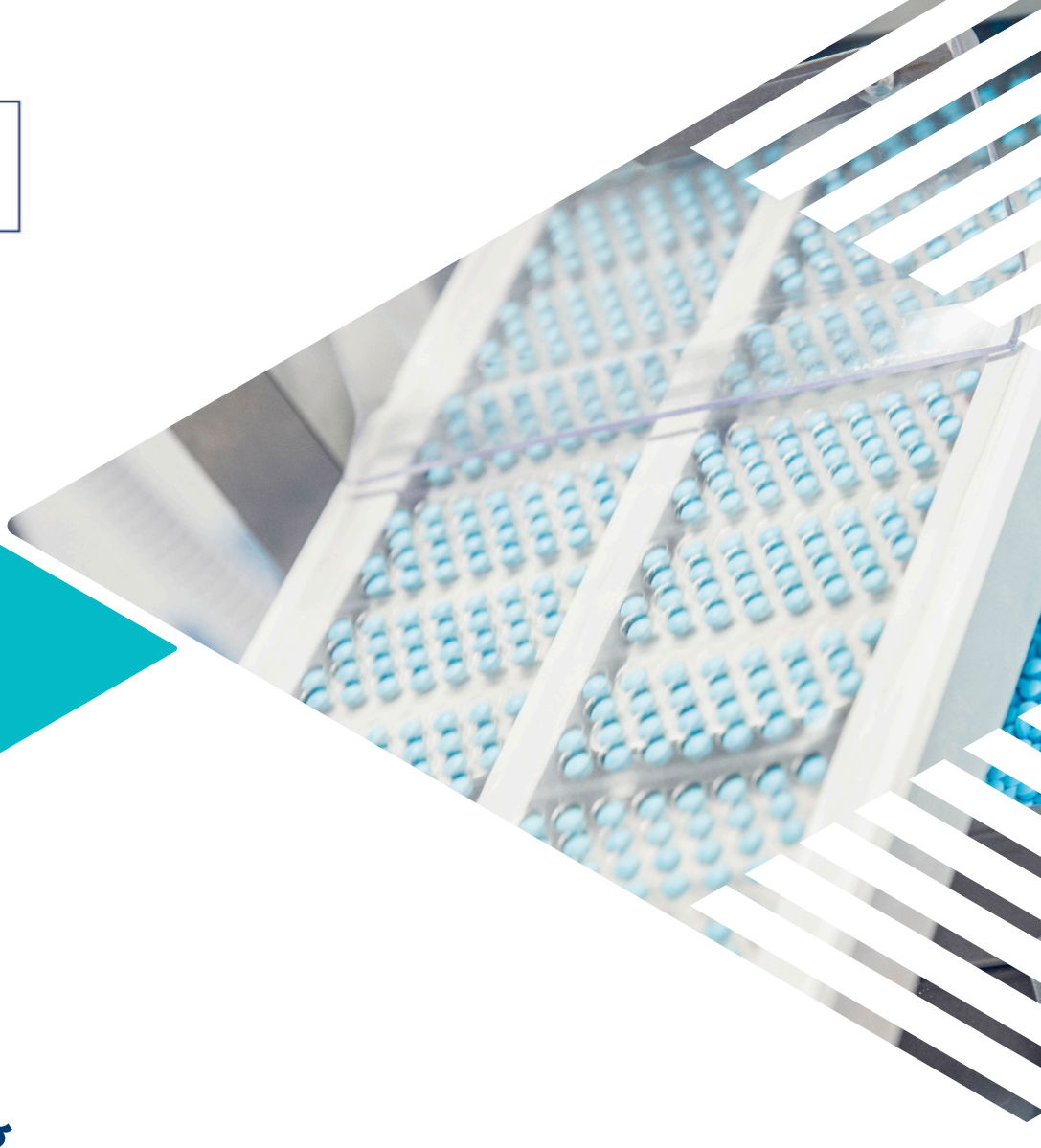
Imperial College London

Enterprise



IBP briefing
AI and pharmaceuticals

David Silverman

How AI insights could add value across the pharmaceutical value chain

Imperial Business Partners

Artificial intelligence (AI) and machine learning are presenting new opportunities to the pharmaceutical industry, not only in drug discovery but throughout the value chain.

