

## AI4b.io Webinars 12 & 13 April 2022

You are invited to join a selection or all Artificial Intelligence Lab for Bioscience (AI4b.io) webinars taking place on April 12 & 13. We are organizing this meeting for those interested in and active in the fields of Artificial Intelligence and Bioscience. The full webinar program is included in this document and covers topics ranging from large-scale manufacturing to microbiome-based precision nutrition, going from large to small scale. Experts active in these topics will present their in-depth insights. For each of the 5 webinars, a separate registration form is available. Once you register through one of those forms, an agenda item will be sent to you by e-mail so you can book time in your agenda. Please use the links below provided for each webinar. Please join and participate in the Q&A session.

### Details

**Type of meeting:** webinars

**Software platform:** Teams Live Meeting

**Date:** April 12 & 13

**Time zone:** CET

### *AI4b.io Steering Committee*

Marcel Reinders

Henk Noorman

Hans Roubos

### *AI4b.io Program Manager*

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If you have questions about these webinars, please send an e-mail to [Renger.Jellema@DSM.COM](mailto:Renger.Jellema@DSM.COM).

Webinar	Speaker	Affiliation	Time	Day
<a href="#">1</a>	Marcel Reinders Henk Noorman Hans Roubos	TU Delft + DSM	9:30-10:00	April 12th
	Michael Jensen	DTU	10:00-10:40	
<a href="#">2</a>	Stephan Heijl	Bio-Product B.V.	14:30-15:10	
<a href="#">3</a>	Peter Neubauer	TU Berlin	16:30-17:10	
<a href="#">4</a>	Jens Kober	TU Delft	9:30-10:10	April 13th
	Thomas Gorochowski	University of Bristol	10:10-10:40	
<a href="#">5</a>	Loïc Roch	Atinary	14:45-15:25	

Day 1, April 12<sup>th</sup>

Webinar 1 – register: <https://forms.office.com/r/aPGetu8WKD>

09:30 – 10:00 CET | Advancing Bioscience through Artificial Intelligence

Marcel Reinders<sup>1</sup>, Henk Noorman<sup>2</sup>, Hans Roubos<sup>2</sup>

<sup>1</sup> TU Delft, <sup>2</sup> DSM

Artificial intelligence is recognized as one of the key drivers of modern innovation in many disciplines, including food systems and biomanufacturing. DSM - a global science-based company in Health, Nutrition and Bioscience - has joined forces with Delft University of Technology and established the AI4b.io laboratory to explore new applications of artificial intelligence in bioscience and its industrial applications. Together, five lines of research have been established to explore how AI technologies can be used to optimize biomanufacturing at different scales: from factory unit planning and the development of digital twins of fermentation processes, to self-organizing laboratories and advanced microbial strain building cycles, to understanding the interaction between microbiomes and their hosts. Today, you will learn about the ambitions of AI4b.io and how we plan to solve the challenges.

10:00 – 10:40 CET | Engineering Cellular Metabolism using Machine Learning

Jie Zhang<sup>1</sup>, Søren Petersen<sup>1</sup>, Christine Pedersen<sup>1</sup>, Hector Garcia-Martin<sup>2</sup>, Mike Fero<sup>3</sup>, and Michael Krogh Jensen<sup>1</sup>

<sup>1</sup>Novo Nordisk Foundation Center for Biosustainability, Technical University of Denmark, Kgs. Lyngby, Denmark, <sup>2</sup>Joint BioEnergy Institute, Emeryville, CA, USA, <sup>3</sup>TeselaGen Biotechnology, San Francisco, CA 94107, USA

Leveraging advanced mechanistic modelling and the generation of high-quality multi-dimensional data sets, machine learning is becoming an integral part of understanding and engineering living systems. Among the different types of mechanistic models for simulating metabolism, genome-scale models are one of the most popular approaches. Yet, the predictive power of genome-scale models is often hampered by the limited knowledge and data available for the parameters affecting metabolic regulation. Here we present how mechanistic and machine learning models can complement each other in a combined approach enabling predictive engineering of yeast metabolism. From a single data-generation cycle, we demonstrate that this approach enables successful forward engineering of complex native and heterologous metabolisms in yeast, with the best machine learning-guided design recommendations improving titers and productivities compared to the best designs used for algorithm training. Taken together, this presentation will highlight the power of combining mechanistic and machine learning models to effectively direct metabolic engineering efforts.

