IMP

AI in Process Chemistry

Reality vs Hype

Industry Intelligence White Paper

Process Chemistry | AI & ML | R&D Innovation | B2B Communication

B2B INDUSTRY INTELLIGENCE | IMP INTERMEDIAPARTNERS

IMP InterMediaPartners GmbH

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Contents

01

Executive Summary

> ***AI in process chemistry is real — but the gap between technological possibility and practical deployment remains significant. Understanding where value is created, and where it is not, is the critical first competency.***
>
> — IMP Industry Intelligence

Artificial intelligence is reshaping process chemistry — but not in the way most vendor presentations suggest. Across pharmaceutical development, CDMO operations, and specialty chemical production, AI tools are delivering measurable value in specific, well-defined tasks. At the same time, claims of autonomous discovery, end-to-end synthesis planning, and self-optimising laboratories remain largely aspirational.

This white paper cuts through the noise. It maps where AI genuinely improves experimental efficiency, identifies the structural barriers that limit broader adoption, and draws practical conclusions for R&D; organisations navigating investment decisions. Crucially, it also addresses a challenge that receives far too little attention: how companies in this space should communicate about these technologies — to partners, clients, and the market.

>60%	**3–5×**	**<20%**
of pharma R&D teams have piloted AI tools	faster route scouting with retrosynthesis AI	have integrated AI into core workflows

Sources: Industry surveys, Gartner, McKinsey Chemical Industry Report

1. AI delivers clear value in reaction condition prediction, retrosynthetic pathway exploration, and experimental data mining — none of which eliminates the need for skilled chemists.
2. Structural limitations — data scarcity, model interpretability, infrastructure gaps — explain why most deployments remain at the pilot stage.
3. Organisations gaining competitive advantage are those investing in data infrastructure and human-AI collaboration frameworks before selecting AI platforms.
4. B2B communication in this sector is failing to keep pace with technological complexity. Knowledge-driven formats are now essential, not optional.

02

The AI Moment in Chemistry — Setting the Scene

The emergence of AI in chemical research is not a sudden development. The underlying methods — machine learning, Bayesian optimisation, neural network-based property prediction — have been developing in academic settings for two decades. What has changed is the convergence of three factors: dramatically increased computational power, the digitisation of laboratory data at scale, and the commercial availability of AI tools built specifically for chemistry.

The Catalyst for Change

The pharmaceutical industry's response to COVID-19 accelerated digital transformation in R&D; environments at an unprecedented pace. Compressed timelines and remote collaboration requirements forced organisations to rethink how experimental data was captured, shared, and analysed — creating fertile ground for AI tool adoption.

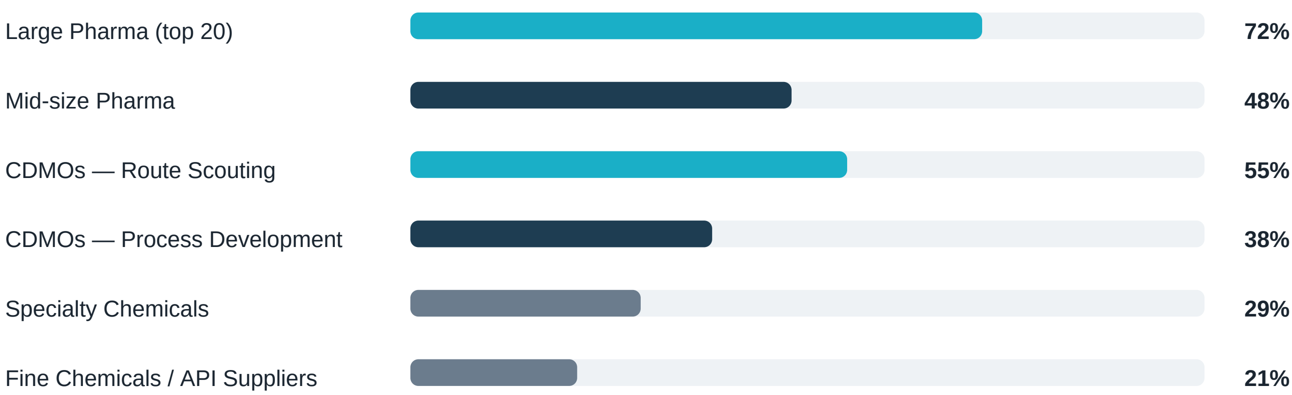
CDMOs — under constant pressure to improve route scouting speed and process robustness — found early-stage AI applications for retrosynthesis and condition prediction directly relevant to their competitive positioning.

