

AiiDA: An online database for sharing and computing ecotoxicity data in the context of REACH

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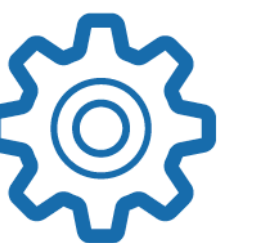
CONTEXT & OBJECTIVE

New environmental regulations such as REACH or the Product Environmental Footprinting require to have a vision of the environmental profile of commercial substances or products. In spite of huge efforts that were done since 30 years to run ecotoxicity tests for thousands of substances, it is still complex and time consuming for scientists to get a clear perception of the potential risk or impact of a chemical substance.

It is the purpose of AiiDA (Aquatic Impact Indicator Database) to provide a quick and clear overview of all ecotoxicity data for more than 22 000 substances and a detailed calculation of the main risk and impact indicators commonly used in the regulation.

- 15 000 HC_{50} , and 13 800 HC_5 with 95% confidence interval
- 38 000 $PNEC$ with assessment factor
- All tests sources and documentations **traceable**
- 27 500 SSD and PSD interactive representations
- **Select** and **compare** up to 5 substances
- Presenting **relative toxicity** of substances or group of substances among all reported substances

Indicators provided by AiiDA & Methods associated



Substance Description (for 22 270 chemicals)

Quick Find Q: CAS or Echemumber Substance name

Molecule Type: All OSAR Class: All Use: All

CAS	EC Number	Type	Chemical Name	Phyla	View	Comp.
7758-98-7	231-847-6	Inorganic	copper sulphate	34	Q	+
10108-64-2	233-296-7	Inorganic	cadmium chloride	26	Q	+
1912-24-9	217-617-8	Pesticide	atrazine	26	Q	+

Id: 4120
 CAS: 7758-98-7
 Echemumber: 231-847-6
 Name: copper sulphate
 Smiles: O[S(=O)](=O)[Cu]
 OSAR:
 Weight: 159.61 (g/mol)
 Solubility: 96200 (mg/L)
 Type: Inorganic
 Use: Agricultural chemical, Antidotes, Autonomic agents, Central nervous system agents, Emetics, Fungicide, bactericide, wood preservative, Gastrointestinal agents, Human data, Mutation data, Peripheral nervous system agents, Protective agents, Reproductive effect, Tumor data
 ECHA: Link ECHA for copper sulphate

HC_5 and HC_{50} (Hazardous Concentration)

HC_5 Phyla/Species comparison
 CAS : 1135995

HC_5 Based on Aldenberg (2000) and US-EPA method
 HC_{50} Based on A.M.I method (Assessment of the Mean Impact)

$PNEC$ (Predicted No Effect Concentration)

Description HC_{50} HC_5 $PNEC$ Figure

$PNEC$ and Assessment Factor

$PNEC$ (mg/L)	AF	Most Sensitive Species	Phylum	Acute Tests	Chronic Tests	Species	Phyla
7.8	1	desmodium sphenos	Chlorophyta	12530	694	31	3285
5.2	1					281	26

$PNEC$ or Predicted No-Effect Concentration is the concentration below which exposure to a substance is not expected to cause adverse effects.

$PNEC$	Unit	AF	Type	Conclusion	Extrapolation Method	Source
7.8	µg/L	1	Freshwater	$PNEC$ aqua (freshwater)	statistical extrapolation	Source ECHA
5.2	µg/L	1	Marine water	$PNEC$ aqua (marine water)	assessment factor	Source ECHA
220	µg/L	1	STP	$PNEC$ STP	statistical extrapolation	Source ECHA
87	mg/kg sediment dwt	1	Sediment (freshwater)	$PNEC$ sediment (freshwater)		Source ECHA
676	mg/kg sediment dwt	1	Sediment (marine water)	$PNEC$ sediment (marine water)	partition coefficient	Source ECHA

Data Source $PNEC$

Base	Endpoint	Water Type	Test Duration	Conc. (mg/L)	Source	Author	Title	Year	Remarque
ECOTOX - USEPA	EC50	FW	5 d	2.0E-5	ECOTOX Database	US-EPA		2014	Link to USEPA database

