

IMP

Automation in Chemical R&D

From Robotics to Closed-Loop Discovery

Industry Intelligence White Paper

Lab Automation

High-Throughput

Flow Chemistry

Digital R&D

B2B INDUSTRY INTELLIGENCE | IMP INTERMEDIAPARTNERS

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01

Executive Summary



Laboratory automation is not about replacing chemists. It is about removing the experimental bottlenecks that prevent chemists from doing the work that requires chemical intuition — which machines cannot replicate.

— IMP Industry Intelligence

Chemical R&D is in the middle of a transformation that will fundamentally change what it means to conduct experimental work. Robotic liquid handling, automated flow chemistry platforms, high-throughput analytical systems, and AI-driven experimental design are converging to create laboratory environments that can run, analyse, and learn from experiments at speeds and scales that manual workflows cannot approach.

Yet automation adoption remains uneven and often underperforms expectations. The organisations realising transformative value are not those that have invested the most in hardware — they are those that have redesigned their experimental workflows around automation capabilities, built the data infrastructure to capture and act on automated experiment outputs, and aligned their scientific culture with the changed role of the human chemist.

10x

throughput increase
reported in leading
HTE implementations

40%

reduction in process
development timelines
with full automation

65%

of R&D labs plan
automation investment
increase by 2026

Sources: Deloitte Life Sciences R&D; Report, Nature Chemistry Automation Review

- 1 High-throughput experimentation and automated condition screening are delivering the clearest and most reproducible value across the broadest range of chemistry applications.
- 2 Closed-loop discovery — where AI systems design experiments, robots execute them, and algorithms interpret results to design the next round — is moving from research concept to commercial reality.
- 3 The primary barriers to automation value realisation are organisational and informatic, not technological: workflow redesign, data architecture, and change management determine outcomes more than hardware specification.
- 4 Vendors communicating through application-focused technical content significantly outperform those leading with platform specifications in R&D purchasing decisions.

02

The Automation Imperative in Chemical R&D

The commercial pressures driving automation investment in chemical R&D are not primarily about cost reduction. They are about speed, throughput, and the ability to explore chemical space at a depth that manual experimentation cannot provide.

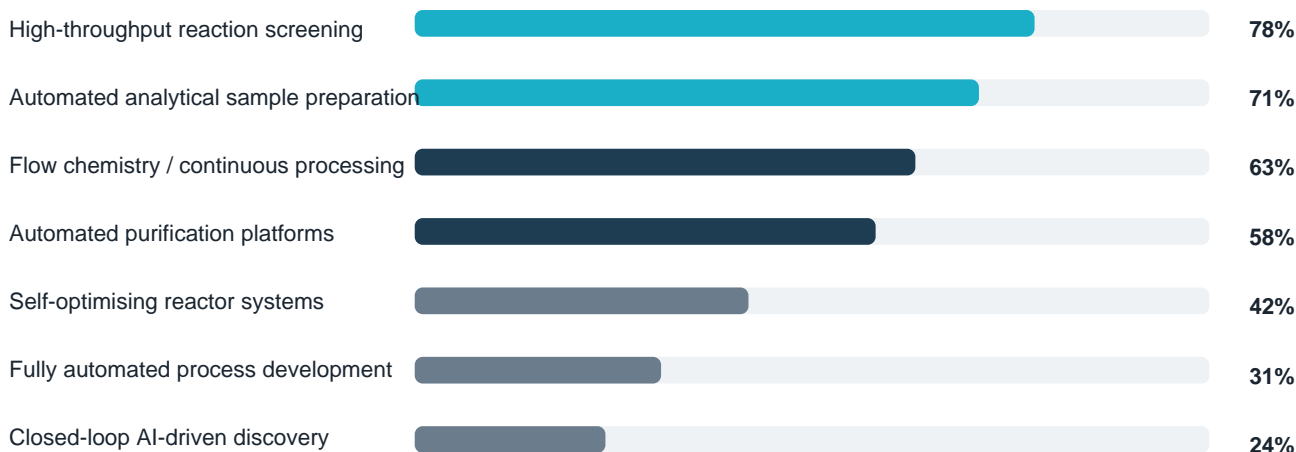
Why Now?

Three converging forces have made 2024-2026 the critical window for automation investment. First, the cost of robotic and analytical hardware has fallen dramatically. Second, the software layer connecting automation hardware to data systems has matured. Third, competitive pressure from organisations that have already invested is beginning to show up in development timelines.

The Throughput Gap

A skilled synthetic chemist can rigorously evaluate 20–30 reaction conditions per week. An automated high-throughput experimentation platform can evaluate 500–2,000 conditions in the same time window. This is not a marginal efficiency difference — it is a fundamentally different approach to chemical space exploration that changes what questions can be asked and answered within a development programme.

