

AIIDA: ONLINE DATABASE FOR SHARING AND COMPUTING ECOTOXICITY DATA

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Abstract

Currently, industries that want to obtain ecotoxicological data on a substance of interest are facing different problematics, such as the inexistence of ecotoxicological data on the substance, the difficulty to obtain an efficient and global view on data sources and databases, and the complexity for calculating ecotoxicological impacts indicators used in the context of life cycle assessment or environmental risk assessment.

The AiiDA tool provides more than 500 000 ecotoxicological bioessays on more than 3600 species and belonging to 30 phyla. This global database is used to automatically calculate different ecotoxicological endpoints and their uncertainties according to the Technical Guidance Document (*TGD*) from the European Union. AiiDA provides data on 7500 molecules from which 5400 are covered with data on 3 phyla or more.

The following ecotoxicological endpoints are proposed in AiiDA:

- HC₅₀ calculated with the AMI (*Assessment of Mean Impact*) method provided with it confidence interval for more than 10 000 HC₅₀ Acute and Chronic. This endpoint is used in USEtox™ model for the calculation of the effect factors in context of LCA.
- HC₅ and confidence interval 95% based on the Aldenberg review (2000) or based on US-EPA method.
- PNEC calculated with the recommendations of the Technical Guidance Document on Risk Assessment (2003)

The calculated endpoints are available in the interactive platform that provides the results and the traceability of all the calculation steps of the endpoints. This traceability doesn't exist in the usual tools of ecoconception and ensure the consistency of the aquatic indicators. The comparison of the substances and the calculation of the Species Sensitivity and Phyla Sensitivity Distributions are provided to the user.

Keywords:

Ecotoxicology, Database, Aquatic Impact Indicators, Traceability, SSD, Web-based Platform

1. INTRODUCTION

The development of chemistry and increase of chemicals use and application has led to a decrease of the global ecological health of surface waters. In France, in 2011, pesticides have been found in 93% of the tested samples of water, 30% of which containing more than 10 substances [1].

While the importance of ecotoxicological impacts of industrial chemicals have been proved, these impacts rarely have been taken into account for the ecological conception of products. Methods to quantify these impacts exist and are internationally well-recognised. However, they are today neglected, for three main reasons:

- The data are lacking in the main world databases
- The data are not traceable and documented
- The ecotoxicological endpoints are not easily calculable

Ecotoxicological tests are tools that have been developed in order to assess the impact of chemicals on ecosystems. These experimental data are primary variables that can be used as input models such as USEtox, from which are calculated potential ecotoxicological impacts in life cycle impact assessment, environmental footprinting and ecological risk assessment. There is therefore an important need in order to unit and normalize these ecotoxicological data.

In the context of the REACH regulation, more than 150 000 substances have been pre-registered by the European Chemicals Agency, and tests on more than 30 000 substances should be available in 2018 [2].

2. OBJECTIVE OF THE PROJECT

New environmental regulations such as REACH or 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 7500 substances and a detailed calculation of the main risk and impact indicators commonly used in the regulation.

2.1 Creation of a global ecotoxicity database: AiiDA

Tools for environment has created a database that groups together ecotoxicological tests results available in various databases so as to create a world database of ecotoxicological data as exhaustive as possible.

Table 1 – The main ecotoxicity databases in 2012

Name	Organization	Update	Tests	Substances	Species	Access
Aquire	USEPA	Regular	330.000	4.800	3.000	Free
OPP	USEPA+OPP	2009	20.000	800	300	Free
USGS	CERC	1995	5.000	400	60	Free
EAT	ECETOC	2008	5.000	500	250	Private
eChemportal	ECHA+ IUCLID	Regular	100.000	4.000	300	Free
All tests considered			460.000			

2.2 Automatic calculation of aquatic indicators

This general database allows the automatic calculation of the main ecotoxicological aquatic endpoints and their uncertainties following the official European Technical Guidance Document, with the objective of regular updates so as to improve the ecological representativeness and decrease the uncertainty of these endpoints. The automatic update of the AiiDA database directly allows the endpoints update for each molecule.

2.3 Comparison and Substitution of dangerous substances

In the context of Ecodesign of products, the best method is to avoid the use of unsafe products and to replace it by a less hazardous substance. The AiiDA platform allows comparing the toxicity of these different molecules on the basis of the calculation of Species Sensitivity Distributions, allowing the identification of less hazardous substances and substituting them by other molecules with less impact on the aquatic environment.

