

B-IT/ PICB Workshop “Computational Life Sciences”

January 25, 2010, 11:00 – 17:00 hours

Venue: B-IT, Dahlmannstraße 2, 53113 Bonn, Rheinsaal, organised by: B-IT Research School
Contact for the workshop registration: Dr. Alexandra Reitelmann, alexandra.reitelmann@bit.uni-bonn.de

Program

- 11:00 **Introduction**
Prof. Dr. Armin B. Cremers, University of Bonn
- 11:10 **Biomolecular Simulations of Proteins at PICB/Shanghai**
Prof. Dr. Klaus Gerwert, University of Bochum and PICB Shanghai
- 11:35 **QM/MM Simulations on the Hydrolysis Mechanisms of RAS**
Till Rudack, University of Bochum
- 12:00 **Insights into Odorant Recognition via Molecular Dynamics Simulations**
Dr. Steffen Wolf, University of Bochum
- 12:25 **Coffee Break**
- 12:40 **Efflux Pump-mediated Antibiotics Resistance - Insights from Computational Structural Biology**
Dr. Christian Kandt, University of Bonn
- 13:05 **Navigating Biological Activity Landscapes**
Prof. Dr. Jürgen Bajorath, University of Bonn
- 13:30 **Lunch at Deutsche Welle**
- 14:45 **The Challenge of Multi-Scale Modeling from High Content Imaging Data**
Prof. Dr. Thomas Berlage, Fraunhofer FIT and RWTH Aachen
- 15:10 **Tree Assignments and their Application in Bioimaging**
Dr. Axel Mosig, PICB Shanghai
- 15:35 **Coffee Break**
- 15:50 **Conditional Random Fields: Feature Modelling and Applications in Named Entity Recognition**
Roman Klinger, Fraunhofer SCAI
- 16:15 **Learning from Perturbation Effects**
Prof. Dr. Holger Fröhlich, University of Bonn
- 16:40 **Closing Statements**
Prof. Dr. Armin B. Cremers and Prof. Dr. Klaus Gerwert