PRESS RELEASE

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Enamine and Chemspace Join IHI Project LIGAND-AI to Advance Artificial Intelligence (AI)-Driven Drug Discovery

[FOR IMMEDIATE RELEASE]

January 28nd, 2026

Frankfurt, Germany / Kyiv, Ukraine, 28 January 2026 –

The new multi-sector public-private partnership funded by the Innovative Health Initiative (IHI) brings together 18 partners across nine countries to generate large open, high-quality datasets of protein–ligand interactions and use them to train artificial intelligence (AI) models capable of predicting candidate molecules as suitable binders for thousands of human proteins.

- Experts across academia, industry, technology companies, and research organizations will collaborate over the next five years to generate open and accessible, high-quality, AI-ready protein-ligand data at scale as a public resource.

This project is supported by the Innovative Health Initiative Joint Undertaking (IHI JU) under grant agreement No 101252959. The JU receives support from the European Union's Horizon Europe research and innovative programme, COCIR, EFPIA, EuropaBio, MedTech Europe, Vaccines Europe, Enamine, and The Hospital for Sick Children. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the aforementioned parties. Neither of the aforementioned parties can be held responsible for them.

- With a budget of more than €60 million, the project aligns with IHI's mission to foster international, cross-sectoral collaboration and advance medicine discovery by bringing the power of data science to hit identification technologies.

Led by Pfizer and the Structural Genomics Consortium (SGC), LIGAND-AI consortium will interrogate thousands of proteins relevant to existing and unmet disease areas including rare, neurological, and oncological conditions.

Early drug discovery is a long, expensive, and uncertain process. Scientists spend years testing thousands of molecules to find just one that binds to a disease-related protein. LIGAND-AI aims to change this by combining advanced laboratory technologies with computational methods to create a seamless pipeline from experiment to prediction. The consortium will generate billions of data points using complementary screening technologies, enabling researchers worldwide to develop, train, and benchmark AI models that predict molecular interactions.

"This project brings together scientists and companies from across disciplines within an open science ecosystem. It is heartening to see these diverse scientific communities coalesce around a common vision to generate and share valuable chemical data openly with the world," said Aled Edwards, PhD, CEO of the Structural Genomics Consortium and project coordinator.

Beyond data generation, LIGAND-AI will foster an open discovery ecosystem by inviting the scientific community to co-develop and refine predictive models through open challenges

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and benchmarking campaigns. All data generated through LIGAND-AI will be shared according to FAIR principles, ensuring they are findable, accessible, interoperable, and reusable by the global scientific community. By integrating expertise in protein science, structural biology, chemistry, and machine learning, the project will build a dynamic network where experimental and computational discoveries evolve together, ensuring that progress is cumulative, transparent, and accessible.

Sven Wagner, PhD, Vice President of Partnerships at Enamine: "We are aligning Enamine's profound knowledge of chemical space and its IDD-platform of integrated drug discovery with the paradigm shift of AI-driven hit finding and optimization. Being a member of this world-class LIGAND-AI project gives us the chance to accelerate pharmacological research in an open-access mode towards medicines for patients in need."

Olga Tarkhanova, PhD, CEO at Chemspace: "For us, LIGAND-AI project represents a unique opportunity to contribute our approach to exploration of chemical space through DNA-encoded library (DEL) technologies to achieve a truly global impact. It is much in line with Chemspace' commitment to support open science initiatives that build shared infrastructure for the global research community."

Tim Schober, PhD, General Manager at Enamine Germany, added: "LIGAND-AI represents a paradigm shift towards AI-driven drug discovery with its foundation and benchmarks in the real world of patient-centric research pursuits. Our Frankfurt-based Enamine researchers, in sync with our global Enamine R&D infrastructure and Enamine's unrivaled chemical space exploration, are determined to contribute innovative technologies for faster and more effective design–make–test–analyze cycles for open science discovery."

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By establishing a shared, open-science infrastructure for AI-driven drug discovery, LIGAND-AI will not only advance early-stage research but also train a new generation of interdisciplinary scientists fluent in both computation and experimentation. The project represents a major step toward the mission of Target 2035 — to discover chemical modulators for every human protein by the year 2035. LIGAND-AI is a major milestone toward realizing this vision, catalyzing global collaboration, reducing fragmentation across sectors, and advancing data-driven discovery.

For more information, visit www.target2035.net

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About LIGAND-AI:

LIGAND-AI is a flagship project of the Target 2035 initiative, funded by the Innovative Health Initiative, a public-private partnership (PPP) between the European Union and the European life science industries, represented by COCIR, EFPIA (including Vaccines Europe), EuropaBio and MedTech Europe.

The LIGAND-AI Consortium is formed by the following partners:

Structural Genomics Consortium, European Molecular Biology Laboratory, Goethe University Frankfurt, Universidade Estadual de Campinas, University College London, University Health Network, Vall d'Hebron Institute of Oncology (VHIO), Abcam Limited, AstraZeneca UK Limited, Chemspace LLC, Enamine Germany GmbH, IBM Research Israel – Science and Technology LTD, Novo Nordisk, Nuvisan ICB GmbH, Pfizer Inc, The Hospital for Sick Children in Toronto, Thermo Fisher Scientific GmbH, and Vernalis (R&D) Limited.

About Chemspace:

Chemspace is a global provider of drug discovery services. We can streamline hit finding by integrating our Computational Chemistry tools, Bioinformatics, and Machine Learning-based services for smarter drug discovery. By exploring ultra-large chemical spaces, we deliver high-quality hit molecules for discovery projects. Our integrated projects combine hit identification services with biological validation, providing a seamless path from hit identification to pre-clinical studies.

For more information, please visit: https://chem-space.com

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About Enamine:

Enamine is the leading provider of chemical compounds and a scientifically driven, integrated discovery Contract Research Organisation for integrated discovery with unique partnering opportunities in exploring new chemical space. The company combines access to the in-house produced screening compounds (4.5 million in stock) and building blocks (350,000 in stock) with a comprehensive platform of integrated discovery services in bioinformatics, biology, and chemistry to advance and accelerate the efforts in drug discovery.

For more information, please visit: www.enamine.net/

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