Where We Stand in 2025

The current landscape is characterised by a significant gap between the most sophisticated AI deployments — concentrated in a handful of large pharmaceutical companies and well-capitalised startups — and the average adoption level across the broader industry.

Most organisations are in an evaluation or early-piloting phase. The questions being asked are no longer 'Is this technology real?' but rather 'What does it take to make this work in our environment?'

Adoption Maturity by Sector



AI tool adoption rate (pilot or active deployment) — indicative estimates based on industry surveys

03

Technology Landscape: What Is Actually Available

The AI-for-chemistry ecosystem is fragmented across academic tools, commercial platforms, and embedded modules within existing laboratory informatics systems. Understanding these categories is essential for evaluating options without getting lost in marketing claims.

Technology	Primary Capability	Maturity	Typical Application
Reaction Prediction	Predict reaction outcomes & selectivity	★★★★■	Feasibility screening, scale-up risk
Retrosynthesis AI	Identify multi-step synthetic pathways	★★★★■	Route scouting, patent navigation
ML Process Optim.	Suggest improved conditions	★★★■■	Yield and purity improvement
Data Mining / NLP	Analyse literature and internal data	★★★★■	Prior art, competitive intelligence
Lab Automation + ML	Closed-loop experimental cycles	★★■■■	High-throughput screening
Predictive Analytics	Model process robustness at scale	★★★■■	Process validation, DOE
Digital Twins	Simulate entire process environments	★★■■■	Scale-up simulation, risk reduction

★ = Deployment maturity (★★★★★ = widely deployed · ★■■■■ = emerging)

The Vendor Landscape

The market comprises three distinct tiers. At the top sit pure-play AI chemistry companies — firms like Chemify, Iktos, and Insilico Medicine — offering platforms built from the ground up for chemical AI applications. A second tier consists of established laboratory informatics vendors — IDBS, Dotmatics, LabVantage — embedding AI into existing ELN and LIMS platforms. The third tier is open-source and academic tools, including IBM's RXN for Chemistry and the Open Reaction Database ecosystem, which offer high customisability at the cost of vendor support.

04

Where AI Delivers Measurable Value

Cutting through vendor claims requires focusing on evidence. In the areas below, there is consistent, reproducible evidence of value creation — not from isolated case studies but from patterns observable across multiple organisations.

Reaction Condition Prediction	Machine learning models trained on large reaction databases can predict optimal conditions — solvent, temperature, catalyst, stoichiometry — with sufficient accuracy to substantially narrow the experimental space. Instead of exploring 50+ conditions, chemists work from a prioritised shortlist of 8–12. Time savings of 30–50% in condition screening have been documented across multiple pharma settings.
Retrosynthetic Pathway Analysis	AI-driven retrosynthesis tools, now operating with transformer-based architectures similar to those underpinning large language models, can generate credible multi-step synthetic routes within seconds. The value is rapid generation of route options — including routes outside the chemist's immediate knowledge — for human evaluation and selection.
Experimental Data Mining	Perhaps the most immediately deployable application: AI-assisted analysis of historical internal reaction data and scientific literature. NLP models can identify yield-limiting patterns, flag successful condition combinations from past experiments, and surface relevant prior art. Particularly valuable for CDMOs with decades of proprietary process data that remains underanalysed.
Process Robustness Modelling	In late-stage process development, statistical ML models trained on experimental design data can predict process sensitivity to parameter variations — critical information for manufacturing scale-up and regulatory submissions. This application has a clear, measurable impact on development timelines and regulatory risk.

05

Structural Limitations — The Honest View

Any credible analysis of AI in process chemistry must address the substantial barriers that explain the persistent gap between pilot projects and operational deployment. These are not temporary technical glitches but structural characteristics of the domain.

> *The bottleneck is almost never the algorithm. It is the absence of structured, reliable, machine-readable experimental data that the algorithm could learn from.*
>
> — Senior Process Development Scientist, major European CDMO

01 Data Scarcity and Quality

Chemistry generates data at a fraction of the volume available in image recognition or natural language processing. Experimental data is often unstructured, recorded inconsistently, or embedded in PDF reports inaccessible to machine learning systems. Negative results — which carry high informational value for AI training — are routinely not reported.

02 Reaction Complexity

Heterogeneous catalysis, solid-liquid systems, and flow chemistry involve physical phenomena not adequately captured in reaction SMILES representations. Models trained predominantly on homogeneous solution chemistry generalise poorly to the industrial reaction classes where the economic stakes are highest.

