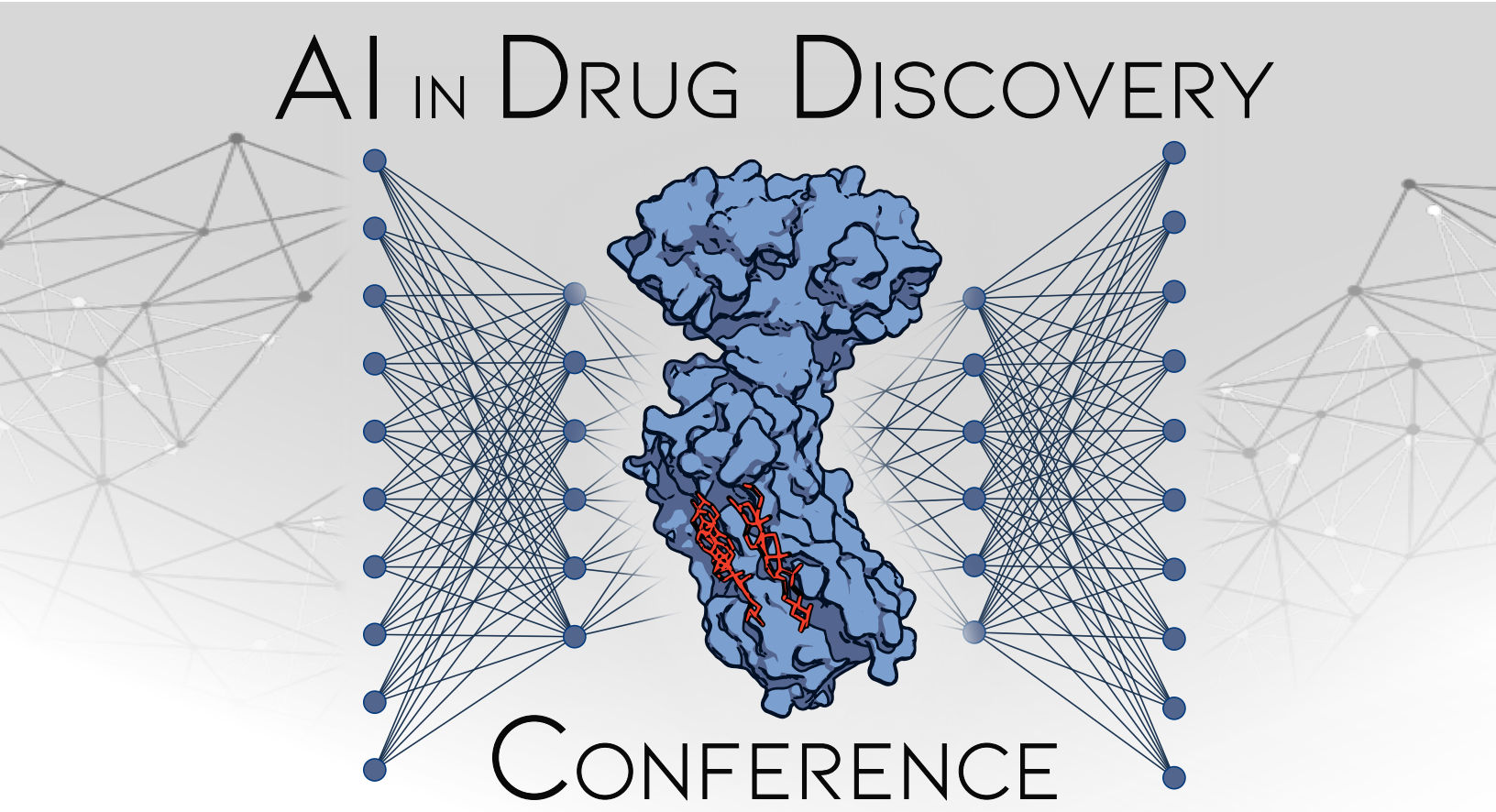
Imperial College
Computational Biology Society

AI in Drug Discovery Conference:

Delegate Handbook

27th February 2021



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Chair's Address

It is our pleasure to welcome you to the Imperial College Computational Biology Society's first AI in Drug Discovery Conference!

The field of AI in Drug Discovery is growing at an unprecedented rate to meet the challenges presented to us in this day and age. From reducing development costs by designing better therapies to the rapid re-purposing of existing drugs to treat rare and emerging diseases, AI seems set to cause a revolution in nearly every part of the Drug Discovery process. Today, we hope to give you a glimpse into the field to decide for yourself whether this excitement is based in reality.

