Modeling complex protein-ligand interactions and drug action

Mini-symposium preceding Ruben Vosmeer's thesis defense

Thursday 2 April, Main Building of VU University (6th floor, room HG-06A05), De Boelelaan 1105, Amsterdam

Program:

10.15 h Coffee

10.30 h Introduction (Daan P. Geerke, Molecular and Computational Toxicology, VU)

Part I *The Viennese connection: exploring protein conformational and open data space*

10.35 h Chris Oostenbrink (Molecular Modeling and Simulation, BOKU, Vienna, Austria)
Biomolecular simulations of Cytochrome P450 enzymes ... and some other proteins

11.15 h Gerhard F. Ecker (Pharmacoinformatics, University of Vienna, Austria)
The Open PHACTS Discovery Platform - Integrated open data for drug discovery

11.55 h Lunch

Part II *Down under and up again: from force field optimization to end point predictions*

12.50 h Alan E. Mark (Molecular Dynamics group, University of Queensland, Brisbane, Australia)
Single step perturbation approaches in ligand design and force field parameterization

13.30 h Scott Boyer (Swedish Toxicology Sciences Research Center, Södertälje, Sweden)
Being more certain about uncertainty in modeling toxicology data

14.10 h Closure mini-symposium

15.45 h In the VU University Aula, C. Ruben Vosmeer will defend his thesis
Improved description of complex plasticity and interactions in protein-ligand simulations