

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"> Click the Create Structure or Reaction Drawing box. Create the substance structure drawing. For more information on using the Marvin JS structure editor see: <ol style="list-style-type: none"> The Structure drawing 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, click Search.
Query builder (See page 5 & 6)	<ol style="list-style-type: none"> 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 Drag & Drop from one of these options <ol style="list-style-type: none"> Fields: search for properties using the Search properties field. Forms: use a Predefined Form such as Physical Data, Reactions, etc. History: use a Recent or Saved search. 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 Show fields to enter specific search values.

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"> Click the Create Structure or Reaction Drawing box. Create the reaction structure drawing. For more information on using the Marvin JS structure editor see: <ol style="list-style-type: none"> The Structure drawing workflow. Create a Reaction Query in the Search for Reactions 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, click Search.
Query builder (See page 5 & 6)	<ol style="list-style-type: none"> 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 Drag & Drop from one of these options <ol style="list-style-type: none"> Fields: search for properties using the Search properties field. Forms: use a Predefined Form such as Physical Data, Reactions, etc. History: use a Recent or Saved search. 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. Reactions. Note: Click Show fields to enter specific search values.

Search (continued)

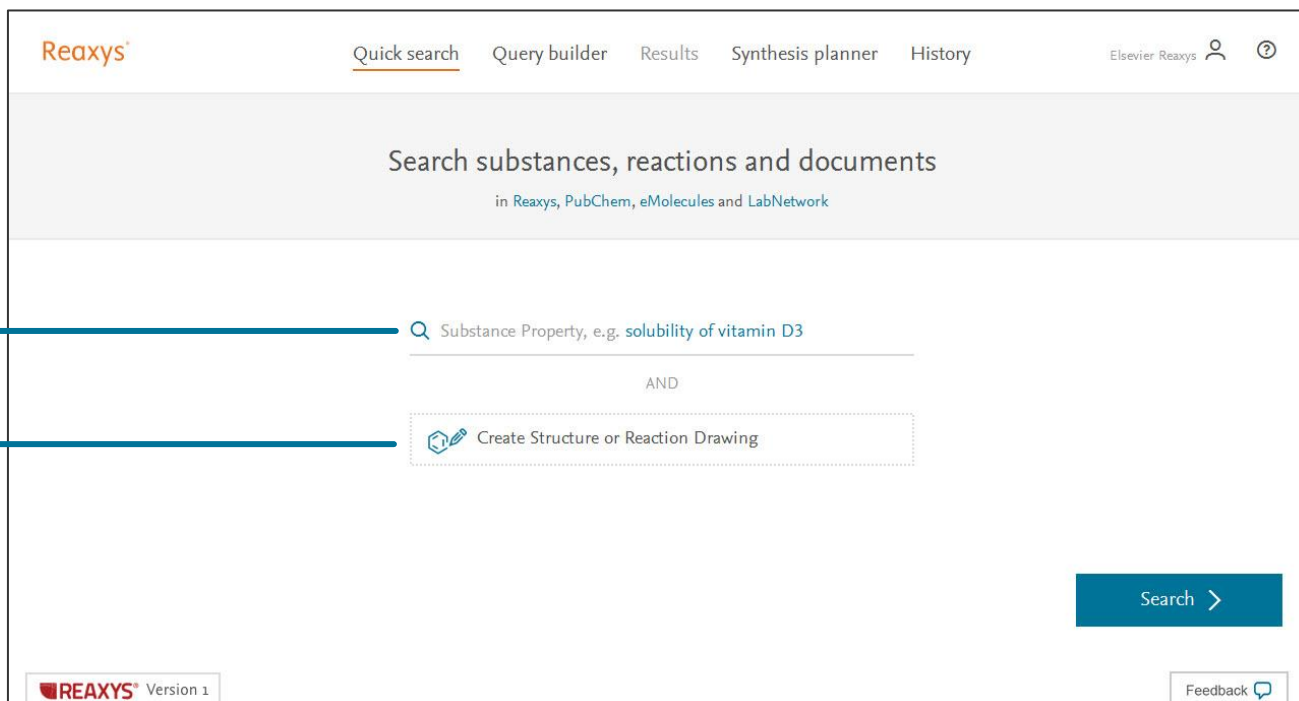
LITERATURE	
FEATURE	COMMENT
Quick search (See page 3)	Enter a term(s) in the Search Reaxys field and click Search . Examples: <ul style="list-style-type: none"> publications about quasicrystals Tetrahedron, 2014, 70, 2343 published by Schrock
Quick search with Structure or Reaction Drawing (See page 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"> 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 Drag & Drop from one of these options <ol style="list-style-type: none"> Fields: search for properties using the Search properties field. Forms: use a Predefined Form such as Physical Data, Reactions, etc. History: use a Recent or Saved search. 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 Show fields to enter specific search values.

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"> Click the Create Structure or Reaction Drawing box. Create the substance structure drawing. For more information on using the Marvin JS structure editor see: <ol style="list-style-type: none"> The Structure drawing workflow. 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 Reaxys field. Click Search.
Query builder (See page 5 & 6)	<ol style="list-style-type: none"> 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 Drag & Drop from one of these options <ol style="list-style-type: none"> Fields: search for properties using the Search properties field. Forms: use a Predefined Form such as Physical Data, Reactions, etc. History: use a Recent or Saved search. 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 Show fields to enter specific search values.

