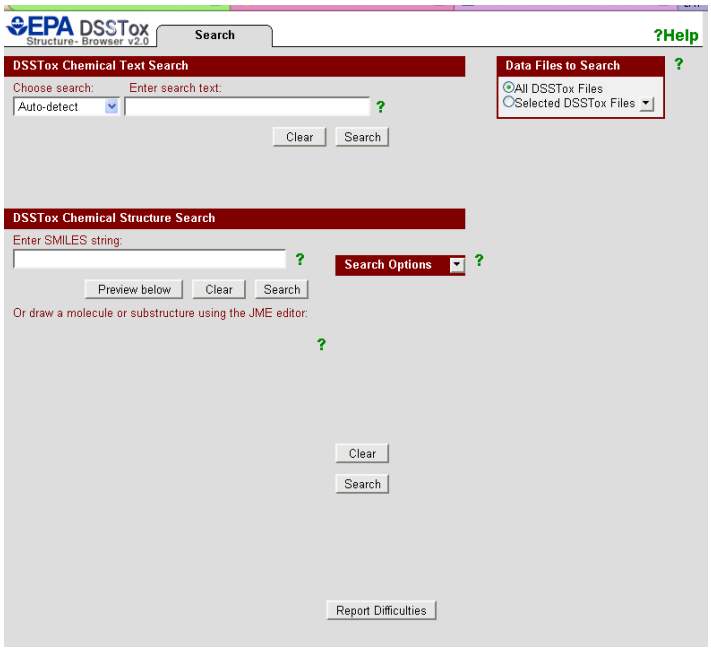


SHORT DESCRIPTION	The Toolbox is a software application intended to be used by governments, chemical industry and other stakeholders in filling gaps in (eco)toxicity data needed for assessing the hazards of chemicals. The Toolbox incorporates information and tools from various sources into a logical 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/



