

Enamine and ChemPass Collaborate to Accelerate Hit Discovery

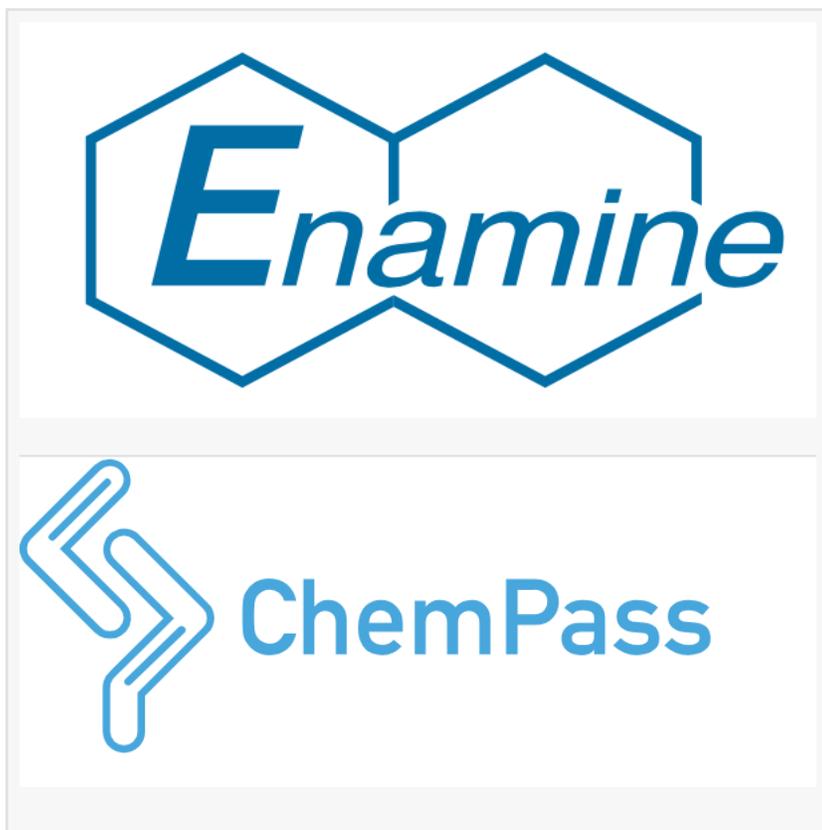
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[/EINPresswire.com/](https://www.einpresswire.com/) -- Enamine, the leading provider of chemical compounds and drug discovery services, and ChemPass, a contract research organization for computational and AI-assisted software, today announced their start of strategic partnership to provide hit discovery solutions to their customers.

The joint effort between the two companies aims to expand significantly efficient fragment hit discovery and to shorten the fragment-to-lead development cycle for challenging biological targets. ChemPass, applying its Universal Fragment Library Design Platform, will provide target-specific

fragment libraries based on the customer's biological target of interest. Enamine's team will support the screening of the fragment libraries, the expansion of the obtained fragment hits into lead-like analogues from Enamine REAL[®] Space, the development of structure-activity relationship (SAR) by a few rapid rounds of screening of REAL[®] catalog compounds. Overall, the application of the ChemPass Library Design Platform, Enamine's REAL[®] combined with its extensive medicinal chemistry expertise, and Enamine's screening facilities in discovery biology will result in optimized hits in five months, a true acceleration of early phase drug discovery.

Dr. Yurii Moroz, Vice President of Sales and Marketing, Enamine, said: "Fragment-based drug discovery is a highly successful and indispensable tool of drug discovery today. For the discovery of novel chemical matter modulating a manifold of modes-of-action against the most challenging targets, fragment-based drug discovery needs to be adapted in the context of exploiting ultra-large chemical space. Fast identification of hits and their potential for rapid optimization is important for a successful discovery project. Application of the ChemPass technology and



Enamine expertise in synthesizable chemical space of the REAL[®] molecules will support both.”

Dr. Greg Makara, CEO, ChemPass, mentioned: “Challenging target classes have evaded hit finding efforts by many organizations. We built - in collaboration with the lab of Professor György Keserű at the HUN-REN Research Centre for Natural Sciences in Hungary - the unique Universal Fragment Library Platform that uses vast protein-ligand binding knowledge from structural databases to further enhance the success rate of fragment-based hit discovery against difficult targets. Hole-filling of existing sets, or general and targeted library designs are all made possible by the technology. Linking it to Enamine’s popular REAL[®] space is an exciting natural extension of the approach that will be a game changer for rapid target to lead campaigns for our customers.”

This collaborative initiative will bring speed and promising results to the joint customers to shorten their DMTA cycle.

Discover our Universal Fragment Library: <https://enamine.net/services/ufrag-library>

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Enamine is a scientifically driven integrated discovery Contract Research Organisation with unique partnering opportunities in exploring new chemical space. The company combines access to the in-house produced screening compounds (4.5M in stock) and building blocks (350K in stock) with a comprehensive platform of integrated discovery services to advance and accelerate the efforts in Drug Discovery. For more information visit: <https://enamine.net>

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Enamine REAL[®] Space contains 64.9 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. For more information visit: <https://enamine.net/compound-collections/real-compounds>

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ChemPass is a developer of computational in silico software tools and platforms for accelerating lead discovery. Apart from the Universal Fragment Library Platform, ChemPass has developed the AI-assisted design software SynSpace for lead finding and optimization, the AI-assisted AID Platform for rapid multiparameter lead optimization, the PoseValidator software for the analysis of in silico predicted small molecule poses, the CovMap tool for covalent drug discovery, and recently a generative lead-like macrocycle design and structure-based analysis platform. For more information on ChemPass’ tools and services visit: <https://chempass.ai>

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