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Getting Started with Lab Automation: Requirements, Misconceptions, and Practical Workflows

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Abstract: We herein provide a practical introduction for chemists with limited prior experience in automation, highlighting requirements, frequent misconceptions and common pitfalls encountered while setting up automated workflows. Key topics include the distinction between automation and autonomy, the development and integration effort typically required, and the central role of robust data capture and handling beyond the bench. Selected literature examples illustrate how substantial benefits can already be achieved with targeted automation of key elements, before moving to more connected end-to-end platforms.

Keywords: Digital chemistry · High throughput experimentation · Lab automation · Self-driving labs

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1. Introduction: Why Automate?

In recent years, rapid advances in machine learning and artificial intelligence (AI) have driven a surge in data-intensive applications. As a consequence, the demand for large volumes of standardized and reproducible data has increased, not only in disciplines closer to computer science, but also across the natural sciences, including chemistry.[1–6] While many IT applications can rely on digitally generated data collected at scale, chemistry still depends largely on experimental data that are labour-intensive to produce, often noisy, and typically available only in limited quantity. Lab automation technologies have therefore gained increasing attention as a means to address these limitations by enabling standardized execution and higher-throughput data generation, while also reducing time spent on repetitive, low-value tasks and contributing to improved reproducibility and data quality. Nevertheless, despite these advantages, practical challenges are often underestimated, complicating effective adoption. This perspective is intended as a practical starting point for chemists with little to no background in lab automation who aim to introduce automation into their laboratory. The most common requirements, pitfalls, and misconceptions encountered when setting up automated workflows are discussed, followed by selected examples of practical applications. Although the focus of this mini guide is on chemistry, many of the principles presented are applicable to other experimental disciplines within the natural sciences. In addition, the literature on laboratory automation is rich in comprehensive reviews and detailed articles covering high-throughput experimentation, self-driving laboratories, and digital workflows, which we leave here as a reference for readers who wish to explore the topic more deeply.[7–23]

2. Requirements and Pitfalls of Lab Automation

To successfully harness the power of automation, one should be aware of a few requirements. While the needs of each lab are different, there are common prerequisites that are shared and essential (Fig. 1). We will now proceed to list here what we believe are the most important ones.

2.1 People and Funding

Sitting at the intersection of engineering, science, and information/operation technologies (IT/OT), the successful adoption of lab automation requires a non-negligible effort. The most prominent requirement is access to the right talent, equipped with the interdisciplinary skills needed to understand the scientific workflow and translate it into automation-ready procedures. At the same time, it is important to develop a solid understanding of the automation technology in use, together with a fundamental awareness of IT/OT considerations.

While these interdisciplinary skills are often associated with the automation expert, an equally important requirement concerns end users. Adoption depends on culture and mindset: end users need to be willing to adopt new ways of working and, as we will see, to invest time in standardization and change.

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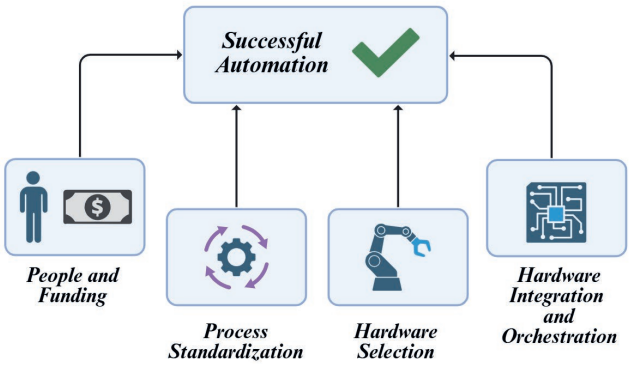


Fig. 1. Schematic overview of the main factors leading to successful automation, encompassing people and funding, process standardization, hardware selection, as well as hardware integration and orchestration.

In addition to skills and mindset, capital investment is an obvious enabling factor. Automation hardware, service contracts, software licenses, and the development or adaptation of custom software represents significant upfront costs. As a result, budget constraints often dictate both what can be implemented and the speed at which adoption can proceed.