Quick search

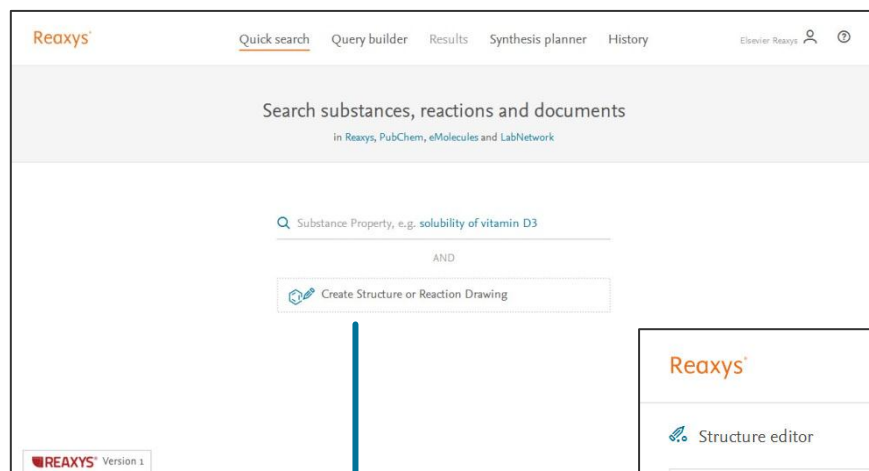
The text search option allows you to enter natural language terms (terms may be left, right or middle truncated using an asterisk (wildcard searching)).

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



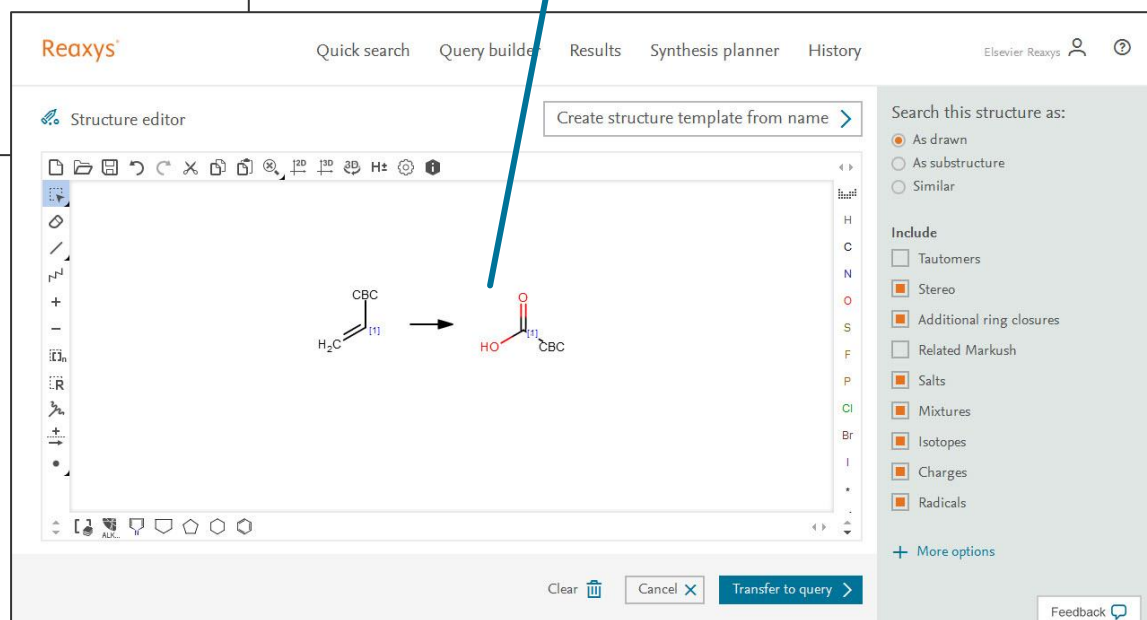
The screenshot shows the Reaxys Quick search interface. At the top, there is a navigation bar with the Reaxys logo, a 'Quick search' tab (which is underlined), and other tabs: 'Query builder', 'Results', 'Synthesis planner', and 'History'. On the right side of the navigation bar, there is a user profile icon and a help icon. Below the navigation bar, the main heading is 'Search substances, reactions and documents' with a subtitle 'in Reaxys, PubChem, eMolecules and LabNetwork'. The search area contains a text input field with the placeholder text 'Substance Property, e.g. solubility of vitamin D3'. Below the input field, there is a dashed box containing a pencil icon and the text 'Create Structure or Reaction Drawing'. A blue 'Search >' button is located at the bottom right of the search area. At the bottom left of the page, there is a footer with the Reaxys logo and 'Version 1'. At the bottom right, there is a 'Feedback' button with a speech bubble icon.

