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Drug discovery and development may never be the same — the life sciences are embracing AI

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CAS president Manuel Guzman addresses the crowd at a recent STAT event.

Every year, life science companies spend billions of dollars to develop new drugs, but the return on investment often disappoints.

Artificial intelligence (AI) holds the promise of making drug discovery and development less expensive and more effective. The ability to process huge stores of data is enabling drug makers to identify the precise mechanisms of disease, target new therapies to address them, and build more-detailed biological profiles of the types of patients who could benefit.

STAT recently convened a panel of industry experts to discuss how drug developers, doctors, and bioinformatics researchers are using AI to enhance the search for breakthrough therapies. The session, part of Boston's HUBweek, was moderated by STAT national correspondent Casey Ross and featured the following panel members:

- Niven Narain, Berg co-founder, president and CEO
- Mariana Nacht, Vivid Biosciences chief scientific officer
- Chrisoph Lengauer, Celsius Therapeutics president and co-founder, and venture partner at Third Rock Ventures
- Donald Bergstrom, Relay Therapeutics head of research and development

It starts with a robust data foundation

Session sponsor CAS released a white paper, "Building a Foundation for Profitable Digital Transformation in Sci-Tech R&D," at the STAT event. Among other topics, the paper examines the importance of having a robust data foundation to implement AI and other digital technologies. It cites a survey in which respondents identified access to data and data quality as two of the biggest barriers to successful digitalization projects.

In his introduction to the session, CAS president Manuel Guzman noted that many life science companies struggle to attain a positive return on their digital technology investment due to shortcomings in content management, knowledge management, and predictive/cognitive capabilities.

"At CAS, we specialize in providing those types of services to large commercial, government and academic organizations in the sci-tech space to help them make their AI vision a reality," Guzman said.

What does AI mean to you?

Although AI is a hot topic in the life sciences, not everyone seems to agree on its meaning.

"How we're applying it actually defines what AI is to us," Nacht said. "I'd call it a computer algorithm. You're feeding in large amounts of data and through some iterative algorithm, you're getting some answers out that then get fed back in. And you keep refining and redefining the algorithm based on the iterative responses and the validation of those responses."

A broad definition of AI would include any machine making an independent analysis of data without any human oversight, said Narain. "As it pertains to healthcare," he added, "the core of the definition is the processing of large, iterative datasets that are subject to mathematical algorithms that then result in either a verifiable result or not."

Finding the right patient population

Contrary to the hype, Nacht cautioned, AI isn't necessarily capable of accelerating drug discovery. It can, however, fulfill another critical objective: streamlining the challenge of finding the right patient population for a clinical trial.

Echoing that sentiment, Narain elaborated on how AI helped Berg create a biological map of patients at various points of a phase I trial of a cancer drug. Following the completion of that phase, Berg's analytics and cancer teams collaborated to single out the key components in patients who responded to the drug.

"We could then choose our clinical indications more specifically as we went into our phase IIs," Narain said. "Now that we're anticipating our phase IIIs, we have a causal map of response that's potentially going to be used for the inclusion criteria or to validate this as we anticipate our NDA.

"So we've really been able to leverage the biological narrative of responses by using AI along the clinical journey of development. That's been exciting for us because it really personifies what precision medicine is."

Expediting compound design

Relay Therapeutics is applying AI and machine learning not to identify targets or patient populations, but rather in compound design. Bergstrom outlined how the company set out to improve on the one-micromolar potency of its lead compound.

The process began with building predictive models to detect compounds with greater potency. "Instead of going into the lab and making a thousand compounds, cataloging and testing them, we ran in silico over two weeks and ended up with 18 molecules that were predicted to be more potent," Bergstrom said.

After synthesizing 15 of those molecules, the Relay team found eight were already sub-hundred nanomolar. Another round of optimization reduced those further to single-digit nanomolar.

"So in the course of a month, we went through a cycle where we started at one micromolar and then very quickly in silico jumped down into compounds that were single-digit nanomolar compounds," Bergstrom said. "That was the real eye-opening, 'a-ha' moment for us because it said these models are correct."

What's needed to realize AI's potential

For the purposes of drug discovery and development, AI is most effective when it can work with a few data points collected from many patients. The problem is, in fields like oncology, clinical trials tend to generate many data points from a relatively small number of patients.

That amount of data is "too big for a human to be able to discern pattern recognition, but not big enough for most AI algorithms to make sense of it," Bergstrom said. "It's the perfect setup to make false discoveries."

In order to realize AI's vast potential, investigators need not only a sufficiently large and diverse dataset, but also human expertise and well-structured processes to ensure the data's on-going reliability. That's where a partner like CAS can provide real value, Guzman explained.

"Scientific data is uniquely challenging from the standpoint of content management and technology integration," he said. "Going well beyond just text and numbers, the datasets these organizations are focused on include elements such as chemical names and structures, reaction data, graphs, DNA and protein sequences, and screening libraries.

"With over 110 years' experience managing and curating large scientific data collections and building technology solutions to derive insight from them, CAS is uniquely positioned to help life science organizations maximize the value of their data assets and deliver on the promise of new technologies to help them achieve better patient outcomes more efficiently."

To learn how CAS can help progress your digitalization strategy forward, download the white paper.