# Better Drugs Faster: Cambridge Molecular, Enamine and Chemspace Announce DEL-based Collaboration

CAMBRIDGE, ENGLAND, AND KYIV, UKRAINE, December 20, 2021 / EINPresswire.com/ -- Cambridge Molecular, a leading provider of machine learning and data science services for DNA-Encoded Libraries, announces a collaboration with Enamine, a pioneer in the creation of ultra-large chemical spaces of highly feasible compounds. Enamine is supported by the highly capable IT platform of Chemspace, an online chemical marketplace leader and experienced provider of compound sourcing and procurement services. The partners will apply Cambridge Molecular's deep learning DEL follow-up tool DeepDELve 2 to the world's largest catalogue of small molecules provided by Chemspace including 20 billion compounds from Enamine's REAL® Space.

The collaboration includes the integration of the comprehensive collection of small molecules maintained by Chemspace with the DeepDELve 2 platform, allowing the platform to recommend diverse and quickly available high-affinity hits against the target of a DEL screen. Chemspace will provide ultra-fast access to its catalogue of off-the-shelf compounds and Enamine REAL® Compounds to quickly populate pricing, purity, and availability information and support fast turnaround time through Cambridge Molecular's systems. Both Enamine and Chemspace will offer an exclusive discount to DeepDELve users, and Enamine commits to short synthesis times of the selected compounds to accelerate the process of confirming leads.

The companies will also create a schedule of joint events to showcase the capabilities of DeepDELve 2 in conjunction with Enamine synthetic capabilities and the Chemspace platform. In addition, Cambridge Molecular and Enamine will collaboratively explore the generation of DEL follow-up catalogues that can be synthesised and delivered faster. Chemspace will work on enabling fast search in these catalogues and arranging the logistics for the selected compounds allowing DeepDELve 2's machine learning models to move numerous and diverse leads into clients' labs as quickly as possible.

The collaboration reflects the companies' shared view that a combination of deep learning and access to large chemical space is central to the future of DEL follow-up. Compared to a resynthesis paradigm, DeepDELve 2 reduces compound acquisition costs by more than 90%, while increasing the speed of the follow-up process and the diversity of confirmed binders. It is currently the only commercially available DEL- follow-up machine learning system, and the culmination of two and a half years of research and development.

"This collaboration marks a milestone for DEL. For the first time, there is a commercially available option to follow up DEL screens with a high-fidelity virtual screen into many billions of readily available molecules, making novel chemical space easy to search robustly, and accelerating both hit identification and lead optimisation. It is a privilege to bring together the world-leading expertise within the three companies to increase the number, diversity, delivery speed, and cost-effectiveness of DeepDELve clients' hits," said Dmitry Foxham, CEO of Cambridge Molecular.

Andrey Tarnovskiy, Sales Director, Europe at Enamine, commented: "Our REAL® Space has been proven to be an essential source of new screening compounds and analogues for hit expansion. Still, there is a constant demand for computational tools enabling more efficient and quick exploration of the REAL® Space, which now counts 20 billion synthetically feasible structures. The DeepDELve 2 platform opens new scope for convenient selection of the most relevant structures for hit follow-up in such enormous chemical space."

"With a fast and efficient search technology implemented on the Chemspace platform, we are able to give accurate information on price and availability for the REAL® billions listed in our catalogue," adds Dr. Yurii Moroz, CEO of Chemspace. He continues: "Linking DeepDELve 2 and Chemspace enables a workflow that combines a discovery tool and a procurement platform. This combination is another step to speed up chemical sourcing and thus make the discovery process faster."

Cambridge Molecular Ltd.

Cambridge Molecular is a leading provider of machine learning and data science services for DNA-Encoded Libraries, based in Cambridge, England. The company's specialised algorithms and large-scale computational infrastructure fully leverage DEL datasets, enabling clients to quickly and robustly explore novel chemical space. These systems are used by industry-

leading partners of all sizes and include tools specific to low-data screens, selectivity screens, and excessively noisy screens.

About Enamine https://enamine.net/

Enamine is a global leading designer and largest producer of building blocks (240,000+) and screening libraries (2.7M+ compounds). REAL® Database https://enamine.net/compound-collections/real-compounds/real-database is a collection of 4.1 billion enumerated compounds that can be synthesized within just 3 weeks with over 80% success rate. REAL® Space https://enamine.net/compound-collections/real-compounds/real-space-navigator is a database of synthons and reactions that have been prepared to enable searches in around 20 billion possible combinations using infiniSee by BioSolveIT. MADE® Building Blocks https://enamine.net/building-blocks/make-on-demand-building-blocks are a catalogued collection of 210 million highly feasible building blocks. Enamine provides expertise in advanced organic synthesis, library synthesis, and medicinal chemistry. In 2011 Enamine established a pre-clinical service unit including ADME, in-vivo PK studies and High Throughput Screening under the brand name “Bienta”, allowing the company to tackle since that time fully integrated or à-la-carte research programs.

About Chemspace https://chem-space.com/

Chemspace was launched in 2016 to create a specialized comprehensive catalog of screening compounds and building blocks. It is powered with the latest IT technologies in chemical structure data storage and searches. Today Chemspace is the largest online catalog of small molecules. Users can perform a convenient and fast search in 20 billion building blocks, fragments, and screening compounds provided by the most trustful suppliers of in-stock and unique make-on-demand molecules. Chemspace also provides sourcing and procurement services.

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