

ExaWizards and Daiichi Sankyo Achieve Results in AI Drug Discovery, Joint Project Identified Hit Compounds on Challenging Target Proteins in a Short Period of Time

ExaWizards, Inc. (“the Company”) and Daiichi Sankyo Company, Limited (Chuo-ku, Tokyo; President: Hiroyuki Okuzawa; hereinafter “Daiichi Sankyo”) announced that their joint AI-based drug discovery project discovered a hit compound on a challenging disease-causing target protein. The two companies started a joint development project on data-driven drug discovery in 2019, and started a project to create hit compounds in 2023.

ExaWizards aims to solve social issues in the medical field by utilizing AI to develop drug discovery support, medical device programs, and services for consumers and patients.

1. Outcomes of this project

【Outcomes of this project】

ExaWizards has developed an innovative approach to drug discovery that combines AI technology and structure-based drug discovery (SBDD¹). This project conducted an ultra-large scale virtual screening² (ULVS) to identify potential hit compounds from a set of approximately 6 billion compounds. The project succeeded in filtering and selecting approximately 400 promising compounds for a target protein (for which it has been difficult to obtain high-quality hit compounds) in two months.

From the selected compounds, the concentration (IC₅₀) required to inhibit the reaction (activity) of a specific protein by 50% was below the set criterion, showing good activity as a hit compound.

Daiichi Sankyo will continue to study these compounds.

1 SBDD: Structure-Based Drug Design

2 A method of filtering a large number of compounds to those that show favorable activity via computer or other means. High-throughput screening, which evaluates millions of compounds, was the prior mainstream method.

【The Strengths of ExaWizards and Daiichi Sankyo】

The success of this project was a result of the combined strengths of ExaWizards’ AI engineers and Daiichi Sankyo’s researchers.

The project benefitted from a workflow that combined AI technology developed by ExaWizards’ engineers with docking simulations of compound-protein interactions, the expertise required to design and implement annotations, the ability and provide detailed descriptions of compound properties. Daiichi Sankyo’s research team then used their extensive knowledge of pharmaceuticals to develop a new method to create the new compound.

ExaWizards and Daiichi Sankyo have built a relationship based on knowledge and trust since the start of their collaboration in 2019 by combining their AI and data utilization technologies with pharmaceutical expertise. This has established an innovative approach to drug discovery and has created a faster and more efficient method for compound discovery.

2. Future Plans

The two companies will build on the results of this project by continuing their joint research on multiple target proteins, accumulating more successful results, and creating innovative drugs. ExaWizards will continue to develop their AI technology to contribute to efficient drug development through data-driven drug discovery research.

This collaboration will establish innovative approaches to drug discovery and create new methods for faster and more efficient compound discovery, contributing to the acceleration of drug research.

3. Impact on Business Performance

Although the impact of the results of this project on our business performance is still under scrutiny, we believe that it will contribute to improving our business performance in the medium to long term. When a reasonable calculation becomes possible, and when it is determined that there will be a significant impact on our business performance, we will promptly disclose such information.

(Reference) Consolidated earnings forecast for the current fiscal year (announced on August 14, 2023) and consolidated results for the previous fiscal year.

(Millions of Yen)

	Consolidated Sales	Consolidated Operating Income	EBITDA
Consolidated Earnings Forecast for the Current Fiscal Year (Year ending March 31, 2024)	8,500	(290)	600
Consolidated Results for the Previous Fiscal Year (Year ending March 31, 2023)	5,591	(378)	72

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