AI Makes Drug Discovery Faster

Software Saves Time and Costs in Early-stage Drug Development

The effect of a drug starts after a few minutes. The headache disappears, the stomach calms down, or the fever drops. What an effective opportunity for mankind: We are used to medication helping us when we are sick. However, the development of a drug usually takes a decade. The Dresden, Germany-based start-up PharmAI has found a way to significantly speed up the process. To do so, they use artificial intelligence and rely on the capabilities of smart algorithms. Joachim Haupt, co-founder and CEO, and Florian Kaiser, co-founder and CTO, explain PharmAI's technology and describe the company's options and steps ahead.

Joachim Haupt, PharmAI

Florian Kaiser, PharmAI

CHEManager: Mr. Haupt, which challenges is drug research currently facing?

Joachim Haupt: The two most important challenges are certainly time and budget. The development of new drugs normally takes a decade. This is associated with high costs. Therefore, finding solutions for rare diseases is unfortunately not lucrative for many companies. PharmAI would like to solve these problems. We see the PharmAI technology as an enabler and are convinced that we can help to accelerate drug development with our approach.

Mr. Kaiser, how does it work?

Florian Kaiser: Artificial intelligence (AI) and smart algorithms are the foundation of our software DiscoveryEngine. It uses information about the composition of proteins in the human body, viruses, or diseases. Using a combination of smart algorithms to process protein structures and AI to detect significant features, the software builds specific fingerprints of the binding site of a protein target. These fingerprints are the essential component, allowing our DiscoveryEngine to identify suitable drugs from libraries with billions of small molecules. You can think of it like a big jigsaw puzzle—with millions of pieces.

What are the concrete advantages of this method for drug research?

F. Kaiser: Our proprietary method is fast, cost-efficient and very effective. It also conserves resources. By using our method, our customers only need to test a few hundred molecules in vitro to obtain hits for their drug target—in contrast to several tens of thousands with classical high throughput screening (HTS). The positive implications are manifold: Timelines are reduced from 12 months to 3 months, assays, which would not work with HTS, can be used, and the chemical diversity of the identified molecules is very high.

When did the idea of founding your own company arise from this approach?

J. Haupt: Important preliminary work for this took place at Biotechnology Center (Biotec) of TU Dresden several years ago. It was clear to us that this new development could revolutionize early-stage drug discovery. That's why we founded our start-up in 2019. A lot has happened since then. We all learned a lot and our software became so much better and much more flexible with respect to the use cases.

Who is interested in your work? What important projects have there been since the founding?

F. Kaiser: There have been quite a few. One wonderful project was part of the ongoing cooperation with 2Bind from Regensburg. We combined AI and highly efficient biophysical tests to a new method. This makes it possible to detect undesirable side effects of drugs in record time and very early in the development process. Previously, it took many months to confirm these effects in the laboratory. With our new approach, results are available after only eight weeks.

J. Haupt: NanoTemper Technologies from Munich is also an important partner. Together with their team, we published the tool Proto at the beginning of 2022. Proto assists scientists in their decisions on how to label proteins. The resulting web app uses more than half a billion protein structures, many of them from AlphaFold.

Together with NanoTemper you have decided to offer Proto for free. Is that smart? As a start-up, don't you also have to earn money?

J. Haupt: Whether this decision is considered smart or not really depends on the perspective. We understand PharmAI as enabler of a faster and more cost-effective drug discovery. And I think that we are on the same page with NanoTemper here. However, it was NanoTemper's decision to offer Proto for free and I think that was a smart decision. To attract more small laboratories into drug research, these need tools that make their work easier and reduce costs. This is the only way to develop therapies for many more rare diseases. Every patient deserves help. AI helps us to help them.

What role will AI play in the laboratories of this world in the future?

F. Kaiser: I think a big one. It holds enormous potential. We will only need days or hours to find answers to questions that previously took us years. That means we can devote ourselves to many more topics. It's going to be exciting. Our work will definitely not be boring in the future.

Personal Profile

Joachim Haupt is CEO and co-founder of PharmAI. He graduated with honors in Bioinformatics from Martin-Luther-University and holds a PhD in computer science from TU Dresden. His career in drug discovery started at the Leibniz Institute of Plant Biochemistry. Since then, he has built a long scientific track record in the areas of cheminformatics, computational drug discovery, and structural bioinformatics. Apart from his scientific career, he founded a number of companies. And he casted church bells.

Florian Kaiser is CTO and co-founder of PharmAI. He holds a PhD in computer science from TU Dresden. During his academic career at Biotec, he contributed to algorithmic development for large-scale protein structure analysis. Florian is heavily involved in the application of AI to biological problems and always keen to identify and tackle new challenges. At PharmAI, he puts cutting-edge AI technology to the test to accelerate drug discovery.

Business Idea

Structure to Knowledge

Over the past five years, PharmAI has built and fine-tuned the DiscoveryEngine—a software for drug discovery with cutting-edge machine learning techniques and bioinformatics algorithms based on the latest scientific research. Originally developed for virtual screening, the DiscoveryEngine was extended to off-target search and prediction of properties of proteins. PharmAI is offering smart services for pharma and biotech research, allowing easy access to advanced computational tools for clients without cheminformatics capacities. Over the last year, PharmAI established a software-as-a-service (SaaS) toolchain, which can be easily combined to a custom solution fitting the needs of platform providers.