2.2 *Process Standardization*

To reap the benefits of lab automation, it is fundamental to start with a well-defined process. A common example in synthetic chemistry is reaction condition scouting. The same transformation is often screened across a matrix of bases, solvents, catalysts or ligands, and temperatures. This is a repetitive task, typically carried out with small volumes, and it benefits strongly from standardized dispensing and mixing. In practice, the process can be defined as a sequence of simple, discrete steps: preparation of stock solutions (substrate, coupling partner, catalyst system), dispensing into a multi-well plate, addition of base, sealing and shaking, incubation, quenching, dilution, and preparation of liquid chromatography-mass spectrometry (LC-MS) vials or an analysis plate. When these steps are written down with unambiguous parameters (volumes, order of addition, mixing time, temperature, plate type, seal type), the process becomes automation ready.

As discussed later, automation does not require automating the full workflow from start to end. Oftentimes, automating only the most repetitive and error-prone parts already delivers most of the benefit. This modular approach reduces complexity and shortens setup time, while still improving repeatability and throughput. Conversely, 'over automation' can lead to unnecessarily complex processes, making adoption even more difficult for end users.

2.3 *Hardware Selection*

Once the processes have been identified and described in detail, the next step is to select the appropriate hardware. Numerous manufacturers already supply automation-ready devices, which ensure compatibility with American National Standards Institute/Society for Laboratory Automation and Screening (ANSI/SLAS) standard consumable formats and allow external software to access their main functions. The heterogeneous landscape of vendors and models can pose challenges for a successful choice. In many cases, a simple liquid handler is sufficient to cover routine pipetting operations. Given the number of available models, selection should be guided by the intended applications. For instance, when aggressive chemicals are handled, chemical compatibility of exposed parts becomes a key constraint. When sterility or an inert atmosphere is required, practical considerations include whether the system can operate in an enclosed environment (*e.g.* under laminar flow or inert atmosphere). Further selection criteria typically include the nature of the liquids to be transferred and the required pipetting technology (air displacement versus positive displacement), as well as tip strategy (fixed versus disposable tips). Given the landscape of possibilities, obtaining clear specifications and support information from a trusted manufacturer is of fundamental importance. Likewise, many suppliers offer the possibility to test their equipment with in-house samples, which reduces the risk of committing to costly purchasing decisions.

Beyond liquid handlers, several other devices are commonly encountered in chemistry automation:

- **Robotic arms**: used to move consumables in ANSI/SLAS format between instruments.
- **Centrifuges**: used for a wide range of applications, for example filtration, sedimentation of solids, removal of bubbles in solution, phase separation, *etc*.
- **Shakers**: used to shake multi-well plates, with or without heating.
- **Sealers**: used to seal plates to prevent material loss during shaking, incubation, or transport.
- **Peelers**: used to remove seals, often *via* an adhesive roll mechanism.
- **Plate readers**: used for optical readouts in plate format, typically to assess analyte concentration or to assess pipetting precisions.
- **Solid dispensers**: used to dose powders into vials or wells.

It should be noted that this list is not exhaustive and does not include stand-alone analytical instruments, which can often be adapted to become compatible with automation. Several other devices are available on the market depending on the specific workflow requirements, which stresses even more the importance of having well-defined processes.

2.4 *Hardware Integration and Orchestration*

The main advantage of having multiple pieces of equipment is the possibility of making them work together, typically with a task scheduler or orchestrator. There is in fact a large amount of software which facilitates task orchestration between devices, both commercial and open source, and their choice is dependent on specific needs of the user. Physical placement in the lab space is of equal importance. Hence, it is paramount to plan properly the placement of each equipment in space, so that samples can be effectively and reliably moved from one device to another, typically *via* a robotic arm.

