

1. Search

SUBSTANCES	
FEATURE	COMMENT
Quick search as text (See page 3)	Enter a substance name, molecular formula or CAS number in the search 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 3 & 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. Create a Structure Query in the Search for Substances 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)	<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. OR 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. Note: Click Exist to enter specific search values.

REACTIONS	
FEATURE	COMMENT
Quick search as text (See page 3)	Enter a term(s) in the search 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 3 & 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. Create a Reaction Query in the Search for Reactions 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)	<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. OR 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. Note: Click Exist to enter specific search values.

Search (continued)

LITERATURE	
FEATURE	COMMENT
Quick search (See page 3)	Enter a term(s) in the search bar 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 3 & 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)	<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. OR <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. Note: Click Exist to enter specific search values.

PROPERTIES	
FEATURE	COMMENT
Quick search (See page 3)	Enter terms in the search bar 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 3 & 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. Create a Structure Query in the Search for Substances 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. 4. Enter property (e.g. boiling point) in the search bar. 5. Click Search.
Query builder (See page 5)	<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. OR <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. Note: Click Exist to enter specific search values.

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

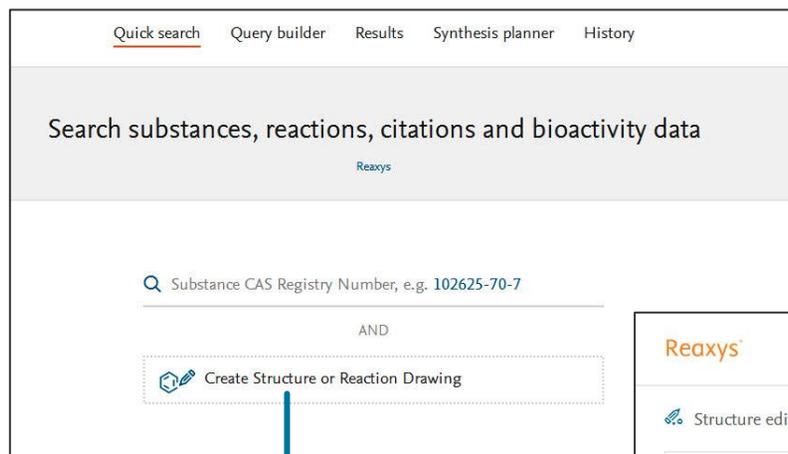
AND

 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.

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

Structure editor

Create structure template from name >

Structure editor toolbar: File, Edit, Copy, Paste, Undo, Redo, Zoom, Rotate, H±, etc.

Reaction shown: C=C → CC(=O)N

Search this structure as:

- As drawn
- As substructure
- Similar

Include:

