DeepLife
deeplife.co

How digital twins of human cells are accelerating drug discovery

Designed to reshape drug discovery and drug repositioning, systems biology company DeepLife has created a data-driven technology platform that creates digital twins of human cells, to evaluate response to new drug candidates.

The rapid proliferation of omics data, which provides essential information regarding biomolecular activity within cells, is transforming drug discovery. Equipped with this data, DeepLife, a next generation systems biology company, has established a platform for creating digital twins of human cells, enabling scientists to rapidly evaluate how unhealthy cells respond to drug candidates in silico. DeepLife has deployed and established proof-of-concept for its platform, and is now actively seeking partners for target identification and drug repositioning projects enabled by its digital twin technology.

All diseases, and efforts to treat them, start at the cellular level. Small changes in the trillions of chemical interactions that make up human cells, which can be triggered by mutations or external forces, can cause cells to enter pathological states that ultimately manifest in diseases. The massive scale and complexity of the inner workings of cells has traditionally impeded efforts to identify the drivers of diseases through the iterative reconstruction of cell mechanisms, but science is now taming the challenge.

"The convergence of recent technological advances in high-throughput sequencing to measure cell activity at the single cell resolution and deep learning is opening new opportunities to model cell behavior at unprecedented levels and DeepLife is leading the way," said Jean-Baptiste Morlot, co-founder and CTO at DeepLife.

However, the life sciences sector has yet to realize the full potential of the rapidly growing trove of multi-omics data. The fast growth of data repositories is outstripping the capacity of humans to generate insights from these resources, and drug discovery remains a largely siloed, iterative process, in which data is interpreted, accessed, and analyzed by distinct teams of wet-lab biologists, bioinformaticians, and engineers.

The shortcomings of the current approach are clear. Traditional target development can take four years and cost $300 million, making it a significant contributor to the time and money needed to develop new medicines. Even after this expensive, time-consuming process, the chances of the project resulting in an approved medicine are slim. A better approach is needed.

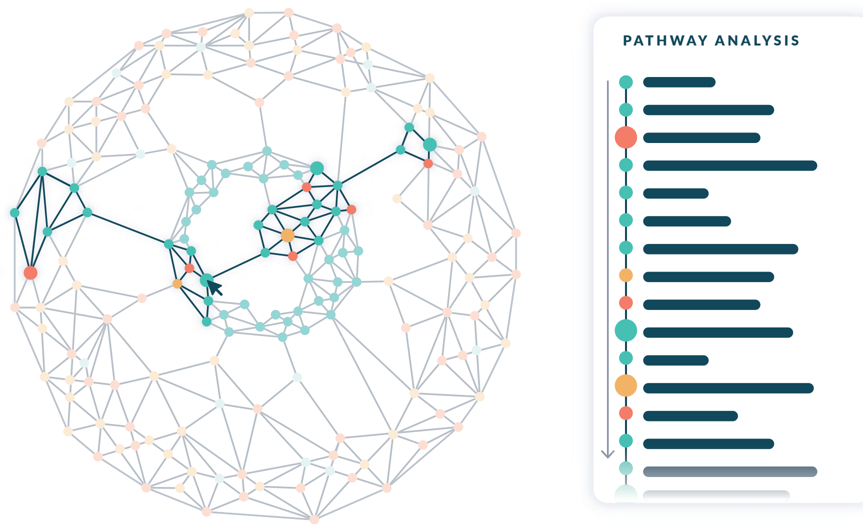

Fig. 1 | The DeepLife Digital Cell technology platform. With the digital cell technology developed by DeepLife, biologists can access interpretable representation of cell mechanisms highlighting pathways and most probable druggable targets.

Building an omics data and discovery platform

Two years ago, DeepLife set out to develop its digital twin technology (Fig. 1). The experience showed DeepLife the value of, and need for, improved data analysis, leading it to establish a data-as-a-service offering. Working out of sites in Paris and Boston, DeepLife has gone on to create a platform that supports both sides of its business, with single-cell data services offered alongside digital twins of human cells that could reshape drug discovery.