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

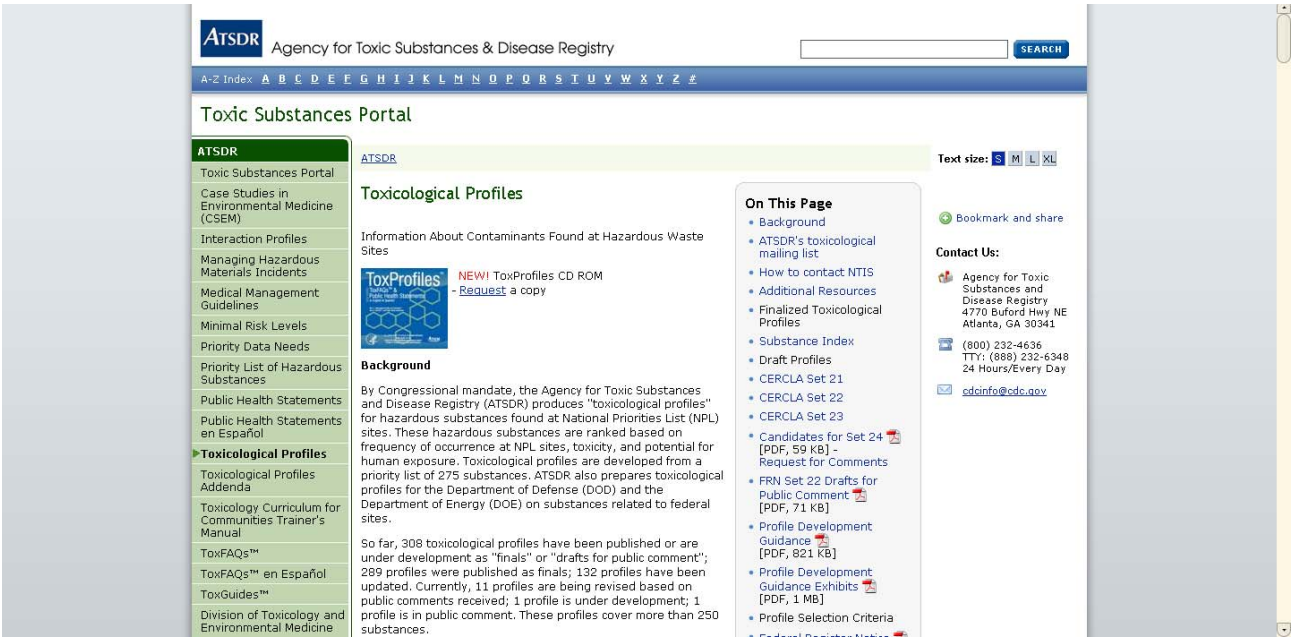
3 Toxicological database

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

3.1 ATSDR

Name ATDSR – 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

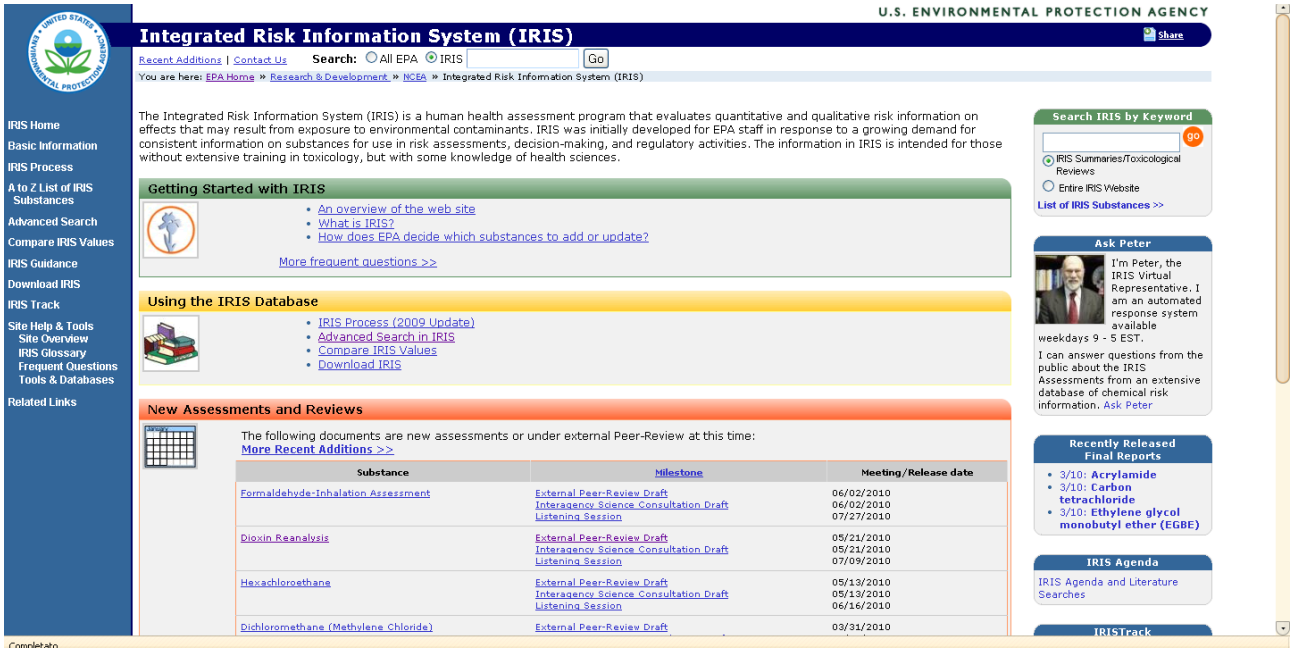
Nr of CHEMICALS 275

QUALITY CONTROL Very probably yes

3.2 IRIS

Name IRIS – Integrated risk information system

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



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

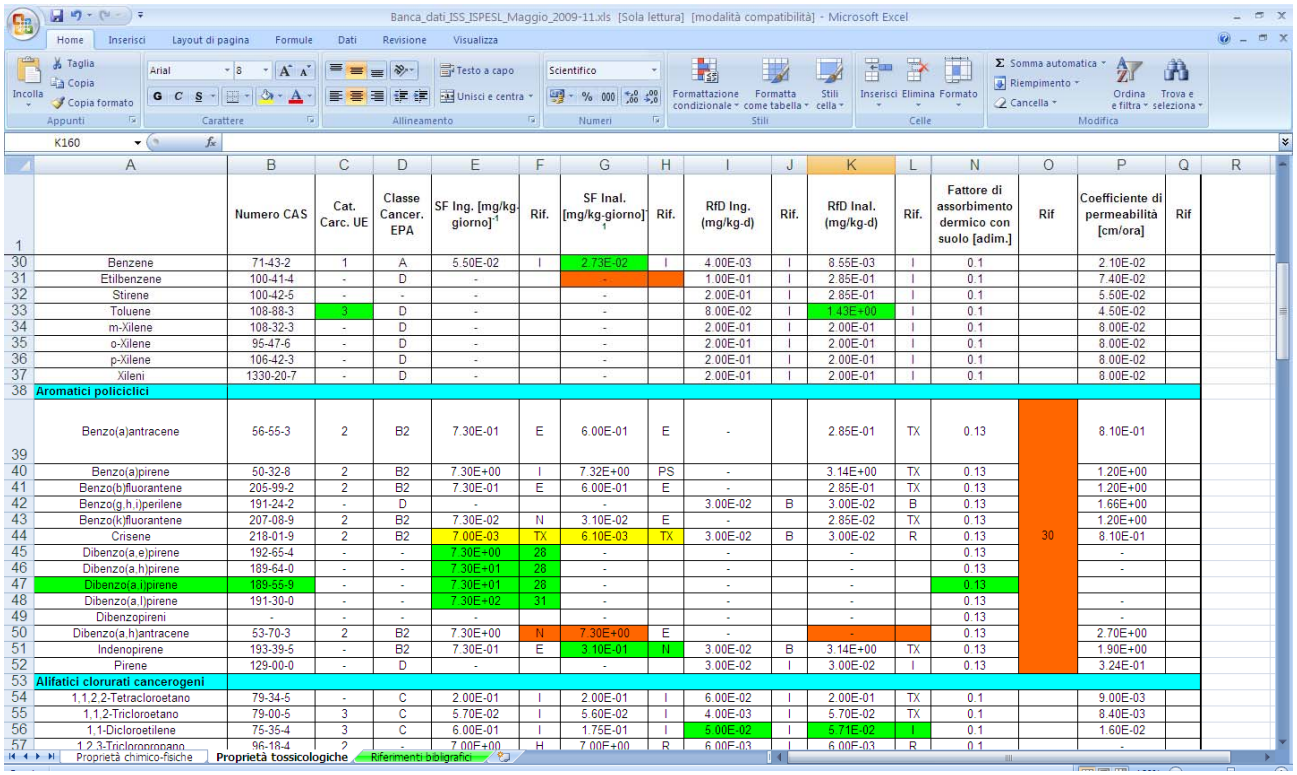
Nr of CHEMICALS >1000

QUALITY CONTROL Accurance 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
1		Numero CAS	Cat. Carc. UE	Classe Cancer. EPA	SF Ing. [mg/kg-giorno]$^{-1}$	Rif.	SF Inal. [mg/kg-giorno]$^{-1}$	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	-	-	-		-		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	Xileni	1330-20-7	-	D	-		-		2.00E-01	I	2.00E-01	I	0.1		8.00E-02		
38	**Aromatici policiclici**																
39	Benzo(a)antracene	56-55-3	2	B2	7.30E-01	E	6.00E-01	E	-		2.85E-01	TX	0.13		8.10E-01		
40	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		
41	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		
42	Benzo(g,h,i)perilene	191-24-2	-	D	-		-		3.00E-02	B	3.00E-02	B	0.13		1.66E+00		
