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University of Münster Corrensstraße 36
Institute of Organic Chemistry 48149 Münster

6TH INTERNATIONAL MINI-SYMPOSIUM

ON

MOLECULAR MACHINE LEARNING

JANUARY 18TH 2024 | 3:00 PM (UTC +1)

Francesca Grisoni *Eindhoven University of Technology*, NL
Jens Meiler *University of Leipzig*, GER; *Vanderbilt University*, USA
Franziska Schoenebeck *RWTH Aachen*, GER
Fred Manby *Iambic Therapeutics*, USA

Chair:
Frank Glorius *University of Münster*, Germany

SPEAKERS

Francesca Grisoni received her Ph.D. in the group of Prof. Roberto Todeschini (University of Milano-Bicocca). After working in industry for a year, she joined at ETH Zurich (Prof. Gisbert Schneider's group) as a postdoctoral researcher and worked on scaffold hopping approaches and generative deep learning. In 2021, she was appointed as an Assistant Professor at TU/e. Her current team works at the intersection of chemistry, biology, and computer science, to advance the potential of machine learning for drug discovery.

Jens Meiler obtained his PhD working in the laboratory of Christian Griesinger at the Goethe University in Frankfurt. In January 2020, with an Alexander von Humboldt Professorship, Jens Meiler became director of the newly founded Institute for Drug Discovery at Leipzig University. Simultaneously, he continues in his role as Professor at Vanderbilt University. In his research he fuses computational and experimental efforts to investigate proteins, and their interactions with small molecule substrates, therapeutics, or probes.

Franziska Schoenebeck received her PhD in 2008 from the University of Strathclyde (Glasgow, UK) working with Prof. J. A. Murphy. After a postdoctoral stay with Prof. K. N. Houk at UCLA, she started her independent career at the ETH Zürich in 2010. In 2013 she was appointed Professor at the RWTH Aachen University, where she was promoted to Full Professor and Chair in 2016. Her research is based at the interface of organic, mechanistic and computational chemistry with an emphasis in homogeneous metal catalysis.

Fred Manby is Co-founder and CTO at Iambic Therapeutics. After a BSc and PhD in Chemistry at the University of York, he pursued a 20-year academic career, much of it as Professor of Theoretical Chemistry at the University of Bristol. His research on predicting properties of molecules spanned high-level quantum chemistry, dynamics and machine learning, together with creation of software to translate discoveries to impactful applications. platform, and its application in finding new medicines.

SCHEDULE: THURSDAY, JANUARY 18TH 2024

3:00 pm Introduction

3:10 pm **Francesca Grisoni**
Deep Learning for Drug Discovery in Low-Data Scenarios
Deep learning has had an incredible impact in various fields of science and technology, such as protein structure prediction and organic reaction planning. However, its success is more prominent when large-scale datasets are available. Drug discovery, on the other hand, is often a low-data endeavor, which limits the potential of 'out-of-the-box' deep learning approaches. This talk will reflect on the limitations of deep learning for drug discovery in low-data scenarios, and will illustrate some ongoing research to alleviate some of these challenges.

3:40 pm **Jens Meiler**
Artificial Intelligence, Ultra-Large Library Screening, and Citizen Scientists in Small Molecule Drug Discovery
I will summarize new technologies on small molecule drug discovery using artificial neural networks and ultra-large library screening. I will also review some of our efforts to develop Drugit, a citizen scientist game for drug discovery.

4:10 pm Break

4:30 pm **Franziska Schoenebeck**
Accelerated Catalyst Identification through Machine Learning
A machine learning workflow is discussed that requires as little as a handful of experimental data points by employing generalized parameter databases that are complemented with problem-specific in-silico data acquisition and clustering. The predictive power of this strategy for the challenging problem of speciation of catalysts will be shown as well as the ability to predict suitable ligands from virtual ligand space that has never been synthesized or tested before.

5:00 pm **Fred Manby**
Dealing with the Data Shortage for Machine Learning in Drug Discovery
"AI" is becoming ubiquitous in the space of drug discovery, as in so many other domains. A key challenge is that data points needed to train the most impactful models are expensive to obtain. Here I will talk through three primary strategies for addressing this, and how they're manifested at Iambic: (1) design of data-efficient algorithms; (2) automated generation of large datasets; (3) accessing broader classes of data through multimodal architectures.

Universität Münster

SPP 2363

Starting Times	
Beijing	9:00 pm
New Delhi	6:30 pm
Paris	3:00 pm
London	2:00 pm
New York	9:00 am

Please find the registration and
Zoom invitation using the following link:
www.uni-muenster.de/Chemie.oc/glorius/symposium_mml.html