

## 1. Search

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

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

## Search (continued)

LITERATURE	
FEATURE	COMMENT
<b>Quick search</b> (See page 3)	Enter a term(s) in the search bar and click <b>Search</b> . Examples: <ul style="list-style-type: none"> <li>• publications about quasicrystals</li> <li>• Tetrahedron, 2014, 70, 2343</li> <li>• published by Schrock</li> </ul>
<b>Quick search</b> with Structure or Reaction Drawing (See page 3 & 4)	<b>Note:</b> 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.
<b>Query builder</b> (See page 5 & 6)	<ol style="list-style-type: none"> <li>1. Click <b>Query builder</b> (See page 6).</li> <li>2. Select one of the Quick Querylets (Structure, Molecular Formula, CAS RN or Doc Index) under the search button.</li> </ol> <p><b>OR</b></p> <ol style="list-style-type: none"> <li>2. Search for properties using the <b>Search properties</b> field and Drag &amp; Drop the property onto the <b>Query builder</b>.</li> <li>3. If you have multiple search fields, use the appropriate Boolean operator (see page 7).</li> <li>4. Click <b>Search</b> at the top of the screen and select the desired target content: e.g. <b>Documents</b>.</li> </ol> <p><b>Note:</b> Click <b>Exist</b> to enter specific search values.</p>

