

1. Search

SUBSTANCES	
FEATURE	COMMENT
Quick search as text (See page 3)	Enter a substance name, molecular formula or CAS number in the Search Reaxys field and click Search . Examples: <ul style="list-style-type: none"> • Atenolol • Pt(PPh₃)₃ • 102625-70-7
Quick search with Structure or Reaction Drawing (See page 4)	<ol style="list-style-type: none"> 1. Click the Create Structure or Reaction Drawing box. 2. Create the substance structure drawing. For more information on using the Marvin JS structure editor see: <ol style="list-style-type: none"> a. The Structure drawing workflow. b. View our Tips for using ChemAxon Marvin JS. c. Visit the ChemAxon Marvin JS website which includes a MarvinJS User's Guide. 3. Click Transfer to query, click Search.
Query builder (See page 5 & 6)	<ol style="list-style-type: none"> 1. Click Query builder (See page 6). 2. Select one of the Quick Querylets (Structure, Molecular Formula, CAS RN or Doc Index) under the search button. <p>OR</p> <ol style="list-style-type: none"> 2. Search for properties using the Search properties field and Drag & Drop the property onto the Query builder. 3. If you have multiple search fields, use the appropriate Boolean operator (see page 7). 4. Click Search at the top of the screen and select the desired target content: e.g. Substances. <p>Note: Click Show fields to enter specific search values.</p>

REACTIONS	
FEATURE	COMMENT
Quick search as text (See page 3)	Enter a term(s) in the Search Reaxys field and click Search . Examples: <ul style="list-style-type: none"> • preparation of porphyrine • phosphorylation • Suzuki coupling • Adler phenol oxidation
Quick search with Structure or Reaction Drawing (See page 4)	<ol style="list-style-type: none"> 1. Click the Create Structure or Reaction Drawing box. 2. Create the reaction structure drawing. For more information on using the Marvin JS structure editor see: <ol style="list-style-type: none"> a. The Structure drawing workflow. b. Create a Reaction Query in the Search for Reactions Workflow. c. View our Tips for using ChemAxon Marvin JS d. Visit the ChemAxon Marvin JS website which includes a MarvinJS User's Guide 3. Click Transfer to query, click Search.
Query builder (See page 5 & 6)	<ol style="list-style-type: none"> 1. Click Query builder (See page 6). 2. Select one of the Quick Querylets (Structure, Molecular Formula, CAS RN or Doc Index) under the search button. <p>OR</p> <ol style="list-style-type: none"> 2. Search for properties using the Search properties field and Drag & Drop the property onto the Query builder. 3. If you have multiple search fields, use the appropriate Boolean operator (see page 7). 4. Click Search at the top of the screen and select the desired target content: e.g. Reactions. <p>Note: Click Show fields to enter specific search values.</p>

Search (continued)

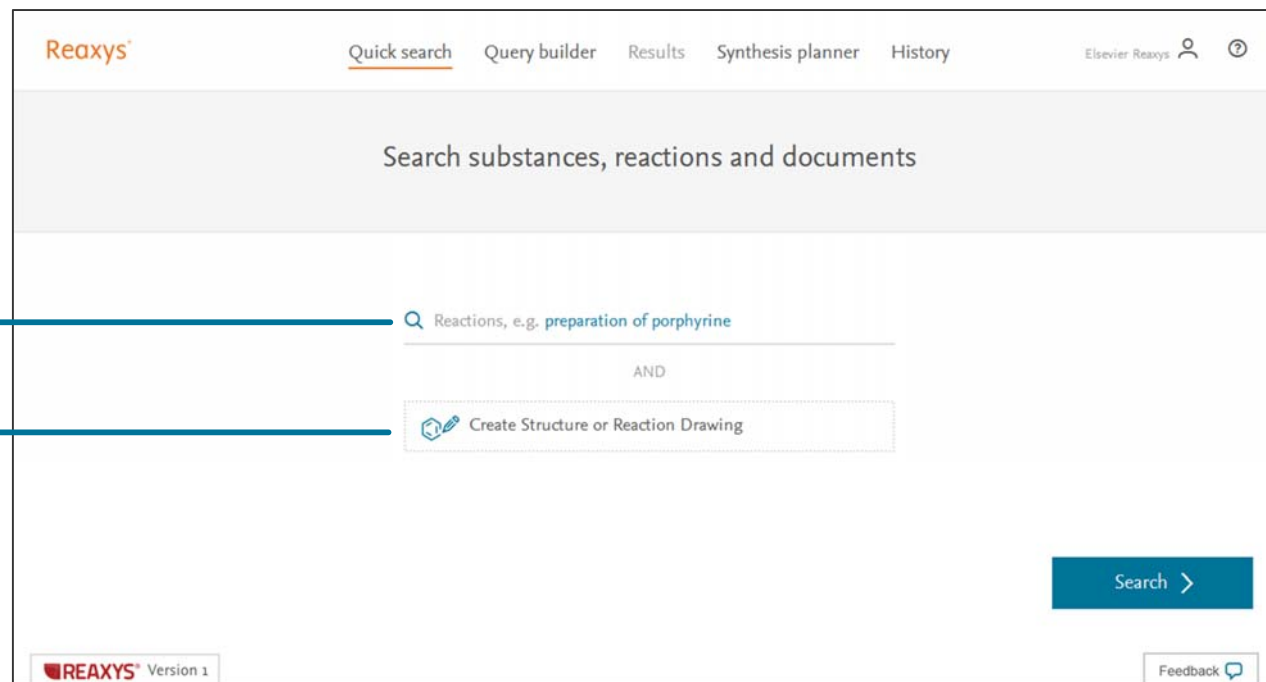
LITERATURE	
FEATURE	COMMENT
Quick search (See page 3)	Enter a term(s) in the Search Reaxys field and click Search . Examples: <ul style="list-style-type: none"> • publications about quasicrystals • Tetrahedron, 2014, 70, 2343 • published by Schrock
Quick search with Structure or Reaction Drawing (See page 4)	Note: Any structure or reaction query (see page 1) will primarily find substances or reactions. Any data point in those results has a reference, which provides additional links to documents. In addition you may click the documents link at the top of the page to view documents for the result set.
Query builder (See page 5 & 6)	<ol style="list-style-type: none"> 1. Click Query builder (See page 6). 2. Select one of the Quick Querylets (Structure, Molecular Formula, CAS RN or Doc Index) under the search button. <p>OR</p> <ol style="list-style-type: none"> 2. Search for properties using the Search properties field and Drag & Drop the property onto the Query builder. 3. If you have multiple search fields, use the appropriate Boolean operator (see page 7). 4. Click Search at the top of the screen and select the desired target content: e.g. Documents. <p>Note: Click Show fields to enter specific search values.</p>

