SNAPS

applied technologies

# Off-target identification using Discovery Engine technology

The use of artificial intelligence in the healthcare industry is increasingly proving to be a lucrative technology by reducing the R&D gap in the drug manufacturing process and facilitating the targeted production of drugs. In drug discovery, AI helps solve complex challenges and problems in the development process through machine-simulated human intelligence.

In drug development, it is not uncommon for manufactured compounds not to do what researchers expected. A large number of new drug candidates in the testing phase fail clinical trials due to undesirable and potentially harmful side effects. This results in not only scientific risk, but also significant economic risk.

Discovery Engine technology assists researchers in drug discovery by screening hundreds of thousands of proteins and existing drugs for associations and off-targets. It does this by using a future-changing combination of 3D protein structure data and AI technology. Information about the nature of various proteins in the human body, as well as information from viruses or other pathogens, is used to extract knowledge of how proteins interact with already known drugs and other small molecule compounds. Based on AI and smart algorithms, the software searches for matching compounds between the respective proteins and active ingredients among the candidates available in the database.

The technology provides unprecedented accuracy in mapping drug-target complexes. To optimize the prediction of binding site similarities, the technology uses both a geometric comparison of binding sites based on local alignments and incorporates non-covalent interactions. The technology, which has been continuously improved in the past, has found application in repositioning already known drugs for new targets against, for example, cancer or malaria.

To find off-targets, the technology proceeds in three steps: (1) analysis of the binding sites to characterize their geometry in atomic detail, (2) performing an interaction analysis to detect non-covalent interactions and finally (3) a calculation of unique fingerprints. The uniqueness of the technology is that geometric binding site properties and non-covalent interaction patterns are used, making it possible to generalize ligand binding. By translating protein-ligand complexes into individual fingerprints, there is the possibility to quickly calculate similarities between arbitrary chemical libraries and thus ultimately predict novel compounds as well as use them for predicting potential off-targets.

## INNOVATIVE TECHNOLOGICAL APPROACH

- **Company:** PharmaAI (Spin-off of the TU Dresden)
- **Technological basis:** Artificial intelligence & 3D protein structure data
- **Field of application:** Off-target identification in drug discovery

  Analysis of protein structure data
- **Advantages:** Level of detail in the representation of drug-target complexes

  Binding site analysis

  Prediction of new Drug-Target-scaffolds

  Translation of protein-lingand complexes into unique fingerprints
- **Website:** https://www.pharm.ai/

**Off-Targets = undesirable drug targets that lead to side effects**