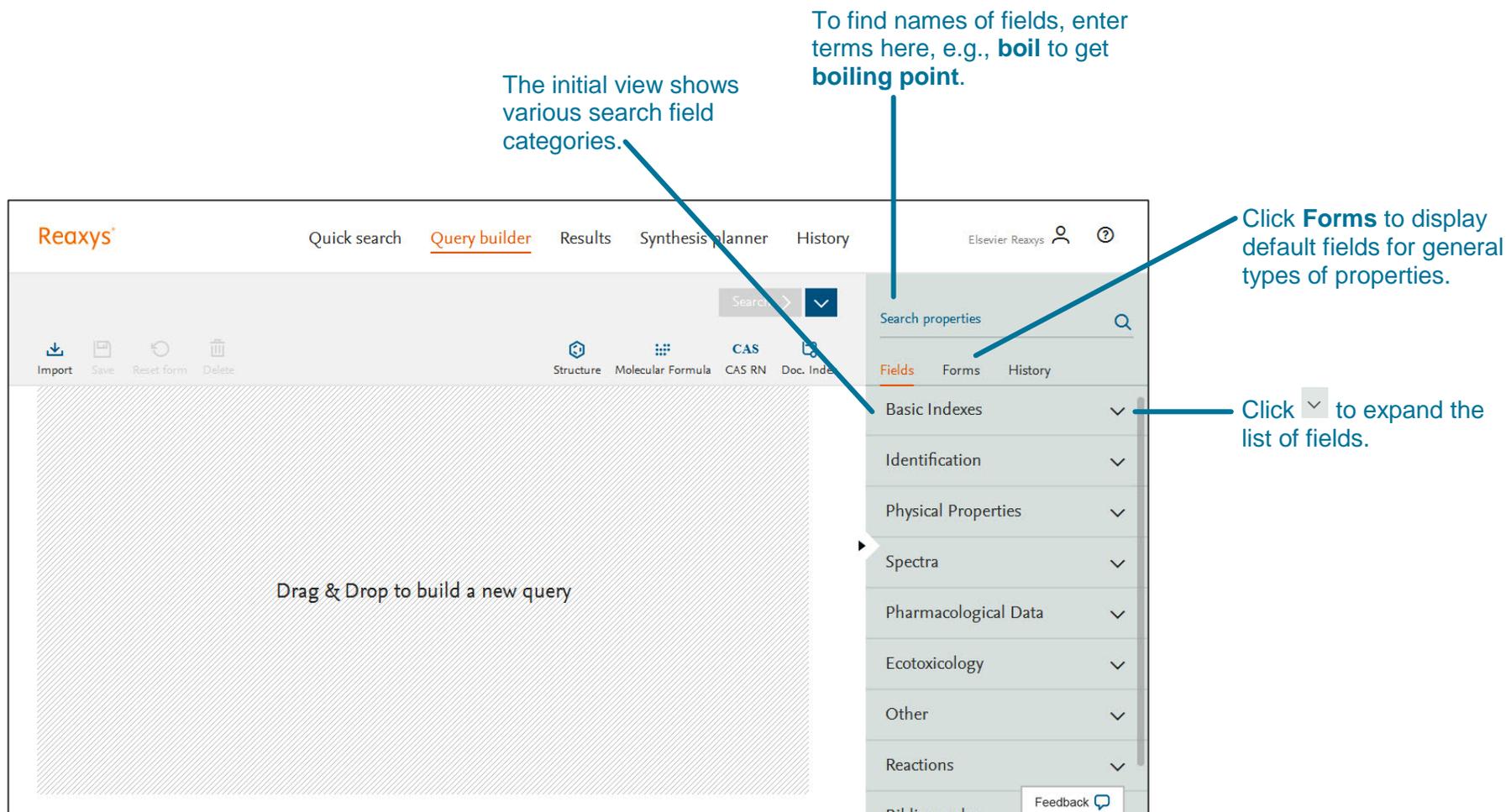
- Tautomers
- Stereo
- Additional ring closures
- Related Markush
- Salts
- Mixtures
- Isotopes
- Charges
- Radicals