Quick search with Structure or Reaction Drawing

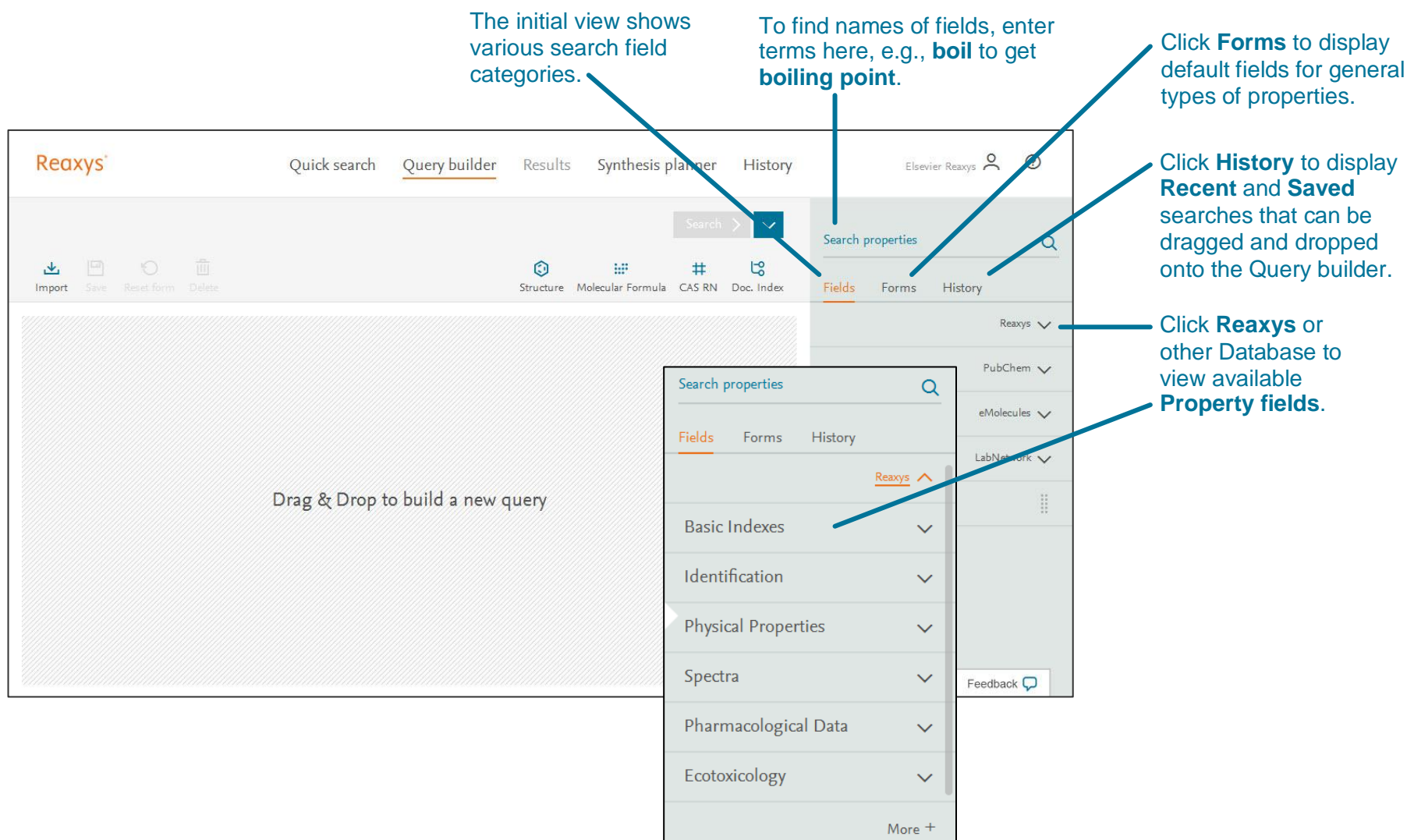


1. Click the **Create Structure or Reaction Drawing** box.

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



Query builder Fields, Forms & History 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 **History** to display **Recent** and **Saved** searches that can be dragged and dropped onto the Query builder.

Click **Reaxys** or other Database to view available **Property fields**.

