DrugSpace 2023 Programme

BioSolveIT
expect actives!

Time (CEST)	May 24th (Wednesday)	May 25th (Thursday)
15:00-15:15	**BioSolveIT – Christian Lemmen** Welcoming Address	**BioSolveIT – Christian Lemmen** Welcoming Address
15:15-15:45	**Philippe Schwaller** École Polytechnique Fédérale de Lausanne "AI-Accelerated Organic Synthesis"	**Lewis Martin** OpenBench "Fast and Economical Hit Finding with Active Learning"
15:45-16:15	**Quentin Perron** Iktos "Yes, You Should Use AI for Medicinal Chemistry"	**Francesca Grisoni** Eindhoven University of Technology "Deep Learning for Drug Discovery: Challenges and Opportunities"
16:15-16:45	**Marcus Gastreich** BioSolveIT "Claw Machines for Exploding Chemical Spaces"	**Christoph Grebner** Sanofi "AI-Driven Mining of Accessible Chemical Spaces"
16:45-17:15	**Yurii Moroz** Chemspace "Making Virtual REAL: Creation and Use of the Giga-Scale Chemical Spaces"	**Lea El Khoury** Qubit "Application of Absolute Binding Free Energy Calculations to Predict the Binding Modes and Affinities of Protein-Protein Inhibitors"
17:15-17:45	**Daniel Kuhn** Merck "You Can't Improve What You Don't Measure –Measuring ML/AI Impact in Drug Discovery Projects"	**Nick Antonopoulos** DeepLab "Scalable and High-Throughput Deep Neural Virtual Screening"
17:45-18:15	**Dusan Petrovic** Nuvisan "Virtual Screening for Multiple Modalities"	**Connor Coley** Massachusetts Institute of Technology "Learning to Navigate Synthetically Accessible Chemical Space"
18:15-18:45	**Henry van den Bedem** Atomwise "An Efficient Graph Generative Model for Navigating Ultra-Large Combinatorial Synthesis Libraries"	

- Machine Learning
- Artificial Intelligence
- Neural Networks
- Big Data

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