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Assessment and pilot lab automation solution for pRED Building 12

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Master thesis, Bioanalytics

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INTRODUCTION

Laboratory automation has progressed rapidly over the last decade, driven by high-throughput screening technologies, advanced robotic platforms and the need to provide patients with potentially life changing treatments in a fast and cost effective manner [1]. Although these advancements have improved quality and reproducibility, many R&D settings still rely on a mix of manual, semi-automated and fully automated processes, often using proprietary implementations or various vendor specific software [2]. This thesis evaluates whether current standards, such as Standardization in Lab Automation (SiLA 2) and Laboratory and Analytical Device Standard (LADS), can meet diverse instrumentation needs, streamline device integration, and reduce vendor lock-in. Additionally, the thesis provides strategic recommendations for laboratory automation in the laboratories of Building 12, planned to open in 2029.

CONCEPT

To assess whether SiLA 2 and LADS will remain relevant until Building 12's planned opening in 2029 and beyond, a comparative framework was developed. This framework was constructed using the results of a historical analysis of three established standards: USB, OPC Classic, and Ethernet. The common success factors identified through this analysis enabled these standards to achieve long-term success despite strong competition in their respective areas. Next, data from device manufacturers regarding standard adoption and future development plans were gathered. This was accomplished by performing a survey at the Ilmac 2024 trade fair, with a specific focus on manufacturers that produce tabletop equipment for R&D laboratories, such as currently in use within the user groups scheduled to move into Building 12. In parallel, key representatives from the SiLA consortium and the LADS initiator were interviewed and surveyed to understand their long-term strategies and further development. Additionally, integrators and solution providers who have worked with Roche, either currently or in the past, were interviewed and surveyed to gather insights into real-world usage, financial impacts and challenges. For evaluating the practical implementability, a pilot use case was defined by analyzing common workflows and equipment within the department planned for Building 12. A buffer preparation workflow was chosen as a representative example, which involved a Mettler Toledo AX 205 balance, a Mettler Toledo SevenCompact S220 pH meter and a Universal Robots UR3e collaborative robot. For the pilot implementation, servers were developed to connect and control the instruments via SiLA 2. Commands from each instrument were restructured into a standardized format, as defined by the corresponding specification. The business logic, consisting of the information on what each command should perform, and how the outputs should be used, was implemented using Python. Figure 1 illustrates the development process for a SiLA 2 server.

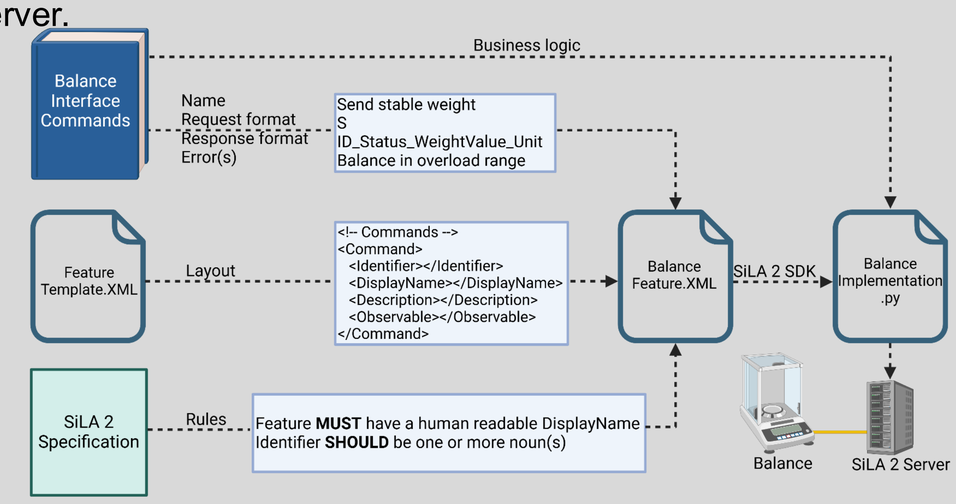


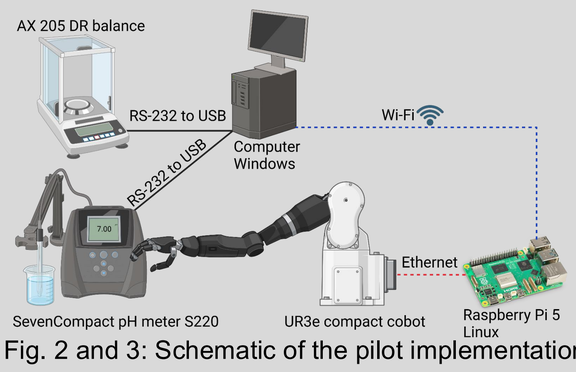
Fig. 1: Process of SiLA 2 server generation. Balance interface commands are transformed into a SiLA 2 compliant format following the SiLA 2 specification.

