

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



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

Substances (Grid)Substances (Table)Citations

1 substances out of 528 citationsgo to PagePage 1 of 1

Limit to SelectionOutputSort byMolweight

Structure

Chemical Name

Available Data

Nº of ref.

Nº of prep.

Boiling Point

Structure

Chemical Name

Available Data

Nº of ref.

Nº of prep.

Boiling Point

5-methoxy-2-[[[(4-methoxy-3,5-dimethyl-2-pyridinyl)-methyl]sulphonyl]-1H-benzimidazole (-)-5-methoxy-2-[[[(4-methoxy-3,5-dimethyl-2-pyridinyl)methyl]sulfinyl]-1H-benzimidazole 5-methoxy-2-[[[(4-methoxy-3,5-dimethyl-2-pyridyl)methyl]sulfinyl]-1H-benzimidazole 5-methoxy-2-[[[(4-methoxy-3,5-dimethyl-2-pyridyl)methylsulphonyl]-1H-benzimidazole 2-[[[(3,5-dimethyl-4-methoxypyridin-2-yl)methylsulfinyl]-5-methoxybenzimidazole rac-omeprazole

Identification Physical Data (41) Spectra (26) Bioactivity/ECotox (690) Use/Application (1040)

528

15 prep out of 80 reactions.

Structure/Compound Data

Reaxys Registry Number: 3628192 CAS Registry Number: 73590-58-6 119141-88-7 119141-89-8 131959-78-9 326602-80-6 Molecular Formula: C₁₇H₁₉N₃O₃S Linear Structure Formula: C₁₇H₁₉SN₃O₃ Molecular Weight: 345.422 InChi Key: SUBDBMMDZJVOS-LILDFLRNCA

Identification

Physical Data

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)

Solubility (MCS) (2)

Adsorption (MCS) (1)

Association (MCS) (6)

Spectra

NMR Spectroscopy (8)

Description	Nucleus	Solvents	Temperature	Frequency	Original Text
Chemical shifts	1H	tetradeuteriomethanol			
	1H	chloroform-d3		300MHz	1H NMR (300 MHz, CDCl3): δ 8.24 (1H, s), 7.58 (1H, mbroad), 7.06 (1H, s), 6.96 (1H, dd), 4.78and4.60 (2*1H, system AB,, 3.87 (3H, s), 2.25 (3H, s), 2.23 (3H, s)
Chemical shifts	13C	acetone-d6	26.9°C		
Chemical shifts	1H	acetone-d6	6.9 - 26.9°C		

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

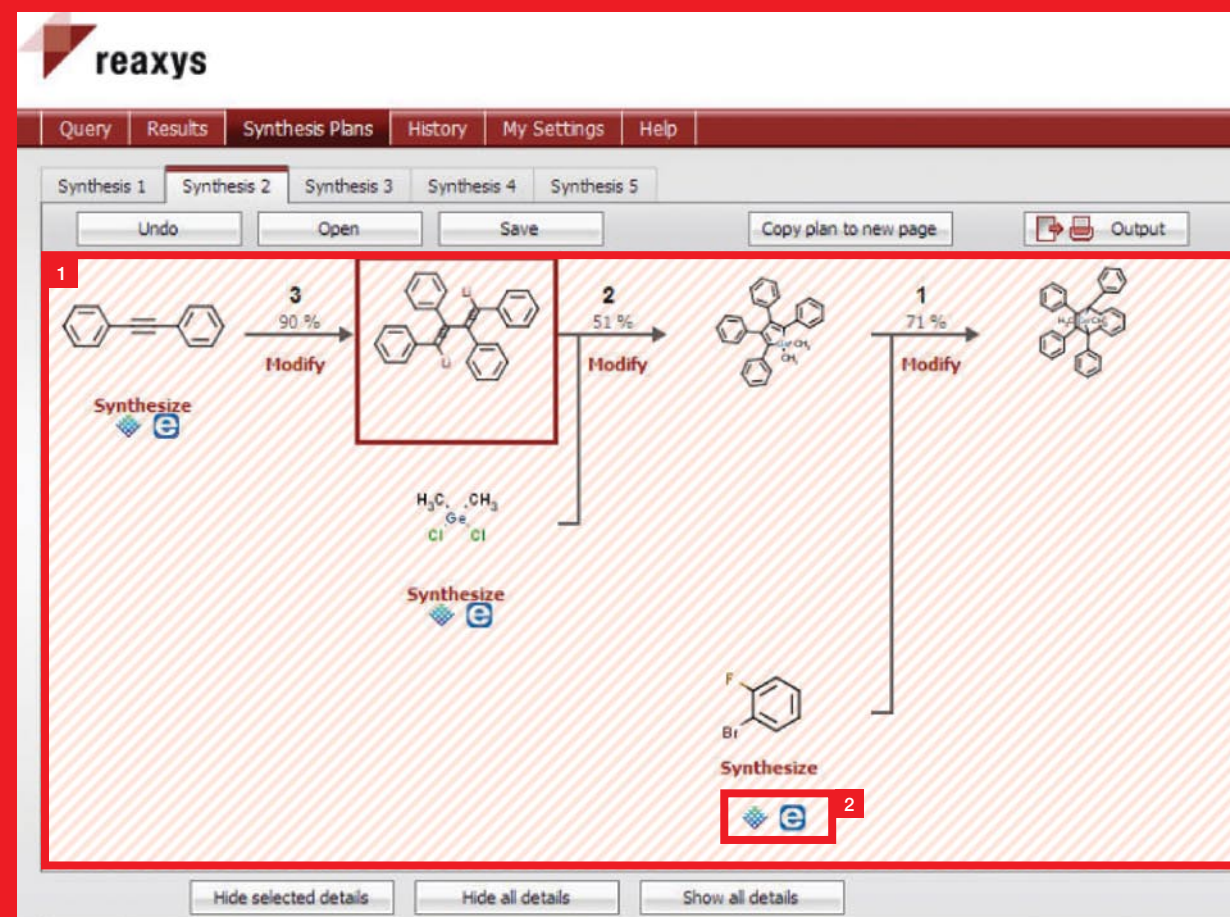
With flat-rate access, the chemists in your institution can get the information they need immediately and simultaneously. Reaxys is web-based, so they can work anytime and from anywhere. And, because there's no software rollout required and no limits on access, it's less administrative work for you.

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



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 application interface. At the top is the Reaxys logo and a navigation bar with links: Query, Results, Synthesis Plans, History, My Settings, and Help. Below this is a sub-navigation bar with tabs: Reactions, Substances and Properties (selected), and Text, Authors and more. The main content area is divided into two sections. The top section, labeled 'Generate structure from name' (marked with a red '1'), contains a large frame with a red border and diagonal lines, labeled 'Double click this frame and draw structure query' (marked with a red '2'). Inside this frame is a chemical structure of Geldanamycin. To the right of this frame is a modal dialog box titled 'Please enter a chemical identifier and then click "Submit"'. It contains a text input field with 'Geldanamycin' entered, and three example entries: 'Example 1: aspirin', 'Example 2: BSYNRYMUTXBXSQ-WXRBYKCCW', and 'Example 3: 50-78-2'. There are 'Submit' and 'Cancel' buttons. Below the modal dialog is a 'Search' button. The bottom section, labeled 'Hide further search conditions', contains a list of search criteria: Substance Data, Search text in all facts, Identification Data, Physical Data, Spectroscopic Data, Bioactivity Data, Ecotoxicological Data, and Bibliographic Data. There are also buttons for 'Clear Query', 'Load Query', and 'Save Query'.

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

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