Day 1, April 12<sup>th</sup>

Webinar 2 – register: <https://forms.office.com/r/g1PWz7aJqS>

14:30 – 15:10 CET | Helix engineering: combining the power of 3DM with AI to disrupt protein engineering

Stephan Heijl, Jeanine Boot, Bastiaan Brier, Tom van den Bergh, Bas Vroling, Henk-Jan Joosten  
Bio-Product B.V.

The high dimensionality and practically infinite size of the sequence space requires effective techniques to explore, navigate and improve proteins. Current techniques are underwhelming in their accuracy and ability to find novel variants. With its 3DM technology Bio-Product has long been at the forefront of providing protein engineering solutions. We automated 3DM-based search strategies to smartly select positions to mutate initially. We also developed a deep learning based ensemble architecture for the next rounds. Using multiple datasets we showed that this pipeline outperforms legacy machine learning methods on average by 71.5% when mutations were selected randomly and by 115% when the 3DM-based initial selection step was used. We have shown that with our technology, even as few as 50 initial mutations yield competitive hit rates.

Day 1, April 12<sup>th</sup>

Webinar 3 – register: <https://forms.office.com/r/s7vYErXqgj>

16:30 – 17:10 CET | From Screening to Production: a Holistic Approach of High-throughput Model-based Bioprocess Development

Peter Neubauer, Mariano Nicolas Cruz Bournazou  
Technische Universität Berlin, Germany

A significantly more efficient development of bioprocesses can only be achieved through a higher degree of automation and digitalisation. With the ultimate goal of generating a digital twin that describes the dynamics of the cell system across scales: (i) informative experiments (often fed-batch high-cell-density cultivations) must be optimally designed on a parallel scale, (ii) these experiments need to be optimally operated with advanced control tools, and combined with comprehensive process analytics, which in turn (iii) require automated operation of complex robotic systems running difficult nonlinear dynamic bioreactor processes.

In the KIWI-biolab, we integrate these sub-strategies using process control and optimization, AI and machine learning and demonstrate the advantages on different microbial bioprocesses to produce recombinant proteins.

Day 2, April 13<sup>th</sup>

Webinar 4 – register: <https://forms.office.com/r/ysEy51cMLz>

09:30 – 10:10 CET | Robots Learning (Through) Interactions

Jens Kober

TU Delft

The acquisition and self-improvement of novel motor skills is among the most important problems in robotics. I will discuss various learning techniques we developed that enable robots to have complex interactions with their environment and humans. Complexity arises from dealing with high-dimensional input data, non-linear dynamics in general and contacts in particular, multiple reference frames, and variability in objects, environments, and tasks. A human teacher is always involved in the learning process, either directly (providing data) or indirectly (designing the optimization criterion), which raises the question: How to best make use of the interactions with the human teacher to render the learning process efficient and effective?

10:10 – 10:40 CET | End-to-end experimental and machine learning workflows for predictive genetic design

Pierre-Aurelien Gilliot, Matthew J. Tarnowski and Thomas E. Gorochowski

School of Biological Sciences, University of Bristol, UK

High-throughput experiments combined with emerging machine learning (ML) technologies are enabling data-centric biological design workflows for synthetic biology. In this talk, I will introduce some of the ways my group are contributing to this area, both from an experimental perspective, where nanopore sequencing is being used to characterise diverse libraries of genetic parts, to improved data processing pipelines and the rigorous optimisation of machine learning models for predicting the function of genetic parts from sequence alone. I aim to show the value of considering these workflows from end-to-end and how this can help improve quality and reproducibility of results.

Day 2, April 13<sup>th</sup>

Webinar 5 – register: <https://forms.office.com/r/SvezTUZjqH>

14:45 – 15:25 CET | Atinary SDLabs: Revolutionize R&D with Machine Learning

Loïc Roch

Atinary, Lausanne, Switzerland

Atinary Technologies is a Swiss-American deeptech startup that develops market-leading ML algorithms and technology tools to revolutionize R&D and innovation of advanced materials.

In his talk, Dr. Roch will describe how Atinary SDLabs accelerates R&D by orders of magnitude by putting Machine Learning (ML) at the heart of the innovation process. Atinary's cloud-based platform SDLabs can integrate with off-the-shelf robotics and lab equipment to enable the Self-Driving Labs. Companies and users can deploy our ML solutions seamlessly in the cloud, starting with simulations or straight in wet labs.



AI4b.io is the Artificial Intelligence Lab for #Bioscience which was founded in 2021 by TU Delft and is funded by DSM. This laboratory is the first of its kind in Europe to apply artificial intelligence to full-scale #biomanufacturing, from microbial strain development to process optimization and factory scheduling. The lab is led by Professor Marcel Reinders, Director TU Delft Bioengineering Institute.