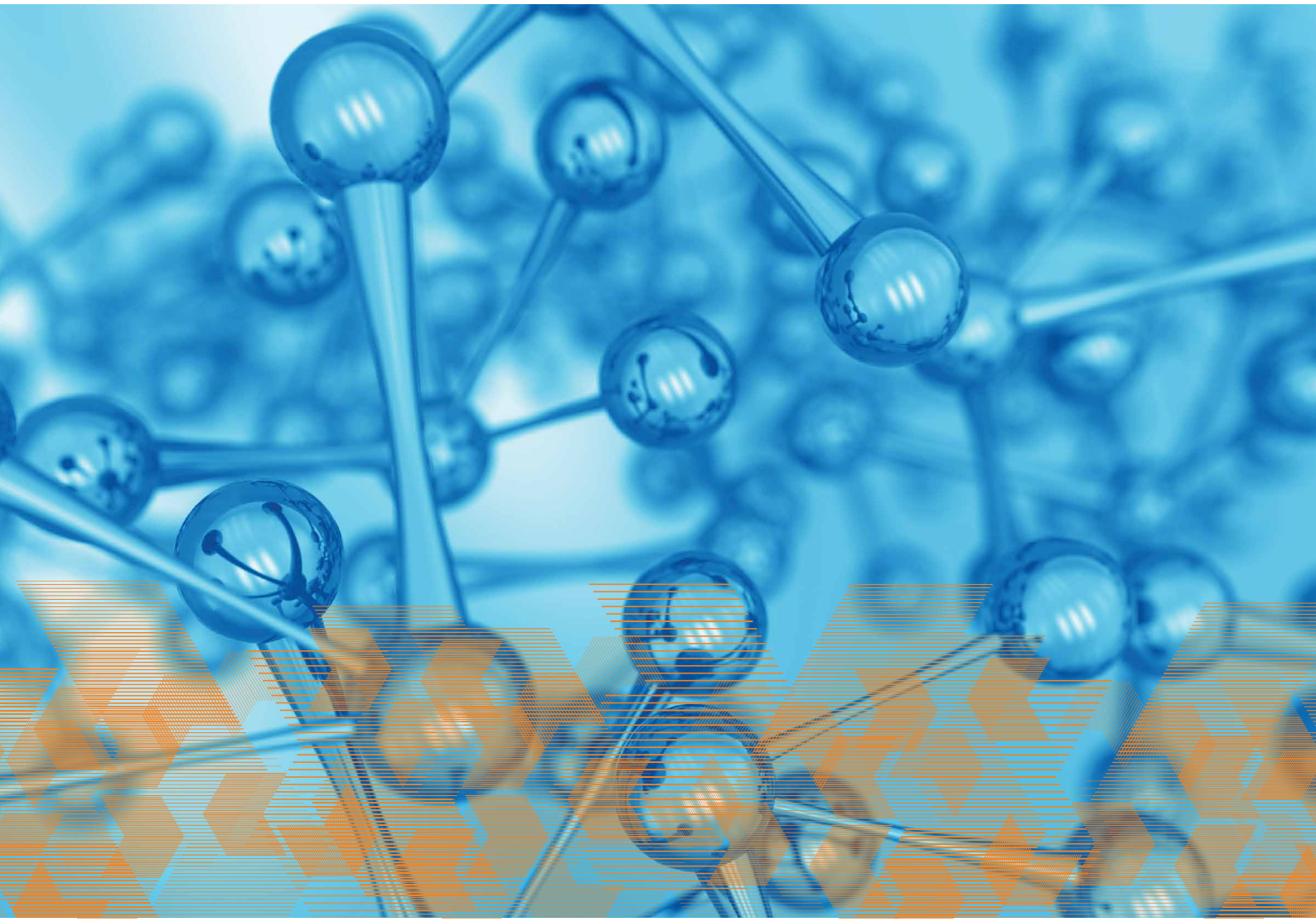
Reaxys®

Fact Sheet



DATA FOR INFORMED DECISIONS IN CHEMICAL R&D

Reaxys is a web-based research solution that improves R&D productivity by delivering experimental facts on chemical structures, properties, reactions and procedures.

