

Short Term Marie Curie Fellowship for PhD students (STR2 a, b und c)

*Evaluation of QSAR/QSPR modeling
performance of some novel molecular descriptors*
12 months (3 positions of 4 months each)



Several new molecular descriptors have been defined in the last few years; however, their role in QSAR/QSPR modelling was not explored at all or was evaluated only by means of simple few benchmark datasets.

Therefore, some efforts need to be addressed to obtaining more knowledge about chemical information encoded by these molecular descriptors, their correlation with other well-known descriptors and their ability of predicting some properties of substances.

The molecular descriptors that are going to be considered in this study are:

- 1) some topological indices calculated from generalized graph-theoretical matrices based on different weighting schemes of molecular graphs;
- 2) TDB descriptors, which are autocorrelations that also incorporate geometrical distances between atoms;
- 3) ETA descriptors, that encode electronic information;
- 4) surface and volume descriptors;
- 5) new substructure descriptors and fingerprints.

These molecular descriptors may hopefully improve models for prediction of environmental properties of interest. Therefore, experimental data will be collected from literature or existing open databases for different partition coefficients, vapor pressure, water solubility, bioconcentration factor, biodegradation, atmospheric oxidation, and so forth. Predictive models will be developed and compared with the models based on the EPA software (Episute).

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.

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