

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: • Atenolol • Pt(PPh₃)₃ • 102625-70-7
Quick search with Structure or Reaction Drawing (See page 3 & 4)	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: 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)	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: • preparation of porphyrine • phosphorylation • Suzuki coupling • Adler phenol oxidation
Quick search with Structure or Reaction Drawing (See page 3 & 4)	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: 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)	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)

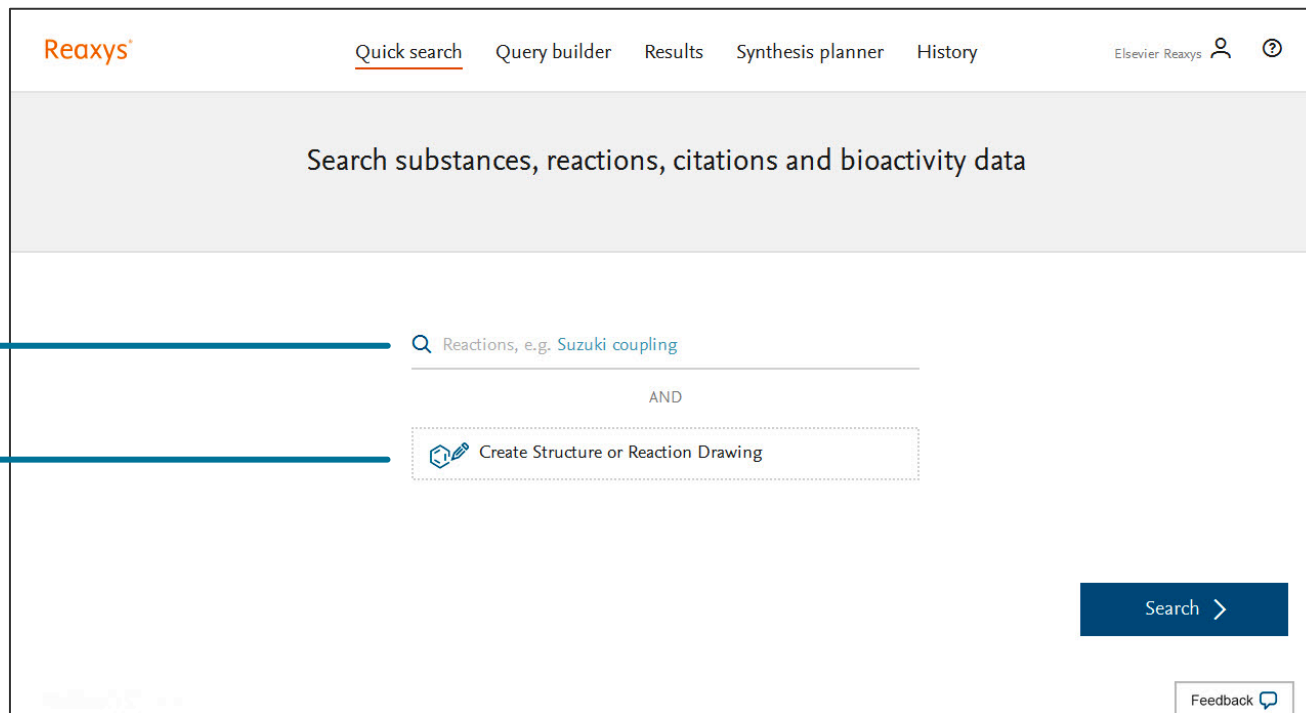
LITERATURE	
FEATURE	COMMENT
Quick search (See page 3)	Enter a term(s) in the search bar and click Search . Examples: - publications about quasicrystals - Tetrahedron, 2014, 70, 2343 - published by Schrock
Quick search with Structure or Reaction Drawing (See page 3 & 4)	Note: Any structure or reaction 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)	- Click Query builder (See page 6). - Select one of the Quick Querylets (Structure, Molecular Formula, CAS RN or Doc Index) under the search button. OR - Search for properties using the Search properties field and Drag & Drop the property onto the Query builder. - If you have multiple search fields, use the appropriate Boolean operator (see page 7). - 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: - boiling point of benzene - density of quinolone
Quick search with Structure or Reaction Drawing (See page 3 & 4)	- Click the Create Structure or Reaction Drawing box. - Create the substance structure drawing. For more information on using the Marvin JS structure editor see: - Create a Structure Query in the Search for Substances Workflow. - View our Tips for using ChemAxon Marvin JS - Visit the ChemAxon Marvin JS website which includes a MarvinJS User's Guide - Click Transfer to query. - Enter property (e.g. boiling point) in the search bar. - Click Search.
Query builder (See page 5)	- Click Query builder (See page 6). - Select one of the Quick Querylets (Structure, Molecular Formula, CAS RN or Doc Index) under the search button. OR - Search for properties using the Search properties field and Drag & Drop the property onto the Query builder. - Repeat for other properties as necessary. - If you have multiple search fields, use the appropriate Boolean operator (see page 7). - 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

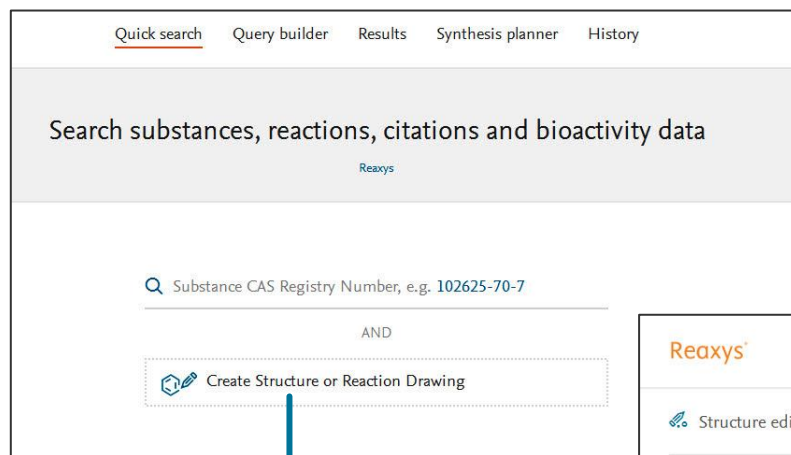
The text search option allows you to enter natural language terms (terms may be left, right or middle truncated using an asterisk (wildcard searching)).

