This press release is an English translation of a Japanese-language press release. The official language of this press release is Japanese, and the Japanese version takes precedence over the English version in terms of content and interpretation.

<Press Release>
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Announcement Regarding Publication of Research Demonstrating on AI-Driven Generation of Novel Molecular Scaffolds

Chordia Therapeutics Inc (Head Office: Fujisawa City, Kanagawa Prefecture; CEO: Hiroshi Miyake, "Chordia") today announced research findings on the generation of novel molecular scaffolds using artificial intelligence (AI), conducted as part of the Company's preclinical research activities. The study was carried out in collaboration with research teams from Institute for Theoretical Medicine Inc.. and Axcelead Drug Discovery Partners, Inc.

The results of this research have been published online in *ChemMedChem* on July 8, 2026.

Overview of the Research

The discovery of novel chemical scaffolds is an important challenge, enabling the expansion of chemical space and the generation of new intellectual property. However, transforming existing bioactive compounds into structurally distinct scaffolds while retaining biological activity remains difficult and continues to be a major challenge in medicinal chemistry. This study was conducted as part of the research activities for the Company's fifth novel pipeline program in the preclinical stage, with the objective of evaluating the feasibility of AI-driven molecular scaffold generation technology. As a model case, phosphoinositide 3-kinase (PI3K)/mammalian target of rapamycin (mTOR) inhibitors were selected. Although numerous PI3K/mTOR inhibitors have been reported, many are concentrated within a limited number of chemical scaffold classes, making them a suitable model for demonstrating the generation of novel scaffolds.

Using the AI-assisted molecular design platform DeepSARM, the research team generated a diverse library of virtual compounds based on the clinically investigated PI3K/mTOR inhibitor samotolisib. Promising candidates were then selected through ligand-based virtual screening, leading to the design and synthesis of a compound incorporating a structurally distinct scaffold compared with existing PI3K/mTOR inhibitors.

The synthesized compounds demonstrated inhibitory activity against PI3Kα in enzymatic assays. Furthermore, analyses using Boltz-2, a state-of-the-art AI-based molecular modeling technology, suggested a plausible binding mode between the compounds and the target protein. Notably, the newly generated scaffold was confirmed to retain PI3K inhibitory activity despite having a much simpler structure than the complex tricyclic scaffold of the starting compound, samotolisib.

These findings demonstrate the potential of combining AI and computational science to efficiently generate novel chemical structures that may be difficult to identify through conventional drug discovery approaches. The Company expects that applying this technology to therapeutic targets within its novel pipeline programs may contribute to the discovery of new compounds and improve the efficiency of drug discovery research.

Publication Details

Integrative Molecular Scaffold Generation of PI3K/mTOR Inhibitors Using DeepSARM and Ligand-Based Virtual Screening Approaches
ChemMedChem, Jul. 8, 2026
URL：https://doi.org/10.1002/cmdc.70362

About the Journal

ChemMedChem is an international peer-reviewed journal in the field of medicinal chemistry, published by Wiley in partnership with Chemistry Europe. The journal publishes a broad range of research covering compound design and synthesis, pharmacological evaluation, computational chemistry, chemical biology, and other drug discovery-related fields.

Glossary of Terms

Term	Explanation
Boltz-2	Boltz-2 is an AI-based structural modeling technology developed primarily by researchers at the Massachusetts Institute of Technology (MIT), United States. It predicts the three-dimensional structures of proteins as well as protein–small molecule complexes, helping researchers understand potential binding interactions and supporting rational compound design in drug discovery research.
DeepSARM	DeepSARM is an AI and machine learning-based molecular design technology developed by Dr. Yoshimori at Institute for Theoretical Medicine Inc. and his colleagues. By learning from the chemical structures of existing drugs and biologically active compounds, DeepSARM can propose new chemical structures and molecular scaffolds.
PI3K/mTOR Inhibitors	PI3K/mTOR inhibitors are targeted therapeutic agents that act on the PI3K/AKT/mTOR signaling pathway, which regulates cell growth and survival. Since PI3K and mTOR are known to be abnormally activated in many cancers, inhibition of these targets is expected to suppress the proliferation of cancer cells.
Virtual Screening	Virtual screening is a computational technique used to evaluate large numbers of compounds and efficiently identify candidates that are likely to interact with a target protein. By prioritizing

	promising compounds before experimental testing, virtual screening can improve the efficiency of drug discovery research and reduce development timelines.

About Chordia Therapeutics

Chordia Therapeutics is a research and development-stage biopharmaceutical company specializing in oncology with clinical-stage assets, headquartered in Fujisawa City, Kanagawa Prefecture. Chordia's lead asset, rogocekib (CLK inhibitor CTX-712), is under Phase 1/2 clinical study in the US. Rogocekib potentially targets the vulnerability of cancer and is expected to deliver benefits to patients of various types of cancer. In addition to rogocekib, Chordia is engaged in the research and development of several assets, including ocipumaltib (MALT1 inhibitor CTX-177), CTX-439, a CDK12 inhibitor, and GCN2 inhibitors. For more information, please visit our website https://www.chordiatherapeutics.com/en/.