2.4 Traceability and sharing platform of ecotoxicity data

The calculated endpoints are available in the AiiDA Web platforms, with the description of all the calculation step and documentation on the data sources. This traceability is of main importance for Ecodesign by allowing the user to analyse each endpoint. The AiiDA platform also can be improved by the user, for example by adding new ecotoxicity data after administration. This last step will allow obtaining a sourced and checked world ecotoxicological database.

3. INDICATORS PROVIDED BY AIIA & METHODS ASSOCIATED

3.1 HC₅₀ (Hazardous Concentration for 50% of species)

The calculation of HC₅₀ is based on A.M.I (*Assessment of the Mean Impact*) method (Payet and Jolliet 2004). All the EC_{50s}, NOECs, and LOECs concerning the given chemical are collected. When data are lacking, the EC₅₀ can be extrapolated from NOEC or LOEC data. A list of test results covering several species is then available for the chemical, covering all sorts of effect and all test durations available. For a given chemical, the Log (HC_{50EC50}) is calculated as the mean of the Log(EC₅₀) values. The EC₅₀ values must cover at least three different taxa.

A Confidence Interval is associated with HC₅₀. Indeed, in a comparative assessment, as required in LCIA, it is crucial to identify whether chemicals present a difference in terms of toxicity. For this purpose, the 95% Confidence Interval on the HC₅₀ is calculated using the Student method. The Confidence Interval is dependent on the number of species considered in the calculation. The size of the Confidence Interval for a chemical can be reduced by the inclusion of data concerning new species [3].

The AMI method enables the assessment of numerous substances with an indicator based on several species, and providing a Confidence Interval. The AMI method is already implemented in the IMPACT 2002 model for the assessment of toxicological impacts on human and ecosystems in Life Cycle Assessment.

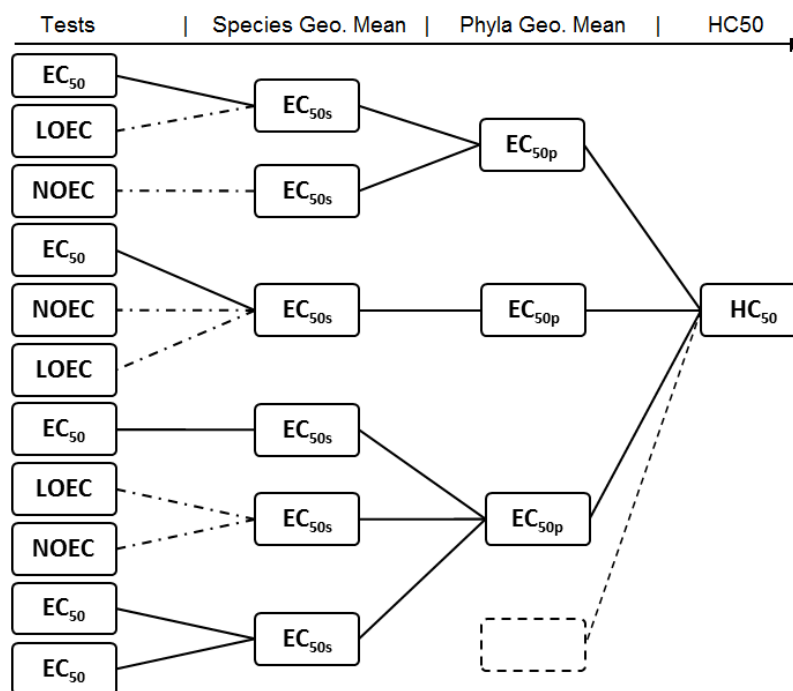


Figure 1: Principle of the A.M.I method

3.2 HC₅ (Hazardous Concentration for 5% of species)

The calculation of HC₅ and its confidence interval 95% are based on the Aldenberg review (2000) or on US-EPA method [4][5]. AiiDA Web platform allows the calculation of the HC₅ and its confidence interval for phyla or species with these two different methods and automatically draw graphs for comparison.