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

Reactions, e.g. Suzuki coupling

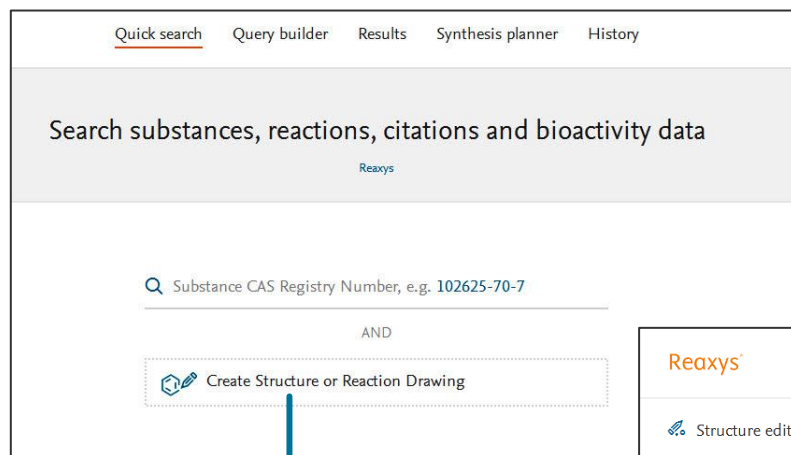
AND

Create Structure or Reaction Drawing

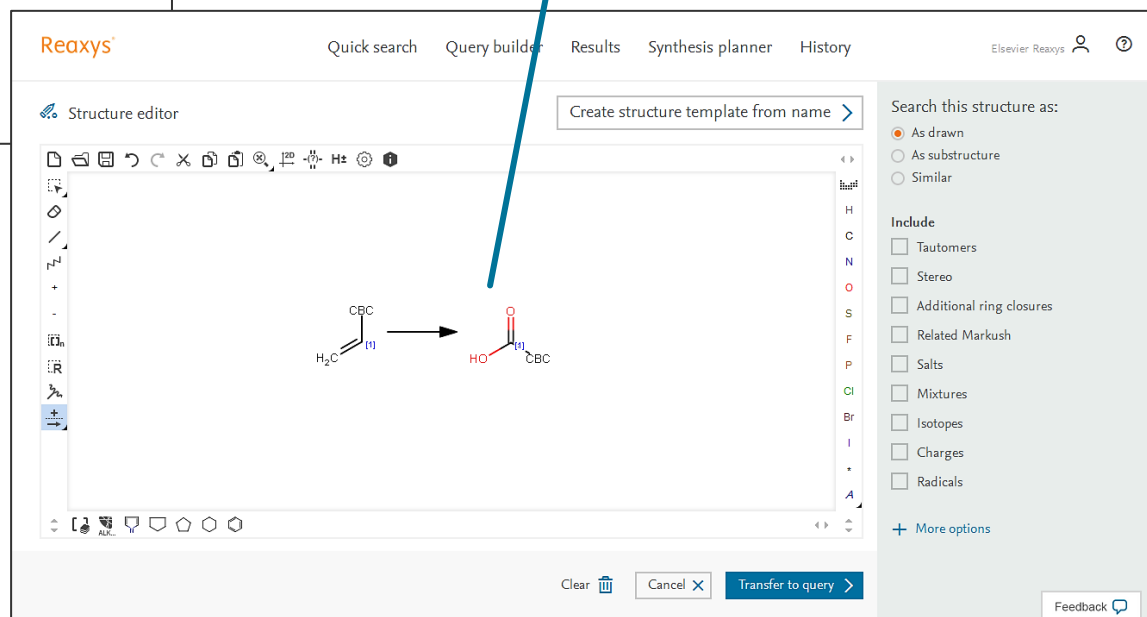
Search >

Feedback

## Quick search with Structure or Reaction Drawing

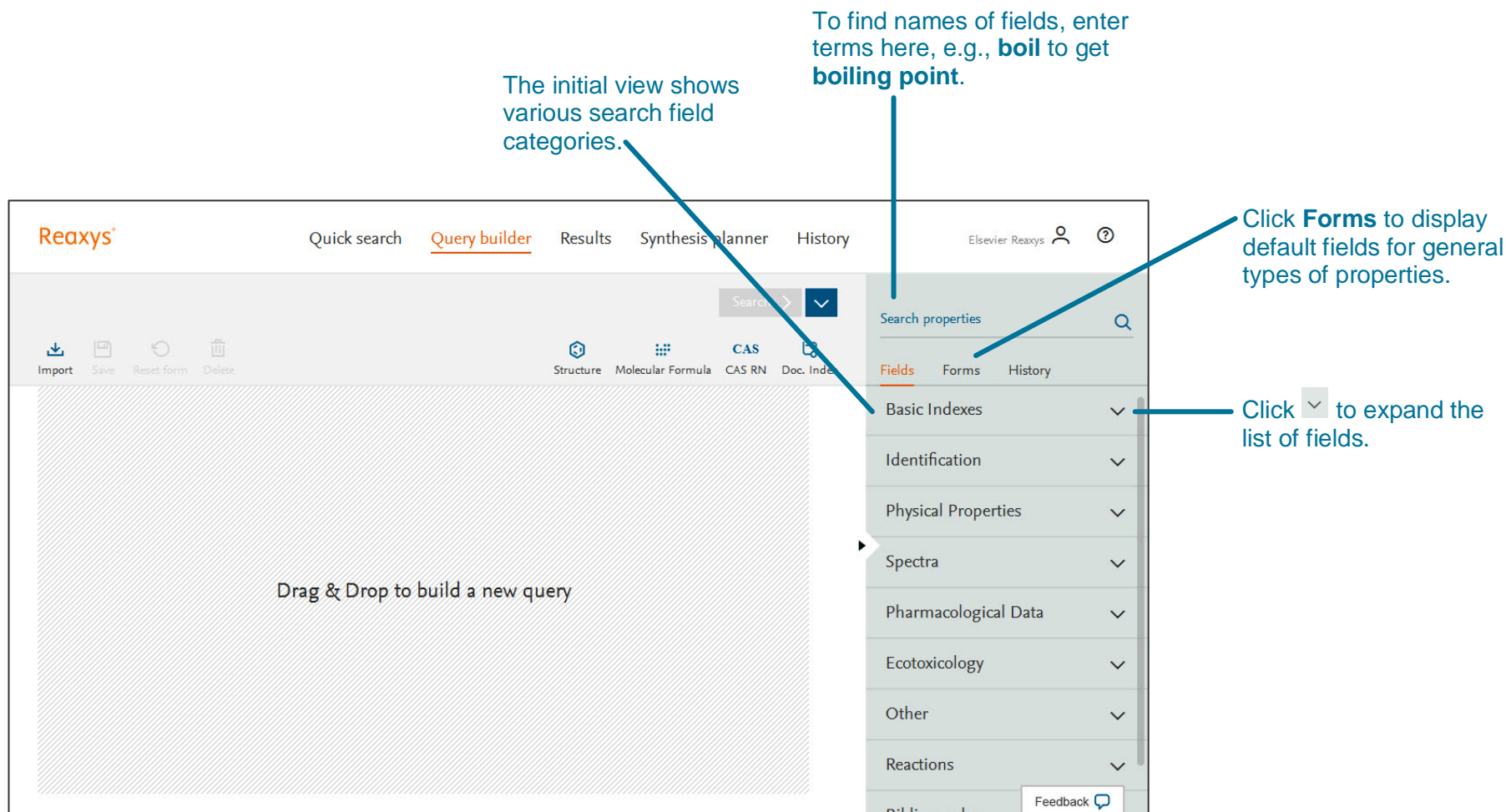


1. Click the **Create Structure or Reaction Drawing** box.



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  
