ECHA
EUROPEAN CHEMICALS AGENCY

The NEW OECD QSAR Toolbox version 4.0

The new OECD QSAR Toolbox v.4 simplifies the correct use of non-test methods. Users with a sufficient understanding of (eco)toxicology can now focus on the content while being guided in their choices by the software

More user friendly

Toolbox v.4 highlights with colours the profilers, metabolic simulators and databases that are relevant for the endpoint you are working on.

Relevant profilers

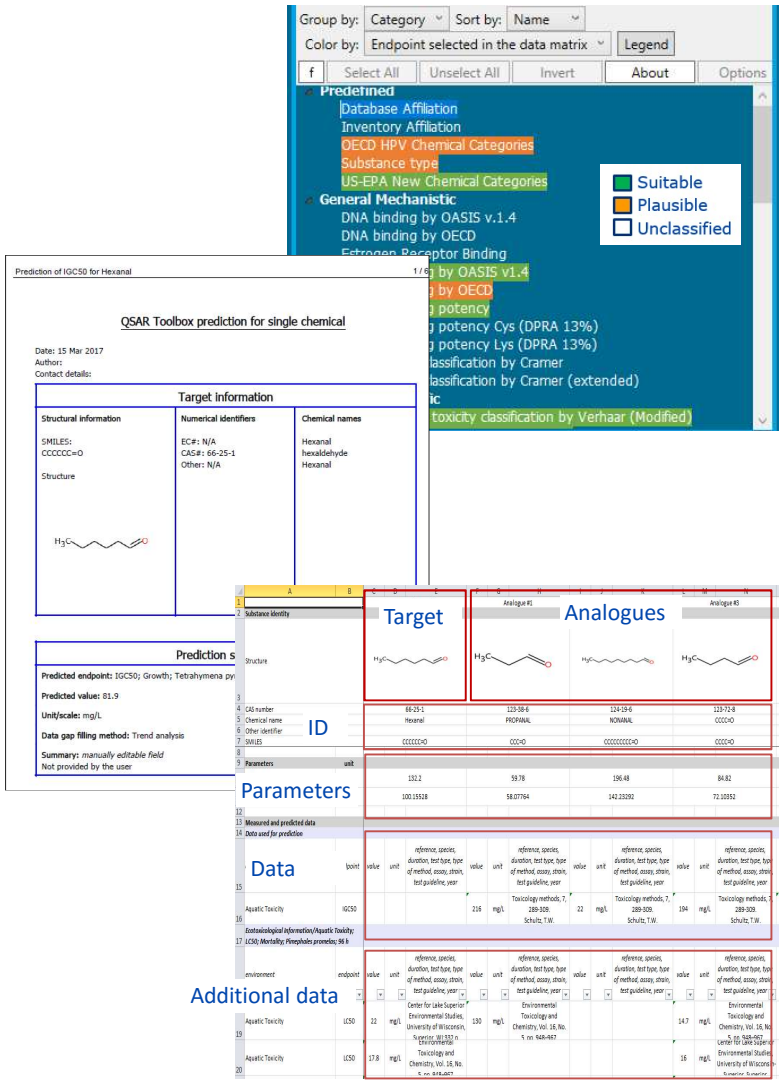
Profilers are considered "Suitable" and are coloured in green if they have been developed using data for the endpoint of interest. "Plausible" profilers (in orange) are also somehow related to the endpoint of interest (e.g. the functional groups profilers, which are useful for finding structural analogues).

Relevant databases

Databases containing data for the endpoint of interest are coloured in green.

Relevant metabolic and transformation simulators

Metabolic and transformation simulators related to the endpoint of interest are coloured with the same logic of the profilers.



Improved reports

Reports have been completely revised to make the most important information readily accessible and understandable. The possibility to export the data matrix to Excel simplifies the preparation of read-across and category documentations.

Prediction report

Target information and prediction summary are all available in the first page of the report. Details are described from the second page onwards, starting from the most relevant ones.

Data matrix in Excel format

The preparation of the data matrix listing structures and properties of the category members has always been a time consuming operation. Now, you can automatically generate and customise such a matrix for any prediction run with the Toolbox.

Guided predictions

The automated and standardised workflows guide you in the prediction of selected endpoints straight after the input. In Toolbox v 4.0 these workflows are available for skin sensitisation and aquatic short-term toxicity.

Automated workflow: input the chemical and obtain a prediction

Input the chemical and select the workflow for the endpoint you want to predict.

Standardised workflow: input the chemical and be guided in each step

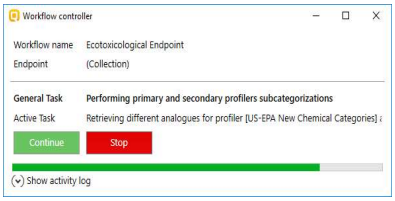
You can choose among the options proposed by the Toolbox.

Manual prediction: as in Toolbox v.3, it is all up to you

If you are familiar with the previous version, you can still use the Toolbox in the classical way. Nevertheless, you can now select an endpoint and activate colour coding for getting help in the selection of databases and profilers.

How to run the new workflows?

