

## 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 readily biodegradable	readily biodegradable
not readily biodegradable	385	13
readily biodegradable	11	113

### Validation set


Experimental values	QSAR predictions	
	not readily biodegradable	readily biodegradable
not readily biodegradable	158	17
readily biodegradable	24	29

Parameters	Training	Validation
Accuracy	0.95	0.82
Sensitivity / recall	0.91	0.55
Specificity	0.97	0.90
Precision	0.90	0.63
Negative predictive value	0.97	0.87
F-score	0.90	0.59
Matthews Correlation Coefficient	0.87	0.47
Critical Success Index	0.82	0.41
Area under the ROC	0.94	0.73

ProtoREACH is part of



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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