

Lecture with practical training: Theoretical and Computational Biophysics by Helmut Grubmüller (HG), Bert de Groot (BdG), and Jochen Hub (JH)

Winter Term 2013/2014

Mondays 16:15-17:45 in HS3 (A0.105) or SR1 (A1.101), Physics Faculty

Date	Topic	Type
2013-10-21	Introduction, protein structure and function, molecular dynamics, approximations, numerical integration (HG)	L = Lecture in lecture hall 3
2013-10-28	Introduction, protein structure and function, molecular dynamics, approximations, numerical integration (JH)	P= Practical training in seminar room SR1
2013-11-04	Tertiary structure, force field contributions, efficient algorithms, electrostatics methods, protonation, periodic boundaries, solvent, ions, NVT/NPT ensembles (JH)	L
2013-11-11	Tertiary structure, force field contributions, efficient algorithms, electrostatics methods, protonation, periodic boundaries, solvent, ions, NVT/NPT ensembles (BdG)	P
2013-11-18	Protein data bank, structure determination by NMR / x-ray, refinement (JH)	L
2013-11-25	Protein data bank, structure determination by NMR / x-ray, refinement (BdG)	P
2013-12-02	Monte Carlo, normal mode analysis, principal components (HG)	L
2013-12-09	Monte Carlo, normal mode analysis, principal components (BdG)	P
2013-12-16	Bioinformatics: Sequence alignment & evolution (JH)	L
Christmas Holidays		
2014-01-06	Bioinformatics: Sequence alignment & evolution (BdG)	P
2014-01-13	Structure prediction, homology modeling (HG)	L
2014-01-20	Structure prediction, homology modelling (BdG)	P
2014-01-27	Aquaporin / ATPase: two examples from current research (HG)	L
2014-02-03	Aquaporin / ATPase: two examples from current research (BdG)	P