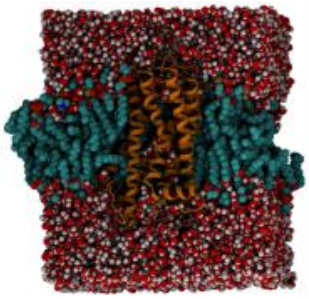
proteinformatics

Molecular Modeling Course WS 2021 / 8 SWS

AG Prof. Dr. Peter Hildebrand, special guest: Dr. Georg Kuenze (AG Meiler)



We are pleased to offer a course in Molecular Modelling, which includes a lecture series at the beginning of the semester **(Tue 17:00-18:30)** and a three-week practical course **(22.11.-10.12.2021).** The focus of the course is on modelling the 3D structure of (mainly membrane) proteins and studying their dynamics. The key technology you will be introduced to is **molecular dynamics simulations**, which link structure to dynamics by allowing exploration of the conformational energy landscape accessible to protein molecules. After a three-day introduction into molecular modeling with the well-established ROSETTA software, which is used for structure determination and protein design, you will be introduced to molecular dynamics simulations at both a theoretical and practical level. Not only will you use a standard method to perform molecular dynamics simulations, but you will also learn the importance of analyzing the obtained trajectory data using a number of different tools, including visualisation, advanced sampling or machine learning methods. In order to be able to interpret the simulation data, you will gain insights into the kinetics of biological systems and their application to the pharmacology of **G protein-coupled receptors**. Finally, we will relate the insights gained from computational analysis to experimental biophysical or biochemical methods. We are happy to provide all students with pre-loaded software that will be required during the course. The practical course is accompanied by a lecture series. All dates and topics are detailed in the attached table. Familiarity with Linux and analysis tools is an advantage, but not a must.

Contact:

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Theoretical lectures:

Date	Time	Topic	Lecturer
Tuesday 19.10.2021	17:00-18:30	Proteins are dynamic I	Prof. Dr. Peter Hilderbrand
Tuesday 26.10.2021	17:00-18:30	Proteins are dynamic II	
Tuesday 02.11.2021	17:00-18:30	Proteins are dynamic III	
Tuesday 09.11.2021	17:00-18:30	Proteins are dynamic IV	
Tuesday 16.11.2021	17:00-18:30	Introduction to Rosetta	Dr. Georg Kuenze

Practical courses:

Date	Time	Topic	Lecturer
Monday 22.11.2021 (Day-1)	10:00-10:30	Introduction, handing laptops	Dr. Hossein Batebi
	10:30-12:00	Short talk: Rosetta input/output & Navigating Rosetta Short talk: Rosetta energy function	Dr. Georg Kuenze
	13:00-14:30	Tutorial 1: Structure preparation and scoring	
	15:00-16:30	Tutorial 2:Comparative modeling of a G protein-coupled receptor	

Date	Time	Topic	Lecturer
Tuesday 22.11.2021 (Day-2)	10:00-12:00	Short talk: Protocol development with Rosetta Scripts Tutorial 3: Protein-small ligand docking	Dr. Georg Kuenze
	13:00-14:30	Short talk: Model evaluation	
	15:00-16:30	Tutorial 4: Antibody-antigen docking	

Date	Time	Topic	Lecturer
Wednesday 23.11.2021 (Day-3)	10:00-12:00	Tutorial 5: Single-state and multi-state protein design	Dr. Georg Kuenze
	13:00-14:30	Short talk: Using experimental data with Rosetta	
	15:00-16:30	Tutorial 6: Scaffolding and epitope grafting	

Date	Time	Topic	Lecturer
Thursday 25.11.2021 (Day-4)	10:00-12:00	Key concepts in machine learning. Regression and classification. Artificial neural networks as main example	Dr. René Staritzbichler
	13:00-14:30	Simple but useless example: a sinus predictor. A first and straightforward try.	
	15:00-16:30	Identification of limitations/problems. A second and more efficient approach.	

