

# Automating sample transport and instrument control to improve inter-lab workflows

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## Overview

Orion, a global pharmaceutical company based in Finland, develops, manufactures, and markets human and veterinary pharmaceuticals and active pharmaceutical ingredients. The Medicine Design department within Orion R&D has several synthesis laboratories spread across two floors of the Espoo Research Center. Around 30 chemists and research assistants work in the synthesis labs every day and are supported by a 5-person analytical group that performs chromatographic analyses and preparative purifications to support the day-to-day synthesis work.

Good analytical support is crucial for chemists working in a synthesis laboratory. Monitoring the progress of reactions and getting instant feedback is essential for speeding up synthesis and providing new research compounds to different studies as quickly as possible. The key aim for the Medicine Design department was to streamline its system for transporting samples between labs, and rapidly deliver the results from the analytical laboratories back to the synthesis lab.

## The drawbacks of manual sample transport

Under the previous system, samples were brought to the analytical laboratory in person, where processes were carried out by hand. Manual transportation was incredibly time consuming, interrupting progress to synthesis work.

**The total time spent transporting approximately 150 samples every day was equivalent to one FTE.**

An analyst then had to run each sample manually, which left them restricted to the lab while waiting for the analysis to complete.

When reviewing this workflow, the department's aim was to ensure fewer interruptions for the experts working in the synthesis labs, while also freeing up highly skilled professionals in the analytical lab to do more critical and value-adding work. The department needed its analytical services to be fully operational throughout the evening and overnight, even when no staff were present. The team wanted a fully automated workflow and eventually chose SPT Labtech's novel lab2lab system.

## The lab2lab sample and data transfer network

lab2lab is a site-wide integrated sample transport and instrument control network that offers a unique pneumatic system for transporting samples in 2D-barcoded vials. It transports vials to instruments, where lab2lab's combined mechanical and software integration initiates analysis. Vials are registered in a standardized way regardless of the type of instrument required. A single vial can be sent sequentially to multiple instruments.

