BCB-Seminar

Time: Thursday, July 12th 2007, 3 - 5 pm

Place: Max Planck Institute for Molecular Genetics, Ihnestr. 63 – 73, 14195 Berlin (lecture hall)

Speaker: **Gisbert Schneider**, Beilstein-Stiftungsprofessur Chemieinformatik, Chem- & Bioinformatics, Johann Wolfgang Goethe-University Frankfurt / Main and
Michael Schmuker, Neuroinformatics/Theoretical Neuroscience, Inst. for Biology, Neurobiology, Free University Berlin

Abstracts

The rational design of focused compound libraries: A journey through chemical space

Gisbert Schneider, Johann Wolfgang Goethe-University Frankfurt / Main

Drug discovery relies on new pharmacologically active chemotypes. Computer-assisted drug discovery methods assist the medicinal chemist in this endeavor. These “rational” approaches complement high-throughput “random” screening. We will present and discuss techniques for structure- and ligand-based chemical similarity searching, “fuzzy” pharmacophores, and automated molecular *de novo* design. Case studies include the development of machine-learning systems for estimation of structure-activity relationships, molecular representation schemes for the purpose of “scaffold-hopping”, the prediction of cross-activity of bioactive molecules, and the design of natural-product derived compound libraries.

Principles of olfactory coding applied to pattern recognition in cheminformatics

Michael Schmuker, Free University Berlin

Olfaction, the chemical sense, has evolved to encode and classify odorants. Thus, the neural circuits in the olfactory system are likely to implement an efficient method for coding, processing and classification of chemical information. Olfactory receptor neurons (ORNs) provide the interface between the chemical world of odorants and the brain. Aiming to understand the olfactory code at this level, we established a predictive model for ORN activation from odorant structure and derived structure-activity-relationships. Based on computational principles that govern subsequent processing stages in the olfactory system, we designed a method for coding and processing chemical data. This method is suited for prediction of bioactivity of pharmaceutical compounds.

Guests are welcome!