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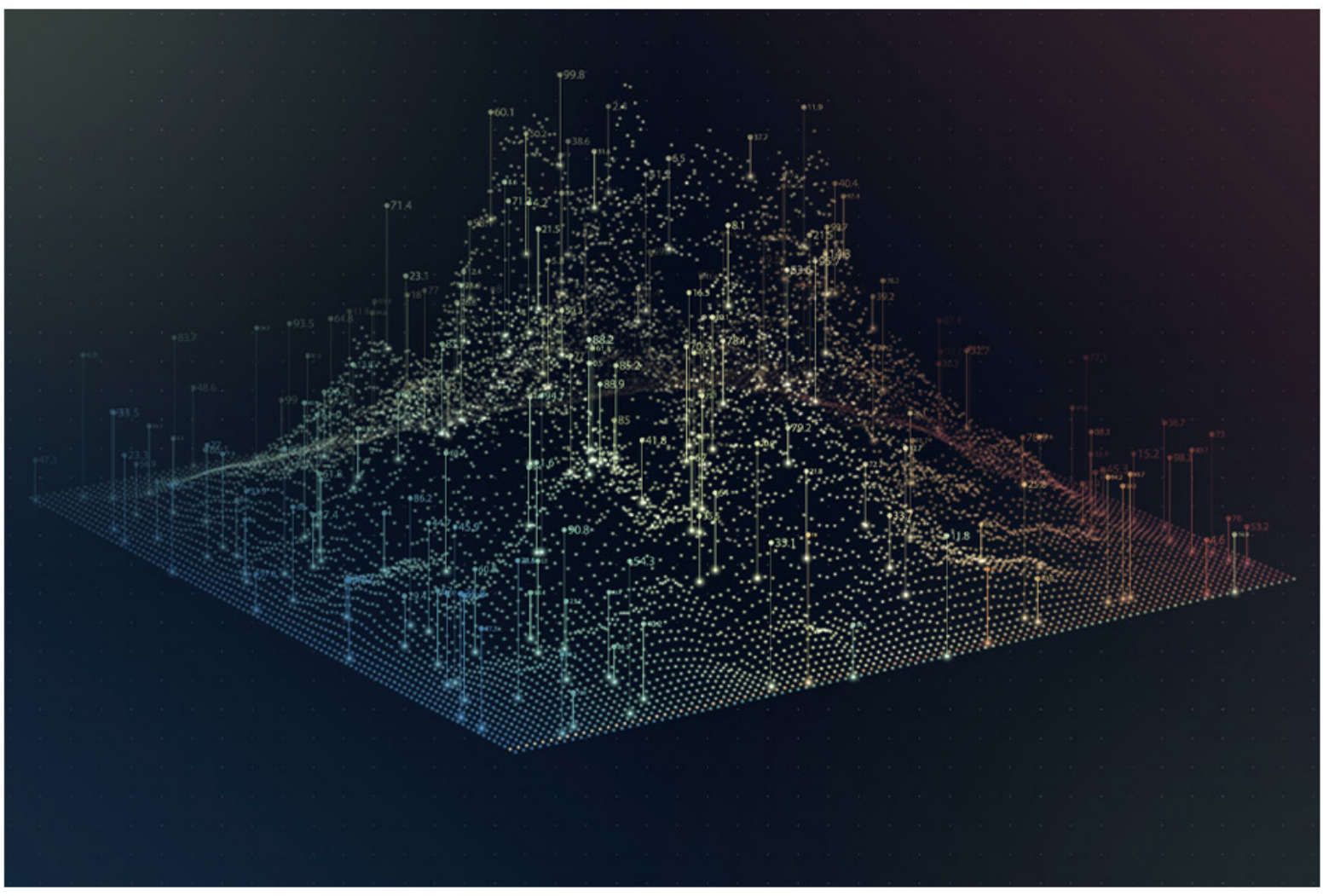
The value of scientific intelligence in drug discovery



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Leif Pedersen, President, Software, and David Lowis, Executive Director of Scientific Informatics at Certara, explain how scientific intelligence can refine 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 life cycle.

When biopharmaceutical companies set out to build a new therapeutic, they already know what they want to achieve, and they have defined their target product profile (TPP). But faced with pressure to shorten drug development timelines, all drug discovery research activities need to be focused on optimising analytics for faster, critical decision making. Utilising scientific intelligence capabilities to provide conclusive analysis and find the best possible candidate substance or molecule to reach the TPP is essential.

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, remove noise, clean the data, and align them with standards and ontologies. Furthermore, with new modalities in today's drug development, such as peptides, oligonucleotides, antibodies, and antibody-drug conjugates (ADC), the data complexity increases even further, and that needs to be taken into account.

The scientific intelligence platform needs to have a set of capabilities for data aggregation, cleansing, preparation, contextualisation, reporting, analysis, intelligence, segmentation, and visualisation of outcomes. It must also be able to integrate with all other scientific data sources, workflows, and applications within the drug discovery life cycle.

The scientific intelligence platform should be open from the architectural, software integration, and leverage standpoint. For example, while the scientific intelligence platform would not secure IP protection for the final molecule, which meets the TPP, it should interface with the application that does.

When a biopharmaceutical company's scientists identify a promising drug candidate, laboratory and *in vitro* work is required to investigate and verify that it is the right substance or molecule. Therefore, the platform needs to be able to support a workflow to ensure that the scientific project can progress smoothly. Ideally, it should integrate with the compound ordering system so scientists can request the synthesis of a new batch of the chosen molecule, order a set of tests, and receive the test results in the same place.

In general, scientists must break up the workflow and determine points of scientific decision-making, which for example, will reduce the number of target compounds. Once a chosen target compound is identified, scientists need to be able to view information within the context of the target molecule. The ability to move between data visualization, insight, and analysis is necessary for efficient drug discovery.

Biopharmaceutical discovery research is leveraging artificial intelligence (AI) today. Therefore, the platform has to enable, embed and integrate multi-level machine learning (ML) and AI capabilities for data modeling and prediction.

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

Today, biologics make up about half of all research into new therapies. Yet, the scientific informatics systems that support them lag behind small molecule drug development. Data capture systems for small molecules are mature and well featured, whereas, for biologics, the situation is vastly different.

There are also more new 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 decide whether it is better to pursue a small molecule, antibody, or an ADC therapeutic.

Looking forward, there needs to be more advanced use of ML and AI on 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 ML and AI algorithms needs to go further into the field of unsupervised AI and bring in topological approaches to deep learning. This will, at the same time, require scientists to be trained to work with these models and systems.

As much drug discovery and other research is performed outside the biopharmaceutical company 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 those capabilities, but they are still in their infancy.

As part of all the above, migration to and adoption of scalable cloud technology is essential. A key element of cloud leverage is to make sure that security standards like ISO 27001 are met since the data are often highly proprietary and confidential.

Conclusion

Scientific intelligence has the power to dramatically improve the effectiveness and efficiency of the drug discovery process and should be an essential part of a scientific informatics strategy. It is empowering scientists to build their own data views from diverse data sources so they can test their theories and design new molecules. All this while working with an even more complex network of partners. Scientific intelligence platforms also encourage pre-competitive collaboration between companies and facilitate better use of resources.

About the authors

Leif Pedersen is President of Software, and David Lowis, DPhil, is Executive Director of Scientific Informatics at Certara. Certara uses biosimulation and scientific informatics software and technology to transform traditional drug discovery and development. Its clients include more than 1,650 global biopharmaceutical companies, leading academic institutions, and key regulatory agencies across 61 countries. The company is based in Princeton, New Jersey, USA.

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