Institut für Verfahrenstechnik, Umwelttechnik und techn. Biowissenschaften
Institute of Chemical Engineering, TU Vienna

Workshop "Molecular Descriptors"

Introduction – Theory – Applications

Monday, 5th December 2011, 14:00

TU Wien, Getreidemarkt 9, Chemiehochhaus (BA), 8th floor, seminar room

Programme

14:00 – 15:00 **Roberto Todeschini**
Milano Chemometrics and QSAR Research Group, Department of Environmental Sciences, University of Milano-Bicocca, Milan, Italy; http://michem.disat.unimib.it/chm
Introduction to QSAR/QSPR strategies, the role of chemometrics and molecular descriptors

15:00 – 15:20 Break

15:20 – 15:50 **Matthias Dehmer**
Institute for Bioinformatics and Translational Research, UMIT - The Health and Life Sciences University, Hall in Tirol; www.dehmer.org
On the uniqueness of structural graph measures

15:50 – 16:20 **Peter Filzmoser**
Department of Statistics and Probability Theory, TU Vienna; www.statistik.tuwien.ac.at/public/filz
Finding relevant descriptors

16:20 – 16:50 **Bettina Liebmann**
Institute of Chemical Engineering, TU Vienna; http://institute.tuwien.ac.at/vt
A QSPR example in practice

16:50 – 17:05 **Kurt Varmuza**
Institute of Chemical Engineering, TU Vienna; www.lcm.tuwien.ac.at
Binary substructure descriptors and software *SubMat*

17:05 – … Discussion

Organisation

Bettina Liebmann, Kurt Varmuza, Anton Friedl
bettina.liebmann@tuwien.ac.at, kvarmuza@email.tuwien.ac.at, anton.friedl@tuwien.ac.at

Institute of Chemical Engineering | Thermal Process Engineering and Simulation |
Sustainable Process Engineering & Chemometrics
http://institute.tuwien.ac.at/vt