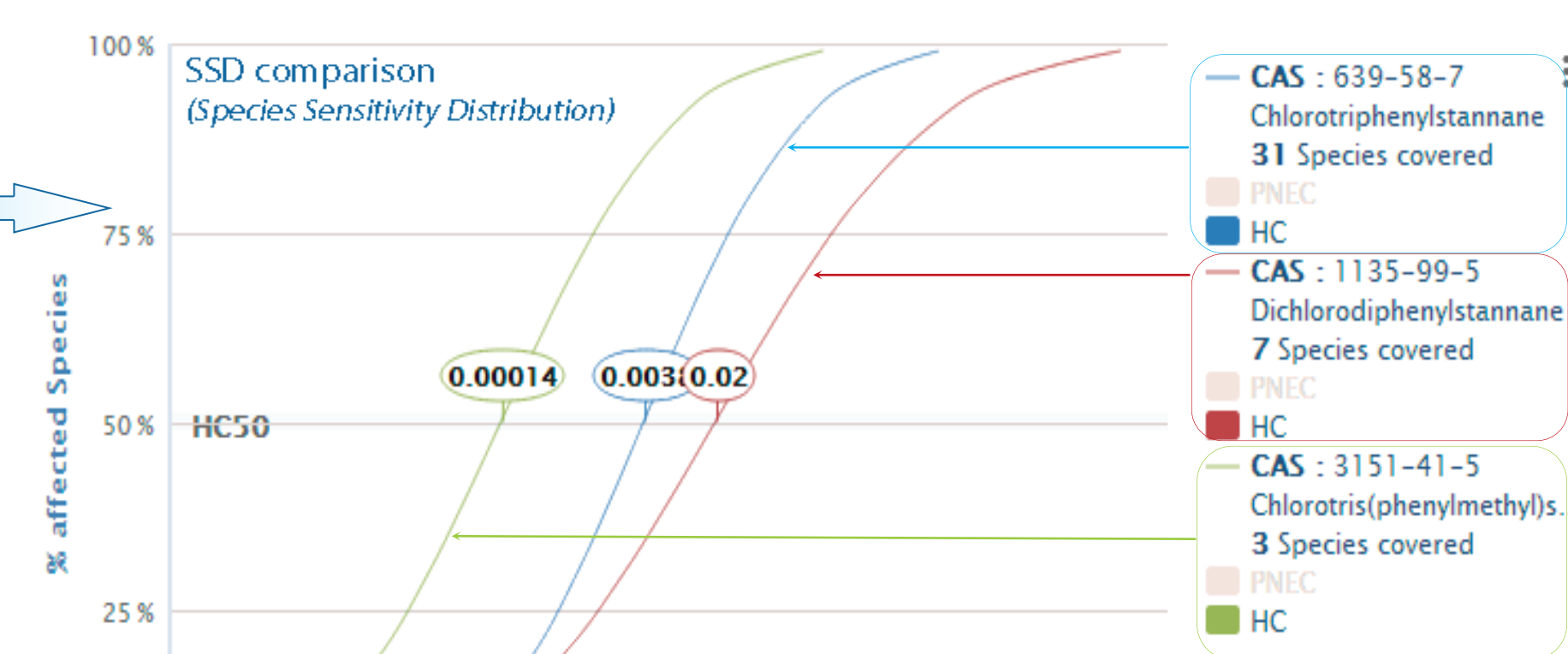
Based on Technical Guidance Document (TGD 2003)

Case Study



Comparison of 3 substances

CAS : 639-58-7	Name : Chlorotriphenylstannane
CAS : 1135-99-5	Name : Dichlorodiphenylstannane
CAS : 3151-41-5	Name : Chlorotris(phenylmethyl)stannane



Key Points



Representativity

- 500 000 ecotoxicity tests on more than 8432 species and belonging to 34 phyla.
- 22 270 molecules from which 13 783 are covered with data on 3 phyla or more.
- 30 000 SSD and PSD representation (Species/Phyla Sensitivity Distribution).

