

Chemspace boosts Enamine's drug discovery platform

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Chemspace, an expert in the generation and exploration of ultra-large chemical datasets, and Enamine, a global leader in supplying small molecules and early drug discovery services, are excited to announce a collaboration to unveil the real potential of Enamine's chemistry capabilities and deliver unparalleled discovery solutions. By combining their unique strengths, both companies aim to accelerate and enhance the process of identifying and developing new active molecules.

Enamine offers integrated drug discovery services empowered by its unique chemical tools – an unparalleled collection of modern compound libraries and building blocks. The company provides access to an ultra-large virtual chemical space of REAL Compounds, enabling the fast advance of identified hits into lead series. However, it's only now, in the new partnership with Chemspace, that Enamine has exposed its complete chemical resources exceeding 2.7 trillion REAL compounds to its customers. This jump into trillions is expected to accelerate the discovery of potent compounds having desirable ADME/T PK profiles.

Chemspace constantly advances its approaches in virtual screening and machine learning-assisted data processing, providing cutting-edge solutions for hit finding and optimization. Their expertise lies in utilizing computational methods, preparatory chemoinformatics tools, and ML algorithms to screen vast chemical libraries, including virtual libraries and DNA-encoded libraries, and perform the prediction of promising drug candidates.

Olga Tarkhanova, Ph.D., the CEO of Chemspace, expressed enthusiasm about the collaboration with Enamine, stating, "We are thrilled to expand our long-lasting partnership with Enamine to leverage our accumulated expertise and effective computational resources for identifying novel active compounds and performing their optimization within the tera-scale xREAL Space. We can help Enamine's clients navigate this vast space more efficiently in their quest for new medicines."

"Chemspace's ability to explore colossal chemical spaces maximizes the value of Enamine's synthetic resources and significantly enhances the probability of identifying novel previously unknown active compounds, potentially leading to breakthroughs in various areas of medical research," concluded Vladimir Ivanov, Ph.D., Executive Vice President at Enamine.

About Chemspace. Chemspace is a leading platform for drug discovery solutions, offering access to over 50B compound Freedom Space and now to 2.7T xREAL Compounds. Utilizing Computational Chemistry, Bioinformatics, and Machine Learning, Chemspace supports researchers in hit discovery, optimization, and expanding molecular exploration. With end-to-end services spanning the Drug Discovery process up to pre-clinical studies, Chemspace helps identify, source, deliver, and test molecules. For more information, visit <https://chem-space.com>

About Enamine. Enamine is a scientifically driven integrated discovery Contract Research Organization with unique partnering opportunities for exploring new chemical space. The company combines access to the in-house produced screening compounds (4.4M 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. For more details, visit <https://enamine.net>.

About Enamine REAL. Enamine REAL Space contains make-on-demand molecules that can be synthesized at Enamine extremely fast (3-4 weeks), with high feasibility (over 80%), and at affordable prices. The REAL compounds are created by compiling in-house qualified building blocks via in-house validated parallel synthesis protocols, underlying Enamine's approach to designing make-on-demand compounds to maximize synthesis success rate.