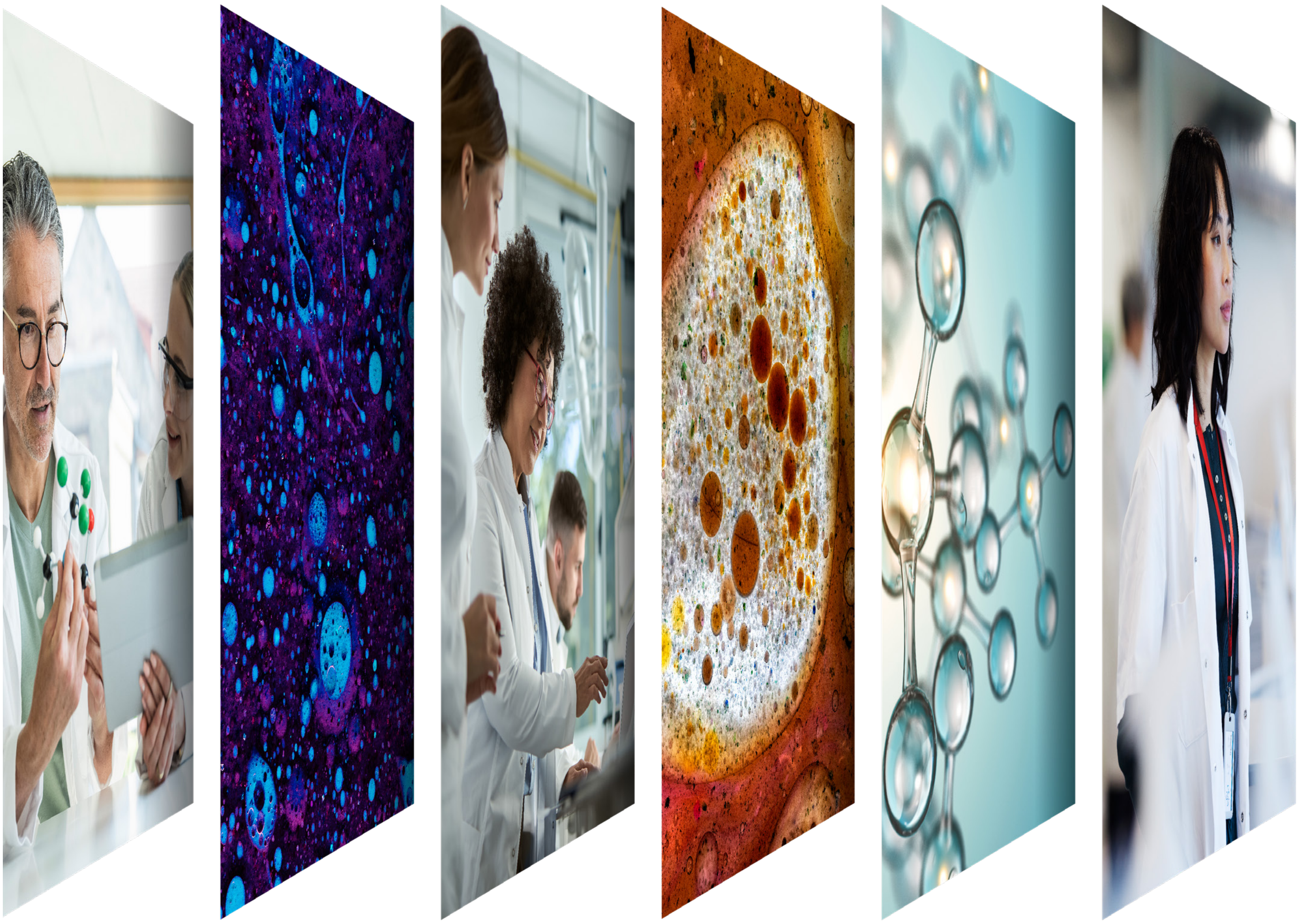
Reaxys

The *hidden costs* of chemistry workflows

And how AI can help



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Advancing human progress together

Contents

It's time to replace fragmented workflows with intelligent, chemistry-aware platforms that unify substance, synthesis, literature and patent data — reducing cognitive friction and enabling deeper, faster discovery.

Executive summary

Academic chemists today are under pressure from growing expectations and shrinking time. Increased global research output and fierce competition for funding intensify the push to publish, patent and collaborate more than ever. Yet despite unprecedented access to data, discovery workflows remain fractured, and researchers increasingly find themselves navigating inefficiencies instead of insights.

On average, chemists lose up to **9 hours** per week: the equivalent of **22 working days** per year[1], looking for and verifying information across multiple tools. This structural bottleneck directly impacts research momentum, novelty validation and grant competitiveness, yet these losses often go unnoticed. Chemists remain confident in their patchwork of tools, under a cognitive illusion that their current process is as efficient as it can be.

