The value of scientific intelligence in drug discovery

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Leif Pedersen, President; Software, and David Lewis, Executive Director of Scientific Information at Certara, explain how scientific intelligence can enhance and increase the effectiveness of critical decision points in drug discovery.

Strong scientific intelligence capabilities are essential building blocks for a scientific informatics strategy, and will increase the effectiveness of the drug development lifecycle. When biopharmaceutical companies set out to build a new therapy, they already know what they want to achieve, and they have defined (at least in part) a rationale and a plan. But what is the best approach to drug development timelines? All drug development efforts, no matter how well planned and executed, need to be focused on optimizing analytics for faster, better, and more effective drug discovery.

How can scientific informatics help drug discovery?

One of the primary challenges is the integration of data in many different formats, with varying degrees of quality, from a plethora of different sources. It requires a platform that can connect those sources, review, refine, cleanse, and align them with standards and analytics. Futhermore, with new innovations in today’s drug development, such as peptides, oligonucleotides, and antibodies, and antibody drug conjugates (ADCs), the data complexity increases even more, and that needs to be taken into account.

The scientific intelligence platform needs to be able to support all data aggregation, cleansing, preparation, contextualization, reporting, analysis, intelligence, implementation, and visualization of outcomes. It must be also be able to integrate with all other scientific data sources, workflows, and applications within the drug discovery lifecycle.

How do you see the technology landscape for scientific informatics platforms changing?

Today, biology makes up around half of all research into new drugs. Yet, the scientific informatics systems that support them lag behind small molecule drug discovery (SMD). Data capture systems for small molecule programs are more well developed, whereas, for biology, the situation is very different.

There are also more emerging modalities being researched. While candidates are not often compared at the individual substance level, it is important to compare them at the project level to determine whether it is better to pursue a small molecule, antibody, or an ADC therapeutic.

Looking forward, there needs to be more advanced use of AI, and all data available experimental data. Rather than just showing scientists data, the platform will present them with models, concepts and data to support their research decisions. The blended use of AI, and AI algorithms that not only expand further into the field of unprocessed AI, and bring in translational approaches to drug learning. This will, as a whole, improve scientists to be trained to work with these models and systems.

As much drug discovery and other research is performed outside the biopharmaceutical companies today, there needs to be a smoother, more integrated workflow approach across companies that work together providing different disciplines for projects. Some scientific informatics platforms today provide some of these capabilities, but they are still in their infancy.

About the authors

Leif Pedersen is President of Software, and David Lewis, PhD, is Executive Director of Scientific Informatics at Certara. Certara uses bioinformatics and scientific informatics software and technology to transform traditional drug discovery and development. Its clients include more than 1,450 global biopharmaceutical companies, leading academic institutions, and key regulatory agencies across 61 countries. The company is based in Princeton, New Jersey, USA.