1. Input your target
2. Go to data gap filling
3. Select automated or standardised workflow
4. Follow the wizard



And much more…

www.qsartoolbox.org

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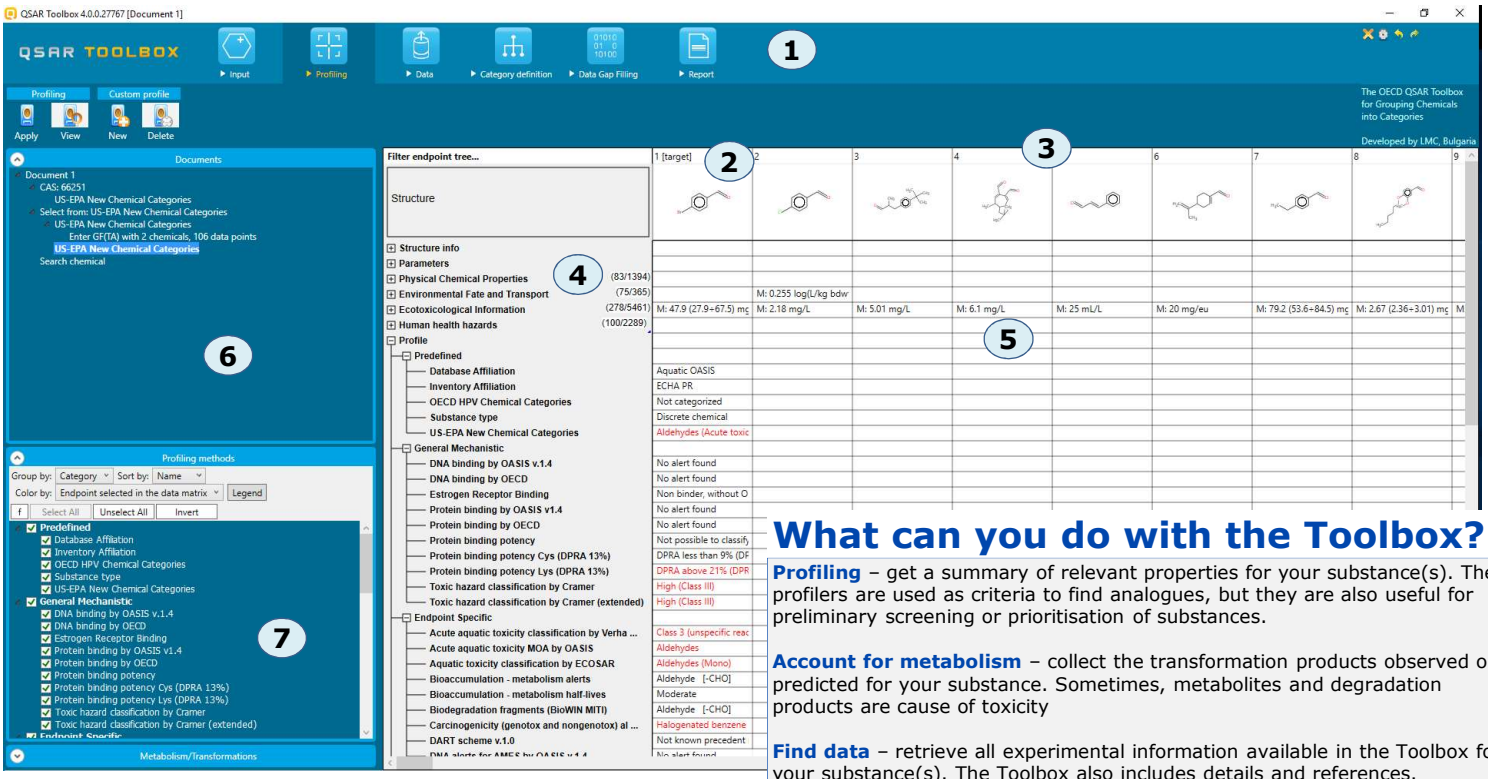
QSAR TOOLBOX

What is the OECD QSAR Toolbox?

The QSAR Toolbox is a decision-support tool to find experimental data for chemicals, group substances into categories based on chemical and mechanistic similarity, and predict substance properties without testing



Key elements:

1. Modules
2. Target chemical
3. Analogues
4. Endpoint tree
5. Data Matrix
6. Document tree
7. Profilers

What can you do with the Toolbox?

Profiling – get a summary of relevant properties for your substance(s). The profilers are used as criteria to find analogues, but they are also useful for preliminary screening or prioritisation of substances.

Account for metabolism – collect the transformation products observed or predicted for your substance. Sometimes, metabolites and degradation products are cause of toxicity

Find data – retrieve all experimental information available in the Toolbox for your substance(s). The Toolbox also includes details and references.

Grouping - find analogues for your substance and the available experimental data for them. It is useful for identifying analogues and data gaps

Predict – fill a data gap for your substance by using trend analysis, read-across and existing QSAR models

Over two million data points!

The Toolbox gathers a large number of publicly available databases

Database Content	Chemicals	Data points
Physical Chemical	45 238	177 258
Environmental Fate and Transport	9 446	97 469
Ecotoxicological	17 649	856 473
Human Health	30 447	912 687
Total number	**79 204**	**2 043 887**

The terminology

Definitions in the QSAR Toolbox context:

NON-TEST METHODS – methods that do not require performing a new experiment (QSAR, read-across, trend analysis) to fill a data gap

TARGET CHEMICAL - chemical of interest

MODULE – the Toolbox consists of six modules, each of them performing some specific actions useful for data gap filling

PROFILER - algorithm (rule set) for the identification of specific features of chemicals. Several types of profilers are available, such as structural (e.g. organic functional groups) and mechanistic (e.g. Protein binding by OECD) ones

CATEGORY – "group" of substances. Usually it consists of a target chemical and its analogues gathered according to the selected profilers (e.g. same functional groups)

ENDPOINT TREE – The Toolbox organises endpoints in a branched scheme, from a general level (Physical Chemical properties, Environmental Fate and transport, Ecotoxicology, Human health hazard) to a more specifc one (e.g. EC3 in LLNA test under Human health hazard-Skin sensitization). The levels can be re-arranged by the user

DATA MATRIX – Table reporting substances, data and profiler outcomes. The first row shows the structures. Each chemical defines a column

WORKFLOW – the use, in combination, of the different modules (e.g. prediction workflow: from input to report)