Pharos iBio Co., Ltd.
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The Chemiverse platform: AI and big data-based drug discovery and development

Chemiverse provides a quicker route to 'the best target, the best chemical,' according to the Korean biotech Pharos iBio. With its first AI-based drug currently undergoing clinical trials, the company is demonstrating the broad value AI can provide from discovery to clinical development.

Unlike other artificial intelligence (AI)-based discovery platforms, Chemiverse, developed by South Korean biotech Pharos iBio, is useful in all aspects of the drug discovery process, from new drug target searches to candidate selection for clinical development. It uses a variety of algorithms, 10 distinct modules and more than 230 million big data entries. "Our Chemiverse platform is allowing us to expedite the long R&D cycles common in drug discovery and development, and enable us to quickly deliver life-saving drugs for tough-to-treat diseases," said Pharos iBio chief development officer, June Han. The company has already demonstrated the power of its proprietary platform with the first South Korean AI-based drug, PHI-101, currently undergoing clinical trials.

"The Chemiverse AI platform is unique and multifunctional, accurately identifying hit compounds based on 3D target protein structure and quantum mechanical energy calculations, assessing toxicity and analyzing bio-activity," said the company's chief technology officer, Ky-Youb Nam. The platform optimizes every part of the process, discovering novel binding sites in target proteins and predicting intermolecular interaction energies between proteins and inhibitors, faster and more precisely (Fig. 1).

"Chemiverse helps to design novel drug candidates using chem-informatics, structure- and ligand-based analysis, and then proposes compounds with entirely new scaffold structures and lead compounds," added Han, "while simultaneously factoring in currently registered patents, drug efficacy, cellular activity, cardiac toxicity, predicted pharmacokinetics, and synthesis potential." The company harnesses the Chemiverse platform to develop 'first-in-class' or 'best-in-class' therapeutics through AI translating massive chemical and genomic information with effectiveness and speed.

Founded in 2016 by Jeong-Hyeok Yoon, an expert in computational chemistry and a biotechnology industry veteran with more than 20 years of experience in building and running companies, Pharos iBio currently has 18 employees based in Seoul and 21 patents across 13 countries. The company now has 8 ongoing drug discovery and development programs, to treat relapsed or refractory diseases, one of which is PHI-101. In addition, Pharos iBio has four additional drug candidates in its pipeline, discovered using Chemiverse. These all target highly aggressive and difficult-to-treat tumors. The focus of the firm remains on R&D, including drug discovery, clinical development, and AI technologies that support its broad ambitions to create 'the best target, the best chemical'.

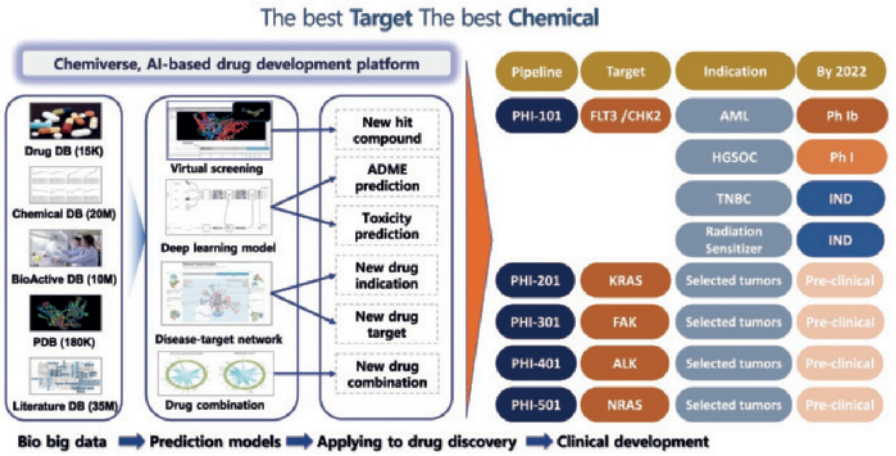

Fig. 1 | Transforming big data to healthcare with an AI-powered drug discovery and development platform. The power of computational molecular modeling and the prediction algorithm of the Chemiverse platform can be applied across all drug discovery stages including target identification-hit and lead generation, new drug candidate optimization-scoring potential and further development into clinical stages. AI, artificial intelligence; AML, acute myeloid leukemia; HGSOC, high-grade serous ovarian carcinoma; IND, investigational new drug; TNBC, triple-negative breast cancer.

Development candidates

The company's first drug candidate, PHI-101 is an orally available, small molecule drug, now in two phase 1 clinical trials for acute myeloid leukemia (AML) and high-grade serous ovarian carcinoma (HGSOC). Designed as a next generation FLT3 tyrosine kinase inhibitor, PHI-101 has a novel mechanism of action to overcome resistance to AML. In preclinical studies, it showed higher anti-leukemic activity and selectivity while having lower toxicity than current FLT3 inhibitors such as midostaurin (Rydapt) and gilteritinib (Xospata). The ongoing global clinical trial in Australia and South Korea with relapsed and refractory AML patients is expected to report this year.

Chemiverse is also equipped with an algorithm to uncover alternative modes of action for compounds, to expand their indications. These insights enabled Pharos iBio to initiate phase 1 clinical trials for PHI-101 to treat platinum-resistant, HGSOC, after validation. The company also plans to start clinical trials next year for PHI-101 to treat triple-negative breast cancer and for use as a radiation sensitizer, which enhances tumor cell death on irradiation.

Collaborations and open innovation

The company is already working with several hospitals and academic laboratories in Korea and the US and is open to new collaborators as well as strategic investors, to expand and co-develop its current clinical and preclinical pipelines and to constantly look for cutting-edge solutions. "Open innovation is a very important part of our business model," stressed Han, "we are seeking partners who share our values and commitments to save lives."

Pharos iBio is looking for partners who are interested in licensing the assets derived from the Chemiverse platform. "Out-licensing or industrial partnerships should expedite the whole process of clinical development and increase the possibility of successfully launching an innovative product," said Pharos iBio chief business officer, Kyu-Tae Kim.

Whilst AI is now becoming part of the drug discovery landscape, "our capabilities extend beyond discovery," noted Kim "Chemiverse provides tools for the entire development pathway, we can cover all stages from target to drug candidate selection and drug repurposing to expand clinical development."

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