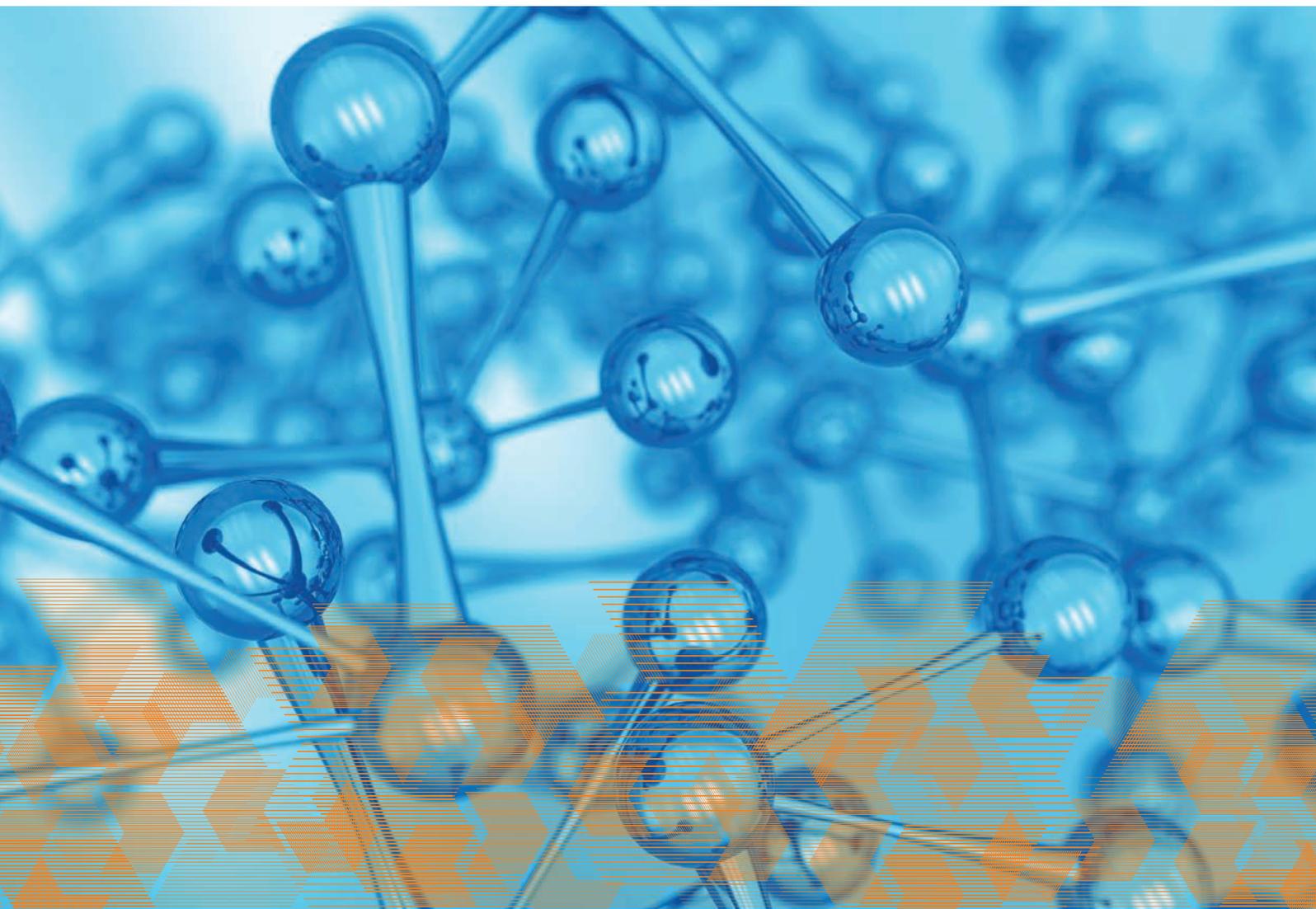


Reaxys[®]

Fact Sheet



THE SHORTEST PATH TO CHEMISTRY DATA AND LITERATURE

Designed to support the full range of chemistry research, including pharmaceutical development, environmental health & safety work and material science, Reaxys puts every scientist, from beginner to expert, on the shortest path to answers. Chemistry queries are launched from the highly intuitive search interface to quickly retrieve relevant literature, patent information, valid compound properties and experimental procedures. Finding answers has never been easier.



