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AI Driving Innovation: Insights From Exscientia CEO Andrew Hopkins

by Lucie Ellis-Taitt

Andrew Hopkins, founder and CEO of Exscientia, invented and championed an algorithmic approach to drug design and drug discovery. He talks to *In Vivo* about artificial intelligence in the biopharma industry today and what lies ahead.

Founded back in 2012, *Exscientia plc* went public on Nasdaq in October 2021, raising over $300m – a huge amount for a biotech that is yet to bring a drug into the clinic on its own. However, it was ahead of the game being the first company to automate drug design and the first to have an AI-designed molecule enter clinical trials (albeit a partnered asset).

The company's most advanced, wholly owned drugs are in IND-enabling studies. EXS74539 is a selective, reversible and brain penetrant LSD1 inhibitor being studied in both hematology and solid tumors. EXS73565 is a selective MALT1 protease inhibitor with potential applications in hematology.

ANDREW HOPKINS

Exscientia's most advanced drug programs are partnered. EXS21546, of which it has majority ownership, is in development with *Evotec SE*. The companies are enrolling patients in the Phase I/II IGNITE study in relapsed/refractory renal cell carcinoma and non-small cell lung cancer. Co-owned with *Apeiron Biologics AG*, GTAEXS617 is in Phase I/II trials for the treatment of solid tumors. And EXS4318, a PKC-theta inhibitor licensed by *Bristol Myers Squibb Company*, entered Phase I earlier this year.

Prior to founding Exscientia, CEO Andrew Hopkins spent 14 years at *Pfizer Inc.* and in academia, pioneering projects using data mining and machine learning in the pharmaceutical industry.

Q ***In Vivo:*** **Exscientia was founded on the notion of innovation, but how do you foster a culture of innovation within an organization?**

A Andrew Hopkins: The primary driver essential to building a culture and an ecosystem of innovation inside a company is the question of 'How can you learn faster no matter where you're starting from?' You're feeling your way in the dark to understand a new problem. The fundamental building block is learning faster as a key competitive advantage.

One important element that helps you do that is diversity amongst your teams because different experiences allow for different viewpoints. I originally started work in the steel industry, you know, before I moved into computational drug design. But I learned what it meant to deliver in a very competitive environment, and the innovation required to stay ahead of the game. I never had any assumptions when moving into another industry and I had a very different concept of competitive behavior.

Exscientia is a global company now, well over 400 people. And we have bases from Miami to Boston, Vienna, Dundee in Scotland, Osaka in Japan. And we have, I think, over 45 different nationalities. A very large proportion of our workforce in Oxford, UK, is from all over the world. And that brings a very different set of perspectives. That's one of the beauties of science, it is such an international pursuit. Our teams consist of biologists, they consist of software developers, AI scientists and hardware engineers ... It creates a very different environment for innovation. The pharmaceutical industry is really an information industry, the questions are: 'How do we use these new techniques of manipulating and learning from information?' And 'How do we apply them to improve the industry?'

Q **How do you balance the pursuit of innovation with the need for investor**

returns and sustainability of a business?

A We have found it to be a virtuous cycle as we have been pushing ourselves to deliver more value and move up the value chain. Every time we approach a new problem, we ask ourselves 'How can we do this differently?' We've built a drug discovery engine using a model-driven adaptive design as one of our key philosophical approaches. What we are finding now, as we move into the clinic, is that it is really important how we build our techniques. For example, of how we run simulation guided clinical trials, where we can actually run 10s of 1000s of variations. And how a clinical trials can be run *in silico*, before we actually enact it.

This concept of model-driven adaptive learning has been an overarching philosophy for our evolution and continuous learning, not just in drug discovery, but also in development. As our pipeline moves forward into the clinic and as we face new problems, we want to think about them in a new way as well. We don't just want to be innovative in drug discovery, we want to continue to be innovative as we ourselves push forward into the clinic and ultimately onto the market.

Q **How do you work with industry partners?**

A We started collaborating with pharma partners almost from day one of the company forming. Partnerships have been essential and are important to our innovation because they allows us to test out our algorithms and our approaches on real-world problems that matter to people. We've learned greatly from our past collaborations with *Sumitomo Pharma Co., Ltd.*, and current relationships with Bristol Myers Squibb Company and *Sanofi*. Working with partners has exposed us to a wider variety of problems to test with our algorithms, which we believe has made them much more robust. (Also see "*Exscientia And Sanofi Will Search For 15 Novel Oncology, Immunology Drugs Under New Pact*" - Scrip, 7 Jan, 2022.)

Q **Which areas of drug development do you see AI having the biggest impact?**

A The area, I believe, where we will see the greatest impact is truly making personalized

medicine a reality. We are seeing that in our own work. I'll give an example of how we are using AI technologies to help select the right drug for patients. Last year, we published results from a clinical trial called EXALT-1, it was a real milestone. I think it might be the first clinical trial that really showed how an AI process improved clinical outcomes in oncology.

EXALT-1 was the first-ever prospective interventional study of its kind. Predictions made by the platform proposed which therapy would be most effective for late stage hematological cancer patients based on testing drug responses ex vivo in their own tissue samples. When we looked at results, about 25% of the patients four years later were progression free. And within the control group, within a year everyone was progressing. We saw an objective response rate of around 55%.

This was actually an AI driven technique, in basically getting the algorithm to select the right drug for a patient. What you can start to imagine is that an AI created drug is not just about how you can use AI to help drug hunters design a molecule, it's not about just precision engineering of the molecular structure, but also about precision selection of the right patients for the treatments.

Q **What are your predictions for the future of AI and the biopharma industry?**

A I envisage a world where all drugs will be designed using AI approaches. It will become an integral technology for drug discovery and development. The question now is 'How do we integrate the different algorithms into a full end-to-end process?' Where we'll invest, is in the integration of AI with automation, and then in how AI and laboratory operations come together. The next quantum leap and productivity enhancement will come from the interaction of AI with the physical world of experimentation.