PROPERTIES	
FEATURE	COMMENT
Quick search (See page 3)	Enter terms in the Search Reaxys field and click Search . Examples: <ul style="list-style-type: none"> • boiling point of benzene • density of quinolone
Quick search with Structure or Reaction Drawing (See page 4)	<ol style="list-style-type: none"> 1. Click the Create Structure or Reaction Drawing box. 2. Create the substance structure drawing. For more information on using the Marvin JS structure editor see: <ol style="list-style-type: none"> a. The Structure drawing workflow. b. Create a Structure Query in the Search for Substances Workflow. c. View our Tips for using ChemAxon Marvin JS d. Visit the ChemAxon Marvin JS website which includes a MarvinJS User's Guide 3. Click Transfer to query. 4. Enter property (e.g. boiling point) in the Search Reaxys field. 5. Click Search.
Query builder (See page 5 & 6)	<ol style="list-style-type: none"> 1. Click Query builder (See page 6). 2. Select one of the Quick Querylets (Structure, Molecular Formula, CAS RN or Doc Index) under the search button. <p>OR</p> <ol style="list-style-type: none"> 2. Search for properties using the Search properties field and Drag & Drop the property onto the Query builder. 3. Repeat for other properties as necessary. 4. If you have multiple search fields, use the appropriate Boolean operator (see page 7). 5. Click Search at the top of the screen and select the desired target content: e.g. Substances. <p>Note: Click Show fields to enter specific search values.</p>

Quick search

The text search option allows you to enter natural language terms (terms may be left, right or middle truncated using an asterisk (wildcard searching)).

Structure Search allows you to search for substances and reactions by drawing.



