

Cresset® expands collaboration with Enamine to extend targeted protein degrader library

Cresset, an in silico solutions provider for drug discovery, has extended its collaboration with Enamine.

Cresset and the chemical and biological CRO are looking to develop targeted protein degraders (TPDs), which can be used to develop therapeutic interventions for a number of diseases.

A major class of these protein degraders are proteolysis-targeting chimeras (PROTACs), which can be highly challenging to optimise for use as degraders owing to their physicochemical and ADME properties.

Enamine's TPD linkers to feature on Spark

Enamine has synthesised a library of 5,400 TPD-related linkers, while the company has also developed another 13,000 linkers to be available through quick synthesis.

The Enamine Linker Library was also incorporated into Cresset's Spark, a bioisostere replacement tool used for hit and lead optimisation.

Integration of the new Enamine TPD-related Linker Library in Spark enables searching for known degrader linkers, which are usually larger and more flexible than typical fragments found in existing libraries. Early experiments show very promising results, suggesting these libraries could be key in designing heterobifunctional molecule linkers.

Enamine's Executive Vice President, Dr Vladimir Ivanov, commented: "We are happy to continue our productive collaboration with Cresset. Furthermore, providing streamlined access to Enamine TPD-related Linker Library in Spark gives our joined customers a great solution for bioisosteric replacement and scaffold hopping. Moreover, finding analogs to the linkers of interest is available via Enamine MADE building blocks, deliverable within 4-6 weeks, and via Enamine contract chemistry services."

Cresset's Chief Scientific Officer, Dr Mark Mackey, commented, "The addition of these linker libraries will expand the utility of Spark to an even wider set of small molecule drug discovery programmes. We are excited to continue working with Enamine to help our customers advance their projects by designing the best molecules they can."

The two companies will also run a collaborative webinar in September, with more details on this being announced in due course.



For more information about the collaborators visit <u>www.cresset-group.com</u> and <u>www.enamine.net.</u>





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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 <u>CADD Software</u>, collaborative <u>Torx® DMTA</u> design-make-test-analyze platform, and expert <u>Discovery CRO</u> 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. <u>www.cresset-group.com</u>



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 (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 MADE Building Blocks

Enamine MADE (MAke-on-DEmand) building blocks are a catalog of 1 billion chemical building blocks that can be synthesized within several weeks using short pre-validated experience and starting materials from Enamine stock in 2-4 steps with a 75% success rate. For more information visit: https://enamine.net/building-blocks/made-building-blocks

About Enamine Fast MADE Building Blocks

Enamine Fast MADE building blocks is a special set of Enamine MADE building blocks. The Fast MADE catalog contains 78.7 million molecules that can be synthesized in ultra-short terms (within 7 to 10 days), through 1-3 commonly utilized procedures with an 80% success rate. For more information visit: https://enamine.net/building-blocks/fast-made-building-blocks