

Program

Welcome and Introduction

Chris Luebke, Arup Foresight

Talks

Drug Design of the Future

Gisbert Schneider, ETH Zurich

Enhancing Drug Discovery through In Silico Modelling

Jasmin Fisher, Microsoft Research and University of Cambridge

AI Guiding the Exploration of Chemical Space by DNA-encoded Chemistry

Robert Goodnow, Pharmaron

AI-Driven Smart Search through Design Space

Jennifer Listgarten, UC Berkeley

The Philosophy of (Artificial) Intelligence

Norman Sieroka, ETH Zurich

Q&A

Networking Reception

Social Media: @eth_en, #ETH2CAL

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«RETHINKING Drug Design»

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swissnex San Francisco

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Presented by ETH Zurich

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The challenges of discovering new pharmaceutical therapies present a multi-dimensional problem. Identifying viable drug candidates requires optimization – in parallel – of both efficacy and safety. In the midst of The Fourth Industrial Revolution, much excitement surrounds the potential of AI to further digital healthcare. How might we define “intelligent behavior” in the context of drug discovery? Essentially, an intelligent agent – either man or machine – demonstrates an ability to solve problems, to learn from experience, and to deal with new situations. With regard to these three central criteria, certain machine learning modalities, specifically autonomous adaptive systems, may constitute instances of AI.

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Speakers



Chris Luebke's interest in the built environment propelling him to pursue a multi-faceted education, beginning with engineering and culminating in a Doctorate in Architecture from ETH in Zurich, a city to which he remains deeply connected. Chris gained valuable experience as the protégé of esteemed Spanish Architect, Santiago Calatrava. He subsequently turned to his other love, education, by accepting teaching positions at several prestigious universities. In 1999, Chris joined Arup as the co-Director for Research and Development. A couple of years later, he formed the Foresight, Innovation and Incubation team, which has evolved into its present form as Research + Foresight + Innovation.



Gisbert Schneider is a full professor at ETH Zurich, holding the Chair for Computer-Assisted Drug Design, and the Associate Vice President for ETH Global. He received his PhD in Biochemistry from Freie Universität Berlin. He then joined Roche Pharma in Basel as a cheminformatics group leader. From 2002 to 2009, he was a full professor at Goethe-University in Frankfurt (Beilstein Endowed Chair). His research focuses on the integration of artificial intelligence into practical medicinal chemistry.



Norman Sieroka is the managing director of the Turing Centre Zurich and belongs to the core team of ETH's critical thinking initiative. He studied philosophy, physics, and mathematics in Heidelberg and Cambridge and received doctorates in both physics and philosophy. Norman Sieroka held positions as a guest professor at the Universities of Notre Dame (U.S.) and Bremen. His research focuses on conceptual questions regarding the exact sciences, the mind, and time.



Robert Goodnow completed his BS in chemistry at Georgetown University followed by a Ph.D. in natural products organic/ bioorganic chemistry at Columbia University. He continued research in oligosaccharide synthesis at Princeton University as an NIH Postdoctoral Fellow. Rob began his industrial career at Hoffmann-La Roche. In addition to many medicinal chemistry project leadership responsibilities, Rob has managed multiple outsourcing collaborations for pre-clinical discovery chemistry on a local and global level, eventually becoming the Global Leader of Medicinal Chemistry Outsourcing. Rob's research has also focused on the implementation of several chemistry platform technologies. These include small molecule targeted delivery of siRNA for therapeutic applications, analytical chemistry and DNA-encoded chemistry. Rob's efforts in medicinal chemistry have been focused on projects in oncology, inflammation and metabolic diseases. He has authored or co-authored more than 80 scientific papers, book chapters and patent applications. He edited a book entitled "A Handbook of DNA-Encoded Chemistry"; recently he edited Annual Reports in Medicinal Chemistry Vol. 50. In 2013, Rob joined AstraZeneca as the Executive Director of the Discovery Sciences Chemistry Innovation Centre leading efforts in chemical biology, fragment-based lead generation and computational chemistry. Rob joined Pharmaron as Vice President Innovation Chemistry in October 2016 responsible for shared risk research programs. Rob has a few hobbies: piano, running, and study of Asian languages.



Since Jan. 2018, **Jennifer Listgarten** is a Professor in the Department of Electrical Engineering and Computer Science, and Center for Computational Biology, at the University of California, Berkeley. She is also a member of the steering committee for the Berkeley AI Research (BAIR) Lab, and a Chan Zuckerberg investigator. From 2007 to 2017 she was at Microsoft Research, through Cambridge, MA, Los Angeles, and Redmond, WA. Before that, she completed her PhD in the machine learning group at the University of Toronto after an undergraduate degree in Physics from Queen's University in Kingston, Ontario. Jennifer's research interests are broadly at the intersection of machine learning, applied statistics, and molecular biology.



Jasmin Fisher is a Principal Researcher at Microsoft Research Cambridge. She is also an Associate Professor of Systems Biology in the Department of Biochemistry at the University of Cambridge. She is a member of the Cancer Research UK Cambridge Centre, Cambridge Systems Biology Centre and the Wellcome Trust-MRC Cambridge Stem Cell Institute. In 2016 she was elected Fellow of Trinity Hall, Cambridge. Jasmin received her Ph.D. in Neuroimmunology from the Weizmann Institute of Science in 2003. In 2007, Jasmin joined the Microsoft Research Lab in Cambridge. In 2009, she was also appointed a Research Group Leader in the University of Cambridge. Jasmin has devoted her career to develop methods for Executable Biology. She is a pioneer in using formal verification methods to analyse mechanistic models of cellular processes and disease. Her research group focuses on the development of computational models to study the molecular mechanisms of cancer in order to identify new and improved treatments for cancer patients. In 2017 Jasmin was named one of the Top Outstanding Female Leaders in the UK Healthcare by BioBeat. In 2018 she was elected Fellow of the Royal Society of Biology.