In this environment, AI is not a luxury, but a necessity. Forward-looking labs are no longer accepting business-as-usual inefficiencies. They're replacing fragmented workflows with intelligent, chemistry-aware platforms that unify substance, synthesis, literature and patent data — reducing cognitive friction and enabling deeper, faster discovery.

This paper explores why fragmented systems are no longer sustainable in academic research and how modern AI tools, when thoughtfully integrated, are reshaping what's possible in chemistry.

We demonstrate how unified platforms can help researchers reclaim time, surface overlooked insights, and advance both academic excellence and institutional success.

By focusing on the real challenges researchers face, from wasted time to lost momentum, we explore how AI-powered tools can transform traditional chemistry workflows for institutions that want to lead, not lag, in the next era of scientific discovery.

Chapter 1

Data overload and workflow fragmentation

Chemistry has reached a turning point. The issue is no longer access to data. In fact, today's researchers are inundated with information, from data on reactions, to pathways, substances, patents and more.

The bottleneck is not access to this wealth of information, but navigating how to manage, integrate, and extract meaningful insights from a mass of fragmented data. What should be a golden age of data-driven discovery too often becomes an exercise in intellectual triage: sorting, switching, duplicating and second-guessing.

The data overload challenge

Chemistry researchers are overwhelmed with a huge volume of datasets from multiple sources, all stored in different places. For a single investigation, a chemist could work with substance properties, reaction data and conditions, bioactivity data, spectra, and text from journal articles, books and patents, to name just a few. This information rarely sits in a single home. Instead, it is scattered across disconnected databases, bespoke lab notebooks, cloud storage, literature platforms, and local software tools.

A chemist may find a reaction condition in one database, substrate properties in another, and related synthetic pathways in a third. Stitching these fragments together is a manual, time-consuming effort, often involving repetitive searches and cross-referencing between incompatible interfaces.

Valuable research time is squandered with this fragmented approach, and mission-critical insights risk being missed entirely.

Cognitive friction: the daily strain of switching between tools

The challenge is not only data fragmentation but also workflow fragmentation, as chemistry researchers regularly switch between various disconnected tools.

Consider the modern chemistry student's approach: they might start with a simple keyword search on Google Scholar or a basic database query (unaware of more advanced structural searches which they could use). In practice, researchers often perform three or four separate searches in sequence; a quick literature keyword query, then a manual lookup of compound properties, followed by a search in a chemistry database, and perhaps a separate patent search, all before getting the full picture for a single investigation[2].

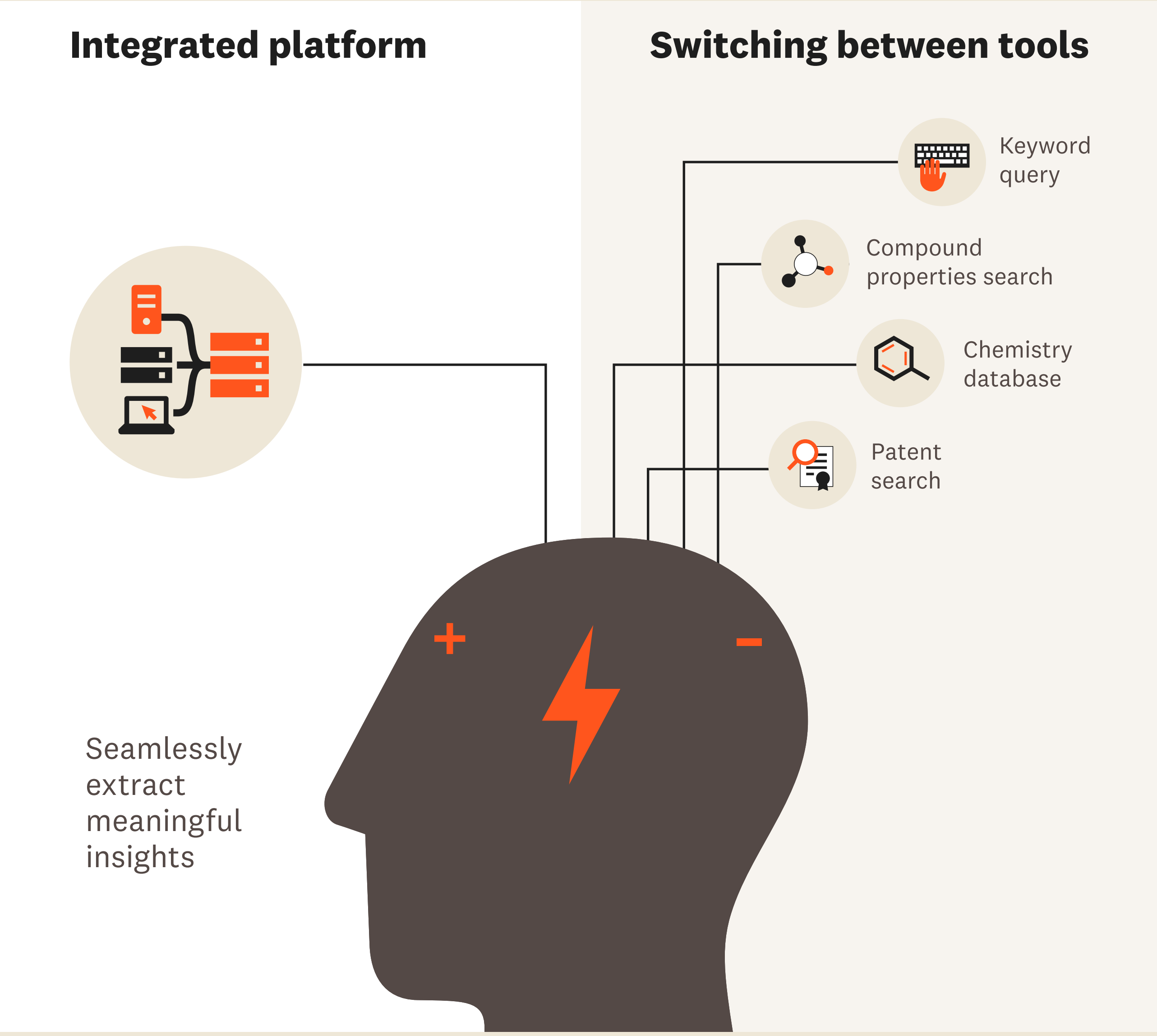
As one senior faculty member observed, students frequently just "look up compound names and synthesis routes" without realizing what more sophisticated, integrated tools could offer[2].