Automation Investment Priority by Application



R&D automation investment priority (current or planned) — indicative estimates based on industry surveys 2024

03

Technology Landscape: Platforms and Capabilities

The automation technology landscape spans from discrete laboratory instruments to fully integrated robotic platforms. Understanding the value proposition and operational requirements of each tier is essential for making investment decisions that match organisational capability.

Platform Type	Core Capability	Maturity	Key Consideration
Liquid handling robots	Parallel reaction setup, reagent dispensing	★★★★★	Throughput vs. flexibility
HTE platforms	Miniaturised parallel screening, nano-scale	★★★★■	Data capture integration
Flow chemistry systems	Continuous synthesis, parameter screening	★★★★■	Scale-up translation
Automated HPLC/MS	High-throughput analytical characterisation	★★★★★	Throughput-quality balance
Self-optimising reactors	Real-time feedback, parameter adjustment	★★★██	AI integration required
Robotic synthesis platforms	Multi-step synthesis, library generation	★★★██	Chemistry scope limitation
Closed-loop AI systems	Autonomous experimental design and execution	★★███	Data infrastructure critical

★ = Platform maturity (★★★★★ = widely deployed · ★★★██ = emerging)

Note: While full closed-loop systems remain 'emerging', core components like Bayesian optimization have already reached commercial maturity.

The Integration Layer: Where Value Is Won or Lost

The most significant insight from organisations that have successfully scaled automation is this: hardware is rarely the limiting factor. The software layer connecting automation platforms to structured data environments — enabling the outputs of automated experiments to be captured, organised, and made available for analysis — determines whether automation delivers transformation or simply accelerates the generation of unstructured data that cannot be acted upon.

04

Where Automation Delivers Measurable Value

Automation value is concentrated in specific workflow stages. Organisations that have targeted investment at these high-impact points consistently outperform those that have pursued broad automation coverage.

■ Reaction Condition Screening

The application with the clearest and most consistently documented value. Automated parallel screening of catalysts, solvents, temperatures, and additives in miniaturised format reduces the time and material required to identify optimal conditions by 80–95% compared to manual sequential screening contributing to the overall 40% reduction in timelines mentioned earlier. Critically, it also enables exploration of condition space that manual workflows cannot practically address — identifying optima that would never be found through sequential experimentation.

■ Analytical Sample Processing

Automated sample preparation for HPLC, LC-MS, and NMR analysis eliminates a significant human bottleneck in high-throughput workflows. The throughput limitation in most R&D laboratories is not synthetic — it is analytical. Automated sample handling and injection dramatically improves the analytical throughput that limits the practical utility of high-throughput synthesis.

■ Flow Chemistry Optimisation

Automated flow chemistry platforms enable rapid, systematic screening of reaction parameters — residence time, temperature, concentration, stoichiometry — under continuous processing conditions. The data generated has direct relevance to scale-up, making automated flow chemistry particularly valuable in process development contexts where the gap between laboratory and manufacturing conditions is a critical challenge.

■ Library Synthesis for SAR

For discovery chemistry applications, automated parallel synthesis platforms enable the generation of compound libraries for structure-activity relationship studies at scales and speeds that fundamentally change the scope of chemical space that can be explored. The downstream impact on the quality of candidates reaching development is well-documented across multiple therapeutic areas.

05

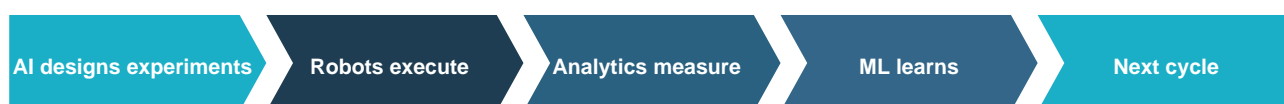
Closed-Loop Discovery: The Self-Optimising Laboratory

The concept of the self-optimising laboratory — where AI systems design experiments, robotic platforms execute them, and machine learning algorithms interpret results to design the next experimental round — has moved from academic novelty to commercial reality. Understanding what this means in practice, and where it is and is not applicable, is essential for R&D strategy.



We ran 1,200 experiments in six days and found a reaction condition that no one in the team would have proposed based on intuition. The system explored a region of chemical space that our mental models told us wouldn't work — and it did.