We will be hearing from seasoned practitioners of Drug Discovery about how they are integrating AI into their pipelines, as well as from computer scientists leveraging the cutting edge of Deep Learning to tackle major problems in medicine and biology. Topics covered include molecular design, literature screening, using data to uncover novel proteins from nature, Geometric Deep Learning and much more!

I would like to thank all of you for coming today, the excellent organising committee that made this possible and most importantly to all of our guest speakers and panellists for all their tremendous support. We hope you enjoy this event as much as we did putting it together and that you learn as much as possible!

With kind regards,

Charles Harris

About us

The Imperial College Computational Biology Society was founded in the Spring of 2020 in order to create a cross-discipline community that shares a fascination for data, machine learning and the application of artificial intelligence (AI) to life science research and medicine. Since October 2020, we have gained over 350 members to become one of the largest academic societies at Imperial. Our members are a diverse group of students from the Departments of Computing, Life Sciences, Bioengineering and Medicine who are interested in learning about machine learning technologies relevant to healthcare and developing their programming skills. Throughout the Autumn term we have organised webinars on the use of AI in drug discovery and high-throughput technologies in single-cell transcriptomics and proteomics. Our educational agenda includes weekly events such as webinars, journal clubs, coding classes, as well as organisation of biohackathons, which we hope will inspire students to join the exciting field of computational biology.

Conference sub-committee 2021:

- Charles Harris – Society Chair
- Rebeca Ianov Vitanov — Industry Liaison Officer
- Joseph Ellaway – Treasurer
- Laura Dyamond – Secretary
- Julia Dabrowska — Society Vice Chair, Events and Promotional Officer
- Abhranil (Riju) Maiti – AV Officer

SCHEDULE

Session*	Time	Event
Session 1 Link	10:00 – 10:10	*Welcome address, Introduction to the conference* and foreword by **Prof Michael Sternberg FRSB** | Imperial College London
	10:10 – 10:40	*Using Artificial Intelligence to Optimise Small-Molecule Drug Design* | **Dr Nathan Brown FRSC** | BenevolentAI | UK-SQAR and Chemoinformatics Group
	10:40 – 11:20	*Curating truths with AI* | **Dr Daniel Jamieson FRSB** | Biorelate
	11:20 – 11:40	**Break**
Session 2 Link	11:40 – 12:30	*Geometric Deep Learning: From Euclid to Drug Design* | **Prof Michael Bronstein** | Imperial College London | Twitter | Relation Therapeutics
	12:30 – 13:10	*Novel Proteins from Nature* | **Dr Philipp Lorenz** | BaseCamp Research
	13:10 – 14:00	**Lunch break**
Session 3 Link	14:00 – 14:40	*Artificial Intelligence in Drug Discovery: Where are we today? What else is needed to advance further?* | **Dr Andreas Bender** | University of Cambridge | Nuvisan Pharma Services | HealX | PharmaEnable
	14:40 – 15:20	*Building a biology-driven AI platform focused on mechanistic interpretability* | **Dr Neel Madhukar** | OneThree Biotech
	15:30 – 15:30	**Break**
Session 4 Link	15:30 – 16:30	*Business panel discussion* | **Dr Daniel Jamieson FRSB, Dr Neel Madhukar, Prof Noor Shaker, and Dr James Field**
Session 5 Link	16:30 – 17:30	*Science panel discussion* | **Prof Sir Tom Blundell FRS FRSC FMedSci MAE, Prof Michael Bronstein, and Dr Andreas Bender**

Wonder.me - Networking platform:
https://www.wonder.me/r?id=63de89bd-f6a4-4734-97c0-35f416935437

* full session URLs are provided at the end of the handbook.

Speaker Biographies

Dr Nathan Brown. *Director of Chemoinformatics and Computational Chemistry at BenevolentAI and Chair of UK-SQAR and Chemoinformatics group.*

DR NATHAN BROWN FRSC

Dr Nathan Brown is a leader in the field of Chemoinformatics and computational drug discovery and is the inventor of the first multi-objective *de novo* molecular design system. He joined BenevolentAI in 2017 from The Institute of Cancer Research, London where he founded and led the In Silico Medicinal Chemistry team for over ten years, with significant scientific impact on drugs in active clinical trials, and the development of new algorithms for drug discovery. Dr Brown has published over 40 papers and three books, is a Fellow of The Royal Society of Chemistry and is the 2017 recipient of the Corwin Hansch Award.