Each new tool requires context switching: reorienting one's thinking, adapting to different user interfaces, and manually transferring data to the next platform. In reality, every context switch carries a cost. Fragmented workflows create cognitive friction, a well-documented phenomenon where frequent task changes reduce concentration, memory, and overall productivity.

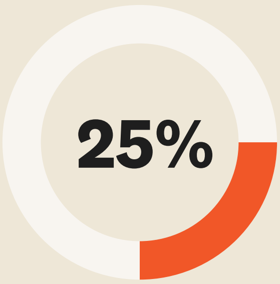
Research shows that such task switching can reduce memory recall by up to **25%**[3] and consume as much as **40%** of productive time[4].

These are not edge cases: they are structural faults embedded in how discovery is done.

Fragmented workflows create cognitive friction



Task switching can **reduce memory** recall by up to



Task switching **consumes** as much as

of **productive time**

The real cost of complexity: innovation impeded

Many chemists don't realize how much is slipping through the cracks in their current workflows. They've built workarounds by manually stitching tools together, transferring data, redoing searches, bouncing between interfaces and adapted to the friction. But that very adaptation has created a false sense of control: a "cognitive illusion" of efficiency.

However comforting this illusion of efficiency may be, the impacts are all too real. Researchers report losing about **19%** of their week searching for information across multiple platforms[5]. That equates to nearly one month every year lost to non-experimental tasks, when that time could be better spent designing and executing experiments, or interpreting the results.

Ultimately, the toll is deeper than hours. Fragmented workflows reduce reproducibility and complicate collaboration, as data and insights are trapped in isolated silos or personal workflows. This fragmented way of working slows the very research that leading institutions are relying on to attract funding, advance innovation, and drive success.

This cognitive illusion of efficiency leads many researchers and labs to operate as if these costs are unavoidable, but they're not. They're the result of outdated systems being used in a new era of research. These workflows are stuck in manual, disconnected processes that can't keep pace with the demands and complexity of modern science.

Forward-looking institutions are beginning to confront this disconnect.

They're no longer asking, "How do we make current systems work better?"

They're asking, "Why are we still relying on systems that hold us back?"

The answer is clear: if chemistry is to keep pace with its own ambitions – in speed, in innovation, in sustainability, in impact – the way researchers discover must fundamentally change. Leading institutions must look beyond patching old systems, and adopt truly integrated AI platforms that meet the needs of modern research.

Chapter 2

Navigating novelty in chemistry innovation

A fundamental challenge for today's chemistry researchers lies in confidently establishing the novelty of their discoveries. Demonstrating that a new compound, synthesis route or methodology is truly original requires a deep knowledge of the published academic literature, including the complex patents landscape. However, patents currently represent a significant gap in the workflow for many chemistry researchers.

A missed opportunity

Despite containing crucial information, researchers admit they rarely explore patent data, either because they're uncertain where to look or because existing interfaces are too complex to navigate efficiently. Only 22% of chemists surveyed said they consistently review patent data when designing new synthetic routes[2].

Yet patents can reveal reactions not found in academic literature, surface competitive intelligence, and provide early signals of innovation direction, all of which are needed when assessing novelty.

