Chemspace, Enamine, and Paul Scherrer Institute Launch a Joint Service for Fragment-Based Lead Discovery

Kyiv, Ukraine and Villigen, Switzerland, April 7, 2026. Chemspace, a drug discovery engine providing machine learning-guided support for hit identification, hit-to-lead, and lead optimization using the largest purchasable collection of chemicals and biologics, Enamine, a leading provider of small molecules and drug discovery services, and the Paul Scherrer Institute (PSI), the largest research institute for natural and engineering sciences in Switzerland, have announced today a strategic collaboration aimed at creating an efficient platform for fragment-based drug discovery in the ultra-large chemical space.

Enamine's REAL composing of trillions of easy-to-make virtual compounds provides enormous opportunities to accelerate drug discovery. The efficient navigation in this chemical space is still challenging. The partners joined their efforts to apply the power of fragment-based drug discovery to quickly produce promising lead compounds. Chemspace has recently developed the REAL Crystallographic Library (REAL Fragment Library | Chemspace) to enable a hit finding tool with straight analogues in Enamine's REAL. This library will be screened against protein targets in the Fast Fragment and Compound Screening (FFCS) Facility of the Swiss Light Source, by soaking its 524 compounds into protein crystals and solving the structure to detect binding of fragments and to identify their binding poses. Based on this information, options for follow-up compounds in Enamine REAL can rapidly be identified. Further iterative crystallographic studies and compound development in a close collaboration between the partners will offer a streamlined pathway for lead generation.

"*With the creation of the REAL Crystallographic Library, we provide our customers with a powerful new tool for fragment-based drug discovery. In partnership with Enamine and PSI, we now offer a seamless, end-to-end solution: from fragment hit identification to the synthesis and experimental validation of small molecule hits, accelerating the path from idea to discovery,*" said Olga Tarkhanova, PhD, CEO of Chemspace.

May Sharpe, PhD, Paul Scherrer Institute, added: *"Fragment-based Drug Development has proved to be a very effective method for generating potent lead compounds with favourable properties for further development into drug candidates. One of the stumbling blocks for wider uptake of this approach has been the need for extensive cooperation between the biomedical experts who identify a protein target, structural experts who detect and characterise fragment binding, and medicinal chemistry experts who provide fragments as a starting point as well as develop hits into potent lead compounds. It is amazing to be able to combine our capabilities of the Swiss Light Source at the PSI, with the world-famous expertise, richness and quality of synthetic chemistry provided by Enamine. We hope that this will encourage many scientists who need small molecule binders and drug-like lead compounds to try to find them using a fragment-based approach."*

Vladimir Ivanov, PhD, Executive Vice President at Enamine, stated: "*Enamine has built the world's most extensive purchasable chemical dataset, Enamine REAL. Fragment growing within this chemical space opens unprecedented opportunities. We are proud to partner with Chemspace and PSI, accelerating the journey from fragments to tomorrow's medicines.*"

About the REAL Crystallographic Library. The REAL Crystallographic Library was created based on the REAL Fragment Library, specifically for crystallographic fragment screening. It contains 524 fragment-like molecules selected to provide fast access to follow-up compounds within Enamine xREAL Space. The library comprises fragments that can be evolved in several directions while offering broad chemical diversity. In practice, fragment hits can be quickly advanced into full compounds that can be synthesized in 3-4 weeks with an 80 % synthesis success rate. Combining crystallographic precision with direct synthetic accessibility, the library offers a powerful and practical tool for systematic structure-activity relationship and rational hit optimization across the 5 trillion xREAL compounds.

About Chemspace. Chemspace is a global platform for discovering, designing, and delivering small molecules, providing integrated solutions for early-stage drug discovery through both online and offline platforms.

The Chemspace online platform offers a comprehensive solution for molecule discovery, purchasing, and procurement, enabling exploration of trillions of small molecules. With customizable catalog access, flexible purchasing options, and advanced compound management tools, the platform delivers a streamlined experience from search to synthesis.

The Chemspace offline platform provides end-to-end discovery services, including AI/ML-driven design, virtual screening, cheminformatics, chemistry, and biology services. This integrated approach supports hit identification, optimization, and biological validation within a coordinated workflow. For more information, visit https://chem-space.com/search

About Enamine. Enamine is the leading provider of chemical compounds and a scientifically-driven, integrated discovery Contract Research Organization (CRO) with unique partnering opportunities in exploring new chemical spaces. The company combines access to the in-house produced screening compounds (4.7M in stock) and Building Blocks (350K in stock) with a comprehensive platform of integrated discovery services in bioinformatics, biology, and chemistry to advance and accelerate the efforts in drug discovery. For more information, visit: enamine.net

About Enamine REAL®: Enamine REAL (**RE**adily **A**ccessib**L**e) contains trillions of synthetically feasible 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 200,000 in-stock building blocks via 172 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

About PSI. The Paul Scherrer Institute PSI develops, builds and operates large, complex research facilities and makes them available to the national and international research community. The institute's own key research priorities are in the fields of future technologies, energy and climate, health innovation and fundamentals of nature. PSI is committed to the training of future generations. Therefore about one quarter of our staff are post-docs, post-graduates or apprentices. Altogether PSI employs 2300 people, thus being the largest research institute in Switzerland. The annual budget amounts to approximately CHF 460 million. PSI is part of the ETH Domain, with the other members being the two Swiss Federal Institutes of Technology, ETH Zurich and EPFL Lausanne, as well as Eawag (Swiss Federal Institute of Aquatic Science and Technology), Empa (Swiss Federal Laboratories for Materials Science and Technology) and WSL (Swiss Federal Institute for Forest, Snow and Landscape Research). For more information, please visit: https://www.psi.ch

About the FFCS pipeline. The fast fragment and compound-based screening (FFCS) pipeline at the Swiss Light Source (SLS) is an integrated next-generation pipeline for crystal soaking, handling and data collection. The integrated robotics setup in combination with the lims software suite allows for fast crystallography-based screening of protein crystals against hundreds of fragments and compounds.

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