Dr Daniel Jamieson. *CEO/Founder at Biorelate.*

Dr Daniel Jamieson founded Biorelate during his PhD in computational biology at the University of Manchester. After having supported the successful identification of drug repurposing opportunities with Pfizer, Dr Jamieson is now focusing on growing Biorelate into a world leading enterprise, helping pioneering companies in their mission to develop life-saving innovations. He co-developed Galactic AI™, a supercomputing platform that automatically curates biomedical research to dramatically improve the understanding of a particular research area in drug discovery. By connecting obfuscated evidence, Biorelate's goal is to accelerate development of important new therapies.

DR DANIEL JAMIESON FRSB

Prof. Michael Bronstein. *Chair of Machine Learning at Imperial College London, Head of Graph Machine Learning at Twitter and Scientific Advisor at Relation Therapeutics.*

PROF MICHAEL BRONSTEIN

Professor Michael Bronstein joined the Department of Computing of Imperial College London as Professor in 2018. His main expertise is in theoretical and computational geometric methods for machine learning and data science, and his research includes computer vision, pattern recognition, geometry processing, computer graphics, and their applications in biomedicine. Prof Bronstein has authored over 200 papers and was awarded various awards, including five ERC grants, two Google Faculty Research awards and the Royal Academy of Engineering Silver Medal. Besides academic work, Prof Bronstein has held technological leadership positions in multiple startup companies, is the Head Of Graph Learning Research at Twitter and was one of the key developers Intel RealSense 3D camera technology.

Dr Philipp Lorenz. *Head of Data Science at BaseCamp Research*

DR PHILIPP LORENZ

Dr Philipp Lorenz obtained his PhD from Oxford, focusing on the development of novel Bioinformatics and Next Generation Sequencing approaches to expand human genome annotations. A former iGEM team founder and gold medalist, Dr Lorenz has been involved in business development, data science and bioinformatics in the pharmaceutical and biotech industry and is now leading the Data Science division at BaseCamp Research. His work at BaseCamp Research involves identifying, building and maintaining a suite of computational tools for the characterisation of industrially-relevant protein properties from the company's unique, internal datasets. This protein screening will be used to understand how these previously undiscovered proteins can be used as starting candidates for many sectors, including food, pharma, biotech and agriculture.

Dr Andreas Bender. *Reader for Molecular Informatics at Cambridge, Co-founder of HealX and PharmaEnable, Director of Digital Life Sciences at Nuvisan Pharma Services*

DR ANDREAS BENDER

Dr Andreas Bender leads a research group in the Centre for Molecular Informatics at University of Cambridge, focusing on data-driven chemical and biological screenings for detecting mechanisms of action and adverse drug reactions, especially related to cancer. He has previously been affiliated with the Lead Discovery Informatics group of Novartis in Cambridge/MA and the department of Clinical Pharmacology and Artificial Intelligence at AstraZeneca in Cambridge/UK. He has recently become the Director of Digital Life Sciences at Nuvisan Pharma Services. He is also the co-founder of the Healx and PharmEnable startups which specialise in AI-driven small molecule discovery for various disease areas, including neurodegenerative, inflammation and rare diseases.

Dr Neel Madhukar. *CEO and Co-Founder of OneThree Biotech*

Dr Neel Madhukar received his PhD from the Weill Medical College of Cornell University, using data analytics and machine learning to study cancer systems biology and to help improve precision patient care. He authored numerous scientific publications in the fields of machine learning, pharmacology, and precision medicine. To date, his work has led to the development of new AI prediction methods, the discovery of a novel class of cancer therapeutics, and the start of new clinical trials. During his postdoctoral studies at Cornell, he established OneThree Biotech, which develops machine learning technologies for providing insights across multiple parts of the drug development pipeline.

DR NEEL MADHUKAR

Prof. Sir Tom Blundell. *Honorary Director of Research and Emeritus Sir William Dunn Professor of Biochemistry at University of Cambridge*

PROF SIR TOM BLUNDELL FRS, FRSC, FMEDSCI, MAE

Professor Blundell leads the Structural biology, bioinformatics and drug discovery group within the Department of Biochemistry at the University of Cambridge. He was a member of the team of Dorothy Hodgkin that solved in 1969 the first structure of a protein hormone, insulin. In 1999 he co-founded the oncology company Astex Therapeutics, which has moved ten drugs into clinical trials. Prof Sir Blundell's Group at University of Cambridge now focuses on machine learning as well as databases to underpin drug discovery and to understand cancer and drug resistance. He has also played central roles in restructuring British research councils and, as President of the UK Science Council in developing professionalism in the practice of science.

