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

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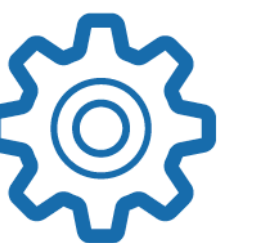([1]Tools4Env, [2]Cycleco, [3]EPFL)

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 assesment 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)

HC_5 and HC_{50} (Hazardous Concentration)

HC_5 Based on **Aldenberg (2000)** and **US-EPA method**
HC_{50} Based on **A.M.I method** (Assessment of the Mean Impact)
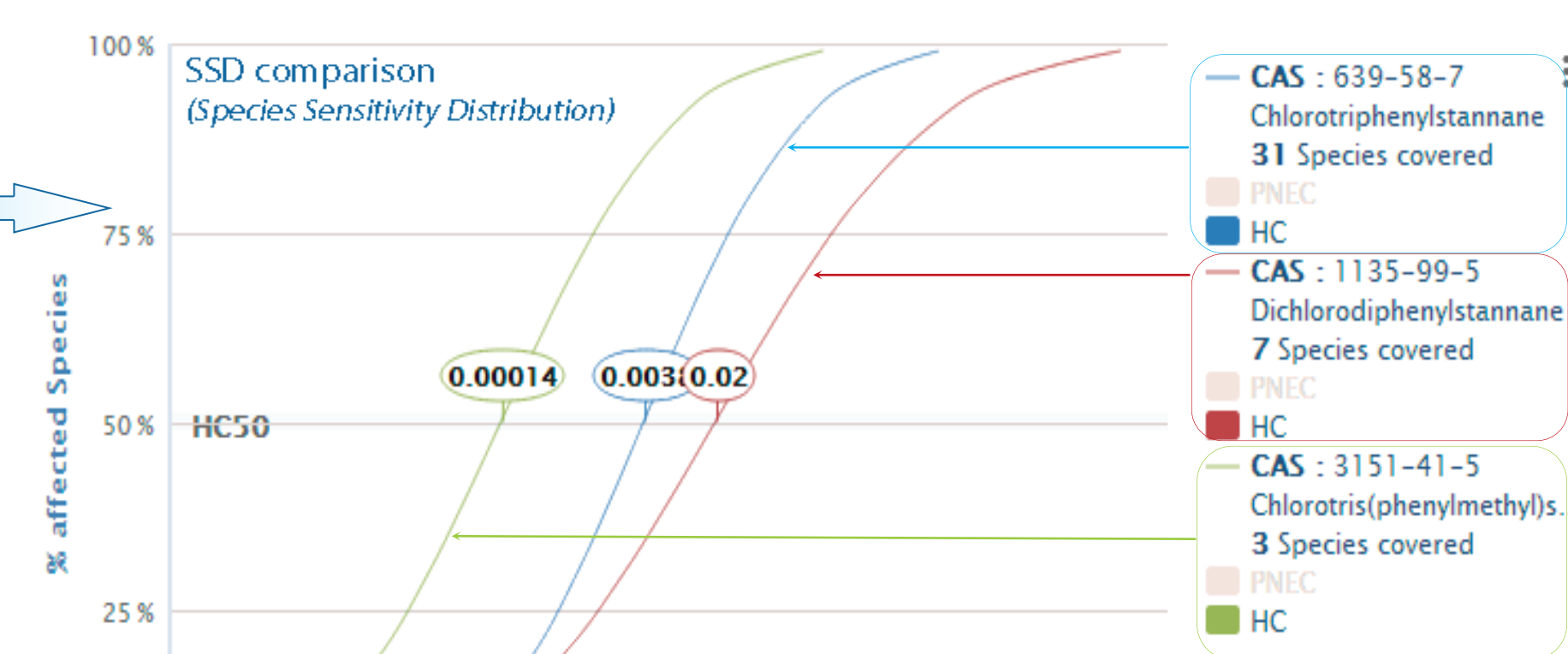
PNEC (Predicted No Effect Concentration)