Reaxys

Quick search Query builder Results Synthesis planner History Elsevier Reaxys

Search substances, reactions and documents

Reactions, e.g. preparation of porphyrine

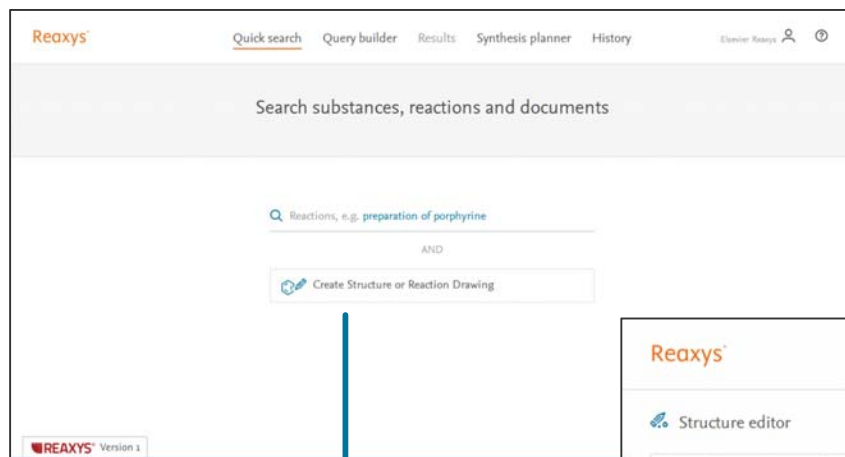
AND

Create Structure or Reaction Drawing

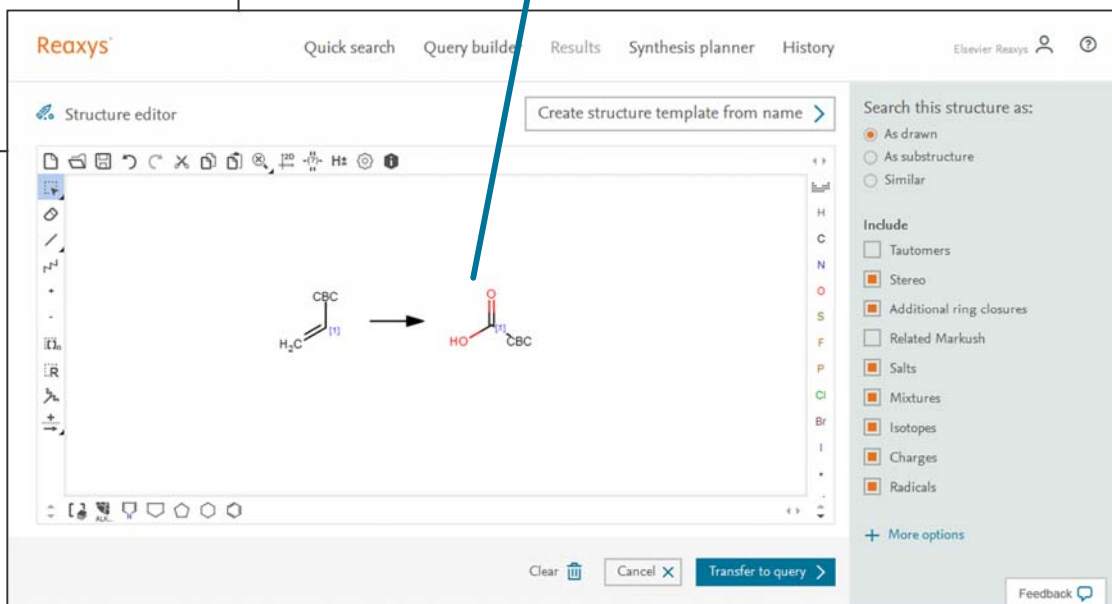
Search >

REAXYS Version 1 Feedback

Quick search with Structure or Reaction Drawing

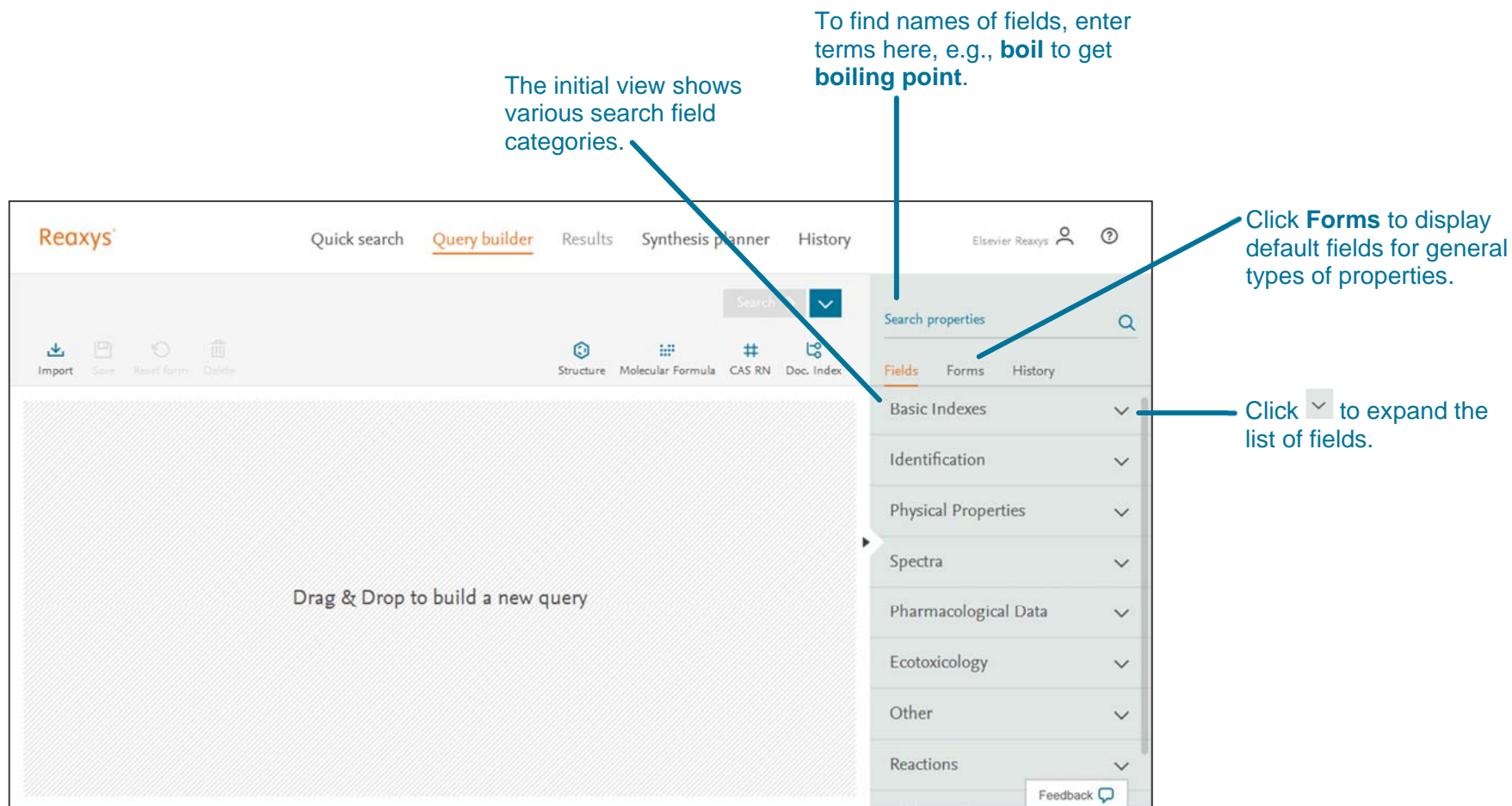


1. Click the **Create Structure or Reaction Drawing** box.



2. Use ChemAxon's Marvin JS tools to create a structure or reaction drawing.

Query builder Fields & Forms Panel



The initial view shows various search field categories.

To find names of fields, enter terms here, e.g., **boil** to get **boiling point**.

Click **Forms** to display default fields for general types of properties.

Click to expand the list of fields.

