**Dr. Andrea Gissi - ECHA**



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**Title of the presentation:**   
The OECD QSAR Toolbox – a software to support chemical hazard assessment

**Abstract:**   
The Toolbox is a free software application that supports reproducible and transparent chemical hazard assessment. As a freely available computational tool, it promotes the use of non-test methods and minimizes unnecessary animal testing without reducing the safety of human health and environment. It is intended to be used by governments, chemical industry and other stakeholders.

Using the Toolbox, the users can:

* Find experimental data - With over 2 500 000 data points for almost 100 000 structures from around 60 databases, the Toolbox is an invaluable tool to find publicly available experimental data including details on the experimental test
* Find analogues, build and assess categories - the Toolbox can be used to find data-rich analogues based on the knowledge for structural characteristics (alerts from profilers) and chemical properties. The Toolbox can be also used to assess the consistency of a category, the starting point for read-across justification.
* Account for metabolism - The assessment of metabolism and transformation products is a crucial step in chemical risk assessment. The Toolbox can be used to explore experimental metabolic maps or to simulate the metabolism and degradation of chemical substances in different organisms and conditions.
* Fill data gaps from analogues – the toxicity of a substance can be predicted by using data from analogues. Classical read-across or trend analysis can be used for this purpose. Furthermore, the Toolbox also includes external QSAR models.

The presentation will give an overview of the above functionalities.

**About the training:**   
During the practical session will be showed functionalities mentioned in the presentation using the Toolbox and the participants can try to run them on their computers if they have the Toolbox installed.

**Short bio:**   
Dr Gissi has been working in the computational assessment unit of the European Chemicals Agency since 2013. His main activities include the assessment of the reliability of QSAR studies submitted in REACH registration and the project and product management of the OECD QSAR Toolbox. Dr Gissi has a PhD in computational ecotoxicology and a master degree in medicinal chemistry.

**Additional materials for participants:**

* ***QSAR Toolbox for download:*** https://qsartoolbox.org/download
* [***Manuals***](https://qsartoolbox.org/download/)*:* <https://qsartoolbox.org/support>
* ***Additional information on QSAR Toolbox***: <https://www.oecd.org/chemicalsafety/risk-assessment/oecd-qsar-toolbox.htm>