DTU Food
National Food Institute

New free online Danish (Q)SAR predictions database with >600,000 substances

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The Danish (Q)SAR Database was published in November 2015 and replaces the previous version from 2005.

Predictions are included from more than 200 (Q)SARs covering a wide range of hazardous properties relevant for human health and the environment such as acute toxicity to rat, mouse, fish, daphnia and algae, as well as many physical-chemical and environmental fate properties, skin irritation, sensitization, mutagenicity, cancer, reproductive toxicity including potential for endocrine disruption.

Commercial, free and DTU-developed models using CASE Ultra, Leadscope PDM, SciQSAR, ACD/Tox Suite and EPI Suite are included in the database. Battery calls based on models in three software systems are included where possible.

The database with its >600,000 substances, including ~72,000 REACH pre-registered substances, is one of the most comprehensive freely available (Q)SAR tools for substance evaluations and large-scale screenings.

It is developed by the National Food Institute, Technical University of Denmark, in cooperation and with financial support from the Danish Environmental Protection Agency and the Nordic Council of Ministers.

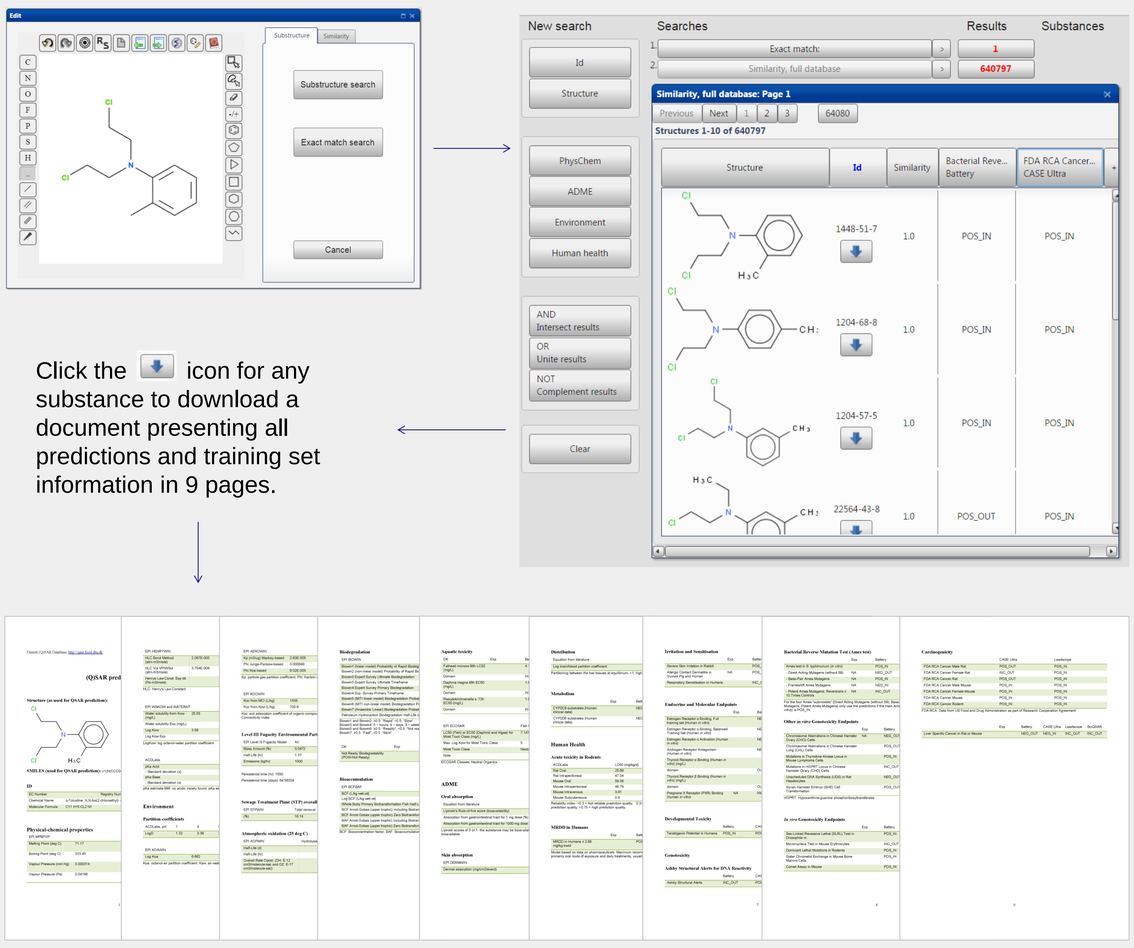
(Q)SAR predictions can be used in regulatory contexts for many types of chemical substances and their metabolites, e.g. REACH, the Biocidal Products Regulation, the Pesticides and Cosmetics Regulations, as well as the ICH M7 guideline for pharmaceutical impurities.

