Companies are given new tool to check for harmful chemical substances

November 23 2015

New database containing more than 600,000 chemical structures gives companies a unique opportunity to quickly get an overview of the harmful effects associated with substances they are considering using.

When a company wants to replace a harmful chemical substance in its production it is often a major challenge that possible alternatives have not been sufficiently tested for harmful effects. However, a new (Q)SAR database, which the National Food Institute, Technical University of Denmark, and the Danish Environmental Protection Agency are behind, now makes it possible to do a search on a chemical substance and quickly find out if there are indications that it has potential carcinogenic effects or other harmful health or environmental effects.

"When companies are able to more quickly get an indication as to whether the substances they want to use are harmful, they can save a lot of time and resources and they can avoid investing blindly. For example, a paint manufacturer can use the (Q)SAR database to choose the least harmful chemical substances when testing and developing a new product. This way it is easier for the industry to focus on the environment and health, and this will ultimately benefit consumers," Danish Minister for the Environment and Food Eva Kjer Hansen says.

The (Q)SAR predictions are based on advanced computer models which look at whether the chemical structure resembles other chemical substances that have been tested for example for endocrine disrupting,

allergic or carcinogenic effects. If a new chemical structure is sufficiently similar to that of a known harmful substance it is highly probable that the new substance is also harmful.

"This advanced expert system is the fruit of a long research effort here at the Technical University of Denmark. It has great application potential for innovative companies, authorities and others who wish to make chemical use safer," Director at the National Food Institute Christine Nellemann says.

Available to all companies

The (Q)SAR database which is made publically available to companies and others contains information about more than 600,000 chemical structures. Companies can easily do a search for a substance in the database and get an overview of the (Q)SAR predictions of a wide range of harmful effects.

"The chemical industry wants REACH to deliver on all its goals. (Q)SAR tools, such as the Danish (Q)SAR Database, will clearly contribute to this by increasing our knowledge on hazardous properties of substances put on the market and by allowing an early screening in the research and development phase," says Erwin Annys, Director REACH/Chemicals Policy at the European Chemical Industry Council.

The (Q)SAR database has been developed by a research group at the National Food Institute in cooperation with and with financial support from the Danish Ministry of Environment and Food (The Danish Chemicals Initiatives and Eco-Innovation Program) and the Nordic Council of Ministers.

The (Q)SAR database is available from today via (Q)SAR's website: qsar.food.dtu.dk.

FACTS ABOUT (Q)SAR

- (Q)SAR stands for (Quantitative) Structure–Activity Relationship
- The database includes computer calculations for the hazardous effects of more than 600,000 chemical structures
- The database is available to all companies, universities, research institutions and NGOs who want to use the information in their work on chemical safety
- The database give opportunities for companies to find less harmful alternatives
- Ultimately (Q)SAR could help reduce the number of tests on animals as it will be possible to target animal testing at properties that are already suspected of having harmful effects. (Q)SAR predictions can in some cases be used in conjunction with other information to replace animal testing
- Authorities can use (Q)SAR to target resources at substances which are most likely to be harmful. Consumers stand to benefit from this because as a result such substances will be identified more quickly and subjected to a thorough assessment before eventually being phased out of various products.

Provided by Technical University of Denmark