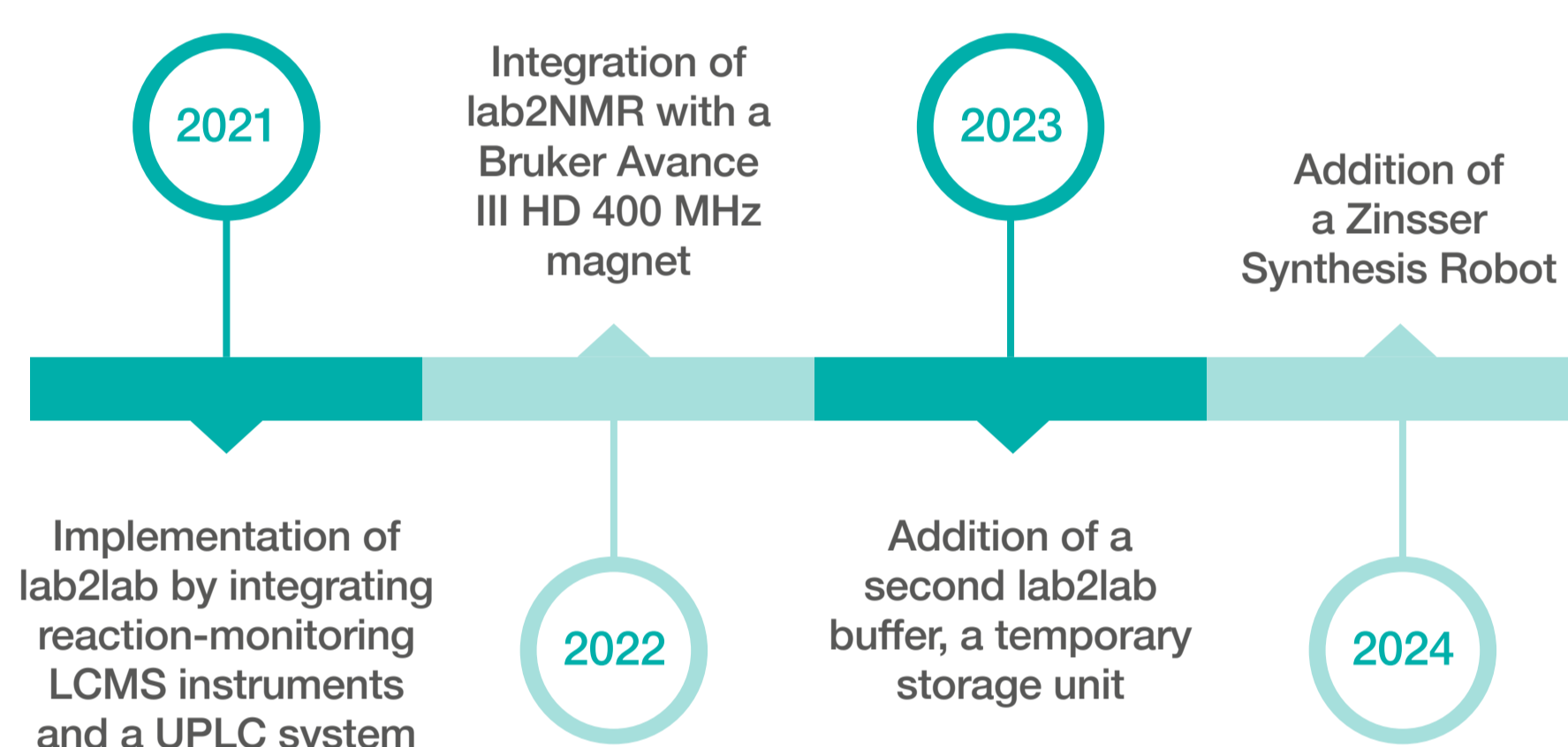


Figure 1: The lab2lab set up in Orion Pharma's chromatography laboratory.

## lab2lab offers numerous advantages over conventional Open Access arrangements:

- Instrument utilization rates are much higher and the instruments themselves have much lower downtime.
- The amount of human intervention required is reduced. Lab productivity is increased as researchers can submit samples for analysis much more quickly and easily.
- As well as removing bottlenecks, lab2lab greatly enhances the traceability of samples as each vial can be registered with a sample reference.
- Analytical results are formatted consistently, and their repeatability is improved due to the tighter control over instruments.
- lab2lab integrates with instruments from Agilent, Bruker and Waters, as well as SPT Labtech's own sample storage solutions. The system allows laboratories to cluster instruments more closely, freeing up valuable bench space and reducing background noise.

## Improving sample flows from synthesis labs to analysis tools: A timeline



Orion implemented lab2lab in October 2021 by integrating reaction-monitoring LCMS instruments and a UPLC system for chromatographic purity analyses. Once set up, the team quickly got to grips with the system and appreciated its 24/7 availability. lab2lab has simplified and streamlined the sample analysis process, reducing training requirements and chances for human error through manual handling and coding. While initial training investment is still needed for key users, the system is easier to learn overall, saving time for end users compared to historical manual processes.

