



## Does your work flow?

Reaxys supports the workflow of your researchers, increases their productivity and elevates the output of your organization.



Reaxys fuels discovery and innovation by integrating reaction and substance data search with synthesis planning.

Easy access to relevant and actionable results means chemists can move more quickly through the steps in their workflow and deliver superior outcomes.

# 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?

## Integrated workflow tools

Reaxys integrates reaction and substance data search with synthesis planning, so researchers can move more quickly through the steps in their workflow.

## Relevant information

Reaxys offers unsurpassed depth of quality information in combination with excellent analysis tools, so researchers can be confident that they can find exactly what they need.

## Productive processes

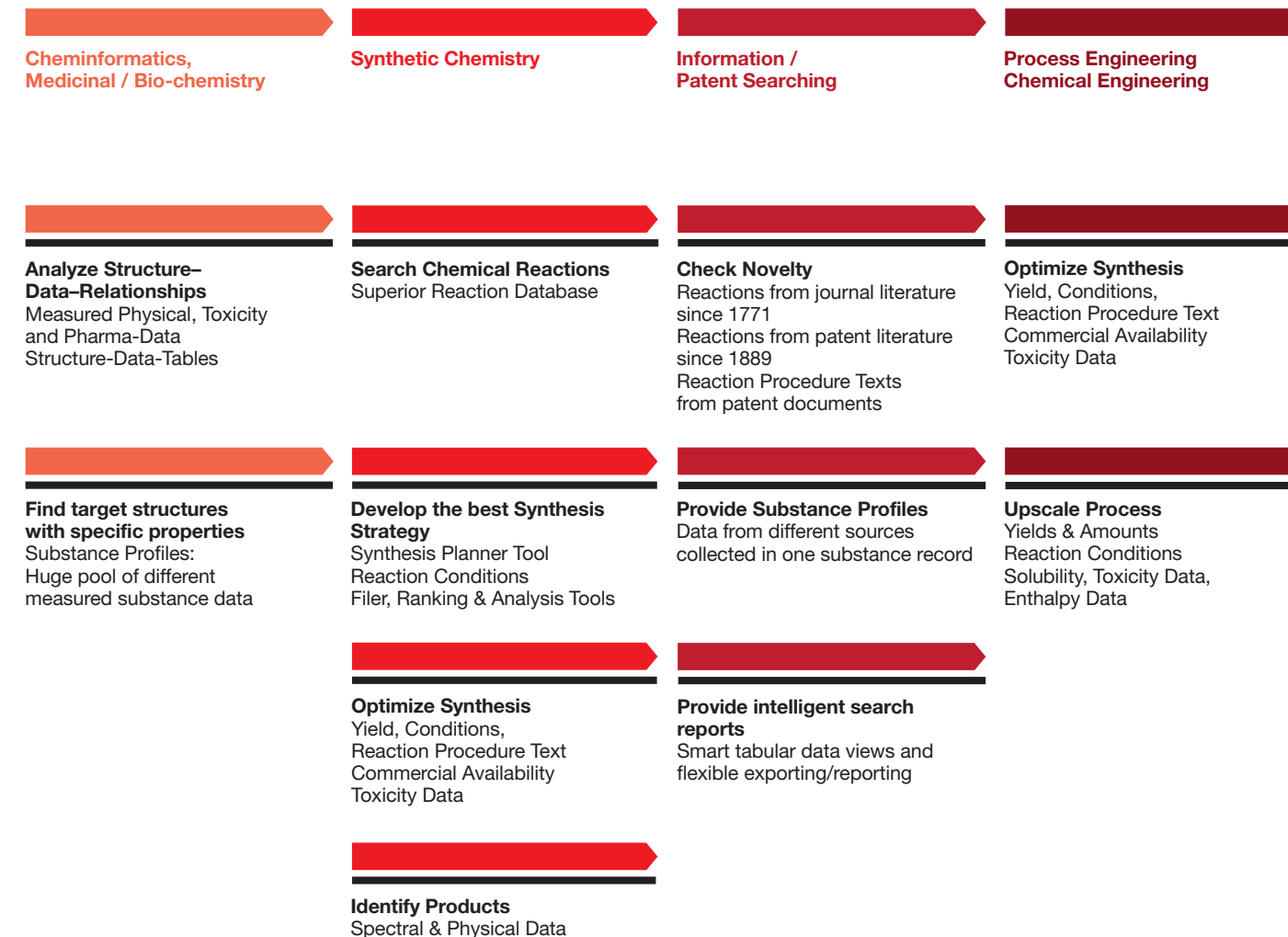
Reaxys saves valuable time by integrating relevant and actionable information, so researchers can expect improved outcomes.

