Data availability and IT tools for chemicals management

Green Chemistry Change Manager Course

17th September 2024

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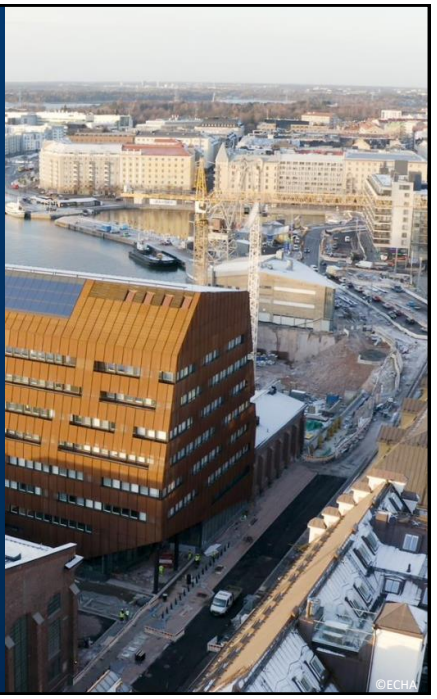

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- → IUCLID
  - IUCLID data tools
- → Making data available
  - ECHA CHEM
  - Data available for download
  - eChemportal
- → Chesar
- → OECD QSAR Toolbox

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What is IUCLID?

International Uniform ChemicaL Information Database

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IUCLID 6

- A software application used to record, store, maintain and exchange data on intrinsic and hazard properties of chemical substances.
  - Company information
  - Substance identity, including composition, Classification (GHS and CLP) and PBT assessment.
  - Use and Exposure, Hazard information, Possibility to attach documents
- OECD project, using OECD harmonised templates as the main structure
  - Hazard templates are based on OECD test guidelines, but also fit for other ways of information generation (e.g. QSAR, read-across)
- Configurable for specific needs
- Main repository to capture and exchange data on chemicals, with possibility to connect to other systems

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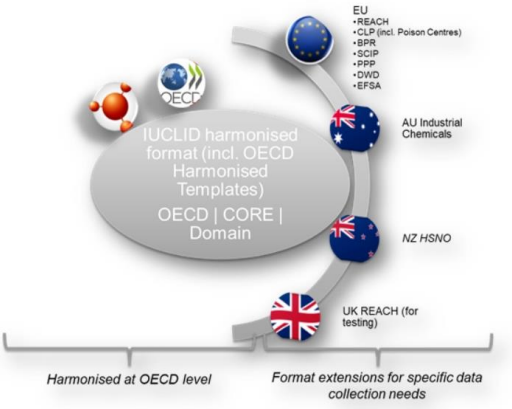
IUCLID 6 format

OECD contains the set of documents harmonised at the OECD level to report studies done on chemicals to determine their properties or effects on human health and the environment.

CORE (IUCLID) contains the main documents of IUCLID such as the substance identification, the classification and labelling information or the endpoint summaries.

DOMAIN, contains the main entities of the IUCLID application. It is a mandatory module containing all entities used in IUCLID.

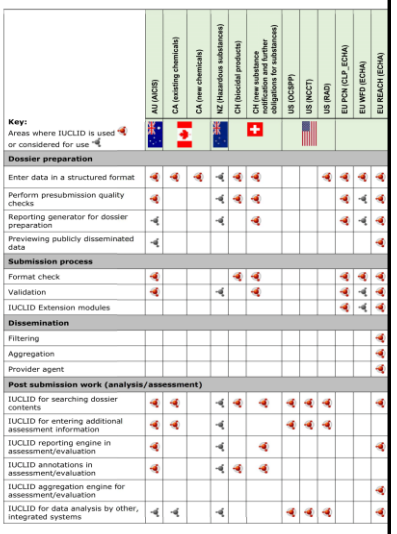
e.g. legal entity: company information



More information:
https://iuclid6.echa.europa.eu/project-iuclid-6
https://iuclid6.echa.europa.eu/format

Who is using IUCLID?