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

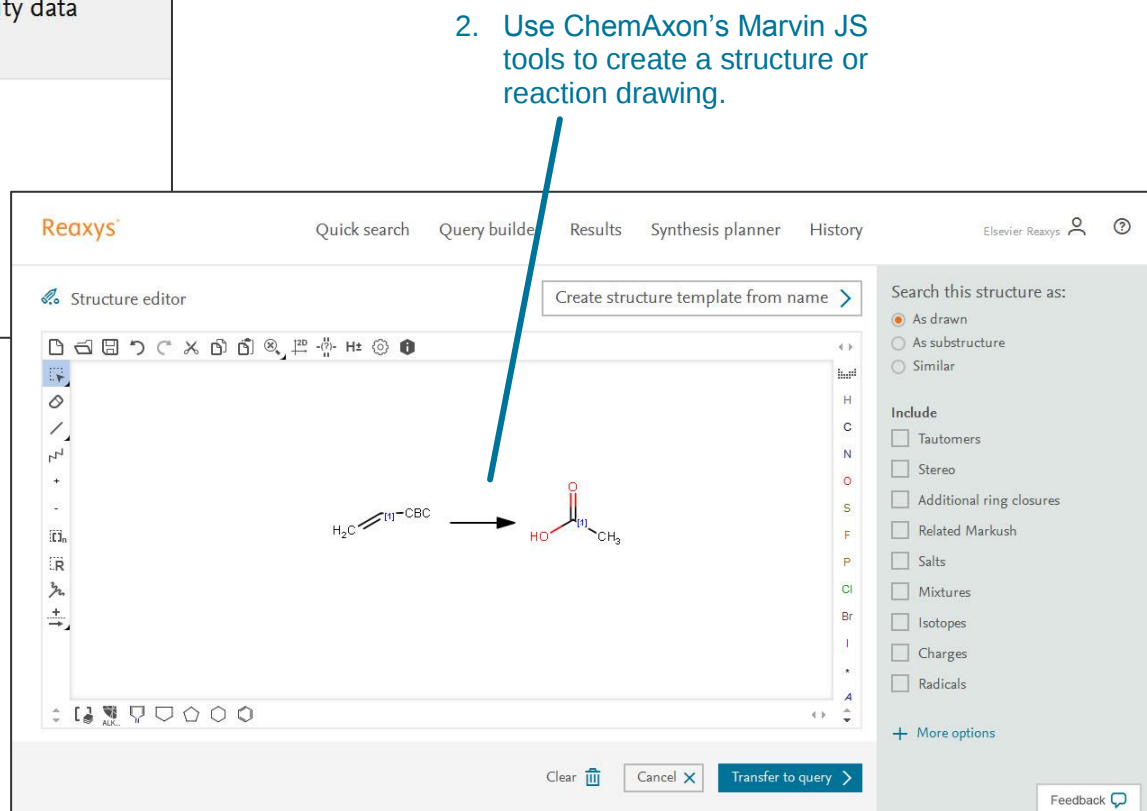


The screenshot shows the Reaxys Quick search interface. At the top, there is a navigation bar with the Reaxys logo, a 'Quick search' link (underlined), and other links: 'Query builder', 'Results', 'Synthesis planner', and 'History'. On the right side of the navigation bar, there is a user profile icon and a help icon. Below the navigation bar, there is a large grey header area with the text 'Search substances, reactions, citations and bioactivity data'. Below this header, there is a search input field containing the text 'Reactions, e.g. Suzuki coupling'. Below the input field, there is a dashed box containing a pencil icon and the text 'Create Structure or Reaction Drawing'. To the right of the search input field, there is a blue button with the text 'Search >'. At the bottom right of the interface, there is a 'Feedback' button with a speech bubble icon.

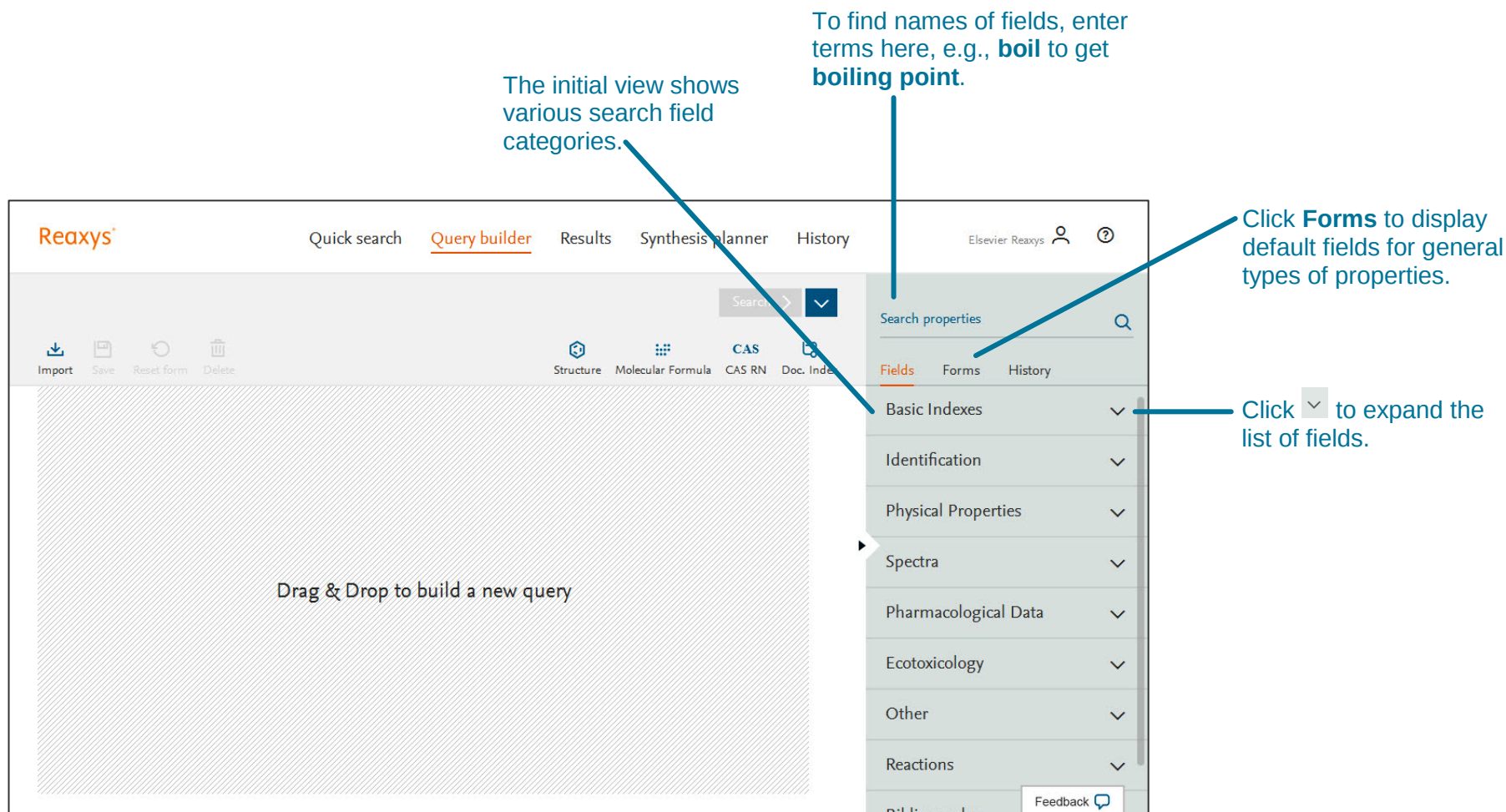
Quick search with Structure or Reaction Drawing