43	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		
44	Crisene	218-01-9	2	B2	7.00E-03	TX	6.10E-03	TX	3.00E-02	B	3.00E-02	R	0.13	30	8.10E-01		
45	Dibenzo(a,e)pirene	192-65-4	-	-	7.30E+00	28	-		-		-		0.13		-		
46	Dibenzo(a,h)pirene	189-64-0	-	-	7.30E+01	28	-		-		-		0.13		-		
47	Dibenzo(a,i)pirene	189-55-9	-	-	7.30E+01	28	-		-		-		0.13				
48	Dibenzo(a,l)pirene	191-30-0	-	-	7.30E+02	31	-		-		-		0.13		-		
49	Dibenzopireni	-	-	-	-		-		-		-		0.13		-		
50	Dibenzo(a,h)antracene	53-70-3	2	B2	7.30E+00	N	7.30E+00	E	-		-		0.13		2.70E+00		
51	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		
52	Pirene	129-00-0	-	D	-		-		3.00E-02	I	3.00E-02	I	0.13		3.24E-01		
53	**Alifatici clorurati cancerogeni**																
54	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		
55	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		
56	1,1-Dicloroetilene	75-35-4	3	C	6.00E-01	I	1.75E-01	I	5.00E-02	I	5.71E-02	I	0.1		1.60E-02		
57	1,2,3-Tricloropropano	96-18-4	2	-	7.00E+00	H	7.00E+00	R	6.00E-03	I	6.00E-03	R	0.1		-		

Proprietà chimico-fisiche | Proprietà tossicologiche | Riferimenti bibliografici

SHORT DESCRIPTION Database on Human toxicological and phisico-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.