Drug discovery

The use of machine learning to accelerate drug discovery is well known, with billions of dollars invested annually into companies that are using machine learning algorithms to help identify promising targets and compounds and to automate the lead optimisation process that refines these into drug candidates.

Imperial College London is also active in this area, drawing on its partnerships with external organisations, its multidisciplinary expertise across medicine, chemistry, life sciences and AI, and large data sets such as millions of patient records held by the Imperial College Healthcare NHS Trust and 500,000 records from ten countries in Europe by the European Prospective Investigation into Cancer and Nutrition. Its work is brought together through centres such as the new **Institute for Digital Molecular Design and Fabrication** and the **UKRI Centre in AI for Healthcare**.

In a long-term partnership with Bayer, Imperial researchers led by Professor Declan O'Regan are using machine learning to discover new pathways for treatment of heart diseases by applying machine learning to 3D images of the heart alongside genetic data from the UK Biobank, a public resource containing health data from 500,000 patients.

In economic terms, the advantage of AI for drug discovery is that it reduces the cost of target validation and compound screening. "If you can deliver these early stages very cheaply, you can evaluate thousands of drug candidates, and it doesn't matter if you only end up pursuing a small proportion of those," says Professor Aldo Faisal, Director of the AI for Healthcare Centre.

Drug approval

While AI is proving its value for drug discovery, it is not necessarily in this part of the value chain that it has the greatest potential.

"There is a question of whether efforts are being focused on the right parts of the pipeline," Professor Faisal continues. "Candidate generation is not the most expensive part of drug development – it's at the clinical trial stage that costs stack up." With only around 10% of the candidates that enter clinical trials eventually approved, around 60% of drug development costs occur at clinical trial stage.

"Another important area of work concerns using AI to find ways that drugs can be repurposed," says Professor Faisal. By avoiding the costs of both candidate generation and early-phase clinical trials, drug repurposing can bring significantly lower costs, lower risk and shorter timescales.

This is being pursued at Imperial through initiatives such as a partnership with Vodafone Foundation that is using the crowd-sourced computing power of volunteers' smartphones to process huge volumes of data and learn about the anti-cancer properties of existing medicines. It has recently revealed anti-cancer properties of anti-diabetic drug Metformin and anti-microbial Rosoxacin.

Manufacturing

Looking further along the pharmaceutical value chain, Imperial researchers are working with partners from industry to use machine learning and other digital technologies to improve the efficiency of medicine manufacturing.

One challenge they have addressed is that of producing hard-to-manufacture large molecule drugs such as peptides. At Imperial's **Sargent Centre for Process Systems Engineering**, Professor Claire Adjiman is leading a Prosperity Partnership with Eli Lilly and Company, University College London and Queen Mary University London that is using digital tools including AI to find more efficient and sustainable manufacturing techniques that deliver large molecule drugs at high purity and with fewer waste products.

As part of a strategic partnership with chemical company BASF, Professor Ruth Misener in the Department of Computing alongside colleagues at Imperial and BASF are developing machine learning techniques for optimising the design of experiments in chemical manufacturing R&D. The researchers have developed algorithms that make better predictions than humans about experimental manufacturing settings – for example the flow rates and temperatures – most likely to yield the desired performance.

In addition to providing valuable new techniques, this work, theoretically significant enough to yield three papers at the prestigious machine learning conference NeurIPS, has shown the potential of collaboration with academia to help non-tech companies position themselves as leaders in AI and attractive destinations for machine learning talent.

Prescribing and use

Once a medicine has entered the market, several new challenges present themselves to industry. In addition to the need to continue to monitor their safety, effectiveness, and their potential to be used for new indications (as addressed above), these often concern the ways that the medicines are being prescribed and used.

"Post launch of a product, we think about educational marketing, work to help shape policy, and work with the NHS – for example identifying social determinants of health," says Dr Antonia Solomon, Head of Digital Excellence, Medical Innovation & Information at MSD UK, which has recently joined the Imperial Business Partners membership network.