Too often, researchers discover late in the process that a route has already been published or patented. This is a frustrating and recurrent obstacle for chemists, and one that reflects a deeper problem.

> As one doctoral researcher puts it, "Because I missed information across multiple platforms, I only discovered after months of work that someone had already published the same compound" (Synthetic Chemist and PhD Scholar)[2].

This scenario highlights a crucial mindset challenge: chemists often feel they've been thorough, until a missed reference proves otherwise. It's a stark example of cognitive illusion in action. The false sense of security afforded by manual, fragmented searches can lull researchers into thinking all bases were covered, when in fact critical leads were hiding in overlooked sources.

A new solution

When patents are excluded from chemistry searches, the result can be duplicated effort, missed opportunities, and gaps in novelty assessment. By contrast, integrated, AI-powered tools can help make patent data not just searchable, but genuinely usable — turning an underused resource into a strategic advantage, and helping to ensure that months of work aren't derailed by something that was knowable from the start.

AI-powered tools make patent data more accessible by connecting structural queries with experimental precedents, reaction conditions and jurisdiction-specific filings.

As a result, researchers can now assess novelty earlier, reduce duplication and design experiments that are both strategically and scientifically informed.

> *A recent study demonstrates that large language models (LLMs) can mine chemical patents to extract 26% more reaction data and correct errors present in manually curated datasets.*[6]

Chapter 3

AI-powered search aligned with the chemistry mindset

Traditional search systems require chemists to translate their questions into ultra-precise queries, relying on exact keywords and Boolean logic. This forces researchers to think like computers, often needing multiple query reformulations to gather information.

These searches potentially omit critical information and data points because of syntax errors or missing and inaccurate keywords. The impact of this goes beyond frustration and wasted time: ultimately, it can cause researchers to overlook essential insights, impacting the accuracy and efficiency of their work.

Beyond keywords: semantic understanding

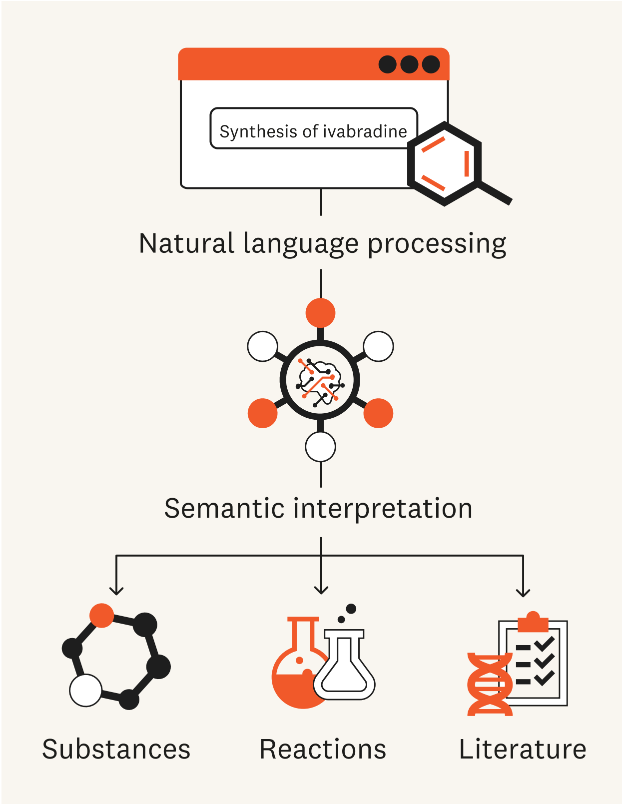
In contrast, AI tools built specifically for chemists are transforming how they search – making it faster, more intuitive, and more aligned with how researchers naturally think.

Not all AI tools offer the same transformative benefits for chemistry searches. AI designed with chemists in mind, with a deep level of chemistry awareness, can be game-changing in unlocking the insights that generic AI tools simply can't provide.

Moving beyond rigid text queries, AI-enabled search that understands chemical context and structure, allows chemists to ask complex questions effortlessly and uncover richer insights from literature, structures and patent data.

With natural language search and intelligent ranking, researchers can explore complex topics and receive precise, relevant results. As this chemistry-specific technology evolves, AI-based natural language search is being developed to interpret queries which are open-ended, using everyday phrasing, like "synthesis of ivabradine", instead of researchers needing to build a complex query using keywords and Boolean logic.

These natural language queries will be able to return ranked results that meaningfully connect substances, reactions, and literature, because AI has interpreted the intent behind the query (for example, is the user doing a background search, or exploring a synthesis need?) and prioritized the right results for the user.



Ultimately, AI-enabled search means researchers can put less effort into their search queries, and have more confidence in the results. This reduces the trial-and-error loop, freeing chemists to focus on analysis rather than syntax.

