CDD Vault Integrates Enamine Compound Collection into AI-Powered Structural Similarity Searches

KYIV, UKRAINE, August 16, 2024 /EINPresswire.com/ -- Collaborative Drug Discovery (CDD), a leader in providing scientific informatics solutions, announced today that its flagship platform, CDD Vault, now includes the complete compound collection of Enamine, a leading provider of chemical compounds and early discovery services, within its AI module for structural similarity searches. This integration enhances the platform's capabilities, offering users an unprecedented breadth of chemical diversity and precision in their research endeavors.

The incorporation of the Enamine commercial compound collection into CDD Vault's AI module underscores CDD's commitment to empowering scientists with the best tools for accelerating drug discovery. Enamine, recognized for synthesizing the world's largest and most diverse collections of small molecules, enables "SAR by catalog" to CDD Vault's ultra-fast deep learning structural similarity search functionality. This vast database, now accessible within CDD Vault, enables researchers to explore over 4.3 million compounds in stock at Enamine, optimizing their search for novel drug candidates with unparalleled speed and accuracy. Additionally, because Enamine has the synthetic methods for fast delivery of novel compounds from vast Enamine REAL Space, hits and leads are well positioned for rapid lead optimization.

"We are pleased to securely offer our users access to Enamine's extensive library directly within CDD Vault with their proprietary structures," said Dr. Barry Bunin, CEO of Collaborative Drug Discovery. "This integration allows researchers to pinpoint relevant compounds to every structure in their Vaults. Combining AI-driven insights with the most comprehensive chemical

libraries available provides an indispensable resource for modern drug discovery. Individuals not using these modern capabilities, will be at a competitive disadvantage over time. The deep learning technology also suggests bioisosteres of all molecules for new IP."

The AI module in CDD Vault supports researchers managing and interpreting complex datasets, predicting compound behavior, and identifying potential leads with greater precision, and is directly integrated with the Visualization module for multiparameter optimization. With the addition of the Enamine commercial library, users now benefit from a richer dataset, expanding the possibilities for innovative drug development.

"Enamine is delighted to build on our existing collaboration with CDD," said Dr. Vladimir Ivanov, Executive Vice President at Enamine. "Together we will help deliver the right compounds to the hands of researchers who are driving innovation that makes a difference in the world."

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.

About Enamine
Enamine is a scientifically driven integrated discovery contract research organization with unique partnering opportunities in exploring new chemical space. The company combines access to the in-house produced screening compounds (4.33M in stock) and building blocks (300K in stock) with a comprehensive platform of integrated discovery services to advance and accelerate the efforts in Drug Discovery.

About Enamine REAL
Enamine REAL Space contains 48 billion make-on-demand molecules that can be synthesized at Enamine extremely fast (3-4 weeks), with high feasibility (over 80%), and inexpensive. The REAL compounds are created by parallel chemistry through the compilation of 143,000 building blocks via more than 167 well-validated parallel synthesis protocols, underlying Enamine's approach to design make-on-demand compounds to maximize synthesis success rate.

Oleksii Gavrylenko
Enamine Ltd
email us here
Visit us on social media:
Facebook
X
LinkedIn
Instagram