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ASIA EDITION

Speeding up drug discovery process with Artificial Intelligence

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Experts say, Artificial Intelligence saves half the time and money needed for discovery of new drugs



Singapore: It's estimated that, on average, to bring one new drug to the market can take 1,000 people, 12-15 years, and up to $1.6 billion. Pharmaceutical companies are grappling with these scandalous costs and constantly in search for inefficiencies in the drug discovery process, and hope to fasten the process by focusing on key elements, like management models, new technologies and creative study approaches. With many new viruses and bacteria daunting the globe there is an increased necessity to innovate and develop new drugs and safeguard public health. Also with patent cliff looming large, pharma companies need to evolve their R&D efforts to ensure that the core of their business keeps pace with the changes. With increasing competition, experts are looking at newer methods to speed up and increase accuracy rates. One such approach is using Artificial intelligence in drug discovery.

The technology aims to streamline the initial phase of drug discovery, which involves analyzing how different molecules interact with one another—specifically, scientists need to determine which molecules will bind together and how strongly. They use trial and error and process of elimination to analyze tens of thousands of compounds, both natural and synthetic. "Many large pharma companies are starting to realise the potential of this approach and how it can help improve efficiencies," said Mr Andrew Hopkins, chief executive of Scotland-based Exscientia, which announced the new tie-up with GSK. Mr Hopkins, who used to work at Pfizer, said Exscientia's AI system could deliver drug candidates in roughly one-quarter of the time and at one-quarter of the cost of traditional approaches.

Exscientia also signed a 250 mn Euros deal with Sanofi in May. As part of this agreement, Exscientia will be responsible for all compound design, whilst chemistry synthesis will be delivered by Sanofi. With its unique AI platform, Exscientia is delivering a pipeline of efficacious, bispecific small molecules, as well as highly selective single target candidates, for multiple indications.

In an interaction with Mr Andrew Hopkins, CEO, Exscientia. Please check below for Excerpts:

What is artificial intelligence (AI) and how does it speed up drug discovery process?

AI, if used correctly, is a new approach to drug discovery, that uses computer algorithms to search create original solutions to the questions a drug discovery scientist might ask when designing a new medicine. These systems are uniquely able to learn from existing data resources, much in the way that a human would learn and then apply the knowledge gained on a new project. However the amount of data now available is so vast that it is beyond a human's capability. For AI focused towards drug design, where Exscientia focuses its expertise, the typical sources of information could be the vast resources of chemical structure, pharmacology, bioassays data as well as other supporting literature and patent information. The AI algorithms then apply the distillation to the design of new small molecules. Successful molecules will hit the desired target whilst at the same time avoiding known selectivity, toxicology or pharmokinetic issues (among many other parameters). Further refinement can lead to completely new and optimized molecules (and IP) for advancing towards the clinic. AI is also being applied to many areas of drug development. For example AI approaches might look at better patient stratification for clinical trials, thereby fitting the patient to the treatment being tested better, enabling quicker recruitment and increasing the likelihood of getting the required clinical response for regulatory approval.

- **What are the key trends that will drive the growth of AI in drug discovery for the next 5 years?**

  The need to reduce R&D costs is a major drive. Lead optimisation is the highest cost per launched drug due to the number of projects researched that never reach the market. Improving discovery efficiency through high quality candidates that are discovered effectively would dramatically improve these metrics. Exscientia's deal with GSK is looking at this exact problem, designing candidates in a highly productive manner.

  Also, the need to reduce healthcare costs – combination therapies (e.g in cancer) looking to become prohibitively expensive – AI approaches can be used to design drugs that could modulate multiple biological process (e.g blocking tumour signalling and survival mechanism, boosting immune response), in a cost-effective manner. Exscientia is looking to tackle efficacy directly by design a breed of small molecules that we call bispecific small molecules. These are single small molecules with carefully designed dual pharmacology. Exscientia projects focus on I/O (with Evotec) , diabetes (with Sanofi) and psychiatric diseases (Dainippon Sumitomo Pharma).

  • What factors will play a critical role in the success of AI driven drug discovery projects?

  Delivery on the promise.

  Exscientia has already demonstrated the delivery of a clinic-ready candidate from the start of a project in a quarter of the time and a quarter of the cost compared to traditional metrics.

  Exsicentia's goal is to improve this still further – 10x improvement – and then AI approaches could become dominant

  • In your opinion what are the major challenges in the traditional drug discovery process and how does AI help to address them?

  Drug discovery is fundamentally expensive and time consuming. Therefore AI has the potential - if well designed – to positively impact a variety of areas such as those already described. However AI alone will not solve the problem and the approach needs to be driven by highly knowledgeable domain experts. At Exscientia we have some of the best medicinal chemists working alongside the technologists to develop 'best of breed' approaches. Combining human expertise with AI power is creating 'centaur' drug design capabilities – derived from 'centaur' chess – a term coined by chess grandmaster Garry Kasparov for the teaming up of chess experts with AI, which have the ability to beat either human or AI players.

  • Please tell us more about Exscientia, its portfolio and unique AI platform

  Exscientia is at the forefront of Artificial Intelligence (AI)-driven drug discovery and design. By fusing the power of AI with the discovery experience of seasoned drug hunters, we are the first company to automate drug design, surpassing conventional approaches. Our innovative platform enables breakthrough productivity gains as well as new approaches to improve drug efficacy. Novel compounds prioritised for synthesis by Exscientia's AI systems simultaneously balance potency, selectivity and pharmacokinetic criteria in order to deliver successful experimental outcomes. By applying a rapid design-make-test cycle, the Exscientia AI system actively learns from the preceding experimental results and rapidly evolves compounds towards the desired candidate criteria. Exscientia first developed their platform to design efficacious, selective single-target compounds, whilst further innovation now allows the same platform to design small molecules with dual pharmacology, as well as more complex target product profiles guided by high content phenotypic

data. Exscientia is now collaborating with several leading pharmaceutical companies. Current partners include Evotec (immuno-oncology), Sanofi (metabolic disease), Sumitomo Dainippon Pharma and Sunovion Pharmaceuticals (CNS) and GSK.

- **What according to You are the risks associated with use of AI technologies in drug discovery?**

  In the case of our company specifically we have no concerns as we are secure in our knowledge that we are domain experts and have carefully developed the approaches over a 5 year period, during which it has been tested and refined in real-world drug discovery situations for partners. However for the broader industry there is a risk that those with insufficient experience will suddenly expect generic AI algorithms to be a magic bullet and solve complex tasks even in the absence of domain expertise. This is unrealistic. As an analogy, it is well known that the Deepmind AI algorithm alphaGO beat the reigning GO world champion. What is often overlooked is that the group tasked with developing the alphaGO AI algorithm actually had multiple GO experts working in the design team. At Exscientia, we have human drug discovery experts working alongside the AI – and the highest profile among these is Andy Bell, a co-inventor of Viag*ra and other drugs while at Pfizer

- **Are pharma companies ready to adopt these technologies and revolutionize healthcare?**

  Most are exploring the use of AI now, as evidenced by our own experience and deals. There are many areas in which to apply them so we expect their use to increase.
  In our own case, delivering consistently and demonstrating the efficiencies makes other companies more likely to explore.

  - **How has AI assisted drug discovery taken off in Asia?**

  Our initial focus was solely Japan and Dainippon Sumitomo was actually one of our first partners. Now interest is clearly growing in the broader Asia region, where we see strong potential.