Drag & Drop to build a new query

Reaxys Quick search **Query builder** Results Synthesis planner History Elsevier Reaxys

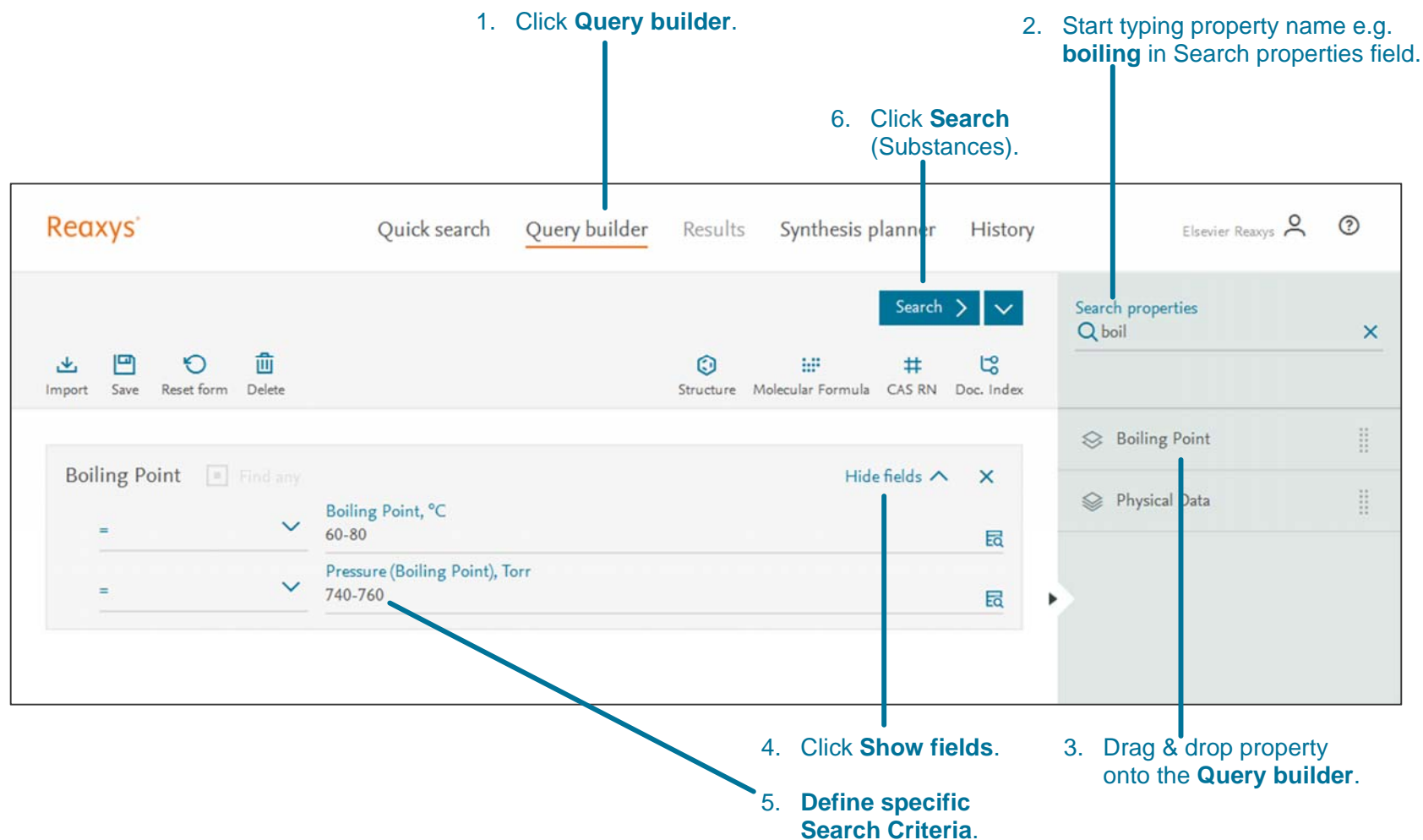
Search Search properties

Fields Forms History

Basic Indexes Identification Physical Properties Spectra Pharmacological Data Ecotoxicology Other Reactions

Import Save Reset form Delete Structure Molecular Formula CAS RN Doc. Index Feedback

