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News Alert

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QSAR Toolbox version 3.0 now available

The new generation of the QSAR Toolbox is a more complete tool to predict reliably properties of chemicals.

Helsinki, 31 October 2012 - The QSAR Toolbox helps companies and authorities to use Quantitative Structure-Activity Relationship ((Q)SAR) methodologies to group chemicals into categories and to fill data gaps by read-across, trend analysis in order to assess the (eco)toxicity hazards of chemicals to be registered under REACH. This helps to reduce costs and unnecessary testing on vertebrate animals.

The QSAR Toolbox 3.0 contains many new features, of which the most important ones are:

- Inclusion of additional data sources including study results from the REACH dissemination website;
- IUCLID 5.4 compatibility;
- Quantitative mixtures toxicity prediction;
- Tautomeric set prediction and metabolism simulator;
- Implementation of Adverse Outcome Pathways (AOPs) related to skin sensitisation supplemented by three new databases containing AOPs data for skin sensitisation.

In addition, the QSAR Toolbox contains improved search functionalities, 22 new mechanistically and endpoint specific profiling schemes and an enhanced reporting engine to handle mixtures, tautomers and metabolites.

With the QSAR Toolbox, the user can:

- Identify analogues[1] for a chemical, retrieve experimental results available for those analogues and fill data gaps by read-across or trend analysis;
- Categorise large inventories of chemicals according to mechanisms or modes of action;
- Fill data gaps for any chemical by using the library of (Q)SAR models;
- Evaluate the robustness of a potential analogue for read-across;
- Evaluate the appropriateness of a (Q)SAR model for filling a data gap for a particular target chemical;
- Build (Q)SAR models;
- Predict metabolites or generate tautomers for the target chemical.

Version 3.0 is a final release of a four-year collaborative project between the OECD and ECHA. It is now available for downloading.

[1] An analogue specifies a chemical for which read-across may be applied (see also the REACH guidance document on QSARs and grouping of chemicals).

Further information

Free download and supporting material:

QSAR Toolbox
http://www.qsartoolbox.org/

Guidance on information requirements and chemical safety assessment
Chapter R.6: QSARs and grouping of chemicals
http://echa.europa.eu/documents/10162/13632/information_requirements_r6_en.pdf