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



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**.

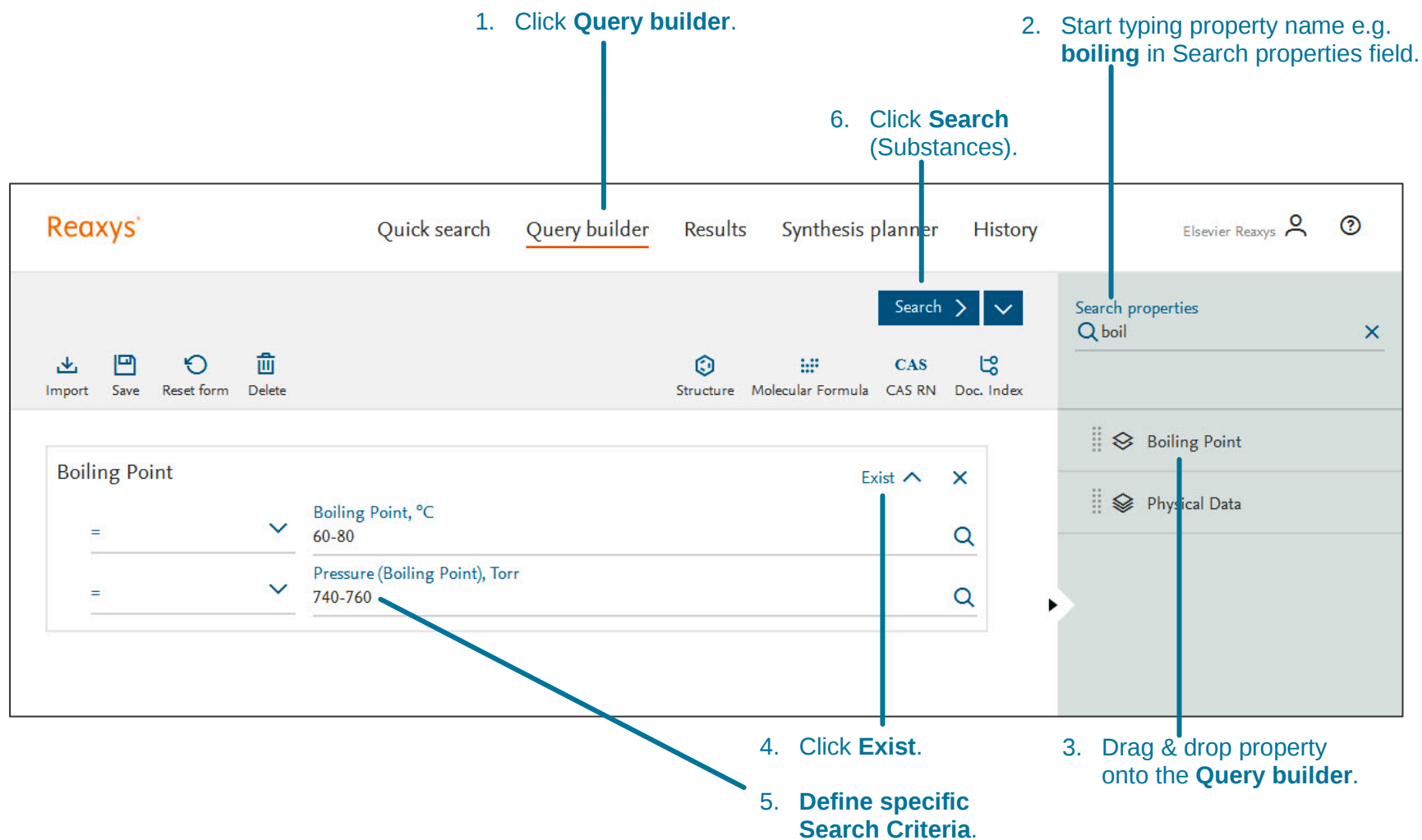
Click **Forms** to display default fields for general types of properties.

Click **▼** to expand the list of fields.

Drag & Drop to build a new query

The screenshot shows the Reaxys interface with the 'Query builder' tab selected. The main area is a large grey box with the text 'Drag & Drop to build a new query'. On the right, there is a sidebar with a search bar and a list of categories: Basic Indexes, Identification, Physical Properties, Spectra, Pharmacological Data, Ecotoxicology, Other, Reactions, and Publications. The 'Fields' tab is selected in the sidebar. A dropdown arrow is visible next to the 'Basic Indexes' category. The top navigation bar includes 'Quick search', 'Query builder', 'Results', 'Synthesis planner', and 'History'. The top right corner shows 'Elsevier Reaxys' and a user profile icon.