Query builder Steps



1. Click **Query builder**.

2. Start typing property name e.g. **boiling** in Search properties field.

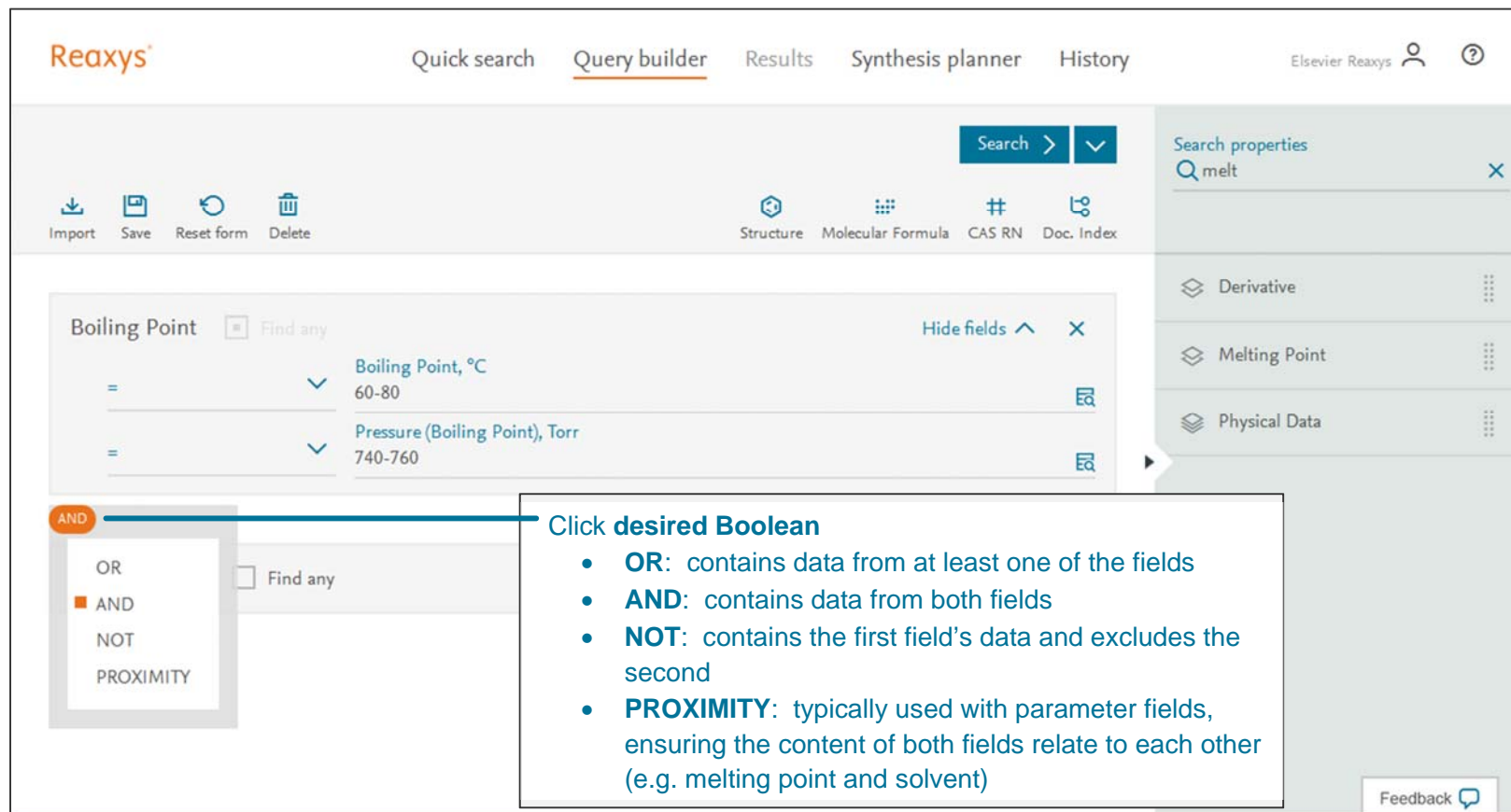
3. Drag & drop property onto the **Query builder**.

4. Click **Show fields**.

5. **Define specific Search Criteria.**

6. Click **Search (Substances)**.

Query builder: Multiple Properties and Booleans



The screenshot shows the Reaxys Query Builder interface. At the top, there are navigation tabs: Quick search, **Query builder**, Results, Synthesis planner, and History. On the right, there is a user profile for Elsevier Reaxys and a help icon. Below the navigation, there are utility icons for Import, Save, Reset form, and Delete. A search bar contains the text "Search" and a dropdown arrow. Below the search bar, there are icons for Structure, Molecular Formula, CAS RN, and Doc. Index. The main query area shows two conditions: "Boiling Point" with a value of "60-80" and "Pressure (Boiling Point), Torr" with a value of "740-760". A dropdown menu is open, showing Boolean operators: OR, **AND** (selected), NOT, and PROXIMITY. A callout box titled "Click desired Boolean" provides definitions for each operator.

Click desired Boolean

- **OR**: contains data from at least one of the fields
- **AND**: contains data from both fields
- **NOT**: contains the first field's data and excludes the second
- **PROXIMITY**: typically used with parameter fields, ensuring the content of both fields relate to each other (e.g. melting point and solvent)

2. Results

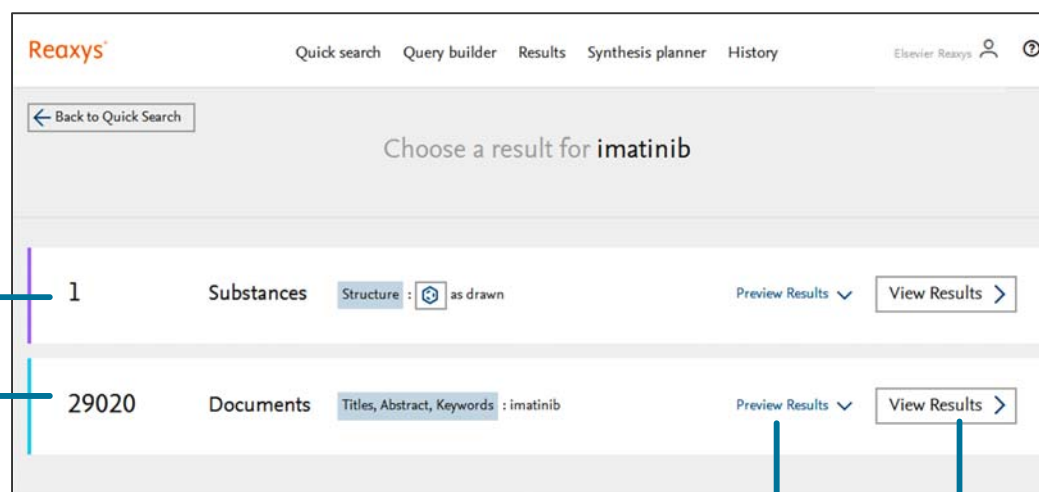
Quick search Results Preview

Reaxys analyzes the **Quick search** query input and returns result sets in a Results Preview (note: only **Quick search** queries will present a results preview, because of the nature of query interpretation).