ELSEVIER

Reaxys®

Fact Sheet

Introduction

Reaxys provides rapid and easy access to experimental facts to empower chemistry research, chemical discovery and scientific education. Finding relevant literature, retrieving precise compound properties and reaction data, and incorporating that information into research workflows has never been easier.

REAXYS IMPROVES R&D PRODUCTIVITY BY PUTTING SCIENTISTS ON THE SHORTEST PATH TO RELEVANT ANSWERS.

QUESTION

- Does this compound exist?
- What do we know about it?
- How can I obtain it?
- Is it involved in novel research?
- Who else is working on it?

ANSWERED WITH

- The latest chemistry literature and patents
- Excerpted data on properties, reactions & more
- Excerpted synthesis plans & purchase information
- Patent data from every relevant patent office
- Direct links to Scopus for detailed information

>105 MILLION
organic, inorganic
and organometallic
compounds

>42 MILLION
chemical reactions

>500 MILLION
published experimental
facts

>16,000
chemistry-related
periodicals

>240
years of chemistry
knowledge

6
indexing sources for a
cross-disciplinary view
of chemistry

FEATURES

SMART INDEXING FOR MAXIMUM DISCOVERABILITY

To ensure that Reaxys fully facilitates discoverability in the far-reaching and complex discipline of chemistry, two indexing processes occur alongside each other. The core chemistry journals, textbook chapters and patents undergo deep manual indexing and exception of compound properties, reactions and synthesis procedures. In addition, a process of rules-based automated content enrichment is applied to a broader range of chemistry-related periodicals.

Because different scientists approach articles from different perspectives, each record is indexed with terms from 6 sources: Authors (from Scopus®), Compendex®, Embase®, GeoBase®, MEDLINE® and Reaxys itself. This supports a truly cross-disciplinary view of chemistry information.

GET STARTED QUICKLY

The streamlined user interface means it's easy for even beginners to get started. Quick searches for literature or compound properties are possible using natural language-based keyword queries, structure or reaction drawings, or a combination of the two (Figure 1). The full query builder enables construction of complex queries using a streamlined drag-and-drop interface that includes all the essential search input, including structure drawing, molecular formula building and basic indexes (Figure 2).

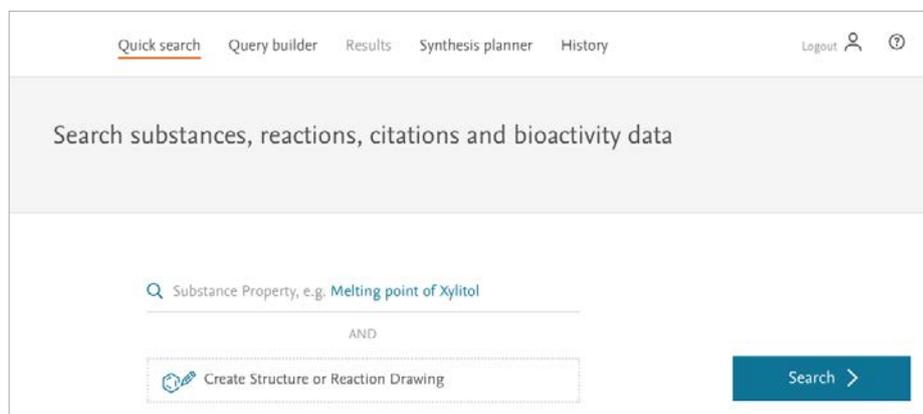


Figure 1. The Reaxys home screen gives two intuitive quick search options.