Besides replacing experimental tests, (Q)SARs can for example be used

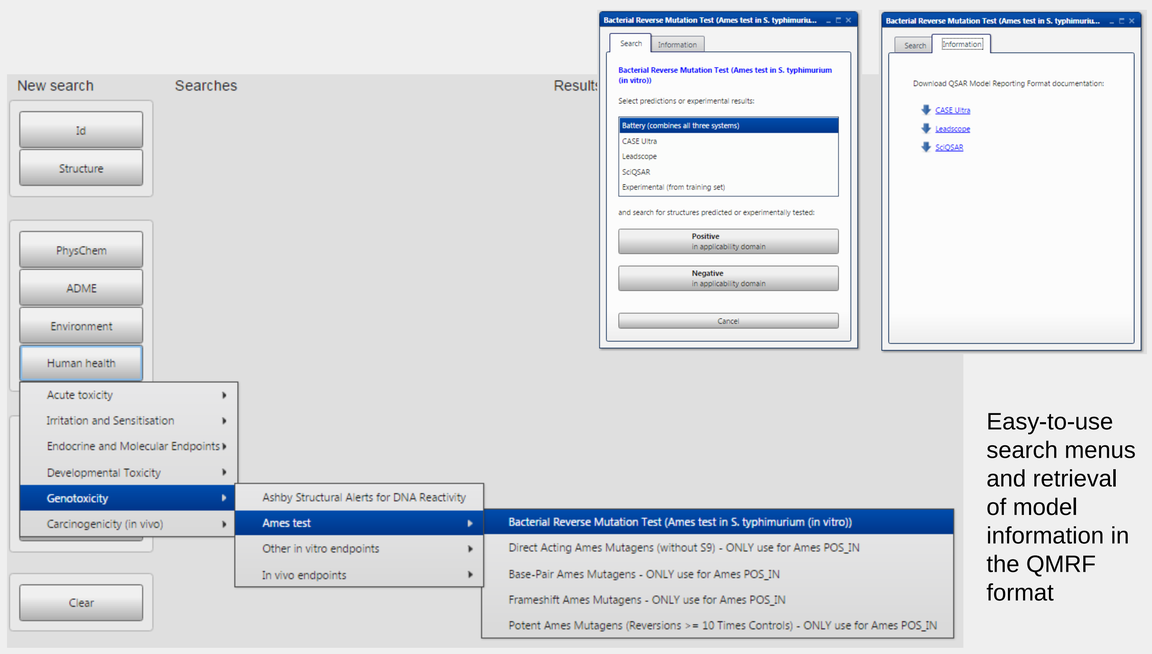
- to identify suspected hazardous substances for priority setting
- in weight-of-evidence assessments
- to improve evaluation of existing test data
- to provide mechanistic information
- in the design of testing strategies
- in development of read-across cases
- in the design of safer substitution chemicals
- to provide information beyond the standard regulatory information requirements.

The database content can be searched by:

- Chemical name and registry numbers (single or list)
- Structure (exact match, substructure, similarity)
- All contained predictions and training set information
- Combinations of searches with ‘AND’, ‘OR’, ‘NOT’



Click the icon for any substance to download a document presenting all predictions and training set information in 9 pages.



Easy-to-use search menus and retrieval of model information in the QMRF format

‘The Danish (Q)SAR Database is a valuable tool that is used by ECHA to screen among thousands of chemicals and identify those that are most likely to be of concern.’
Mike Rasenberg, Head of Computational Assessment and Dissemination Unit, ECHA

‘The Danish (Q)SAR database will surely play a key role in the implementation of 21st Century toxicology which is increasingly based on the use of prediction tools that are not only scientifically robust, efficient and cost-effective, but which also avoid the need for animal testing.’
Prof. Maurice Whelan, Head of Systems Toxicology Unit, and the EU Reference Laboratory for Alternatives to Animal Testing (EURL ECVAM).

‘With the use of (Q)SARs, innovative companies can identify early on in the R&D process those new chemicals that are most likely to be safe and thereby contribute to sustainable chemistry.’
Bob Diderich, Head of the Environment, Health and Safety Division, OECD

‘The chemical industry wants REACH to deliver on all its goals. (Q)SAR tools 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.’
Dr. Erwin Annys, Director REACH / Chemicals Policy, Cefic European Chemical Industry Council

DTU Food, Technical University of Denmark

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Danish (Q)SAR Database - http://qsar.food.dtu.dk