Structure-aware discovery

One of the most powerful applications of AI-enabled search in tools designed specifically for chemists is the seamless integration of text-based and structure-based queries, so researchers don't have to choose between ease and precision. Modern platforms allow seamless toggling between name-based or drawn molecule queries, letting researchers move from a scaffold search to related literature and back again in one continuous flow.

> *"Students begin with simple keyword searches, but once shown how to use structure filters, they find better, more relevant results."* [2]
>
> **Senior Faculty and Researcher**
> in Nucleic Acid Chemistry

Fragmented workflow
(Traditional)

Tool 1: Name-based search

↓

Tool 2: Structure editor

↓

Tool 3: Literature database

↓

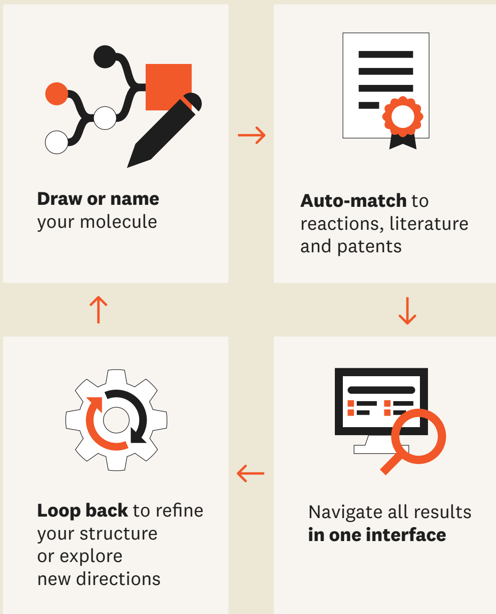
Tool 4: Patent search

↓

Manual Notes/Export

Disconnected tools. Repetitive queries. Slow decisions.

Seamless workflow
(Modern)



Better search for better science

Traditional search platforms often prioritize broad access to information over relevance, leaving researchers to manually filter high-volume results, re-verify data across sources, and navigate siloed patent archives. This manual overhead reduces both the speed and precision of scientific inquiry, particularly when novelty validation is at stake.

By contrast, AI-driven search systems for chemists that combine semantic understanding, structure recognition, and intelligent ranking can deliver results that are context-aware and decision-ready. Instead of just returning more data, these platforms help chemists surface the right data – and do so faster, with more confidence.

> The result isn't just better search. It's better science: more reproducible workflows, reduced rework, and greater agility in both academic and applied research settings.

Chapter 4

How AI transforms route planning

Traditional route planning in chemistry can be a lengthy manual process with a trial-and-error approach, often lacking critical contextual insights like cost, safety, and sustainability. AI-powered retrosynthesis technology can transform this workflow by providing faster, data-driven guidance that incorporates these important factors, enabling chemists to design more efficient, safer and greener synthetic routes, quickly and easily.

From days to hours: accelerated route planning

Predictive retrosynthesis tools dramatically accelerate planning. Comparing hundreds of reactions manually once took days or weeks, but can now be done in minutes.

Advanced algorithms can rapidly analyze thousands of known reactions, evaluate multiple synthetic pathways simultaneously, and rank viable routes based on predicted yield, selectivity, cost, and safety considerations.

Predictive technologies can suggest optimal routes, flag greener or safer alternatives, and help chemists evaluate trade-offs up front, thereby reducing uncertainty and rework. This shift not only saves time but also opens up new possibilities for more sustainable, high-impact chemistry.

Real-world results

Academic and industrial researchers alike are seeing tangible results from these new technologies. At the University of Wrocław, PhD researchers are using retrosynthesis tools to explore synthesis routes that haven't even been published yet. Their work, focused on impurity profiling for active pharmaceutical ingredients, shows how AI can support cleaner, more efficient research from the outset.[7]

In one industrial case, researchers shortened a seven-step synthesis to just four [8], saving valuable time and resources. These tools also highlight alternative reagents, cheaper precursors, or lower-energy pathways, reducing both cost and risk.

These examples are not outliers, but signals that a better chemistry approach exists, and that teams willing to challenge traditional planning workflows can achieve more with fewer resources.

Before vs. after transformation

Traditional approach	AI-enhanced process	Outcomes for chemists
Manual literature search (2-3 days)	Automated route suggestions (minutes)	Frees up hours of work and accelerates the start of experimental planning. Researchers can explore more options in less time, without sacrificing depth.
Sequential route evaluation	Parallel pathway comparison	Enables chemists to evaluate multiple viable synthesis paths at once — helping them identify the most efficient, cost-effective, or sustainable option early.
Limited precedent analysis	Comprehensive database mining	Reduces the risk of missing critical prior work, improving novelty validation and grant-readiness.
Reactive optimization	Predictive condition recommendations	Shifts synthesis from trial-and-error to insight-driven planning.

Integration with experimental design

The most advanced AI systems go beyond route suggestions, to support full experimental design — from sourcing reagents to recommending optimal conditions and flagging regulatory or safety risks. This is an even smarter way to plan chemistry, freeing up researchers to focus on strategy, creativity, and scientific insight.