- **European Union and its entities:** The main users are ECHA, the Departments and Executive agencies, the Joint Research Centres, Member States and industry.
- **Switzerland (authority and companies):** notifications new chemicals and database existing chemicals
- **Türkiye**: the new chemicals regulation makes the use of IUCLID mandatory (industry and authority)
- **Canada:** central database for their assessment work (existing chemicals), discussions on acceptance of new chemicals on-going
- **Japan**: has used IUCLID in support to their programme.
- **New Zealand:** used as hazardous substance database of the New Zealand EPA
- **US Environmental Protection OPPC/OPPT and the US Office of Research and Development (ORD):** have implemented IUCLID as a database for non-submission information on chemicals.
- **Taiwan** and **South Korea:** accept IUCLID files, and their systems are IUCLID compatible
- **Australia**: uses IUCLID and is making their own configurations



IUCLID data tools

IUCLID data tools

Data Uploader

- Supports the transformation of data into IUCLID format.
- Useful for conversion of legacy toxicity data into harmonised templates.
- Developed as a KNIME Analytics Platform plug-in.

Data Extractor

- Advanced tool that extracts data from IUCLID in accordance with a set of user-defined rules.
- Own web-based user interface modelled on the IUCLID data structure.
- MS Windows and Linux packages available.

Text Analytics

- Search engine for IUCLID data and attachments.
- Searches can be carried out on both structured data such as picklists and dates, and on unstructured data such as free text fields and attachments.
- Runs on MS windows and Oracle database or PostgreSQL

Making data available

IUCLID 6

ECHACHEM
ECHA CHEMICALS DATABASE

IUCLID data available for download

eChemPortal
https://www.echemportal.org/echemportal/

QSAR Toolbox
Freely available at qsartoolbox.org

ECHA chem

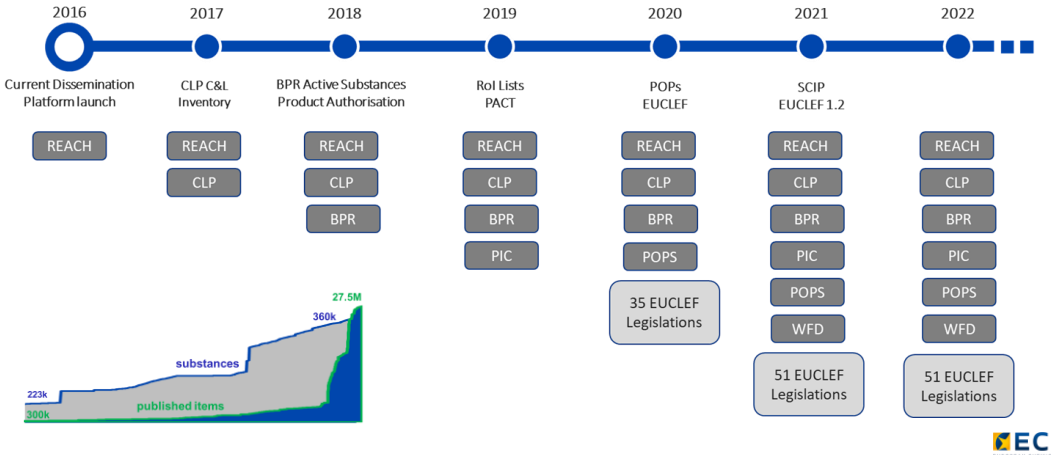
ECHA's data availability activities

- Legislation sets out explicit obligations for services and agencies to make data publicly available
- For ECHA, obligations included in the various chemicals regulations and directives allocated to it

REACH CLP BPR PIC POP WFD DWFL

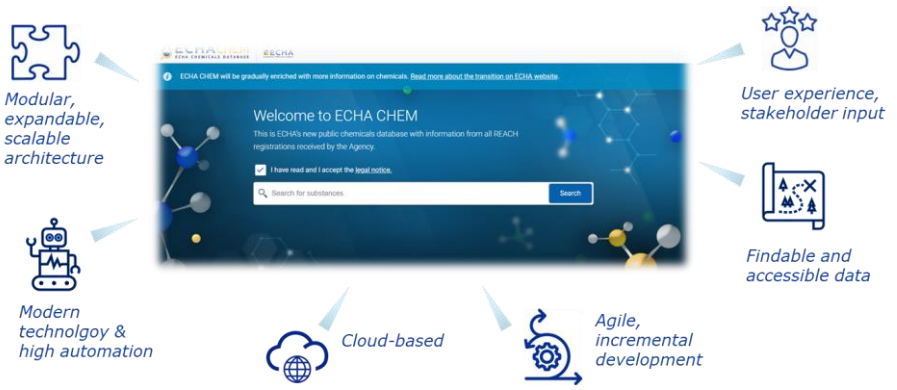
- Since 2016, ECHA has operated its current dissemination platform making available information on chemicals and regulatory work
- As of 2024, information gradually moved to new data availability system ECHA CHEM