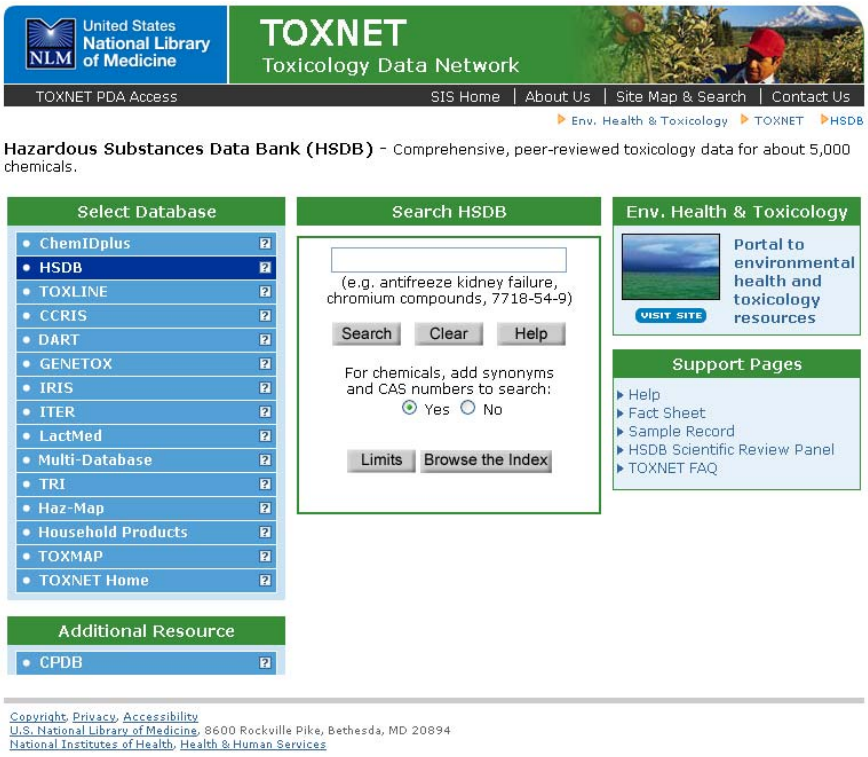
Nr of CHEMICALS 150

QUALITY CONTROL updated

3.4 HSDB

Name HSDB - Hazardous Substances Data Bank

URL http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB



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

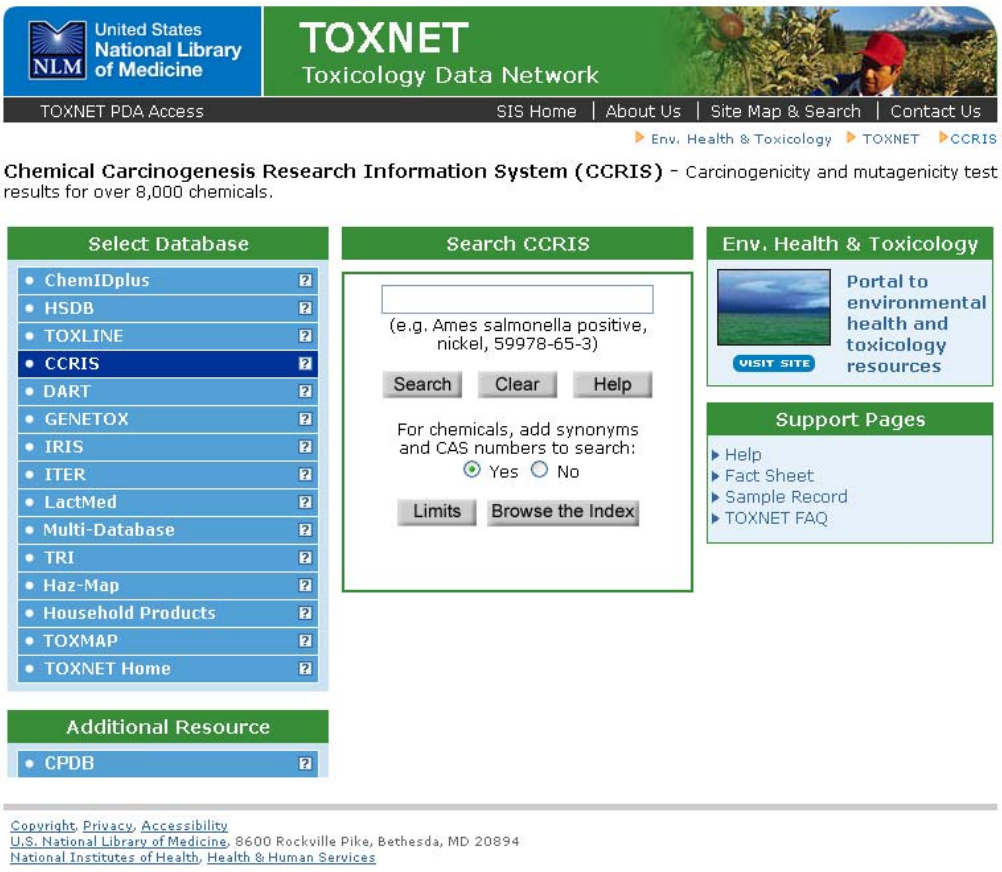
Nr of CHEMICALS 5000

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



SHORT DESCRIPTION

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

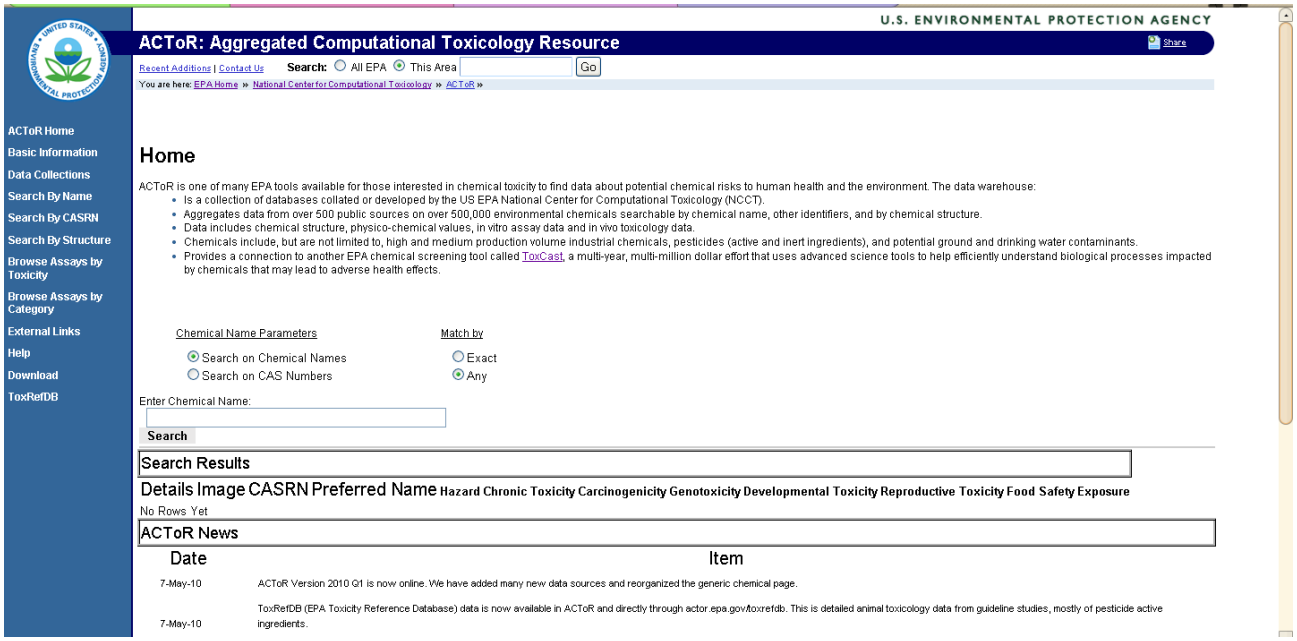
Nr of CHEMICALS 9000

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

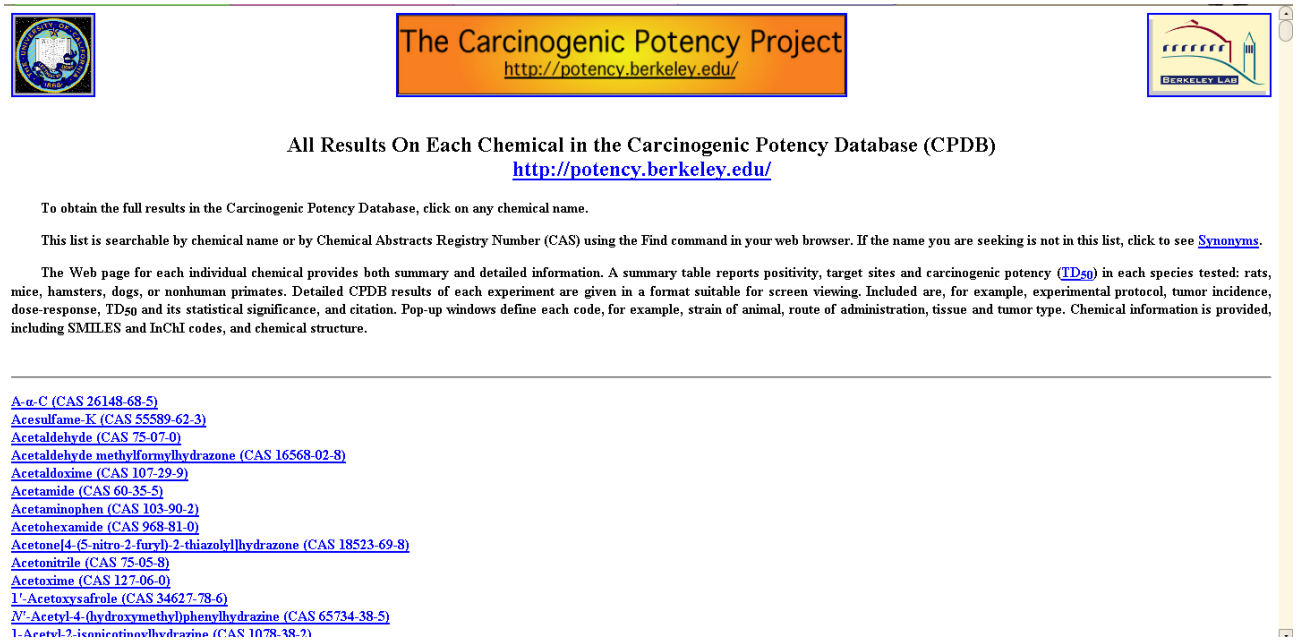


