

ProtoTOX

ProtoTOX is a computational (*in silico*) tool focused on the prediction of endpoints related with the toxicity of chemical substances. It includes a variety of *in vitro* and *in vivo* tests in humans, animals, microorganisms and cell lines.

ProtoTOX 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.

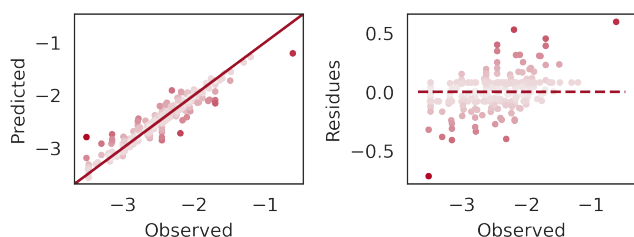
Endpoint

Human health effects: Neurotoxicity.

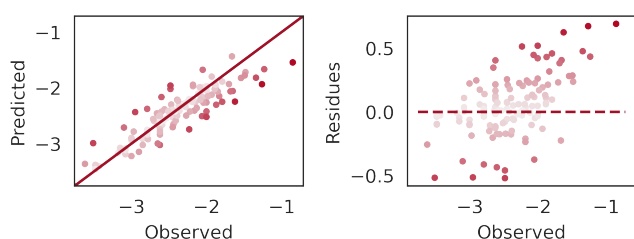
Neurotoxicity is the induction by a substance of adverse effects in the central or peripheral nervous system, or in sense organs. It is useful for the purpose of hazard and risk assessment to differentiate sense organ-specific effects from other effects which lie within the nervous system. A substance is considered neurotoxic if it induces a reproducible lesion in the nervous system or a reproducible pattern of neural dysfunction.

Metrics

Training set



Validation set




Parameters	Training	Validation
R ² score	0.92	0.79
Mean absolute error (MAE)	0.10	0.18
Mean squared error (MSE)	0.02	0.06
Median absolute error	0.08	0.12
Explained variance	0.92	0.80

ProtoTOX 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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