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, increasing their productivity and elevating the output of your organization. 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 the workflow in chemistry-related R&D



# Experimentally validated reaction and substance data

The chemists 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
- Commercial availability tags

### 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 prestigious databases **CrossFire**, **Beilstein**, **CrossFire Gmelin** and the **Patent Chemistry Database**. With such a rich, time-tested heritage, chemists 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 Information

Filter by:

Molecular Weight

Number of Fragments

Physical Data

Spectroscopic Data

Bioactivity

Document Type

Authors

Patent Assignee

Journal Title

Publication Year

Substances (Grid)

Substances (Table)

Citations

Limit to Selection

Output

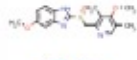
Sort by: Molweight

1 substances out of 528 citations

go to Page

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Hide Details

Structure	Chemical Name	Available Data	Nº of ref.	Nº of prep.	Boiling Point
	5-methoxy-2-[[[4-methoxy-3,5-dimethyl-2-pyridinyl)methyl]sulfinyl]-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)methyl]sulfinyl]-1H-benzimidazole 5-methoxy-2-[[[4-methoxy-3,5-dimethyl-2-pyridin-2-yl)methyl]sulfinyl]benzimidazole 2-[[[3,5-dimethyl-4-methoxypyridin-2-yl)methyl]sulfinyl]-5-methoxybenzimidazole rac-omeprazole	Identification Physical Data (41) Spectra (26) Bioactivity/Ecotox (590) 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

Chemical Name: 5-methoxy-2-[[[4-methoxy-3,5-dimethyl-2-pyridinyl)methyl]sulfinyl]-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)methyl]sulfinyl]-1H-benzimidazole, 5-methoxy-2-[[[4-methoxy-3,5-dimethyl-2-pyridin-2-yl)methyl]sulfinyl]benzimidazole, 2-[[[3,5-dimethyl-4-methoxypyridin-2-yl)methyl]sulfinyl]-5-methoxybenzimidazole, rac-omeprazole

Type of Substance: heterocyclic

Molecular Formula: C<sub>17</sub>H<sub>23</sub>N<sub>3</sub>O<sub>5</sub>

Linear Structure Formula: C<sub>17</sub>H<sub>23</sub>N<sub>3</sub>O<sub>5</sub>

Molecular Weight: 345.422

InChi Key: SUEDEP#0023VOS-LILDFLRNCA

Identification

Physical Data

Adsorption (MCS) (1)

Association (MCS) (6)

Spectra

NMR Spectroscopy (8)

Description	Nucleus	Solvents	Temperature	Frequency	Original Text
Chemical shifts	1H	tetradecuteriomethanol			
	1H	chloroform-d3		300MHz	1H NMR (300 MHz, CDCl3): δ 8.24 (1H, s), 7.58 (1H, mbroad), 7.01 (1H, s), 6.96 (1H, dd), 4.78 and 4.60 (2*1H, system AB), 3.87 (3H, s), 2.25 (3H, s), 2.23 (3H, s)
	1H	chloroform-d3		300MHz	1H NMR (300 MHz, CDCl3): δ 8.24 (1H, s), 7.58 (1H, mbroad), 7.01 (1H, s), 6.96 (1H, dd), 4.78 and 4.60 (2*1H, system AB), 3.87 (3H, s), 2.25 (3H, s), 2.23 (3H, s)
Chemical shifts	13C	acetone-d6	25.9°C		
Chemical shifts	1H	acetone-d6	5.9 + 25.9°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 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

A single-result record – from all available data for the queried compound or reaction – removes barriers between separate information sources. Reactions with the same reactant and product, but with different reagents, solvents and conditions, are merged into one, single-reaction record. From this same record, researchers can assess other properties, evaluate optimum synthesis routes and spend less 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 organization 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, it's less administrative work for you.

