



December 20, 2024

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

Alivexis announces publication of a research article on its ground-breaking ModBind™ simulation technology

News – December 20, 2024 – Alivexis, Inc. (Headquartered in Minato-ku, Tokyo; CEO S. Roy Kimura, “Alivexis”) a preclinical-stage computation-driven drug discovery firm, announces that a research article entitled “ModBind, a Rapid Simulation-Based Predictor of Ligand Binding and Off-Rates” by William Sinko et. al. has been published in the Journal of Chemical Information and Modeling. This article describes the methodology, validation, and application results of the initial version of the company’s ground-breaking simulation technology that enables accurate absolute ligand efficacy predictions at up to ~1,000s x faster speeds than existing methods. ModBind™ has been used extensively to accelerate drug discovery and has delivered pharma collaborations and multiple clinical candidate molecules in the company’s pipeline.

Publication information

Title: ModBind, a Rapid Simulation-Based Predictor of Ligand Binding and Off-Rates

Authors: William Sinko, Blake Mertz, Takafumi Shimizu, Taisuke Takahashi, Yoh Terada and S. Roy Kimura (Alivexis, Inc.)

Journal: Journal of Chemical Information and Modeling

DOI: [10.1021/acs.jcim.4c01805](https://doi.org/10.1021/acs.jcim.4c01805)

Publication date: December 16th, 2024 (online)

【CEO S. Roy Kimura’s Comments】

“We are very excited to announce the publication of our research article on our novel ModBind™ technology. Over the past several years, we have developed this unique technology and have applied it successfully to our discovery programs and collaborations with biopharma partners, resulting in accelerated discovery of multiple clinical candidate molecules. Our method is based on a statistical thermodynamic theory that is distinct from the industry state-of-the-art, and has major advantages including enabling >100-1,000-fold shorter simulation times required for convergence and accurate predictions. We hope that



this publication will stimulate discussions and innovations that would enable the efficient discovery of drug candidates for diseases with high unmet need.”

About Alivexis, Inc.

Name: Alivexis, Inc.

Headquarter: Daiichi Hibiya Building 7F, Shimbashi 1-18-21, Minato-ku, Tokyo 105-0004, Japan

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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