

Elix and University of Vienna Enter Joint Research Agreement for AI Drug Discovery

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/EINPresswire.com/ -- Elix, Inc. (CEO: Shinya Yuki / Headquarters: Tokyo; hereinafter "Elix") and University of Vienna, Austria (represented by the Dean of the Faculty of Life Sciences, Prof. Mag. Dr. Karl-Heinz Wagner; hereinafter "U. Vienna"), are pleased to announce the signing of a joint research agreement aimed at advancing drug discovery using AI technologies.



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Traditional drug discovery methods require considerable time and cost to identify promising compounds from a large number of candidates yet still face low success rates as a key obstacle. In this context, AI's emergence is attracting interest as a game-changing tool for the efficiency of drug discovery research. Specifically, the application of AI to molecular design and property prediction makes it possible to more accurately design drug candidates and narrow down synthesis and evaluation targets, thereby accelerating development and reducing costs from the early discovery stage onward.

Elix (<https://www.elix-inc.com/>) is a Japan-based AI drug discovery company committed to "Rethinking Drug Discovery." Aiming to cut the substantial time and cost of drug development while enhancing success rates, Elix leverages AI and machine learning in collaborations with pharmaceutical companies, universities, research institutes, and biotech startups.

One of Elix's business models is the provision of its integrated AI drug discovery platform, Elix Discovery™, developed under the concept of "medicinal chemists can truly use it." Elix Discovery™ offers an intuitive graphical user interface (GUI) that automatically constructs predictive models for optimal compound profiling. It also features diverse structure generation capabilities, with a unique strength in "proposing structures that humans would not conceive." By integrating curated structure generation models, including proprietary ones, with predictive models and parameters built into the intuitive GUI, researchers can rapidly and intuitively refine molecular design. The platform supports both ligand-based drug design (LBDD) including pharmacophore modeling and structure-based drug design (SBDD), the latter utilizing docking simulations and other methods, thus enabling exploration across a broader range of

approaches.

The second business model focuses on collaborative drug discovery research with pharmaceutical companies, biotech ventures*1, and academia*2. By combining its vast knowledge of pharmaceutical research with state-of-the-art AI, Elix continues to pursue the discovery of innovative drug candidates.

Led by Associate Professor Julien Orts at the University of Vienna, this research group specializes in pioneering NMR spectroscopy techniques to decode the atomic-resolution structures, dynamics, and interactions of biomacromolecules. The lab's primary focus involves studying protein conformational switches and allostery in signaling, utilizing groundbreaking methodologies they developed such as INPHARMA for validating small-molecule binding modes and NMR² for the automated determination of protein-ligand structures. By applying eNOE distance measurements with 0.1 Å accuracy to resolve protein ensembles, the Orts Lab provides the thermodynamic insights necessary to tackle "undruggable" targets and advance modern structure-based drug design.

In this joint research project, Elix will collaborate with the research group of Associate Professor Julien Orts. This partnership merges Elix's proprietary expertise in chemoinformatics-based approaches and AI-driven molecular generation with the Orts group's cutting-edge capabilities in structural dynamics and NMR-validated molecular interactions.

The collaboration aims to design and develop novel compounds against traditionally "undruggable" targets, with a specific focus on intrinsically disordered proteins (IDPs) and proteins implicated in epigenetic signaling and cancer. By integrating AI's predictive power with experimental atomic-resolution data, the project seeks to bypass the limitations of traditional drug discovery, delivering new therapeutic insights and next-generation candidates for complex diseases.

Comment from Associate Professor Julien Orts of the University of Vienna

We are thrilled to partner with Elix to bridge the gap between advanced structural biology and artificial intelligence. My laboratory has always been driven by the desire to push the boundaries of what NMR can achieve in drug discovery. By combining our ability to resolve protein dynamics at atomic precision with Elix's sophisticated AI-driven generation, we can move beyond static structures and begin to target the complex, transient behaviors of proteins that were once considered out of reach. This synergy is exactly what is needed to accelerate the discovery of transformative medicines for the next generation.

Comment from Shinya Yuki, CEO of Elix, Inc.

At Elix, our mission is to rethink drug discovery by bridging cutting-edge AI with experimental innovation. Collaborating with the group led by Associate Professor Julien Orts at the University of Vienna allows us to pursue this mission on a global scale, uniting expertise in AI drug discovery with world-leading structural biology. We believe this partnership will open new possibilities for targeting diseases that have long remained beyond the reach of traditional drug

discovery.

Reference:

*1 April 15, 2025 press release: "Elix and PRISM BioLab Join Forces to Accelerate AI-Driven Drug Discovery for Challenging Protein-Protein Interaction Targets"

URL: <https://www.elix-inc.com/news/news-release/2117/>

*2 October 2, 2025 press release: "Elix and Tohoku University Enter Joint Research Agreement to Advance AI Drug Discovery"

URL: <https://www.elix-inc.com/news/news-release/2198/>

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