— Director of Process Chemistry, global pharma company



What Closed-Loop Systems Can and Cannot Do

Capability	Current State	Limitation
Bayesian optimisation of reaction conditions	Mature — commercially deployed*	Defined parameter space required
Active learning for HTE	Mature — widely available	Training data quality critical
Multi-objective optimisation	Advanced — limited deployment	Objective weighting complex
Retrosynthesis-to-execution	Emerging — research stage	Chemistry scope constrained
Autonomous process development	Emerging — pilot deployments	Regulatory acceptance unclear

While the broader framework is emerging, Bayesian optimization within closed-loop AI has matured more rapidly.

06

Integration Challenges and Organisational Barriers

The gap between automation potential and automation reality is primarily organisational, not technological. The barriers that prevent organisations from realising full automation value are well-characterised and addressable — but they require explicit attention.

01 Workflow Redesign Deficit

Automation delivers its full value when workflows are redesigned around automated capabilities — not when robots are inserted into existing manual workflows. The most common failure mode is acquiring high-throughput equipment and using it to run the same experiments that would have been run manually, simply faster.

02 Data Architecture Gaps

High-throughput experimentation generates data at volumes that overwhelm traditional laboratory data management approaches. Without structured data capture, automated annotation, and integration with downstream analysis tools, the data generated by automation becomes a burden rather than an asset.

03 Scientific Culture Resistance

The role of the chemist in an automated laboratory is fundamentally different from the role in a manual laboratory — and this change requires explicit management. Scientists who define their professional identity through bench skills may experience automation as a threat rather than a tool. Organisations that invest in training and role redefinition alongside hardware investment consistently outperform those that do not.

04 Vendor Ecosystem Fragmentation

Most R&D automation environments involve multiple vendors with incompatible data standards, proprietary software layers, and limited integration capabilities. Managing this fragmentation requires either significant internal software engineering capability or explicit vendor partnership strategies that prioritise interoperability.

05 Return on Investment Measurement

Automation investments are frequently justified on throughput grounds but evaluated on cost grounds — a mismatch that creates persistent tension between R&D leadership and finance functions. Organisations that define automation ROI in terms of scientific outcomes — compounds characterised, conditions explored, development timeline compression — make more effective investment decisions.

Industry Signals: Who Is Leading and Why

Large Pharma — Infrastructure Investment

Leading pharmaceutical companies are treating laboratory automation as infrastructure rather than instrumentation — making multi-year, multi-site investments in robotic platforms, data integration layers, and scientist training programmes. The companies achieving the greatest productivity gains are those that have invested in the data and workflow layer with the same rigour applied to the hardware layer.

Biotechs — Speed as Competitive Advantage

Innovative biotechs are using automation as a competitive differentiator, compressing early-stage discovery and process development timelines to outpace larger competitors in specific therapeutic niches. For resource-constrained organisations, automated high-throughput screening dramatically extends the scientific reach of small chemistry teams.

CDMOs — Automation as Service

Forward-looking CDMOs are positioning automated process development capability as a premium service offering, allowing sponsors to access high-throughput experimentation capabilities without capital investment. This model is particularly attractive to mid-size sponsors and creates a meaningful differentiator in competitive CDMO evaluations.

Instrument Vendors — Platform Thinking

The instrument vendors gaining market share are those that have evolved from selling discrete instruments to offering integrated platform solutions — hardware, software, data management, and application support in a configured package. Platform thinking reduces the integration burden for customers and creates stickier commercial relationships.

08

Strategic Questions for R&D Leadership

Effective automation investment requires strategic clarity before hardware selection. These questions address the dimensions most frequently underweighted in automation planning.

Q1

What is the actual bottleneck in your R&D workflow?

Before selecting automation platforms, have you mapped where experimental time is actually spent? Is the bottleneck synthesis, analysis, data management, or decision-making? Automation investments aligned to the actual bottleneck deliver orders of magnitude more value than general-purpose investments.

Q2

What is your data architecture for automation outputs?

High-throughput experimentation generates data at volumes that require structured capture and management. Do you have an ELN infrastructure capable of handling automated experiment data? How will results be linked to compounds, conditions, and downstream decisions?

Q3

How will scientist roles change?

Automation fundamentally changes what chemists spend their time on. Have you explicitly addressed what scientists will do differently in an automated environment? Organisations that invest in role redefinition alongside hardware investment consistently achieve better outcomes.

Q4

What is your integration strategy?

How will new automation platforms connect to your existing laboratory informatics infrastructure? Who owns the integration challenge — internal IT, the vendor, or a systems integrator? What are your requirements for data format interoperability?

Q5

How will you measure success?

Have you defined automation success metrics in scientific terms — conditions screened, development timeline compression, compound library coverage — rather than purely operational terms? Without predefined scientific success criteria, automation investments cannot be properly evaluated.

09

The Communication Gap in Automation Marketing

Laboratory automation vendors face a persistent challenge: R&D purchasing decisions are made by scientists, but vendor communication is typically structured around product specifications that address the concerns of procurement rather than the questions of bench scientists.



