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Nikolov, Nikolai Georgiev; Wedebye, Eva Bay

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Recent developments of the Danish (Q)SAR Database: Updates, statistics and link to the OECD QSAR Toolbox

Nikolai G. Nikolov¹ and Eva B. Wedebye¹

¹*Technical University of Denmark, National Food Institute*

Division of Diet, Disease Prevention, and Toxicology

Kemitorvet, Building 201, 2800 Kongens Lyngby, Denmark

The Danish (Q)SAR database is a free searchable online repository of structural information and (Q)SAR predictions for more than 650,000 discrete organic substances, including about 80,000 REACH pre-registered and registered substances. Endpoints include physical-chemical properties, environmental fate, bioaccumulation, eco-toxicity, absorption, metabolism and toxicity. The results are made freely available via a web portal (<http://qsar.food.dtu.dk>) with an advanced search system including search by predictions, structure, similarity and experimental data from training sets. Since the new database was published in November 2015, it has been used by 4,000 unique IP addresses worldwide from regulators, academia, industry and NGO. Recent work on the database includes adding 10,000 new structures, correcting some structural information and adding new endpoints. The (Q)SAR predictions from the database are donated to the OECD and are being linked to the OECD QSAR Application Toolbox via a hotlink for dynamic data retrieval.

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