## Reaxys®

### 2025 Fact Sheet for Researchers

Reaxys reimagines the research environment by replacing fragmented tools with a single integrated platform designed to accelerate breakthroughs. It eliminates repetitive, time-consuming tasks through centralized data access, breaking down information silos to drive faster discoveries and amplify research impact.

#### How Reaxys helps researchers accelerate discovery with integrated tools

#### Faster and more accurate results with AI-powered search capabilities

Reaxys accelerates scientific discovery by integrating **comprehensive chemical data** with **machine learning**, empowering researchers to uncover insights faster and with greater precision. Developed in collaboration with AI pioneers and academic experts, it streamlines literature searches and supports complex research inquiries. The **advanced author search** improves name disambiguation, providing accurate results and reducing manual verification with up-to-date affiliations. The **enhanced relevancy** ranking surfaces pertinent research first and a **new tab-based navigation system** allows quick switching between substance databases, facilitating rapid cross-referencing and efficient research support.

ELSEVIER

#### **Accelerated research using Predictive Retrosynthesis**

Reaxys offers highly improved, multiple **state-of-the-art predictive retrosynthesis models** that accelerate research for synthetic, medicinal, computational, and process chemistry teams. Current improvements include an updated model trained using recent Reaxys reaction data that leads to faster processing time and improved diversity of synthesis routes. The system is built on **neural networks** and **Monte Carlo Tree Search**, enabling it to learn transformation rules from reaction data, prioritize the most relevant rules, predict feasible synthetic routes, and apply efficient search algorithms to identify optimal pathways. Researchers can also access the largest library of commercial building **blocks**, exceeding **110 million compounds** with **enhanced commercial substance integration**.

#### Seamless data access and efficient research workflows

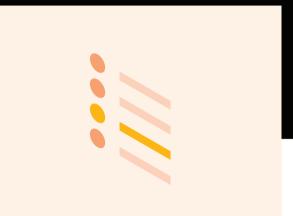
Reaxys integrates with **ScienceDirect** and **Scopus**, enabling researchers to seamlessly navigate substance properties, commercial availability, reactions, and bioactivity data directly from article pages. Researchers can extract chemical entities, biological targets, and key concepts from patents and journals to support **SAR studies** and off-target assessments. **Expanded Asian patent coverage** (CN, KR, JP, TW) and **enhanced bioactivity visualization exports** ensure faster insights with smooth data integration into research tools.

#### Integrated data for cross-disciplinary research



- Reaxys empowers research and innovation with seamless access to **268 million substances**, **47 million bioactivities**, and **43,000 pharmaceutical targets**, spanning chemistry, biology, and materials science.
- Enhanced patent discoverability features include patent family clustering via LexisNexis, weekly updates on patent assignees and owners, and expanded IPC coverage in high-growth areas like batteries, organic solid-state devices, and natural large molecules.
- Users can also avail integrated access to historical resources like the **Beilstein** and **Gmelin Handbooks**, alongside **19,000+ periodicals** and data from **105 patent offices**—all within a unified platform for interdisciplinary exploration and analysis.

# Improvements and updates planned for 2025



#### New technological advancements for precision and accuracy

- Upgradation of Reaxys data excerption engine to improve the quality and precision of the extracted data.
- Launch of 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.
- 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 contexts and ensure tailored predictions and exclusive access based on the contexts.

#### **Enhanced user experience**

- New similarity sorting capabilities for both substances results and commercial products
- Auto-saving of search queries for logged-in users, to access search history and re-run searches.
- Customer usage data will be accessible through EPIC, ensuring smooth usage reporting across the users' Elsevier portfolio.
- For users of Predictive Retrosynthesis: Fewer zero-result cases, improved route diversity, and a better experience with branded Building Block Integration.



#### Expanded and refined content for accelerated innovation and discovery

 The addition of 43 million make-on-demand analogues from Enamine, alongside the existing 300 million commercial products, expands the searchable chemical space. 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.

#### Experience it firsthand—request your trial today!

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