

**Reaxys**®

# **Navigating Reaxys**

A short guide showing how to find your favorite features and functionality in the new and improved user interface

# Introduction

This is the first edition of a new guide to help Reaxys users get used to the upgraded user interface. The guide content is based on questions we have received from users. Answers use screenshots from the both user interfaces.

New editions of this guide will be created as we receive more questions from users.

Want more information on Reaxys? Don't forget to download the Quick User Guide!

### Old Reaxys user interface

Query	Results Synthesis Plans	History Report	My Alerts	My Settings	Help		Logout			
							Timport 🔛 Save			
	Ask Reaxys e.g. Ask Reaxys for 'publications about quasicrystals' Smart searching with Ask Reaxys. See examples >									
	Find substances, reactions, bioactivity data, citations, patents, and more from Reaxys, PubChem, eMolecules, LabNetwork, and SigmaAldrich           Reactions         Substances, Names, Formulas         Medicinal Chemistry         Literature         ReaxysTree									
	Å	••			<u>O</u>					
	Start by specifying common ID fields such as CAS Registry number and more.									
	You can also search directly by these common property groups:									

### Reaxys user interface

Reaxys	Quick search Query builder Results Synthesis planner History	õ	Ŷ	0
Import 🛓	Search substances, reactions, documents and bioactivity data in Reaxys, Reaxys Medicinal Chemistry. PubChem, eMolecules, LabNetwork and SigmaAldrich			
	Q Substance Properties, e.g. solubility of vitamin D3			
	AND			
	Create Structure or Reaction Drawing			

## **Search features**

Where can I find Ask Reaxys, the Reactions query form, the Literature query form, etc.?

All the query forms from the old Reaxys user interface are now contained within Quick Search and Query Builder.

Figure 1. How search options in the old user interface map to search interfaces in the upgraded user interface Old Reaxys user interface

Query Results Synthesis Plans	History Report	My Alerts M	ly Settings	Help		Logout					
						Timport 📄 Save					
Ask Reaxys	Search										
Find substance	s, reactions, bioactivity	y data, citations,	patents, and	more from Reaxys, Pub	Chem, eMolecules, LabNetwork, and S	SigmaAldrich					
Reactions	Substances, N Formula	ames,	Medicir	al Chemistry	Literature	ReaxysTree					
▲	ေစ့		(	$\bigcirc$							
	Start	by specifying cor	mmon ID field	ds such as CAS Registry	number and more.						
		You can also se	arch directly	by these common prop	erty groups:						
	🙅 Phys	ical 🛛 曼 S	pectra	🕑 Natural Produc	t Advanced						
	Reaxys' Quick search Query builde Results Synthesis planner Asistory A Q O										
	actic ns, documents and bi emistry, ubChem, eMolecules, Lainetwork			import 🔜 📑	S E Sincher Metsaler Formule	#         U2           CAS MN DOC Index         Failuble           Ratic Indexes         Names A					
Q Substance Prope	ties, e.g. solubility of vitamin D3					Hernfuton v Popula Propertis v Spectra v KedChern v					
Q₽ Create S	tructure or Reaction Drawing				Drag & Drop to build a new query	Diter v Resolver v Robingraphy v Robingraphy Robingra					
						Labitesenik 🥪					

Quick Search enables keyword\*- and structure-based searches. Quick Search retrieves information on reactions, substances, bioactivities, literature literature and a full range of properties. Query Builder facilitates the creation of all query types from the old UI and adds the possibility to easily combine them.

The old user interface had a number of query forms, each focused on a different aspect of chemistry searching: reactions, substances, physical properties, spectra, etc. Clicking on an option on the home screen opened a dedicated query form. It also offered the option to perform a keyword-based search using Ask Reaxys.

Now, Reaxys offers two search approaches: Quick Search and Query Builder. Between them, they contain all of the search options of the multiple query forms in the old interface, along with powerful new options that increase the search power available to users.

Quick Search offers keyword-based searching similar to Ask Reaxys. Users can enter keywords\* to create their query. In addition, Quick Search offers the possibility to create structure-based searches, which can be combined with keywords or run on their own.

**\*What counts a keyword?** In the new Quick Search, the names or descriptors of properties, substances, experimental procedures and reactions (including named reactions), author names, journal titles, and 'ordinary' words all count as keywords. Therefore, users do not need to use specialized forms or fields to make queries about properties, substances, etc. For example, if a user wanted to find all substances with NMR specta, they could simply type NMR in Quick Search and then choose the results for substances in the results preview (see Figure 2).

As mentioned above, queries run with Quick Search can retrieve information on substances, reactions, targets and documents. After submitting a query, a preview of the results that match the keyword(s), phrase(s) and/or structure(s) is shown, allowing the user to select the results they need.

