July 15, 2025

Company Name Alivexis, Inc.
C E O Suguru Roy Kimura

**Notice of Selection for the Ministry of Economy, Trade and Industry's Domestic Generative AI Development Strengthening Project "GENIAC"**

News – July 15, 2025 – Alivexis, Inc. (Headquartered in Minato-ku, Tokyo; CEO S. Roy Kimura, "Alivexis") a preclinical-stage computation-driven drug discovery firm, is pleased to announce that it has been selected for the third round of the Ministry of Economy, Trade and Industry (METI) and the New Energy and Industrial Technology Development Organization (NEDO)'s Generative AI Accelerator Challenge (GENIAC) project, which aims to strengthen domestic development capabilities in generative AI.

The GENIAC project primarily provides high-performance computational resources to support the development of foundational models, which are core technologies in generative AI, and provides support for proof-of-concept investigations into the practical application of data and AI. The first round of the project was implemented starting in February 2024, and the second round began in October of the same year. In this third round, Alivexis aims to utilize the computational resources provided to develop a generative AI foundational model for use in drug discovery that can predict the biological activity of small molecule compounds with world-leading accuracy by integrating our proprietary simulation technology ModBind™ into the process of AI model training. Through the implementation of the AI model supported by this GENIAC project, we hope to further contribute to the development of innovative medicines and the improvement of drug discovery research productivity.

**Background**

In the field of small molecule drug discovery, physics-based simulations for biological activity prediction have been widely applied and have delivered many successful outcomes. While AI is expected to play an increasingly important role, its use in this area faces several challenges, including the vast structural diversity of small molecule compounds and the limitations in the quality of datasets available for AI training, particularly those found in public domain. As a result, current AI models are not yet capable of delivering sufficiently high performance in this field.

In contrast, AI has made significant advances in other fields, such as autonomous driving,

by leveraging not only real-world data but also synthetic data generated through simulation. This has enabled practical applications with high performance. Drawing on this success, it is expected that simulation-generated data can similarly accelerate progress in AI-driven drug discovery.

However, traditional bioactivity prediction methods rely heavily on compounds with known activity to achieve high accuracy. These methods have struggled to significantly improve prediction speed while maintaining precision. To date, no simulation technology has successfully combined the quality, volume, and wide range of adaptability required for effective AI training in this field.

In response to these challenges, our proprietary simulation technology, ModBind™, enables high-speed, high-accuracy prediction of absolute biological activity without the need for compounds with known experimental data. This technology has already led to the identification of five clinical candidate compounds. Based on these results, we believe that integrating ModBind™ with AI holds strong potential as an innovative solution to the current limitations of AI-driven small molecule drug discovery. As a result, we have launched the GENIAC initiative to demonstrate this potential in practice.

**Key Features of the Small Molecule Drug Discovery Foundational AI Model to Be Developed in This Project**

In this project, we will use ModBind™, our independently developed physics-based simulation algorithm for predicting the biological activity of small molecules, as an "oracle" in an active learning workflow. This approach will allow us to generate highly accurate biological activity prediction data for new compounds, which will serve as additional training data for the foundational AI model. By incorporating active learning techniques into this training process, we will efficiently expand the learning scope across a wide range of compound spaces. This is expected to enhance the adaptability of the model and significantly improve its predictive accuracy.

Through this initiative, we aim to develop a foundational AI model for small molecule drug discovery that achieves unprecedented prediction accuracy across multiple drug targets.

**About Alivexis' proprietary drug discovery platform ModBind™**

ModBind™ is a proprietary physics-based simulation technology developed by Alivexis that enables high-speed, high-accuracy prediction of the absolute binding strength between small molecule compounds and target proteins, without the need for experimental activity data.

By leveraging ModBind™ along with other platform technologies, we have already identified 5 clinical candidate compounds. One of these led to a licensing agreement with a Swiss company last year valued at approximately 42.5 billion yen, demonstrating the practical and commercial utility of our technology.

In addition, we have conducted multiple joint research projects with pharmaceutical companies, with ModBind™ serving as the central technology in these collaborations.

**Reference:** NEDO Project Announcement Page (Japanese only)
https://www.nedo.go.jp/koubo/CD3_100397.html

**About Alivexis, Inc.:**

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Representative directors: S. Roy Kimura, Ph.D., CEO / Kazuki Ohno, Dr. Eng. COO
Established: August 8, 2016
URL: https://alivexis.com
Business Description: A network-based drug discovery company utilizing cutting-edge technologies.

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