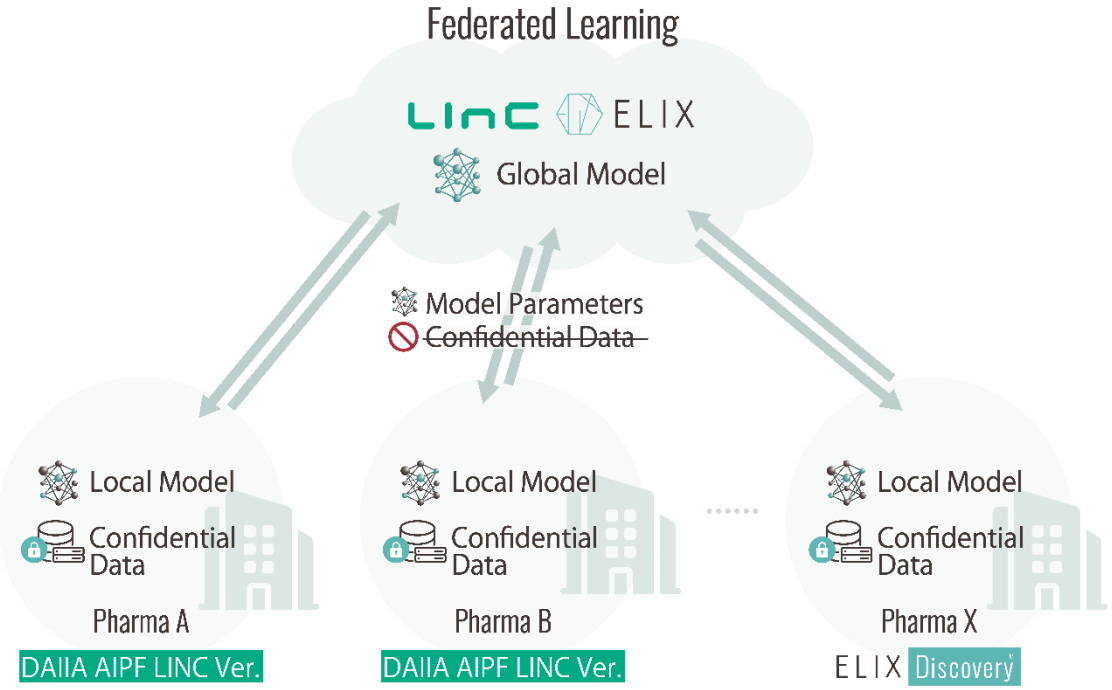
PRESS RELEASE

# LINC and Elix Become the First in the World to Commercialize an AI Drug Discovery Platform Incorporating Federated Learning-Based AI Models Trained on Data from 16 Pharmaceutical Companies

OSAKA, Japan — Life Intelligence Consortium (Representative Director: Yasushi Okuno / Headquarters: Osaka, hereinafter “LINC”) and Elix, Inc. (CEO: Shinya Yuki / Headquarters: Tokyo, hereinafter “Elix”), an AI drug discovery company with the mission of "Rethinking Drug Discovery” are pleased to announce that for the first time in the world we have commercialized an AI drug discovery platform that incorporates multiple AI models trained using federated learning on data provided by 16 pharmaceutical companies.




The key to AI drug discovery lies in high-quality and sufficiently large datasets. Diverse and abundant data are indispensable for building superior AI models; however, pharmaceutical companies are generally limited to utilizing their own proprietary data and public datasets, resulting in significant data shortages that have posed major challenges to progress. Federated learning technology provides a solution to this challenge.

Elix, in partnership with the Department of Biomedical Data Intelligence, Graduate School of Medicine, Kyoto University, developed the federated learning library kMoL*[2] through “Development of a Next-generation Drug Discovery AI through Industry-academia Collaboration” (DAIIA) *[1], an industry-academia collaborative program under the Project Promoting Support for Drug Discovery led by the Japan Agency for Medical Research and Development (AMED). Using this library, Kyoto University developed “Compound profile prediction AI” that was trained on public data as well as data held by 16 pharmaceutical companies without disclosing their

confidential data externally.

“Compound profile prediction AI” and “New compound proposal AI” which is developed through the same project under DAIIA are now implemented on DAIIA AIPF LINC version and Elix Discovery™, Elix’s proprietary AI drug discovery platform.

To ensure the continued operation and advancement of the innovative models and mechanisms cultivated in DAIIA, Elix—which already operates its own AI drug discovery platform—and LINC—a consortium supporting industry-academia collaboration in AI for life sciences with participation from many DAIIA member companies, have joined forces to commence the world’s first commercialization of an AI drug discovery platform serving models pre-trained with federated data, subsequently starting from April 2025. Through this initiative, we expect to see further adoptions of these technologies in real-world drug discovery settings.

Initially, the primary users will be the pharmaceutical companies that participated in DAIIA. However, as more companies join, the pool of available data will expand, further improving the accuracy and usability of the AI models for all users. We also plan to actively open the platform to companies that were not part of DAIIA. If you are interested in this initiative, please reach out to us via the contact information below.

