QSAR model for ready biodegradability (v1.1)

ProtoREACH by ProtoQSAR

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

Environmental fate parameters: Persistence: Biodegradation. Ready/not ready biodegradability.

Biodegradation is a naturally occurring process where microorganisms, such as bacteria, feed themselves by breaking-down (organic) substances into smaller fragments which may themselves be further degraded to even smaller fragments. When 'complete' biodegradation takes place, all that will be left of the substance is water, carbon dioxide and salts.

Metrics

Training set

Experimental values	QSAR predictions	
	not ready biodegradable	ready biodegradable
not ready biodegradable	565	28
ready biodegradable	25	229

Validation set

Experimental values	QSAR predictions	
	not ready biodegradable	ready biodegradable
not ready biodegradable	236	20
ready biodegradable	41	68

Parameters	Training	Validation
Accuracy	0.94	0.83
Sensitivity / recall	0.90	0.62
Specificity	0.95	0.92
Precision	0.89	0.77
Negative predictive value	0.96	0.85
F-score	0.90	0.69
Matthews Correlation Coefficient	0.85	0.58
Critical Success Index	0.81	0.53
Area under the ROC	0.93	0.77

ProtoREACH is part of

ProtoPRED

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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