Reaxys Value Proposition Corporate

Audience

Roles: Synthetic, medicinal, organic, computational, process, polymer, inorganic, analytical, environmental and materials chemists; researchers, engineers, scientists, specialists, analysts, technologists and technicians
Senior job titles: Managers, seniors, principals, heads, leads, leaders, directors and VPs in R&D, drug discovery, chemistry and innovation
Companies: Pharmaceutical, CRO, chemical, agrochemical and related industries

Internal Statement/value statement

For chemists in pharmaceutical and chemical R&D, Reaxys provides comprehensive, diverse and trusted data, seamless in-house data integration and AI tools to optimize chemistry workflows. Advanced analytics on over a billion chemistry and bioactivity data points enable quick, critical insights for informed decision-making throughout the innovation process.

Customer Context (Internal)

Chemists in both pharmaceutical and chemical R&D are expected to accelerate innovation, reduce development costs and meet evolving expectations around sustainability and competitiveness.

The main challenges they need to address are:

- **Accelerate time to market and reduce the cost** of research and development, which includes streamlining the design-make-test-analyze (DMTA) cycle, overcoming fragmented or incomplete data sources, and breaking down data silos that slow research workflows.
- **Discover and implement new approaches**, including more sustainable methods, and efficiently select optimal synthetic routes based on feasibility, cost and environmental impact.
- **Stay informed about the evolving competitor landscape** and intellectual property space, ensuring a competitive edge by maintaining up-to-date knowledge of emerging drug candidates, targets and therapeutic areas (specific to pharmaceutical R&D).
- **Identify new applications for existing compounds and whitespace opportunities** in chemical manufacturing and materials discovery, supporting market expansion and product diversification (specific to chemical R&D).
- **Empower teams across the organization with easy access to high-value information** by leveraging AI technologies to lower barriers to information discovery and drive innovation.
- **Upscale lab chemistry protocols** for practical, large-scale application.

Addressing these challenges is essential for organizations to enhance decision-making, improve efficiency and maintain a competitive edge in a rapidly advancing R&D landscape.

Short Description - 25 Words or less (External)	Long Description - 50 Words or less (External)
Accelerate chemistry research with Reaxys, a comprehensive database delivering critical insights from over a billion trusted data points combined with innovative technology.	Optimize chemistry research with Reaxys, a comprehensive database delivering critical insights from over a billion data points combined with innovative technology. Easily explore chemical, bioactivity and toxicity data from literature and patents. Reaxys helps you accelerate synthesis planning, competitive analysis and the DMTA cycle, so you can go further, faster.

Principles

Best Portfolio: Strengthen confidence through trusted quality	Best Portfolio: Deliver critical insights	Best Partner: Enhance through technology & innovation
Benefits Reaxys provides access to diverse, comprehensive and trusted information, including over a billion chemistry and bioactivity data points from chemical patents and literature. So you can discover, innovate and develop with confidence.	Benefits Combining comprehensive data with analytical and AI-powered predictive tools, Reaxys delivers critical scientific insight. So you can make informed decisions at critical moments in the innovation process.	Benefits We continually enhance Reaxys through data transformation and technological innovation. So, your R&D teams and your organization can stay ahead in an ever-changing world.

