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Exploring Biomolecules in 3D: Principles and Applications of Computational Structural Biology

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13.-20. August 2021 I virtually via Zoom I Lecture: 3-6pm CEST I Lab: 7-10pm CEST

Program

Date	Program	
13.08.2021	Computer setup • introduction to the Linux command line • shells • Linux filesystem • text editors • data processing tools	Lab
16.08.2021	Fundamentals of protein structure and protein structure determination • data representation and databases • visualization of protein structures	Lecture
	De novo protein structure prediction with ROSETTA • scoring and analysis of protein structures with ROSETTA • protein structure prediction with EPR data	Lab
17.08.2021	Prediction of protein structure in 1D (secondary structure, membrane regions, solvent accessibility) • Homology modeling • De novo protein structure prediction • Loop closure problem	Lecture
	Sequence alignment • structure-based alignment • threading • comparative modeling of membrane proteins with ROSETTACM • ROSETTA membrane scoring function	Lab
18.08.2021	The ROSETTA scoring function • Comparison and evolution of protein structures • Protein-protein docking	Lecture
	Protein-protein docking with ROSETTADOCK • low-resolution docking and high-resolution refinement • experimental restraints	Lab
19.08.2021	Protein-ligand docking • structure-based virtual screening	Lecture
	Protein-ligand docking with ROSETTALIGAND • generation of small molecule conformers and ROSETTA parameter files	Lab
20.08.2021	Protein engineering • Antibody and immunogen design	Lecture
	Protein design with ROSETTA • single-state and multi-state design	Lab

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