ELSEVIER

Reaxys®
Fact Sheet

Introduction

Reaxys provides access to over 500 million published experimental facts to empower chemical discovery and development. The focus on structures, properties and reactions supports early drug discovery, material selection and synthesis planning and the data export possibilities allow harmonized analysis of in-house and external data.

REAXYS IMPROVES R&D PRODUCTIVITY BY DELIVERING ANSWERS THE WAY CHEMISTS NEED THEM.

- Does a compound exist?
- What do we know about this compound?
- How can I obtain this compound?
- Who else is working on this compound?

The Reaxys database contains:

>74.9 MILLION organic, inorganic and organometallic compounds	**>40.7 MILLION** chemical reactions	**>500 MILLION** published experimental facts
>16,000 chemistry-related periodicals	**>130** subject themes — more than any other research solution	**>240** years of chemistry knowledge (1771–present)

FEATURES

COMPREHENSIVE, HIGHLY ORGANIZED CONTENT

Reaxys excerpts experimental structure, reaction and property data from essential journals, patents and textbook chapters. The core of the database is a comprehensive set of chemistry literature selected for relevance. A further 16 thousand periodicals taken from a broad range of chemistry-related journals, textbooks and conference proceedings complete the picture. To increase searchability, all of the information is indexed and organized according to the principles of chemistry taxonomy.

ASK REAXYS

This innovative single-click search option provides an intuitive way to quickly find chemical property and reaction data, concepts and citations. **Ask Reaxys** understands and interprets text (Figure 1) and retrieves specific information in the most relevant form. By bridging the user-friendly input that resembles natural language and the abstract technical language of the database, it makes information more accessible.

Figure 1. Ask Reaxys accepts and interprets text queries

FLEXIBLE SEARCH QUERY CONSTRUCTION

The Reaxys start page (Figure 2) provides the choice of search categories: **reactions; substances, names, formulas; medicinal chemistry;** and **literature** (Figure 2). The customizable query themes support text-, numeric- and chemical structure-based input and include 500 searchable fields covering more than 130 subject themes that include concepts as varied as physico-chemical data, spectra, thermodynamics, electrochemistry and magnetochemistry.

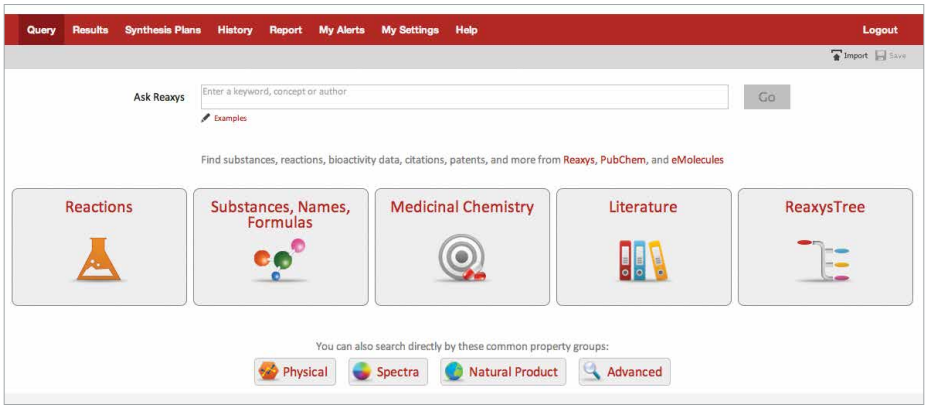


Figure 2. The Reaxys start page with the main search categories

It also includes a periodic table-based **Formula Builder** (Figure 3) to facilitate inorganic and organometallic chemistry searches, based on complete or partial chemical formulas.