+ More options

Clear | Cancel | Transfer to query >

Feedback

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 properties

Fields Forms History

Basic Indexes ▼

Identification ▼

Physical Properties ▼

Spectra ▼

Pharmacological Data ▼

Ecotoxicology ▼

Other ▼

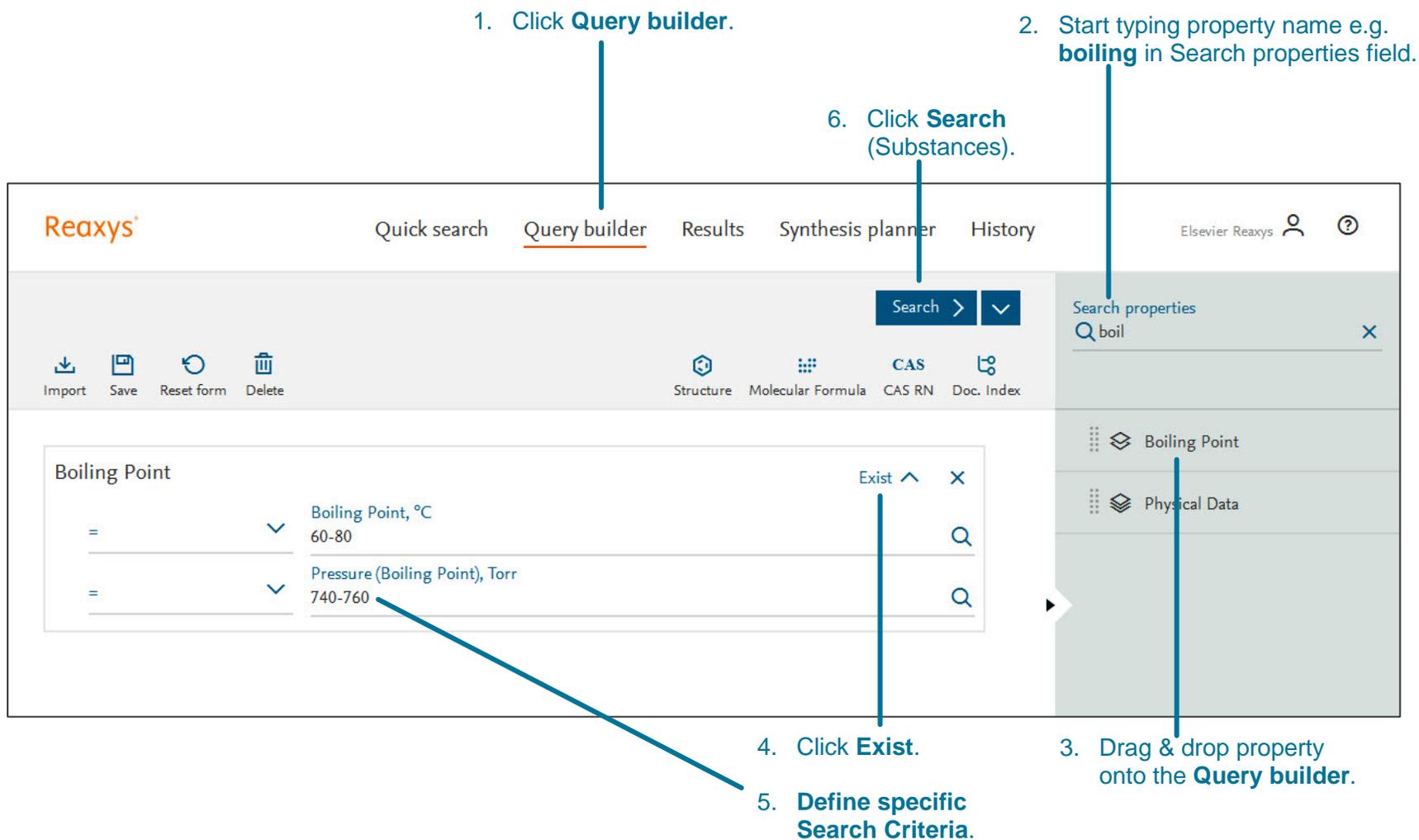
Reactions ▼

Publications Feedback

Import Save Reset form Delete

Structure Molecular Formula CAS RN Doc. Index

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. 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 icons for Import, Save, Reset form, and Delete. In the center, there are icons for Structure, Molecular Formula, CAS RN, and Doc. Index. A search bar contains the text 'melt'. Below the search bar, there are two filter boxes. The first is 'Boiling Point' with a dropdown menu showing 'Boiling Point, °C' (60-80) and 'Pressure (Boiling Point), Torr' (740-760). The second is 'Melting Point'. A dropdown menu for logical operators is open, showing 'AND' (selected), 'OR', 'NOT', and 'PROXIMITY'. A blue arrow points from the 'AND' option to a text box on the right.

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.

The screenshot shows the Reaxys interface with a search for 'imatinib'. The results are divided into two sections: 'Substances' and 'Documents'. The 'Substances' section shows 0 results with a search filter of 'Structure : as drawn'. The 'Documents' section shows 28898 results with a search filter of 'Titles, Abstract, Keywords : imatinib'. There are two buttons at the bottom right: 'Preview Results' and 'View Results'.

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.

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.

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).