The result sets depend on the term(s) entered. In this case, Reaxys identified the name of a substance and searched for the substance by structure in Substance Records and by name in Document Records.

This option indicates there is 1 **Substance Record** – found through an exact search of the structure.

This option indicates there are over 29,000 **Document Records** – found through a search on the text term.



The screenshot shows the Reaxys search results page for the query 'imatinib'. The page title is 'Choose a result for imatinib'. There are two result sets listed:

Count	Record Type	Search Criteria	Preview Results	View Results
1	Substances	Structure :  as drawn	Preview Results ▾	View Results >
29020	Documents	Titles, Abstract, Keywords : imatinib	Preview Results ▾	View Results >

Click **Preview Results** to view the top three results of a result set.

Click **View Results** to view all results from a result set.

In other cases, **Search Reaxys** may give options that display **Reaction Records** or **Document Records** with different combinations of search terms entered.

Quick search or Query builder Results – Substances

Use **Filters and Analysis** to narrow your results.

Keep track of the session through the 'breadcrumbs'.

Default display is by number of references, but other options are available. Slider enlarges the structure diagram.

Click links to see Preparation and Reaction information, and Documents (literature).

Click to expand filters.

Click links to view specific information on the substance.

Quick search or Query builder Results – Reactions

Use **Filters and Analysis** to narrow your results.

Keep track of the session through the 'breadcrumbs'.

The screenshot displays the Reaxys search results for reactions. On the left, a sidebar titled 'Filters and Analysis' lists various filter categories such as 'By Structure', 'Yield', 'Reagent/Catalyst', 'Solvent', 'Catalyst Classes', 'Solvent Classes', 'Product Availability', 'Reactant Availability', 'Reaction Classes', 'Document Type', and 'Publication Year'. A '1,762' count is shown at the top of the sidebar. The main content area shows '1,762 Reactions out of 4,573 Documents containing 6 Substances'. Below this, there is a chemical reaction scheme showing a reactant with a methyl group and a hydroxyl group reacting to form a product with a methyl group and a hydroxyl group. Below the reaction scheme, there is a table with columns for 'Yield', 'Conditions', and 'Reference'. The table shows a yield of 97%, conditions of 'With water; sodium hydroxide In 1,4-dioxane at 60°C for 2h; pH=10 - 14 Torr', and a reference to 'Lanzhou Institute of Chemical Physics, Chinese Academy of Sciences; Huang, Hanmin; Xia, Chungu; +1 other - US2013/303798, 2013, A1'. There are also links for 'Full Text' and 'Show details'. A 'Feedback' button is located at the bottom right of the interface.

Default display is by Reaxys Ranking, but other options are available.

Click links to view Full Text, details and more.

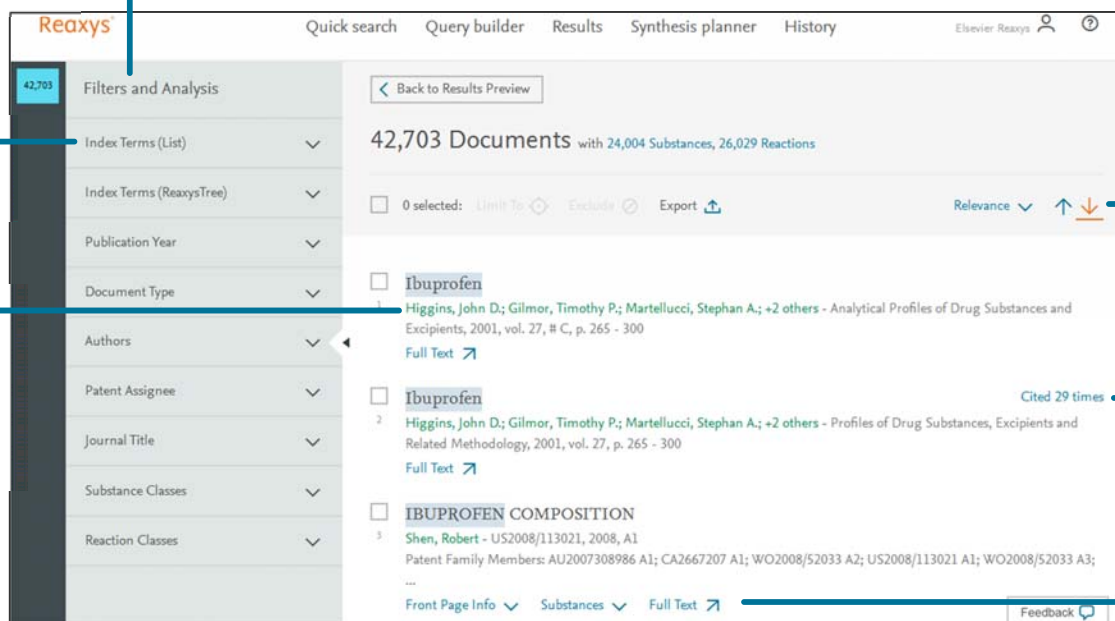
Click to expand filters.

Quick search or Query builder Results – Documents

Use **Filters and Analysis** options to narrow your results.

Use **Index Terms** to narrow documents by topics.

Click links for **author(s)** to explore details about their publications and additional analysis options in Scopus.



The screenshot shows the Reaxys search results page for 'Ibuprofen'. The interface includes a top navigation bar with 'Quick search', 'Query builder', 'Results', 'Synthesis planner', and 'History'. A left sidebar contains a 'Filters and Analysis' section with a '42,703' count and various filter categories: Index Terms (List), Index Terms (ReaxysTree), Publication Year, Document Type, Authors, Patent Assignee, Journal Title, Substance Classes, and Reaction Classes. The main content area displays '42,703 Documents with 24,004 Substances, 26,029 Reactions'. It shows a list of results for 'Ibuprofen' with checkboxes, document titles, authors, and 'Full Text' links. A 'Relevance' dropdown and sorting arrows are visible. At the bottom, there are links for 'Front Page Info', 'Substances', and 'Full Text', along with a 'Feedback' button.

