

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

**Nikolov, Nikolai Georgiev; Cross, Kevin P.; Quigley, Patrick; Dybdahl, Marianne; Reffstrup, Trine Klein; Abildgaard Rosenberg, Sine; Wedebye, Eva Bay**

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DTU Food
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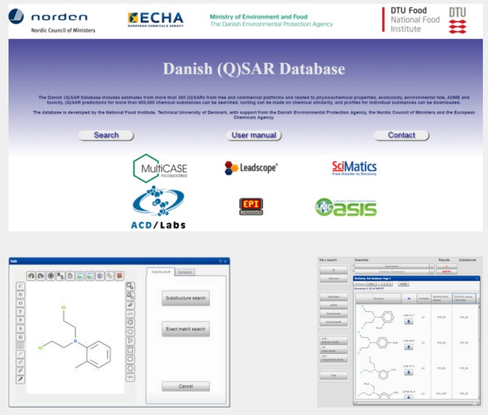
# A free online DTU QSAR predictor powered by Leadscope

**Nikolai G. Nikolov[1], Kevin P. Cross[2], Patrick Quigley[2], Marianne Dybdahl[1], Trine K. Reffstrup[1], Sine A. Rosenberg[1], Eva B. Wedebye[1]**
[1]Technical University of Denmark, [2]Leadscope Inc.

**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



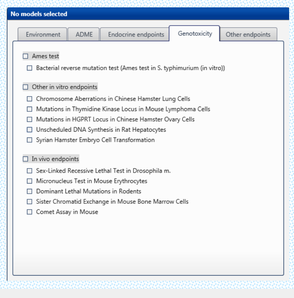

- Single substance look-up by ID or structure: profiling
- Screening across all QSAR-predicted and experimental properties and structures
- Sort on chemical similarity for read-across purposes
- Free for everyone to use

## 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*)



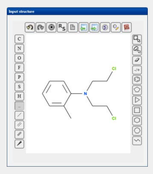


On-the-fly prediction generation:

- 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

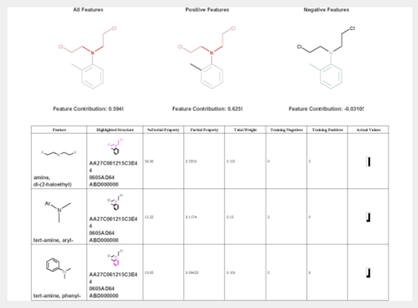
**Draw, enter SMILES, MOL/SDF or look up by name:**



### Predictions and reports download

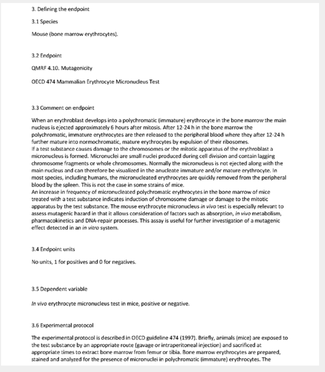
**QSAR Results**

| 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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