To evaluate platform neutrality, the servers were tested using different operating systems (Windows/Linux). To assess device agnostic properties, the balance server was tested with two additional balance models. Due to unavailability of LADS reference implementations in Python, a minimal OPC Unified Architecture (OPC UA) server for the balance was developed instead, as the LADS standard uses OPC UA communication technology as its foundation. The development was performed using the FreeOpcUA Python library, mirroring the core functionality and communication logic of the SiLA 2 server. Similar to the SiLA 2 server, each function and each error state was tested to assess the functionality.

To reduce the time and effort required to convert laboratory device command descriptions into standardized formats, an automated method using the Large Language Model (LLM) Claude 3.5 Sonnet was developed. Relevant documents, such as the balance command set and the SiLA 2 specification were loaded and preprocessed to extract command structures, parameters and error handling information. Based on this information, a knowledge graph and a schema definition template were created for validating feature definition files.

RESULTS

From the historical analysis of USB, OPC Classic and Ethernet, five success factors were identified: Industry collaboration, cost effectiveness, vendor neutrality, scalability and flexibility, and backward compatibility. Evaluating SiLA 2 and LADS against these criteria revealed that both standards can address current R&D needs but differ significantly in maturity and market adoption. Survey data from laboratory device manufacturers indicate growing SiLA 2 support, whereas LADS remains less established. Interviews with integrators and standard organizations highlighted cost benefits when standardized interfaces are implemented and pointed out a strong influence of user demand towards manufacturer adoption. Using SiLA 2, all planned devices could be integrated for the simulated buffer preparation workflow. Figure 2 shows the schematic of the pilot implementation, whereas Figure 3 shows the actual setup.



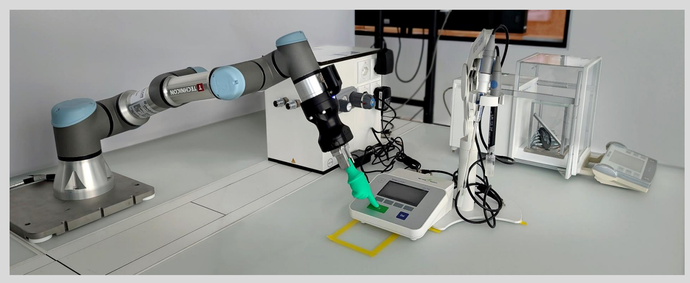


Fig. 2 and 3: Schematic of the pilot implementation and image of the implementation

Although retrofitting older instruments presented challenges, the results confirmed that standards such as SiLA 2 effectively integrate devices. The implementation of a collaborative robot demonstrated that even instruments which were not designed for automation can be integrated seamlessly into automated workflows. On the other hand, the OPC UA server confirmed a similar integration possibility. Finally, the LLM approach showed promising results but still required manual oversight and improved documentation to work efficiently.

CONCLUSION

Evaluating SiLA 2 and LADS against the established success criteria suggests that both standards can remain relevant until the planned opening of Building 12 in 2029 and beyond. SiLA 2 offers greater commercial availability and has proven retrofitting options for legacy equipment, making it well suited for agile R&D laboratories. LADS builds on robust OPC UA infrastructure and therefore seems promising for regulated or production associated laboratories. The current lack of commercially available solutions and reference implementations for programming languages other than C++ and C# shows a need for further investigation.

Based on these findings, it is recommended for Building 12 to adopt SiLA 2 as the primary interface standard, especially in requests for proposals for new laboratory devices. This can help to address the current fragmentation in automation, motivate manufacturers to provide native SiLA 2 support and reduce the overall integration costs. At the same time, LADS should be monitored for potential benefits once products become commercially available. External integration projects should use SiLA 2 to ensure consistency across different departments. Finally, the creation of a legacy integration guideline and carefully evaluating scheduling software which supports both standards will help to maintain a future-proof environment.

By following this approach, Building 12 can minimize vendor lock-in, simplify maintenance and support flexible, emerging automation solutions.

REFERENCES

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[2] C. Hawker et al., Tietz Textbook of Clinical Chemistry and Molecular Diagnostics, 2017, 6, p370-370.e24