SHORT DESCRIPTION	a collection of databases collated or developed by the US EPA National Center for Computational Toxicology (NCCT) Chemical structure, physico-chemical values, *in vitro* assay data, and *in vivo* toxicology data
Nr of ENDPOINTS/TESTS	Whatever available
Nr of CHEMICALS	500,000
QUALITY 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 (TD_{50}) 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, TD_{50} 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-isopicotinoylhydrazine (CAS 1078-38-2)

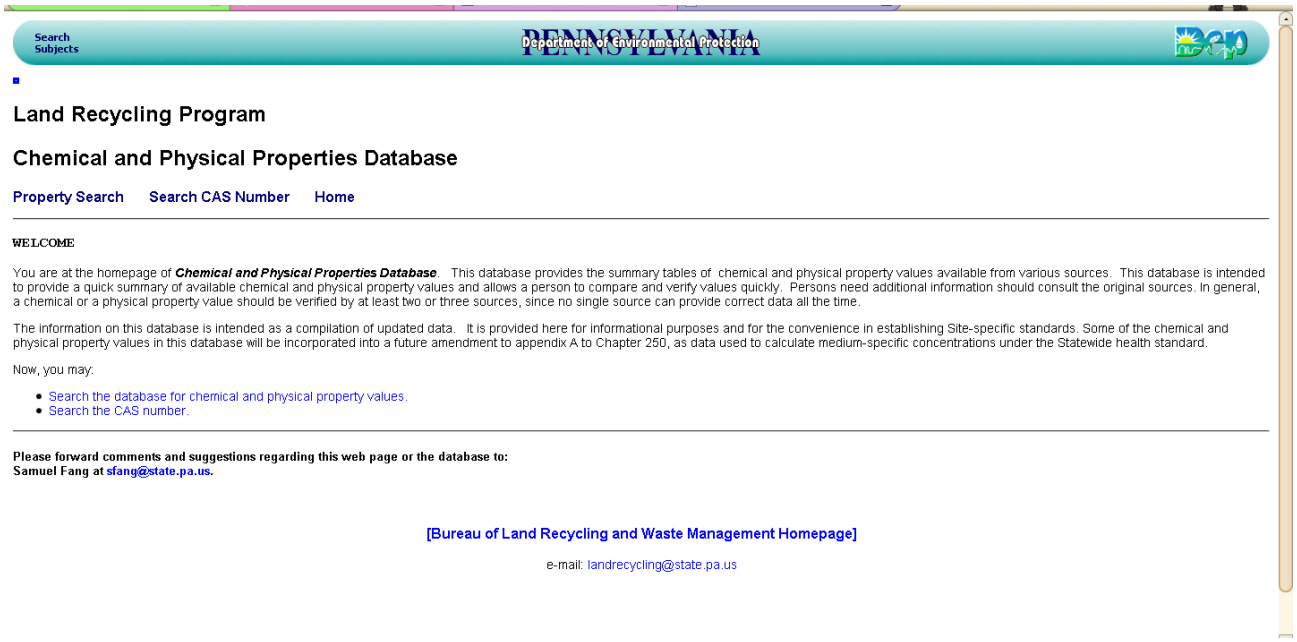
SHORT DESCRIPTION	The Carcinogenic Potency Database (CPDB) is a unique and widely used international resource of the results of 6540 chronic, long-term animal cancer tests on 1547 chemicals.
Nr of ENDPOINTS/TESTS	TD50
Nr of CHEMICALS	1547
QUALITY CONTROL	

