

Science Newsflash:
New ECETOC manuscript addresses the relationship between activity and toxicity for non-polar narcotic chemicals

Brussels, October 2015

In a Nutshell:

The relationship between the toxicity of narcotic chemicals and the octanol water partition coefficient (KOW) has been widely explored. An alternative but closely related property can be used to directly frame toxicity within the concept of phase equilibrium thermodynamics. This property, termed chemical activity, is inversely proportional to solubility, proportional to toxicity and should be applicable for the prediction of effects in aquatic species.

This manuscript employs an extensive set of existing data, and provides a proof of concept for the relationship between chemical activity and toxicity for narcotic chemicals. The authors used published methodology and freely available software to classify the data according to Mode of Action 1 (MOA). The analysis of MOA 1 (non-polar narcosis or baseline toxicity) substances shows promise as an alternative to KOW-based predictions of effect.

This Open Access paper has been published in *Environmental Science & Technology*:

Thomas P, Dawick J, Lampi M, Lemaire P, Presow S, van Egmond R, Arnot JA, Mackay D, Mayer P, Galay Burgos M. 2015

Application of the Activity Framework for Assessing Aquatic Ecotoxicology Data for Organic Chemicals
Environ. Sci. Technol 49(20):12289-12296 (Open Access) DOI: 10.1021/acs.est.5b02873

ECETOC Direct Link to the web page of the Article: <http://bit.ly/ecetoc-art2015-thomas-et-al>

Supporting information for this manuscript can be found in the ECETOC Technical Report 120: *Activity-Based Relationships for Aquatic Ecotoxicology Data: Use of the Activity Approach to Strengthen MoA Predictions*. Published in December 2013 by the same ECETOC Task Force, TR120 can be downloaded from the ECETOC website and via the following direct link: <http://bit.ly/ecetoc-tr120-pdf>

The article has been published in the run up to an ECETOC / RIFM Workshop on *Defining the role of chemical activity in environmental risk assessment within the context of mode of action: Practical guidance and advice*, to be held 29-30 October 2015 back-to-back with the SETAC North America meeting in Salt Lake City. The Workshop was a recommendation of ECETOC Technical Report no. 120 and follows the work of Cefic LRI project [ECO16](#). It will assess the applicability of using chemical activity in the interpretation of effects data within the context of environmental risk assessment.

Abstract:

Toxicological research in the 1930s gave the first indications of the link between narcotic toxicity and the chemical activity of organic chemicals. More recently, chemical activity has been proposed as a novel

exposure parameter that describes the fraction of saturation and that quantifies the potential for partitioning and diffusive uptake. In the present study, more than 2000 acute and chronic algal, aquatic invertebrates and fish toxicity data, as well as water solubility and melting point values, were collected from a series of sources. The data were critically reviewed and grouped by mode of action (MoA). We considered 660 toxicity data to be of acceptable quality. The 328 data which applied to the 72 substances identified as MoA 1 were then evaluated within the activity-toxicity framework: EC50 and LC50 values for all three taxa correlated generally well with (subcooled) liquid solubilities. Acute toxicity was typically exerted within the chemical activity range of 0.01 – 0.1, whereas chronic toxicity was exerted in the range of 0.001 – 0.01. These results confirm that chemical activity has the potential to contribute to the determination, interpretation and prediction of toxicity to aquatic organisms. It also has the potential to enhance regulation of organic chemicals by linking results from laboratory tests, monitoring and modelling programs. The framework can provide an additional line of evidence for assessing aquatic toxicity, for improving the design of toxicity tests, reducing animal usage and addressing chemical mixtures.



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Founded in 1978, ECETOC is an industry-funded, scientific expert not-for-profit think tank that enhances the quality of chemicals risk assessment so that chemicals management decisions are informed, reliable and science-based.

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