Drag & Drop to build a new query

Search properties

Fields Forms History

Reaxys

Basic Indexes

Identification

Physical Properties

Spectra

Pharmacological Data

Ecotoxicology

More +

Reaxys

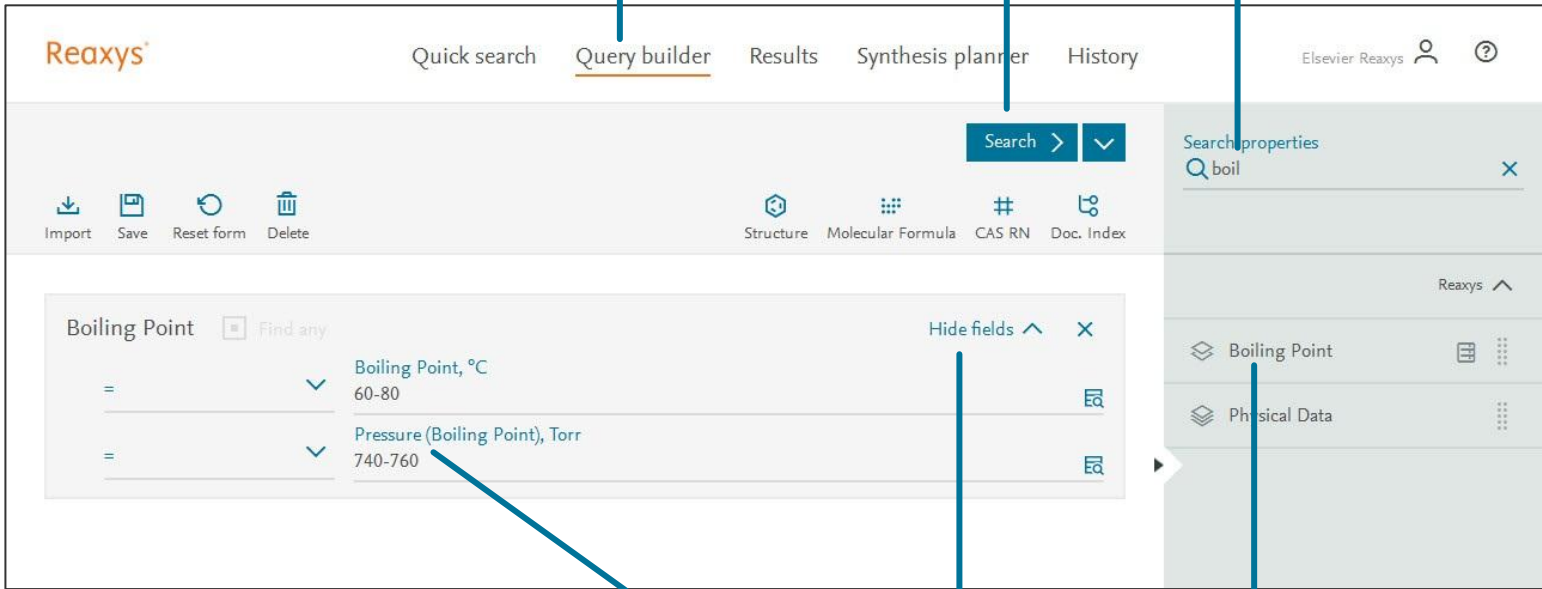
PubChem

eMolecules

LabNetwork

Feedback

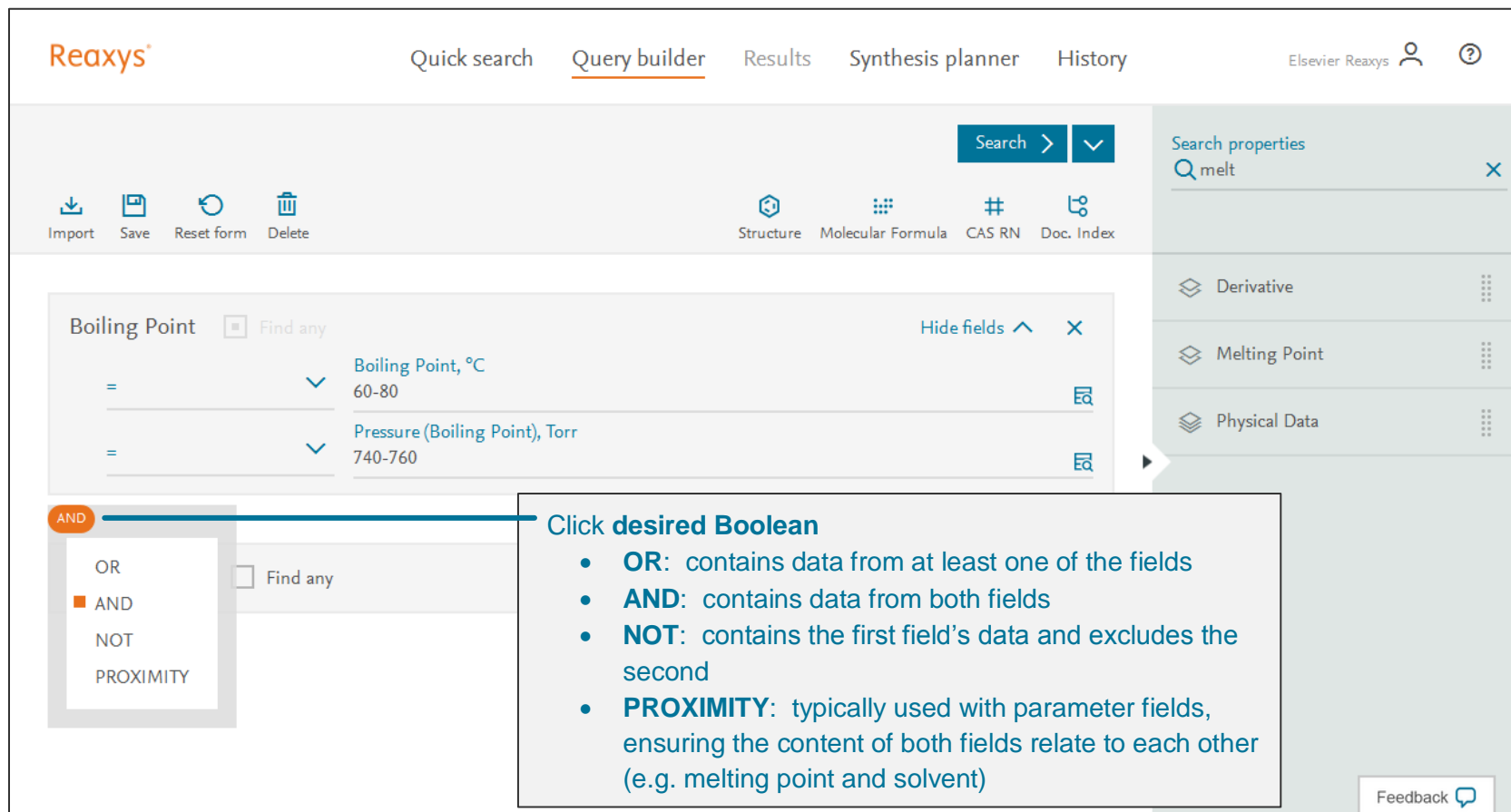
Query builder Steps



The screenshot shows the Reaxys Query builder interface. The top navigation bar includes 'Quick search', 'Query builder' (highlighted), 'Results', 'Synthesis planner', and 'History'. Below this is a toolbar with 'Import', 'Save', 'Reset form', and 'Delete' buttons, followed by search filters for 'Structure', 'Molecular Formula', 'CAS RN', and 'Doc. Index'. A 'Search' button with a dropdown arrow is also present. On the right, a 'Search properties' sidebar shows a search for 'boil' with results for 'Boiling Point' and 'Physical Data'. The main query builder area displays a table with columns for property names and values. The table contains two rows: 'Boiling Point, °C' with a value of '60-80', and 'Pressure (Boiling Point), Torr' with a value of '740-760'. A 'Hide fields' button is visible in the top right of the table. Numbered steps are overlaid on the interface: 1. Click Query builder. (points to the 'Query builder' tab), 2. Start typing property name e.g. boiling in Search properties field. (points to the 'Search properties' sidebar), 3. Drag & drop property onto the Query builder. (points to the 'Boiling Point' property