Announcement

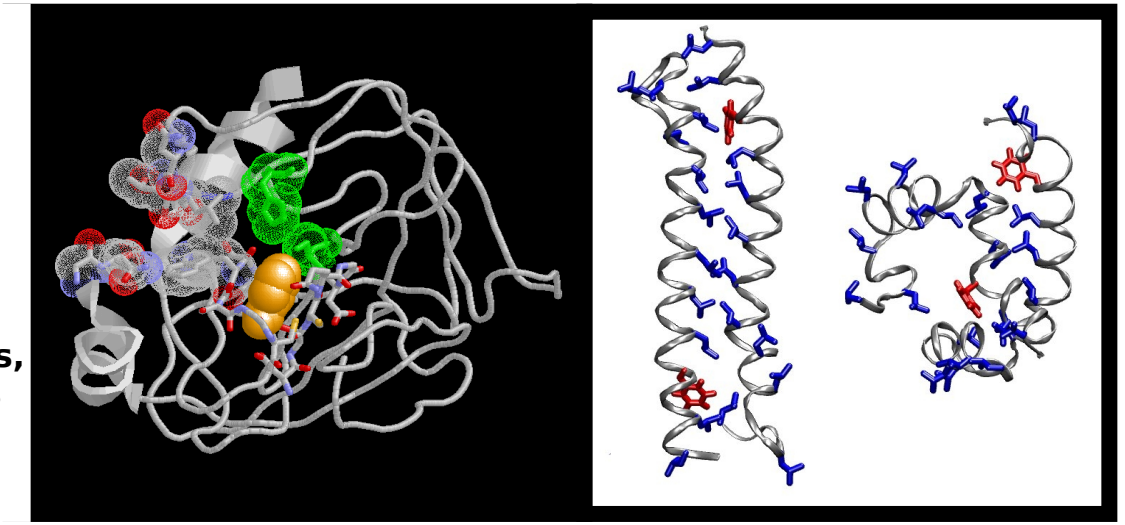
Molecular Dynamics Simulations

Lecture (2 SWS) and Computer exercise (2 SWS)

H. Gohlke (Molecular Bioinformatics) and A. Villa (Theoretical Chemistry)

Tentative agenda:

- **Model systems and force fields**
- **Treatment of long-range interactions**
- **Neighbor lists and cell structures**
- **Molecular dynamics simulations: Equations of motion, FD techniques**
- **Basics of statistical mechanics**
- **Simulation in different ensembles**
- **Analyses of results: Geometric parameters, time correlation functions, error estimates**
- **Free energy calculations**



Informative meeting:
Thursday, April 19st 2007, 2.00 pm in the Beilstein Computer Center (BCC) / Biocenter

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