 Import Save Reset form Delete  
 Structure Molecular Formula CAS RN Doc. Index  
 Search properties  
 Fields Forms History  
 Basic Indexes  
 Identification  
 Physical Properties  
 Spectra  
 Pharmacological Data  
 Ecotoxicology  
 Other  
 Reactions  
 Feedback

## Query builder Steps

1. Click **Query builder**.

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

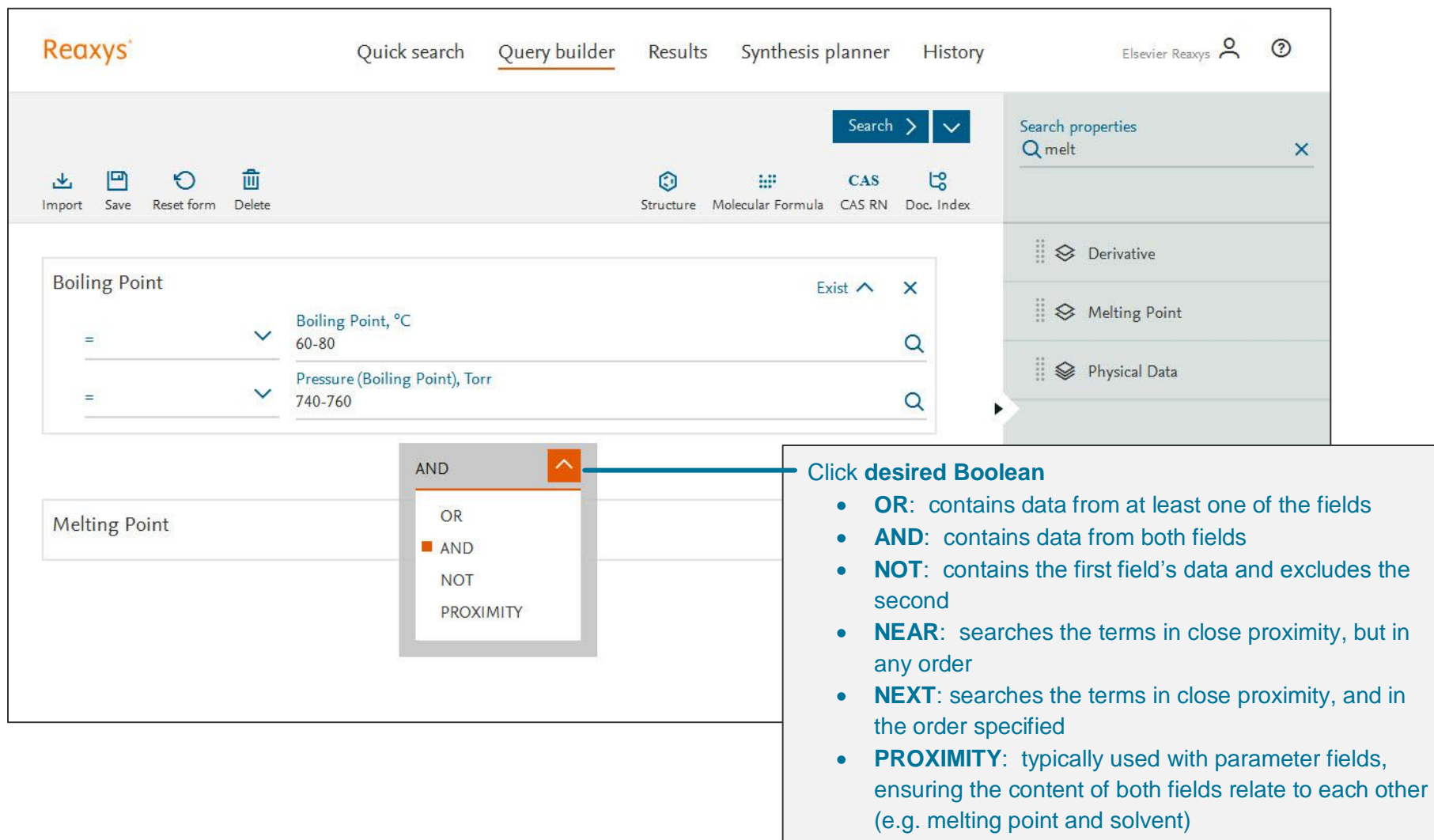
3. Drag & drop property onto the **Query builder**.

