Advisory self-classifications for 54,135 substances based on (Q)SAR predictions from the Danish (Q)SAR database, VEGA QSAR and the OECD QSAR Toolbox

Nikolov, Nikolai Georgiev; Tyle, Henrik; Løfstedt, Magnus; Wedebye, Eva Bay

Publication date:
2018

Document Version
Version created as part of publication process; publisher's layout; not normally made publicly available

Advisory self-classifications for 54,135 substances based on (Q)SAR predictions from the Danish (Q)SAR database, VEGA QSAR and the OECD QSAR Toolbox

Nikolai Georgiev Nikolov[1], Henrik Tyle[2], Magnus Løfstedt[2], Eva Bay Wedebye[1,*]

[1]*Technical University of Denmark, National Food Institute, Division of Diet, Disease Prevention, and Toxicology, Kemitorvet 2, 2800 Kongens Lyngby, Denmark*

[2]*The Danish Environmental Protection Agency, Chemicals Division, Haraldsgade 53, 2100 Copenhagen Ø, Denmark*

Lack of experimental data on toxicological properties make it difficult for companies to self-classify the chemical substances they import or produce. To address this issue, 80,085 pre-registered and/or registered REACH substances from the Danish (Q)SAR Database were evaluated by (Q)SAR. For this purpose predictions primarily from the Danish (Q)SAR Database were used, supplemented with predictions from VEGA QSAR and a number of the profilers available from the OECD QSAR Application Toolbox. The following classification endpoints were addressed:

- Mutagenicity: Muta. 2
- Carcinogenicity: Carc. 2
- Reproductive toxicity (possible harm to the unborn child): Repr. 2
- Acute oral toxicity: Acute Tox.1-4
- Skin irritation: Skin Irrit. 2
- Skin sensitisation: Skin Sens. 1
- Danger to the aquatic environment: Acute 1, Chronic 1-3

Algorithms were developed for each classification endpoints to combine predictions to reach a final call in an attempt to reach further reliability and to best comply with the classification criteria. No advisory predictions were based on a positive prediction from a single system, and if only based on a battery prediction (majority vote from 3 systems) the third system was required not to give a negative prediction in applicability domain. This resulted in a list with a total of 54,135 substances with one or more advisory self-classifications. The list is available

from the Danish Environmental Protection Agency homepage.

Specify the topic of your contribution and type of presentation (mark with **X**):

Section

x	(Q)SAR models for regulatory use
	Models for human health effects
	Models for ecotoxicological and environmental effects
	Protein-ligand interactions, *in silico* studies related to toxicological effects
x	Software and tools

Presentation

	oral
x	poster