P-A1-022

QSPR MODELS FOR ENVIRONMENTAL FATE ASSESSMENT AND PRODUCT DEVELOPMENT IN SMALL AND MEDIUM SIZED CHEMICAL COMPANIES

W. M. M. Mahmoud[1,2], C. Leder[1], C. Rücker[1], K. Kümmerer[1], D. Schwartz[3]

[1]*Sustainable Chemistry and Material Resources, Institute of Sustainable and Environmental Chemistry, Leuphana University Lüneburg, Scharnhorststr. 1, 21335 Lüneburg, Germany.*
[2] *Analytical Chemistry Department, Faculty of Pharmacy, Suez Canal University, Ismailia 41522, Egypt.*
[3]*Bruno Bock GmbH, 21436 Marschacht, Germany*
Presenting author: waleed.ahmed@inkubator.leuphana.de

REACH (Registration, Evaluation, Authorisation and Restriction of Chemicals) is a regulation of the European Union, adopted to improve the protection of human health and the environment from risks that can be posed by chemicals, while enhancing the competitiveness of the EU chemical industry [1].

Often information on compound properties available to small companies is insufficient for REACH registration. Experimental testing of compounds is expensive and time consuming. Alternative methods for hazard assessment such as QSPR/QSAR (Quantitative structure − property/activity relationships) are expressly recommended by regulatory authorities. However, there are at least two problems with this approach: i) Available computer programs for compound property prediction may be not appropriate for the particular compounds of interest. ii) Small chemical companies may not have personal sufficiently familiar with such programs to realistically estimate their limitations.

Our project "Use of Cheminformatics models for the development and optimization of chemical products" is intended to alleviate this situation by supporting small companies in using appropriate computer programs. For example, a compound property of fundamental importance is biodegradability or not so. If a compound is readily biodegraded in the environment, there will be no major concern on bioaccumulation or long-term toxicity. Biodegradability is often predicted using the Biowin models of the U. S. EPA. However, the Biowin models are primarily based on the presence of certain substructures in molecules that are recognized by the program, for each such substructure a certain numerical contribution is added to a predicting function. If a compound structure is devoid of these substructures, and perhaps contains other substructures important for biodegradation, the Biowin predictions are based on the molecular mass only. A user unfamiliar with the programs may take such predictions literally, not realizing that his compounds are outside the domain of applicability of the programs.

The approach will be to use a variety of biodegradability prediction software on particular classes of compounds containing less familiar functional groups, and to generate experimental biodegradation data for certain compounds with the aim to use these in establishing "local" biodegradation models for these compound classes in contrast to existing models that claim "global" applicability but were trained on compound classes containing the most fundamental functional groups only.

This is a joint research project of Leuphana University Innovation Incubator and Bruno Bock GmbH, a leading producer of organosulfur compounds. Biodegradation tests for selected compounds will be performed according to OECD guidelines such as the Closed Bottle test (CBT).

Reference:

(1) http://echa.europa.eu/web/guest/regulations/reach/ (accessed May 13, 2014).