Proof points	Proof Points	Proof Points
Content coverage - Documents: Reaxys provides access to title, abstract, claims and extracted data from over 122M documents, 19,000 journals and textbooks, and 47M patents (from 105 patent offices and 173 IPC subclasses). Reaxys covers diverse fields offering twice as many documents as are currently available in SciFinder. - Unmatched substance coverage: Reaxys provides access to 350M substances (as of July 2025), more than any other chemical database, according to Christopher Southan, Honorary Professor at the University of Edinburgh. - Trusted patent data: Through the collaboration with LexisNexis PatentSight, Reaxys delivers a comprehensive view of patent ownership and inventorship, enabling customers to scout chemistry technologies and identify key players in the field. **Integration with Scopus** Researchers value the seamless workflow between Reaxys and Scopus: "*Reaxys compound search results can be easily transferred to Scopus literature search results, making it a useful way to obtain literature related to compounds of interest in one go"*. — Researcher at chemicals company, verbatim from (NPS 2024) **Trusted quality data**	**Synthetic route design and optimization** - To overcome challenges in synthetic route design, **Lonza** selected ***Reaxys Predictive Retrosynthesis*** for its computer-aided synthesis planning. On average, Reaxys reduces the number of synthesis steps by 17%, accelerating the journey from discovery to market and helping to avoid costly late-stage redesigns and delays. - Boehringer Ingelheim identified Reaxys Predictive Retrosynthesis as a key driver in rapidly identifying high-quality, reference-supported synthetic routes: "*Reaxys outperformed basically any other tool because of the combination of quality (of the prediction) and reference quality*." — Bart Herle, Senior Scientist at Boehringer Ingelheim (*video link, timestamp 12:02* at Global Reaxys User Day 2023*).* - Sygnature Discovery selected Reaxys to equip *"its scientists with a powerful, unified platform supporting reaction chemistry, synthesis, and drug discovery innovation. As Sygnature Discovery continues to push the boundaries of scientific innovation, the integration of Reaxys will provide the foundation for more efficient workflows, accelerated timelines, and deeper insights into chemical reactions and compound data."* **Accelerating target assessment**	**Advanced predictive retrosynthesis** - Reaxys offers two predictive retrosynthesis models developed with leading AI companies Iktos and Pending.AI. Each model has unique algorithms and features, so customers can choose the option that best fits their workflows and research needs, improving synthetic planning. - Reaxys Predictive Retrosynthesis won an International Life Sciences Award from Global Health & Pharma for Best Chemistry Predictive Analytics, 2020 (page 23). The award recognizes Reaxys being taken to the next level with "*an AI solution for drug discovery - the best-in-class Predictive Retrosynthesis software that combines reaction data with deep learning algorithm to support innovation in synthetics and medicinal chemistry*." - "*As AI continues to shape the future of scientific research, we are confident that Reaxys offers the most advanced retrosynthesis technology available*," said Colin Sambrook Smith, Sygnature Discovery's Director of Computational Sciences and Informatics. Evaluation of Reaxys Predictive Retrosynthesis: Twenty chemists from the Carreira Research Group at ETH Zurich evaluated the Reaxys Predictive Retrosynthesis, finding it user-friendly and intuitive, with robust and innovative predictions for drug-like molecules. They determined that the tool offers significant time savings in designing synthesis routes and provides useful

- Award-winning data engineering: Reaxys won the CYPHER Data Engineering Excellence Award (2022) for its content processing and enrichment platform, which extracts chemistry knowledge from patents at scale.
- *Data quality one can trust: "These are what I pay for when I license a Reaxys database: normalization of data and quality assurance." — Senior Knowledge Manager, leading pharmaceutical company*

Strengthening confidence for safer chemistry decisions

"Sometimes some reagents have toxic effect on the environment and in searches from Reaxys we can find alternate reagents which are more compliant by comparing their safety data."— Senior researcher, chemical manufacturer (NPS 2024)

- "*Sygnature Discovery selected Reaxys, Elsevier's chemistry database, for its curated patent and structural data, transparent search capabilities and reliable excerpted content. Reaxys is one of a suite of purpose-built solutions that enable Sygnature to accelerate target assessments across the business*." **Sygnature case study- WIP_DO NOT USE THIS EXTERNALLY, AS it IS CURRENTLY WITH SYGNATURE FOR APPROVAL**

AI-powered search across disciplines

- *Reaxys AI Search* delivers results based on user intent and context, accelerating information discovery across chemistry and interdisciplinary fields such as materials science, drug discovery (including IP insights), chemical engineering and polymer science. "*I'm entering into an unknown research area, this type of tool would save tons of time*." — Materials engineer and Reaxys AI Search tester

Content Integration: Integrating internal and external knowledge

- Lundbeck chose Reaxys for its comprehensive chemistry content, properly interpreted and curated data, and integration of in vitro and pharmacology information. Reaxys now serves as the single point of access for literature references and ideas for reaction conditions.