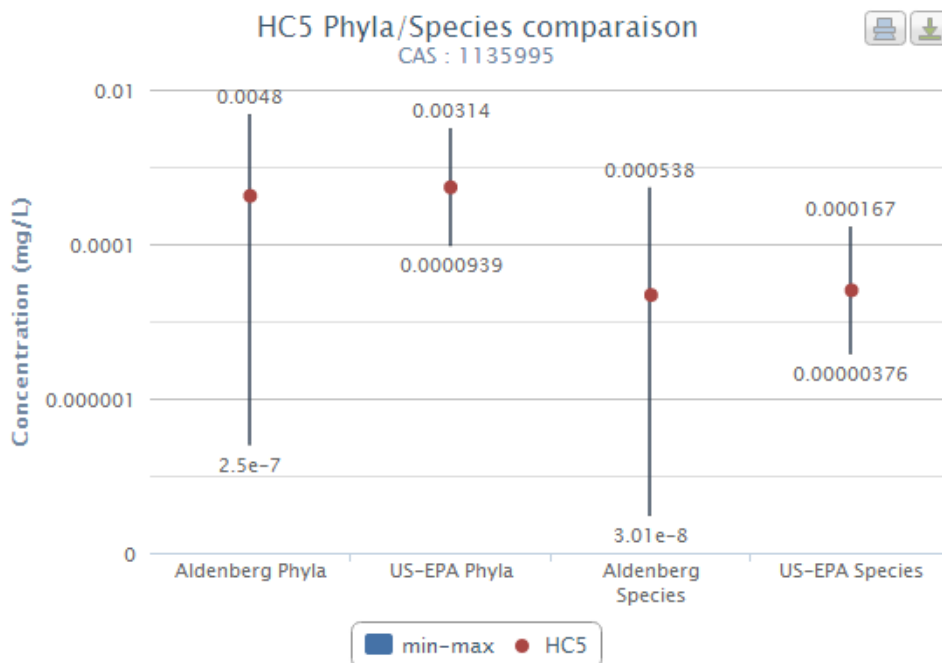


Figure 2: HC₅ of Dichlorodiphenylstannane, source AiiDA platform

3.3 PNEC (Predicted No Effect Concentration)

The calculation of PNEC and its assessment factor are based on Technical Guidance Document (TGD 2003) [6].

4. KEY FEATURES AND CONCLUSION

The AiiDA Web platform includes 500 000 ecotoxicity tests on more than 3600 species and belonging to 30 phyla. 7500 molecules with their 95% confidence interval are available from which 5400 are covered with data on 3 phyla or more. The platform provides 12.000 SSD and PSD representation (*Species/Phyla Sensitivity Distribution*).