Date	Time	Topic	Lecturer
Friday 26.11.2021 (Day-5)	10:00-12:00	Biological example: predicting helices from protein sequence. Data collection/inspection.	Dr. René Staritzbichler
	13:00-14:30	Data representation: translating amino acids into descriptors.	
	15:00-16:30	Training. Evaluation: the confusion matrix. Optimization: develop own concepts.	

Date	Time	Topic	Lecturer
Monday 29.11.2021 (Day-6)	10:00-12:00	Bridging the Microscopic and Macroscopic	Dr. Hossein Batebi
	13:00-14:30	What makes molecular dynamics work?	
	15:00-16:30	From Quantum mechanics to force field	

Date	Time	Topic	Lecturer
Tuesday 30.11.2021 (Day-7)	10:00-12:00	Setup of a GPCR MD simulation	Dr. Alexander Vogel
	13:00-14:30		
	15:00-16:30		

Date	Time	Topic	Lecturer
Wednesday 01.12.2021 (Day-8)	10:00-12:00	From minimization to equilibrium and production runs.	Dr. Hossein Batebi
	13:00-14:30	How to run MD simulations on cluster?	
	15:00-16:30	Sanity check of minimization and equilibrium.	

Date	Time	Topic	Lecturer
Thursday 02.12.2021 (Day-9)	10:00-12:00	Visualization of MD trajectory (VMD).	Dr. Hossein Batebi
	13:00-14:30	Initial analysis checking stability and sanity of production runs.	
	15:00-16:30	How to look at the trajectory? What we can learn from generated dynamics?	

Date	Time	Topic	Lecturer
Friday 03.12.2021 (Day-10)	10:00-12:00	How can we run MD simulations so fast?	Dr. Alexander Vogel
	13:00-14:30	Example from actual science: Comparison of MD simulations with experiments.	
	15:00-16:30	Example from actual science: Comparison of MD simulations with experiments.	

Date	Time	Topic	Lecturer
Monday 06.12.2021 (Day-11)	10:00-12:00	Adaptive sampling and kinetic models.	Dr. Guillermo Pérez Hernández
	13:00-14:30	Basic MD trajectory analysis.	
	15:00-16:30	Our lab-made tool (MDCIAO)	

Date	Time	Topic	Lecturer
Tuesday 07.12.2021 (Day-12)	10:00-12:00	General introduction to enhanced sampling methods in molecular dynamics simulations with focus on metadynamics simulations	Dr. Passainte Ibrahim
	13:00-14:30	General setup of metadynamics simulations	
	15:00-16:30	Analysis of metadynamics simulations	

Date	Time	Topic	Lecturer
Wednesday 08.12.2021 (Day-13)	10:00-12:00	Electron transfer? Introduction to multiscale modelling QM/MM.	Dr. Hossein Batebi
	13:00-14:30	Introduction about protonation states and pKa values, methods to evaluate pKa values like constant pH simulations	Florian Seufert
	15:00-16:30	Generating an APBS surface with PDB2PQR and APBS. Evaluating protonation states with PropKa.	

Date	Time	Topic	Lecturer
Thursday 09.12.2021 (Day-14)	10:00-12:00	How to write a scientific report based on computational analysis?	Dr. Hossein Batebi
	13:00-14:30	Programing and data analysis in computational techniques.	Dr. Guillermo Pérez Hernández
	15:00-16:30	Computational approaches in natural science, yesterday, today and tomorrow.	Dr. René Staritzbichler

Date	Time	Topic	Lecturer
Friday 10.12.2021 (Day-15)	10:00-12:00	Computational techniques and drug design.	Dr. Passainte Ibrahim
	13:00-14:30	From experiments to computational techniques.	Florian Seufert
	15:00-16:30	Final remarks and conclusion	Dr. Hossein Batebi