[P32] New QSAR Models Concerning (Eco)Toxicological Endpoints: Acute toxicity, Bioaccumulation and Biodegradability

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REACH and CLP regulations demand significant data generation for all substance in the market. In this context, in-silico methods are valid alternatives for data gap filling [1, 2]. Freely available tools [2], don't have always good performances in the industrial context, especially being tested on chemical substances of interest of SOLVAY. The goal of this project is thus to develop new QSAR models on three (eco)toxicological endpoints (rat oral acute toxicity, bio-concentration factor and ready biodegradability) and to validate them on industrial data.

Experimental data were prepared using a standardization workflow implemented in Knime [3] and ChemAxon Environment [4]. ISIDA Property-Labelled Descriptors were chosen to encode molecular structures [5]. Best descriptor spaces and optimized model parameters were selected by Genetic Algorithm using in-house scripts [6]. Employed machine learning algorithms include Support Vector Machine, Random Forest and Naive Bayesian. Models were generated with Weka and LIBSVM.

Each individual model was both internally and externally validated according to the OECD principles [7]. Only models respecting OECDs criteria were retained and used for consensus calculations. Validation on industrial data demonstrated that developed models perform better than already existing tools.

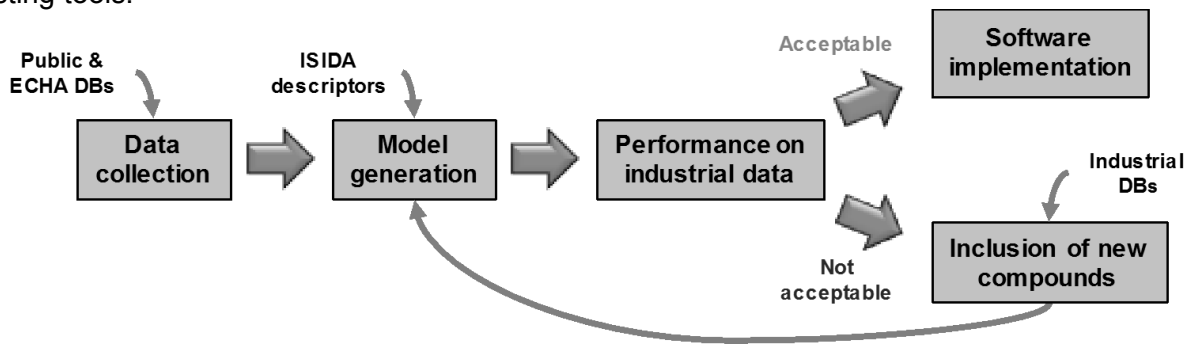

Figure 1 - Modeling workflow overview

Bibliography:

[1] ECHA Guidance on information requirements and CSA, Chapter R.6, (2008).
[2] ECHA Practical guide: How to use and report (Q)SARs, Version 3.1, (2016).
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[7] ENV/JM/MONO(2007)2, Guidance on the validation of QSAR models, (2007).