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).
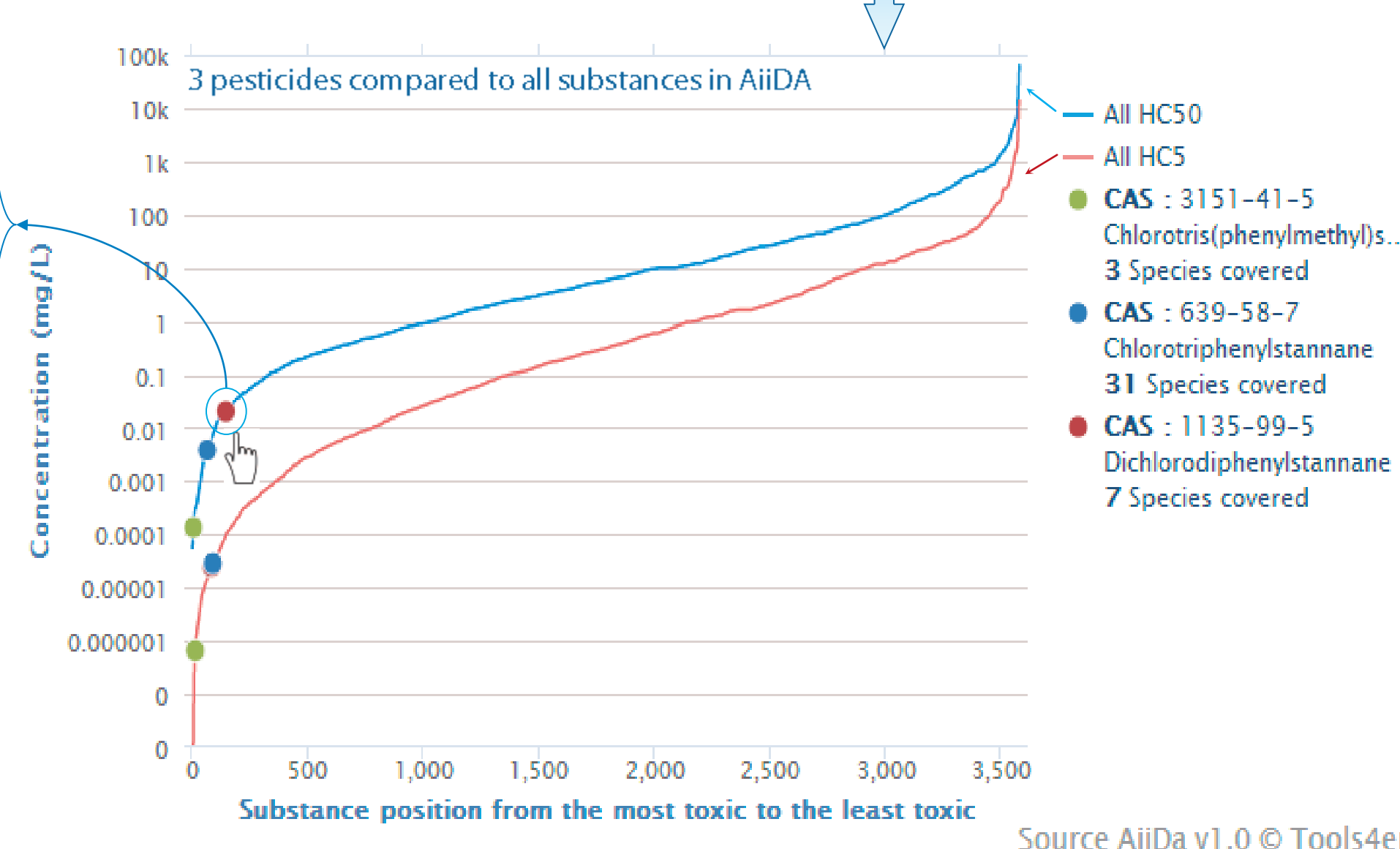