DeepCure, Google and CWX Demonstrate the Potential For Chemistry LLMs To Increase Productivity In Medicinal Chemistry

BOSTON, MA, UNITED STATES, March 3, 2025 /EINPresswire.com/ -- DeepCure, a therapeutics company using AI to discover novel drugs for immune and inflammatory diseases, announced today the successful completion of a pilot program with Google Cloud Platform (GCP) and CloudWerx (CWX) to build an AI-driven workflow that can extract chemical insights from unstructured literature to answer complex queries on organic chemistry.

DeepCure specializes in discovering innovative small molecule therapies for undrugged protein targets to transform the lives of patients with autoimmune and inflammatory diseases. DeepCure's MolGen™ system uses AI to design molecules that can bind to proteins that have historically been very challenging to drug. Each AI design is supported by physics-based analyses, such as molecular dynamic simulations and quantum mechanical calculations. Chemists often require up-to-date, open-access data to complement internally generated datasets for drug design. However, this data is often in publications as unstructured text or images, which requires scientists to spend hours manually reading and documenting the information. There is a pressing need for a workflow to capture specific data from recent documents in response to queries and then structure the data so it is easily interpretable to scientists and AI tools.

DeepCure, CWX and GCP created a workflow that uses a fine-tuned LLM model trained with data extracted from public chemistry literature and a set of data harmonization instructions from DeepCure, and the output is in a format that is both understandable to chemists and directly interpretable by robotic systems. The workflow increased researcher productivity seven-fold, and additional optimization of the system could further increase productivity by an order of magnitude.

"Our new Google Cloud-based solution streamlined our chemical data harmonization process. What used to take hours of manual work now takes just minutes. We've seen over a seven-fold reduction in data processing time. This frees up our scientists to focus on complex, high-value

activities such as problem-solving and more creative aspects of drug design," Thras Karydis, Chief Technology Officer and Co-Founder, DeepCure.

Google Cloud has expressed excitement about DeepCure's use of the Google cloud-based architecture built by CWX to expand the applications of AI tools into R&D and explore new types of reasoning, and believe this will be a new frontier in innovation for many industries.

"CWX is proud to have supported DeepCure in bringing this vision to life with custom model development that parses dense scientific papers, extracts insights and chemical notations using custom LLMs and enables the DeepCure science team to accelerate discovery" said Sidhant Gupta, Chief Technology Officer, CWX. "We've demonstrated how quickly and effectively powerful AI tools can be deployed to augment scientists' ability to gather and process data."

The partnership demonstrates the potential value of using Google Cloud tools like BigQuery and VertexAI to process and analyze large volumes of data from public scientific literature, including extracting key chemical reaction details such as reactants, conditions, and molecular structures. This streamlined pipeline efficiently organizes the data for future scalability, supporting DeepCure's internal drug discovery efforts. Google's expertise in real-time patent searches, publications, images, and language translation, combined with its custom Gemini AI chatbot created by CWX, enables scientists to interact with AI and receive reasoned, data-backed responses.

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About DeepCure
DeepCure is a therapeutics company focused on advancing novel drugs with the potential to transform the treatment of inflammation and autoimmune diseases. The company was founded by researchers at MIT to accelerate breakthrough therapies using artificial intelligence (AI) and AI-enabling technologies for small molecule drug discovery. The company is based in Boston, MA, and its engineers, chemists, and biologists collaborate to find solutions to hard problems that will have an enormous impact on patient health. For more information, visit www.deepcure.ai.

About CWX
CWX is a Google Cloud solutions provider built with a global force of engineering experts, laser-focused on conquering your toughest challenges. With a team of elite tech talent and an unwavering commitment to next-level customer service, they empower businesses to accelerate and thrive in even the most complex Google Cloud environments. As a Google Cloud Premier Partner, the 2023 North American Sales Partner of the Year, and the recipient of Google Cloud's 2024 North American Breakthrough Partner of the Year, they are not just keeping pace with cloud innovation—they are setting the pace. Ready to break boundaries and achieve the impossible? For more information, visit https://www.cwx.tech/.

About Google Cloud
Google Cloud is the new way to the cloud, providing AI, infrastructure, developer, data, security, and collaboration tools built for today and tomorrow. Google Cloud offers a powerful, fully integrated and optimized AI stack with its own planet-scale infrastructure, custom-built chips, generative AI models and development platform, as well as AI-powered applications, to help organizations transform. Customers in more than 200 countries and territories turn to Google Cloud as their trusted technology partner.

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