



Cresset® Announces Global Collaboration with Enamine on New Virtual Screening Drug Discovery Technology

February 21st 2024 – Cambridge, UK – Cresset, an innovative provider of integrated in silico solutions for drug discovery announces a collaboration with Enamine, the world's leading provider of chemical building blocks and drug discovery services to develop innovative new solutions for the early drug discovery process.

The newly announced collaboration involves the development of groundbreaking technology to enable the screening of ultra-large chemical spaces, as part of the virtual screening process in drug discovery. Virtual screening is a technique used to search libraries of small molecules to identify those structures, which are most likely to bind to a drug target.

It has traditionally been performed by generating 3D conformations of the molecules to be screened and then computational processes on each conformation. However, this approach becomes unfeasible when it is used to screen ultra-large chemical spaces, as the storage costs quickly become astronomical as the number of compounds in the space increases.

Ignite™ is a form of virtual screening technology developed by Cresset that utilizes knowledge of the construction of these ultra-large chemical spaces, in terms of reagents as synthons and reactions, that allows the rapid screening of the space. Efficiency gains of more than a hundredfold can be achieved, allowing 3D virtual screening with relatively modest resources.

After being successfully developed as part of a bespoke client library screening project, Cresset extended the capability to collaborate with a commercial vendor, Enamine. The technology has been successfully applied to Enamine's REAL Space, a library of over 38 billion make-on-demand molecules, and currently the largest collection of commercially available compounds.

Commenting on the collaboration, Vladimir Ivanov, Enamine's Executive Vice President said, "Chemical space is countless and we, at Enamine, have developed an approach to its synthetically accessible parts like Enamine REAL Space. We are always happy to see an application of our make-on-demand compounds to speed up delivering new medicines."



Cresset's Chief Executive Officer, Rob Scoffin, added, "virtual screening on ultra-large chemical spaces is currently mostly performed using 2D methods, Ignite provides a novel strategy for fast 3D screening of billions of compounds enabling our clients to access novel chemical starting material for their research programmes in collaboration with our Discovery CRO scientists."

A collaborative webinar, 'New modalities for 3D virtual screening of ultra-large chemical spaces' will take place on 5th March.

For more information about the collaborators visit www.cresset-group.com or <https://enamine.net/>



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About Cresset

Chemists in the world's leading research organizations use Cresset solutions to discover, design, optimize, synthesize and track the best small molecules. Our patented CADD Software, collaborative Torx[®] DMTA design-make-test-analyze platform, and expert Discovery CRO scientists, enable chemists to enhance efficiency and win the race to scientific success in industry sectors including pharmaceuticals, agrochemicals, fine chemicals and flavors and fragrances. www.cresset-group.com



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 in-house produced screening compounds (4M 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 over 38 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 137,000 building blocks via 167 different synthesis protocols, underlying Enamine's approach to design make-on-demand compounds to maximize synthesis success rate.