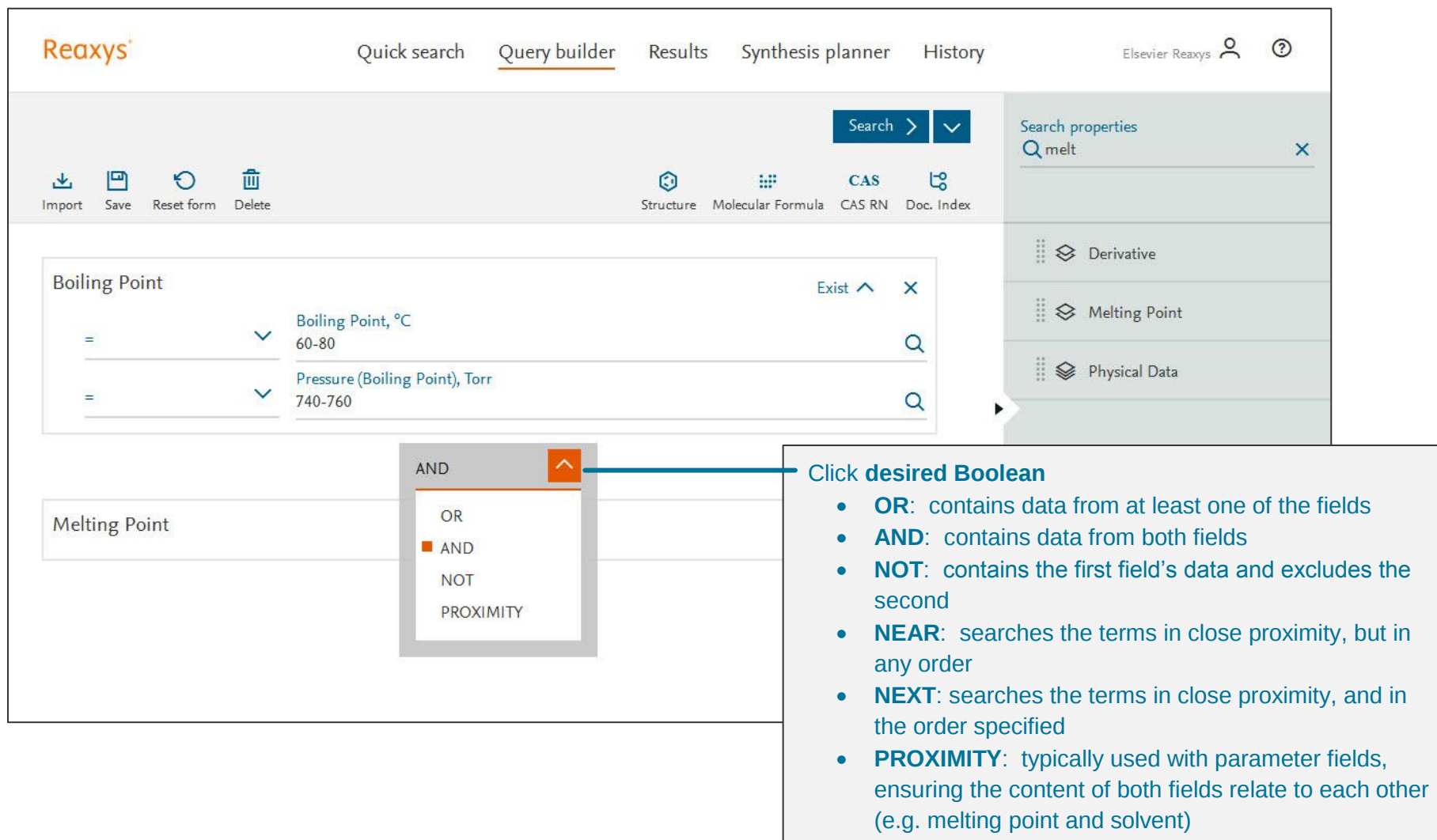
Query builder Steps



The screenshot shows the Reaxys Query Builder interface. The top navigation bar includes 'Quick search', 'Query builder' (highlighted), 'Results', 'Synthesis planner', and 'History'. On the right, there is a user profile and a help icon. Below the navigation bar, 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' button with a dropdown arrow is located above the 'CAS RN' icon. On the left, a 'Boiling Point' section contains two input fields: 'Boiling Point, °C' with a value of '60-80' and 'Pressure (Boiling Point), Torr' with a value of '740-760'. To the right of these fields is an 'Exist' button with an upward arrow and a close 'X' button. On the right side of the interface, a 'Search properties' panel is open, showing a search bar with 'boil' and a list of properties including 'Boiling Point' and 'Physical Data'. Arrows from numbered steps point to various elements: Step 1 points to the 'Query builder' tab; Step 2 points to the 'boil' text in the search properties bar; Step 3 points to the 'Boiling Point' property in the list; Step 4 points to the 'Exist' button; Step 5 points to the '60-80' value in the boiling point input field; and Step 6 points to the 'Search' button.

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 'Query builder' section has a 'Search' button and a dropdown menu. Below the search bar, there are icons for 'Import', 'Save', 'Reset form', and 'Delete'. The main query area shows two properties: 'Boiling Point' and 'Melting Point'. The 'Boiling Point' property is set to 'Boiling Point, °C' with a range of '60-80'. The 'Melting Point' property is set to 'Pressure (Boiling Point), Torr' with a range of '740-760'. A dropdown menu is open for the 'Boiling Point' property, showing 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