Default display is by **Relevance**, but other options are available.

Click link to view citations in **Scopus**.

Click links to view **Full Text**, **Front Page info** (for patent records), **Substances**, **Reactions**, **Abstract** or **Index Terms**.

3. Analyze and Filter

Use the Filter & Analysis panel to narrow your results:

Use **Filters and Analysis** to narrow results. Index Terms are systematic and are a good way to filter records.

3. Applying this filter will reduce the original 302 Reactions to 81.

1. Click to expand the Catalyst Classes Filter

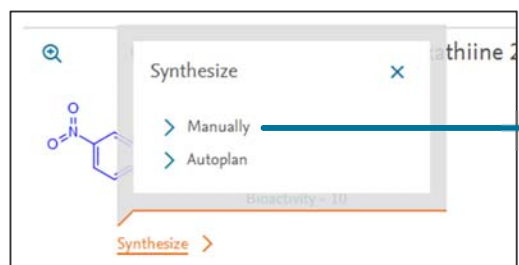
2. Click **More** to display additional filter options.

The screenshot shows the Reaxys interface with the 'Filters and Analysis' panel on the left. The panel is expanded to show 'Catalyst Classes' with a 'More' button. A detailed view of the 'Catalyst Classes' filter is shown, listing various catalysts and their counts. The 'active center' filter is selected, and the 'Mn' sub-filter is also selected, resulting in 81 reactions.

Filter	Count	Sub-filter	Count	Sub-filter	Count
active center	203	Mn	81	potassium permanganate	
heterogeneous	8	Ru	49	permanganate(VII) ion	
		Os	42	manganese (VII)-oxide	
		Cr	27	Manganese (II) acetate	
		B	11		
		Ni	11		
		Fe	10		
		Pd	6		
		Si	5		

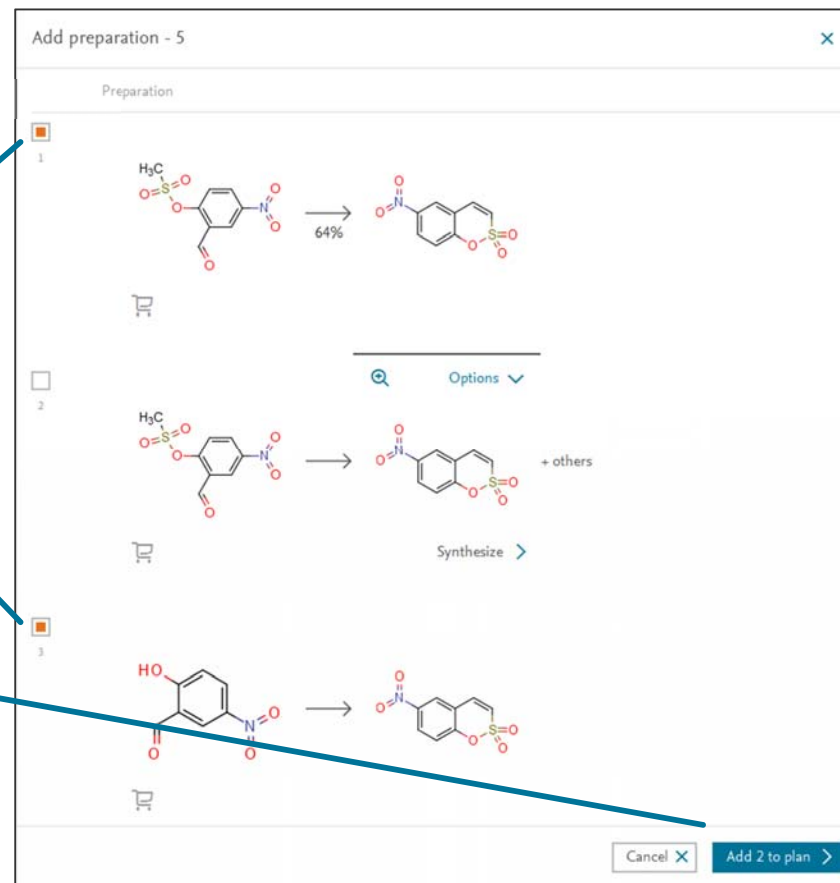
4. Synthesis planner - Manually

Build a synthesis pathway manually or let Reaxys do it automatically (see page 15). To begin, click **Synthesize** below a structure.



1. Click **Manually**.

2. In the **Add preparation** window, select reactions to add to your plan. Note: the product structure is not shown because it is the same as the starting structure.



3. Click **Add # to plan**.

Synthesis planner – Manually (continued)

1. From the **Synthesis planner**, click the Synthesis plan to view.

3. Click **Show conditions**.

Experimental details for the selected preparation step is displayed, scroll up or down to view details of other steps in the synthesis plan.

