

ProtoREACH

ProtoREACH is a computational (*in silico*) tool specially focused on 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.

REACH also promotes alternative methods for the hazard assessment of substances in order to reduce the number of tests on animals. The requirements for registering a chemical substance are organized as annexes of the REACH regulation. Different annexes must be used depending on the substance mass produced or imported by each company.

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

ProtoREACH is part of



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

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