PISTOIA ALLIANCE

UX Pistoia Alliance Pharma and Life Sciences AI/ML training program
20 May - 15 July 2025

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Format: one hour length sessions, each starting at 3pm UK time. Sessions available on demand.
Provisional agenda, subject to change.

#	Date	Topic	Content
1	20 May	Introduction to AI for drug discovery	**Marina Borozna, Head of AI Strategy, IPSEN** A concise introduction to key AI technologies, including definitions of Artificial Intelligence (AI), Machine Learning (ML), Generative AI, Large Language Models (LLMs), and other relevant technologies mentioned in the course. Includes an overview of the most promising AI use cases across the pharmaceutical value chain — covering R&D, Operations, Commercial, Medical Affairs, and Corporate Functions — with a focus on AI applications in R&D: in Drug Discovery, Preclinical Research, Clinical Development, and Regulatory Affairs. This session provides participants with a clear perspective on how AI is transforming the pharmaceutical industry, while offering a solid foundation for the in-depth applications explored later in the course. **Prof. Mike Barnes, Queen Marys University** Broad overview based on the review wrote with MSD. **Varun Shivashankar, Associate Director, Machine Learning, Parabilis Medicines** Screening better: How we use AI/ML approaches to screen smarter across therapeutic modalities
2	27 May	Generative AI for Drug Development	**Dr. Moe Elbadawi, Queen Mary University** GANs for generating novel medicines LLMs for simulating drug development **Matthieu Dagommer, Machine Learning Scientist, AbbVie** Internal deployment of REINVENT as a CLI tool available on High-Performance Computational (HPC) resources for an audience of computational chemists at AbbVie. Recurring discussions with an academic lab from Northwestern University on LLM-based de novo design (prompt-engineering with chemical expert models such as Chemcrow/LLasmol), although nothing was transferred so far.
3	29 May	Computer vision	**Prof. Greg Slabaugh, Queen Marys University** Introduction to computer vision Deep learning Image classification

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			Object detection Segmentation (semantic and instance) Outlook / Future Trends **Hrishikesh Deshpande, AI Consultant** This session will explore how computer vision is driving real-world impact in pharma and life sciences, highlighting key application areas, development strategies and critical success factors. We will also examine how emerging trends are reshaping the future of innovations in this field.
4	9 June	Multimodal Deep Learning	**Prof. Greg Slabaugh, Queen Marys University** Introduction to multimodal deep learning Encoders for different modalities Discriminative multimodal approaches (fusion) Generative multimodal approaches Foundation models Challenges Outlook / future trends
5	17 June	LLMs in early discovery	**Prof. Dan Crowther, University of Dundee** Introduction to target identification Knowledge extraction from literature (embedding, clustering, chatbots) Reducing the hallucinations (RAG, Graph RAG) Accessing structured data: impact on scripting and next-gen tools **David Brett, Associate Director of LLMs, Recursion**
6	30 June	LLMs as Agents in Drug Discovery	**Prof. Mike Barnes, Queen Marys University** LLM agents Automating DD tasks **Anniek Myatt Recursion, Recursion**
7	01 July	AI in Computational Medicinal Chemistry	**Prof. Mike Bodkin, University of Dundee** The MedChem task & multimodal discovery Protein structure prediction Druggability assessment Virtual screening Actives assessment & hit expansion (Exploration) Lead Optimisation & ADMET approaches (Exploitation) Generative Design strategies **Rajarshi Guha, Senior Director, Data & Computational Sciences, Vertex** AI/ML is ubiquitous across the pharma industry, at least as a label. Do all AI/ML activities actually represent artificial intelligence? I will first frame AI and ML separately, and describe why we might want one or the other. With a definition in place, I will highlgiht examples of ML/AI applications across the entire drug discovery & development pipeline and discuss opportunities as well as limitations when appling AI/ML methods to drug discovery problems.

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8	08 July	Knowledge graphs	**Prof. Conrad Bessant, Queen Marys University** Knowledge graphs as a heterogeneous data store Analysis of knowledge graphs Graph RAG Graph neural networks **Brian Martin, Senior Research Fellow, AbbVie** (details to follow) **Tankred Ott, Senior Data Scientist - AI & Analytics CoE, Novo Nordisk** Understanding complex biological mechanisms of action (MoA) for drugs and diseases is crucial for effective ORC prioritization and target identification. MIDAAS, our Multi-modal Integrated Data, Analytics & Agentic System, leverages GenAI-powered multi-agent systems to enhance this biological understanding. However, rigorously evaluating the performance of such systems is essential. This session will introduce MIDAAS and its capabilities in MoA explanation, while also showcasing LEMuR, an inner-source Python tool we developed to streamline the benchmarking of LLMs and multi-agent systems. We will demonstrate how LEMuR addresses the specific evaluation needs of MIDAAS and similar LLM-based systems, ensuring reliable performance.
9	15 July	Digital pharmaceutical manufacturing	**Dr. Moe Elbadawi, Queen Marys University** Automating Drug Development via AI and 3D Printing NLP in Drug Development