4. Click **Exist**.

5. Define specific Search Criteria.

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

## Query builder: Multiple Properties and Booleans



The screenshot shows the Reaxys Query Builder interface. The top navigation bar includes "Quick search", "Query builder" (selected), "Results", "Synthesis planner", and "History". The user is logged in as "Elsevier Reaxys". The main area displays a query for "Boiling Point" with two conditions: "Boiling Point, °C" (60-80) and "Pressure (Boiling Point), Torr" (740-760). Below this, a "Melting Point" field is visible. A dropdown menu is open, showing Boolean options: "AND" (selected), "OR", "NOT", and "PROXIMITY". A callout box on the right explains the Boolean options.

**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
- **NEAR**: searches the terms in close proximity, but in any order
- **NEXT**: searches the terms in close proximity, and in the order specified
- **PROXIMITY**: typically used with parameter fields, ensuring the content of both fields relate to each other (e.g. melting point and solvent)

## 2. Results

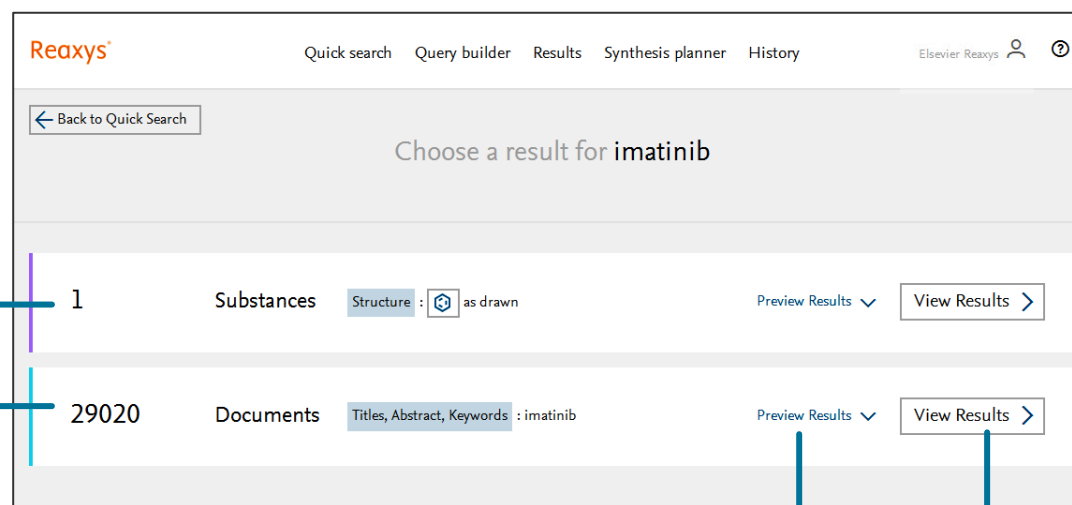
### Quick search Results Preview

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 28,000 **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 main result categories:

- Substances:** 1 result. Search criteria: Structure :  as drawn. Action: Preview Results (dropdown), View Results >
- Documents:** 29020 results. Search criteria: Titles, Abstract, Keywords : imatinib. Action: Preview Results (dropdown), 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'.

