

CASE STUDY

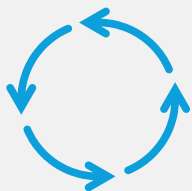


# Rail-Based Automation Fortifies an AI-Enabled Drug Discovery Learning Loop



# Re-imagining drug discovery to improve patient outcomes

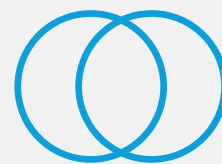
## Exscientia Drug Discovery Automation Goals



Increase the learning loop rate



Build economies of scale




Support workflow reliability and repeatability



Traditional drug discovery methods yield limited progress over long periods of time. Exscientia recognized this as a major roadblock and sought to reimagine this critical step in developing therapies to improve patient lives. As a pioneering artificial intelligence (AI)-driven precision medicine global company, Exscientia leverages generative AI and machine learning with experimental innovation in its drug discovery strategy. As a result, it was the first company to have an AI-designed molecule enter clinical trials.





“We are aiming at multiple assets on the system per day, which requires considerable automation flexibility.”

Martin Redhead, Ph.D.  
Executive Director, Primary Pharmacology

## Looping in Automation

Automation is a key component of Exscientia's process, facilitating high throughput screens (HTS) along with biochemical and cell-based assays. Automated workflows are known to improve reliability and repeatability of assays, but the Exscientia team was equally motivated by increasing the rate of its learning loop and enabling a scalable process.

Martin Redhead, Executive Director Primary Pharmacology at Exscientia recalls that when the company looked into automation providers, they wanted a relationship-minded supplier who clearly understood Exscientia's requirements and design ethos. “It was clear, upon speaking

to HighRes, that they were listening and keen to understand our requirements,” Martin recalls. “They turned out to be highly collaborative, and in some cases, they even changed their established way of working in order to suit our needs.”

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# All-in-One Nucleus® Automated Ecosystem



Four multi-device Nucleus Work Cells, each with a defined function, form the basis for the automated drug discovery processes installed. The Nucleus Work Cells are interconnected as one large multitasking system through an overhead rail-based sample conveyance structure. The rails use electromagnetic force to gently yet quickly move Exscientia's 96-, 384-, or 1536-well plates around the automated ecosystem without the need for human intervention.

Once the system is in full operation, it is expected to be in nearly constant use to support design, make, test, and analyze the team's discovery efforts. Unlike typical high-throughput systems (HTS), where up to one hundred or more plates are processed in tandem, Exscientia's Nucleus system is specifically designed for flexibility. Here, fewer plates may be processed each day, but the plates each contain different multiplexed assays.



# Orchestrating Control through Cellario®

This system, including all devices on the application-specific Work Cells and the rail structure, is controlled by Cellario whole lab automation software and its corresponding remote-enabled CellarioOS™ software. Together, these overarching software platforms, in concert with Exscientia's own proprietary systems, enable remote management of reagent storage, assay development and more. These systems can direct the Nucleus system to prepare everything needed for a particular assay or set of assays without active involvement from a team member.

An open application programming interface (API) architecture eases communication between Cellario and Exscientia's databases. "In our survey of schedulers, Cellario was the best one to work with our existing database and tools and manage our scale of different experiments," explains Martin. On top of this, Exscientia users speak positively about Cellario's usability and reinforce that it is fast, intuitive, and straightforward to send instructions from Exscientia's own proprietary systems to the automation platform using the Cellario API.



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# Tangible Automation Benefits

With walkaway convenience, the entire team can focus on high-value tasks while the Nucleus system operates. Experimental time is expected to decrease while maintaining high-quality results. Compounds can be made and tested within hours for an efficient learning loop. On top of that, detailed experimental protocols are stored and easily recalled at any time as projects ebb and flow via a combination of Exscientia's own proprietary systems and CellarioOS.

"One thing that surprised me was how quickly we were able to operationalize the Nucleus system," notes Martin. "I was expecting six to nine months of coming up to speed, but within a month and a half, we were using it for some of our use cases.

The team appreciates the collaborative robotics for their small footprint and safe interaction. They also like the dynamic aspects of the scheduler that allow them to queue up several assays at a time and have them run across the system at the same time to maximize device use and overall efficiency.





# A Nod to HighRes Service

Martin gives praise to the HighRes support staff throughout this project. Examples include intensive Cellario training courses to create highly skilled super users as well as regular meetings and onsite visits from HighRes experts as needed to ensure that the Nucleus system meets Exscientia's expectations and is running as smoothly as possible.

Martin and his team aim for "true automation"



## The Automation Journey Continues

As the Nucleus automated ecosystem nears full operation, Martin and his team aim for "true automation" which does not require human input and where experiments can revolve around the science rather than personnel schedules.

The system is also expected to strengthen the bond between Exscientia's programmers and scientists, each with their unique perspectives. By having a very collaborative automation, everyone can see the workflow and the experiments take on a more tangible quality for those unfamiliar with biology.



# Conclusion

By encoding and automating the workflow loop, Exscientia has been able to significantly increase its learning loop rate. Its own proprietary systems, under the supervision of Exscientia researchers, generate assay conditions and develop assays. Team members are now freed up to focus on mechanism of action (MOA) mysteries and other priorities to further drive project value.



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