Journal of
Cheminformatics

POSTER PRESENTATION

Open Access

Fingerprint-based detection of acute aquatic toxicity

Luca Pireddu[1*], L Michielan[2], M Floris[1], P Rodriguez-Tomé[1], S Moro[2]

From 5th German Conference on Cheminformatics: 23. CIC-Workshop
Goslar, Germany. 8-10 November 2009

In this work we show the effectiveness of 2D structural fingerprints in the prediction of aquatic toxicity of chemical compounds, creating a self-contained system for structure-based aquatic toxicity classification. Using the data from the U.S. Environmental Protection Agency Fat Head Minnow (EPA-FHM) dataset [1] we build a non-linear RBF SVM [2] classifier that distinguishes acutely toxic compounds from less toxic compounds, loosely according to the criterion stipulated by the E.U. Reach legislation [3]. The classifier achieves up to 86% accuracy in leave-one-out validation using 580 of the dataset's 614 compounds. This performance is comparable with models built from the same dataset using more sophisticated molecular descriptors, such as AutoMEP and Sterimol descriptors [4]. We apply our classification model to predict the aquatic toxicity of 3M compounds in the MMsINC database [5]. Furthermore, we create a linear SVM model using the same technique and apply it to the MMsINC data, with the additional integration of the EXPLAIN system [6] which allows us to show which structural features are responsible for the model classifying a molecule as less toxic or acutely toxic.

Author details
[1]CRS4, Pula, Italy. [2]University of Padova, Padova, Italy.
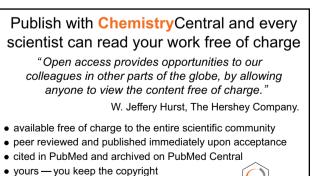
Published: 4 May 2010

References
1. Russom CL, Bradbury SP, Broderius SJ, Hammermeister DE, Drummond RA: Predicting modes of action from chemical structure: Acute toxicity in the fathead minnow (Pimephales promelas). *Environmental Toxicology and Chemistry* 1997, **16**(5):948-967.
2. Boser B, Guyon I, Vapnik V: **A Training Algorithm for Optimal Margin Classifiers.** *Computational Learning Theory* 1992, 144-152.
3. EU: **Corrigendum to Regulation (EC) No 1907/2006 of the European Parliament and of the Council of 18 December 2006 concerning the Registration, Evaluation, Authorization and Restriction of Chemicals (REACH).** *Off J Eur Union L136* 2007, 50.
4. Michielan L, Pireddu L, Floris M, Bacilieri M, Rodriguez-Tomé P, Moro S: 2009.
5. Masciocchi B, Frau G, Fanton M, Sturlese M, Floris M, Pireddu L, Palla P, Cedrati F, RodriguezTomé P, Moro S: **MMsINC: a large-scale chemoinformatics database.** *Nucleic Acids Research* 2008, , **37** Database: D284-90.
6. Poulin B, Eisner R, Szafron D, Lu P, Greiner R, Wishart D, Fyshe A, Pearcy B, Macdonell C, Anvik J: **Visual Explanation of Evidence in Additive Classifiers.** *Innovative Applications of Artificial Intelligence* 2006.

[1]CRS4, Pula, Italy