



Pharmacelera to partner with Enamine for the screening of ultra-large chemical libraries

Barcelona, Spain, and Kyiv, Ukraine, 15 December 2022. Pharmacelera, the leading provider of computational tools for hit discovery, and Enamine, the developer of REAL Database – the world’s largest virtual library of highly feasible compounds, have announced a partnership to jointly provide an efficient solution for hit finding. Ultra-large chemical libraries are observed as one of the key paradigms to access an unexplored chemical space. How to traverse these enormous spaces accurately is a research area that has raised the interest of the pharmaceutical industry, since finding novel hits with chemical diversity is a fundamental pillar in drug discovery.

In this context, Pharmacelera and Enamine have reached an agreement to plug the Enamine Real Database - over 5.5 billion highly feasible compounds - into the new version of Pharmacelera’s virtual screening flagship tool **PharmScreen®**. The resulting joint solution will allow the accurate screening of the ultra-large chemical library, providing its users not only with access to the physical compounds for testing from Enamine but also with new Intellectual Property (IP) for their targets of interest.

*“Pharmacelera offers an original, scientifically sound, and meaningful way of reading and interpreting the molecules, with excellent further applicability for virtual screening in Drug Discovery programs. We are happy to partner with Pharmacelera, to enable a more straightforward connection of **PharmScreen®** to the real test compounds”, said Michael Bossert, Head of Strategic Alliances at Enamine.*

“This agreement is extremely aligned with Pharmacelera’s strategy to work with leading institutions in the fields of Drug Discovery that have complementary technology and expertise”, says Rémy Hoffmann, Chief Business Development Officer at Pharmacelera. “We are thrilled to start this collaboration with Enamine, the prominent compound provider, as it will allow us to apply our accurate Quantum-Mechanics (QM) and Machine Learning (ML) algorithms to mine the Enamine’s REAL Database”, said Enric Gibert, Pharmacelera’s CEO.

ENDS

About Enamine

<https://enamine.net/>

Enamine is a global leading designer and the largest producer of building blocks (280,000+ compounds in stock) and screening libraries (3M+ compounds in stock). REAL® Database is a collection of currently 5.5 billion enumerated compounds that can be synthesized within only 3 weeks with more than 80% success rate. This database is complemented with REAL® Space providing access to over 32 billion REAL Compounds through the compilation of 137,000 building blocks used in 167 different synthesis protocols. Enamine offers integrated drug discovery services with seamless and efficient hit follow-up support.

About Pharmacelera

<https://pharmacelera.com/>

Pharmacelera develops advanced computational tools for the discovery of novel hits using accurate Quantum-Mechanics (QM), Artificial Intelligence (AI), and High-Performance Computing (HPC). The company's products **PharmScreen®** and **PharmQSAR** use 3D molecular descriptors derived from Quantum-Mechanics (QM) calculations to mine an unexplored chemical space and to identify hits uncovered by traditional algorithms. Pharmacelera is a private company founded in 2015 and based in Barcelona, Spain. The company works with several big pharma and biotech organizations across Europe and the United States.

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