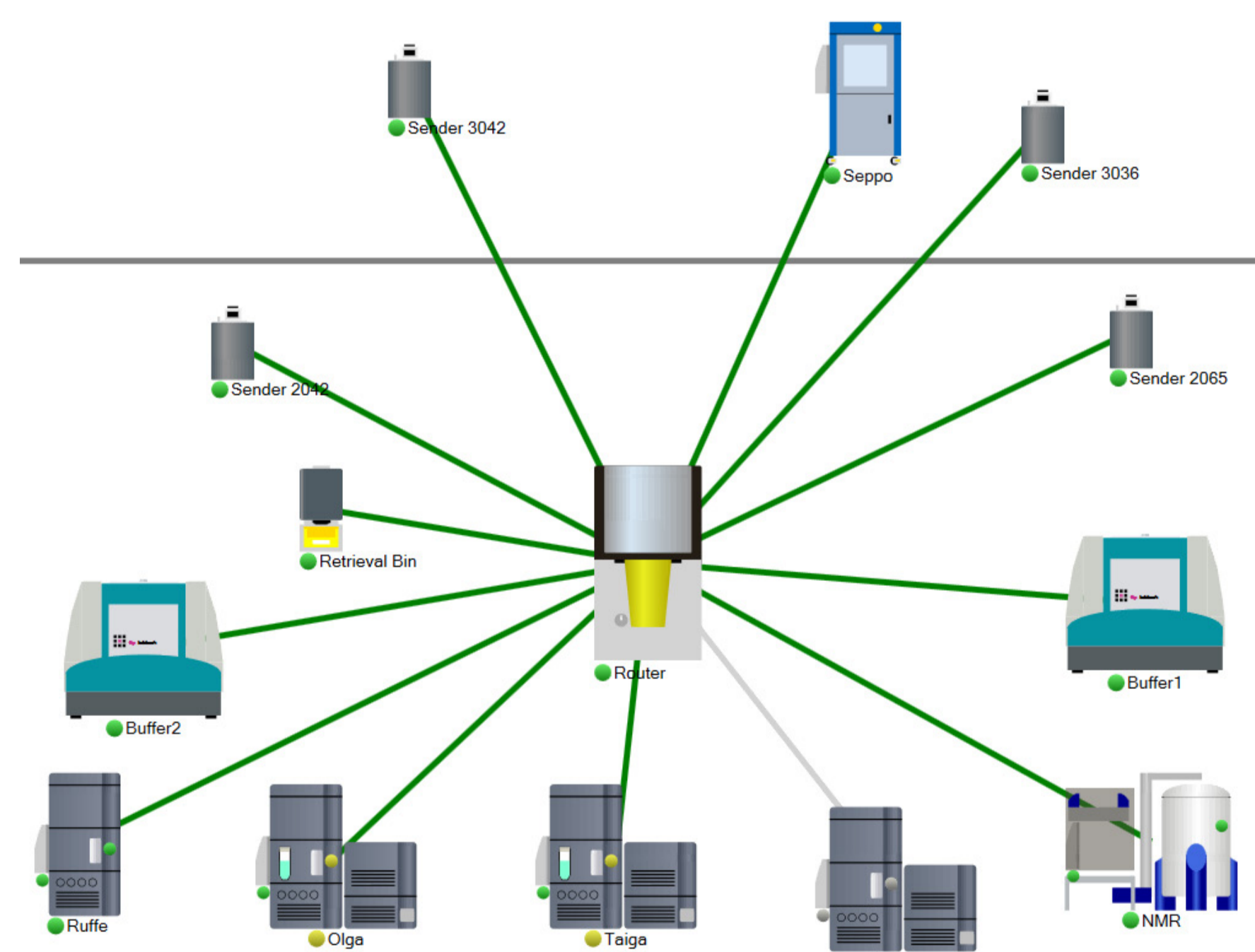


Figure 2: A schematic representation of the lab2lab set-up in Orion.

In 2022, Orion integrated lab2NMR setup with a Bruker Avance III HD 400 MHz magnet. In this workflow, sample vials in NMR solvent (DMSO-d<sub>6</sub>) are transported via lab2lab to the SampleProTube pipetting robot. Samples are then transferred into NMR tubes and to the magnet for measurement. <sup>1</sup>H experiments are run during the day, while others are run overnight. With the lab2NMR setup, <sup>1</sup>H NMR analysis starts immediately as soon as the instrument is free, and results are quickly available. This is a significant improvement on the old system, where scientists often had to wait for results as the NMR operator had to balance other duties.