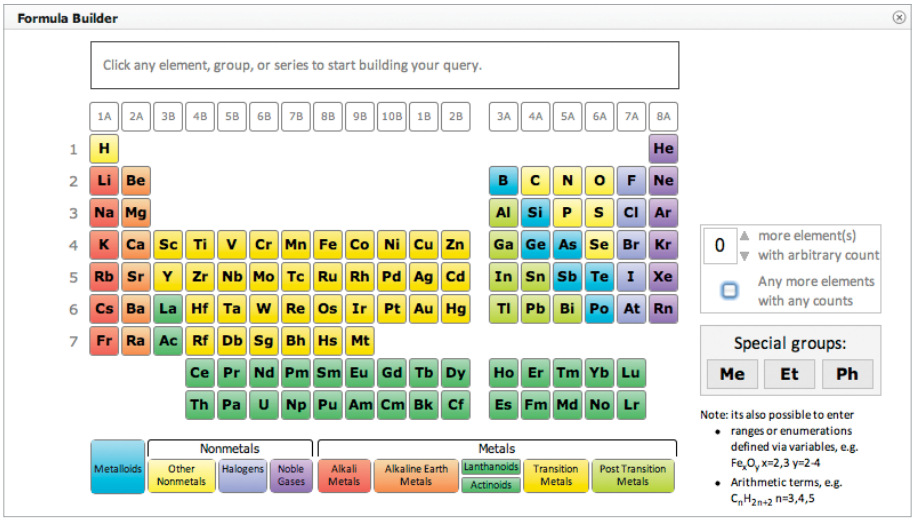


Figure 3. Formula Builder facilitates searching for inorganic and organometallic compound data

BROWSE THE DATABASE

ReaxysTree visualizes the Reaxys taxonomy (Figure 4). Users can browse hierarchies of terms, particularly those relating to chemical transformations and substance properties. This helps users to make connections between seemingly disparate aspects of chemistry.

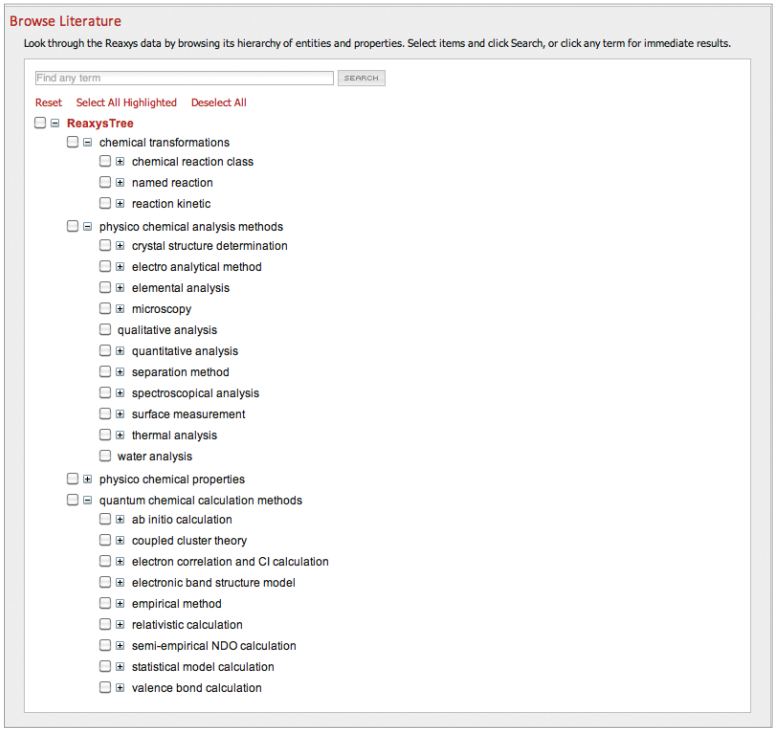


Figure 4. Browse the database taxonomically using ReaxysTree

FOCUS ON RELEVANT RESULTS QUICKLY

To help identify the most relevant results, Reaxys has a comprehensive set of filters for hitsets. Users can filter by **structure and properties**, **reaction parameters**, **bioactivity parameters**, **publication type** and more.