## Keywords

*1 DAIIA: “Development of an integrated drug discovery AI platform combining multi-target prediction and structure generation models using state-of -the art AI technologies” project (R&D Principal Investigator: Teruki Honma, RIKEN) under DAIIA was launched in FY2020 with the aim of establishing a drug discovery support infrastructure leveraging AI, the project involved 17 pharmaceutical companies, research institutes such as RIKEN, Kyoto University, Nagoya University, along with about 10 IT companies with AI expertise. The project concluded at the end of March 2025.
https:// www.amed.go.jp/program/list/11/02/001_02-04.html

*2 kMoL: kMoL is a library for building machine learning models for the drug discovery and life science fields, and is the only publicly available library for AI drug discovery that has a “federated learning” function.
https://www.elix-inc.com/news/newsrelease/1470/

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**Comment from Yasushi Okuno, Ph.D., Representative Director, LINC; Professor, Department of Biomedical Data Intelligence, Graduate School of Medicine, Kyoto University; Division Director, HPC- and AI-driven Drug Development Platform Division, Center for Computational Science, RIKEN; and Co-Investigator of the AMED DAIIA Project**

On the occasion of commercializing the AMED project, I would like to express my heartfelt gratitude to AMED and to all the pharmaceutical companies that have cooperated with us.

This commercialization has two points of significance. First, while many government-funded projects fail to reach practical implementation after their funding period ends, this initiative will be utilized by pharmaceutical companies, thereby contributing directly to real-world drug discovery. Second, multiple pharmaceutical companies will continue to share data across the industry through federated learning, aiming to develop highly accurate AI. In an industry where the pursuit of individual corporate profit often takes precedence, the effort by each of these companies to share data for the benefit of patients and to build and utilize high-performance drug-discovery AI is profoundly meaningful and a source of great pride.

I sincerely hope that this project will become a cornerstone for enhancing Japan's drug-discovery capabilities and, ultimately, contribute to the health of patients around the world.

**Comment from Shinya Yuki, Ph.D., Co-Founder and CEO, Elix**

Data scarcity remains one of the biggest challenges in AI drug discovery. By jointly developing federated learning technology, kMoL, with the Department of Biomedical Data Intelligence, Graduate School of Medicine, Kyoto University, we have created a system that enables learning from the data held by 16 pharmaceutical companies while preserving the confidentiality of data such as compound structures.

Commercializing the predictive models we have built and deploying them on an AI drug discovery platform is a world-first initiative. This accomplishment was only possible through the collaboration of pharmaceutical companies, academia, AMED, LINC, and AI/IT enterprises involved in the project, and represents an important milestone that advances the use of AI in the pharmaceutical industry to a new stage. I believe that this will make Elix Discovery™ the de-facto standard of AI drug discovery platforms.

This federated learning based initiative is just the starting point for further progress. By encouraging even greater participation and data contributions from pharmaceutical companies, we aim to further expand and strengthen this initiative, enhancing our contribution to the pharmaceutical industry as a whole and ultimately to patients.

**Comment from Teruki Honma, Ph.D., Team Director, Molecular Design Control Research Team, Center for Biosystems Dynamics Research, RIKEN; and R&D Principal Investigator of the AMED DAIIA Project**

I am delighted that the AI models for on/off-target prediction, ADMET prediction, and molecular generation produced by the AMED DAIIA project will now be commercialized by LINC and Elix.

DAIIA's predictive AIs were built using chemical structure data provided by pharmaceutical companies, and training on structural data covering more than 1 million compounds and over 10 million data points, is unprecedented on a global scale. This training was made possible by a dedicated system capable of stable federated learning, allowing collaborative model development while preserving confidentiality.

Regarding the generative AI, we plan to extend ChemTS and incorporate advanced functions such as DyRAMO, which enables efficient multi-objective optimization. This will make it possible to create novel compounds and evaluate their activity profiles with higher accuracy and speed than ever before.

Continuous updates are indispensable when leveraging technologies such as federated learning and generative AI. Through this commercialization, I expect the achievements of DAIIA to keep evolving and, delivered as long-term software for pharmaceutical companies, to greatly contribute to the acceleration and innovation of drug discovery research.

## About LINC

The Life Intelligence Consortium aims to advance and implement applications of AI, big data, IoT, and related technologies in the life-science field, promoting the field's development, human-resource cultivation, digital transformation, and economic growth. For details, please visit https://linc-ai.jp.

## About Elix

Elix is an AI drug discovery company with the mission of "Rethinking drug discovery". Through our flagship software platform, Elix Discovery™, and collaborative consulting engagements, we work with leading pharmaceutical companies and biotech startups to reduce the enormous costs and time associated with drug discovery, while improving the rate of successful outcomes. We achieve these goals via our company's unique blend of AI engineering and medicinal chemistry expertise that allows us to stay at the forefront of development in both fields, and offer the solutions of tomorrow to the problems of today. https://www.elix-inc.com/.