The shift from traditional synthesis planning to AI-enhanced workflows isn't just about speed, but also about confidence. Researchers no longer need to rely on fragmented searches or sequential guesswork. AI systems now surface literature and patent data, propose alternative routes, and even recommend likely reaction conditions – all within a unified, chemistry-aware environment.

For academic labs under time constraints and publication pressure, this transformation enables better decisions earlier. It reduces false starts, accelerates validation, and helps ensure the research being planned is not only feasible, but fundable and novel.

Practical implementation success stories

At pharmaceutical company Shionogi, researchers used the Computer-Assisted Synthetic Planning (CASP) system developed by the cheminformatics company CDI (Chemical Design Inc.) in partnership with Reaxys to develop a new synthesis that resulted in "a shorter, greener, and more efficient synthesis route compared to the benchmark route filed in a patent." [9]

This demonstrates how AI-powered green chemistry tools translate directly into measurable improvements in both sustainability and efficiency.

The practical value can be demonstrated across diverse research environments. One pharmaceutical company reported using AI tools to identify greener synthetic routes that reduced solvent usage by 40% while improving overall yield.[10]

Academic institutions are embedding these capabilities to help researchers align projects with institutional sustainability commitments and develop competitive grant proposals.

OECD's sustainable chemistry framework stresses "designing chemicals with reduced hazard potential and production routes that consume fewer resources." AI makes these principles actionable at the laboratory level.[11]

> *"This technology can accelerate and facilitate route scouting exercises by providing overviews of routes avoiding halogenated solvents and reagents… A distinguishing feature of this tool is the possibility to select routes that maximize the use of renewables and/or reagents that can be easily derived from renewables."* [9]
>
> **Senior Scientist II**
> Nutritional Products, DSM-Firmenich

Chapter 5

The librarian lens

The librarian lens: enabling institutional AI adoption

The way chemists are trained is evolving because the demands of industry are evolving too. Today's chemistry students are entering a profession that expects more than technical knowledge: they must be able to navigate digital research ecosystems, work with predictive AI tools, and collaborate across disciplines.

Institutions that treat AI fluency as optional risk leaving their graduates behind. That's why leading institutions are embedding AI-powered tools into undergraduate and graduate curricula – not just to teach the how, but to explore the why. From undergraduates learning to run structure-aware searches, to PhD candidates using predictive retrosynthesis in thesis work, AI is moving from optional skillset to core competency.

Librarians often lead the charge when it comes to successful AI adoption, serving as bridges between technology capabilities and research needs. Their unique position makes them essential partners in transforming how institutions (and their students) approach AI-powered chemistry research.

The librarian's strategic role

The interdisciplinarity of modern research requires AI tools that enable smooth collaboration between chemists, data scientists and librarians. At many institutions, librarians serve as AI literacy champions, training faculty and students in new tools, curating institutional metadata and helping align systems.[7] Modern platforms, with unified interfaces and customizable search layers, support this alignment by reducing rework and communication breakdowns.

Increasingly, global publishers like Elsevier are supporting librarians with targeted professional development around AI. Their Library Connect Academy offers peer-developed courses in GenAI literacy, project management, and data-driven impact. These programs offer librarians tools and resources to help them better serve their communities, not just as enablers of AI, but as strategic AI leaders within research institutions.

These programs also underscore a broader industry recognition: empowering librarians with GenAI fluency is essential for responsible and effective AI integration at scale.

Using GenAI responsibly in research and education

As GenAI tools become part of everyday academic work, institutions face new questions: What tasks are safe to automate? How do we ensure ethical use of AI tools? And how do we guide students through it all?

Elsevier's Responsible AI Principles offer a clear foundation focused on fairness, transparency, and accountability.

For educators, librarians and research leaders, building AI literacy and responsible usage is becoming part of day-to-day work. From crafting prompts to evaluating GenAI outputs, students are asking for guidance – and institutions that provide it will be ahead of the curve.

To support this shift, Elsevier has also launched a free GenAI Literacy Program for Librarians, equipping them with practical frameworks to assess AI outputs, mitigate bias, and ensure ethical use. These resources are part of a growing GenAI Hub for librarians, bridging the gap between technical innovation and academic integrity.

For institutions already navigating GenAI adoption, such external resources complement internal AI literacy strategies and provide ready-made materials for onboarding, training, and policy development.

If your team is evaluating new tools, this practical guide to selecting GenAI can help. It breaks down what matters most: transparency, trust, and fit for purpose.

Key responsibilities in AI integration

Training and skill development: Often, the biggest barrier isn't the tool, it's just knowing what's possible. Institutions that offer hands-on support see better adoption and outcomes.[2] In surveys, users who received just a short walkthrough were twice as likely to use advanced features like retrosynthesis and patent mining.

