

[SC4] Applicability domain and confidence in predictions: Towards a more formal framework

Thierry Hanser¹, Barber Christopher¹, Guesne Sébastien¹,
Marchaland Jean-François¹, Werner Stéphane¹, Williams Richard¹

¹ *Lhasa Limited (UK)*

Applicability domain and confidence in an individual prediction are important aspects in QSAR modelling in general and key concerns when it comes to human safety assessment. Many approaches have been elaborated in order to estimate the validity and the confidence in a prediction; however there is no clearly unified definition of the concept of applicability domain and even less so a common framework for assessing the confidence in a prediction. In this presentation, we will explore a new methodology that aims to clarify and formalise the assessment of a prediction. This new framework relies on the separation of concerns into three independent and staged aspects of the concept of confidence: applicability domain, reliability domain and decidability domain. We hope that this new staged definition will provide the end user with a clear and easy to interpret information describing the confidence in a prediction and initiate a good will of convergence towards a common framework within the QSAR community¹.

Bibliography :

[1] SAR QSAR Environ Res. 2016; 27(11):893-909.