"AI is a useful tool to do a lot of the heavy lifting," she continues. "If you get the algorithms right to pick up the unknowns, we uncover data that could have signals for us such as data gaps. Analysis on demographics and other information allow greater insight on how medicines are likely to be the most effective for a given patient. For example, in Oncology, depending on the indication, there are effective treatments on the market, however we are still presented with challenges of late diagnosis. We try to find out what is behind that."

One need is to verify that doctors are being consistent in how they prescribe a particular medicine. The use of machine learning algorithms combined with patient data makes it possible to identify incorrect or inconsistent prescribing decisions.

AI can also be leveraged to identify the benefits and disadvantages of polypharmacy. These include the risks that medicines are being inadvertently prescribed alongside other drugs that reduce their benefit, or are being prescribed inappropriately to counter side effects of other drugs, and the potential advantages of using multiple drugs in a complementary way.

Using AI to study drug uptake, interactions and patient trajectories offers pharmaceutical companies the opportunity to refine the information they provide to doctors and policymakers. It could also allow them to develop digital tools to offer as services alongside pharmaceutical products that offer optimal and dynamic dosage recommendations.

At Imperial, the vast electronic healthcare databases held by the Imperial College NHS Trust's **Discover-NOW** hub with millions of detailed electronic patient records, are providing an unprecedented resource for understanding how drugs are combined used and interact using data science methods.

This data is being analysed for a multitude of projects with industry and academic partners that are uncovering, for example, the potential of metformin to prevent weight gain as a side effect of antipsychotics, and predicting the onset of complications in Type 2 Diabetes patients.

Other questions are whether there are socioeconomic factors that are preventing the benefits of medicines such as vaccines from being realised, and the ways these are distributed among varying demographic groups. This can be important from the perspective of diversity and inclusion.

Unlocking new opportunities

In comparison to controlled clinical trials, rich real-world data sets present unique opportunities to gain new insights, with concomitant challenges.

Some of these challenges are technical in nature. Other concern risks like privacy and algorithmic bias. Still more concern creating innovative and adaptable organisational cultures, compliance and governance structures and skill sets required to take advantage of new opportunities.

"As an industry we are on a journey," says Dr Solomon. "We need to think about our capabilities and keep leveraging the fact that there may be solutions that can serve as an adjunct – whether these are internal tools or collaborating with tech companies and academic centres. Challenges include data regulation and privacy, confidence in AI, and a mindset change. Nevertheless, I am confident that ongoing research and development, is likely to uncover additional ways that AI can be used to improve patient outcomes."

"Our main message to the pharmaceutical industry is that we have just started to realise the benefits of AI, and it's not just in drug discovery," says Professor Faisal. "At Imperial, we have the population data and the means and models to analyse them. We also have a strong track record as a nexus of collaboration between partners in academia, healthcare, industry and government to help the community take advantage of the evolving opportunities that AI affords."

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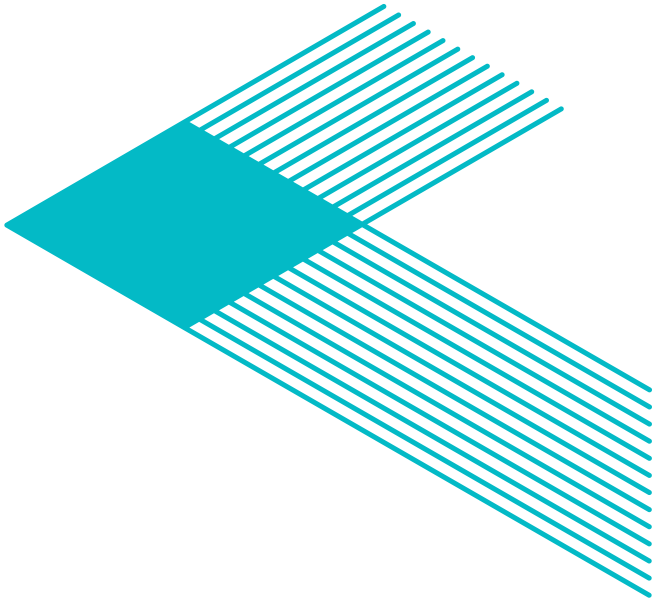

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ibp@imperial.ac.uk | **imperial.ac.uk/ibp**

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