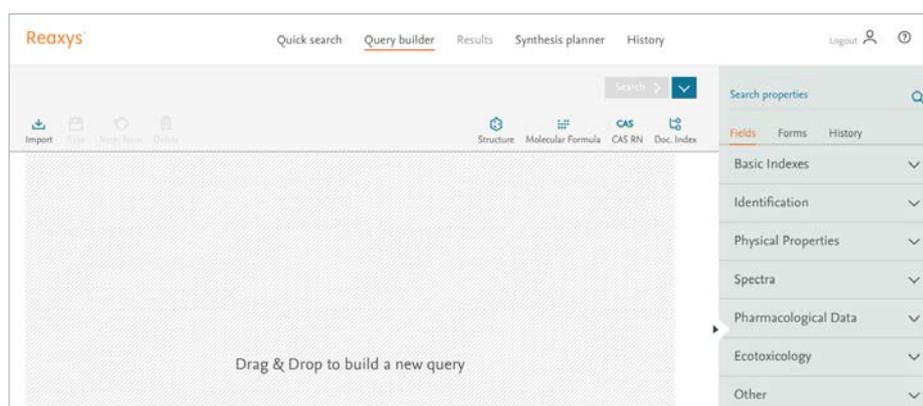


Figure 2. The query builder screen puts all the most important search features in one place.

SEARCH PEER-REVIEWED ARTICLES, PATENTS AND MORE

Each query starts a search of a comprehensive database of literature covering every type of literature. Reaxys enables users to retrieve precise data points (compound properties, reactions and synthesis routes) excerpted from the full text of core chemistry literature; or quickly find relevant articles, patents and textbook chapters of interest.

The database covers:

- ~450 core chemistry journals and textbooks
A carefully curated collection of essential titles in organic, inorganic and physical chemistry as well as material science, petrochemistry, pharmacology, and medicinal and computational chemistry
- >16,000 chemistry-related periodicals, including conference abstracts
A broad range of content that is relevant for chemists, including minor publications in core fields and major publications in related fields
- Patents from all the major world offices, including the US and Asia
A global range that goes beyond the WO, US and EP content to include Asian-language patents from the China, Taiwan, Japan and South Korea offices

FOCUS ON RELEVANT RESULTS

Designed in a user-centric process to ensure that scientists' needs are met, Reaxys has a streamlined interface for selecting the desired results view (Figure 3) and filtering and refining hitsets (Figure 4).

Choose a result for Preparation of Ritalin

Count	Category	Search Criteria	Preview Results	View Results
146	Reactions	Product: Ritalin (Exact Search)	Preview Results ▾	View Results >
56	Documents	Document Basic Index : Formation; Formations; Make; Making; Manufacture; Prep; Preparation; Preparation; Preparations; Prepare; Prepared; Preparing; Preps; Synthesis; Synthesise AND Document Basic Index : Ritalin	Preview Results ▾	View Results >
552	Documents	Document Basic Index : Ritalin	Preview Results ▾	View Results >

Figure 3. Users select the result set based on relevance to their query.

Filters and Analysis Apply

Yield

- >95 - 100: 3
- >90 - 95: 5
- >85 - 90: 5
- >80 - 85: 2
- >75 - 80: 2
- >70 - 75: 1
- >65 - 70: 1

Catalysts Classes

- active center: 2
- heterogeneous: 1

Solvent Classes

- Low boiling (<100°C): 9
- Green: 9

146 Reactions out of 49 Documents containing 110 Substances

0 selected: Limit To Export

Reaxys Ranking

Find Similar Reactions

Yield	Conditions	Reference
	Stage #1: (R)-phenyl-pyridin-2-yl-acetic acid methyl ester With perchloric acid; hydrogen; acetic acid palladium on	IPCA Laboratories Limited - EP1607388, 2005, A1

Figure 4. Reaxys offers multiple options to filter and refine hitsets.

PLAN SYNTHESIS ROUTES

Reaxys AutoPlan (Figure 5) 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.

Reaxys AutoPlan includes links to the eMolecules®, Biovia® ACD and PerkinElmer® ChemACX databases to provide more information, including the best options for buying the compounds.

