Short Term Marie Curie Fellowship for PhD students (STR3)

Methods for selection of structural features that influence substance toxicities.
8 months (1 position) (4 months more, if possible)

Nowadays, substances can be computationally represented by several thousands of molecular descriptors which are numbers encoding structural features of them. Thanks to this huge amount of molecular descriptors, more chemical information is available to study substances from different points of view; however, when the aim is to generate robust predictive models for properties of substances, these are usually based on a few molecular descriptors and thus the problem here is how to select the most predictive ones. To this concern, it must be noted that the presence in a model of not relevant molecular descriptors doesn't play a neutral role, i.e. no influence in the model quality, but, on the contrary, it contributes to increase noise in the model and then to lower its predictive ability.
Two basic approaches are defined in literature: variable reduction and variable selection. The former is based on reduction techniques of descriptors without considering the response being modelled and are, basically, founded on the analysis of internal correlation among descriptors.
In the latter approach, descriptors are selected considering the response being modelled. Genetic algorithms, in their different forms, step-wise procedures, descriptor annihilation in latent variable techniques are some of the algorithms used to select the most relevant descriptors in QSAR/QSPR modelling.
The main goal of this STF will be to study toxicological properties of substances by using both variable reduction and variable selection approaches. In particular, the study will focus on binary endpoints like active / no active and different techniques will be applied and compared, such as logistic regression, GA-KNN, sub-structural analysis, cluster significance analysis, together with the most common ones.
The choice of the environmental properties of interest will be performed considering the data produced from the other Partners of the ECO Project.

Type of job Full time
Application deadline (date of receipt) 30.09.2010
How to apply Please apply online at http://www.eco-itn.eu
Formal applications should be exclusively send electronically and should include:
- Full CV and non Italian citizenship
- A statement of motivation (not more than one page)
- Copies of relevant exams, grades, master thesis work or publications
- Contact information of two reference persons

This position is funded by EU and the applicants should check their eligibility as indicated at the web site of the project.

Company name Department of Environmental Sciences, University of Milano-Bicocca **Address** P.za della Scienza, 1 **Zipcode/City** 20126 Milano **Country** Italy **Website** http://www.eco-itn.eu **Contact person** Prof. Roberto Todeschini **Contact phone** +39 02 64482820 **FAX contact** +39 02 64482839 **email** roberto.todeschini@unimib.it