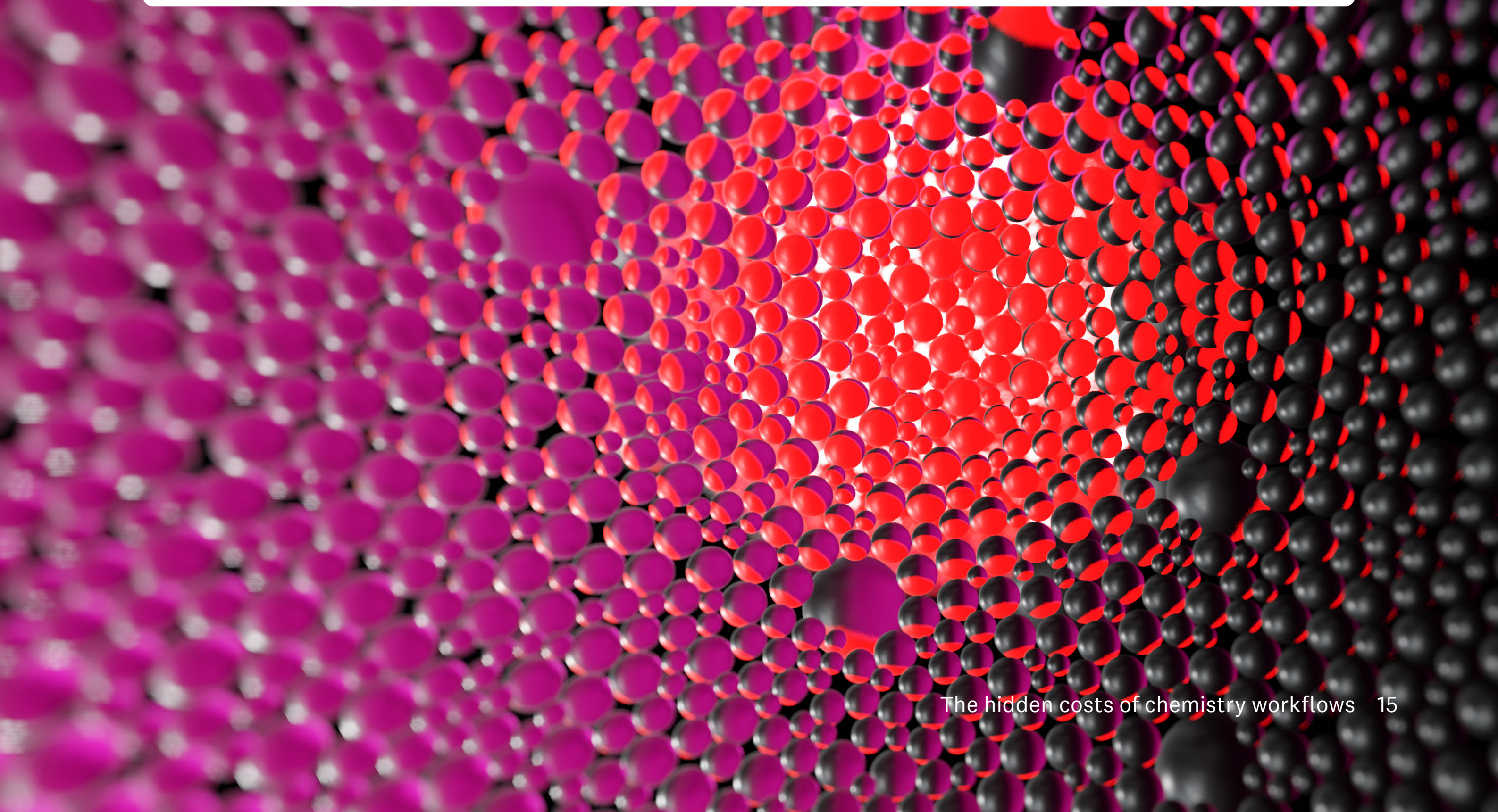
Data quality stewardship: AI systems are only as good as the data they process. Librarians ensure institutional data quality through careful metadata management and database curation.

Cross-departmental coordination: Librarians coordinate AI tool adoption across departments, reducing platform fragmentation and ensuring consistent approaches throughout the institution.

Measuring impact and success: Researchers and librarians at leading institutions report significant productivity improvements. Users save about three hours a week just by reducing the time spent switching between systems.[7,12] They also praise the intuitive visuals and search hierarchies, which help them get to relevant results faster.[12]

A senior professor at the University of Milan noted that modern AI-powered platforms serve "as cost- and time-efficient tools that support both teaching and research needs effectively."[2]

Success factors: The most successful implementations combine technical capability with human support. Librarians who understand both the technology and the research culture can dramatically improve adoption outcomes.