Integrating customer building blocks into Reaxys allows chemists to easily identify available compounds and ensure that proposed synthetic pathways are immediately actionable with in-house resources**.** "*So you can be very focused in what type of building blocks you're using to deconstruct a molecule… And you can rest assured that the pathways that are predicted in this retrosynthetic planning optimization are aware of the building blocks that are available for you*." Pushkar Ghanekar, Senior Advisor - Frontier AI, Eli Lilly and Company (Global Reaxys User Day 2025, min:10.40

Collaboration with LG-AI: Elsevier has partnered with LGAI Research to develop AI-based vision model technology to enhance the Reaxys substance extraction engine and enable the deployment of a new reaction extraction engine. This collaboration allows programmatic extraction of both substance and chemical reactions, significantly expanding the breadth and depth of Reaxys comprehensive content (not yet released!). Elsevier and LG: Turning data into action - ECHEMI

ReactionFlash app: Developed in collaboration with ETH Zurich, the ReactionFlash app leverages high-quality Reaxys data to help R&D teams quickly learn and review named chemical reactions.

	internal and external data, increasing efficiency and effectiveness while simplifying and streamlining data flows. (Bio-IT-presentation_lundbeck 2019.pptx) **Greener, more efficient synthesis with PSG and Reaxys data** The CDI-CASP system, developed by CDI and powered by Reaxys data, was tested in the development of a new synthesis of S-Zanubrutinib. Using a "human-in-the-loop" interactive strategy, CDI-CASP delivered a shorter, greener and more efficient synthesis route compared with the benchmark patent route **(10.26434/chemrxiv-2024-f0kcq).** **Powering predictive models with datasets** Evotec uses Reaxys data as a core building block in its knowledge graph and data framework, which integrates internal, external, open-source, imaging and full-text data. This knowledge graph enables Evotec scientists to build predictive models, interpret screening results and prioritize targets effectively. (Evotec presentation at Global Reaxys User Day 2025; timestamp: 12.45)	
Features **Content** - Documents: Reaxys offers comprehensive coverage of authoritative information in organic, inorganic and organometallic chemistry, providing	Features **Reaxys Retrosynthesis** • . Reaxys Predictive Retrosynthesis models are available via the web interface or API,	Features **Reaxys Predictive Retrosynthesis** Reaxys provides two predictive retrosynthesis models, developed with leading innovators Iktos and Pending.AI. Each model uses distinct AI algorithms

access to the most recent content as well as archival data dating back to 1771 (from Gmelin and Beilstein).
Reaxys includes over 121M documents from:

- 19,000 journals and textbooks
- 47M patents from 105 patent offices and 173 IPC subclasses, with all non-English patent abstracts and claims translated into English

Comprehensive data:

- Reactions: 70M
- Substances: 350M
- Commercial products: 431M
- Physical properties: 28M facts
- Spectral information: 40M facts
- Other data points including thermodynamic properties, EHS data, safety data and more
- Pharmacokinetic, efficacy, toxicity, safety and metabolic profiles, as well as data from in vivo animal studies (over 49M bioactivities and 45K targets)

PubChem: Reaxys also hosts PubChem content (structures and table of contents) within its secure environment. Structure searches in Reaxys are run across all integrated PubChem databases.