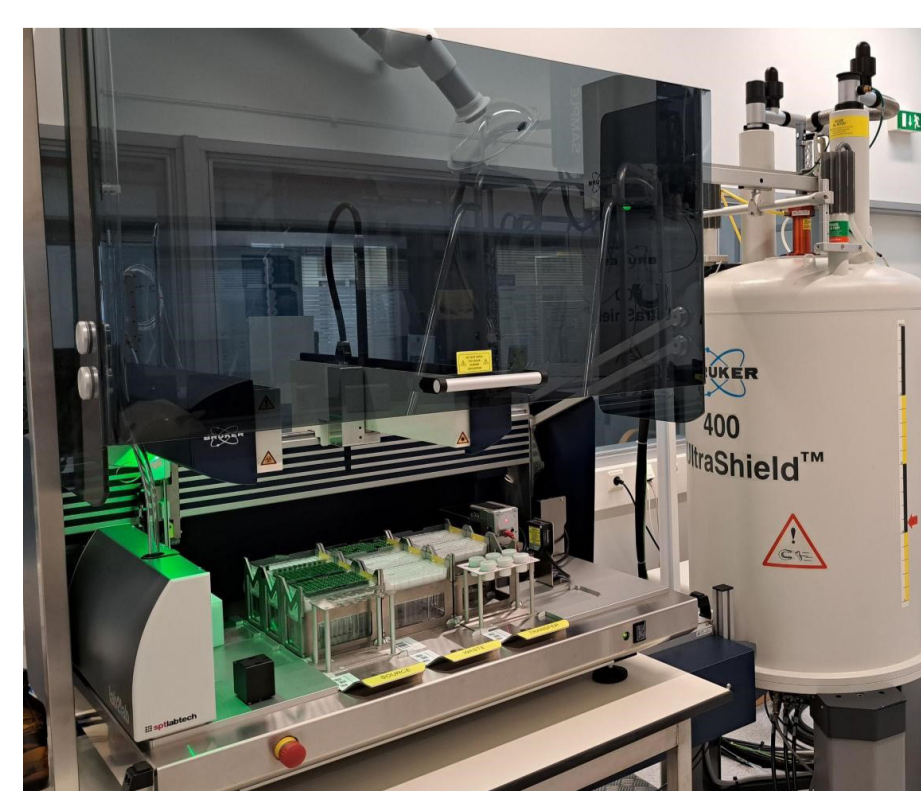


Figure 3: The Lab2NMR setup in Orion.

In autumn 2023, a second storage unit the lab2lab buffer was added to meet the expected increase in sample demand. These two units are connected to one PC. Once the first unit is at full capacity, samples are then stored in the second unit. It is very common and highly appreciated to store analyzed sample in the lab2lab buffer for 24 h in case an additional analysis is needed.

At the beginning of 2024, a Zinsser synthesis robot was added to the setup to increase sample analysis throughput. Samples from the robot reactions are pipetted into pre-capped lab2lab vials and transported by one of the robotic arms to the lab2lab receiver unit. Lower priority samples are typically stored in the lab2lab buffer and sent for analysis when there is no queue of reaction monitoring samples.

