UNIVERSITÄT LEIPZIG

SFB1423

VANDERBILT UNIVERSITY

MKF / SFB1423 Module

Computational Design and Directed Evolution of Therapeutic Peptides

AIMS

Teach theoretical and practical aspects of computational design and directed evolution of therapeutic peptides.

COURSE DESCRIPTION

Peptides as therapeutics are an emerging class of therapeutics modalities, due to their high binding affinities and specificities. Here we will discuss their characteristics as therapeutic class and give an overview on recent and future developments. Furthermore, we highlight strategies for identification and optimization of peptide therapeutics. We will also cover emerging technologies for structure-based computational design of peptides using Rosetta and new AI tools. Specifically, we will train students the theoretical background of computational techniques for peptide design and provide hands-on training with respect to engineering peptides consisting of genetically encoded but also non-canonical amino acids.

METHODS

Molecular visualization of peptide structures with Pymol, prediction of peptide-receptor complexes with AlphaFold, flexible peptide docking with Rosetta, design of peptide binders with ProteinMPNN, design of peptides consisting of non-canonical amino acids with Rosetta

16.-19.12.24

1-5 PM

BBZ, Deutscher Platz 5, Seminar room 1

Registration

Please send an Email to **albrecht@uni-leipzig.de**.

Funded by
Max Kade Foundation
Vanderbilt-Leipzig University Partnership

SCHEDULE

Monday	**Christina Lamers**	**Lecture: Peptide Therapeutics**
24/12/16, 1-5 PM	*Alexander Zlobin*	Lab: "AlphaFold for protein-peptide complexes"
Tuesday	**Allison Walker**	**Lecture: Computational Design and Directed Evolution of Therapeutic Peptides**
24/12/17, 1-5 PM	*Moritz Ertelt*	Lab: "Introduction to Rosetta and FlexPepDock"
Wednesday	**Leonard Kaysser**	**Lecture: Bioactive natural product peptides**
24/12/18, 1-5 PM	**Clara T. Schoeder**	**Lecture: Deep learning versus classical methods for peptide generation and how to combine towards lab experiment**
	Felipe Engelberger	Lab: "Peptide design with ProteinMPNN and BindCraft"
Thursday	**Annette Beck-Sickinger**	**Lecture: Experimental methods to confirm computational methods**
24/12/19, 1-5 PM	*Felipe Engelberger, Moritz Ertelt*	Lab A: "Cyclic Peptide Design"
	Mateusz Skłodowski	Lab B: "Peptide design with non-canonical residues"
Friday		*Exam (optional)*
24/12/20, 9 AM		

Keywords

1 ETCS block Course, 16 hours presence / 60 hours self-study
Exam (optional + 1 ETCS) on Friday December 20, 2024
Literature will be shared with students via email
Venue: BBZ, Seminar Room 1 (Deutscher Platz 5)
Lecture portion virtually via Zoom

REGISTRATION

Students, postdocs, and faculty who wish to audit the class are welcome. Please register online (https://tinyurl.com/238vyzfm) as we have limited seating for the laboratory sections.

CONTACT
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Leipzig-Vanderbilt University Partnership
https://research.uni-leipzig.de/vanderbilt/