Reaxys®

2025 roadmap

Break down information silos and accelerate chemistry research.

The latest Reaxys developments

Patent discoverability improvements

Gain a better understanding of the IP landscape and identify emerging industry players with:

- The new patent family clustering that groups patents based on the extended patent family ID from LexisNexis
- Exclusive weekly updates on Current Patent Assignee and Ultimate Owner information from LexisNexis PatentSight
- Broader coverage of IPC classes in areas like batteries, organic solid-state devices, additives for materials, and natural large molecules

Faster, more precise retrieval of documents, authors and substances

Retrieve more accurate results with any first and last name combinations with the new author search capability and improved "Authors filter", which clearly indicates all the name variation considerations and is tightly coupled with the most up-to-date affiliation.

An improved relevancy ranking ensures that the most relevant results are delivered first, better aligning the content displayed with the query.

You can also toggle between substance databases with a new tab-based design that provides an easy way to navigate results in Reaxys (including ELNs for customer with content integration option).

More target, bioactivity and toxicity insights to design safe and effective compounds

Extensive extraction of chemical names, structures, biological targets, chemistry relevant concepts and keywords from patents and journals support you in SAR studies and assessment of potential off-targets interactions.

Extension of excerption from Asian language patents to include target, bioactivity and toxicity information from CN, KR, JP and TW along with the existing WO, US, EP patent offices.

The Bioactivity visualisation export now provides richer insights in a user-friendly format. Data can be exported and easily ingested into commonly used tools for SAR analysis.

Predictive Retrosynthesis

Reaxys now offer multiple state-of-the-art predictive retrosynthesis models that accelerate research for synthetic, medicinal, computational, and process chemistry teams. The latest improvements include:

- An updated model trained on recent Reaxys reaction data which provides a faster processing time and improves the diversity of synthesis routes
- Enhanced commercial substance integration with the largest library of commercial building blocks, now exceeding 110 million compounds
- New Reaxys Predictive Retrosynthesis API, well suited for batch processing of large molecule sets (additional subscription required)

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Reaxys improvements coming in 2025

At Reaxys, we are committed to continuous improvement. By consistently expanding and refining our content, advancing our technology and elevating user experience, we ensure that researchers have access to the most comprehensive and advanced resources available.

Content expansion and refinement

On top of regular content expansion, Reaxys is adding 43 million make-on-demand analogues of screening compounds from Enamine, adding to the existing 300 million commercial products accessible (see press release for more information). The integration provides chemists with unparalleled access to a diverse array of chemical compounds, facilitating the identification of novel drug targets, biomarkers and screening compounds.

New technological advancements

- Upgrading Reaxys data excerption engine to improve the quality and precision of the extracted data.
- Launching the machine learning optimized reaction flat file to streamline data preparation, and to increase the number of reactions available for training and validating predictive models.
- Offering a customizable retrosynthesis tool with models trained on a combination of Reaxys reactions and unpublished, proprietary customer ELN data. These models consider the specific chemical context of the company and ensure that the predictions are tailored and accessible exclusively to the respective organization.
- Developing a Synthetic Accessibility API, based on Iktos RScore and trained on Reaxys Reactions. This API is designed to assess the synthetic feasibility of molecules, with the potential to process up to 5,000 molecules per hour.

Enhanced user experience

Reaxys users will be able to take advantage of several new upgrades:

- New similarity sorting capabilities for both substances results and commercial products
- Logged-in users will benefit from the auto-saving of search queries, to access search history and re-run searches later
- Customer usage data will be accessible through EPIC, ensuring smooth usage reporting across your Elsevier portfolio

For Reaxys Predictive Retrosynthesis customers:

- Reduce the instance of zero result cases by automatically tweaking parameters to optimize route generation
- Improve user experience with the addition of visible branding for customer with Building Block Integration
- Optimize routes processing to display more routes and increase result diversity

Join us as beta-tester to shape our new AI capabilities

Reaxys is experimenting with vector-driven semantic search to better understand user queries, improve discoverability of unstructured text information and deliver more relevant results.

Reach out to your Customer Consultant to learn more.

For more information, visit:
elsevier.com/products/reaxys

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