To enable programmatic interaction with the device, each vendor utilizes specific communication modes, which might not always be compatible with the scheduling software. Nevertheless, the availability of an application programming interface (API) in a device is one of the most important factors to look for. As the name suggests, an API is an interface between the device and the outside world, enabling access to its main functions from external programs (Fig. 2). For example, a thermal shaker might have an API that allows the user to set the temperature, the shaking frequency, and the duration, while a centrifuge might have an API for setting the rpm and the centrifugation duration. In this way, the user can set those parameters with external software (like the

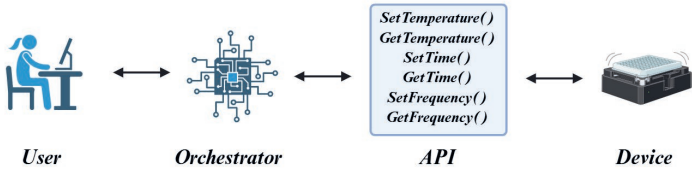


Fig. 2. The availability of a properly documented Application Programming Interface (API) is a key factor for a successful integration of a device into an automated system.

orchestrator), circumventing the need to use its dedicated stand-alone software with a graphical user interface for each device. A good API should not only allow the user to control the instrument but also get status reports from the device (such as idle, running, and error) and recovery options in case of failures. Conversely, when APIs are missing or incomplete, integration may depend on vendor-specific middleware, manual export steps, or the development of custom drivers, increasing both implementation time, costs, and maintenance effort. Drivers' availability is in fact another critical component to consider. As for installing a printer, one needs to install the appropriate drivers on a PC, the same can be applied when incorporating new hardware into a robotic platform, although with slightly different nuances. Hence, while scouting for potential vendors, it is critical to make sure whether a piece of equipment is automation-ready and whether there are already compatible drivers available. While the first requirement is more constraining, the latter can be circumvented with *ad-hoc* driver development, when budget and timelines allow.

3. Common Misconceptions

As a field that has gained significant traction only in recent years, lab automation is often accompanied by misconceptions. While many could be discussed, the following section focuses on those we believe are most frequently encountered.

3.1 *Automation is Autonomy*

An important distinction that needs to be clarified is the difference between automation and autonomy. Automating a process does not necessarily imply that the lab can be autonomous. Even in so-called autonomous systems, routine human supervision and intervention are often still required. Typical examples include loading and replacing reagents and consumables, managing waste, performing maintenance, and troubleshooting errors that the platform cannot recover from automatically. Hence, autonomy is not defined by the absence of humans in the laboratory, but rather by the role humans play in controlling the experimental loop. When humans are involved in decision-making steps, most notably during result interpretation and selection of follow-up actions, we are referring to the so-called human-in-the-loop systems. On the other hand, when one or more applications (typically driven by AI) judge the best next steps in a workflow, based on their interpretation of analytical data, we are referring to closed-loop systems, or self-driving labs. We will provide more examples of both categories in the following parts of this review.

3.2 *Automation Means 'Set and Forget'*

Another common misconception is that lab automation is often seen as a 'set and forget' system. However, devices require regular preventive maintenance and calibration during their lifetime. For example, a liquid handler requires routine checks to ensure that the right amount of liquid is pipetted. Small deviations can go unnoticed until they get bigger, lowering the confidence of the data obtained and putting at risk the validity of experiments. Even 'simpler' devices benefit enormously from preventive maintenance. For example, a plate sealer might decrease its sealing performance over time, resulting in solvent loss during plate storage. Hence, delaying or avoiding maintenance often results in costly consequences that largely impact efficiency and quality. Fortunately, most vendors provide calibration and preventive maintenance workflows and services that help keep downtime to a minimum.

3.3 *Return on Investment is Immediate*

A more subtle aspect concerns the time necessary to have an observable return on investment. In fact, there is typically a 'dead time' between purchasing equipment and obtaining measurable productivity gains. As we have seen in the previous sections, upskilling people, translating existing protocols into automation-ready procedures, integrating the hardware, and testing the workflows requires a considerable amount of time. During this phase, throughput can even temporarily decrease, since routine work continues while the automated method is being developed and validated. As a consequence, automation can be difficult to justify when evaluation is based on short-term metrics, whereas its benefits are more clearly captured over longer time horizons. Accounting for buffer time before the system is up and running is hence of fundamental importance.

