



## Does your work flow?

Reaxys supports the workflows of your researchers and students, increases their productivity and elevates the output of your institution.

[www.info.reaxys.com](http://www.info.reaxys.com)



Reaxys supports research and task-based learning by integrating reaction and substance data search with synthesis planning.

Easy access to relevant and actionable results means researchers and students can move more quickly through the steps in their workflow, improving efficiency and increasing productivity.

# Introducing Reaxys

Time is short, pressure is high and when there's too much information to sort through no one can be effective. Reaxys delivers relevant, actionable results. What more could you want from a workflow tool?

## Relevant information

Researchers and students can be confident that they can find exactly what they need with experimentally validated, not calculated, data and unsurpassed depth of quality organic, organometallic and inorganic chemistry information.

## Integrated tools

Reaxys integrates reaction and substance data search with synthesis planning and excellent analysis tools, so researchers at any level of experience can move more quickly through the steps in their workflow.

## Increased productivity

Reaxys delivers relevant, actionable results displayed so that they can be put into action immediately, supporting the chemists' decision-making process, improving their efficiency and increasing their productivity.

We spend a lot of time with chemists.

Listening to them and watching them work has given us enormous insight into the frustrations they face. Too much effort to find and acquire the data they need to start their experiments, too much time spent validating results, too many false starts.

In the following pages, we'll tell you more about Reaxys and how it can support your researchers and students, increasing their productivity and elevating the output of your institution. You'll learn a bit more about how our tools save researchers' time. We'll tell you about the extraordinary quality of information that we deliver and, last but not least, we'll show you how easy Reaxys is to use.

# How Reaxys supports chemistry-related research

Reaxys supports today's multi-disciplinary approach to modern research with a wealth of experimentally validated data from journals and patents. Researchers and students from all chemistry-related disciplines will benefit from the relevant, actionable results Reaxys has to offer.

## Synthetic chemistry

Experimental reaction and substance data – from organic, inorganic and organometallic chemistry – in combination with the synthesis planner address the needs of synthetic chemists.

## Medicinal chemistry, biochemistry and life sciences

Researchers in medicinal chemistry, biochemistry and the life sciences will find relevant information, for example structure-activity-relationship data.

## Analytical and physical chemistry

Validated spectral data such as NMR shifts and additional physical property data lead to applications in analytical and physical chemistry.

## Environmental chemistry

Reaxys supports environmental chemistry with information such as toxicant uptake in biological systems.

## Materials chemistry

While all scientists benefit from coordination compounds and catalysts – for example in polymer research – alloys, glasses, and ceramics also add value for material scientists. Reaxys' factual data on semi- and superconductivity, magnetism, optical or mechanical properties are essential for developing new materials for modern applications.

# Experimentally validated reaction and substance data

The researchers and students you serve need high quality, relevant information they can trust. With Reaxys, you can give them experimentally validated reaction and substance data so they can spend less time interrogating their results and avoid false starts.

## Extensive coverage

Reaxys has extensive coverage of authoritative information in organic, organometallic and inorganic chemistry including:

- Single and multi-step reaction data
- Information on catalysts
- Experimental substance property data
- Reaction procedure texts

## Multi-step reactions

Reaxys provides more complete information about a reaction pathway. With multi-step reactions, chemists get more insight into the intermediary steps in a synthetic process. Identifying precursor reactions to the target will enhance chemists' workflows.

## Rich heritage

Reaxys combines the content of the prestigious databases **CrossFire**, **Beilstein**, **CrossFire Gmelin** and the **Patent Chemistry Database**. With such a rich, time-tested heritage, your researchers and students can rest assured the information they find meets their quality standards.

## Expert selection

Expert chemists carefully extract high quality, experimentally validated reaction and substance data from selected journals and patent literature.

## Quality and depth of information

The screenshot displays the Reaxys interface for a specific compound. The top navigation bar includes 'Substances (Grid)', 'Substances (Table)', and 'Citations'. The main content area is divided into several sections:

- Structure/Compound Data:** Includes Reaxys Registry Number (3628192), CAS Registry Number (73590-58-6), and the full chemical name: 5-methoxy-2-[[[4-methoxy-3,5-dimethyl-2-pyridinyl]-methyl]sulphonyl]-1H-benzimidazole.
- Identification:** Lists various identifiers and their counts, such as Physical Data (41), Spectra (25), Bioactivity/ECotox (690), and Use/Application (1040).
- Physical Data:** Includes Melting Point (4), Conformation (2), Crystal Property Description (1), Crystal Phase (1), Crystal System (1), Space Group (1), Density of the Crystal (1), Optics (1), Optical Rotatory Power (3), Electrochemical Behaviour (2), Dissociation Exponent (7), Electrochemical Characteristics (2), and Solubility (MCS) (2).
- Spectra:** A table showing NMR data with columns for Description, Nucleus, Solvents, Temperature, Frequency, and Original Text. The table includes data for 1H NMR in CDCl3 and acetone-d6.

Access in-depth, experimentally validated, not calculated, data excerpted from the literature.

# Tools to evaluate hit sets and design synthesis strategies

It's about time. Saving it and maximizing it so your researchers and students can move with confidence and ease from a basic idea to a target compound. And they need to be able to do that at their convenience: anytime, anywhere.

## Single-result records

Reactions with the same reactant and product, but with different reagents, solvents and conditions, are merged into one, single reaction record with a unique tabulated overview. From this same record, chemists can assess other properties and evaluate optimum synthesis routes so they don't have to spend time manually de-duplicating their results.