ASSESS RELATIONSHIPS WITHIN HITSETS

Reaxys Analysis View (Figure 5) lets users select analysis criteria to get a sense of the relationships between results. For example, it permits quick discovery of the individuals and organizations that are active in a particular area of research, sorts results according to yield, or reveals the catalysts or solvents for a particular reaction class.

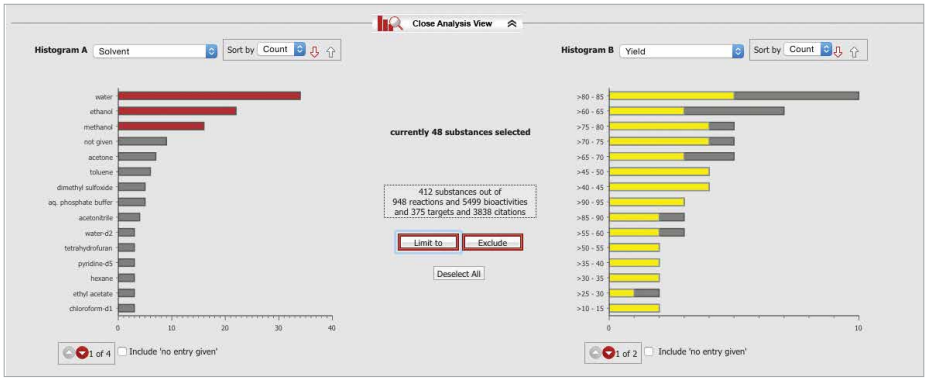


Figure 5. Analysis View is a histogram-based tool for assessing relationships within hitsets

PLAN SYNTHESIS ROUTES

Reaxys AutoPlan removes the time-consuming aspects of synthesis planning by instantly generating multiple, alternative synthesis pathways for compounds of interest. Synthesis plans are constructed from reactions described in multiple source documents, allowing users to build the best synthesis route for their purpose. The tool includes links to the eMolecules, Accelrys ACD and PerkinElmer ChemACX databases to provide more information, including the best options for buying the compounds.

