Artificial intelligence: the key to developing effective drugs quickly

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By recognising patterns in large amounts of data, AI has made huge advances in industries as varied as finance, aviation and customer service. Now GSK are seeing the possibilities of using it to speed up drug discovery and combat intractable diseases

For many people, artificial intelligence, or AI, means intelligent robots taking over the world; Facebook or Google algorithms predicting our wishes before we know them ourselves; or, at the very least, automation replacing all of our jobs.

But behind the doomsday scenarios, AI is increasingly being used to ensure that drugs are being brought to patients more quickly, and more effectively.

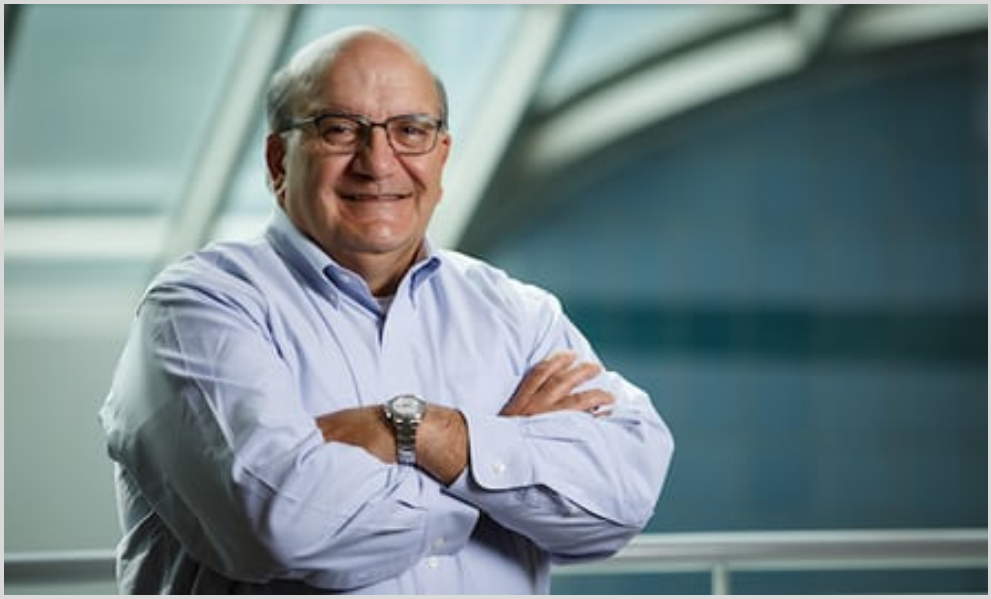
GSK, like other pharmaceuticals companies, generates far more data than it can use – but this is now changing. "Data for a pharmaceuticals company today is its currency – it's like pounds in the bank," says John Baldoni, who leads GSK's drugs discovery unit, Medicines Discovered Using Artificial Intelligence (MEDDAI).

"The drug development process is very complex and not always successful. What success the industry has is predicated by a lot of failure," he continues. But as companies develop drugs, they create huge amounts of data, much of which has never

been used.

"There's a lot of 'dark data' out there – data that is hidden in organisations and research institutes – that is not used for publication and isn't talked about," he says. "For someone who is interested in using that data to create a new way of discovering a drug, there is a vast wealth of information."

Computers have been used in drug development for many years, but recently there has been a significant change in how they are being used. Previously, computing systems, and the humans that run them, did not have the capacity to interpret or investigate unstructured data. As computers become more powerful, however, it becomes possible to analyse that vast quantity of data, which could greatly contribute to drug development.



John Baldoni, head of drug discovery using AI at GSK. Photograph: Alan Brian Nilsen

"Generations of scientists have dedicated their lives to helping people solve intractable diseases. Now the technology is there to enable their data to be realised by society. That's what's the most exciting part to me," Baldoni says.

"There have been so many failed clinical trials. So what if you don't have to run another trial but just give data from those trials that you ran in real life years ago? Then you could run that trial in silico [via computer]," he continues.

The tipping point for GSK was in 2015. Although "machine learning" – where machines apply knowledge from vast data sets, recognise patterns for themselves and make predictions as a result – had been used by pockets of GSK scientists for a number of years, Baldoni recognised that these techniques could be applied more broadly. In particular, he saw that the pattern recognition used in the financial world or for image analysis could also work in drug development.

Using AI will help the pharmaceuticals industry accelerate its development processes hugely. It currently takes around $1.5-1.7bn (£1.1-1.3bn) to develop a drug – and from identifying the biological target in the body to creating the molecule for clinical trials takes five or six years. With AI, this process could be shortened considerably – Baldoni's current goal is to reduce this timescale to one year – and costs would come down too.

In order to do this, GSK has recently announced a range of different collaborations. This summer, it started working with Exscientia, a UK-based AI and machine-learning company.

Exscientia will combine its AI-enabled platform with GSK's research and development expertise. The company is undertaking new discovery programmes for novel and selective small molecules for up to 10 disease-related targets nominated by GSK.

Insilico Medicine, a US-based AI company, is also in partnership with GSK to advance GSK's drug discovery processes. GSK will be sharing its R&D expertise to help validate

the computer algorithms that Insilico is developing.

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GSK is also working with the Hartree Centre, the UK government-backed research centre, which has some of the most technically advanced high-performance computing, data analytics, machine-learning technologies and experts in the UK. GSK is working with them on a supercomputing project that will enable scientists to analyse millions of biomedical research publications to identify patterns and correlations that might act as the starting point for a new medicine.

It is also part of the Accelerating Therapeutics for Opportunities in Medicine (Atom) consortium, a US public-private partnership with the Department of Energy and the National Cancer Institute.

Atom is developing computing models capable of vetting millions of molecules for efficacy and structural relationships. These models will be able to adapt (without human supervision) as they learn from the huge data sets they go through – a process known as "deep learning".

GSK is giving Atom access to more than a million compounds it has screened over the past 15 years, all of which have biological data associated with them.

"I am so proud of GSK because they donated data from all these compounds going into this initiative. Now we will be using some of the fastest computers in the world to trawl through that data, to find out what is hidden in it," says Baldoni.

"Can you imagine if the top 12 pharma companies donated the 12m compounds they have in their libraries? That would be phenomenal! GSK is setting the standard that others should follow."

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