in the sidebar), 4. Click Show fields. (points to the 'Hide fields' button), 5. Define specific Search Criteria. (points to the table), and 6. Click Search (Substances). (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 **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's a user profile icon 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 bar with a 'Search' button and a dropdown arrow is located on the right side of the top bar. Below the search bar, there's a 'Search properties' section with a search input containing 'melt' and a close button. The main query area shows two fields: 'Boiling Point' and 'Pressure (Boiling Point), Torr'. Each field has a dropdown menu with values '60-80' and '740-760' respectively. A 'Find any' checkbox is present next to each field. A 'Hide fields' button is also visible. Below the query area, there's a dropdown menu for Boolean operators: OR, AND (selected), NOT, and PROXIMITY. A callout box titled 'Click desired Boolean' provides a list of the operators and their meanings:

- **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)

A 'Feedback' button is located at the bottom right of the interface.

2. Results

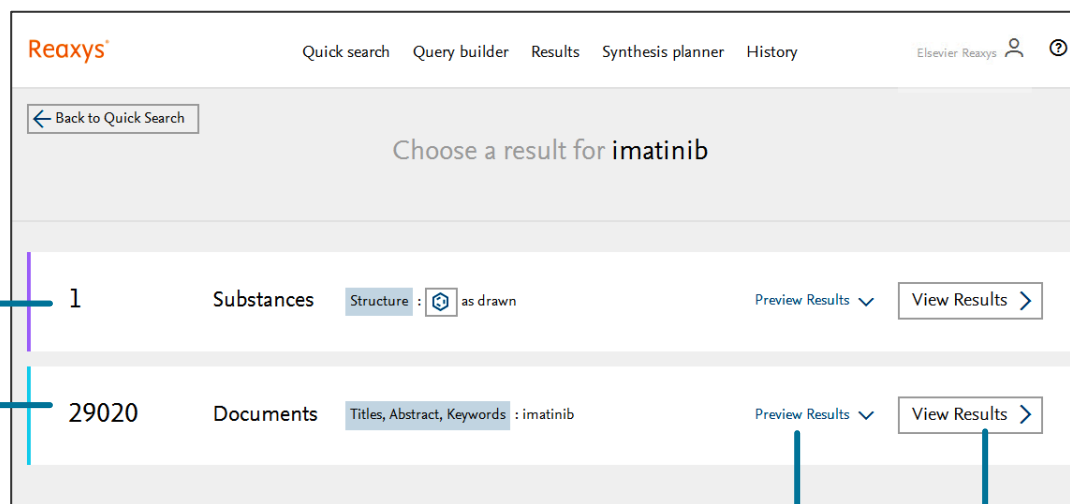
Quick search Results Preview

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.



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

← Back to Quick Search

Choose a result for imatinib

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.

