Danish (Q)SAR Models: A free online DTU QSAR predictor powered by Leadscope

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A free online DTU QSAR predictor powered by Leadscope

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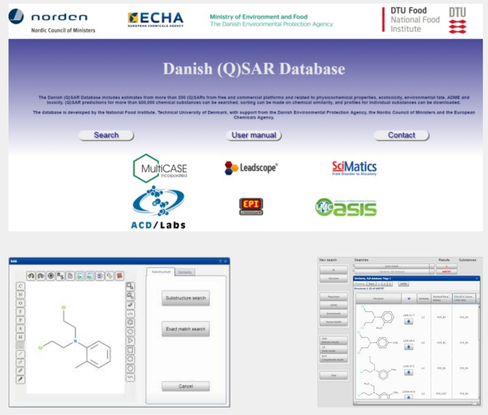
The QSAR team at the Technical University of Denmark, National Food Institute, has recently published a completely rebuilt version of the Danish (Q)SAR Database (http://qsar.food.dtu.dk) with pre-generated predictions from a large number of QSAR models for over 600,000 chemical structures. A selection of more than 20 of these QSAR models of diverse endpoints encompassing acute toxicity, metabolism, endocrine activity, genotoxicity and sensitization have been implemented in a real-time online predictive system. The system generates predictions on the fly for user-submitted structures and uses Leadscope Enterprise software as a back-end to the web server. All models have undergone robust cross-validation, and documentation in the international QMRF format is available from the website.

Danish (Q)SAR Database: Predictions from >200 (Q)SAR models pre-calculated for >600,000 substances

- DTU-developed, commercial and free models
- 72,000 EU REACH chemical substances and 372,000 NIH MLSMR
- Battery predictions: 3 QSAR approaches for the same training set
- Database, client and server software developed by DTU Food



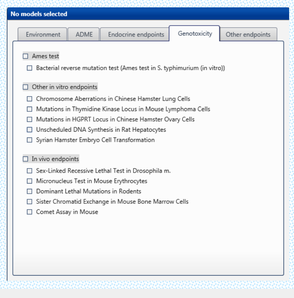
- Single substance look-up by ID or structure: profiling
- Screening across all QSAR-predicted and experimental properties and structures
- Sort on chemical similarity for read-across purposes
- Free for everyone to use

Danish (Q)SAR Models: Online prediction generation from >20 of the Danish (Q)SAR Database models

The Leadscope versions of selected models are made available for real-time prediction. The client/server software is developed by DTU Food and Leadscope Enterprise server is used as a back-end.

Included models

- Acute aquatic toxicity (Fish, Daphnia, Algae)
- Cytochrome P450 substrates (2C9, 2D6)
- Endocrine (ER binding/agonism, AR antagonism, *in vitro*)
- Genotoxicity *in vitro* (Ames test in Salmonella t., Chromosome aberrations in CHL, Mutations in Mouse Lymphoma, Mutations in HGPRT Locus in CHO, Unscheduled DNA Synthesis in Rat hepatocyte, SHE Cell Transformation), *in vivo* (Drosophila m. SLRL, Mouse Micronuclei, Rodent Dominant Lethal, Mouse Sister Chromatid Exchange, Mouse Comet Assay)
- Acute toxicity (Maximum recommended daily dose, human)
- Skin irritation (Severe skin irritation in Rabbit)
- Respiratory sensitization (human)
- Cardiotoxicity (hERG blocking, *in vitro*)

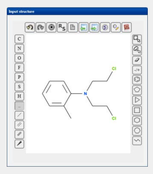


On-the-fly prediction generation:

- Same prediction and domain call as in the Danish (Q)SAR Database
- Positive prediction probability
- Detailed report with structural alerts and training set analogs

Chemical structure input

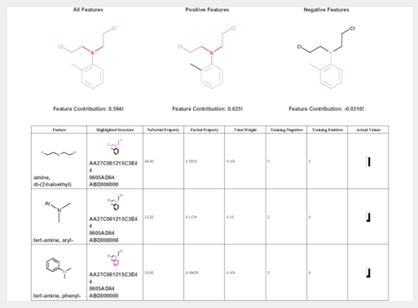
Draw, enter SMILES, MOL/SDF or look up by name:



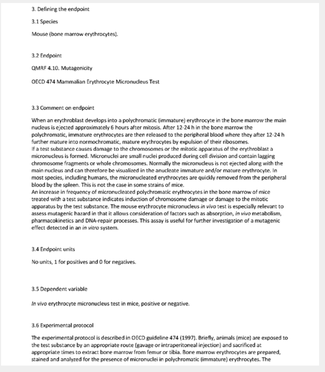
Predictions and reports download

QSAR Results

Model	Probability	Prediction	Report
ER alpha binding (human in vitro), all	0.155	NEG_IN	
ER alpha activation (human in vitro)	0.0186	NEG_IN	
Androgen receptor antagonism (human in vitro)	0.138	NEG_IN	
Unscheduled DNA Synthesis in Rat Hepatocytes	0.308	NEG_OUT	
Micronucleus Test in Mouse Erythrocytes	0.96	POS_IN	
Dominant Lethal Mutations in Rodents	0.979	POS_IN	
Maximum recommended daily dose (MRDD) in Humans	0.51	POS_OUT	



QMRF reports



Works in a browser, no need to install programs, no plugins or add-ons required. All major browsers and operating systems are supported.

Publication in 2016 will be announced on the Danish (Q)SAR Database homepage:

http://qsar.food.dtu.dk

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