3.4 *Automation Ends at the Bench*

Automation should be considered not only as the physical execution of lab work, but also in terms of digital workflows. In more integrated systems, data must flow reliably between instruments and software layers. When data flow is neglected, a new bottleneck is created in which experiments run quickly, but results are transferred, organized, or processed manually.

Even simpler, less connected setups (often centred around a liquid handler) benefit from streamlined data handling, visualization, and analysis. For example, a liquid handler that prepares plates which are then manually loaded into a plate reader can still generate hundreds of data points per day. Working with this volume of results differs substantially from interpreting a small number of manually generated experiments. Simple forms of digital automation can already have a positive impact. In this specific example, automated parsing and visualization tasks can be triggered when new result files appear in a monitored folder of the plate reader, generating standardized plots and summary tables without or with very little manual intervention. Such approaches help ensure that increased experimental throughput translates into immediately usable data rather than fragmented files and *ad-hoc* analyses.

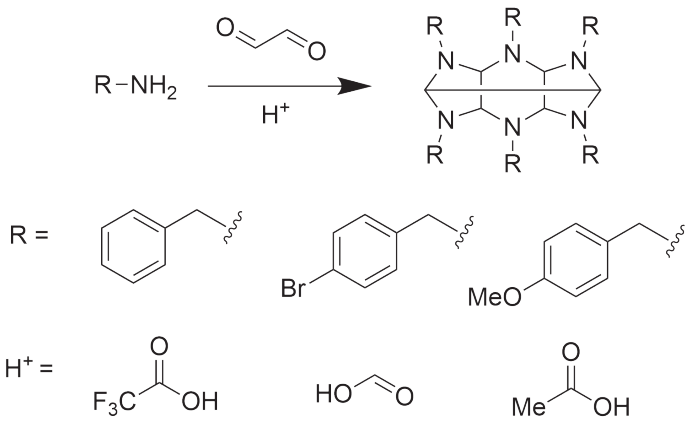
4. Practical Applications

Up to this point, we have mostly focused on best practices and concepts to get started with lab automation. In this section, we will instead present some selected examples of two typical modes of automation: simple stand-alone islands and more connected end-to-end systems.

4.1 *Islands of Automation*

Recent peer-reviewed work demonstrates that automated reaction screening is becoming more accessible, and that useful automation can be introduced without building a fully integrated robotic platform. In practice, the largest benefits often come from automating the most repetitive steps (*e.g.* dispensing, serial dilutions, plate reformatting), as long as the workflow is well defined and the resulting data are handled consistently. For example, Brown and Fedick describe a low-cost workflow in which an automated pipetting robot prepares solutions and spots microliter-scale reaction mixtures onto PTFE-coated glass slides for Desorption Electrospray Ionization Mass Spectrometry (DESI-MS) analysis.[24] The setup relies on dedicated pipetting protocols and custom labware (a 3D-printed slide holder and a labware definition file), while keeping the transfer of the slide to the DESI stage as a manual step. As a demonstration, the platform is used to screen substituted amines and acid catalysts in the condensation reaction leading to the hexabenzylhexaazaisowurtzitane (HBIW) cage precursor, using the MS readout as a rapid indicator of intermediate and product formation, with attention to reproducibility and limited carry-over (Scheme 1). This modular design showcases the power of automation when applied where it is most impactful, without requiring full integration of all devices.