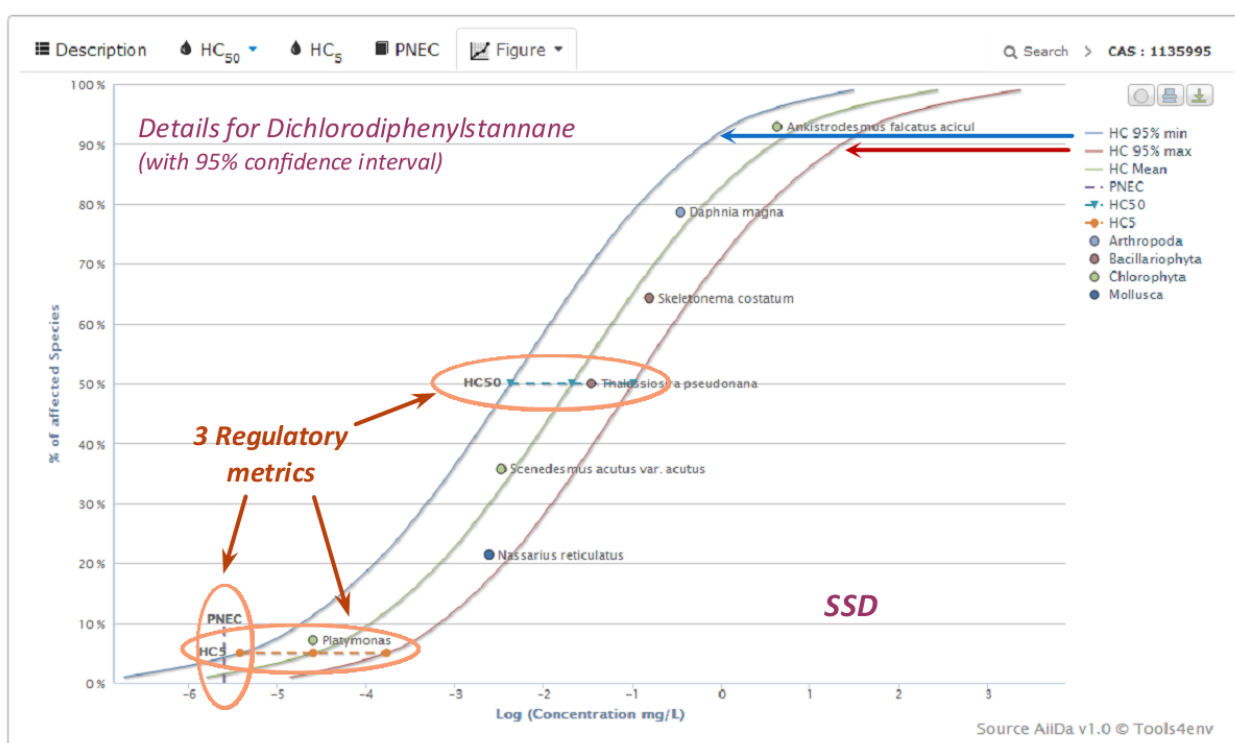


Figure 3: SSD representation for Dichlorodiphenylstannane, source AiiDA platform

The AiiDA platform allows comparing the toxicity of these different molecules. All data are fully traceable, this traceability is of main importance for Ecodesign by allowing the user to analyse each endpoint. In the future, this community platform database will be completed by each user who can suggest improvements.

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AIIDA: BASE DE DONNEES EN LIGNE POUR LE PARTAGE ET L'UTILISATION DES DONNEES ECOTOXICOLOGIQUES

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Résumé

Les nouvelles réglementations environnementales telles que REACH ou l'affichage environnemental nécessitent d'avoir une vision du profil environnemental des substances chimiques ou des produits commercialisés. Bien que d'énormes efforts aient été entrepris depuis 30 ans pour effectuer des tests d'écotoxicité sur des milliers de substances, il est encore long et complexe pour les scientifiques d'obtenir une perception claire de l'impact ou du risque potentiel d'une substance chimique.

Le manque et la difficulté d'accès aux données écotoxicologiques ainsi que la complexité de mise en œuvre des calculs et des méthodes rendent l'utilisation et la représentativité écologique des indicateurs d'écotoxicité aquatique difficilement exploitable. Les grandes entreprises et plus particulièrement les petites et moyennes entreprises (PME) manquent de temps et de compétence en interne pour réaliser ce genre d'étude.

Pour remédier à cette problématique, l'outil AiiDA (*Aquatic Impact Indicators DAtabase*) met à disposition plus de 500 000 tests écotoxicologiques uniques et référencés sur plus de 3600 espèces et 30 phyla. Cette base de données globale est utilisée pour calculer automatiquement les différents indicateurs d'écotoxicité aquatique ainsi que leurs incertitudes en suivant les Technical Guidance Document (TGD) officiels. AiiDA permet de couvrir 7500 molécules dont 5400 avec une représentativité écologique de 3 phyla ou plus.

Les indicateurs regroupés dans AiiDA sont :

- HC_{50} (*Hazardous Concentration 50%*) : calculée à l'aide de la Méthode AMI (*Assessment of Mean Impact*) pour plus de 10 000 HC_{50} chroniques et aiguës.
- HC_5 et $HC_{5-95\%}$ (*Hazardous Concentration 5%*) : calculée à l'aide de la méthode d'Aldenberg (2000) ou de la méthode d'extrapolation SSD (*Species Sensitivity Distribution*) de l'US-EPA (2005).
- PNEC (*Predicted no-effect Concentration*) : calculée selon les recommandations du Technical Guidance Document on Risk Assessment (EU, 2003).

Les valeurs ainsi obtenues sont mises à disposition à travers une plateforme interactive consultable via Internet qui permet de maintenir la traçabilité des calculs et de remonter jusqu'à l'ensemble des tests sources utilisés. Cette traçabilité, jusqu'à lors inexistante, est un atout majeur dans le cadre de l'éco-conception et permet une véritable cohérence des indicateurs. La plateforme permet également de tracer les courbes SSD et PSD (*Phyla Sensitivity Distribution*) des différentes molécules et de comparer leurs toxicités entre elles.

Keywords: Écotoxicologie, Base de données, Indicateurs d'impact aquatique, Traçabilité, SSD, Plateforme Web