



Cyclica Collaborates With Enamine to Use REAL Technology in Its Ligand Design Platform for AI-augmented Drug Design

TORONTO & KYIV, UKRAINE, 05 November 2019. Cyclica, Inc. announced a collaboration with Enamine Ltd., the world's largest chemical supplier, to explore its huge readily accessible chemical space using Cyclica's state-of-the-art AI-driven *Ligand Design*TM platform. The companies aim to empower Cyclica's patented, evolutionary algorithm with new design options based on the 73,000 Enamine's in-stock building blocks and 171 thoroughly validated synthesis procedures. The joint effort is expected to enable Cyclica's *Ligand Design*TM to identify novel molecules with desired polypharmacological properties out of over 11 billion *REAL*TM (readily accessible) compounds. At least 80% of these compounds will be synthesized by Enamine within only 3-4 weeks.

Molecules produced by computers are frequently criticized by chemists who fail to find cost-efficient synthesis pathways to them or even question their existence because of *e.g.* stability issues. Enamine has changed the paradigm in accessing compounds for screening. Because of seamless control of resources (all building blocks need to be in stock at Enamine) and statistical knowledge-based enumeration of the virtual compound libraries, the *REAL* compounds are supplied as if they are from stock.

Cyclica's *Ligand Design* technology will smartly generate *REAL* compounds on the fly which are predicted to bind to one or multiple targets, avoid anti-targets, and have desired ADMET and physicochemical properties, making them excellent future drug candidates. By traversing *REAL* space using a genetic sampling algorithm, a much larger chemical space can be accessed than is possible with conventional compound databases, leading to better candidate molecules.

Dr. Andrii Buvailo, Head of E-commerce at Enamine, commented "the *REAL* technology opens up access to large unexplored territory in the chemical universe of small molecules which are delivered to the bench almost like from stock. It has become a reference among our clients when it comes to virtual screening initiatives." Michael Bossert, Head of Strategic Alliances at Enamine added: "Considering the rapidly evolving field of computational methods and techniques of Artificial Intelligence, such as machine learning and deep learning in virtual screening, we are pleased to enrich Cyclica's approach, conveying in this manner a powerful new toolkit and pool of compounds to the early drug discovery community."

"Bringing together Enamine's *REAL* technology and Cyclica's *Ligand Design* will allow our partners to obtain truly novel molecules without paying the cost of *de novo* synthesis, greatly

increasing the speed and efficiency of drug discovery efforts,” said Dr. Andreas Windemuth, Chief Science Officer at Cyclica.

About Cyclica

Cyclica is a Toronto-based, globally recognized biotechnology company that leverages AI and computational biophysics to reshape drug discovery. Cyclica provides the pharmaceutical industry with an integrated and end-to-end enabling drug discovery platform focused on polypharmacology. Ligand Design and Ligand Express offer a unique AI-augmented platform to design advanced lead-like molecules that minimize unwanted off-target effects, while providing a holistic understanding of a molecule's activity through integrated systems biology and structural pharmacogenomics. By doing more with artificial intelligence, Cyclica aims to revolutionize a system troubled with attrition and costly failures, accelerate the drug discovery process, and develop medicines with greater precision.

About Enamine

Enamine is a science-driven chemical company and provider of the world's largest stock collections of building blocks and screening compounds. The company's medicinal chemistry capabilities are enhanced with on-site HTS, ADMET-DMPK and early preclinical studies to provide an easily customizable integrated service package.

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