

Combine AI and high-quality reaction data to rapidly generate efficient synthesis routes. Monte Carlo tree search and forward synthesis prediction deliver diverse retrosynthetic pathways while accounting for chemo-, regio-, and stereo-selectivity.



16.3M
chemical reactions



453K
retrosynthetic rules



<10
minutes
to get results



150M
commercially
available materials

Scientifically robust predictions

- 1 Link to literature that informed the routes
- 2 End in purchasable starting materials
- 3 Access experimental procedures to execute plans

Intuitive experience

- 4 Published, predicted and custom routes in one view
- 5 Tailor results by editing synthesis routes
- 6 Export easily to collaborate on route design

Customizable

- Integrate reaction data or starting materials
- Select preferred vendors

Explore the intuitive interface of Reaxys Predictive Retrosynthesis

About Advent Informatics

Advent Informatics was founded in 2016 in Pune. Advent Informatics delivers world-leading scientific software solutions for drug discovery and research across India. We also represent the following companies:



AI and Physics bases
Molecular Modeling Software



Cheminformatics and
Chemical Data Solutions



Computational Chemistry
& Materials Modeling

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TRUSTED DATA, TECHNOLOGY AND EXPERTISE TO SUPPORT CHEMICAL, BIOLOGICAL AND PHARMACEUTICAL SCIENCE RESEARCH

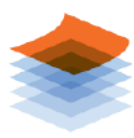
Reaxys is a comprehensive chemical database and chemistry search engine that combines a billion chemistry data points with AI search and retrosynthesis tools.

Reaxys Academic Edition 2026

Empowering multi-disciplinary innovation with cutting-edge data and AI-powered insights and supporting researchers towards groundbreaking discovery.



49M Patents from **125M** Articles
105 patent offices 18K journals



353M
Chemical compounds



44K
Biological targets



500M Phys-Chem
property, bioactivity facts

Reaxys Academic Edition offers an unrivalled value proposition via a seamless upgrade path, to academic institutions. Its unique features propel breakthrough discoveries and sustainable competitive advantage in research innovation.

Content expansion:

- **Enhanced multidisciplinary coverage** — new IPC classes added to programmatic extraction for material science and semiconductors support cross-departmental research.
- **Advanced bioactivity extraction** — extension of manual excerption from Asian language patents boosts drug discovery and chemical biology research.
- **AI-driven substance discoverability** — innovative extractive AI technology increases both the quality and quantity of extracted substances.



Insights discovery and user experience:

- **AI powered search and summaries** — uncover chemistry insights quickly with Reaxys' natural language AI search. Confidently design new compounds using extensive bioactivity data.
- **Author name search** — leveraging Scopus data to support document discoverability and first-time use cases.
- **Accelerated delivery of insights** — faster time to customer by delivering insights more rapidly.

"We always prefer research methods that get us to the answers faster: specific reaction and property searches such as can be done in Reaxys are very useful."

Hironao Sajiki
Professor at Gifu Pharmaceutical University

- **Refined lexical search** — enhanced keyword search with improved relevancy ranking for precise literature and document retrieval.
- **Accelerated delivery of insights** — faster time to customer by delivering insights more rapidly.
- **Seamless releases and accessibility** — regular and frequent product updates and full VPAT compliance ensure continuous innovation and inclusive access.

Reaxys ensures ISO 27001 certified information security standards.

Target & Bioactivity insights

Make informed lead optimization decisions with the world's largest target, bioactivity and toxicology database. Assess the most promising candidates with normalized and accurate SAR and ADMET data.



49M
bioactivity data
points



8.6M
substances with
bioactivity data



44K
biological targets

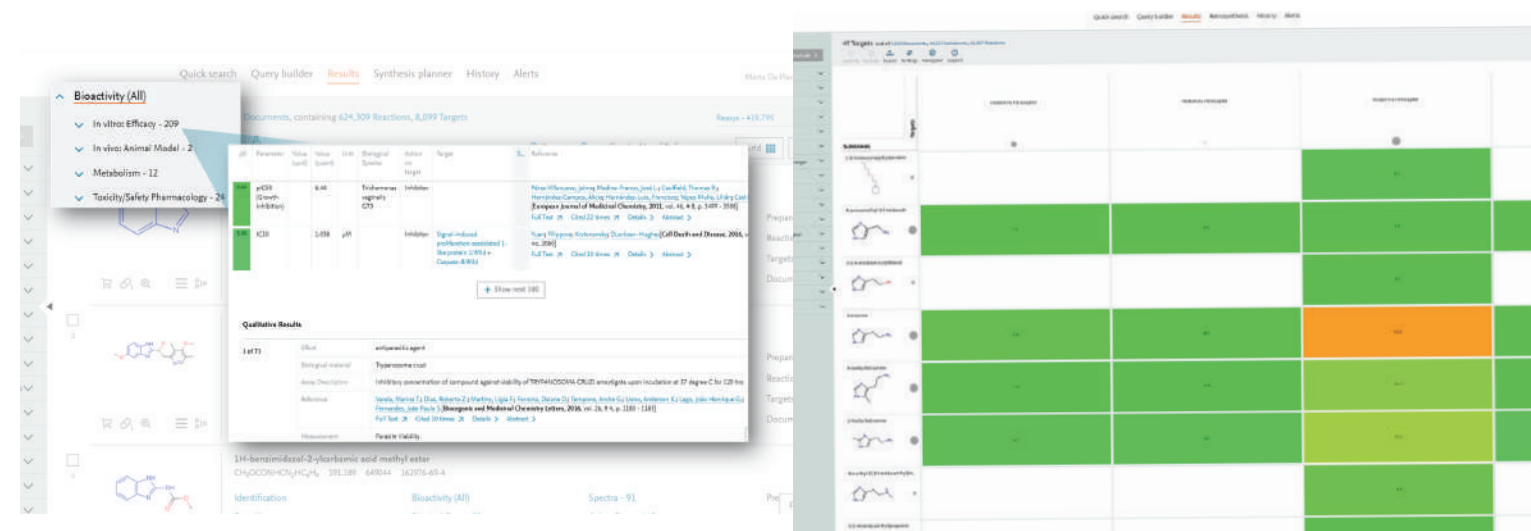


6.6M
assays with
additional insights



26K
celllines from
102K species

Understand SARs to optimize candidates with the highest chance of success



Bioactivity visualization enables easy comparison of relevant data.

Easily compare data points with **normalized pX values** from different publications and locations.

Evaluate substance properties quickly with **druglikeness profiles** based on Lipinski/Verber rules.

Get comprehensive **efficacy, toxicity, pharmacokinetic** and **safety data** from in vivo and in vitro testing.

Integrate high-quality **chemistry datasets** into your custom applications via API.