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



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

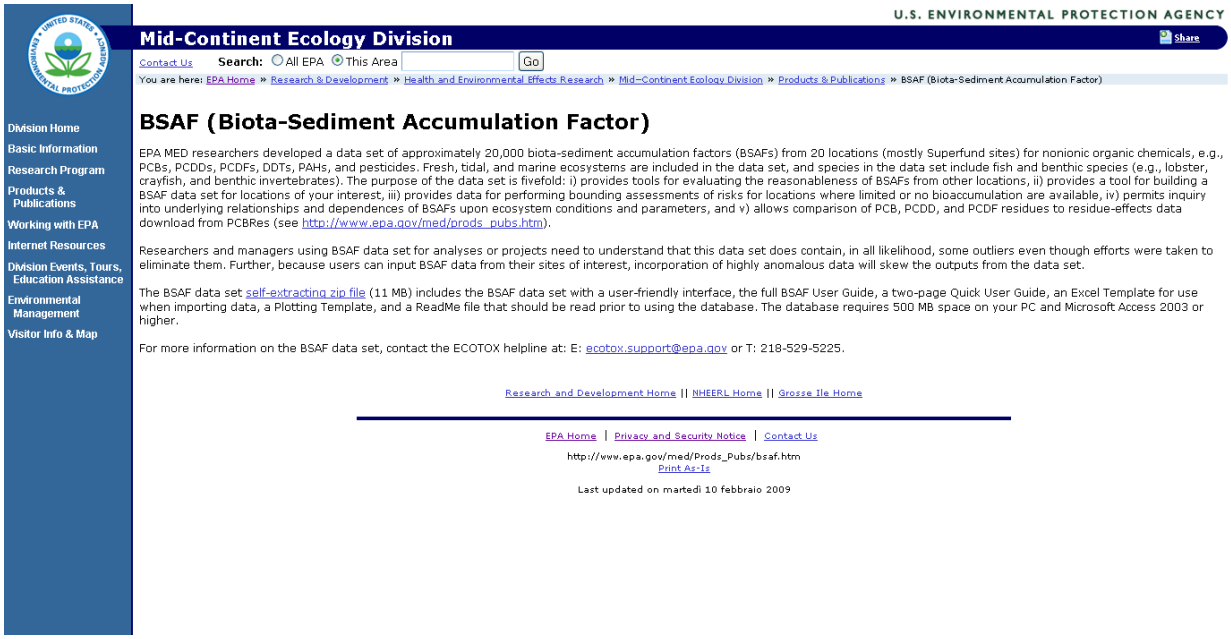
4.2 EPISuite

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

4.3 BSAF

Name BSAF (Biota-Sediment Accumulation Factor)

URL http://www.epa.gov/med/Prods_Pubs/bsaf.htm



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/

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

Nr of ENDPOINTS/TESTS

Nr of CHEMICALS updated

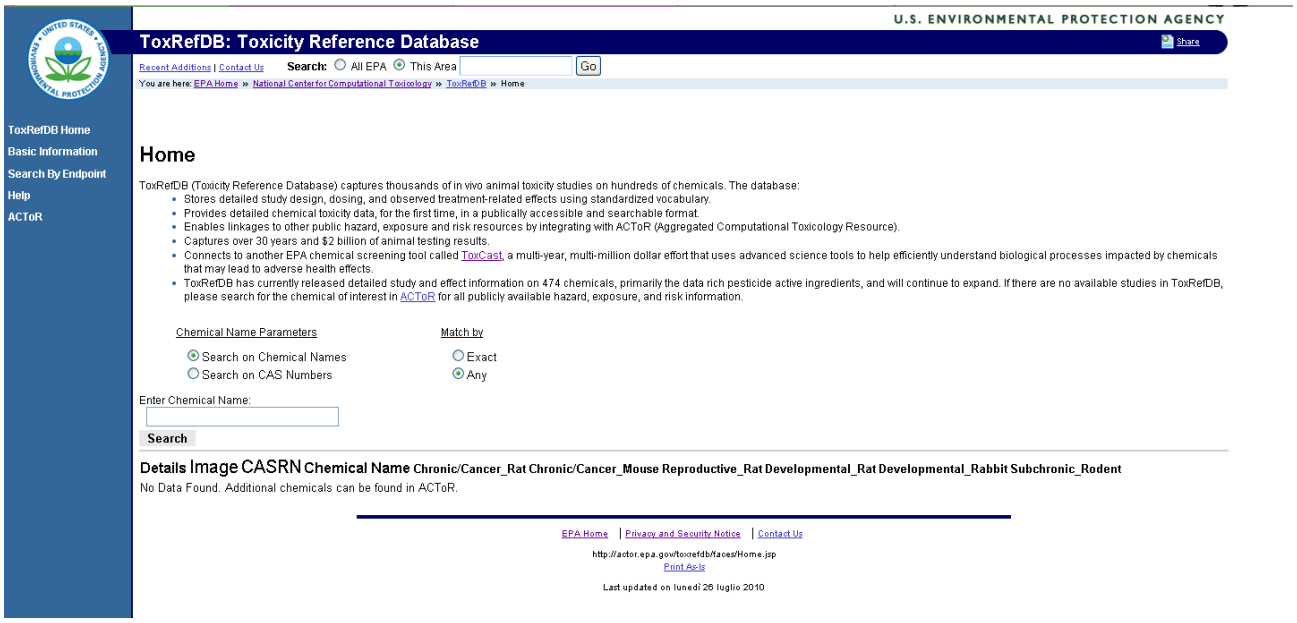
QUALITY CONTROL

5 In vivo studies and bioassays

5.1 ToxRefDB

Name ToxRefDB (Toxicity Reference Database)