Traceability

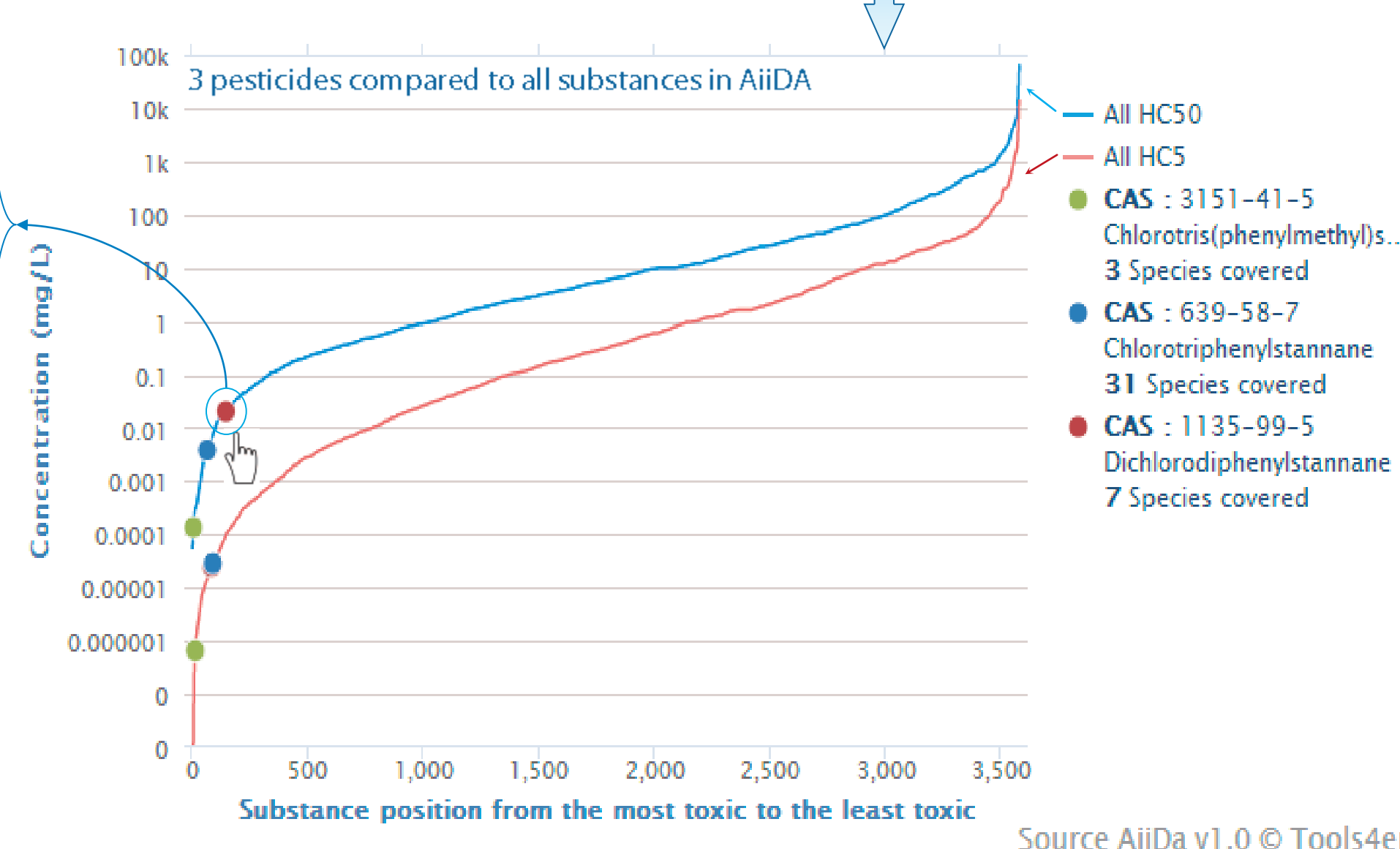
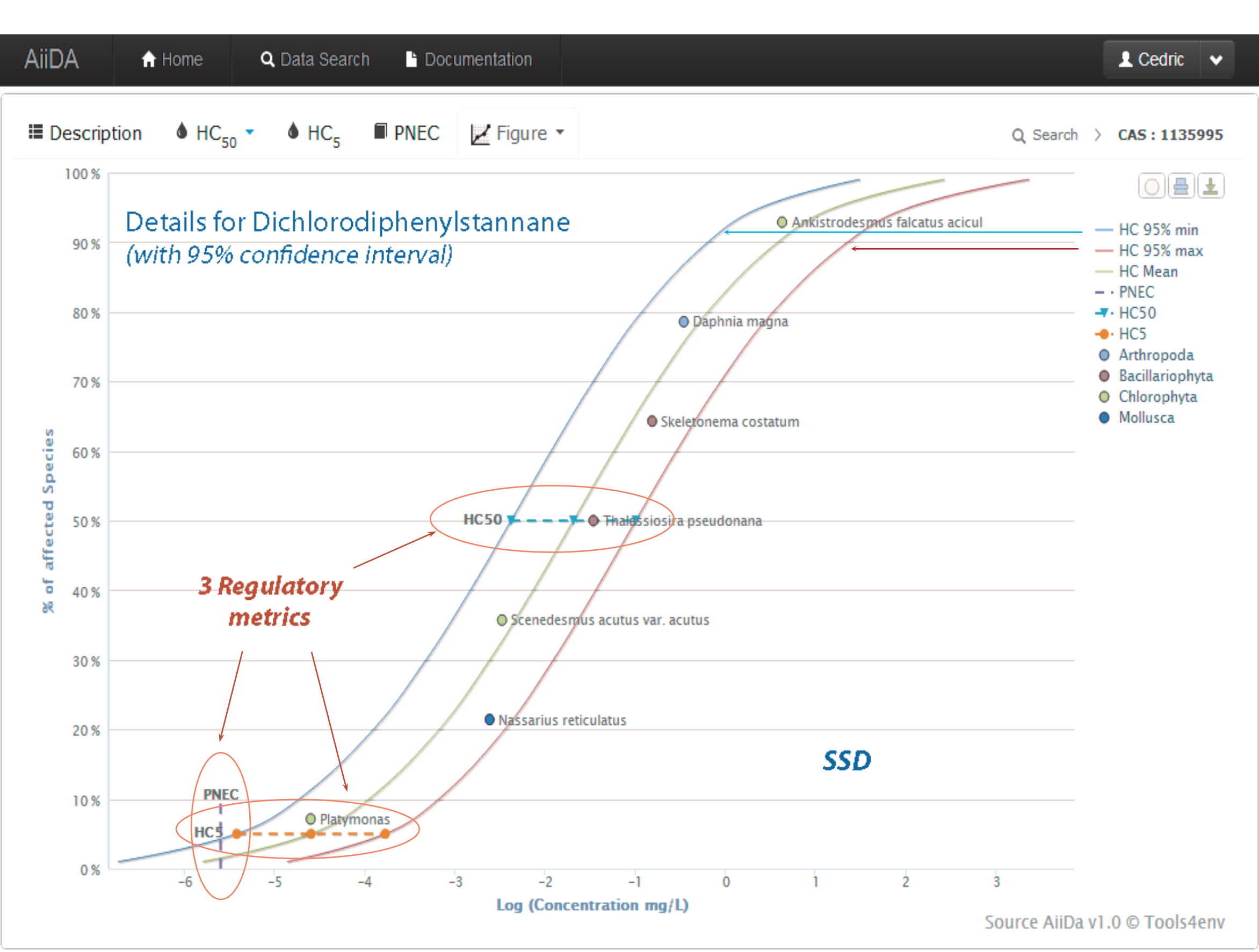
- Fully traceable data.
- Fully traceable methods.
- Fully traceable risk and impact metrics.
- Species taxonomy from the *ITIS* database (Integrated Taxonomic Information System)

Interactivity

- A community Platform where each user can share his data.
- An interactive Database where everybody can propose improvements.

Update

- Data update is provided **regularly** and includes all the available tests of **ECHA** and **US-EPA Ecotox** database.



To learn more about software functionalities please check the different versions of AiiDA (free, standard and premium access)

Create your free account : www.aaida.tools4env.com