Dr James Field. *CEO/Founder at LabGenius*

DR JAMES FIELD

Dr James Field completed his PhD at Imperial College London, when he created the spin-out company LabGenius to commercialise a groundbreaking, new technology: the ability to produce trillions of variations of gene sequences, which can be used to create new biological materials. The company uses artificial intelligence to predict which gene mutations will improve a biological design, enabling scientists to produce new therapeutics or advanced materials. In 2017, Dr Field was awarded the BBSRC Innovator of the Year award for early career impact and one year later he was featured on the Forbes 30 Under 30 list for Science Healthcare. He is also a fellow of the prestigious Synthetic Biology Leadership Excellence Accelerator Program (LEAP).

Prof. Noor Shaker. *CEO/Founder at GlamorousAI*

PROF NOOR SHAKER

Prof. Noor Shaker is a co-founder at GlamorousAI, an AI preclinical drug discovery biotech focusing on first-in-class therapeutics for challenging targets. Prof. Shaker had also founded the drug discovery start-up GTN Ltd before she stepped down in August 2019. She is a former assistant professor at Aalborg university in Copenhagen specialising in machine learning generative models, as well as the author of the book "Procedural Content Generation in Games" and a contributor to over 50 publications. She has received several accolades, including being named a 'Rising Star' among BioBeat's 2018 list of 50 Movers and Shakers in BioBusiness. Representing GTN, she was awarded a CogX UK Rising Star Award in 2018 for her innovative AI techniques for drug discovery and success in securing seed funding and prestigious collaborations.

Prof. Michael Sternberg. Professor Sternberg is the Director of the Centre for Integrative Systems Biology and Bioinformatics (CISBIO) and Chair of Structural Bioinformatics at Imperial College London. Prof. Sternberg's research focuses on protein bioinformatics, an area which he entered after obtaining a first degree in Physics (Cambridge), a Masters in Computing (Imperial College), and a PhD in Biophysics (Oxford). He has worked in protein bioinformatics contributing to the elucidation of new principles of form and function and the development of algorithms for prediction of protein structure, function and interactions. Recently, these approaches have been extended to study protein systems and logic-based drug discovery. He worked at Oxford, Birkbeck College, Cancer Research UK and established the Structural Bioinformatics Group at Imperial in 2001. Fellow of the Royal Society of Biology (FRSB) and the Institute of Biology (FIBiol), Prof. Sternberg has authored and co-authored several books in the field on protein structure and he is also an Associate Editor of the Journal of Molecular Biology.

PROF MICHAEL STERNBERG

Joining Links

Hyperlinks are provided in the schedule table but just in case those do not work we have provided the full links here. We would recommend having the Microsoft Teams client installed but you can view via a web browser too.

Session 1:

https://teams.microsoft.com/l/meetup-join/19%3ameeting_YzMxYTg0YzMtYzAzOC00NmU2LWI3YzUtZmMxM2M0MTNhZjVi%40thread.v2/0?context=%7b%22Tid%22%3a%222b897507-ee8c-4575-830b-4f8267c3d307%22%2c%22Oid%22%3a%22963aad8c-8a6a-4769-89cc-e2466f041e83%22%2c%22IsBroadcastMeeting%22%3atrue%7d

Session 2:

https://teams.microsoft.com/l/meetup-join/19%3ameeting_Y2IzZTVhZGEtMDA0My00YTliLTk0NmUtNjYzY2ZmZjQzMWRi%40thread.v2/0?context=%7b%22Tid%22%3a%222b897507-ee8c-4575-830b-4f8267c3d307%22%2c%22Oid%22%3a%22963aad8c-8a6a-4769-89cc-e2466f041e83%22%2c%22IsBroadcastMeeting%22%3atrue%7d

Session 3:

https://teams.microsoft.com/l/meetup-join/19%3ameeting_YWNmODBlY2ItNWEwYi00NzI2LTk4NGMtOTJiMTAyNDdiM2I0%40thread.v2/0?context=%7b%22Tid%22%3a%222b897507-ee8c-4575-830b-4f8267c3d307%22%2c%22Oid%22%3a%22963aad8c-8a6a-4769-89cc-e2466f041e83%22%2c%22IsBroadcastMeeting%22%3atrue%7d

Session 4:

https://teams.microsoft.com/l/meetup-join/19%3ameeting_MGFjMjRjYjUtZTc0My00NThjLTg5NjctYmI1YTZiY2RmNDIz%40thread.v2/0?context=%7b%22Tid%22%3a%222b897507-ee8c-4575-830b-4f8267c3d307%22%2c%22Oid%22%3a%22963aad8c-8a6a-4769-89cc-e2466f041e83%22%2c%22IsBroadcastMeeting%22%3atrue%7d

