

1 day Soft Skill training “Applying for research positions” will take place in early summer.

6 April, Wednesday

Lectures on Computational Methods in Drug Discovery

The course will comprise lectures covering computational methods as applied to pre-clinical drug discovery. The purpose of the lectures is to provide a detailed view on the role of modern computational technologies, e.g. molecular simulations and machine learning in lead identification and optimization.

Scientific skills: Basic understanding on the key aspects of lead optimization;
Application of basic cheminformatics and structure-based design techniques

14:00-15:00	Artificial Intelligence in Drug Discovery (Nils Weskamp)
15:00-16:00	Computational Chemistry in Drug Discovery at BI (Oliver Hucke)
16:00-17:00	Computational Chemistry and Protein Structures (Christofer Tautermann)
17:00-17:30	Quantum Computing in Drug Discovery (Christofer Tautermann)

Zoom Meeting

7 April, Thursday

Drug Discovery (Medicinal Chemistry and Structural Biology /Biophysics)

The course will consist of presentations and lectures that cover a general overview on modern drug discovery as well as details on a broad range of disciplines and functions. Presentations will be given by senior scientist with multiple years of experience in drug discovery.

- | | |
|----------------------------------|--------------------------------------------------------------------------------------------------------------------------|
| 9-9.40
(Thorsten Oost) | Introduction to Medicinal Chemistry at Boehringer Ingelheim |
| 9.40-11.40
(Marc Grundl) | Basic Principles of Medicinal Chemistry and Lead Optimization |
| 11.40-12.20am
(Thorsten Oost) | Drug Discovery Project: STING Agonists for Immunooncology |
| 14:00-15:15pm
(Herbert Nar) | Role of Structural Biology and Biophysics in Drug Discovery |
| 15:30-16:45 | Crystal structure of CC chemokine receptor 2A provides insights for the design of selective antagonists (Gisela Schnapp) |

Zoom meeting

8 April, Friday

The ESR presentations: 15 min talk, followed by a 10 min discussion.

9:00 – 9:25	Seonwoo Lee (EPFL) - TBA
9:25 – 9:50	Iga Jakóbowska (Intana) - A High-Throughput Cellular Screening Assay for Small-Molecule Inhibitors Binding to PffNT
9:50 – 10:15	Abhinav (UFCH) - pH dependent calcium effects on lipid membrane organization
10:15 – 10:40	Bingxin Chu (EPFL) - TBA
10:40 – 11:00	break
11:00 – 11:25	Nathan Hugo Epalle (CAU) - Investigating the role of proton collecting antenna in lactate transporters
11:25 – 11:50	Satyaranjan Bharambar Biswal (HUJI) - Comparative Analysis of Collagen Hydration from MD simulations with Polarizable and Non-Polarizable Force Fields
11:50 – 12:15	Alejandro Martinez (USAAR) - Binding mode characterization of PffNTinhibitors through Docking and MD simulations
12:15 – 12:40	Bhav Kapur (BI) - GPR68: A Proton Sensing GPCR
12:40 – 13:40	Lunch break
13:40 – 14:05	Stefania Brescia (JKU) - Quantitative assessment of Hv1-mediated proton flux
14:05 – 14:30	Anna Maznichenko (JKU) - Protons waves originating from a membrane transporter
14:30 – 14:55	Honey Jain (FUB) - Dynamic hydrogen-bond networks for proton transfers in Hv1
14:55 – 15:20	Iuliana –Marilena Andrei (CNRS) – TBA
15:20 – 15:40	break
15:45 –	Supervisory board meeting (the members got the Zoom link via Email)

Zoom Meeting