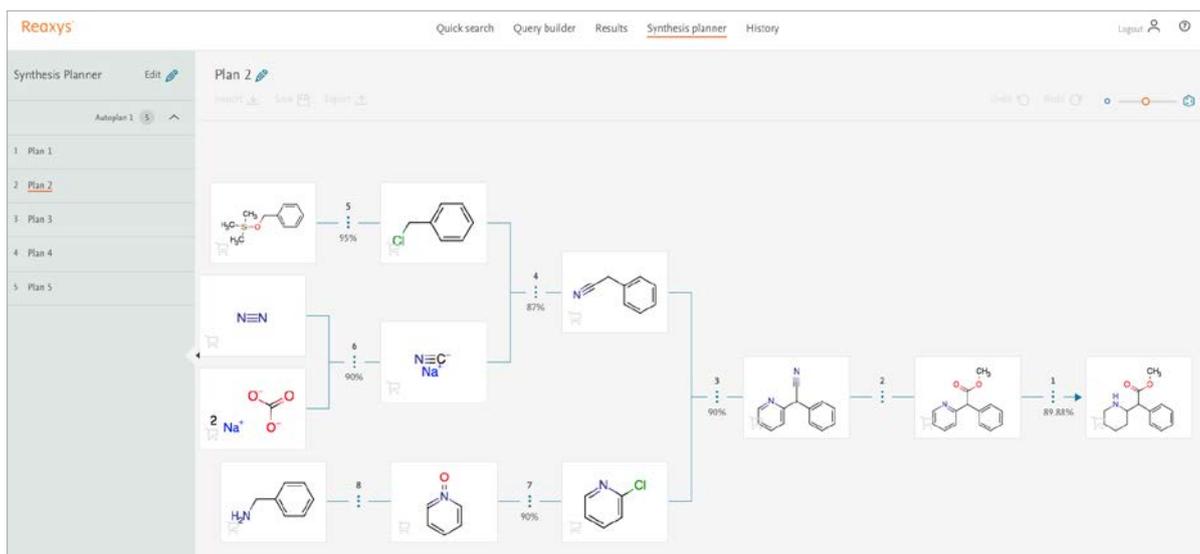


Figure 5. Reaxys AutoPlan generates multiple synthesis pathways.

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.

SHARE FINDINGS WITH OTHER RESEARCHERS

Reaxys Export (Figure 6) is a simple way to export and share search results. Clicking on Export in any result gives numerous format options suitable for any post-processing workflows.

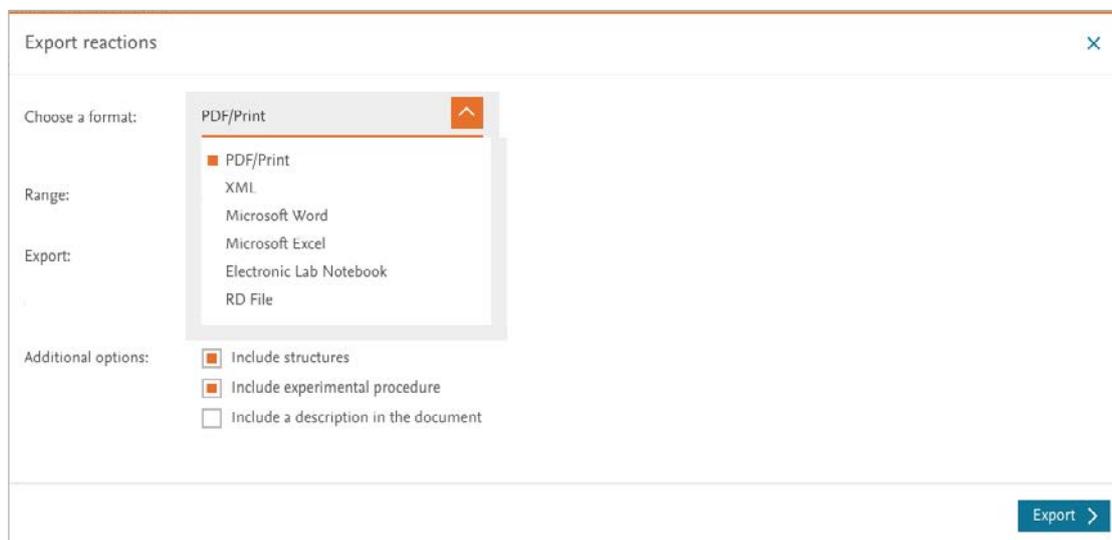


Figure 6. Reaxys Export permits easy sharing of findings.

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. KNIME nodes and Pipeline Pilot components are available to fully support work with those systems. The Elsevier R&D Solutions Professional Services team is prepared to assist in the seamless integration of Reaxys into existing workflows.

