Collaborative Drug Discovery Integrates CDD Vault with NVIDIA BioNeMo NIM For AlphaFold2 and DiffDock Models

BURLINGAME, CA, UNITED STATES, April 2, 2025 /EINPresswire.com/ -- Collaborative Drug Discovery, Inc. (CDD) announces the integration of NVIDIA BioNeMo NIM microservices for AlphaFold2 and DiffDock models into CDD Vault. This integration enriches experimental data within CDD Vault, a

single, intuitive web-based platform, by incorporating predictive, industry-leading models. Researchers can manage, analyze, and securely collaborate on the integrated data with enhanced models, unlocking deeper insights and enabling more informed decision-making.

Scientists engaged in both commercial and humanitarian drug discovery have demonstrated that the integration with BioNeMo NIM for AlphaFold2 and DiffDock significantly enhances CDD Vault's existing AI module. These models are a powerful addition to CDD's chemistry-aware bioisosteric generation for novel structures (IP) and ultrafast deep-learning similarity capabilities. Chemists and biologists can now combine the best of their intuition with generative capabilities for small molecules visualized together with biological proteins.

NVIDIA NIM is a set of easy-to-use microservices designed to accelerate the deployment of generative AI models across the cloud, data center, and workstations. NIM microservices are categorized by model family and on a per-model basis.

"We wanted to give the 690+ research labs that are using CDD Vault effortless access to the powerful BioNeMo NIM tools, enabling them to seamlessly combine over 4 billion experimental data points and 80 million structures with AI-driven insights from these models," said CDD Cheminformatician and Research Informatics Senior Scientist Dr. Peter Gedeck.

Collaborative Drug Discovery empowers CDD Vault users with access to powerful NVIDIA AI tools, BioNeMo NIM for AlphaFold2, a deep learning model that accelerates protein structure determination, and DiffDock, which predicts the 3D orientation and docking interactions of small molecules with proteins. These advanced tools provide a comprehensive structure-based drug discovery (SBDD) extension, enhancing the traditional capabilities of the CDD Vault scientific

informatics platform.

"CDD Vault's strength is biological and chemical activity data management," said Barry Bunin, CEO and Founder of Collaborative Drug Discovery. "With our ELN (electronic laboratory notebook), Inventory, Curves, Automation, and AI modules, it was natural for us to collaborate with NVIDIA, the leading company for biological modeling. Our customers, some of whom are already using AlphaFold2 and DiffDock, are excited to have access to the NIM for these models, to support seamlessly integrating with CDD Vault, and more quickly move to deployment."

"The ability to model biology and generate new chemical structures with AI is a profound breakthrough transforming the healthcare and life sciences space," said Janet Paulsen, Senior Alliance Manager, Drug Discovery, NVIDIA. "The integration of NVIDIA BioNeMo NIM microservices into CDD's Vault platform equips researchers on the forefront of this innovation with the advanced AI tools needed to harness data that can unlock biological insights."

About Collaborative Drug Discovery (CDD)

CDD's (www.collaborativedrug.com) flagship product, CDD Vault®, is a premier hosted database solution for the secure management and sharing of biological and chemical research data. CDD Vault® provides tools for managing chemical and biological registrations, structure-activity relationships (SAR), and organizing experiments. The platform's available modules include Registration, Activity, Visualization, Assays, ELN, Inventory, Curves, AI, and Automation.

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