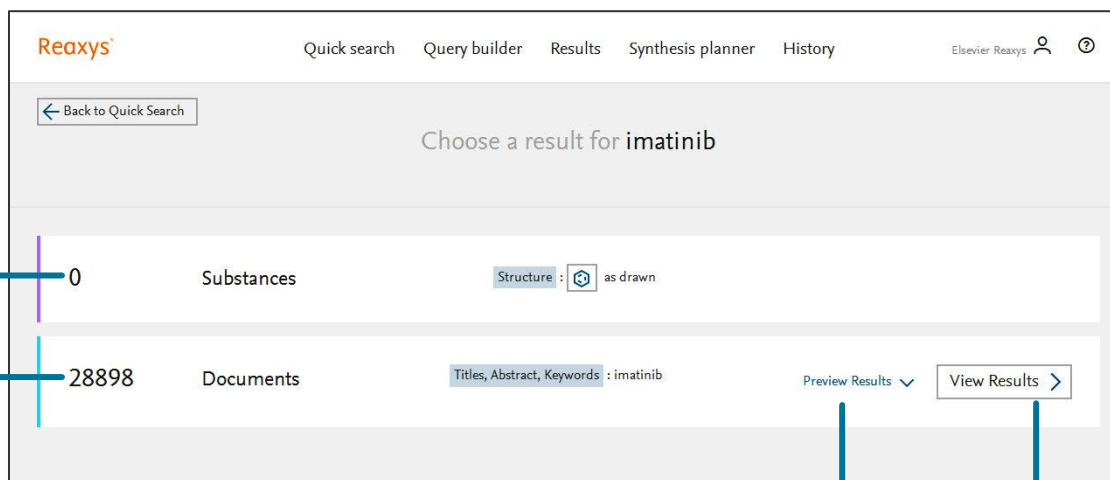
Quick search Results Preview

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 interface with the following elements:

- Navigation Bar:** Quick search, Query builder, Results, Synthesis planner, History. User: Elsevier Reaxys.
- Header:** Choose a result for imatinib
- Results Table:**

Count	Record Type	Search Criteria
0	Substances	Structure :  as drawn
28898	Documents	Titles, Abstract, Keywords : imatinib
- Actions:**
 - Preview Results** (dropdown arrow)
 - View Results** (right arrow)

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

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

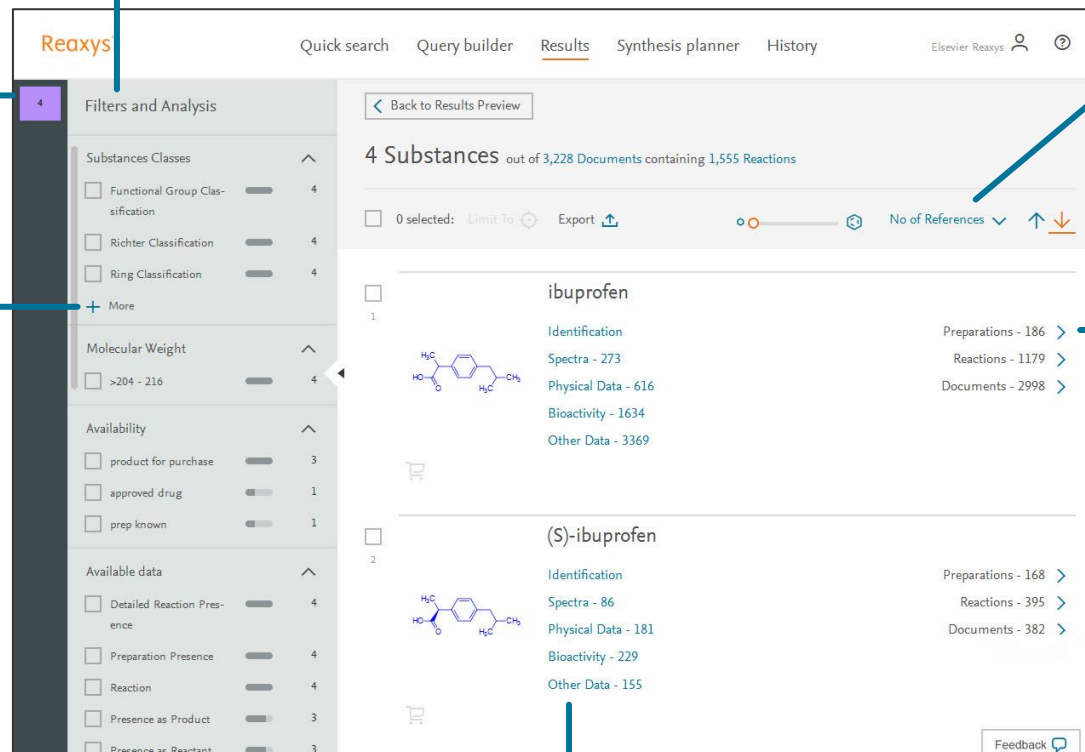
In other cases, **Search Reaxys** may give options that display **Reaction Records** or **Document Records** with different combinations of search terms entered.

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.



Reaxys

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

Elsevier Reaxys

4 Substances out of 3,228 Documents containing 1,555 Reactions

0 selected: Limit To Export

No of References

ibuprofen

Identification
Spectra - 273
Physical Data - 616
Bioactivity - 1634
Other Data - 3369

Preparations - 186
Reactions - 1179
Documents - 2998

(S)-ibuprofen

Identification
Spectra - 86
Physical Data - 181
Bioactivity - 229
Other Data - 155

Preparations - 168
Reactions - 395
Documents - 382

Feedback

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).

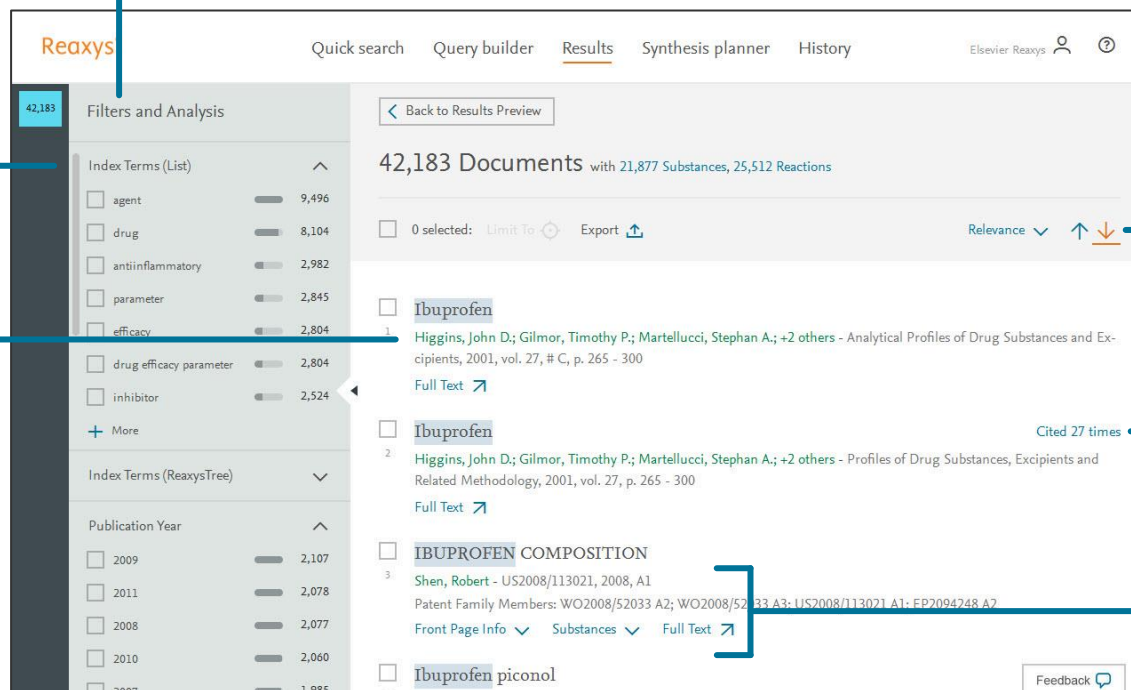
Click links to see specific information on the substance.