Click **More** to display further options.

The screenshot displays the Reaxys search results page. On the left, a sidebar titled 'Filters and Analysis' contains various filter categories such as 'Substances Classes', 'Molecular Weight', 'Availability', and 'Available data', each with a list of sub-filters and counts. The main content area shows '4 Substances' out of 3,228 documents containing 1,555 reactions. Below this, two substance entries are visible: 'ibuprofen' and '(S)-ibuprofen'. Each entry includes a chemical structure, a list of data types (e.g., Identification, Spectra, Physical Data, Bioactivity, Other Data), and links to 'Preparations', 'Reactions', and 'Documents'. A 'Feedback' button is located at the bottom right of the results area.

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).

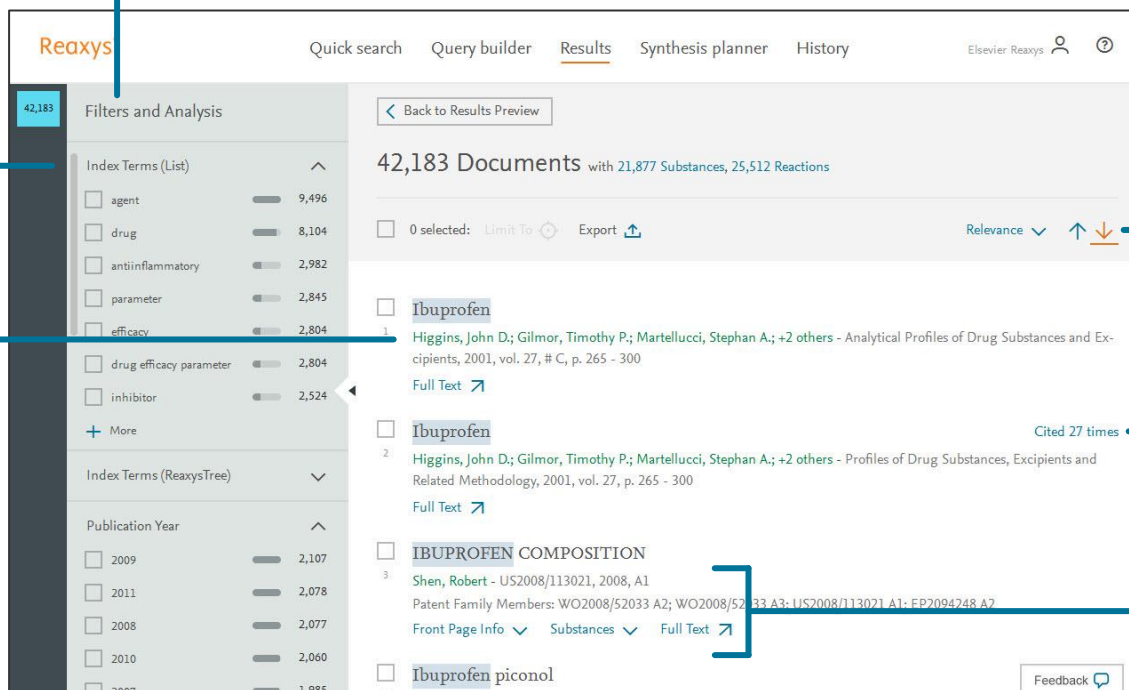
Click links to see specific information on the substance.

## 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 'Filters and Analysis' sidebar on the left shows 42,183 results and various filters like 'agent', 'drug', and 'antiinflammatory'. The main results area displays a list of documents, including 'Ibuprofen' by Higgins, John D.; Gilmore, Timothy P.; Martellucci, Stephan A.; +2 others. Each result has a 'Full Text' link. A 'Cited 27 times' link is also visible. At the bottom, there are links for 'Front Page Info', 'Substances', and 'Full Text' for a patent record.

