

Program: Tuesday, April 29th 2008

8:00-9:15	Registration
9:15-9:20	Welcome remarks / Agenda review
	Session 1, Chair: W. Brandt
9:20-10:20	Plenary Lecture: Hans-Jörg Hofmann <i>Institute of Biochemistry, U Leipzig</i> Prediction of Foldamer Structures Employing Theoretical Methods
10:20-10:50	Coffee break
10:50-11:15	Karel Berka <i>Institute of Organic and Biochemistry, Prague</i> Amino acid side-chain interactions in proteins. Comparison of ab-initio and empirical methods
11:15-11:40	Diana Schulze <i>Leibniz-Institute of Plant Biochemistry, Halle (Saale)</i> Structural Models of Membrane Bound Aromatic Prenyltransferases
11:40-12:05	Christophe Jardin <i>Institute of Biochemistry, U Erlangen</i> The phosphoryl transfer between the IIA and IIB proteins of the Escherichia coli Glucose Phosphotransferase System
12:05-12:30	Jana Selent <i>Computer-Assisted Drug Design Laboratory, U Pompeu Fabra, Barcelona</i> Multi-Receptor Profiling of Antipsychotic Drugs. A Structural Study Based on the new β 2 Adrenergic Receptor Template
12:30-13:30	Lunch break
	Session 2, Chair: H. Bögel
13:30-13:55	Lothar Terfloth <i>Computer-Chemistry-Center, U Erlangen</i> Isoform Specificity of Cytochrome P450 Substrates
13:55-14:20	Sebastian Kruggel <i>Institute of Pharmacy, U Hamburg</i> P-gp substrate differentiation by pharmacophore modelling

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- Session 4, Chair: M. Krug
- 9:15-9:40 **Mateusz Wielopolski**
Computer-Chemistry-Center, U Erlangen
Modeling of Electron-Transfer Properties in Organic π -Conjugated DONOR-WIRE-C₆₀ Systems
- 9:40-10:05 **Rene Meier**
Inst for Pharmaceutical Chemistry, U Halle (Saale)
ParaDockS – An Extensible Framework for Parallel Molecular Docking
- 10:05-10:30 **Tim ten Brink**
Department of Chemistry, U Konstanz
Automated Ligand Preparation for Protein-Ligand-Docking
- 10:30-11:00 Coffee break
- 11:00-11:25 **Michael Hutter**
Center for Bioinformatics, U Saarland
In silico screening of drug-like compounds online: eDrugScan
- 11:25-11:50 **Sina Kazemi**
Computational Pharmaceutical Chemistry, U Kiel
Elastic potential grids - A new paradigm for fully flexible docking
- 11:50-12:00 Conference photo in front of the building
- 12:00-13:15 Lunch break
- Session 5, Chair: T. Clark
- 13:15-14:15 **Plenary Lecture: Pavel Hobza**
Institute of Organic and Biochemistry, Prague
Benchmark Quantum Chemical Calculations on Stabilization Energies in the DNA Base Pairs
- 14:15-14:40 **Jindrich Fanfrlík**
Institute of Organic and Biochemistry, Prague
Interactions of Metallocarboranes with Biomolecules: QM/MM Calculations Refine the Crystal Structure of HIV-1 Protease-Metallocarborane Complex

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- 14:40-15:05 **Wolfgang Wenzel**
Department of Physics, U Dortmund
Free-energy based all-atom protein modelling with
worldwide distributed computational resources
- 15:05-15:20 Coffee break
- 15:20-15:45 **Sebastian Radestock**
Institute of Pharmacy, U Kiel
Constraint network analysis: Exploiting the link
between protein rigidity and thermostability
- 15:45-16:10 **Jan Řezáč**
Institute of Organic and Biochemistry, Prague
“On the fly” ab initio MD simulations of complex
molecular systems
- 16:10-16:30 **Poster & Lecture awards / Closing remarks**



P1	Susanne Aust	A Novel Class of Inhibitors for Prolyl Endopeptidase derived from Docking Analysis and CoMSIA studies
P2	Kristin Engels	Cyclin-Dependent Kinases of Apicomplexan Parasites as Target Proteins for the Rational Design of Antiparasitic Drugs
P3	Stephanie Gulde	Application of MOE's virtual screening for new ligands of a steroid hormone receptor
P4	Anselm H. C. Horn	Dynamics and Binding to a Model Inhibitor of Alzheimer Disease-Related Peptides A β 40 and A β 42
P5	A. Bauer-Mehren	Combination of direct and indirect approaches to study the D2/5-HT2A selectivity of antipsychotic drugs
P6	Monika Nocker	Flexibility of Aldose Reductase: Opening of a novel subpocket upon ligand binding
P7	Mario Dejung	Web interface with advanced query properties for the Binding Interface (BIF) database
P8	Alexander Entzian	Classification of the Amino Acids on the basis of structural data
P9	Volker Hähnke	PhAST – Pharmacophore Alignment Search Tool
P10	A. Koch	Experimental and calculated NMR parameters
P11	Tobias Heintz	Comparing Natural Product (NP) and non-NP Datasets at an Atomic Scale
P12	Anica Lämmermann	NMR and theoretical investigations of intramolecular hydrogen bonding
P13	Björn Loeprecht	Prediction of Blood Brain Distribution with KNIME
P14	Frank Beierlein	QM/MM Binding Free Energy Calculations
P15	Marcel Youmbi Foka	Prediction of the Solvation Free Energy using a Combination of Semiempirical Self-Consistent Reaction Field Calculations and the Local Energy Properties