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 displays the Reaxys search results page. On the left, the 'Filters and Analysis' sidebar shows 42,183 documents. It includes sections for 'Index Terms (List)' with checkboxes for 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 from 2009 to 2007. The main results area shows '42,183 Documents with 21,877 Substances, 25,512 Reactions'. A 'Back to Results Preview' button is at the top. Below the count, it says '0 selected: Limit To Export'. The results list includes three entries for 'Ibuprofen': 1. 'Higgins, John D.; Gilmor, Timothy P.; Martellucci, Stephan A.; +2 others - Analytical Profiles of Drug Substances and Excipients, 2001, vol. 27, # C, p. 265 - 300' with a 'Full Text' link; 2. 'Higgins, John D.; Gilmor, Timothy P.; Martellucci, Stephan A.; +2 others - Profiles of Drug Substances, Excipients and Related Methodology, 2001, vol. 27, p. 265 - 300' with a 'Full Text' link and 'Cited 27 times'; 3. 'IBUPROFEN COMPOSITION' by 'Shen, Robert - US2008/113021, 2008, A1' with 'Front Page Info', 'Substances', and 'Full Text' links. A 'Feedback' button is 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

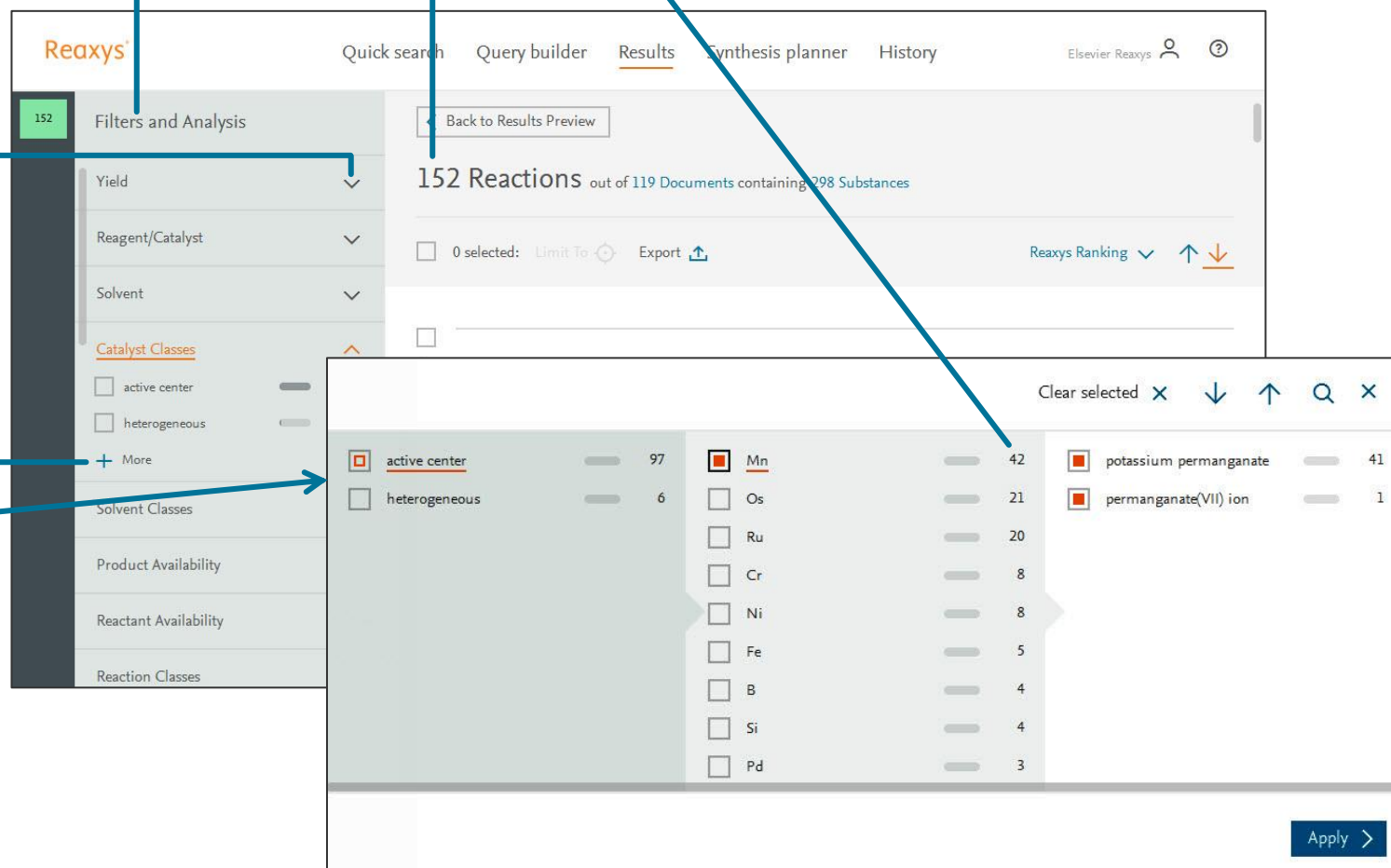
Use the **Filter & Analysis** panel to narrow your results:

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.

