

# Prediction of toxicological endpoints by QSAR modeling

Commonly used acronym: QSAR

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### SCOPE OF THE METHOD

The Method relates to	Animal health, Environment, Human health
The Method is situated in	Basic Research, Education and training, Regulatory use - Routine production, Translational - Applied Research
Type of method	In silico

### DESCRIPTION

### **Method keywords**

predictive modeling multivariate analyses in silico analysis molecular descriptors

## Scientific area keywords

Toxicology Ecotoxicology

## **Method description**

Quantitative Structure Activity Relationship modeling is generally used to construct models in which molecular descriptors of chemical compounds are used to predict endpoints/activities of interest. Commercial packages are available that can be implemented, but new models can be constructed if sufficient data are available.

### Lab equipment

No lab equipment is needed, the methodology aims to use existing data (*in vitro*, *in vivo*) to make predictive models.

#### Method status

Still in development History of use Published in peer reviewed journal

# PROS, CONS & FUTURE POTENTIAL

### **Advantages**

Depending on the strength of the developed models for a specific endpoint, animal experiments can be avoided and new chemicals (within the application domain) can be predicted for the specific endpoint.

# Challenges

Good quality and sufficiently large datasets (containing sufficient chemicals and well performed experiments/measurements) need to be available to start modeling efforts for new endpoints.

#### **Modifications**

Existing models can be improved by adding new experimental datasets.

# REFERENCES, ASSOCIATED DOCUMENTS AND OTHER INFORMATION

#### References

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