ECHA's dissemination system 2016-2023



2024: New data availability system

https://chem.echa.europa.eu



Gradual transfer of data to ECHA CHEM

→ **Jan 2024: REACH registrations**
- substance identification, uses, properties and hazards

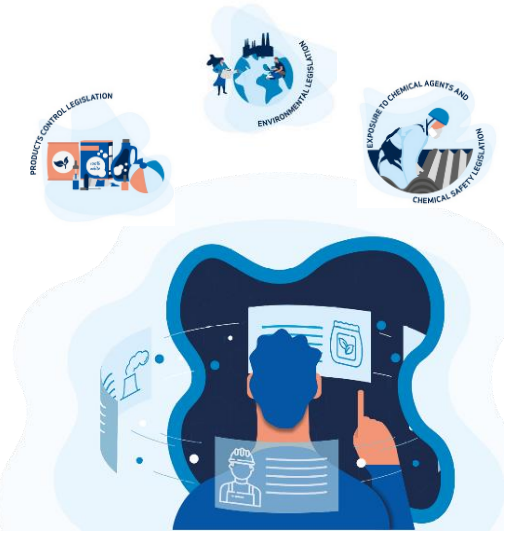
→ **Dec 2024: revamped C&L inventory**
- EU harmonised and company-notified classification and labelling of subtances

→ **Dec 2024: Overview of regulatory processes and their legal outcomes**
- REACH restriction, dossier evaluation, substance evaluation; CLP harmonised classification and labelling
- Restriction list, Authorisation list, Candidate list, List of POPs

→ **2025 – 2026: more data sources and features**
- REACH AfA, REACH CoRAP, DWD, BPR, PIC, Batteries

EU Chemicals legislation finder - EUCLEF

- → Search engine for regulatory information on chemicals
- → Shows how substances are being regulated in the EU and what legal obligations they have
- → Covers 51 pieces of chemicals legislation outside of ECHA's mandate
- → https://echa.europa.eu/legislation-finder



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IUCLID data available for download

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ECHA facilitates access to non-confidential data in IUCLID format

- Development of predictive computational models
- Facilitate correlation and concordance analyses
- Support the development of safety data sheets and classification and labelling of chemicals

ECHA facilitates access to non-confidential data in IUCLID format

REACH study results
Data submitted under REACH registrations for ~ 23 000 substances with studies related to physical-chemical properties, environmental fate and pathways, and ecotoxicology and toxicological information.

US FDA IUCLID dataset
Data on 348 approved pharmaceuticals. Pre-clinical animal data: repeat-dose, carcinogenicity, developmental and reproductive toxicity. And clinical human data. An ontology was also developed.

Industry data contribution project
Previously unpublished data on chemicals tested to develop medicines (94 substances and 517 studies). Project is led by the European Federation of Pharmaceutical Industries and Associations (EFPIA).

OECD eChemPortal

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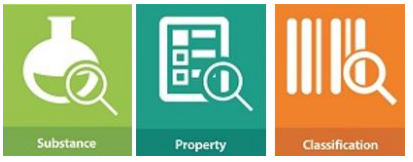
eChemPortal

The Global Portal to Information on Chemical Substances

- Free access to health and environmental effects information prepared for government chemical programs around the world, in a one-stop source
- Features over 800 000 substances records from 34 authorities and international organisation databases on chemicals, pesticides and biocides
- Provides three types of searches



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Chesar
(Chemical safety assessment tool)

Chesar tool

→ **Chesar** is ECHA's chemical safety assessment tool used by REACH registrants for their Chemical Safety Assessment (CSA) and Chemical Safety Reports (CSRs). It includes blocks of functionalities:

