

Theoretische und Computergestützte Biophysik (WS 2018/19)

Theoretical and Computational Biophysics

Helmut Grubmüller (HG), Bert de Groot (BdG)

Tutor for Practical Trainings Leonard Heinz (LH)

Modul B.Phy.5648 (Lehramt: M.Phy.710.Mp)

Mondays 16:00-17:30 in Lecture Hall HS3 (A0.105) and PC-Pool C.00.110, Physics Faculty

Date	Topic	Type/Room
2018-10-15	Introduction, protein structure and function, molecular dynamics, approximations, numerical integration (HG)	L1 = Lecture in lecture hall 3
2018-10-22	Introduction, protein structure and function, molecular dynamics, approximations, numerical integration (BdG)	P1= Practical training in PC-Pool C.00.110
2018-10-29	Tertiary structure, force field contributions, efficient algorithms, protonation, periodic boundaries, solvent, ions, NVT/NPT ensembles (BdG)	Lecture 2
2018-11-05	Protein data bank, structure determination by NMR / x-ray, refinement (HG)	Lecture 3
2018-11-12	Tertiary structure, force field contributions, efficient algorithms, protonation, periodic boundaries, solvent, ions, NVT/NPT ensembles (BdG)	Practical Training 2
2018-11-19	Protein data bank, structure determination by NMR / x-ray, refinement (BdG)	Practical Training 3
2018-11-26	Bioinformatics: Sequence alignment & evolution, structure prediction, homology modelling (HG)	Lecture 4
2018-12-03	Bioinformatics: Sequence alignment & evolution, structure prediction, homology modelling (BdG)	Practical Training 4
2018-12-10	Monte Carlo, normal mode analysis, principal components (HG)	Lecture 5
2018-12-17	Monte Carlo, normal mode analysis, principal components (BdG)	Practical Training 5
2019-01-07	Charge transfer & photosynthesis, electrostatics methods (HG)	Lecture 6
2019-01-14	Charge transfer & photosynthesis, electrostatics methods (BdG)	Practical Training 6
2019-01-21	Aquaporin / ATPase: two examples from current research (HG)	Lecture 7
2019-01-28	Aquaporin / ATPase: two examples from current research (BdG)	Practical Training 7

Exam Dates: Feb/March 2019

11.-15. February 2019

11.-21. March 2019

Lecture period 15.10.2018-01.02.2019

Semester break 22.12.2018-06.01.2019