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University of Münster Correnssstraße 40
Institute of Organic Chemistry 48149 Münster

3rd International Mini-Symposium on Molecular Machine Learning

April 29th 2021 | 3:00 pm (UTC +1)

Industry Edition

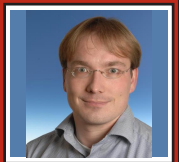
Nadine Schneider *Novartis*, CHE
Ola Engkvist *AstraZeneca*, SWE
Nils Weskamp *Boehringer Ingelheim*, GER
Patrick Riley *Google*, USA

Chair:
Frank Glorius University of Münster, Germany

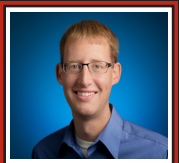
Speakers

Nadine Schneider is a researcher in the Computer-Aided Drug Design team in Global Discovery Chemistry at the Novartis Institutes for BioMedical Research (NIBR), Basel, Switzerland. She obtained her PhD in Molecular Modeling in the group of Prof. Matthias Rarey at the University of Hamburg, Germany after receiving a BSc and MSc in Bioinformatics from the Saarland University. In 2014 she joined NIBR for a postdoc focusing on Cheminformatics and Data Science under supervision of Gregory Landrum and Nikolaus Stiefl.

Ola Engkvist is head of Molecular AI in Discovery Sciences, AstraZeneca R&D. He did his PhD in computational chemistry at Lund University followed by a postdoc at Cambridge University. After working for two biotech companies he joined AstraZeneca in 2004. His main research interests are deep learning based molecular de novo design, synthetic route prediction and large scale molecular property predictions. He has published over 100 peer-reviewed scientific publications.



Nils Weskamp is heading a team of data scientists in the Computational Chemistry group at Boehringer Ingelheim in Biberach, Germany. Together with his colleagues, he applies a broad range of methods to support compound design in drug discovery and builds smart digital tools that support chemists in their daily work. His current research interests focus on explainable machine learning and the user experience of AI. Before joining BI, Nils obtained a PhD in Computer Science from University of Marburg, Germany.



Patrick Riley is a principal engineer and a senior researcher of the Applied Science team at Google Research. His team collaborates with scientists across organizations to apply Google's knowledge and experience in machine learning and data science to important problems in the natural sciences. Much of his recent work has focussed on machine learning applications for the chemistry of small molecules but has worked in fields as varied as materials science, protein design, and nuclear fusion.

Schedule: Thursday, April 29th 2021

3:00 pm Introduction

3:10 pm **Nadine Schneider**
Real-World Application of Machine Learning in Drug Discovery
Machine learning models are becoming more and more relevant for drug discovery. There is a big hope that novel algorithms and models can remedy the challenge of finding new drugs more efficiently. A very important prerequisite for this is better understanding the data before applying new models. Another critical point are the users, to make machine learning models effective and actionable they need to be accessible and integrated into the daily work of the chemists. In addition, education of the users is important to deepen their knowledge and create the right expectations on machine learning models. In this presentation, several of these aspects will be discussed using examples and learnings we made over the past years.

3:40 pm **Ola Engkvist**
Applying Artificial Intelligence for Drug Design
Machine learning (ML) and Artificial Intelligence (AI) have impacted many industrial sectors including the pharmaceutical industry. One area where applying ML/AI is suitable within a pharmaceutical company is drug design. By applying ML/AI together with automation there are opportunities to speed up the delivery of clinical candidates. In this talk there will be overview of AstraZeneca's efforts in applying ML/AI to small molecule drug design. Focus will be on deep learning based molecular de novo design and synthetic route prediction and the in-house developed platforms REINVENT for de novo design and AiZynth for synthetic route prediction.

4:10 pm Break

4:30 pm **Nils Weskamp**
Smart Digital Assistants to Support Molecule Design: Data, Algorithms & User Experience
Three key ingredients are needed to build smart digital tools that support scientists in their daily work: a foundation of well-connected high quality data, smart applications of modern data science methods and excellence in user experience. This talk will discuss the state of the art and remaining challenges in these fields.

5:00 pm **Patrick Riley**
DNA Encoded Small Molecule Libraries Meet Machine Learning
The use of AI/ML methods is often discussed in the drug discovery community. Many modern ML techniques rely on large data volumes, which are often not available. DNA Encoded Small Molecules Libraries (DELs) can provide somewhat noisy binding information for up to 10^{11} molecules, providing an excellent beginning for ML models. In this work, we train graph convolutional neural networks on DEL screening data, make predictions on commercial or easily synthesizable libraries, and use automated or automatable filters to choose compounds. In a large prospective study, we show that this approach is effective with an overall hit rate of ~30% at 30 µM and discovery of potent compounds for every target.

WWU Münster

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