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Statistical inference and extrapolation uncertainty in QSAR predictions

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Applying QSARs to support decision making, such as chemical hazard or risk assessment or drug design, ask for the consideration of two kinds of uncertainties. First, a quantification of uncertainty in the predicted endpoint by a probability distribution is useful information to a decision analysis. Among different statistical principles for predictive inference, Bayesian predictive inference is a good candidate when the purpose is to make predictions using QSAR. Bayesian inference not only gives explicit attention to uncertainty in the model, but allows taking expert knowledge into consideration. I will discuss how various QSAR modeling approaches can be placed into a Bayesian framework. The second kind of uncertainty to consider is to which extent a QSAR prediction is an extrapolation. This provides useful information on the reliability or confidence in a prediction. I will show how the extent of extrapolation can be evaluated by distances to the region in chemical space defined by training data set (also known as the applicability domain), by sensitivity analysis using ensemble predictions, or by performance measures of the accuracy of predictions. I will discuss different ways to consider extrapolation uncertainty in decision analysis based on examples on QSAR informed chemical safety assessment, derived in the EU financed project CAse studies on the Development and Application of in-Silico Techniques for Environmental hazard and Risk assessment (CADASTER).

Biography

Ullrika Sahlin has completed her Ph.D 2010 from Lund University, postdoctoral studies from Linneaus University at the Department of Environmental Science and Technology, and is currently holding a position at the Center of Environmental and Climate Research Lund University. She is the leader of a work package in the EU-funded project CAse studies on the Development and Application of in-Silico Techniques for Environmental hazard and Risk assessment (CADASTER). Here interests are predictive modeling, risk and uncertainty analysis, and robust decision making. She has a Master of Science in Mathematical Statistics, and is working in several research projects with environmental risk assessment and management.

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