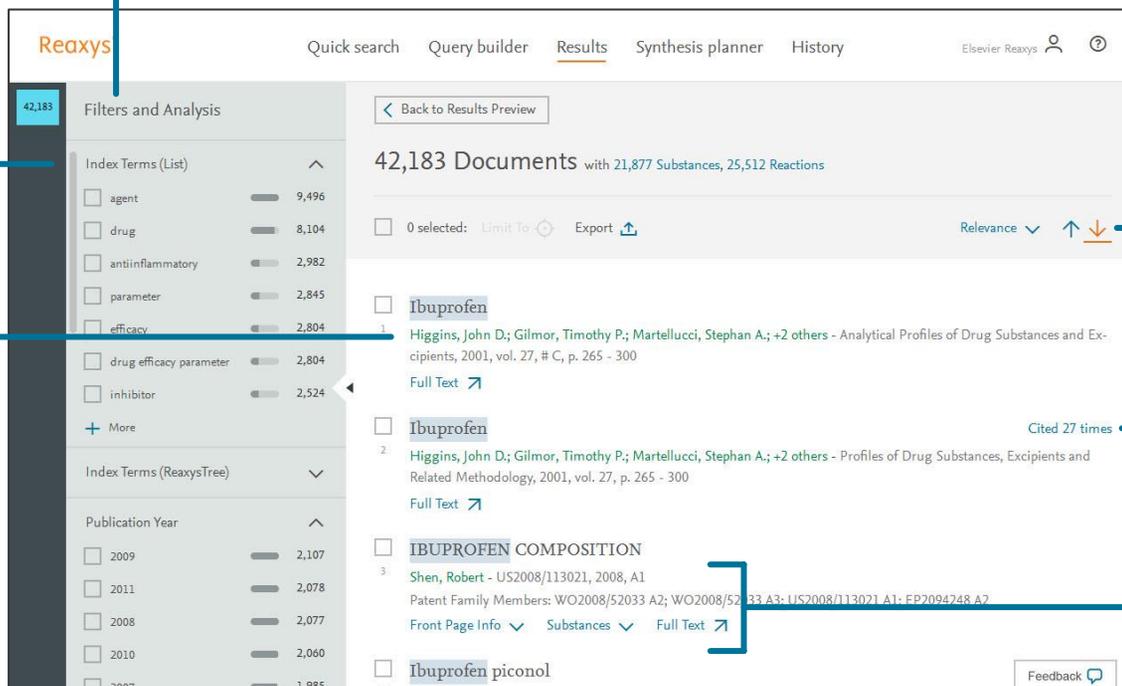
Click links to see specific information on the substance.

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 left sidebar contains the 'Filters and Analysis' section with a count of 42,183 documents. It includes 'Index Terms (List)' with categories like 'agent' (9,496), 'drug' (8,104), 'antiinflammatory' (2,982), 'parameter' (2,845), 'efficacy' (2,804), 'drug efficacy parameter' (2,804), and 'inhibitor' (2,524). Below this is 'Index Terms (ReaxysTree)' and 'Publication Year' with a list of years from 2009 to 2007. The main content area shows '42,183 Documents with 21,877 Substances, 25,512 Reactions'. It lists search results for 'Ibuprofen' with author information and 'Full Text' links. One result is highlighted with a box around the 'Full Text' link. Another result is highlighted with a box around the 'Substances' link. A 'Feedback' button is visible at the bottom right.

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.

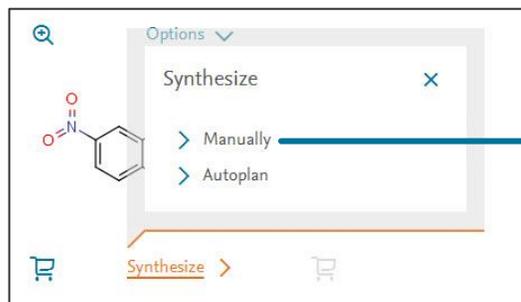
The screenshot shows the Reaxys interface with the 'Filters and Analysis' panel on the left and a detailed filter selection table on the right. The top bar shows '152 Reactions out of 119 Documents containing 298 Substances'. The 'Filters and Analysis' panel on the left has a dropdown menu open, showing 'Catalyst Classes' with options for 'active center' (97) and 'heterogeneous' (6). The 'More' button is highlighted. The detailed filter selection table on the right shows the following data:

Filter Category	Count	Filter Category	Count	Filter Category	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		

An 'Apply' button is located at the bottom right of the filter selection table.

