QSAR model for activated sludge respiration inhibition (v1.0)

ProtoECO
by ProtoQSAR

ProtoECO

ProtoECO is a computational (*in silico*) tool focused on the prediction of endpoints related with ecotoxicity and the environmental effects chemical substances. This includes properties related to the distribution and degradation of substances in the environment as well as their toxic effects in the biota.

ProtoECO mainly includes, but is not limited to, endpoints used by REACH, a European Union regulation, adopted to improve the protection of human health and the environment from the risks that can be posed by chemicals, while enhancing the competitiveness of the EU chemicals industry.

Endpoint

Ecotoxic effects: Microbial inhibition (activated sludge respiration inhibition, inhibition of nitrification, other). OECD 209: Activated Sludge, Respiration Inhibition Test.

Activated sludge that is present in biological sewage treatment plants (STPs), consists mainly of microorganisms that are responsible for breaking down chemicals present in both municipal and industrial wastewater (biodegradation). Toxicity to microorganisms in activated sludge is also generally referred to as 'toxicity to STP microorganisms' or simply 'STP toxicity'.

Metrics

Training set

Experimental values	QSAR predictions	
	non-toxic	**toxic**
non-toxic	91	21
toxic	4	35

Validation set

Experimental values	QSAR predictions	
	non-toxic	**toxic**
non-toxic	34	15
toxic	3	14

Parameters	Training	Validation
Accuracy	0.83	0.73
Sensitivity / recall	0.90	0.82
Specificity	0.81	0.69
Precision	0.62	0.48
Negative predictive value	0.96	0.92
F-score	0.74	0.61
Matthews Correlation Coefficient	0.64	0.46
Critical Success Index	0.58	0.44
Area under the ROC	0.85	0.76

ProtoECO is part of

ProtoPRED

ProtoPRED platform allows the easy, fast and user-friendly prediction of different properties of chemical compounds, using proprietary (Q)SAR models

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