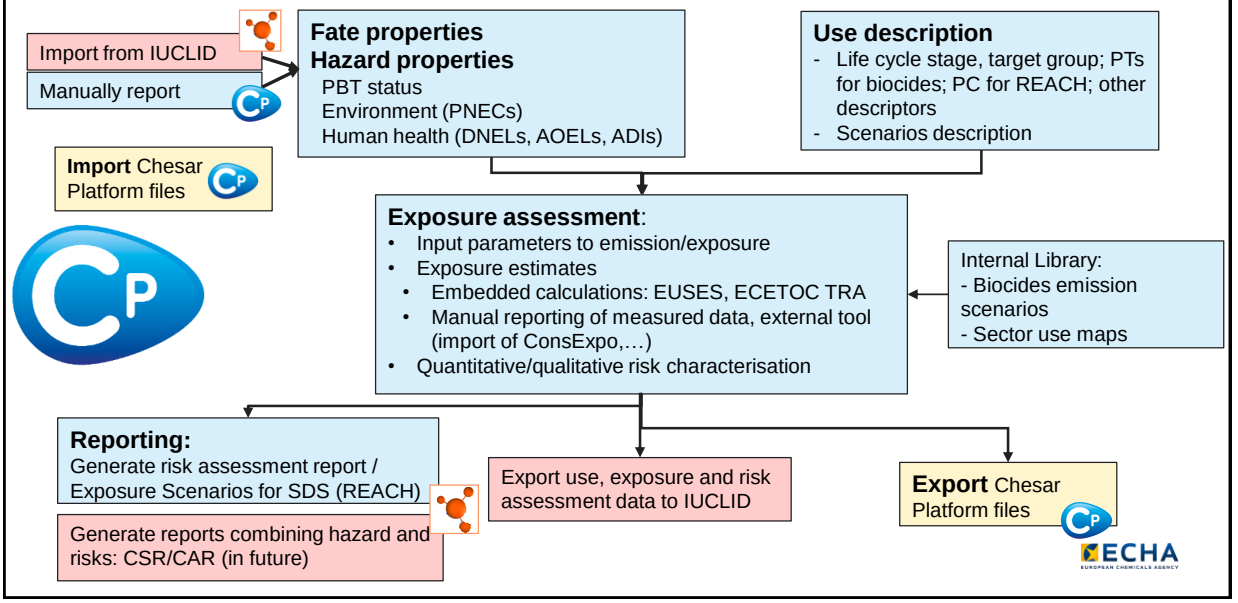
- (Retrieval from IUCLID of) substance data including hazard characterisation
- Use description
- Exposure assessment and risk characterisation; three exposure estimation models embedded
  - Worker, Consumer (ECETOC TRA)
  - Environment (R.16 release module + EUSES for Fate and distribution)
- Generation of CSR and Exposure Scenarios (ES) / Safety Data Sheets (SDS)

Future Chesar Platform

→ Chesar Platform will replace Chesar but can also be extended to other users and for other risk assessment context.

- Chesar Platform will implement the same principles as Chesar, as the aim is to have an assessment that is structured, harmonised, transparent, and easy to update.
- In a first step, it will integrate the **EUSES** models for environmental assessment and will cover **Biocides** risk assessment for the environment.

Workflow in Chesar Platform



QSAR TOOLBOX

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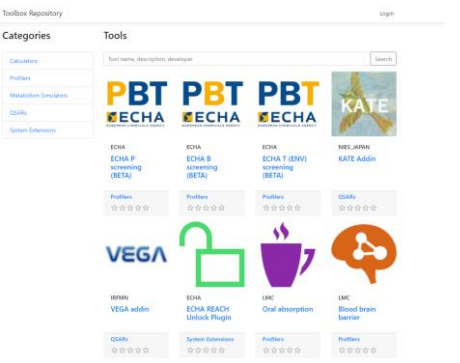
Governance

- ECHA and OECD co-own and co-develop the Toolbox
  - Work executed by LMC
- Activities under the OECD umbrella, core developments contracted by ECHA
  - Coordination group: OECD, ECHA, IT developer
  - Toolbox management group: Coordination group + experts from industry, authorities , NGOs
- Other partners also invest in the development
  - e.g. EPA contracted the link with their tool ONCOLOGIC and Japan developed a plug-in for their QSAR tool KATE
- Now third parties can make their own extensions (e.g. profilers, QSAR models) available through the TB repository.



