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

Tuenter E, Creylman J, Verheyen G, Pieters L, Van Miert S. (2019) Development of a classification model for the antigenotoxic activity of flavonoids. Bioorganic Chemistry 98. Doi: 10.1016/j.bioorg.2020.103705
Van Miert S, Verheyen GR, Creylman J. (2019) Mining a Nanoparticle Dataset, Compiled Within the MODENA-COST Action. International Journal of Quantitative Structure-Property Relationships Vol 4 (1): 1-17. DOI: 10.4018/IJQSPR.2019010101
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
Verheyen GR, Braeken E, Van Deun K, Van Miert S. (2017) Evaluation of existing (Q)SAR models for skin and eye irritation and corrosion to use for REACH registration. Toxicology Letters, 265: 47-52

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