Another example from Gaube and Thomas highlights the use of automated liquid handling in postreaction processing with four case studies.[25] In this approach, automation is deliberately fo-

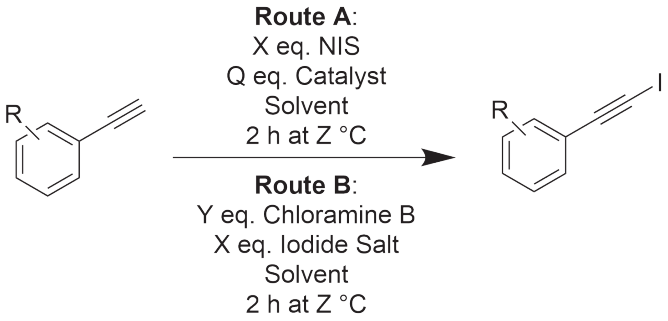


Scheme 1. Synthesis of HBIW cage precursors with different amines and acid catalysts.

cused on repetitive work-up operations: programmed aspiration heights are used to selectively sample organic layers from biphasic mixtures, aqueous washes are implemented with in-vial 'pipette mixing' (aspiration/dispense cycles) to mimic extraction, and crude mixtures are passed through a celite filter plate followed by standardized dilution into analysis-ready plates for gas chromatography-mass spectrometry (GC-MS) or LC–MS. The four case studies cover workflows for Suzuki–Miyaura coupling, Buchwald–Hartwig coupling, Miyaura borylation, and an aqueous wash stability screen of boronated products (to assess degradation during work-up). The authors showed how targeted automation of key, labour-intensive steps can be easily achieved with limited budget and training to accelerate chemical research.

4.2 *End-to-end Systems*

A useful intermediate example between simple applications of automation islands and fully end-to-end platforms is the integration of automated experiment planning with an existing automated synthesis setup *via* a lightweight data interface. Schilter *et al.* demonstrate this by connecting Bayesian optimization to a robotic platform through a custom backend that exchanges reaction parameters and results using a JSON-based protocol.[26] Suggested conditions are translated into robotic actions and executed in standardized fashion in parallel reactors, including automated reagent addition, controlled reaction conditions, quenching, dilution, filtration, and injection into a High-Performance Liquid Chromatography with Diode-Array Detection (HPLC–DAD) setup. In their case study, namely the iodination of terminal alkynes (Scheme 2), three Bayesian optimization algorithms ('optimizers') explored two alternative reaction routes across a parameter space of 12,036 possible condition combinations. Despite the size of this space, the optimizers reached >80% conversion for all substrates within 25 distinct reactions, corresponding to roughly 0.2% of the full space, illustrating how algorithm-driven planning



Scheme 2. Iodination of terminal alkynes with NIS as iodine source (Route A), or with iodide salts and Chloramine B (route B).