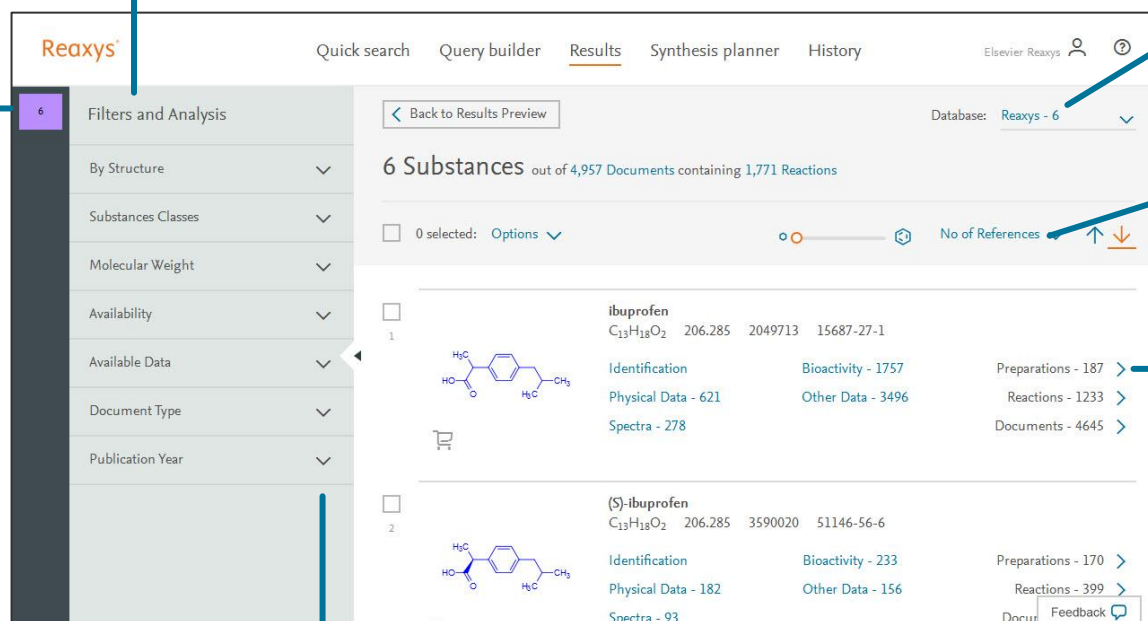
Click **View Results** to view all results from a result set.

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'.




The screenshot displays the Reaxys Results page for Substances. The top navigation bar includes 'Quick search', 'Query builder', 'Results' (selected), 'Synthesis planner', and 'History'. The 'Database' is set to 'Reaxys - 6'. The main results area shows '6 Substances out of 4,957 Documents containing 1,771 Reactions'. The left sidebar contains 'Filters and Analysis' options: 'By Structure', 'Substances Classes', 'Molecular Weight', 'Availability', 'Available Data', 'Document Type', and 'Publication Year'. The results list shows two entries for ibuprofen, with details on identification, physical data, spectra, bioactivity, and other data. The right sidebar provides links to 'Preparations', 'Reactions', and 'Documents' for each substance.

Click appropriate Database: **Reaxys**, eMolecules, LabNetwork, and PubChem.

Sorting option is dependent on the selected Database.

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

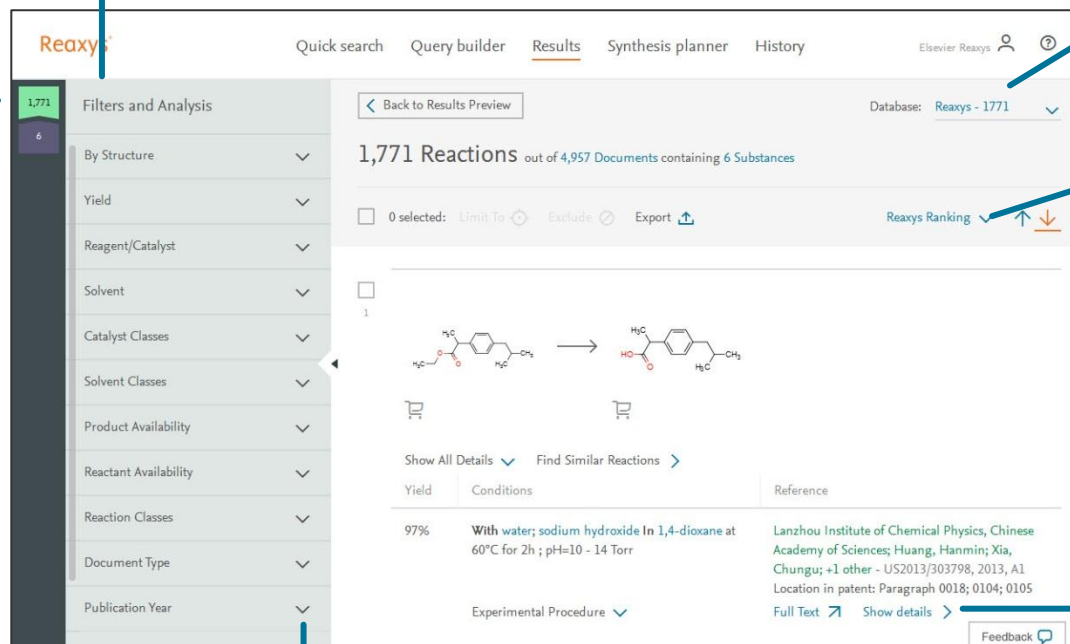
Click  to expand filters.