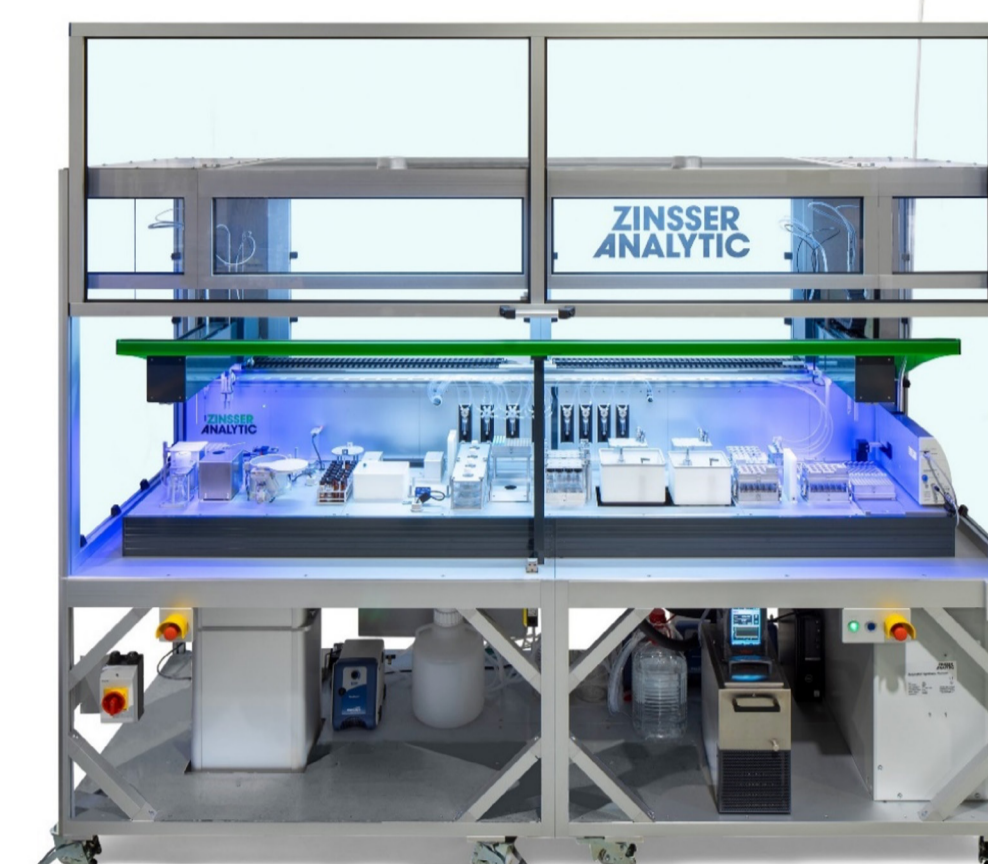


Figure 4: Integration of Zinsser synthesis robot into lab2lab system.

## Advantages of a fully automated workflow

- Submitting samples for analysis is now fast and easy. All manual steps have been automated to minimize the risk of human error. The ability to submit a single sample for multiple analyses saves a significant amount of time and maximizes the reach of every sample.
- Queueing time is minimized as samples are submitted for analysis as soon as an instrument is available. The sender device can select several analyses at once or retain samples in the buffer for later use if more information is needed.
- To date, there are five different analytical LC methods and 13 NMR methods available. Before implementing lab2lab, an analyst had to be contacted whenever additional analyses were required. As the system is fully automated, it is now operational 24/7. Synthesis lab personnel don't need to wait for an analyst to arrive in the morning and can send a sample via lab2lab at any time.
- Chromatographic lab personnel now have more time to conduct other analyses and carry out development tasks. This has a direct effect on the response times of all chromatographic analyses and speeds up research progress.
- Tracking the daily performance of instruments is also easy: Data is collected automatically, statistics are always up to date, and so monitoring is straightforward.

## Increasing throughput: From sample submission to analysis within minutes

At Orion, all reaction monitoring, chromatographic purity samples and NMR samples in DMSO-d<sub>6</sub> are now transported via lab2lab from the synthesis labs to the analytical instruments. The lab2lab software provides easy data tracking possibilities and ready-made templates for data collection.

### The number of samples analyzed increases every year

- In 2022, more than 20,000 vials were sent for analysis via lab2lab with ~30,000 methods.
- In the first 6 months of 2024, almost 15,000 samples have already been analyzed with ~24,000 methods.
- Currently, nearly 200 analyses are performed every day on average, and the median time from submission to analysis is under 5 minutes.