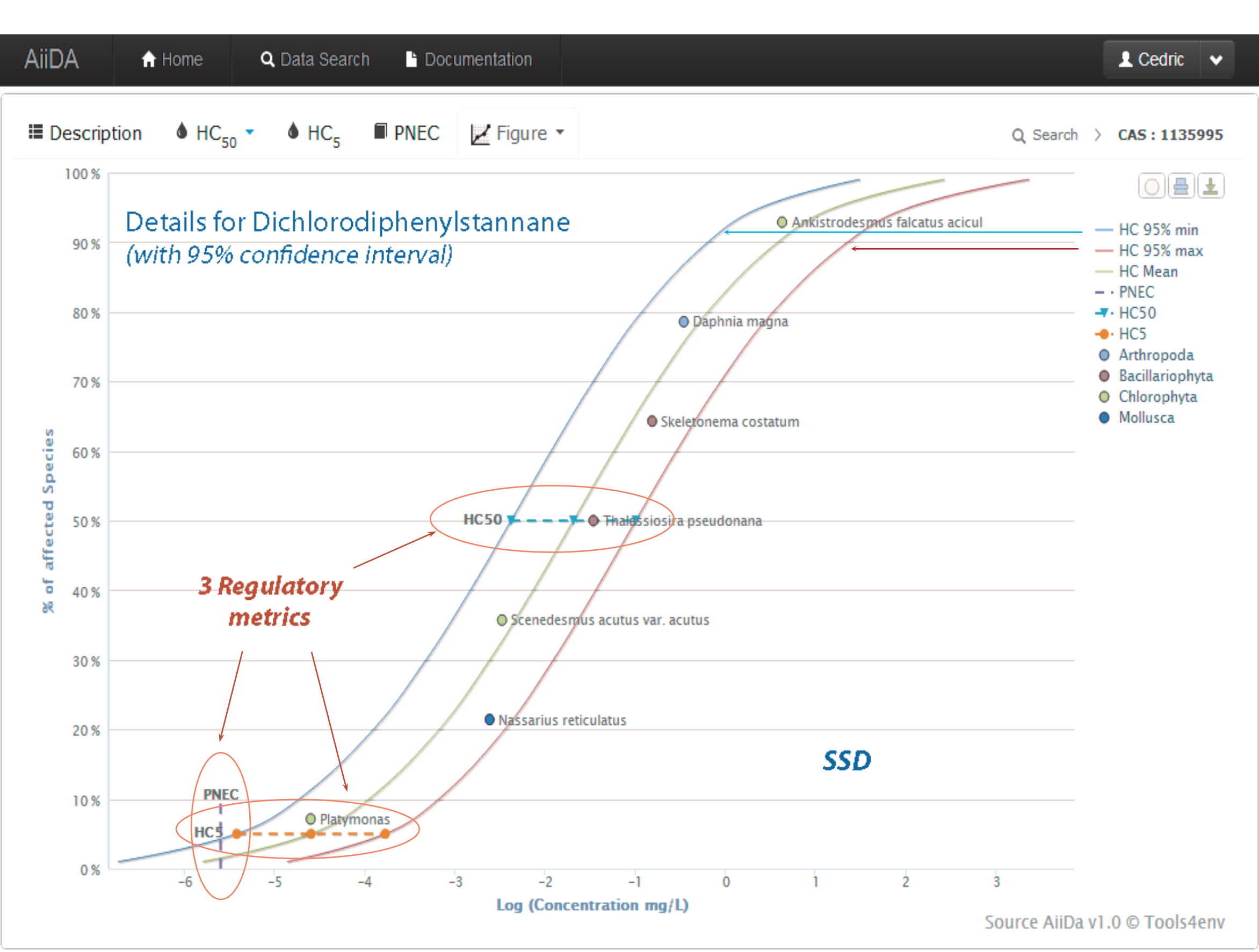
Traceability

- 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.aiida.tools4env.com