4. Synthesis planner - Manually

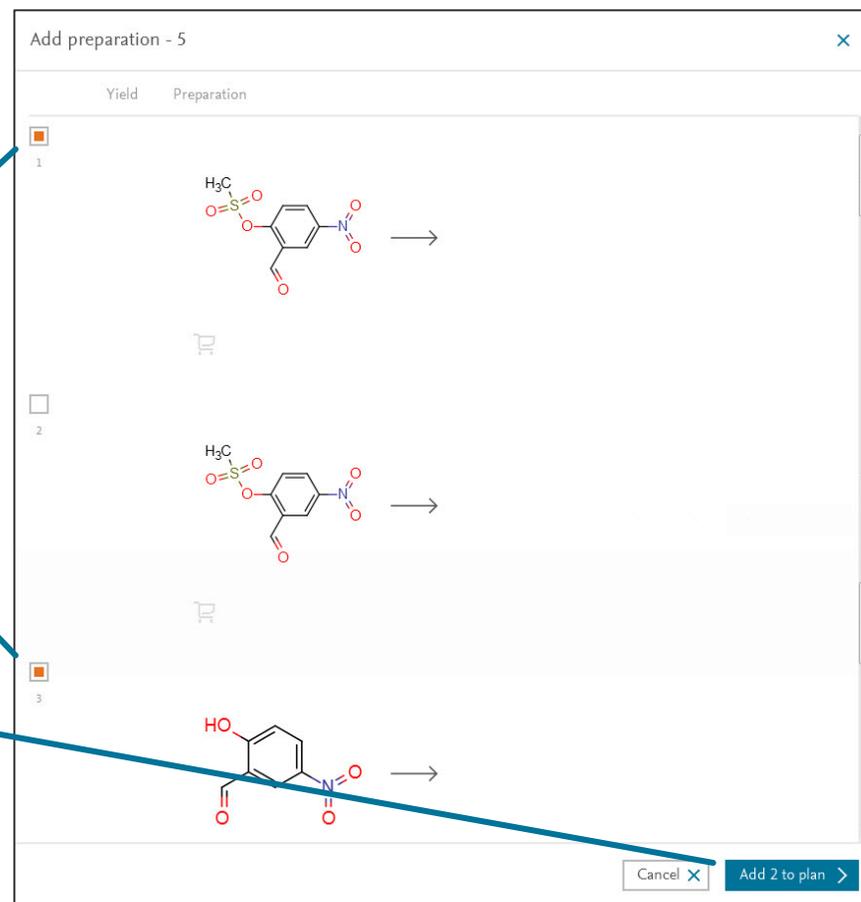
Build a synthesis pathway manually or let Reaxys do it automatically (see page 13). To begin, click **Synthesize** below a structure.



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)

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

- 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.

- Click the **Synthesis step options** () to access:

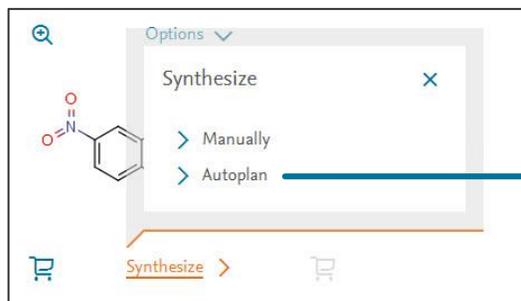
- Show conditions
- Hide preparations
- Add preparations
- Remove preparations

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 13 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	Makrecka, Marina; Zalubovskis, Raivis; Vavers, Edijs; +3 others - Letters in Drug Design and Discovery, 2013 , vol. 10, # 5, p. 410 - 414 Full Text Cited 1 times Show details

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 ×

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

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 2 is highlighted with a blue box and a vertical line pointing to the 'Show conditions' menu. The reaction scheme shows the synthesis of a sulfonamide derivative from a hydroxybenzaldehyde derivative.

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

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

A close-up of the 'Show conditions' menu. The menu is titled 'Show conditions' and has a close button (X) in the top right corner. It contains three options: 'Show conditions' (selected), 'Hide preparation', and 'Remove preparation'.

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'. The dialog has a title bar with a close button (X) and a 'Done' button at the bottom right. The main content is a table with columns for Yield, Conditions, and Reference.

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 5 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 13 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 :	<ul style="list-style-type: none"> • Click Export. • 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.