# 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 |
| **This method makes use of** | Animal derived cells / tissues / organs |

## 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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Verheyen GR, Van Deun K, Van Miert S. (2017) Testing the mutagenicity potential of chemicals. Journal of Genetics and Genome Research, 4:029. DOI:10.23937/2378-3648/1410029
Verheyen GR, Braeken E, Van Deun K, Van Miert S. (2017) Evaluation of in silico tools to predict the skin sensitisation potential of chemicals. SAR and QSAR in Environmental Research, 28: 59-73
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## Associated documents

## PARTNERS AND COLLABORATIONS

### Organisation

**Name of the organisation** Thomas More University of Applied Sciences

**Department** RADIUS

**Country** Belgium

**Geographical Area** Flemish Region

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