NEWS RELEASE

Veritas In Silico

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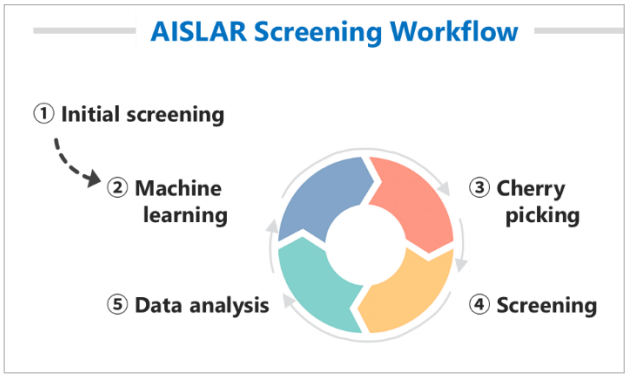
Announcement of the Publication of a Research Article on AISLAR, a Method for Streamlining Screening That Supports Our AI-Driven Drug Discovery

Veritas In Silico Inc. (hereafter referred to as "the Company") is advancing drug discovery research in mRNA targeted small-molecule and nucleic acid medicines through "aibVIS," a platform that integrates specialized AI with experimental technologies. The Company is pleased to announce that a research article, jointly authored by CSO and researchers of the Company, has been published in '*Small Science*', describing a specialized AI-based method for streamlining the screening process.

This method not only improves, by several fold, the efficiency of the initial screening required for small-molecule drug discovery against specific RNA structures, but also enables the efficient identification of chemotypes suitable for the structure–activity relationship (SAR)[*1]-driven development of RNA-binding compounds (SAR-tractable RNA binders).

Small molecules that target RNA are emerging as a powerful therapeutic modality, although deriving structure–activity relationships (SARs) remains a major challenge. Here, we present AI-augmented Iterative Screening of Libraries Against RNA targets (AISLAR), a machine learning–driven strategy that accelerates the discovery of SAR-tractable RNA binders and enables rational analog design. We screened diverse, drug-like chemical libraries against two RNA motifs derived from human p53 mRNA and applied AISLAR within the open-source KNIME platform. The application of AISLAR yielded chemotypes suitable for SAR development. Biophysical assays confirmed direct binding of representative compounds to one RNA motif. Guided by early SAR trends, we developed a pharmacophore hypothesis and designed an analog that retained binding with lower predicted cardiac channel liability. Docking simulations using the crystal structure of the RNA motif revealed a plausible binding mode for the validated hit compound. While further validation across diverse RNA targets and compound libraries will be required, these results

demonstrate how AISLAR can be used as a workflow linking RNA-targeted small-molecule screening with rational analog design.



An example of a machine-learning screening workflow using the proprietary "Specialized Data-Driven AI" AISLAR implemented in aibVIS

● Comments from Ella Czarina Morishita, PhD, Chief Scientific Officer of VIS

Since its founding, Veritas In Silico Inc. have leveraged rule-based AI to develop mRNA targeted small-molecule drugs, with the aim of opening new possibilities for treating diseases that have traditionally been considered difficult to address through drug discovery. As our in-house research and collaborative drug discovery efforts have progressed, we have accumulated a substantial body of data that is unmatched globally. Building on this foundation, we have now begun developing data-driven AI. AISLAR combines these valuable data assets with AI to create new screening methods.

This research represents a long-term effort and was made possible by the contributions of our team across many areas, including experimentation, data acquisition, modeling, and analysis. I would like to express my sincere gratitude to all the researchers who kept the project moving forward despite the challenges posed by the COVID-19 pandemic and made this achievement possible. I would also like to thank everyone, in addition to the authors, who provided feedback and advice on this research.

On a personal note, I am deeply honored to have co-authored this paper with my former senior colleague, Professor Jiro Kondo, Sophia University, Faculty of Science and Technology, Department of Materials and Life Sciences, for the first time in 20 years. We hope this paper will help more people recognize the potential of small-molecule drug discovery targeting mRNA, and we look forward to working with partners to create a wide range of new medicines.

● Glossary for Reference

[*1] structure–activity relationship (SAR): SAR refers to the relationship between the chemical structure of a compound and its biological activity. By systematically analyzing how slight changes in molecular structure affect activity, selectivity, toxicity, and so on, it is an indispensable concept for designing and optimizing more effective and safer drugs, and for elucidating their mechanisms of action.

For Further Information, Contact:
● Veritas In Silico Website Inquiry Form : https://www.veritasinsilico.com/en/contact/