

Lecture: computer assisted procedures

## A logic-based approach for quantitative toxicology prediction

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This talk presents the application of logic-based machine learning for the prediction of toxicology. Our approach starts with the use of inductive logic programming (ILP) which reasons with chemical substructures in a relational framework and learns chemically understandable rules. This is then followed by the use of a support vector machine to extend qualitative ILP-based structure-activity relationships to a quantitative predictor in an approach we term SVILP. The SVILP approach learnt predictive rules from the Distributed Structure-Searchable Toxicity (DSSTox) database from the U.S. Environmental Agency ([www.epa.gov](http://www.epa.gov)). For a diverse dataset of 576 molecules with known fathead minnow fish toxicity, the cross-validated correlation coefficient (R2CV) from SVILP is 0.66 compared to a chemical descriptor approach which yields 0.52. Our SVILP approach has a major advantage that it uses ILP automatically to learn rules, mostly novel, describing fragments that are toxicity alerts. The SVILP approach has general applicability to chemoinformatics, including *in silico* screening to identify novel hits and construction of predictors for ADME properties.

### References

Amini, A., Muggleton, S. H., Lodhi, H. and Sternberg, M. J. (2007). A novel logic-based approach for quantitative toxicology prediction, *J. Chem. Inf. Model.* 47, 998-1006.

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