

OpenEye Scientific Partners with Enamine to Accelerate Early Drug Discovery

OpenEye Scientific's Orion® Molecular Design Platform enables pharmaceutical and biotechnology companies to easily search billions of Enamine's compounds

SANTA FE, N.M., USA, September 9, 2021 /EINPresswire.com/ -- OpenEye Scientific and Enamine, a leading global provider of billions of new screening compounds to the drug discovery market, are partnering to enable faster and more accurate virtual screening of ultra-large compound libraries through access to innovative software.

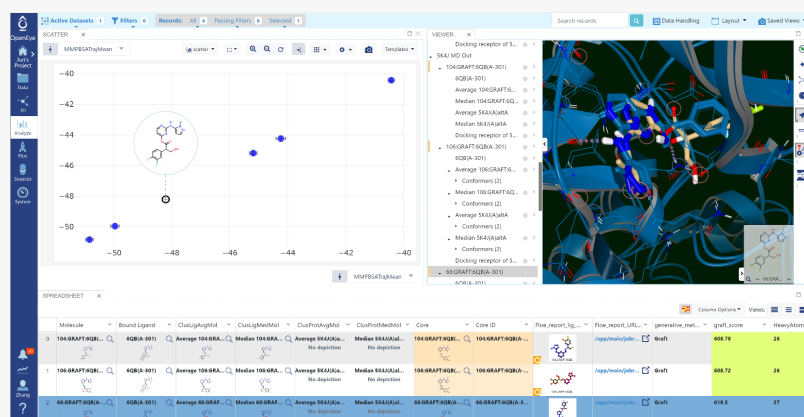
Using Orion®, OpenEye's cloud-native molecular design platform, scientists can:

- Use state-of-the-art 3D and 2D techniques to search and analyze more than 3.6 billion stereo-enumerated molecules with 36 billion conformers, generated from available compounds in Enamine's purchasable [REAL®](#)

[Database](#)

- Identify promising drug-like molecules from billions of compounds in as little as 30 minutes and at a fraction of the cost of in vitro high-throughput screening assays

Enamine commits to manufacture at least 80 percent of any selection from



Scientists now can use FastROCS (shape search) and Gigadock™ (docking) in OpenEye's Orion® molecular design platform to search billions of readily available compounds from the Enamine REAL® library in less than 30 minutes.

those molecules, leading to:

- Completion of the manufacturing process within 3-4 weeks
- Acceleration of the hit-finding process, meaning more new drugs get to market quicker

Matthew Geballe, Vice President of Product at OpenEye Scientific, said:

- "This collaboration brings benefits to everyone involved. When you consider the old-fashioned way of manual screening with a million molecules in plastic trays, what we are doing with Enamine is really revolutionary."

- "Giving OpenEye customers access within Orion® to Enamine's turnkey, professionally prepared, and continuously updated database with billions of compounds will help our customers select candidates much earlier in the discovery process."

□□OpenEye's Orion® molecular design platform uses:

- The power of up to [hundreds of thousands](#) of CPUs and hundreds to thousands of GPUs through Amazon Web Services to provide the fault-tolerant computational capacity required to meet significant scientific and large-scale virtual screening demands

Michael Bossert, Head of Strategic Alliances at Enamine, said:

- "We are happy to partner with OpenEye and conveniently provide our REAL® Database for virtual screenings within Orion®."

- "Complex tasks of finding and optimizing lead compounds can be efficiently performed using various available toolkits in this molecular design platform. However, researchers do need to be sure that their identified valuable molecules will be actually tested in the lab. At Enamine we have worked hard to assure high systematic success rate of synthesis, which in many cases attains 100% within just 3-4 weeks."

-ENDS-□

About Enamine Ltd.

Enamine is a global leading designer and largest producer of building blocks (240,000+) and screening libraries (2.7M+ compounds). □□The REAL® Database is a collection of currently 1.95 billion enumerated compounds that can be synthesized within only 3 weeks with more than an 80% success rate. □□Enamine provides expertise in advanced organic synthesis, library synthesis, and medicinal chemistry. □□In 2011 Enamine established a pre-clinical service unit including ADME, in-vivo PK studies, and High Throughput Screening under the brand name "Bienta," allowing the company to tackle since that time fully integrated or à-la-carte research programs.

About OpenEye Scientific

OpenEye Scientific is an industry leader in computational molecular design, based on decades of delivering rapid, robust, and scalable software, toolkits, and technology and design services.

Our scientific, physics-based approach to molecular design historically focused on molecular shape and electrostatic potential to inform and guide molecular discovery and optimization. OpenEye has now integrated its applications and toolkits into Orion,[®] the only cloud-native, fully integrated molecular design platform. Combining unlimited computation and storage with powerful tools for data sharing, visualization and analysis in an open development platform, Orion offers unprecedented capabilities for the advancement of pharmaceuticals, biologics, agrochemicals, and flavors and fragrances. Founded in 1997, OpenEye is a privately held company headquartered in Santa Fe, N.M., with offices in Boston, Mass.; Cologne, Germany; and Tokyo, Japan. For more information, go to www.openeye.inc.

Contacts

Josh Segal

OpenEye Scientific

+1.617.947.3795

jsegal@punch-pr.com

Michael Bossert

Enamine Ltd.

+380 44 537 3218

m.bossert@enamine.net

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