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

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

Click links to **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.

1. Click  to display Filters and Analysis options for other fields.

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

3. Applying this filter will reduce the original 152 Reactions to 42.

The screenshot shows the Reaxys interface with the 'Filters and Analysis' panel open. The main results area shows '152 Reactions out of 119 Documents containing 298 Substances'. The 'Filters and Analysis' panel is on the left, and a detailed filter selection table is shown in a pop-up window.

**Filters and Analysis Panel:**

- Yield:
- Reagent/Catalyst:
- Solvent:
- Catalyst Classes:
  - active center
  - heterogeneous
  - + More**
- Solvent Classes
- Product Availability
- Reactant Availability
- Reaction Classes

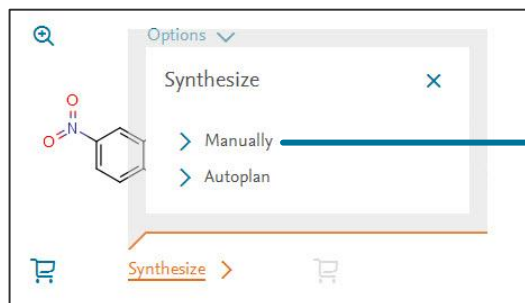
**Filter Selection Table:**

Filter	Count	Filter	Count	Filter	Count
<input checked="" type="checkbox"/> active center	97	<input checked="" type="checkbox"/> Mn	42	<input checked="" type="checkbox"/> potassium permanganate	41
<input type="checkbox"/> heterogeneous	6	<input type="checkbox"/> Os	21	<input checked="" type="checkbox"/> permanganate(VII) ion	1
		<input type="checkbox"/> Ru	20		
		<input type="checkbox"/> Cr	8		
		<input type="checkbox"/> Ni	8		
		<input type="checkbox"/> Fe	5		
		<input type="checkbox"/> B	4		
		<input type="checkbox"/> Si	4		
		<input type="checkbox"/> Pd	3		

Buttons: Clear selected, Back to Results Preview, Limit To, Export, Reaxys Ranking, Apply

## 4. Synthesis planner - Manually

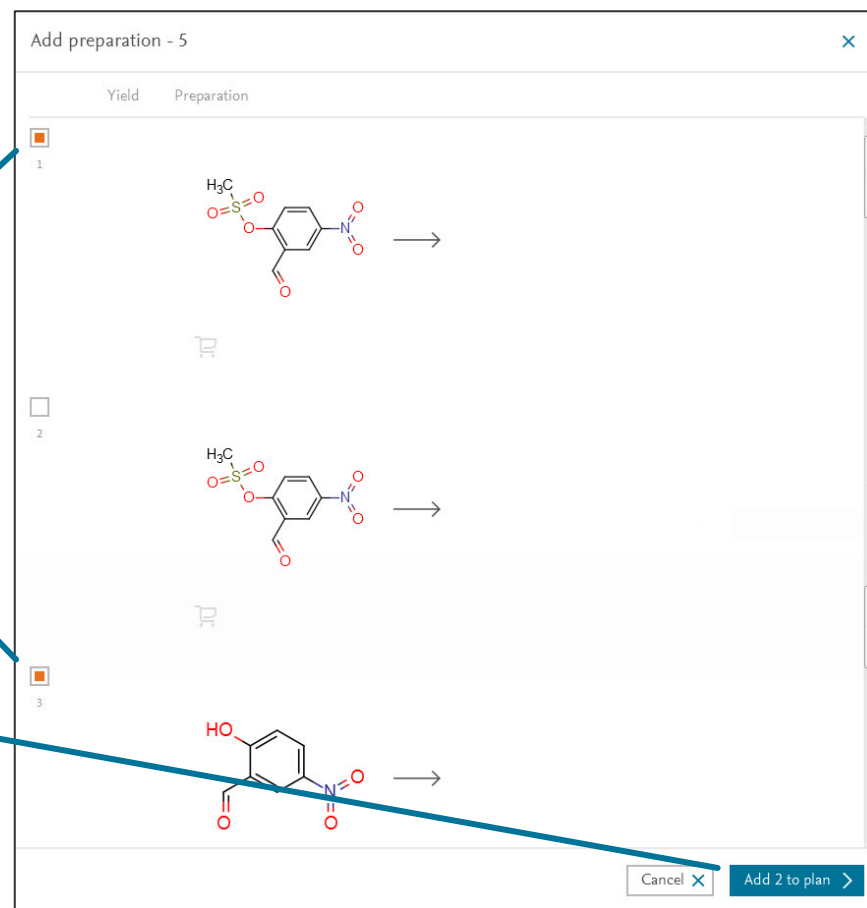
Build a synthesis pathway manually or let Reaxys do it automatically (see page 14). To begin, click **Synthesize** below a structure.



