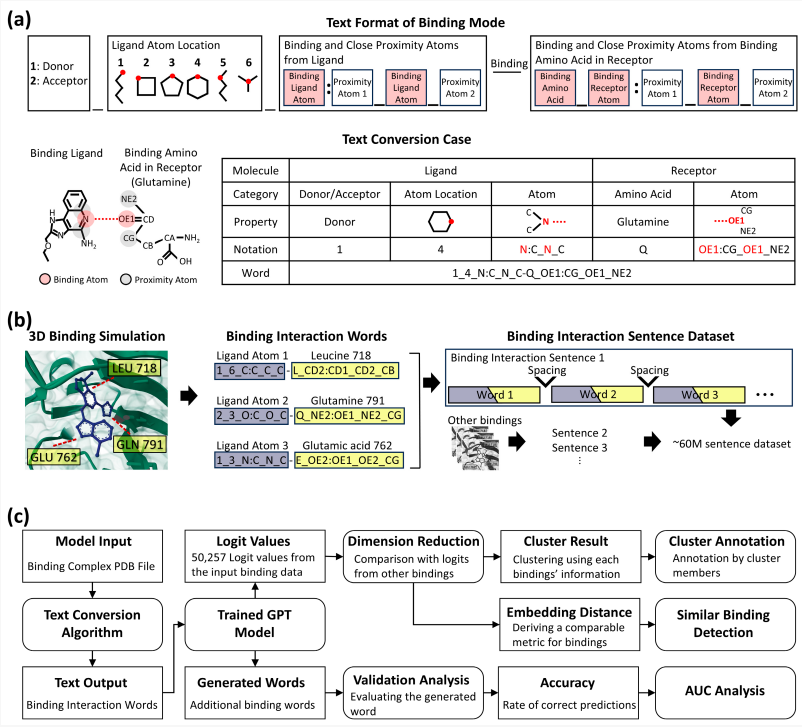
Syntekabio Publishes Peer-Reviewed Study in Molecules on LLM-Driven Small-Molecule Binding Prediction

NEW YORK, NY, UNITED STATES, December 3, 2025 /EINPresswire.com/ -- Syntekabio (KOSDAQ: 226330), a global leader in AI-powered drug discovery, is pleased to announce that its research manuscript, “Systematic Exploration of Small-Molecule Binding via a Large Language Model Trained on Textualized Protein–Ligand Interactions,” has been accepted for publication in Molecules, a peer-reviewed SCI journal published by MDPI.



Overview of the text conversion, dataset generation pipeline, and model application framework

The study introduces 3bmGPT, a large language model that converts 3D protein–ligand interactions into a 1D, language-like format. By translating structural contacts into “binding-interaction sentences,” the model enables scalable and efficient analysis of binding relationship without relying on traditional structural inputs. 3bmGPT also serves as the core engine behind Syntekabio’s LM-VS™ (Language- Model Virtual Screening) platform, providing a practical interface for applying this technology in real-world hit discovery programs.

Key Scientific Highlights

3bmGPT was trained on one of the largest binding-interaction datasets to date: ~ 60 million interaction sentences from 2,900 proteins. The model captures shared binding patterns across major protein families, including tyrosine kinases, serine/threonine kinases, proteases, and nuclear receptors. It clusters proteins based on binding-interaction similarity without sequence or structural information.

3bmGPT identifies structurally similar ligands and known drugs, helping researchers explore drug-repurposing opportunities based on ligand-driven similarity. 3bmGPT correctly positions new protein–ligand interactions (e.g., EGFR) within related functional clusters and maps associated ligand patterns. This study reveals previously unreported protein relationships emerging from shared biochemical binding behavior. A web-based 3bmGPT tool is available to support broader research access and transparency.

“This publication is an important milestone for Syntekabio and a strong validation of our approach to language-model-driven molecular analysis,” said Jongsun Jung, CEO of Syntekabio, Inc. “3bmGPT demonstrates how AI can transform the understanding of protein–ligand interactions, accelerate discovery, and open new opportunities for therapeutic innovation.”

About Syntekabio

Syntekabio is an AI-driven drug discovery company integrating large-scale supercomputing and molecular modeling to accelerate the design and development of small molecules, antibodies, and novel therapeutic modalities. By combining physics-based simulations with proprietary AI platforms such as DeepMatcher® and Language-Model Virtual Screening (LM-VS™), Syntekabio can rapidly explore ultra-large chemical spaces and prioritize high-value candidates with improved developability profiles. The company’s infrastructure and workflows are designed to shorten early discovery timelines, reduce experimental burden, and de-risk portfolio decisions for biopharmaceutical partners across oncology, immunology, and other therapeutic areas.

For more information, visit www.syntekabio.com, for LM-VS™: http://vs.syntekabio.com/ or follow Syntekabio on LinkedIn: https://www.linkedin.com/company/syntekabio.

Suzanne Choi
Syntekabio USA
+1 201-403-5959
suzanne.choi@syntekabiousa.com
