

# ProtoPRED: an innovative platform for the prediction of toxicological properties of small molecules and nanomaterials

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Quantitative Structure-Activity Relationships (QSARs) are mathematical models relating the structure of molecules with a property, through the use of statistical tools and machine-learning algorithms.<sup>1</sup> They can be used to predict toxicological and environmental properties quickly and at a very low cost in comparison to *in vitro* and *in vivo* experiments. Thus, QSAR models are widely applied in different sectors, such as cosmetics and pharmaceuticals.<sup>2</sup>

We have developed a computational platform, ProtoPRED<sup>3</sup>, that allows the reliable, easy, fast and user-friendly prediction of a wide range of toxicological properties of chemical compounds. ProtoPRED only requires the input of the chemical structure (accepting several formats) and performs predictions in seconds, for one or several substances. The predictions come along with detailed reports that provide extensive information about the training and test set, model algorithm, model validation and the quality of the prediction, required to use them for registration purposes.

ProtoPRED includes more than 50 endpoints, grouped in different modules. There are two specific regulation-focused modules (ProtoICH and ProtoREACH) which include models that are linked to the ICH-M7 and REACH regulations, respectively. Other modules are based on the type of endpoints: physicochemical properties (ProtoPHYSCHEM), human toxicity (ProtoTOX), ecotoxicity and environmental fate (ProtoECO) and pharmacokinetics (ProtoADME). In addition, there is a module dedicated to predict the properties of nanomaterials (ProtoNANO).

## References:

1. Tropsha 2010. Best Practices for QSAR Model Development, Validation, and Exploitation. <https://doi.org/10.1002/minf.201000061>
2. Statistics on the use of animals for scientific purposes in the Member States of the European Union and Norway in 2018. Summary Report, European Commission. <https://op.europa.eu/en/publication-detail/-/publication/04a890d4-47ff-11ea-b81b-01aa75ed71a1>
3. <https://protopred.protoqsar.com>