## Time saving

The screenshot displays the Reaxys web interface. At the top, the 'reaxys' logo is visible. Below the navigation bar, the 'Synthesis 1' tab is active. The main workspace shows a synthesis plan with three steps. Step 1 involves the reaction of a starting material with  $\text{HO}^+ \text{CH}_3$  to form an intermediate. Step 2 involves the reaction of the intermediate with  $\text{H}_2\text{C}$  to form another intermediate. Step 3 involves the reaction of the intermediate with  $\text{H}_2\text{C}$  to form the final product. The final product is a substituted benzene ring with a chlorine atom and a nitro group. The interface includes buttons for 'Undo', 'Open', 'Save', 'Copy plan to new page', 'Output', 'Synthesis representation', 'Left to Right', and 'Show Hints'. Below the synthesis plan, there are buttons for 'Hide selected details', 'Hide all details', and 'Show all details'. The 'References' section lists two references: 'Tsuiji, Yasushi; Kotachi, Shinji; Huh, Keun-Tae; Watanabe, Yoshihisa' and 'Tsuiji, Yasushi; Huh, Keun-Tae; Yokoyama, Yasuhiro; Watanabe, Yoshihisa'. The 'Yield' section shows a yield of 92%. The 'Conditions' section lists 'With  $\text{RuCl}_2(\text{PPh}_3)_3$  in toluene, 6 h; Heating; Rate constant;'. The 'References' section lists 'Tsuiji, Yasushi; Kotachi, Shinji; Huh, Keun-Tae; Watanabe, Yoshihisa' and 'Tsuiji, Yasushi; Huh, Keun-Tae; Yokoyama, Yasuhiro; Watanabe, Yoshihisa'. The 'Yield' section shows a yield of 92%. The 'Conditions' section lists 'With  $\text{RuCl}_2(\text{PPh}_3)_3$  in toluene, 6 h; Heating; Rate constant;'. The 'References' section lists 'Tsuiji, Yasushi; Kotachi, Shinji; Huh, Keun-Tae; Watanabe, Yoshihisa' and 'Tsuiji, Yasushi; Huh, Keun-Tae; Yokoyama, Yasuhiro; Watanabe, Yoshihisa'. The 'Yield' section shows a yield of 92%. The 'Conditions' section lists 'With  $\text{RuCl}_2(\text{PPh}_3)_3$  in toluene, 6 h; Heating; Rate constant;'. The 'References' section lists 'Tsuiji, Yasushi; Kotachi, Shinji; Huh, Keun-Tae; Watanabe, Yoshihisa' and 'Tsuiji, Yasushi; Huh, Keun-Tae; Yokoyama, Yasuhiro; Watanabe, Yoshihisa'.

1. Search reactions and plan a synthesis
2. Check commercial availability and supplier data for reaction partners



# An intuitive interface designed by chemists for chemists

With Reaxys, busy chemists 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 pharmaceutical and other chemistry-related industries, universities 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 show the most relevant results. What's more, data is organized in substance and reaction profiles, and data from different publications is merged into one hit record.

## Interoperability

With Reaxys you can export structures and reactions together with their data, for instance, as reaction-data-tables. 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 support with webinars, user guides, FAQs and more.

## Usability

The screenshot displays the Reaxys web application interface. At the top, the 'reaxys' logo is visible. Below it, a navigation bar includes tabs for 'Query', 'Results', 'Synthesis Plans', 'History', 'My Settings', and 'Help'. The main content area has sub-tabs for 'Reactions', 'Substances and Properties', and 'Text, Authors and more'. A red box labeled '1' highlights the 'Generate structure from name' button. Another red box labeled '2' highlights a large drawing area with the instruction 'Double click this frame and draw structure query'. A chemical structure of Geldanamycin is shown within this area. A modal dialog box is open, titled 'Please enter a chemical identifier and then click "Submit"', with a text input field containing 'Geldanamycin'. Below the input field are three example lines: 'Example 1: aspirin', 'Example 2: BSYNRYMUTXBXSQ-WXRBYKCCW', and 'Example 3: 50-78-2'. 'Submit' and 'Cancel' buttons are at the bottom of the dialog. A 'Search' button is located at the bottom right of the main interface. On the left side, there are expandable sections for 'Substance Data', 'Identification Data', 'Physical Data', 'Spectroscopic Data', 'Bioactivity Data', 'Ecotoxicological Data', and 'Bibliographic Data'. At the bottom, there are buttons for 'Clear Query', 'Load Query', and 'Save Query'.

1. Generate chemical structures from a name

2. Draw a structure query

For more information, or to request  
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