PRESS RELEASE

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Nuvisan joins IHI project LIGAND-AI to help advance AI-driven drug discovery through open science

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 organisations 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.

- 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.

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. Funded by the European Union, the private members, and those contributing partners of the IHI JU. 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.

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, 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 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.

"LIGAND-AI represents a transformative step in harnessing artificial intelligence and open science for digital drug discovery. By uniting world-class partners from industry and academia, we are building a foundation of high-quality data and developing innovative AI tools to accelerate the creation of life-changing medicines for patients worldwide," said Franz von Nussbaum, President, Nuvisan.

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Charlotte Kopitz, President, Nuvisan, added: "Nuvisan is contributing to setting a new benchmark for open and standardised data generation in drug discovery. By creating comprehensive, high-quality datasets of protein–ligand interactions across thousands of human protein targets, we help empower researchers and AI innovators to advance the identification of effective therapies — supporting progress in science and society alike."

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 realising this vision, catalysing 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 Institut de Recerca, 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, Thermo Fisher Scientific GmbH and Vernalis (R&D) Limited.

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