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

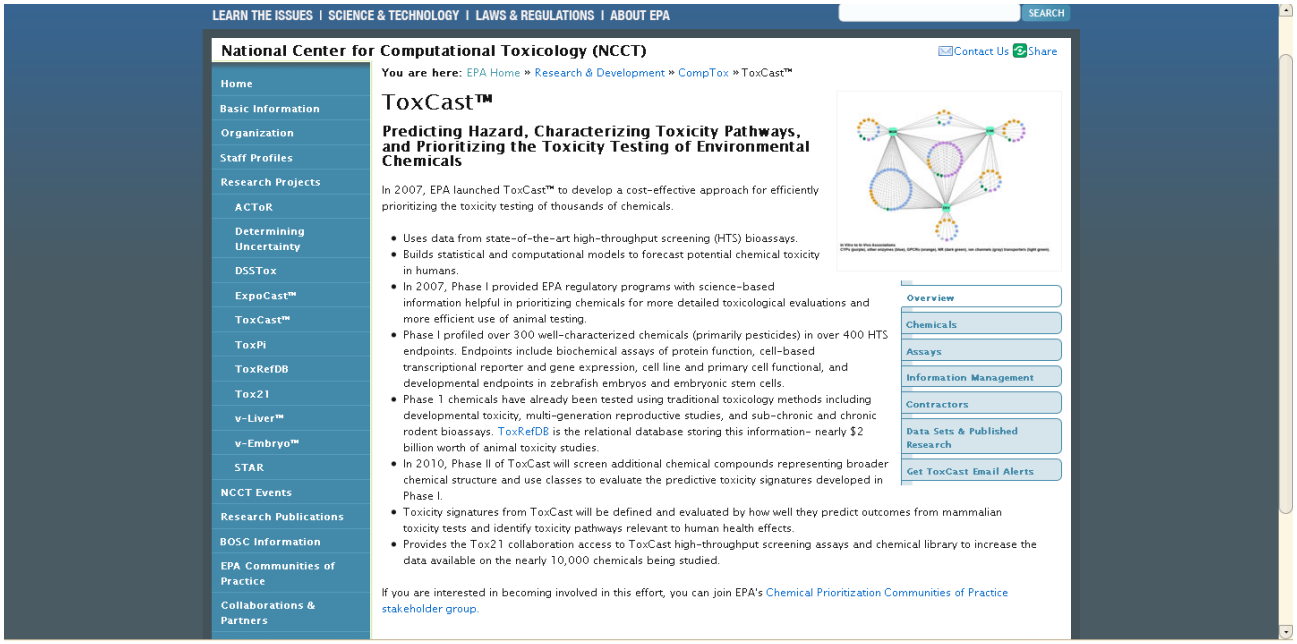


SHORT DESCRIPTION	captures thousands of in vivo animal toxicity studies on hundreds of chemicals
Nr of ENDPOINTS/TESTS	Whatever available
Nr of CHEMICALS	424 (?)
QUALITY CONTROL	updated

