Pharmacelera extends the current partnership with Enamine for the screening of ultra-large chemical libraries

Barcelona, Spain, and Kyiv, Ukraine, 7 May 2024. Pharmacelera, the leading provider of computational tools for hit discovery, and Enamine, the developer of the world's largest and most reputable virtual space: REAL, have announced the extension of their current partnership to explore an extraordinary magnitude of compounds, that has been extended by a 10 fold factor – when compared to the early version. Ultra-large chemical libraries constitute a key paradigm to tap into new and still unexplored chemical spaces, increasing the probability for the researcher to find new and chemically diverse potent hits for Discovery Programs. Efficient handling of the ultra-large compound libraries still remain the main challenge.

In 2022, Pharmacelera and Enamine started their collaboration with the plug-in of Enamine Real Database - over 165 well-validated parallel synthesis protocols applied to over 138,000 qualified reagents and building blocks at this stage- to the new version of Pharmacelera's virtual screening flagship tool. The resulting software product was named ***exaScreen***® . ***exaScreen***® is harnessing the power of Artificial Intelligence (AI) and Quantum-Mechanics (QM) algorithms. The success of this initial phase prompted both partners to create an efficient approach to give their customers an access to more REAL Compounds to find new diverse starting points for drug discovery by allowing the screening of Enamine's REAL Space consisting today of 48 billion compounds. The resulting hits can be synthesized by Enamine within only a 3-4 weeks period with an 80% success rate. More analogues for hit follow-up activities are accessible for Pharmacelera's customers,with Enamine offering an access to several trillions of REAL Compounds, and an even of make-on-demand ("MADE") Building Blocks.

As part of this extended partnership, Enamine will receive a license to use exaScreen® for their internal library research work.

"Screening of ultra-large virtual chemical libraries has shown to be a powerful approach that can give a quick access to potent IP-free hits for a wide variety of targets. We are really delighted to count on Pharmacelera among our armada of talented deep -tech partners, and to extend our current collaboration with Pharmacelera to use their ***exaScreen***® *technology to extract the needles from our exciting expandable 3D space environment, but also being glad to use it in-house for our own screening library development work.», said Michael Bossert, Head of Strategic Alliances at Enamine.*

"This agreement is fully aligned with Pharmacelera's strategy to work with leading institutions in the field of Drug Discovery that have complementary technology and expertise", says Rémy Hoffmann, Chief Business Development Officer at Pharmacelera. "We are thrilled to expand the current collaboration started on December 2022 with Enamine, the prominent compound provider, to apply our accurate Quantum-Mechanics (QM) and Machine Learning (ML) algorithms to mine the Enamine's REAL Space and deliver synthesizable compounds that can be further evaluated in biological assays", said Enric Gibert, Pharmacelera's CEO.

About Enamine

Enamine is a scientifically driven integrated discovery Contract Research Organisation with unique partnering opportunities in exploring new chemical space. The company combines access to the inhouse produced screening compounds (4.2M 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 information visit: https://enamine.net

About Enamine REAL Space

Enamine REAL Space contains 48 billion make-on-demand 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 143,000 building blocks via more than 167 well-validated parallel synthesis protocols, underlying Enamine's approach to design make-on-demand compounds to maximize synthesis success rate.

About Pharmacelera

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®**, ***exaScreen®*** and **PharmQSAR®** use 3D molecular descriptors derived from Quantum-Mechanics (QM) calculations to mine an unexplored chemical space and to identify diverse 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.