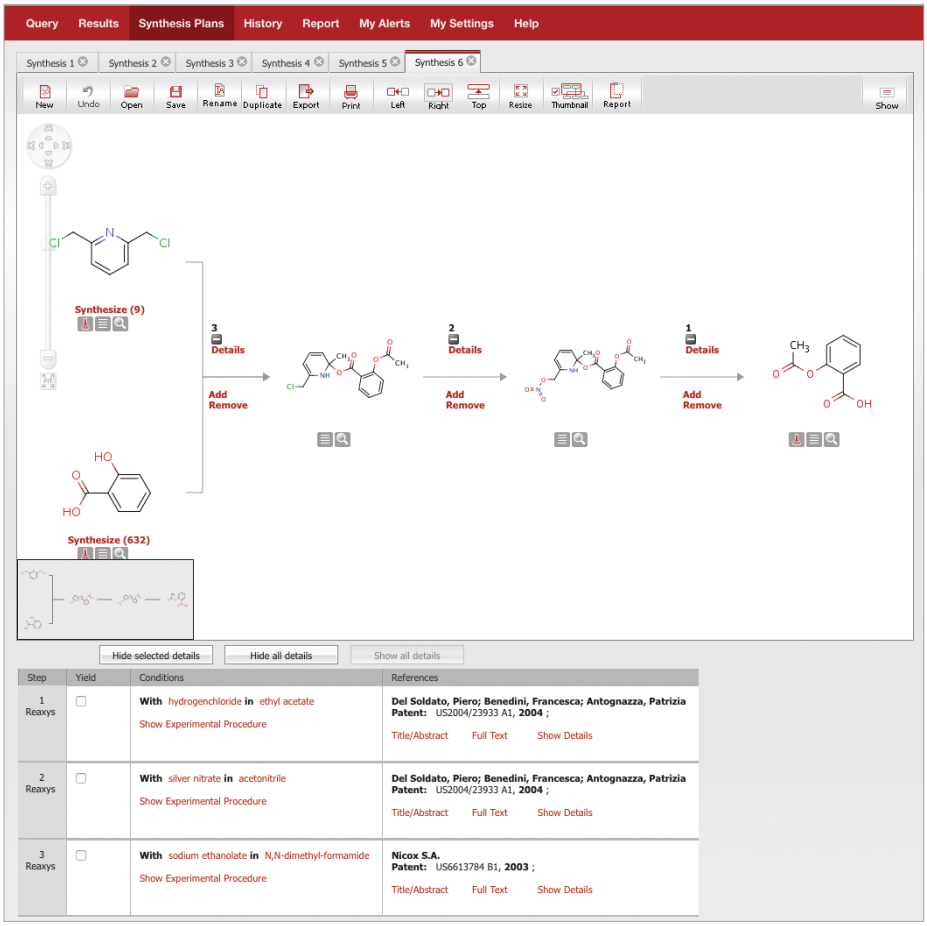


Figure 6. Reaxys AutoPlan generates multiple synthesis pathways

SHARE FINDINGS WITH OTHER RESEARCHERS

Reaxys Report (Figure 7) is a simple way to annotate and export search results. Clicking on any result gives two options for adding it to a report. Annotations can be added to the overall entry or a specific aspect of it. The report can then be emailed to multiple recipients.

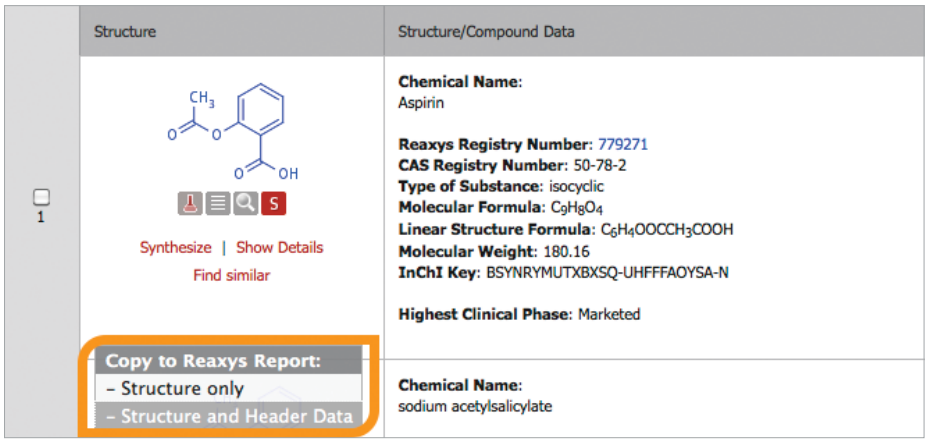


Figure 7. Reaxys Report permits easy sharing of findings

INTEGRATE REAXYS INTO EXISTING WORKFLOWS

Reaxys provides multiple options for the integration of our content into an existing tool and system environment. It is compatible with electronic lab notebooks (ELNs) from major suppliers, including Accelrys, Perkin Elmer and IDBS.

The **Application Programming Interface** allows flexible information delivery and real-time programming access to the Reaxys content and system. The **Structure Flat File** delivers structures, related fact and reaction data and patent information for in-house use, e.g., structural analog searching and assessments of the uniqueness of a compound. The Elsevier R&D Solutions Professional Services team is prepared to integrate Reaxys seamlessly into existing workflows.

INVESTIGATE COMPOUND BIOACTIVITY

Reaxys can be fully integrated with Reaxys Medicinal Chemistry allowing deeper exploration of the relationships between compounds of interest, targets and bioactivity data. Subscribers to both solutions can access them through a single, streamlined user interface.