QSAR TOOLBOX

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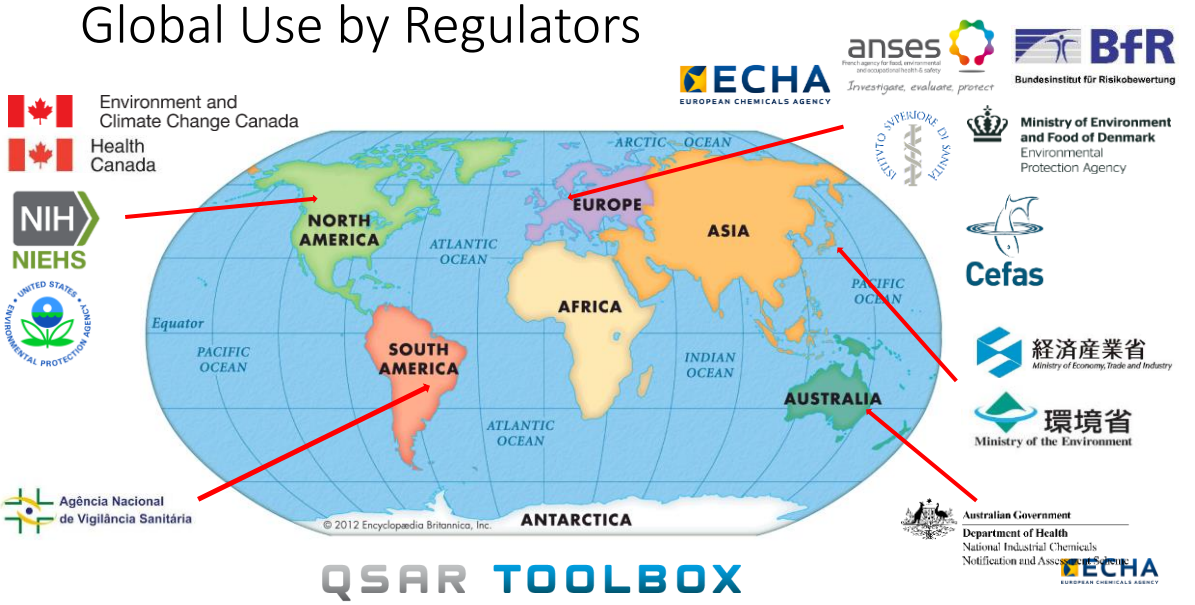
Global Use by Regulators



QSAR TOOLBOX

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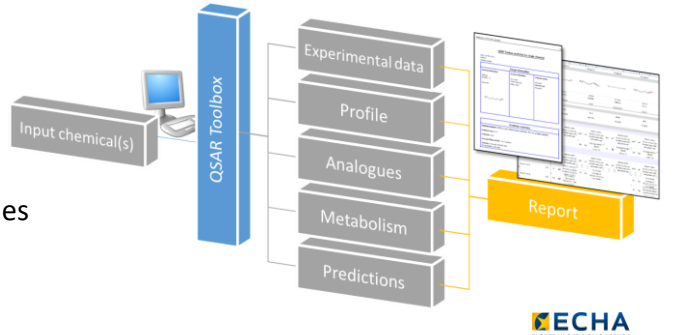
QSAR TOOLBOX

More than QSAR predictions

The QSAR Toolbox is a free software application that supports (eco)toxicologists in performing reproducible and transparent chemical hazard assessment using **non-animal methods**.

Key functionalities:

- retrieve experimental data
- profiling properties of chemical
- simulate metabolism
- identify analogues and build categories
- predict properties



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Experimental data

QSAR TOOLBOX

No need to perform new experimental studies if the information is already (publicly) available.

Toolbox searches **experimental data** on chemicals from 59 databases, including 100 000 chemicals and over 3 million data points.

Experimental data from analogues can also be used for read-across predictions.

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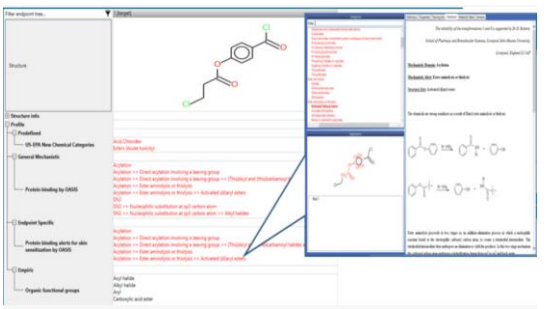
Profiling

QSAR TOOLBOX

Structural profilers support the identification of structurally similar substances.

Mechanistic profilers provide an understanding of the mode of action, which is key to predict the activity of substances or to form mechanistically sound categories.



The results of the profilers in the Toolbox, include descriptions and references to scientific papers to explain the outcome.