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

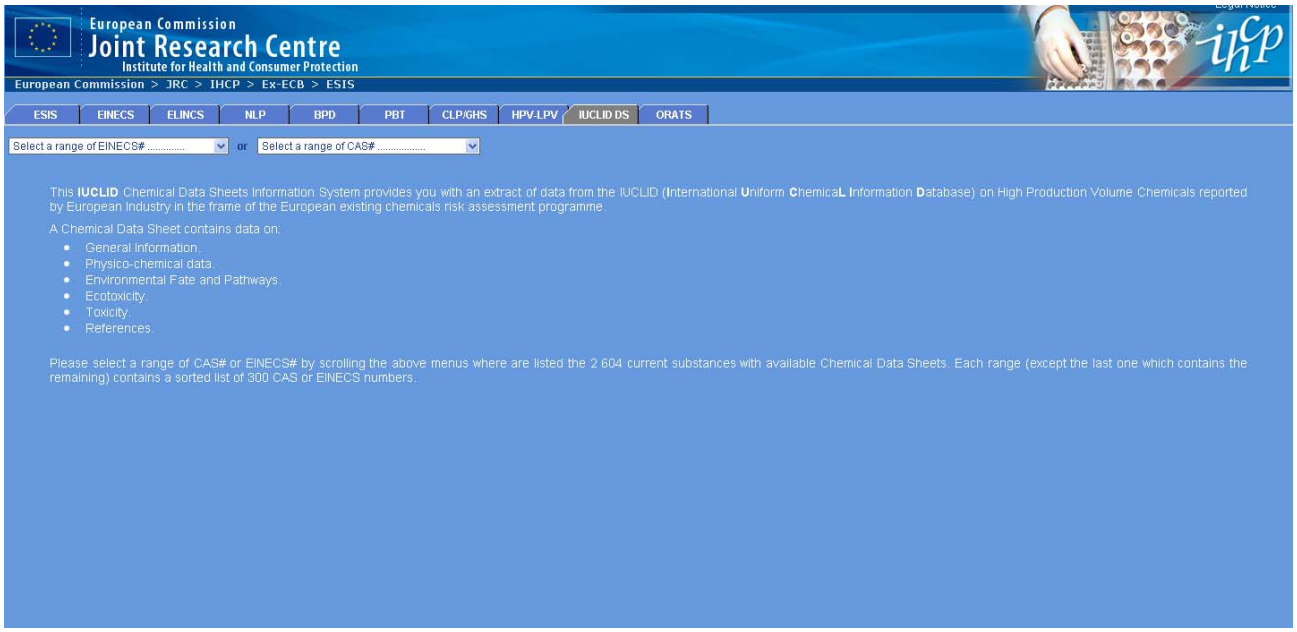
QUALITY CONTROL

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

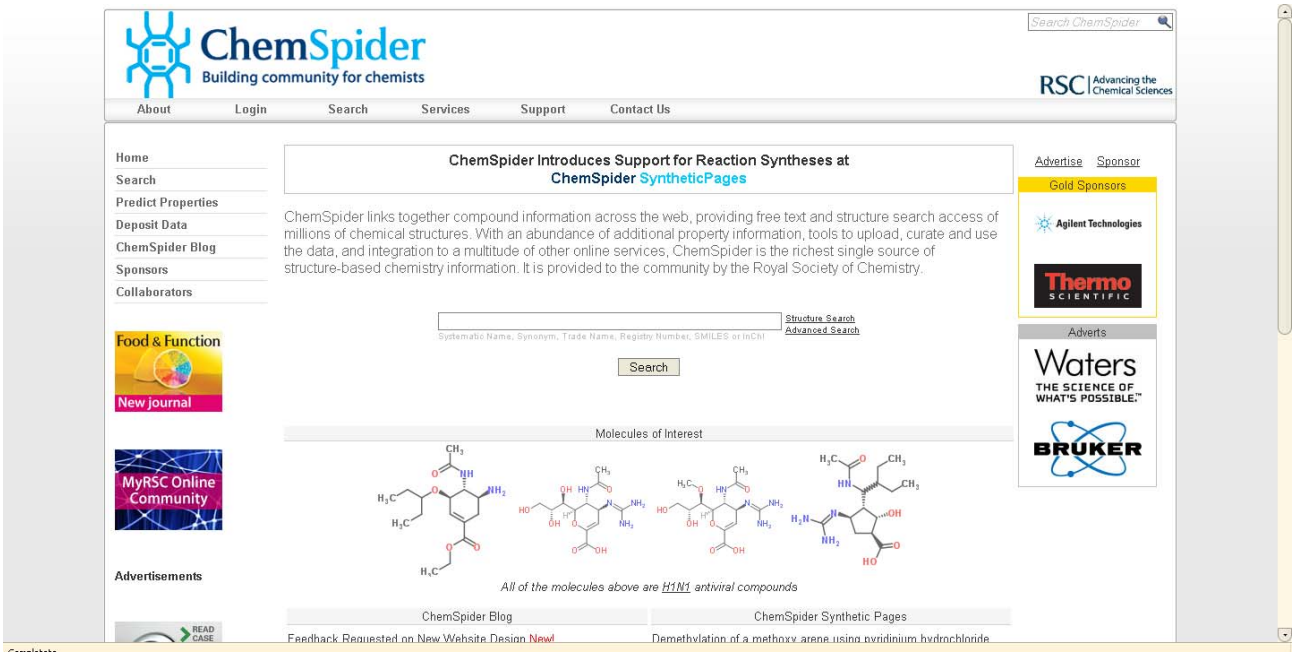
Nr of CHEMICALS 2604

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

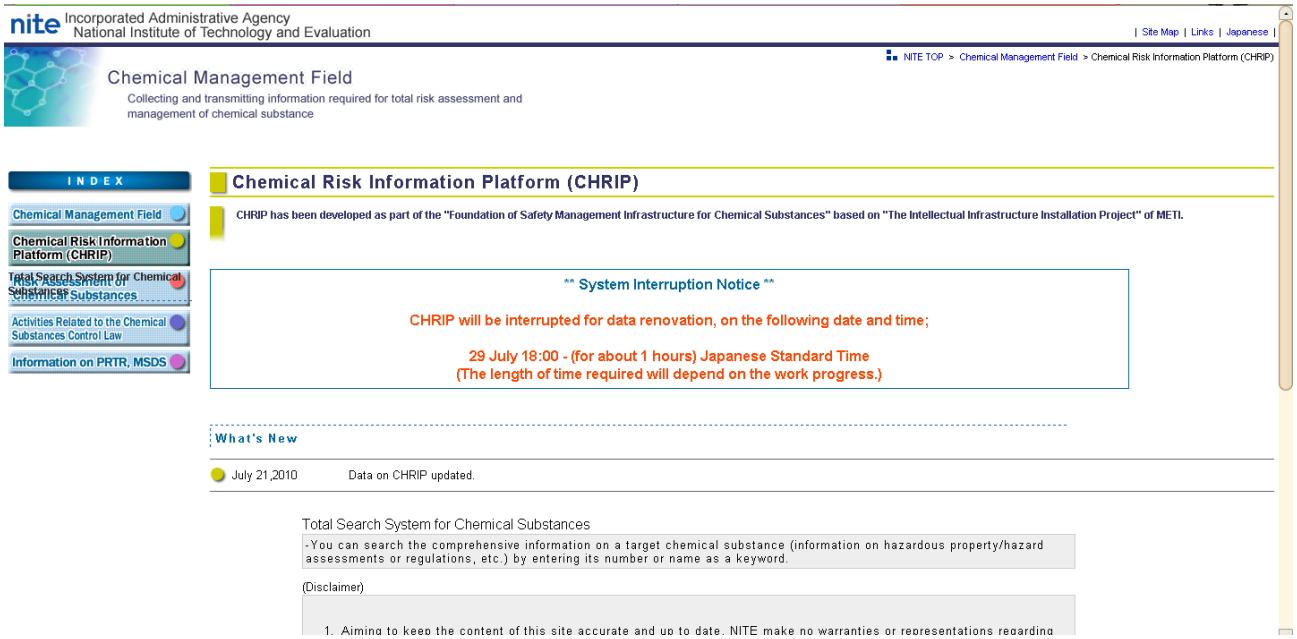
Nr of CHEMICALS 25M

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