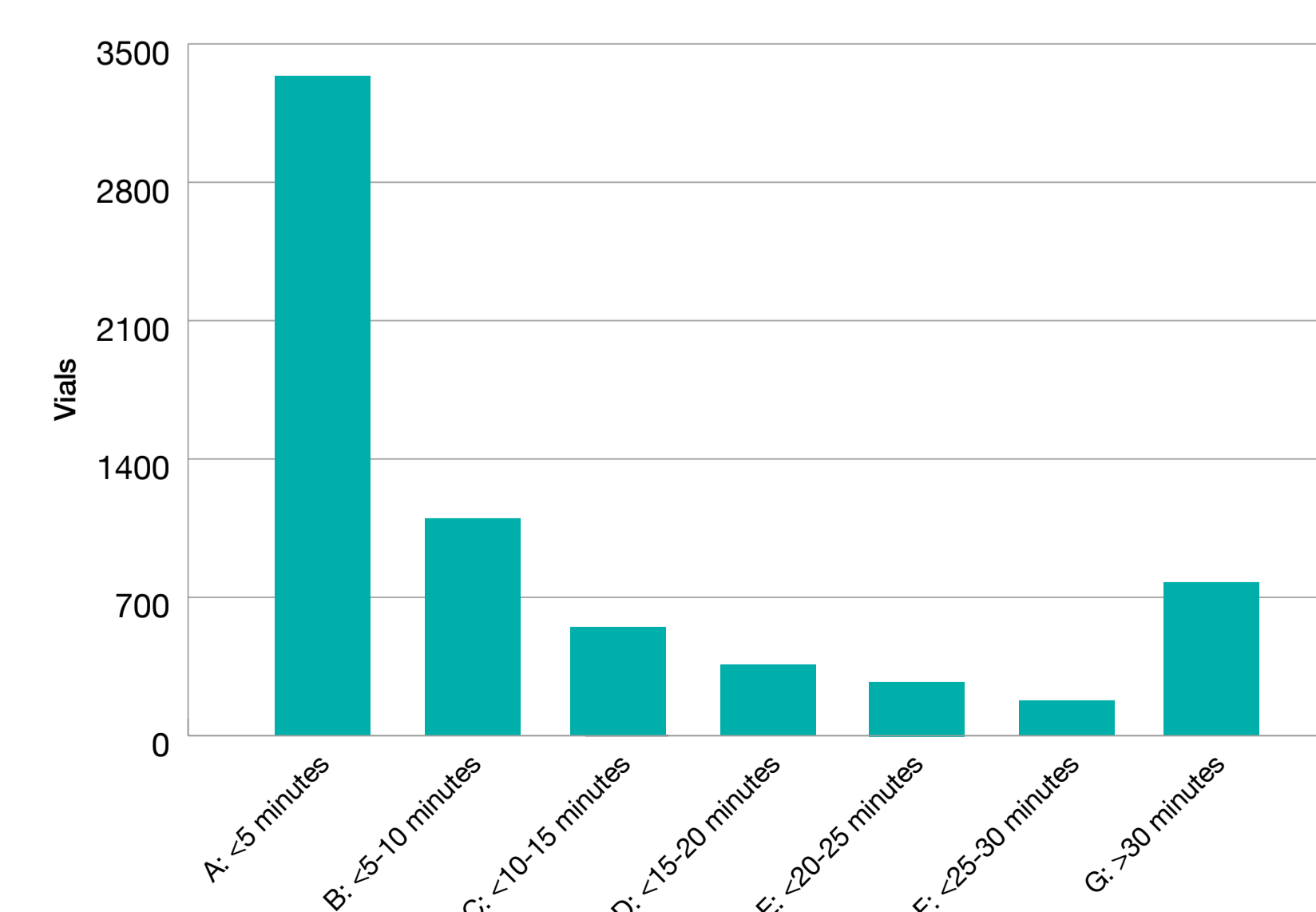


Figure 5: From Physical Submission to Start of Aspiration (2024)