03 Interpretability Deficit

Process chemists want to understand why a model recommends particular conditions. Current deep learning approaches offer limited mechanistic interpretability. 'The model predicts this will work' is insufficient in regulated pharmaceutical development environments where decisions require documented scientific rationale.

04 Integration Friction

Most laboratory environments operate on legacy informatics infrastructure. Connecting AI tools to ELN systems, instruments, and LIMS platforms requires significant IT investment and ongoing maintenance that is consistently underestimated in vendor proposals.

05 Regulatory Uncertainty

In pharmaceutical applications, AI-assisted process development decisions touch on regulatory compliance. Guidance from EMA and FDA on AI-generated process recommendations remains evolving, creating risk aversion among compliance-conscious organisations.

06

Integration into R&D; Workflows

AI tools do not operate in isolation — they are embedded within, and derive their value from, the broader R&D; workflow. Understanding where each technology layer connects to the development lifecycle is essential for implementation planning.

Stage	Primary AI Application	Key Benefit	Readiness
Discovery	Reaction prediction · Retrosynthesis	Route option generation	**High**
Hit-to-Lead	Property prediction · Data mining	Candidate prioritisation	**Medium**
Process Dev	Condition optimisation · DOE analysis	Experimental efficiency	**High**
Scale-Up	Robustness modelling · Digital twins	Risk reduction	**Medium**
Manufacturing	Process monitoring · Anomaly detection	Quality assurance	**Low–Med**

The Human-AI Collaboration Model

The most effective deployments observed in practice follow a consistent pattern: AI systems generate candidates (routes, conditions, experimental designs) and humans evaluate, select, and refine. Neither autonomous AI operation nor simple AI-assisted search captures the value available at this interface. Organisations that design their workflows around this collaboration model — rather than treating AI as a black-box recommendation engine — consistently achieve better outcomes.

07

Industry Signals: What Leading Organisations Are Doing

Pharmaceutical Companies

Major pharma companies are moving AI chemistry from innovation labs into core R&D operations. Investment is concentrated in data infrastructure — building proprietary reaction databases — rather than algorithm development. The strategic logic: models trained on proprietary data are harder to replicate than models running on public data.

CDMOs

CDMOs face a distinctive strategic calculation. AI-accelerated route scouting and process development can be a genuine competitive differentiator in client pitches. The most forward-looking CDMOs are positioning AI capability as a service offering rather than purely an internal efficiency tool.

Laboratory Automation Vendors

Instrument manufacturers and robotics companies are integrating machine learning layers into automated laboratory platforms. The self-optimising reactor — capable of running iterative experiments and adjusting conditions based on real-time data — is moving from concept to commercial product.

Data Infrastructure as Competitive Moat

Across the sector, a consistent insight is emerging: organisations that will extract the most value from AI are those building robust data infrastructure now. ELN adoption, structured data capture, and reaction data governance are becoming strategic investments rather than IT projects.

08

Strategic Questions for Decision-Makers

Organisations evaluating AI investments in process chemistry face a set of strategic questions that are rarely addressed in vendor presentations. These questions determine whether an AI initiative generates lasting value or becomes an expensive proof-of-concept.

Q1

Data Readiness

What is the current state of your experimental data infrastructure? Is reaction data structured, searchable, and machine-readable? If not, what is the cost and timeline to reach a baseline from which AI tools can extract value?

Q2

Workflow Integration

At which specific decision points in your development process could AI recommendations change outcomes? Who makes those decisions, and how would AI-generated information be incorporated into existing review processes?

Q3

Build vs Buy vs Partner

Does your organisation have the data science capability to develop and maintain AI models internally? If not, what vendor relationship model — SaaS platform, embedded consultant, academic partnership — best fits your operational model?

Q4

Measurement Framework

How will you measure the value of AI deployment? Cycle time reduction? Experimental hit rates? FTE hours saved? Without predefined metrics, AI investments cannot be evaluated — or defended to leadership.

Q5

Regulatory Readiness

In regulated development environments, how will AI-assisted decisions be documented in regulatory submissions? Has your quality function been engaged in the AI adoption conversation from the beginning?

09

The Communication Gap: Why B2B Messaging Fails

There is a problem in how the chemical and pharmaceutical industry communicates about technological change — and AI has made it worse. Companies deploy increasingly sophisticated capabilities but communicate about them in formats that were designed for an era of simpler product propositions.

