Atomwise and Enamine to Advance Pediatric Oncology With the World's First and Largest Ten Billion Compound Virtual Screen

SAN FRANCISCO & KIEV, Ukraine, 24th June, 2019 – Atomwise, Inc. today announced the launch of a 10 billion compound AI-powered virtual drug screening initiative, the 10-to-the-10 program, in collaboration with Enamine Ltd., the world's largest chemical supplier. The initiative aims to dramatically increase the discovery of safer small molecule drugs to treat pediatric cancers. Atomwise will use its patented AI virtual screening technology to evaluate the binding of billions of drug-like molecules to cancer target proteins, and Enamine will provide support and access to a virtual library of 10 billion small molecule compounds. The research will be directed by the needs of innovators in cancer research at leading universities.

Cancer is diagnosed in more than 15,000 children and adolescents each year. Many cancers do not have effective treatments and for those that do, it is estimated that 80% have serious adverse effects that impact long-term health.[1] Therefore, new oncology drugs are needed.

The 10-to-the-10 program will search for novel drug candidates by looking at billions of compounds that have never been examined in any drug discovery program. The initiative maximizes the opportunity to develop drugs for novel target proteins to inhibit cancer growth and metastasis. By evaluating truly novel and structurally distinct compounds, the initiative also dramatically increases the likelihood of developing new drugs for existing targets, with less adverse effects.

The enormous screen in the 10-to-the-10 program is possible because of a confluence of technologies: accurate and rapid structure-based drug development with Atomwise's AI algorithms, scalable cloud computing innovations, and large virtual libraries like Enamine's REAL (readily accessible) database of compounds that can be synthesized quickly.

"Many of our partners have successfully identified early drug candidates, including submicromolar hits, by screening only 10 million compounds with our AI virtual screening platform," says Abraham Heifets, CEO and Co-Founder of Atomwise. "We've barely scratched the surface of what is possible – imagine what will be found when we screen a chemical library that is a thousand times larger."

With Atomwise, partners have reported early preclinical success rates more than twice the industry standard. Additionally, average hit rates with Atomwise's AI technology are reported to be a hundred times greater than with traditional screening technologies for comparably difficult targets.[2] Screening hundreds of millions of molecules has already been shown to deliver drugs a thousand times more potent than those found using standard sized libraries[3] – an improvement that could take years to deliver using traditional methods.

Ten billion compounds will provide researchers with many more starting points for drug discovery. Researchers no longer need to sift through the same sets of compounds that have been repeatedly screened in cancer research. With the 10-to-the-10 program, researchers will be able to efficiently test a large and diverse set of compounds, which enables the early identification of solutions to potential roadblocks in drug development. The initiative aims to not only increase the rate of success but also to raise the bar for success and advancement at each step of drug development and to shorten the time needed for preclinical drug discovery.

Dr. Pengda Liu at the University of North Carolina Lineberger Comprehensive Cancer Center, who has had success with Atomwise's AIMS Awards, is hoping to take advantage of this program to advance his research. "In collaboration with Atomwise, we've already found a few inhibitors in just one round of screening. Expanding the chemical space to 10 billion could be an absolute game changer for this research," says Dr. Liu.

The results of this program are to be published in peer-reviewed journals.

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About Atomwise

Atomwise, Inc. invented the first deep learning AI technology for structure-based small molecule drug discovery. Created in 2012, today Atomwise performs hundreds of projects per year in partnership with some of the world's largest pharmaceutical and agrochemical companies, as well as more than one hundred universities and hospitals in more than 20 countries across the world. Atomwise has raised over $50 million from leading venture capital firms to support the development and application of its AI technology.

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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