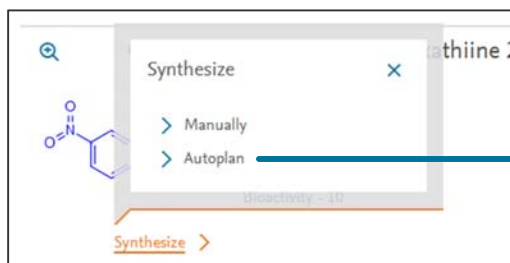
2. Click the **Synthesis step options** () to access:

- Show conditions
- Hide preparations
- Add preparations
- Remove preparations

Yield	Conditions	Reference
64%	Stage #1: 2-formyl-4-nitrophenyl methanesulfonate With DBU In dichloromethane at 0°C for 2h Inert atmosphere Stage #2: With pyridine; phosphoryl chloride at 0 - 20°C Experimental Procedure	Grandane, Aiga; Belyakov, Sergey; Trapencieris, Peteris; +1 other - Tetrahedron, 2012, vol. 68, # 27-28, p. 5541 - 5546 Full Text Cited 14 times Show details
	Stage #1: 2-formyl-4-nitrophenyl methanesulfonate With DBU In dichloromethane at 0°C for 2h Stage #2: With pyridine; phosphoryl chloride at 20°C for 3h Experimental part Experimental Procedure	Makrecka, Marina; Zalubovskis, Raivis; Vavers, Edijs; +3 others - Letters in Drug Design and Discovery, 2013, vol. 10, # 5, p. 410 - 414 Full Text Cited 3 times Show details

Synthesis planner - Autoplan

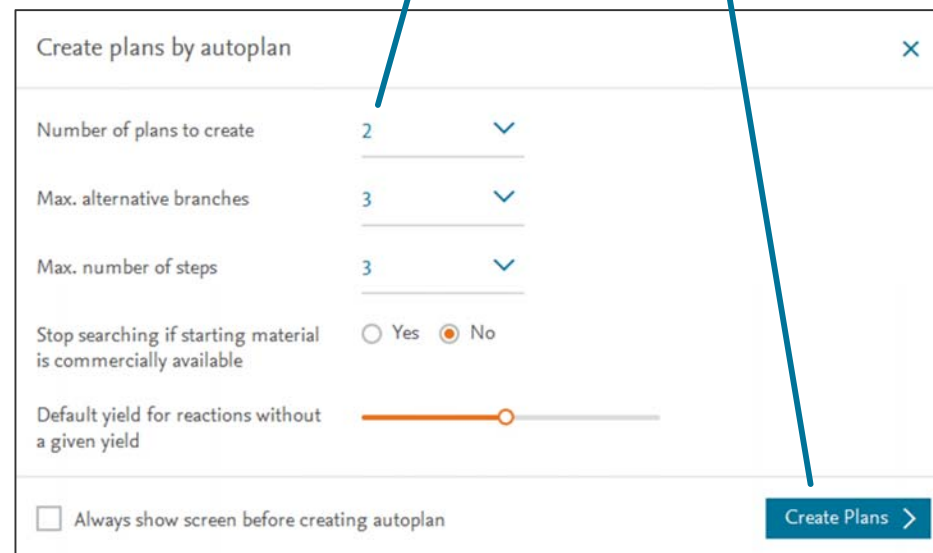
Let Reaxys build a synthesis pathway automatically. To begin, click **Synthesize** below a structure.



1. Click **Autoplan**.

2. Define parameters for automatically generating synthetic pathways.

3. Click **Create Plans**.



Create plans by autoplan	
Number of plans to create	2
Max. alternative branches	3
Max. number of steps	3
Stop searching if starting material is commercially available	<input type="radio"/> Yes <input checked="" type="radio"/> No
Default yield for reactions without a given yield	<input type="range"/>
<input type="checkbox"/> Always show screen before creating autoplan	
Create Plans >	

Synthesis planner – Autoplan (continued)

1. From the **Synthesis planner**, click the plan to view.

2. Click the **Synthesis step options** (**⋮**) to access:

- Show conditions
- Hide preparations
- Add preparations
- Remove preparations

3. Click **Show conditions**.

Experimental details for the selected preparation step is displayed, scroll up or down to view details of other steps in the synthesis plan.

Yield	Conditions	Reference
100%	With triethylamine In dichloromethane at 0 - 20°C for 2h Experimental part	Grandane, Aiga; Tanc, Muhammet; Di Cesare Mannelli, Lorenzo; +4 others - Journal of Medicinal Chemistry, 2015, vol. 58, # 9, p. 3975 - 3983 Full Text ↗ Cited 6 times ↗ Show details >
99%	With triethylamine In dichloromethane at 0 - 20°C for 22.1667h Experimental Procedure v	Grandane, Aiga; Belyakov, Sergey; Trapencieris, Peteris; +1 other - Tetrahedron, 2012, vol. 68, # 27-28, p. 5541 - 5546 Full Text ↗ Cited 14 times ↗ Show details >

5. Saving and Exporting

FEATURE	COMMENT
Saving	
From the Query builder	Define the query; click Save in the upper left. <ul style="list-style-type: none"> The query is saved to a .json file.
From the Synthesis planner	Not yet available.
From the History Page + Recent Tab	The History Page + Recent tab contains a list of searches from your current Reaxys session. Hover over a Recent Search , click Save , Enter a name, click Save . <ul style="list-style-type: none"> The Saved search can now be found under the Saved tab.
Exporting	
From the Results Page:	Select the document(s) you would like to export by ticking the boxes above the number of the search result. <ul style="list-style-type: none"> Click Export. Define Format, Range, Export data and Additional options. Click Export. To view the export progress, click Exports in the lower right corner of the screen. <ul style="list-style-type: none"> When the export is complete, click Download.
From the Synthesis planner:	Click Export . <ul style="list-style-type: none"> Click Export documents or Export reactions. Define Format and Additional options. Click Export. To view the export progress, click Exports in the lower right corner of the screen. <ul style="list-style-type: none"> When export is complete, click Download.