



BIN-06

Interspecies Quantitative Structure–Activity-Activity Relationships (QSAARs):

Development of a global model for predicting the acute toxicity

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Abstract

In silico modelling methods, such as Quantitative Structure-Activity Relationship (QSAR) modelling, are useful for estimating the toxicities. Quantitative Structure- Activity -Activity Relationships (QSAARs) is a hybrid method based on QSAR approach and interspecies modeling, which extrapolate data for one toxicity endpoint to those for another toxicity endpoint, can be used to determine the species-specific toxicity of a chemical.

This study is aimed to develop QSAAR and QSAR models for the acute toxicity data of a huge number of chemical compounds.

Keywords : QSAR, QSAAR, Interspecies, Toxicity.