Hybrid Business Model

PharmAI follows a hybrid business model of service projects on a pure fee-for-service basis complemented by a subscription model for SaaS products. The most popular service is the PharmAI Focused Library, which enables clients to screen chemical libraries with hundreds of millions of compounds. The customer provides information about the target and selects a screening library. PharmAI conducts the virtual screening and delivers a shortlist of some hundred chemically diverse compounds together with a comprehensive report within about a month. Subsequent in vitro tests show hit rates that are several hundred times higher than conventional methods and over ten-fold higher than state-of-the art computer methods. As a result, the customer only needs to test some hundred compounds but obtains hits as if they ran an HTS campaign with tens of thousands of compounds—at a fraction of the conventional timeline.

The SaaS offering allows to deploy solutions in the cloud for customers with specific needs and a high throughput. Due to the rich feature set in structural biology, cheminformatics and AI, the components of the DiscoveryEngine are applied to solve tasks like ADME-T characterization of small molecules, protein sample preparation and virtual screening.

- PharmAI, Dresden, Germany
  www.pharm.ai

Elevator Pitch

Shorten the Timeline

PharmAI's mission is to make early-stage drug development significantly more efficient by increasing success rates while reducing costs. This is achieved through a breakthrough AI-powered platform for 3D protein structure analysis. The DiscoveryEngine technology shortens the timeline for discovering new therapeutic molecules dramatically. PharmAI was founded in 2019 as a spin-off from the Biotechnology Center of the TU Dresden. As of today, 13 members are part of the international PharmAI team.

Milestones

2019
- PharmAI founded as spin-off from TU Dresden, Germany.
- Strategic partnership was established with biophysical screening provider 2Bind.
- PharmAI was awarded member of the TechBoost start-up program of Deutsche Telekom.
- Collaboration with device manufacturer NanoTemper Technologies.
- Extension of business model to Software-as-a-Service (SaaS) solutions.

2020
- PharmAI hosts its own computing infrastructure in a secure datacenter.
- PharmAI was invited to contribute to a long-term drug discovery project for modulation of protein-protein interactions in neurological diseases.
- Collaboration with the Saxon Institute for Computational Intelligence and Machine Learning initiated to enlighten the black box and make PharmAI's machine learning interpretable.

2021
- Transformation of the PharmAI software stack into a cloud-ready and scalable micro service architecture.

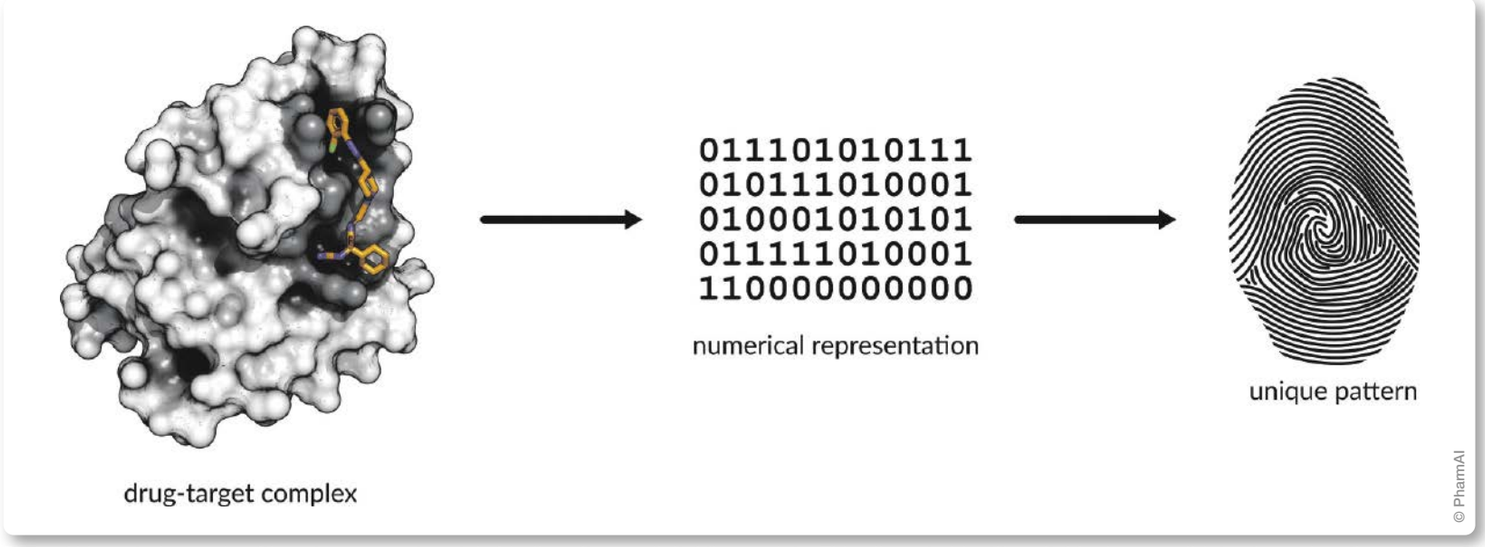
2022
- First SaaS product "Proto" available to the general public in cooperation with NanoTemper Technologies.

Roadmap

2022
- Scale-up of SaaS offering with a new product.

2023
- SaaS solution deployed at platform provider.

2027
- First drug from PharmAI's pipeline in clinical trials.



PharmAI invented new algorithms to represent protein binding sites as digital fingerprints. This allows to identify suitable drug candidates from gigantic compound libraries.