A U S H A N G

FREIE UNIVERSITÄT BERLIN
Fachbereich Mathematik und Informatik

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D I S P U T A T I O N

Montag, 13.02.2023, 13:00 Uhr

WebEx

Disputation über die Doktorarbeit von

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Thema der Dissertation:
Machine Learning for Kinase Drug Discovery

Thema der Disputation:
Virtual screening in computer-aided drug discovery: molecular encodings and deep learning models

Die Arbeit wurde unter der Betreuung von **Prof. Dr. F. Noé** durchgeführt.

Abstract: Drug design is a time-consuming and expensive process that requires several iterations in the "design-make-test-analyse" cycle. In order to save time, costs, and reduce animal testing, computer-aided drug design (CADD) can be helpful in assisting diverse stages of drug campaigns.
In this talk, I will explain how virtual screening (VS), a mature CADD technique, can be applied to prioritize promising compounds. Since VS pipelines require a computational representation of molecular entities, I will describe methods to numerically encode molecular information, from the ligand, protein, and protein-ligand complex perspectives. Special focus will be given to protein kinases, a well-studied family of drug targets. Deep learning models in VS will be presented and open challenges in CADD will be discussed.

Die Disputation besteht aus dem o. g. Vortrag, danach der Vorstellung der Dissertation einschließlich jeweils anschließenden Aussprachen.

Interessierte werden hiermit herzlich eingeladen

Der Vorsitzende der Promotionskommission
Prof. Dr. F. Noé