

AI IN DRUG DISCOVERY

SPEAKER INTERVIEW

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About you – what perspective do you bring to the conference?

I am an Associate Professor at Imperial College London and a Wolfson Fellow at the Royal Society.

I believe a multi-disciplinary approach is crucial to addressing AI for Drug Discovery challenges and my track record reflects this integrative perspective. My training includes an MSc in Neural Networks and a PhD in applied data inference, but I have also developed my career in research centres focusing on computational drug discovery, chemical informatics, structural bioinformatics and cancer research.

What are the biggest challenges you are currently facing as you integrate AI into your existing processes?

To me, the primary challenge lies in selecting the most appropriate AI model for prospective use on a given target, especially when faced with a wide array of available options as it is increasingly the case. In retrospective studies, new models are often presented as superior to their predecessors, with some even being labelled as groundbreaking before any independent peer review. However, the reality is that most AI models, when subjected to rigorous benchmarking, prove to be only incremental improvements at best. This highlights the importance and timeliness of further research into rigorous evaluation and comparison of these models.

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AI is being integrated across the breadth of the pipeline; in which area do you think AI will have the greatest impact?

AI is likely to have the greatest impact first in areas where expert knowledge and relevant datasets can be captured into machine-readable formats quickly, cost-effectively and reliably.

What have been the most exciting advancements and innovations within the field in recent years?

Algorithmic innovations are broadly regarded as the most exciting advancements in AI for Science in general and AI for Drug Discovery in particular. However, with rare exceptions, I believe these are not the most important breakthroughs. In my view, the most impactful innovations often stem from a deep understanding of the data being modelled, the effective integration of domain knowledge into AI workflows, and the development of technologies that can enhance the value, diversity, and scale of molecules with the potential of becoming drugs.

AI has become a major focus in pharma, with significant investment and attention. In your opinion, can AI live up to the current expectations – and what might be the key factors in determining its success?

Whenever I'm asked whether AI is overhyped, my response is always the same: over what time horizon? I believe the key lies in determining whether a given AI technology is currently mature enough to deliver on its promises, especially in an environment saturated with hype. For example, AI has already shown its enormous value in virtual screening and lead optimization, providing potent and novel drug leads for many therapeutic targets previously missing sufficiently promising starting points. In contrast, it seems that more time is needed to achieve reliable predictions of drug toxicity and efficacy in clinical trials.

Why will you be joining the AI in Drug Discovery Conference in March 2026 and are there any presentations you are particularly looking forward to?

I look forward to learning about the latest progress and challenges in AI for Drug Discovery, reconnecting with old colleagues and meeting new ones.