Workshop GPCR-Modeling
Research Training Group GRK1910

Venue: Computer-Chemie-Centrum, Nägelsbachstr. 25, Erlangen
Seminarraum (2.206)

Program

	09:30 - 09:40	Welcome (Tim Clark)	
computational groups	09:40 – 10:00	The Challenges of Simulation	Tim Clark
	10:00 - 10:20	Binding pathway of histamine to the hH4R observed by unconstrained MD simulations	Andrea Strasser *Regensburg*
	10:20 - 10:40	Pharmacophore model optimization via conformer preselection	Thomas Sommer *Erlangen*
	10:40 - 11:00	Coffee break	
	11:00 - 11:20	GPCR-G Protein Modeling	Ralf Kling *Erlangen*
	11:20 - 11:40	Modeling of GPCR Dimerization	Jonas Kaindl *Erlangen*
	11:40 - 12:00	Free-Energy Mapping for the AVP/VR2-system	Noureldin Saleh *Erlangen*
	12:00 - 14:00	Lunch break	
experimental groups	14:00 - 14:30	Bivalent ligands - can computational methods help to investigate the binding mode?	Kilian Kuhn/Andrea Pegoli *Regensburg*
	14:30 – 15:00	Exploration of CXCR3 Functionality via Computational Studies	Lampros Milanos *Erlangen*
	15:00 - 15:30	Coffee break	
	15:30 - 16:00	Mimicking protein-protein interactions through peptide-peptide interactions: HIV-1 gp120 and CXCR4	Johannes Lach *Erlangen*
	16:00 - 17:00	Round Table Discussion – Modeling in GRK1910	
	17:00 – 21:00	Bierkeller-Event	