DeepLife is working to optimize target identification by enhancing in-vitro testing for drug discovery. In trying to achieve that goal, DeepLife has built a collaborative, data-driven ecosystem for drug discovery. The all-in-one solution applies a machine learning (ML)-based data curation pipeline to data taken from DeepLife, its customers, and public sources.

"We use single-cell omics data to shine a light on the inner workings of the human cell, thereby generating the actionable insights scientists need to deliver a sorely needed step change in the speed and quality of target development," said Jonathan Baptista, co-founder and CEO of DeepLife.

The ML-based pipeline curates data from all sources, helping bioinformaticians to cope with the rapid growth of omics data entered into repositories, as well as with the variability of the quality of the omics data across the various repositories. It outputs omics cell, tissue, and organ atlases that are available in DeepLife's multi-omics 'Datastore' data marketplace. The marketplace provides users with one-click access to ML-ready multi-omics datasets, as well as application programming interface (API) access to interoperable data packages.

> **We use single-cell omics data to shine a light on the inner workings of the human cell**
>
> Jonathan Baptista, Co-founder and CEO, DeepLife

DeepLife has mapped more than 30 atlases with more than 20 million single cells (Fig. 2). The atlases span brain, blood, liver, lung, intestines, and other tissues and organs, and DeepLife updates them monthly using more than 20 qualified data repositories.

Yet, DeepLife is much more than a data provider. The atlases also serve as the basis for DeepLife's single-cell 'Analysis' offering. DeepLife Analysis supports large-scale multi-omics data analysis workflows to give scientists and engineers who analyze drug discovery data a scalable ecosystem designed around the intense demands of the omics era. The cloud-based platform has no IT setup and provides a tailored visualization coding environment and graphical interface, empowering users to run large-scale analyses on 10 million cells, and to seamlessly integrate state-of-the-art analysis tools using R and Python.

Developing digital twins

DeepLife's data provision and analysis capabilities form the first phase of its offering. DeepLife uses these capabilities as a launchpad for its digital twin service, establishing itself as a major player in the emerging and groundbreaking field of virtual cell representation.

A digital twin is a virtual model of a physical object or process. The concept, which first emerged outside of life sciences, has enabled companies to model physical objects such as wind turbines in the virtual world. By modeling an object, researchers can simulate how it is likely to respond to different situations, enabling them to generate insights far faster, and at less cost, than would be possible when working with physical objects. DeepLife is leading the effort to apply this concept to drug discovery.

Cells are uniquely complex objects, but the proliferation of omics data has made it possible to generate a comprehensive picture of an unhealthy cell. DeepLife uses omics data to create digital twins of cells in silico. Moving single-cell analysis from in vitro to in silico has profound implications for drug discovery. Because digital twins predict how a cell will react to a molecule, DeepLife can rapidly test billions of drug combinations and use interpretable artificial intelligence (AI) to identify the mechanisms of action which are most likely to restore a cell to its healthy state.

The 'Digital Cell' offering provides comprehensive pathway analysis and supports the identification and prioritization of druggable targets and biomarkers for disease-specific cell models. As DeepLife uses interpretable, rather than black box, AI, its technology does more than just predict how a cell will behave; it also uncovers the mechanism of action that drives the behavior.

DeepLife has generated technical proof-of-concept data to establish many valuable commercial use cases. DeepLife has used its proprietary technology to make predictions about how cells will respond to infection by viruses, to small molecule cancer drug treatments, and to CRISPR and siRNA perturbations, among other examples. These studies are the first steps to validate the use of digital twins in drug discovery, setting the stage for more widespread adoption of this groundbreaking approach.

Drug repositioning is a major application of the digital twin technology. The history of drug development shows that there is potential in repositioning approved medicines for use in new indications. Repositioning cuts the time and money needed to develop new medicines by enabling programs to leverage the studies run to support approval in the primary indication, maximizing the value of molecules. However, the lack of a systematic way to identify additional indications has meant that repositioning has historically relied on serendipity.