Reaxys Commercial Substances (RCS) is a fully integrated supplier database containing over 168M commercial chemical substances and more than 431M associated product items from over 261 suppliers. RCS search results include CAS number, catalogue-specific product ID, price and package size, purity, structure, supplier-specific

Machine learning models trained on over 420,000 rules to reflect real-world chemistry

- Experimental procedures for each synthesis step presented in a single view, based on more than 70 million reactions
- Access to 150 million commercially available starting materials, making routes immediately actionable
- Users can tailor results to project needs with configurable parameters.
  - Set route diversity
  - Define bonds to break and bonds to protect
  - Integrate custom building blocks or select from building block libraries.
  - Edit synthesis routes
  - Include or exclude intermediates to guide predictions and avoid unsuitable compounds
  - Apply chemo-, regio- and stereoselective strategies to design drug-like molecules
  - Filter starting materials by price and shipping time
  - Adjust route length and steps to fine-tune synthetic pathways
  - Export routes to support collaboration

Advanced search capabilities:

- Reaxys supports structure searches, reaction queries, property-based searches and natural language queries (available to registered users for document search via Reaxys AI and Reaxys reaction data. (see column 2 for more details).

Content integration
Customer in-house data can be integrated within Reaxys, including Reaxys Predictive Retrosynthesis, Integration adheres to robust security standards to protect proprietary information.

Reaxys API
The new Reaxys APIs support integration with molecule design tools, ELNs, LLMs and orchestration agents. They can be used with platforms such as Knime or PipelinePilot to aggregate and analyze data efficiently. Users can also leverage tools like Co-pilot, ChatGPT or Gemini to generate queries for the Reaxys API.

Data sharing and export options
Users can share and export data internally or externally with multiple options:

- Formats: PDF/Print, XML, Microsoft Word, Microsoft Excel, Electronic Lab Notebook, RD File and Literature Management Systems (for document results)
- Data types: All available data, identification data only or hit data only. Exportable content may include structures, abstracts, reactions, front-page information, experimental procedures and document descriptions
- Limits: Maximum of 5,000 items per export; up to 25 exports per 24 hours

details, stock availability, shipment time, supplier country and data update label. CAS Registry Numbers (RNs): Reaxys provides access to CAS RNs for both historical and novel compounds via the “retrieve CAS number” function. Each CAS RN uniquely identifies a chemical substance, eliminating confusion from multiple names. **Data extraction** Reaxys combines automated (programmatic) extraction for high-volume coverage of patents and journals with manual extraction for high-quality, detailed data from selected sources. **Dataset:** Reaxys API**:** Provides access to the full Reaxys data corpus, which is updated twice a week. Flat Files: • Reaction Flat File (RFF): 23M ML-ready reactions most relevant for small compound synthesis analytics and predictions. Updated quarterly. • Substance Structure Flat File (SFF): Entire set of Reaxys chemical structures extracted from patents and journals. Updated weekly. • Reaxys Medicinal Chemistry Flat File (RMC FF): Entire Reaxys dataset of reported bioactivities with associated substances, biological targets and assays. Updated weekly.	Search)A quick search for substances, reactions and documents uses text input, structure/reaction drawing or a combination of both across Reaxys content and integrated databases such as PubChem, LabNetwork, eMolecules and SigmaAldrich. - The query builder enables advanced searches across substances, reactions, targets, bioactivities, physicochemical data and documents. - Reaxys AI Search enables document searches using natural language queries and supports long text input. - Bioactivity maps allow visualization of target-substance relationships, with manually curated data from journals and patents available for download and analysis. **Personalized alerts** Keep users informed of the latest content in their area of focus or about specific competitors, supporting optimal competitive intelligence. **Patent ownership information:** Reaxys provides a reliable overview of patent ownership history and current status, (Patent ownership - Reaxys Support Center).	

Color coding labels:
Reaxys Predictive Retrosynthesis
Reaxys Datasets (API and Flat File)
Professional Service group

Key Brand Words:

Advance Human Progress
Support/Help advance
Together
Trusted quality
Strengthen confidence
Impact makers
Mission-critical insights
Transform complexity into clarity
Solutions for better outcomes
Enhance through innovation
Champion inclusion