

ECHA/NA/12/40

## New version of the QSAR Toolbox to be introduced in a workshop in November

The European Chemicals Agency (ECHA), in collaboration with the OECD, invites industry users to a workshop introducing version 3.0 of the QSAR Toolbox on 20 November in Helsinki. Companies are asked to express their interest in participating to the event by 17 October.

**Helsinki, 13 September 2012** - The aim of the workshop is to present the latest version of the OECD QSAR Toolbox. Emphasis will be put on how registrants can use the OECD QSAR Toolbox version 3.0 for filling gaps in (eco)toxicity data to fulfil their information requirements. ECHA and the OECD also wish to collect feedback from industry on the use of the Toolbox and identify needs for implementing additional features in the tool and for providing other kind of support.

Version 3.0 will contain many new features, hence a live demo will be an integral part of the event.

A maximum of **30 participants** is foreseen for this workshop and every effort will be made to have a representative audience from different industry sectors.

We ask you to express your interest in participating to the workshop by filling in the webform no later than the **17 October 2012**.

New features of the QSAR Toolbox 3.0 are:

- Inclusion of additional data sources
- Advanced search engine
- 22 new mechanistically and endpoint specific profiling schemes
- Quantitative mixtures toxicity prediction
- Tautomeric set prediction
- Prediction accounting for metabolism

- Implementation of Adverse Outcome Pathways (AOPs) related to skin sensitisation supplemented by three new databases containing AOPs data for skin sensitisation.
- Four new simulators (autoxidation and hydrolysis)
- Enhanced reporting engine to handle mixtures, tautomers and metabolites

### **What is the QSAR Toolbox ?**

The QSAR Toolbox is an OECD software tool developed for filling data gaps in (eco)toxicity data needed for assessing the hazards of chemicals and for grouping chemicals into categories. It can also be used for the development of integrated testing strategies. Importantly, REACH registrants can use the QSAR Toolbox as a tool to generate an alternative method to animal testing to fulfil their information requirements.

### **Further information**

- Event page  
[https://staging-production.echa.europa.eu/view-article/-/journal\\_content/67f24471-8cd5-4809-9ff1-bfa9c3141bf5](https://staging-production.echa.europa.eu/view-article/-/journal_content/67f24471-8cd5-4809-9ff1-bfa9c3141bf5)
- QSAR Toolbox  
<http://www.qsartoolbox.org>
- For specific questions, please contact:  
[qsar-toolbox@echa.europa.eu](mailto:qsar-toolbox@echa.europa.eu)