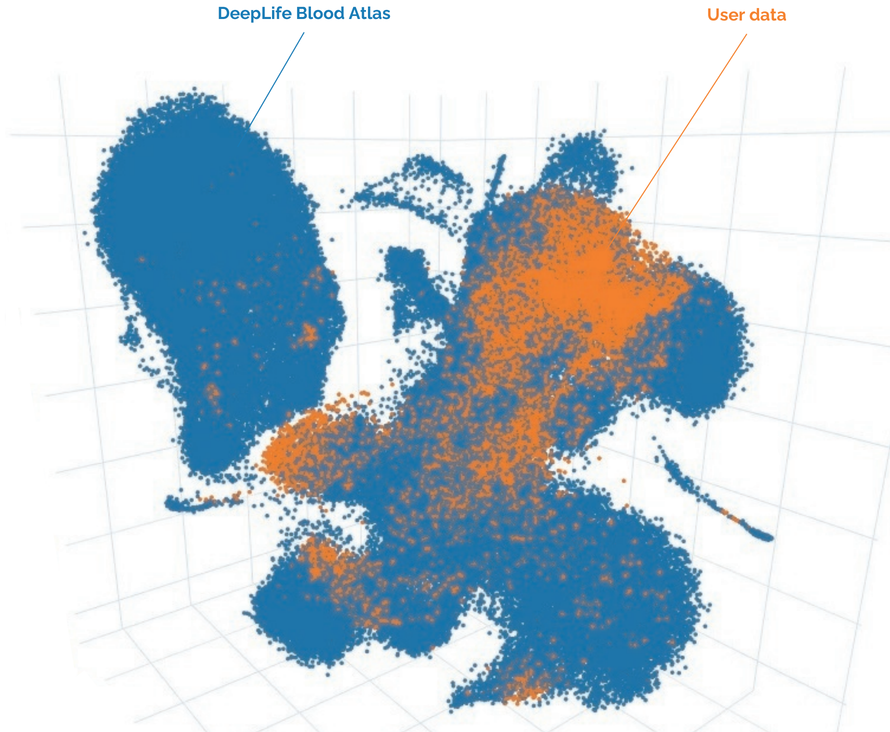

Fig. 2 | A 3D UMAP of the DeepLife single cell Blood Atlas fully annotated. Each dot represents gene expression of a cell associated with metadata of its donor (gender, age, ethnicity, smoking, etc.). Customer data (orange) is automatically mapped on the 2.5 million cells of the DeepLife blood atlas (blue) to virtually expand its cohort size for downstream analysis on the DeepLife platform.

Digital twins stand to enable scalable, systematic searches for repositioning opportunities. By predicting how a cell will react to approved molecules, DeepLife Digital Cell could accelerate repositioning and, in doing so, cut the time it takes to get treatments to patients with unmet medical needs. DeepLife is now showing that its technology can live up to that promise.

"Target identification and drug repositioning are our main focus for 2022 and beyond," said Baptista. "We are actively working with our existing partners to explore how digital twins can accelerate drug development, and remain open to forming new alliances with researchers who want to tap into our transformative technology. The first projects could enable our partners to quickly pick low hanging fruit and show digital twins improve drug repositioning."

> **DeepLife has built a collaborative, data-driven ecosystem for drug discovery**

Partnering to access the platform

Drug repositioning partnerships are one of several ways that researchers can work with DeepLife. The simplest option is the Datastore marketplace, which allows users to access organ omics atlases. With one click, DeepLife provides harmonized repositories of single-cell data and the tools needed to analyze the information, enabling researchers to quickly access and interrogate data as a first step.

DeepLife has made its digital twin capabilities available on a software-as-a-service (SaaS) basis, setting it apart from AI offerings elsewhere in the industry. For select partnerships that DeepLife enters into, it uses its SaaS platform to move rapidly and efficiently, slashing the multi-month and even multi-year setup times that are common in AI collaborations designed to accelerate time to actionable insights.

Companies that partner with DeepLife to work on digital twins will become pioneers in a groundbreaking but now validated field. DeepLife's proof-of-concept studies have validated its digital twin work, cementing its status as a major player in an emerging field, and opening the door to a new methodology for drug discovery. The next step for DeepLife is to more completely leverage the full potential of its technology, embarking on projects that could cut the time and money needed to discover treatments for unmet medical needs.

CONTACT
Jonathan Baptista, CEO
DeepLife
Paris, France
Email: jonathan.baptista@deeplife.co