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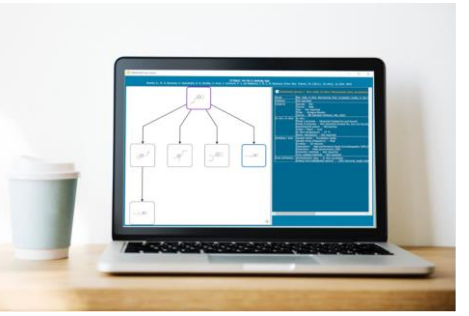
Metabolism

QSAR TOOLBOX

Metabolism influences the activity of substances in many cases. It is important to take it into account when making predictions of forming categories.

Results from 5 experimental metabolic databases and 11 metabolic simulators can be taken into account when assessing a single substance or categories.



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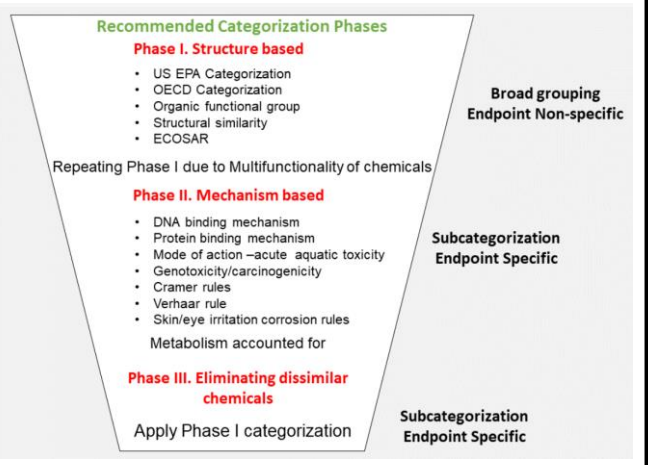
Analogues and categories

QSAR TOOLBOX

Data from analogues can be used to predict the property of a target substance using read-across or trend-analysis.

Toolbox can take into account structural, mechanistic and metabolic aspects to find toxicologically relevant analogues with data on the property of interest.



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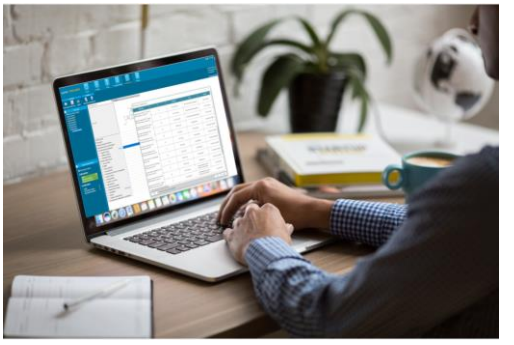
Predict properties

QSAR TOOLBOX

Toolbox can also predict properties by using existing QSAR models, which do not require the (manual) identification of analogues.

Examples of external QSARs included in the Toolbox are:

- EPISuite models by US EPA
- Danish QSAR Database predictions



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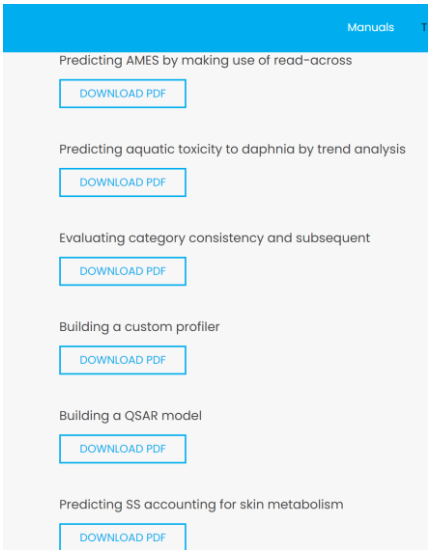
Additional resources

→ Complete Toolbox training ~5 days; today 3 hours. We cannot show everything…

→ Tutorial for specific functionalities:
https://qsartoolbox.org/support/#tutorials

→ Contact the Toolbox Helpdesk for technical questions at qsartoolbox.org



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Final remarks

- → IUCLID is the basis for sharing data on chemicals intrinsic properties, contributing to data harmonisation, interoperability and mutual acceptance worldwide
- → There are several freely available tools to support the manipulation, use and analysis of data in IUCLID format
- → ECHA facilitates the access to non-confidential data to support the development of predictive models and classification of chemicals
- → There will be a gradual transfer of data to ECHA CHEM and deployment of new features
- → QSAR Toolbox is an integrated platform to support regulatory hazard assesment and use of alternative methods

Thank you

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