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**.



Yield	Preparation
<input checked="" type="checkbox"/>	1 <chem>CC(=O)Oc1ccc(cc1[N+](=O)[O-])OS(=O)(=O)C</chem> →
<input type="checkbox"/>	2 <chem>CC(=O)Oc1ccc(cc1[N+](=O)[O-])OS(=O)(=O)C</chem> →
<input checked="" type="checkbox"/>	3 <chem>CC(=O)Oc1ccc(O)cc1[N+](=O)[O-]</chem> →

Cancel X Add 2 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:

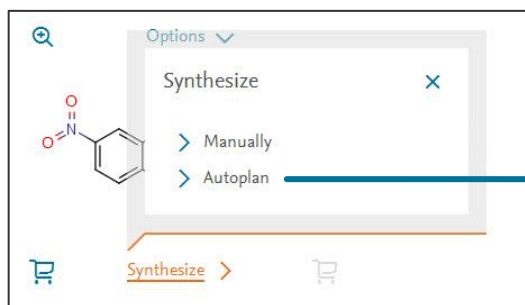
- Show conditions
- Hide preparations
- Add preparations
- Remove preparations

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, <b>2012</b> , vol. 68, # 27-28, p. 5541 - 5546 Full Text  Cited 13 times
	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: t...	Makrecka, Marina; Zalubovskis, Raivis; Vavers, Edijs; +3 others - Letters in Drug Design and Discovery, <b>2013</b> , vol. 10, # 5, p. 410 - 414 Full Text  Cited 1 times

[Done >](#)

## 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
✕

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Number of plans to create 2 ▼

Max. alternative branches 3 ▼

Max. number of steps 3 ▼

Stop searching if starting material is commercially available  Yes  No

Default yield for reactions without a given yield

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Always show screen before creating autoplan
Create Plans >

## Synthesis planner – Autoplan (continued)

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

The screenshot shows the Reaxys Synthesis Planner interface. On the left, there is a sidebar with 'Plan 1' and 'Plan 2'. The main area displays a reaction scheme with four steps. Step 1 is highlighted with a blue arrow pointing to its options menu. The reaction scheme shows the synthesis of a complex molecule from various starting materials, including a phenol derivative, a sulfonamide, and a sulfide.

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

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

A close-up of the synthesis step options menu, which is a small box with a close button (X) in the top right corner. It contains three items: 'Show conditions' with an information icon (i), 'Hide preparation' with a hide icon, and 'Remove preparation' with a trash can icon.

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.

The 'Conditions' dialog box is open, showing experimental details for 'Preparation - 2'. It features a table with columns for Yield, Conditions, and Reference. The table lists two entries with their respective yields, conditions, and references.

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 <a href="#">↗</a> Cited 5 times <a href="#">↗</a> Show details <a href="#">&gt;</a>
99%	With triethylamine In dichloromethane at 0 - 20°C for 22.1667h Experimental Procedure <a href="#">▼</a>	Grandane, Aiga; Belyakov, Sergey; Trapencieris, Peteris; +1 other - Tetrahedron, 2012, vol. 68, # 27-28, p. 5541 - 5546 Full Text <a href="#">↗</a> Cited 13 times <a href="#">↗</a> Show details <a href="#">&gt;</a>

A 'Done' button with a right arrow is located at the bottom right of the dialog box.

## 5. Saving and Exporting

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