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PRESS RELEASE

Dresden start-up de-risks drug development

PharmAI and 2bind discover side effects in record time

Side effects of drugs can have fatal consequences. It is therefore important to detect these side effects at an early stage. This is exactly what a new method developed by the Dresden-based start-up PharmAI GmbH and its partner, 2bind GmbH from Regensburg, is making possible. The two companies' method combines artificial intelligence with highly efficient biophysical testing. The challenge of early side effect detection – which was previously similar to finding a needle in a haystack, requiring considerable time and resources – can now be addressed easily in less than two months thanks to this ground-breaking approach. This leads to a massive risk reduction in drug development.

PharmAI was founded in 2019 as a spin-off from TU Dresden. The company's core software *DiscoveryEngine* is based on the analysis of 3D protein structure data. It uses information about the composition of proteins in the human body, viruses, or diseases and extracts knowledge on how these proteins interact with drugs and other small molecules. Using artificial intelligence-based algorithms, the software searches among hundreds of thousands of proteins and drugs for suitable associations. So far, the PharmAI team has used their technique to develop a new screening workflow for the identification of yet unknown drugs in challenging diseases. "Now, for the first time, we have used our technology to detect so-called off-targets – unwanted protein targets that lead to side effects," explains PharmAI CEO Dr. Joachim Haupt.

In the current project with 2bind, PharmAI is working on a highly relevant protein, the enzyme MAPK14. This enzyme is present in many cell types and is important for DNA repair. In recent years, it has become clear that MAPK14 is also involved in autophagy, cellular waste disposal, and is therefore also of interest in cancer therapy. Using the *DiscoveryEngine*, the PharmAI team identified connections between the kinase inhibitor SB203580 and other proteins. Kinase inhibitors are among the most effective anti-cancer drugs because they can slow down tumor growth significantly. However, they often do

not act selectively and therefore also influence other enzymes. The risk of harmful and even potentially fatal side effects is therefore high. "Together, using our new methodology, we can rapidly find such undesired off-targets," Dr. Haupt continues.

By using the *DiscoveryEngine*, the experts from Dresden discovered 13 proteins that represent potential off-targets which needed further validation in laboratory tests. PharmAI found a competent partner for *in vitro* validation in 2bind, which are experts for validating artificial intelligence predictions. “We take the actual, physical off-targets to the lab, mark them with a special fluorescent dye and test the binding of the kinase inhibitor it all started with, SB203580”, explains 2bind’s CSO Dr. Maximilian Plach. Of the 13 tested proteins, binding was observed for six, which corresponds to an extraordinarily high hit rate of 46 percent.

This method of testing is not only effective, fast and cost-efficient, but it also conserves resources: “Only the tiniest amounts of protein are used to validate the computer-aided predictions in the laboratory” Dr. Plach adds. This is an important point, since there are usually no financial means and time available for the production of large amounts of protein. With this joint effort, PharmAI and 2bind are confident to help revolutionizing the search for undesired side effects in drug research. The presented newly developed methodology makes a significant contribution to de-risk drug development efforts.

The **photo** for the press release can be used free of charge for reporting purposes.

Caption: Christoph Leberecht (Software Engineer), Dr. Joachim Haupt (CEO), and Dr. Florian Kaiser (CTO) are driving the technology development in the international PharmAI team (from left to right).
Credits: Braun-Bunt Photography

About PharmAI

The start-up PharmAI was founded in 2019 as a spin-off from the TU Dresden. The company's core software DiscoveryEngine is based on the analysis of 3D protein structure data. It uses information on the composition of proteins in the human body, viruses, or diseases and extracts knowledge on how these proteins interact with drugs and other small molecules. This is a kind of jigsaw puzzle driven by the unique way how small molecules interact with binding pockets – small cavities on the protein surface. The technology, which is based on artificial intelligence, is used by its customers to find new molecules for the treatment of diseases or to detect undesired side effects in a very short time. PharmAI currently has eight team members.

Contact

PharmAI GmbH
Tatzberg 47
01307 Dresden

Jana Mundus
+49 351-41881626
press@pharm.ai

About 2bind

2bind GmbH was founded in Regensburg in 2011 and provides tailor-made biophysics services and solutions that are perfectly adjusted to precise needs in key, high-value areas of Drug Discovery, Antibody Research, Aptamer Characterization, and Protein Biophysics. A state-of-the-art portfolio of biophysical technologies enables them to provide a complete and comprehensive analysis set from affinity and stability to kinetics and thermodynamics. This method portfolio includes, among others, MicroScale Thermophoresis (MST), nano-Differential Scanning Fluorimetry (nanoDSF), Biolayer Interferometry (BLI), and Isothermal Titration Calorimetry (ITC). Currently, the company has nine team members.

Contact

2bind GmbH
Am Biopark 11
93053 Regensburg

Dr. Thomas Schubert (CEO)
schubert@2bind.com
+49 941 2000 0890