Theoretische und Computergestützte Biophysik (WS 2014/15)

Theoretical and Computational Biophysics

Helmut Grubmüller (HG), Bert de Groot (BdG) and Jochen Hub (JH)

Modul B.Phy.5648

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

Date	Topic	Type/Room
2014-10-20	Introduction, protein structure and function, molecular dynamics, approximations, numerical integration (HG)	L1 = Lecture in lecture hall 3
2014-10-27	Introduction, protein structure and function, molecular dynamics, approximations, numerical integration (JH)	P2= Practical training in seminar room SR1
2014-11-03	Tertiary structure, force field contributions, efficient algorithms, protonation, periodic boundaries, solvent, ions, NVT/NPT ensembles (JH)	L2
2014-11-10	Tertiary structure, force field contributions, efficient algorithms, protonation, periodic boundaries, solvent, ions, NVT/NPT ensembles (BdG)	P2
2014-11-17	Protein data bank, structure determination by NMR / x-ray, refinement (JH)	L3
2014-11-24	Protein data bank, structure determination by NMR / x-ray, refinement (BdG)	P3
2014-12-01	Monte Carlo, normal mode analysis, principal components (HG)	L4
2014-12-08	Monte Carlo, normal mode analysis, principal components (BdG)	P4
2014-12-15	Bioinformatics: Sequence alignment & evolution, structure prediction, homology modelling (JH)	L5
2015-01-05	Bioinformatics: Sequence alignment & evolution, structure prediction, homology modelling (BdG)	P5
2015-01-12	Charge transfer & photosynthesis, electrostatics methods (HG)	L6
2015-01-19	Charge transfer & photosynthesis, electrostatics methods (BdG)	P6
2015-01-26	Aquaporin / ATPase: two examples from current research (HG)	L7
2015-02-02	Aquaporin / ATPase: two examples from current research (BdG)	P7

Exam Dates: February 2015

23.+24.02.2015

2.-5.3.2015