> ***We are trying to explain a five-layer technology stack to procurement managers and R&D directors in a banner ad. Something has gone fundamentally wrong.***
>
> — Marketing Director, European Specialty Chemical Company

What Companies Do	What B2B Audiences Need	The Gap
Product feature claims	Evidence of real-world value	No context or proof
Brand advertising	Technical credibility signals	Wrong format entirely
Press releases	Peer-level dialogue	No engagement mechanism
Trade show presence	Decision-relevant information	Timing mismatch
Sales collateral	Independent validation	Perceived bias

Why Traditional Formats Fail in Technical B2B Markets

The challenge is structural. Chemical R&D; decision-makers are highly educated domain experts who can immediately identify shallow content. In a market where the technology is genuinely complex, marketing messages that oversimplify destroy credibility rather than building it.

The buying process for technology solutions in this sector is long, involves multiple stakeholders (R&D; leadership, IT, procurement, regulatory affairs), and depends heavily on trust built through repeated, substantive interaction. A single well-timed advertising campaign alone does not build this trust. Sustained demonstration of expertise does.

10

Implications for B2B Communication Strategy

Organisations communicating in complex technical B2B markets need to rethink the relationship between marketing and knowledge transfer. In the AI chemistry space, these two functions are not distinct activities — they are the same activity.

Industry Briefings & White Papers ★★★★★	Structured analytical documents that contextualise technology developments for senior decision-makers. Effective when they address genuine pain points rather than product features. The format signals intellectual seriousness and provides a reason for repeated engagement.
Technical Roundtables & Expert Panels ★★★★■	Formats that create peer-to-peer dialogue rather than vendor presentations. High trust-building value when participants include independent voices. Generate content that can be repurposed across multiple channels.
Expert Interview Series ★★★★■	Long-form conversations with practitioners that demonstrate depth of understanding without promotional framing. Particularly effective for CDMOs and technology vendors seeking to establish technical authority.
Webinar Formats (Substantive) ★★★■■	Not product demonstrations — substantive technical discussions of industry challenges. Work best when combined with interactive elements and made available as on-demand content.
Targeted Digital Campaigns ★★★■■	Precise audience targeting through specialist trade media and LinkedIn remains effective for awareness — but requires compelling content to achieve engagement. The bottleneck is content quality, not distribution.
Case Studies with Quantified Outcomes ★★★★★	The most credible format in technical B2B markets — but chronically underutilised due to confidentiality constraints. Even anonymised case studies with specific metrics drive significantly higher engagement than generic claims.

The Content-as-Trust Framework

IMP InterMediaPartners has developed a practical framework for organisations navigating this challenge: a structured three-phase approach moving from awareness to authority to qualified lead generation. In Phase 1, content establishes market presence and signals domain expertise. In Phase 2, deeper formats — briefings, roundtables, expert series — build trust with specific audience segments. In Phase 3, targeted activation converts established trust into measurable commercial engagement.

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.

11

Outlook and Recommendations

The trajectory of AI in process chemistry is clear: over the next five to seven years, AI-assisted decision-making will= become standard across the R&D workflow. Organisations that position themselves now — investing in data= infrastructure, building internal AI literacy, and beginning genuine evaluation of the available tools — will have a= structural advantage over those that wait for the technology to mature further.

But the technology story alone is insufficient. The organisations that will shape industry dialogue — and through= that dialogue attract the partnerships, talent, and commercial relationships that drive growth — will be those that= communicate with clarity, depth, and genuine expertise.

For R&D Organisations

- → Prioritise data infrastructure investment before AI platform selection.
- → Define clear use cases with measurable success criteria before deployment.
- → Design workflows around human-AI collaboration, not AI replacement.
- → Engage regulatory functions from the start in AI adoption planning.

For Technology Vendors & CDMOs

- → Replace feature-based marketing with evidence-based communication.
- → Invest in independent validation — case studies, peer-reviewed publications, third-party audits.
- → Use knowledge-transfer formats to reach technical decision-makers.
- → Build sustained content programmes rather than campaign-based activation.

For B2B Marketing Functions

- → Audit current content against the genuine information needs of your technical audience.
- → Develop a structured content architecture aligned to buying stages.
- → Invest in editorial quality — chemistry audiences will read long-form content if it is genuinely informative.
- → Measure engagement depth, not just reach.

About IMP InterMediaPartners

IMP InterMediaPartners GmbH is a B2B marketing and content strategy firm specialising in complex industrial and technology markets — including chemical R&D;, pharmaceutical manufacturing, 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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