

DATA SCIENCE COLLOQUIUM

Dr. Christoph Grebner

Computational Chemist,
Sanofi-Aventis Deutschland GmbH,
Frankfurt, Germany

Thursday, January 23rd, 2025
@ 10 am | On-Site & Online

Artificial Intelligence in Computer-Assisted Drug Design

Drug design is a resource-demanding process that necessitates mining the incredibly large chemical space and includes expensive and time-consuming experiments. In the last decades, computer-assisted drug design (CADD) has become an indispensable tool to support and facilitate this process. Recent developments in the field include incorporating machine learning models at various steps of the drug discovery process and improving algorithms for searching the chemical universe. The talk will highlight key steps in computer-assisted drug design and discuss upcoming opportunities and challenges for AI technologies in CADD. Dr. Christoph Grebner is a computational chemist at Sanofi with several years of experience supporting drug design projects with CADD.

Chair: Prof. Matthias Rarey

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