I do not buy a robotic platform because of its throughput specification. I buy it because someone showed me data from a real chemistry application that looked like mine, and the results were convincing.

— Senior Process Chemist, European pharmaceutical company

What Vendors Communicate	What Scientists Evaluate	The Gap
Throughput specifications	Performance on relevant chemistry	Specs without context
Platform modularity	Real-world workflow integration	Theoretical flexibility
Software features	Data quality and ELN connectivity	Feature lists vs. data flow
Customer count	Chemistry-specific application evidence	Scale ≠ relevance
Service and support claims	Application scientist quality	Generic service promises

Implications for Vendor and Supplier Communication

Automation vendors that consistently win complex, high-value evaluations share a communication approach: they lead with application evidence, not product specifications. They address the scientific questions their customers are actually asking, and they build credibility through demonstrated chemistry expertise, not commercial claims.

<p>Application-Specific Technical Papers ★★★★★</p>	<p>Detailed accounts of automation performance in specific chemistry contexts — complete with experimental data, comparison with manual workflows, and honest discussion of limitations. These are the content formats that directly address the evaluation questions of scientific purchasers.</p>
<p>Workflow Implementation Case Studies ★★★★★</p>	<p>Accounts of how specific organisations have implemented automation platforms — including workflow redesign, data integration approach, and measured outcomes. The most credible versions include quantified results and honest discussion of implementation challenges.</p>
<p>Scientist-to-Scientist Technical Events ★★★★■</p>	<p>Application seminars, user group meetings, and scientific symposia that create peer-to-peer knowledge exchange around automation. These formats build credibility with scientific audiences in ways that product demonstrations cannot.</p>
<p>Integration Capability Demonstrations ★★★★■</p>	<p>Concrete demonstrations of data integration capability — how platform outputs connect to ELN systems, how data is structured, how it can be accessed for analysis. The growing importance of data architecture in automation evaluation makes this increasingly significant.</p>
<p>Digital Trial Programmes ★★★★■</p>	<p>Structured evaluation programmes that allow prospective customers to apply automation platforms to their own chemistry problems. The willingness to engage in chemistry-specific evaluation demonstrates confidence in application performance and accelerates trust-building.</p>

Strategic Resource Allocation: Investment vs. Expenditure

Implementation of the Content-as-Trust Framework should be viewed as a strategic capital investment in long-term market authority rather than a cyclical marketing expense. The required budget scale is fundamentally driven by two variables: the technical complexity of the underlying solution and the current maturity of the organization's data infrastructure.

While initial pilot phases focus on establishing core technical credibility, full-scale deployment scales proportionally with the breadth of the target audience and the depth of required expert engagement. Organizations typically find that the initial investment is rapidly offset by shortened sales cycles, higher-qualified lead generation, and the reduction of "knowledge-gap" friction in technical procurement.

Outlook and Recommendations

Laboratory automation in chemical R&D is approaching an inflection point. The technology is mature enough to deliver transformative value across a broad range of applications. The organisations that will lead the next decade of chemical R&D productivity will be those that invest now — not just in hardware, but in the workflow redesign, data infrastructure, and scientific culture change that makes automation valuable.

For vendors, the competitive landscape is shifting from hardware performance to application expertise and integration capability. Those that communicate through chemistry evidence rather than specification sheets will define the next generation of the market.

For R&D Organisations

- Map your experimental bottlenecks before selecting automation platforms — align investment to where time is actually lost.
- Build data architecture before or alongside hardware investment; automation without data capture creates noise, not insight.
- Invest explicitly in role redefinition and scientific culture change alongside hardware deployment.
- Define automation ROI in scientific terms — timeline compression, chemical space coverage, candidate quality.

For Automation Vendors

- Lead communication with chemistry application evidence, not platform specifications.
- Develop application-specific technical content for each target chemistry domain.
- Build demonstration programmes that address customers' specific chemistry problems.
- Position data integration capability as a core product value, not an optional add-on.

For B2B Marketing in the Automation Sector

- Audit content against the evaluation questions of scientific purchasers, not procurement.
- Invest in scientist-authored technical content that demonstrates application depth.
- Build event and community programmes that create peer-to-peer scientific dialogue.
- Measure content performance in terms of scientific audience engagement, not reach metrics.

About IMP InterMediaPartners

IMP InterMediaPartners GmbH specialises in B2B marketing and content strategy for complex industrial and technology markets — including pharmaceutical manufacturing, chemical R&D, and laboratory technology.

We help organisations translate technical expertise into market authority through structured demand architecture, knowledge-transfer content, and precision media deployment.

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