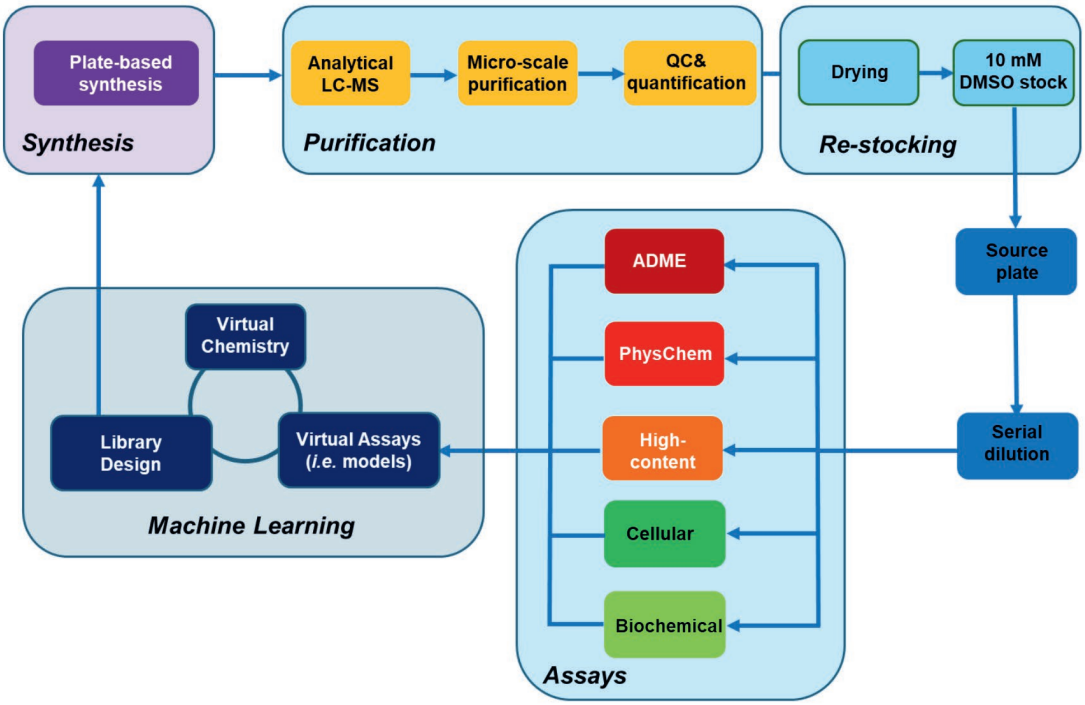


Fig. 3. Schematic overview of MicroCycle, composed of different modules interconnected together in an end-to-end fashion. Adapted with permission from C. E. Brocklehurst, E. Altmann, C. Bon, H. Davis, D. Dunstan, P. Ertl, C. Ginsburg-Moraff, J. Grob, D. J. Gosling, G. Lapointe, A. N. Marziale, H. Mues, M. Palmieri, S. Racine, R. I. Robinson, C. Springer, K. Tan, W. Ulmer, R. Wyler, *J. Med. Chem*. **2024**, *67*, 2118. Copyright 2024 American Chemical Society.

can substantially reduce experimental burden when paired with automated execution and standardized data transfer.

Similarly, MicroCycle represents an end-to-end, integrated automation platform for medicinal chemistry in a pharmaceutical research setting, supporting a design-make-test-analyse (DMTA) cycle (Fig. 3).[27] The workflow combines plate-based microscale synthesis with automated analysis, purification, quantification, and reformatting to generate assay-ready compounds. The resulting compounds are subsequently processed by an integrated module for automated biological and physicochemical profiling, and the data generated are fed into the next DMTA iteration. In a representative project example, iterative cycles enabled potency improvements from 139 μM to 0.22 μM while maintaining high-throughput solubility >0.75 mM and improving log $D_{7.4}$ from 2.0 to 0.8. At the platform level, reported yearly statistics include 81 libraries, 2,744 isolated and registered molecules across 23 projects, and an average of 6.6 data points collected per compound (including 9,393 biological assay data points and 8,850 profiling data points).

5. Conclusions and Outlook

In this perspective, we highlighted that lab automation can be approached effectively by starting from clearly defined, repetitive workflows and translating them into explicit, parameterized steps that are suitable for execution on automated hardware. Key requirements include not only appropriate equipment selection, but also sufficient human and financial resources, robust process definition, and careful integration planning across heterogeneous devices and software ecosystems. Common misconceptions (such as equating automation with autonomy, assuming 'set and forget' operation, or neglecting development time) can hinder adoption if not addressed early, particularly as throughput increases. Finally, examples from the literature illustrate that meaningful benefits can be achieved through modular 'islands of automation' as well as through more connected platforms, with increasing value obtained when experimental execution is coupled to consistent data capture and elaboration across the overall workflow.

Despite the proven advantages, universities often remain anchored to traditional laboratory practices, and only a limited number have updated their training offer accordingly. While traditional chemistry techniques constitute an important basis for a chemist, lab automation becomes increasingly relevant in both academic research and industry environments. There is therefore a growing need to complement conventional chemistry curricula with practical exposure to automation concepts, including basic programming, hardware operation and data handling in high-throughput settings.

In this direction, some institutions have started to expand their educational infrastructure and course offer. In Switzerland, institutions like the University of Zurich, OST, and EPFL have established dedicated teaching activities focused on laboratory automation. Initiatives of this type provide the opportunity for students to gain hands-on familiarity with automated workflows and to develop a skillset that bridges chemistry, engineering, and IT aspects, thereby supporting broader adoption of automation in research laboratories.

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Author Contributions

A. C. was responsible for the conceptualization, drafting, and revision of the manuscript. A. L. contributed to manuscript preparation, review, and revision.

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