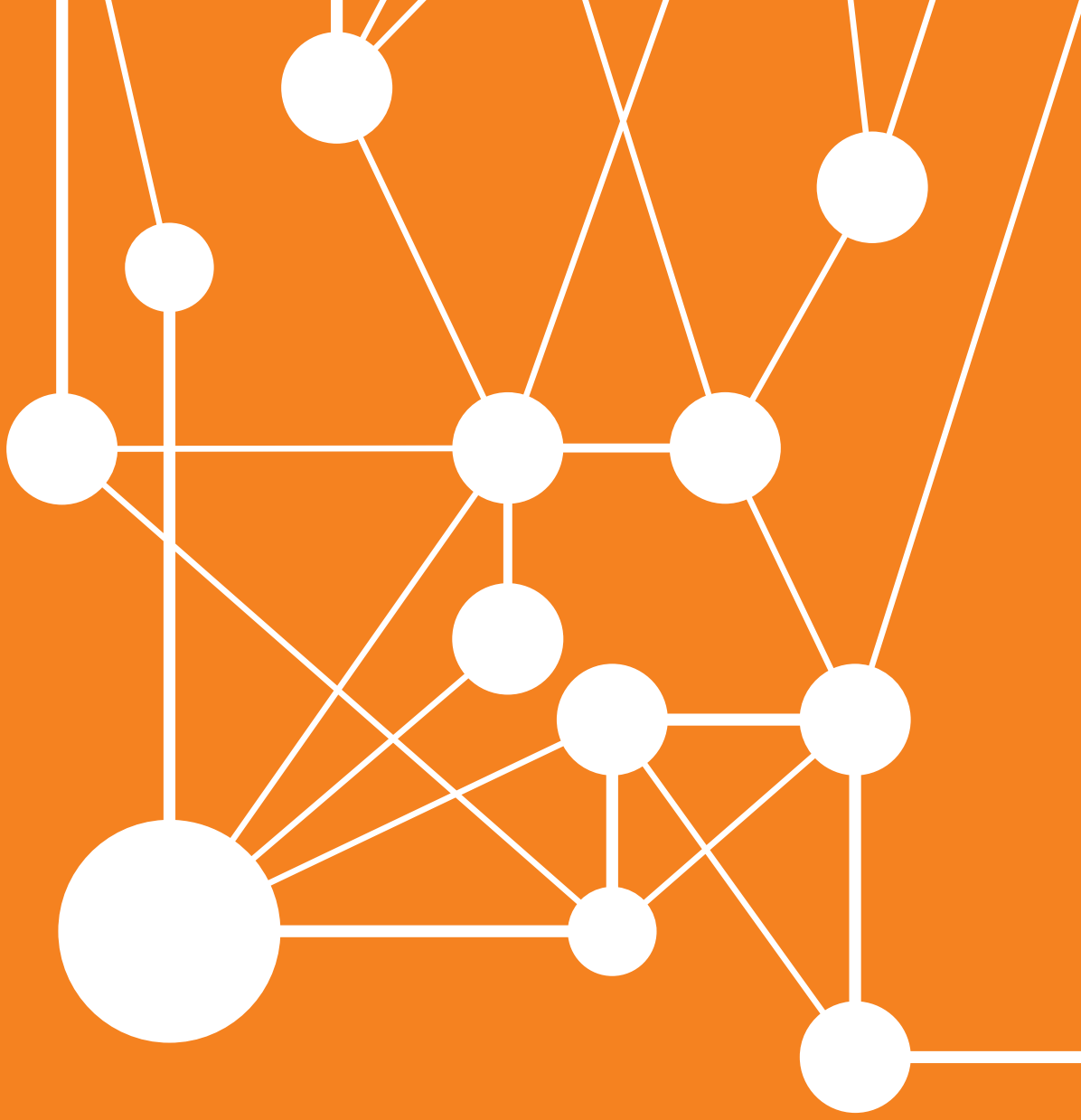
KEY BENEFITS

Reaxys enables researchers to:

- Discover chemical structures, properties and reactions
- Construct flexible queries easily and intuitively
- Assess compound synthesis and purchase options
- Share data within and outside your organization
- Compare in-house and published experimental data

GET STARTED

To learn more about how Reaxys can help your company or institute achieve success in research or education, contact your Elsevier sales representative at **elsevier.com/reaxys**



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