Chapter 6

From insight to action

The real power of integrating AI into chemistry workflows lies in how it allows researchers to focus on what really matters. Whether it is streamlining literature reviews, accelerating synthesis planning, or surfacing sustainability insights, AI works best when it quietly removes friction in the background, allowing scientists to work smarter, not harder.

But impactful AI integration doesn't happen by accident. It takes thoughtful alignment between people, processes, and platforms.

What does effective AI integration look like?

Modern chemistry research demands clarity, reproducibility, and strategic decision-making. The most effective AI-enabled environments support these needs through several key features.

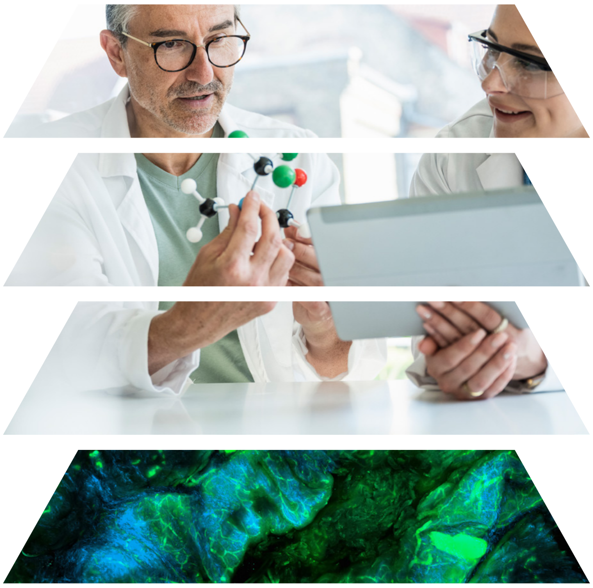
Firstly, they are **integrated** – seamlessly connecting reactions, substances, properties, patents, and literature in a unified view.

They're also deeply **intuitive**, designed to align with how chemistry researchers naturally think and work, minimizing cognitive friction.

Furthermore, these platforms are **predictive**, offering not just data, but practical, useful insights on optimal synthesis routes, greener alternatives, and better reagents.

Flexibility is another crucial factor: the most effective AI tools are designed to fit into existing digital ecosystems and integrate easily with design tools, ELNs, and AI agents.

Finally, they are **aligned with institutional goals** in supporting sustainability, reproducibility and strategic impact, to help institutions drive innovation responsibly and efficiently.



What to look for in a modern chemistry platform

Selecting a research platform today is a strategic decision; one that directly shapes discovery velocity, reproducibility, and competitive positioning.

Chemists need AI-powered systems that streamline synthesis planning, integrate literature and patents, and reduce the cognitive overhead of disconnected workflows. This is more than just technology. This is infrastructure for better science, and it calls for:

Unified insight architecture: Literature, reaction data, substances, and patents should be accessible in a single discovery flow — not across multiple interfaces.

Intelligent, chemistry-aware search: Platforms should accommodate both natural language queries and structure-aware exploration, delivering context-rich results, not raw volume.

Predictive and sustainable retrosynthesis: AI should support faster route design while enabling greener, safer alternatives — aligning scientific impact with ESG goals.

Transparent and interoperable: Outputs must be explainable, sources traceable, and tools integrable with ELNs, molecule design platforms, and AI agents.

To truly embed AI into chemistry research culture, institutions must go beyond tool access. Success hinges on thoughtful onboarding, cross-role collaboration, and alignment with institutional goals like sustainability and reproducibility. That means investing in researcher training, encouraging responsible AI use, and continuously evolving discovery workflows based on feedback.

A new era of AI-powered chemistry research

The role of AI in chemistry is growing and evolving. Where it once helped researchers search a little faster or plan a little more efficiently, it's now becoming a real partner in discovery. Intelligent systems are learning to think more like chemists: spotting patterns, suggesting better routes, even flagging greener alternatives that might have been overlooked.

Emerging AI agents are being designed to plan synthesis routes, critique them, suggest refinements, and predict how molecules might behave — all before any lab work begins. The goal isn't to take scientists out of the loop. It's to give them back time, clarity, and confidence, especially when the stakes are high and the questions are complex.

In the near future, chemistry platforms will offer:

- AI agents for route design and retrosynthesis critique
- Predictive tools for bioactivity, off-target effects, and material properties
- End-to-end automation across synthesis planning, reaction conditions, and green chemistry optimization

But the real transformation isn't just technical. It's cultural. Institutions that prioritize AI literacy, integrate intelligent tools thoughtfully, and build transparent, explainable workflows will lead the next era of chemistry. They won't just publish more. They'll discover faster, collaborate better, and make chemistry more sustainable and reproducible by design.

AI in chemistry is no longer an emerging idea. It's a defining capability. The question is no longer if it belongs in your research environment — but how soon you can put it to work.

Institutions that treat AI as infrastructure, not just innovation, will be best positioned to lead in this next era of chemistry.

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