

Merck teams up with Cyclica for AI-augmented screening Platform

December 7, 2018 | News

Agreement to screen discovery and early development compounds using artificial intelligence and computational biophysics



Merck, a leading science and technology company has entered into a licensing agreement with Cyclica Inc. for the use of Ligand Express®, a cloud-based *in silico* proteome screening platform. Ligand Express® is a structure-based and artificial intelligence (AI) augmented proteome screening platform that is being used to uncover novel targets that are modelled to interact with a small molecule. This year-long agreement will enable Merck to quickly and efficiently elucidate mechanisms of action, evaluate safety profiles and explore additional applications for a number of its investigational small molecules, including those identified in highly disease-relevant phenotypic screens.

"A key part of our R&D strategy is to progress highly promising compounds as efficiently and rapidly as possible," added Friedrich Rippmann, Director of Computational Chemistry & Biology at Merck. "Assessing new technologies is central to how we will advance our discovery programs, and artificial intelligence applications like Ligand Express® will provide important insights to enhance how we think about target identification to support phenotypic screening and off-target profiling in general."

Current experimental protein screening approaches can take up to a year, making it virtually impossible to do this for multiple compounds. We see this as a specific opportunity for cloud-based and AI-augmented technologies to drive drug discovery more efficiently," commented Naheed Kurji, President and CEO of Cyclica. "We are thrilled that Merck will be leveraging the power of our Ligand Express® platform to drive their identification of novel targets."

Traditional development of small molecule therapies focuses on specific, disease-associated protein targets. However, once a drug enters the body, it interacts with dozens, if not hundreds, of proteins before it is eliminated from the body. With Ligand Express®, it is possible to capture a unique panoramic view of the proteome for a given small molecule. As the technology can model the ways in which a small molecule will interact with all proteins (of known structure), it can help identify both 'on-targets' (interactions that may have a desirable effect on a certain disease), as well as 'off-targets' (interactions that may cause an adverse effect).