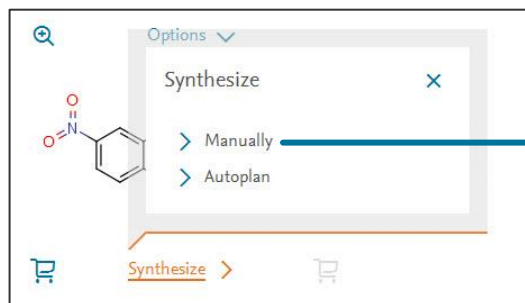


The screenshot shows the Reaxys interface with the 'Results' tab selected. The 'Filters and Analysis' panel is open on the left, showing 152 reactions. A dropdown menu is open for the 'Catalyst Classes' filter, showing options like 'active center' and 'heterogeneous'. A 'More' button is visible. A detailed filter selection dialog is open, showing a list of filters and their counts. The 'active center' filter is selected, reducing the results to 42 reactions.

Filter	Count
active center	97
heterogeneous	6
Mn	42
Os	21
Ru	20
Cr	8
Ni	8
Fe	5
B	4
Si	4
Pd	3
potassium permanganate	41
permanganate(VII) ion	1

4. Synthesis planner - Manually

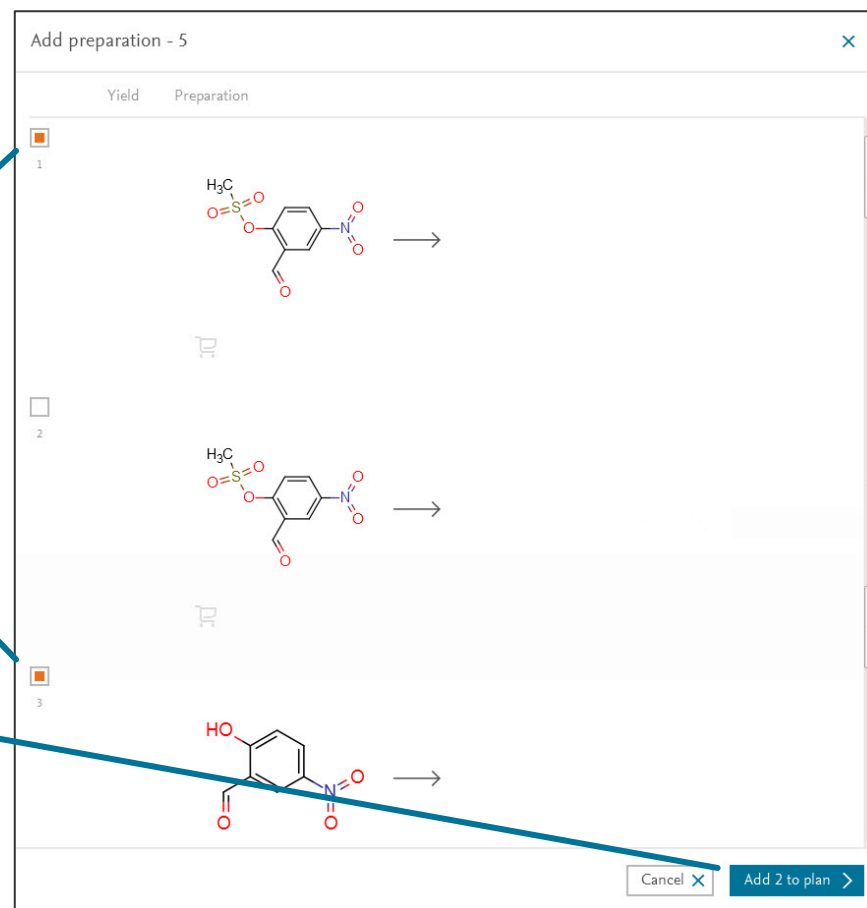
Build a synthesis pathway manually or let Reaxys do it automatically (see page 13). To begin, click **Synthesize** below a structure.



1. Click **Manually**.

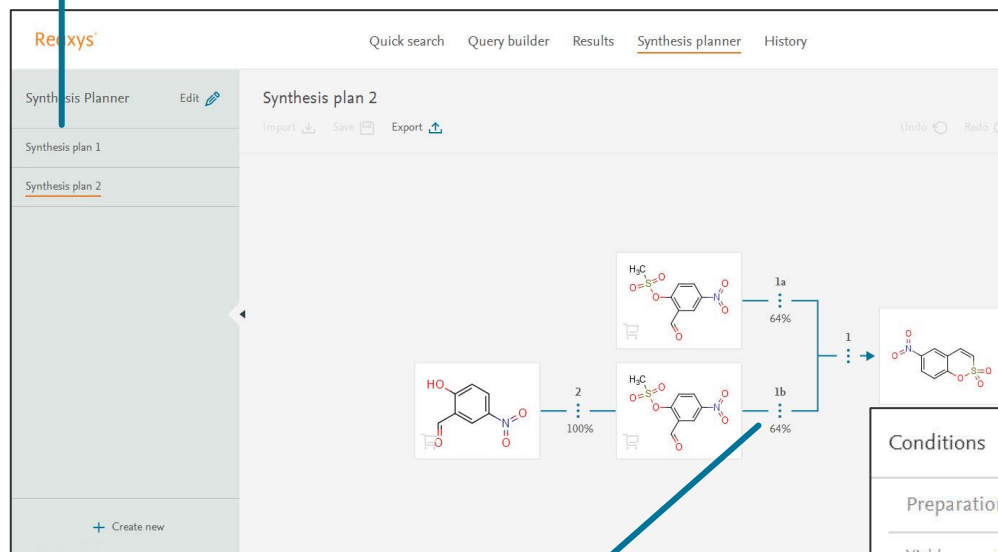
2. In the **Add preparation** window, select reactions to add to your plan.
Note: the product structure is not shown because it is the same as the starting structure.

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



Synthesis planner – Manually (continued)

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



ⓘ Show conditions
 ⌵ Hide preparation
 🗑️ 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.

