

POSTER PRESENTATION

Open Access

Adaptive matrix metrics for molecular descriptor assessment in QSPR classification

Axel J Soto^{1*}, Marc Strickert², GE Vazquez¹

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

QSPR methods represent a useful approach in the drug discovery process, since they allow predicting in advance biological or physicochemical properties of a candidate drug. For this goal, it is necessary that the QSPR method be as accurate as possible to provide reliable predictions. Moreover, the selection of the molecular descriptors is an important task to create QSPR prediction models of low complexity which, at the same time, provide accurate predictions.

In this work, a matrix-based method [1] is used to transform the original data space of chemical compounds into an alternative space where compounds with different target properties can be better separated. For using this approach, QSPR is considered as a classification problem. The advantage of using adaptive matrix metrics is twofold: it can be used to identify important molecular descriptors and at the same time it allows improving the classification accuracy.

A recently proposed method making use of this concept [2] is extended to multi-class data. The new method is related to linear discriminant analysis and shows better results at yet higher computational costs. An application for relating chemical descriptors to hydrophobicity property [3] shows promising results.

Author details

¹Planta Piloto de Ingeniería Química (PLAPIQUI), Universidad Nacional del Sur, Alem 1250, 8000 Bahía Blanca, Argentina. ²Leibniz Institute of Plant Genetics and Crop Plant Research (IPK), Corrensstr. 3, 06466 Gatersleben, Germany.

Published: 4 May 2010

References

1. Strickert M, Keilwagen J, Schleif F-M, Villmann T, Biehl M: **Matrix Metric Adaptation Linear Discriminant Analysis of Biomedical Data.** *Lecture Notes in Computer Science* 2009, **5517/2009**:933-940.

¹Planta Piloto de Ingeniería Química (PLAPIQUI), Universidad Nacional del Sur, Alem 1250, 8000 Bahía Blanca, Argentina

2. Strickert M, Soto AJ, Keilwagen J, Vazquez GE: **Towards matrix-based selection of feature pairs for efficient ADMET prediction.** *Argentine Symposium on Artificial Intelligence, ASAI 2009*, 83-94.
3. Soto AJ, Cecchini RL, Vazquez GE, Ponzoni I: **A Wrapper-based Feature Selection Method for ADMET Prediction using Evolutionary Computing.** *Lecture Notes in Computer Science* 2008, **4973/2008**:188-199.

doi:10.1186/1758-2946-2-S1-P47

Cite this article as: Soto et al.: Adaptive matrix metrics for molecular descriptor assessment in QSPR classification. *Journal of Cheminformatics* 2010 **2**(Suppl 1):P47.

Publish with **ChemistryCentral** and every scientist can read your work free of charge

"Open access provides opportunities to our colleagues in other parts of the globe, by allowing anyone to view the content free of charge."

W. Jeffery Hurst, The Hershey Company.

- available free of charge to the entire scientific community
- peer reviewed and published immediately upon acceptance
- cited in PubMed and archived on PubMed Central
- yours — you keep the copyright

Submit your manuscript here:
<http://www.chemistrycentral.com/manuscript/>



ChemistryCentral



ChemistryCentral

© 2010 Soto et al; licensee BioMed Central Ltd.