Chemspace and the University of Southern California collaborate to make the Giga-scale docking possible, accessible, and affordable!

January 26, 2023. Kyiv (Ukraine), Los Angeles (USA). Chemspace, an online marketplace with billions of items and discovery services to support research projects, and the University of Southern California (USC) signed the Non-Exclusive License Agreement, according to which Chemspace receives access to the V-SYNTHES technology for supporting commercial projects.

The methods to explore giga-scale chemical spaces consisting of billions of molecules have become crucial for drug hunters. While working with such big datasets, the classical virtual ligand screen (VLS) is a bottleneck in the discovery process. To address this issue, the Katritch lab from USC has developed V-SYNTHES, a modular synthon-based approach to perform hierarchical structure-based VLS. This method enables rapid detection of the best-scoring compounds in giga-scale chemical spaces while performing molecular docking of only a small fraction (<0.1%) of the molecules. This technology, in collaboration with Chemspace and Enamine, helped discover high-potency ligands for two prominent GPCR and kinase targets, as published in Nature Journal in 2022 (https://www.nature.com/articles/s41586-021-04220-9)

“With access to the V-SYNTHES, we make the giga-scale VLSs accessible and affordable for the researchers, thus enabling the “the larger and more diverse the library, the better hits you get” statement for chemical spaces of billions of molecules” formulates Chemspace’s CEO Yurii Moroz. He continues: “The Kyiv-based Chemspace provides discovery solutions starting from VLS and ending with the delivery of the molecules for wet screening. The V-SYNTHES approach allows for the simple and highly effective discovery of new hit molecules among billions of molecules. With this approach, we expand our portfolio of services provided to our customers from large pharmaceutical companies as well as small biotechs and research groups at universities.”

“Through V-SYNTHES technology, we can virtually combine building blocks from Enamine REAL Space into the molecules that could fit in a protein pocket. To take full advantage of the library modularity, this iterative algorithm initially tests the pocket fit for millions of molecular fragments strategically representing the whole REAL Space. The best-fitting molecular fragments are then iteratively elaborated with more building blocks, and the resulting molecules are docked again. This process allows efficient selection of best REAL Space compounds fitting the pocket, which can be easily synthesized and tested experimentally”, says Professor Vsevolod Katritch. “V-SYNTHES need thousands of times less computational resources than standard VLS without compromising docking accuracy at any step.”

“Now billion-sized chemical spaces like Enamine REAL space have become more manageable to our customers,” explains Yurii Moroz. “It will immensely simplify the selection and thus the decision-making process, while at the same time improving quality. Ultimately, our customers save money because everything runs more effectively and more swiftly than before.”

Chemspace has already been running commercial projects using the V-SYNTHES technology, and the company plans to increase the number of projects in the coming months significantly. There are a few flexible models available to choose from to make the process suitable for each customer and their needs.

The Extra REAL Space of over 60 billion molecules prepared specifically to run the V-SYNTHES projects is another competitive advantage of accessing this technology via Chemspace.

“We are delighted that Dr. Vsevolod Katritch’s academic discoveries are of broad interest to industry collaborators worldwide,” added Dr. Remo Rohs, Professor and Founding Chair of the USC Dornsife Department of Quantitative and Computational Biology. “Dr. Katritch’s collaboration with Chemspace is very rewarding not only for his own research. It also shows our undergraduate and graduate students that their training in our department can be the basis for a successful industry career.”

About Chemspace

Chemspace was launched in 2015 to create a comprehensive specialized catalog of screening compounds and building blocks. It is powered by the latest IT technologies in chemical structure data storage and searches. Today, Chemspace offers a wide range of services such as Hit Discovery, Sourcing and Procurement, and Compound Management services. The computational team is ready to assist with giga-scale docking, Virtual Screening, SAR, Fragment-based discovery, and Scaffold Hopping. The largest catalog of commercially available chemicals is presented at Chemspace, the largest online catalog of small molecules and biologics. Users can perform a convenient and fast search in over 30 billion chemical building blocks, fragments, and screening compounds provided by the most trustful suppliers of in-stock and unique make-on-demand molecules. Its catalog of biologics includes almost 500,000 antibodies, peptides, and kits.

www.chem-space.com

About USC Dornsife College of Letters, Arts, and Sciences

The USC Dornsife College of Letters, Arts, and Sciences, the academic core of the University of Southern California, works across disciplines to explore fundamental questions facing society, many of which will depend on the life sciences to solve. The Department of Quantitative and Computational Biology is leading the way in training undergraduate and graduate students to be high-level scientists by emphasizing a high-dimensional view of genome organization, cellular function, and data analysis. By approaching biology as a quantitative science, USC faculty are mentoring the next generation of innovation leaders. For more information, please go to https://www.qcb-dornsife.usc.edu/overview

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