2021 World Chemistry Leadership Meeting of 51st IUPAC General Assembly and 48th World Chemistry Congress

"The Future of Chemistry in the World of AI"

Tuesday – Wednesday August 17th – 18th, 2021

PROGRAM THE NETHERLANDS: Wednesday the 18th of August 2021, 09:00 – 12:00h (CET)

Moderator:	Prof. Dr. Timothy Noël, University of Amsterdam, The Netherlands
Panelists:	Dr. Ola Engkvist, AstraZeneca, Sweden
	Dr. Hugo Ceulemans, Janssen Research & Development, Belgium
	Dr. habil. Barbara Zdrazil, University of Vienna, Austria
	Prof. Dr. Maarten Honing, Maastricht University, The Netherlands

PROGRAM

08:50h Open digital room for participants

09:00h Opening and introduction
Welcome to The Netherlands by Prof. Dr. Timothy Noël

09:05h Set-up and introduction of panelists
Moderator explains set-up

Introduction of panelists

- Dr. Ola Engkvist (head of Molecular AI in Discovery Sciences, AstraZeneca R&D)
- Dr. Hugo Ceulemans (Scientific Director Discovery Data Sciences at Janssen)
- Dr. habil. Barbara Zdrazil (University of Vienna)
- Prof. Dr. Maarten Honing (Maastricht University). Please introduce yourself briefly

09:30h Discussing the themes
Short clip of introduction video is shown after which a corresponding statement is discussed.

Discovery: Processes and Tools of the Future
Determination: Candidates for Process Development and Optimization
Development: Products and services using AI in the Future
Impact: R&D Laboratories and Instrumentation of the Future
Information: Informatics, Datasets and Curation of the Future
Insight: Analysis and Modeling Chemical Research of the Future

11:30h General Q&A for remaining questions

11.50 Closing
Hand off to Montreal, inviting everyone in 2 years to join us in The Hague during IUPAC2023: www.iupac2023.org.

BIOGRAPHIES




Dr. Ola Engkvist
Dr. 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. He currently lead the Molecular AI department, where the focus is to develop novel methods for ML/AI in drug design, productionalize the methods and apply the methods to AstraZeneca's small molecules drug discovery portfolio. 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. He is adjunct professor in machine learning and AI for drug design at Chalmers University of Technology and a trustee for Cambridge Crystallographic Data Center.

Dr. Hugo Ceulemans
As Scientific Director Discovery Data Sciences at Janssen, Hugo Ceulemans currently heads a multidisciplinary team that supports drug discovery with machine learning approaches. This team advises on impactful data generation and combines new with existing data to formalize and improve biological and chemical criteria for molecule selection and design and to propose attractive and efficiently synthesizable molecules to make and test. Hugo holds the degrees of MD, MSc in Bioinformatics and PhD in Molecular Biology, and prior to joining Janssen in 2008, he completed postdoctoral fellowships in molecular and computational biology at the University of Leuven and in structural bioinformatics at the European Molecular Biology Laboratories in Heidelberg.

Dr. Habil. Barbara Zdrazil, Priv.-Doz.
Barbara is a group leader at the University of Vienna, and works as a safety data scientist for the European Bioinformatics Institute (EMBL-EBI). Her research is concentrated on integrating Data Science approaches into the Computational Molecular Design process. She focuses on off-targets (mainly SLC transporters), and develops automatized computational techniques to link heterogeneous data sources, perform bioactivity profiling, and generate predictive models – especially for toxicity predictions. In addition, Barbara is interested in large-scale data analyses including time trend analyses by utilizing public domain data. At EMBL-EBI, Barbara is contributing to Open Targets, a project which aims to enable systematic target identification and prioritization. During her PhD, Barbara mainly worked on QSAR models for P-glycoprotein modulators in Gerhard Eckers' lab (University of Vienna). During her postdoc under the supervision of Hans-Dieter Höltje (University of Düsseldorf) she focused on structure-based modelling of DNA polymerase alpha. Barbara contributed to many EU-funded projects (including eTOX, OpenPHACTS, EU-ToxRisk) and led a nationally funded FWF project focusing on modelling of hepatic transporters from 2017 - 2021. In 2020, she accomplished her Habilitation in Pharmacoinformatics. Barbara is also an Associate Editor for the Journal of Cheminformatics.

Prof. Dr. Maarten Honing

Prof. Dr. Maarten Honing graduated (1991) from the University of Amsterdam, with two major research projects; a. gasphase chemistry with FT-MS (Prof. dr. N. Nibbering) and post-column derivatization in LC-MS (Prof. dr. U.A.Th. Brinkman). He obtained his PhD degree (1995) from the VU University (Prof. dr.U.A. Th. Brinkman) with a Thesis studying ionization processes in LC-MS interfacing technologies. Between February 1995 to September 2017 he acted as analytical R&D laboratory manager and principal scientist at Pharma BioResearch, Organon and DSM Research. In addition, he was closely involved in TopInstitute Pharma and treasurer of "Top Institute COAST" (2008 – 2010). In 2013 he was appointed member of the TKI Chemistry Program council "Chemcial Sensing & Enabling Technologies". Currently he is a member of the Dutch Chemistry Council. In 2017 he continued his academic career as professor at the Maastricht University. His academic research interests comprise the design and development of process analytical technology strategies, investigating molecular interactions and conversions, preferably if flow-reactors. AI and ML form an unique tool in the unraveling of molecular interactions and e.g. photo induced ionization processes.