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'.



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

Database: Reaxys - 1771

1,771 Reactions out of 4,957 Documents containing 6 Substances

0 selected: Limit To Exclude Export

Reaxys Ranking

1

Chemical reaction scheme showing the conversion of a reactant to a product.

Show All Details Find Similar Reactions

Yield	Conditions	Reference
97%	With water; sodium hydroxide In 1,4-dioxane at 60°C for 2h ; pH=10 - 14 Torr	Lanzhou Institute of Chemical Physics, Chinese Academy of Sciences; Huang, Hanmin; Xia, Chungu; +1 other - US2013/303798, 2013, A1 Location in patent: Paragraph 0018; 0104; 0105


Experimental Procedure

Full Text Show details Feedback

Click appropriate Database: **Reaxys**, eMolecules, LabNetwork, and PubChem.

Sorting option is dependent on the selected Database.

Click links to view Full Text, details and more.

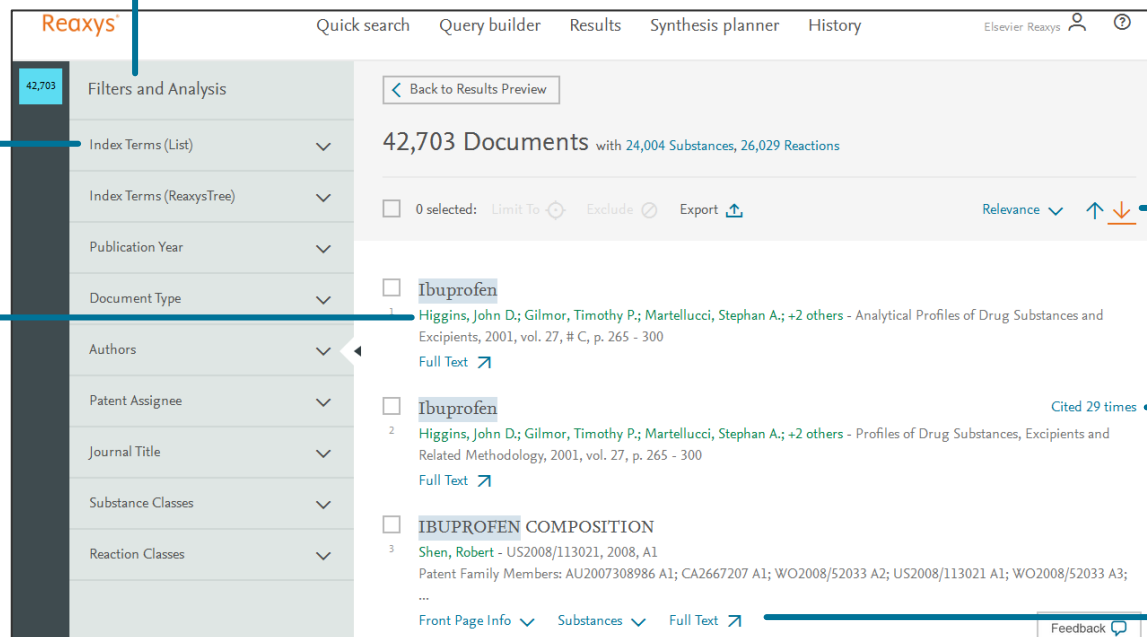
Click  to expand filters.

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 left sidebar contains a 'Filters and Analysis' section with a count of 42,703. Below this are expandable categories: Index Terms (List), Index Terms (ReaxysTree), Publication Year, Document Type, Authors, Patent Assignee, Journal Title, Substance Classes, and Reaction Classes. The main results area shows '42,703 Documents with 24,004 Substances, 26,029 Reactions'. It includes a 'Back to Results Preview' link, a selection status '0 selected', and buttons for 'Limit To', 'Exclude', and 'Export'. The results are sorted by 'Relevance'. Three results are listed, each with a checkbox, a title, authors, and a 'Full Text' link. The first result is 'Ibuprofen' by Higgins, John D.; Gilmor, Timothy P.; Martellucci, Stephan A.; +2 others. The second is 'Ibuprofen' by Higgins, John D.; Gilmor, Timothy P.; Martellucci, Stephan A.; +2 others. The third is 'IBUPROFEN COMPOSITION' by Shen, Robert. At the bottom, there are links for 'Front Page Info', 'Substances', 'Full Text', and 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

