

Lecture: computer assisted procedures

***In silico* estimation tools developed by the Joint Research Centre in support of chemicals legislation**

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To promote the availability of reliable computer-based estimation methods for the regulatory assessment of chemicals, the European Commission's Joint Research Centre (JRC) has developed a range of user-friendly software tools.

Toxtree predicts various kinds of toxic effect by applying decision tree approaches. The set of decision trees includes the Cramer classification scheme, the Verhaar scheme, the BfR rulebases for irritation and corrosion, and the Benigni-Bossa scheme for mutagenicity and carcinogenicity. Additional rulebases are under development.

Toxmatch generates quantitative measures of chemical similarity. These can be used to compare datasets and to calculate pairwise similarity between compounds. Consequently, Toxmatch can be used to compare model training and test sets, to facilitate the formation of chemical categories, and to support the application of chemical read-across.

DART (Decision Analysis by Ranking Techniques) was developed to make ranking methods available to scientific researchers. DART is designed to support the ranking of chemicals according to their environmental and toxicological concern and is based on the most recent ranking theories. Different kinds of order ranking methods, roughly classified as total and partial-order ranking methods, are implemented.

Finally, a web-based inventory of (Q)SAR models (the JRC QSAR Model Database) is under development, which will help to identify relevant (Q)SARs for use in the regulatory assessment of chemicals.

These tools can be downloaded (free of charge) from the following JRC website: <http://ecb.jrc.it/qsar/qsar-tools/>

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