

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

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

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


Validation set

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

ProtoECO is part of



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

 +34 962 021 811

 protopred@protoqsar.com

<https://protopred.protoqsar.com/>

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