C Ne			Results for kinase		
	822,685	Substances	Target(s) : kinase	Preview Results 🗸	View Results >
	4,293	Targets	Target(s) : kinase	Preview Results 🗸	View Results >
	1	Substances	Substance : kinase	Preview Results 🗸	View Results >
	773,136	Documents	Titles, Abstract, Keywords : kinase	Preview Results 🗸	View Results >

Figure 2. An example of the results preview for a Quick Search

Quick Search improves on Ask Reaxys by enabling keyword- and structure-based searches and by providing the possibility to perform the full range of searches in this simple manner.

Query Builder facilitates the creation of queries of all types. Rather than asking users to choose and work with one query form at a time, Query Builder allows users to choose and combine multiple search fields and forms from a comprehensive list, combining them with the chosen Boolean operators. Query Builder includes search forms and fields for physicochemical and bioactive properties, spectra, basic indexes, medicinal chemistry parameters and literature and provides quick access to common search fields like structure, molecular formula, document basic index or CAS RN search.

Reaxys	Quick search Query	v builder Result	s Synthesis p	olanner History		0	Ŷ	0
내 🕑 🏷 🌐 Import Save Reset form Delete all		Structure	Molecular Formula	Search > ~ # CAS RN Doc. Index	Find search fie Q melt	elds and for	rms	×
							Reax	ys 🔨
Boiling Poin	Boiling Point, °C	Hide	ields 🔨 🗙		😞 Derivati	ve		
=	60-80 Pressure (Boiling Point), Television (Boil	orr	民		⊗ <u>Melting</u>	Point		
-	740-760		民		Physical	Data		
AND								
◇ Melting Poir	it 🗌 Find any	Show	ields 🗸 🗙					



Reaxys' Quick search Query builder Results Synthesis planner	History	<u>Α</u> Φ 0	)		
▲ B ○ B 0 # #		Find search fields and forms	Q		
Let C C Let Line Constant Cons		Fields Forms History			
		Reaxys	^	Find search fields and forms	Q
		Basic Indexes	~		~
		Identification	~	Fields Forms History	
		Physical Properties	~	Reaxys Forms	~
		Spectra	~ -		
		MedChem	~	Socuments	
		Other	~	Satural Product	
		Reactions	~		
		Bibliography	~	😂 Physical Data	
		PubChem	×		
	•	eMolecules	~	Reactions	
Drag & Drop to build a new query		LabNetwork	~	😂 Spectra	
		SigmaAldrich	~		
		Structure Structure	1	Substances	

Figure 4. Query Builder showing a selection of the top categories of *Fields* (screenshot on the left) and a close up on a selection of the top categories of *Forms* (screenshot on the right) available for query construction. Each contains multiple options, similarly to the old UI.

### How do I navigate between the tabs?

A very similar navigation bar exists in both user interfaces.

# Navigation in the old UI Query Results Synthesis Plans History Report My Settings Help Logout Navigation now Quick search Query builder Results Synthesis planner History A A O O

Query has been replaced by Quick Search and Query Builder. Results, Synthesis Planner and History are the same. My Settings is now available through the user icon, which appears when the user is logged in. My Alerts is no available through the bell icon, which appears when the user is logged in.

### How do I open the structure editor?

In the old Reaxys user interface, from certain query forms (e.g., the Reaction query form), it was possible to open the structure editor.



Now, users can open the structure editor from Quick Search or Query Builder:



When I am creating a structure or reaction drawing, how do I define the substance as a starting material, product, reagent or catalyst?

In the old user interface, each time you create a structure drawing-based reaction search, it was necessary to select the substance role from a set of defined categories, thus:



Now, this has been simplified so that users just add an arrow in the appropriate position:

Product

#### Starting material







## **Results features**

### Displaying more than 9 hits per page

In the old UI, at the bottom of each Results page, there was the option to change the number of hits per page from 9 (the default, determined as the optimal number for speed of page rendering) to several preset numbers between 1 and 99.

However, unless a user changed their preference settings, they would have to make this selection on every search.



In the new user interface, users change their preferences in their user profile once to select the number of hits per page and then Reaxys will always display this number. Simply open the user profile, select *Preferences*, select *Results per page*, and choose the number that will be set as the account's permanent default.

					Γ	Results per page	
Synthesis planner History	1					Number of results per page	×
and docume & Profile						Number of results per page 99 99	Save >
ork and SigmaAldrich 🕒 Sign out	F	Profile				15 30 60	
	A	Account	Profile	Preferences	7 R	ELX Intellectual Properties SA. Terms an cond • 99	9

Further information on using Reaxys can be found in the user guide in the Reaxys Support Center.

REAXYS is a trademark of RELX Intellectual Properties SA, used under license. Copyright @ 2018, Elsevier B.V.