

## News Release

Your Contact  
Gangolf Schrimpf +49 6151 72-9591  
Investor relations +49 6151 72 3321

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## **Merck KGaA, Darmstadt, Germany, in Agreement with Cyclica for AI-augmented Screening Platform to Expand Research Capabilities**

- **Agreement to screen discovery and early development compounds using artificial intelligence and computational biophysics**
- **Cloud-based *in silico* platform that screens small molecules to determine polypharmacological profiles**
- **Evaluation to include identification of potential mechanisms of action for investigational small molecules**

Darmstadt, Germany, December 6, 2018 – Merck KGaA, Darmstadt, Germany, a leading science and technology company, today announced that it has entered into a licensing agreement with Cyclica Inc. for the use of Ligand Express<sup>®</sup>, a cloud-based *in silico* proteome screening platform. Ligand Express<sup>®</sup> 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 KGaA, Darmstadt, Germany 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.

“With scientific curiosity at the heart of everything we do, the pursuit of state-of-the-art research techniques and technologies is integral to complement our internal discovery engine,” said Belén Garijo, Member of the Executive Board and CEO



Healthcare, Merck KGaA, Darmstadt, Germany. "Artificial intelligence has the power to make the previously unimaginable a reality – we are eager to harness these new possibilities to help drive the discoveries that can transform the lives of people affected by difficult-to-treat diseases."

"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 KGaA, Darmstadt, Germany. "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 KGaA, Darmstadt, Germany 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).

Merck KGaA, Darmstadt, Germany is committed to embracing innovative technologies to help bring a transformational change to patients. This includes those developed by partners who share a similar passion for discovery and advancing human progress.



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#### **About Merck KGaA, Darmstadt, Germany**

Merck KGaA, Darmstadt, Germany, the vibrant science and technology company, operates across healthcare, life science and performance materials. Around 53,000 employees work to make a positive difference to millions of people's lives every day by creating more joyful and sustainable ways to live. From advancing gene editing technologies and discovering unique ways to treat the most challenging diseases to enabling the intelligence of devices – the company is everywhere. In 2017, Merck KGaA, Darmstadt, Germany, generated sales of € 15.3 billion in 66 countries.

The company holds the global rights to the name and trademark "Merck" internationally. The only exceptions are the United States and Canada, where the business sectors of Merck KGaA, Darmstadt, Germany operate as EMD Serono in healthcare, MilliporeSigma in life science, and EMD Performance Materials. Since its founding in 1668, scientific exploration and responsible entrepreneurship have been key to the company's technological and scientific advances. To this day, the founding family remains the majority owner of the publicly listed company. For more information about Merck KGaA, Darmstadt, Germany, visit [www.emdgroup.com](http://www.emdgroup.com).

#### **About Cyclica**

Cyclica is a Toronto-based biotechnology company that is driving drug discovery by empowering scientists in pharma with an integrated cloud-based and AI-augmented platform that enhances how they design, screen and personalize medicines. To learn more, visit [www.cyclicarx.com](http://www.cyclicarx.com).