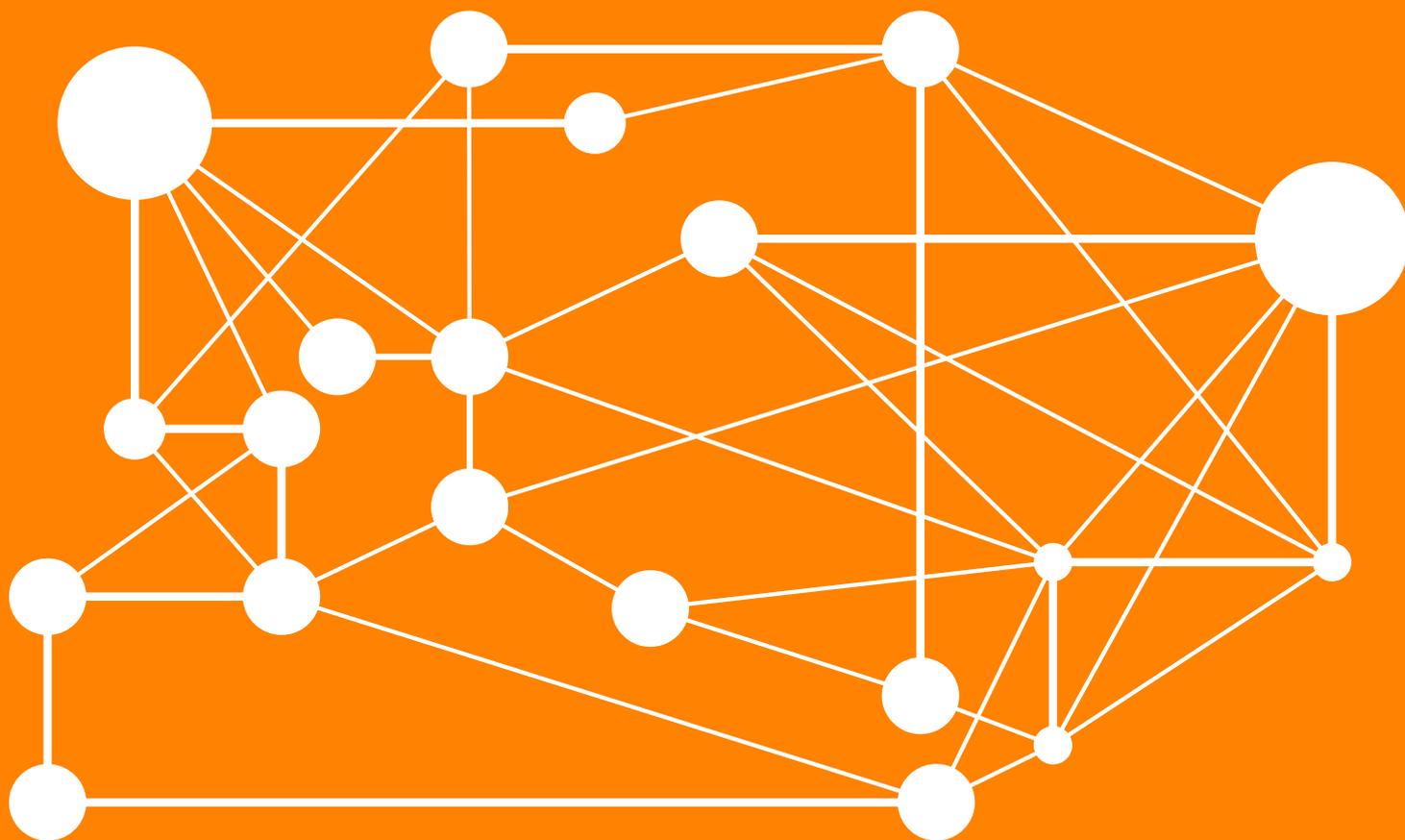
KEY BENEFITS

Reaxys enables researchers to:

- Discover chemical structures, properties and reactions
- Find relevant literature and patents with ease
- Construct queries with streamlined, intuitive interfaces
- Assess compound synthesis and purchase options
- Share data within and outside an organization or institution
- 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



LEARN MORE

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