Session 5:

https://teams.microsoft.com/l/meetup-join/19%3ameeting_NGQ1NzI0MDAtZWU3Ny00MTBhLTljMjgtMDVhMWJhOTAzOTYz%40thread.v2/0?context=%7b%22Tid%22%3a%222b897507-ee8c-4575-830b-4f8267c3d307%22%2c%22Oid%22%3a%22963aad8c-8a6a-4769-89cc-e2466f041e83%22%2c%22IsBroadcastMeeting%22%3atrue%7d

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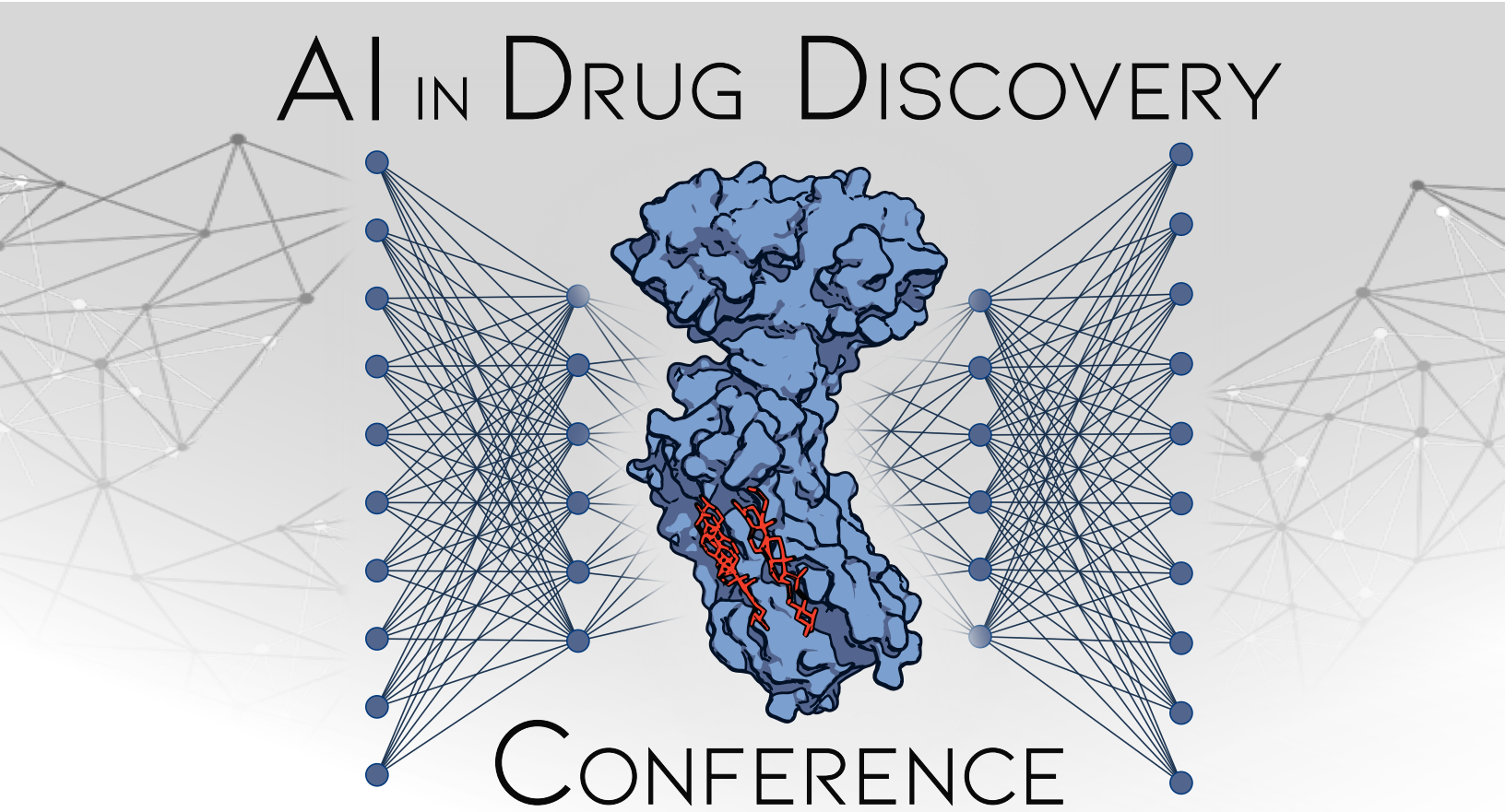
Thank you for attending!



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