Procedure text from patent publications reduces the need to go to the patent full text to check relevance.

## Synthesis planner

A unique synthesis planner supports evaluation of alternative synthetic routes, and allows to identify and combine selected reaction steps to generate the most effective synthesis strategy.

## Anytime, anywhere

With flat-rate access, the chemists in your institution can get the information they need immediately and simultaneously. Reaxys is web-based, so they can work anytime and from anywhere. And, because there's no software rollout required and no limits on access, it's less administrative work for you.

## Advanced search functionality

It's easy to conduct a search on Reaxys. Users can formulate structure and reaction queries using one of the editors provided. They have the option of combining their query with property searches or searching for properties alone using one of the following methods:

- **Form-based Search** provides forms for the most common properties and is suitable for all users.
- **Advanced Search** gives the expert user the opportunity to define property queries by going deeply into the hundreds of data fields available.

## Time saving

The screenshot shows the Reaxys software interface. At the top, there is a navigation bar with 'Query', 'Results', 'Synthesis Plans', 'History', 'My Settings', and 'Help'. Below this, there are tabs for 'Synthesis 1', 'Synthesis 2', 'Synthesis 3', 'Synthesis 4', and 'Synthesis 5'. A toolbar contains 'Undo', 'Open', 'Save', 'Copy plan to new page', and 'Output'. The main workspace displays a reaction scheme with three steps: 1. Synthesis of a starting material (90% yield), 2. Synthesis of an intermediate (51% yield), and 3. Synthesis of the final product (71% yield). Each step is labeled 'Modify'. A 'Synthesize' button is visible for each step. At the bottom, there are buttons for 'Hide selected details', 'Hide all details', and 'Show all details'.

1. Search reactions and plan a synthesis  
or

2. Check commercial availability and supplier data for reaction partners

# An intuitive interface designed by chemists for chemists

With Reaxys, your researchers and students can be confident they'll find what they need quickly and easily. That's because Reaxys was designed in close cooperation with chemists from different disciplines and geographical regions and uses chemistry as an organizing principle.

## Development partners

To ensure that Reaxys supports every step in a chemist's workflow, we work closely with development partners from renowned universities, pharmaceutical and other chemistry-related industries and government institutes.

## Filtering results

It's easy to find, filter and analyze data. Ranked results are displayed in a convenient, tabulated overview, so chemists can see the most important information at a glance. Tools to group, filter and analyze results make it easier to rank hit sets and see what's most relevant.

## Interoperability

With Reaxys you can export structures and reactions together with their data, for instance, as reaction-data-tables. Formats supported, at no additional cost, include: Microsoft Word, Excel, PDF, SD-/RD-/Mol-File, XML, and RIS (Endnote, ReferenceManager).

It's easy to integrate with other systems, so you can load structures/reactions and data/text. Reaxys is interoperable with the Elsevier product suite. Linking to Scopus, the largest abstract and citation database, is as quick as a click of a mouse. And it's just as easy to access primary research found on Elsevier's full-text database: ScienceDirect.

## Training and support

Reaxys is easy to use, so the amount of time you'll have to spend on training is minimal. And we'll be with you, every step of the way, offering you full support, including online training, user guides, FAQs and more.

## Usability

The screenshot displays the Reaxys web interface. At the top, there is a navigation bar with tabs for 'Query', 'Results', 'Synthesis Plans', 'History', 'My Settings', and 'Help'. Below this, there are sub-tabs for 'Reactions', 'Substances and Properties', and 'Text, Authors and more'. The main content area is divided into two sections. The top section, labeled 'Generate structure from name' (1), contains a text input field with 'Geldanamycin' entered. Below the input field, there are three example queries: 'Example 1: aspirin', 'Example 2: BSYNRYMUTXBXSQ-WXRBYKCCW', and 'Example 3: 50-78-2'. A 'Submit' button is located to the right of the input field. The bottom section, labeled 'Double click this frame and draw structure query' (2), contains a chemical structure drawing tool. The structure is a complex polycyclic molecule with various functional groups. Below the drawing tool, there is a 'Search' button. At the bottom of the interface, there are three buttons: 'Clear Query', 'Load Query', and 'Save Query'. A modal dialog box is overlaid on the interface, titled 'Please enter a chemical identifier and then click "Submit"'. It contains a text input field with 'Geldanamycin' entered, and three example queries: 'Example 1: aspirin', 'Example 2: BSYNRYMUTXBXSQ-WXRBYKCCW', and 'Example 3: 50-78-2'. There are 'Submit' and 'Cancel' buttons in the dialog box.

1. Generate chemical structures from a name  
or
2. Draw a structure query

For more information, or to request  
a complimentary trial visit:  
[www.info.reaxys.com](http://www.info.reaxys.com)

**Americas:**

E-Customer Service  
360 Park Avenue South  
New York  
NY 10010-1710  
Toll Free: +1 888 615 4500  
Tel: +1 212 462 1978  
Fax: +1 212 462 1974  
Email: usinfo@reaxys.com

**Europe and all other regions:**

E-Customer Service  
Theodor-Heuss-Allee 108  
60486 Frankfurt/Main, Germany  
Tel: +49-69-5050 4268  
Fax: +49-69-5050 4213  
Email: nlinfo@reaxys.com

**Japan:**

E-Customer Service  
1-9-15 Higashi-Azabu  
Minato-ku Tokyo  
106-0044 Japan  
Tel: +81 3 5561 5034  
Fax: +81 3 5561 5047  
Email: jpinfo@reaxys.com



Reaxys® is a trademark owned and protected by  
Elsevier Properties SA and used under license.