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

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

Conditions

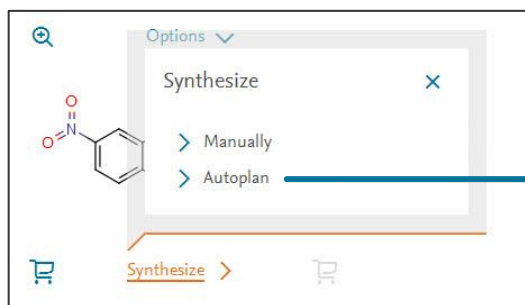
Preparation - 1b

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 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 1 times ↗ Show details ➤

Done ➤

Synthesis planner - Autoplan

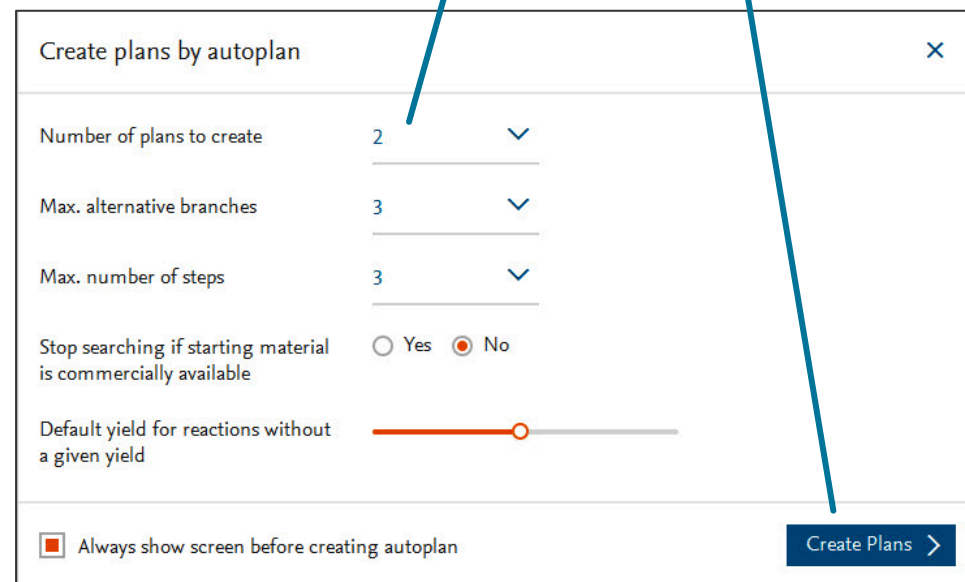
Let Reaxys build a synthesis pathway automatically. To begin, click **Synthesize** below a structure.



1. Click **Autoplan**.

2. Define parameters for automatically generating synthetic pathways.

3. Click **Create Plans**.



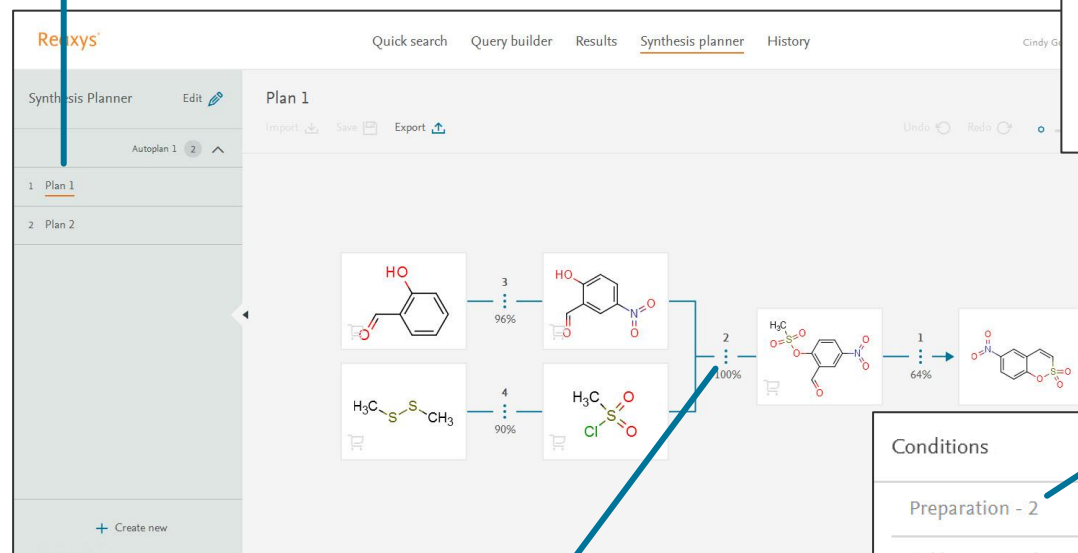
A screenshot of the 'Create plans by autoplan' dialog box. The dialog has a title bar 'Create plans by autoplan' with a close button. It contains several settings:

- 'Number of plans to create': 2 (with a dropdown arrow)
- 'Max. alternative branches': 3 (with a dropdown arrow)
- 'Max. number of steps': 3 (with a dropdown arrow)
- 'Stop searching if starting material is commercially available': Radio buttons for 'Yes' and 'No' (with 'No' selected)
- 'Default yield for reactions without a given yield': A horizontal slider bar.
- 'Always show screen before creating autoplan': A checkbox that is currently checked.

 At the bottom right, there is a blue button labeled 'Create Plans' with a right-pointing arrow.

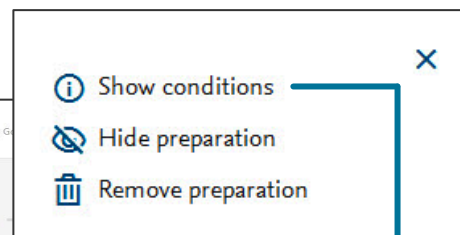
Synthesis planner – Autoplan (continued)

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.

Conditions		
Preparation - 2		
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 ▼	Grandane, Aiga; Belyakov, Sergey; Trapencieris, Peteris; +1 other - Tetrahedron, 2012, vol. 68, # 27-28, p. 5541 - 5546 Full Text ↗ Cited 13 times ↗ Show details ➤
Done ➤		

5. Saving and Exporting

FEATURE	COMMENT
Saving	
From the Query builder	Define the query; click Save in the upper left. • 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 . • 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. • 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. ○ When the export is complete, click Download.
From the Synthesis planner :	• 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. ○ When export is complete, click Download.