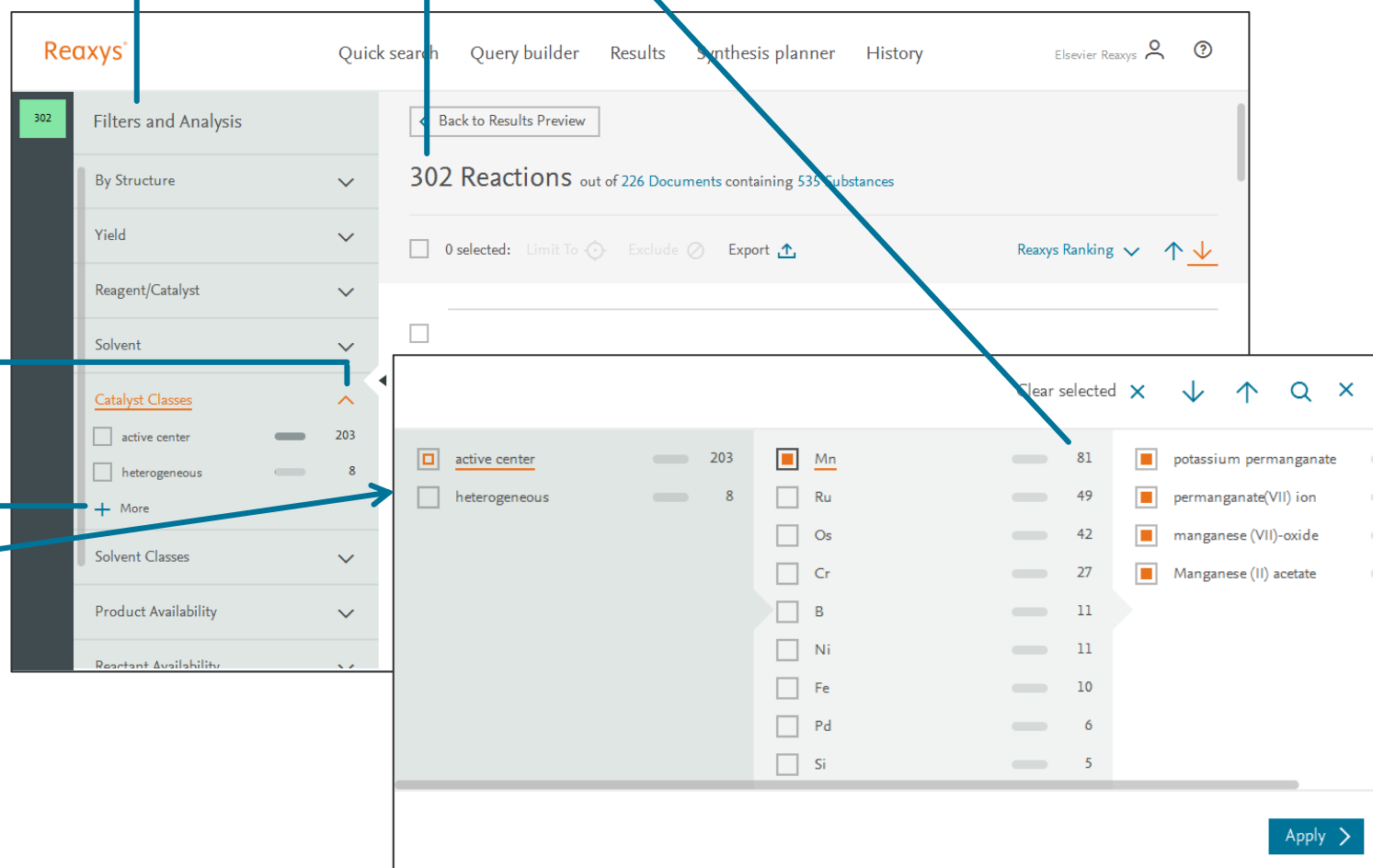
Use the **Filter & Analysis** panel to narrow your results:

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.

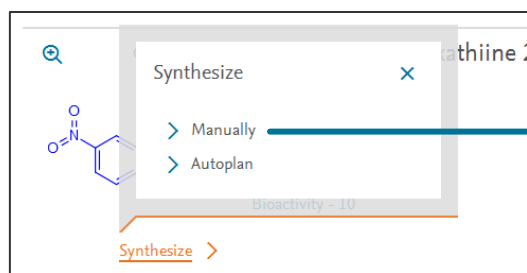


The screenshot shows the Reaxys interface with the 'Filters and Analysis' panel on the left. The panel has a '302' count at the top. Below it are sections for 'By Structure', 'Yield', 'Reagent/Catalyst', 'Solvent', 'Catalyst Classes', 'Solvent Classes', 'Product Availability', and 'Reagent Availability'. The 'Catalyst Classes' section is expanded, showing 'active center' (203) and 'heterogeneous' (8). A '+ More' button is visible. A modal window is open, showing a list of catalyst classes with checkboxes and counts. The 'active center' filter is selected, and the 'Mn' (Manganese) option is highlighted, showing a count of 81. Other options include 'potassium permanganate', 'permanganate(VII) ion', 'manganese(VII)-oxide', and 'Manganese(II) acetate'. The modal window has a 'Clear selected' button and an 'Apply' button at the bottom right.

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

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.

The screenshot displays the Reaxys Synthesis planner interface. The main window shows a synthesis plan titled 'Synthesis plan 1'. The plan starts with a starting material (4-hydroxy-2-nitrobenzaldehyde) reacting with a reagent (2-formyl-4-nitrophenyl methanesulfonate) to form intermediate 1a (64% yield). Intermediate 1a then reacts with another reagent (2-formyl-4-nitrophenyl methanesulfonate) to form intermediate 1b (64% yield). Finally, intermediate 1b reacts with a reagent (2-formyl-4-nitrophenyl methanesulfonate) to form the final product (2-formyl-4-nitrophenyl methanesulfonate).

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

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

Step 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.

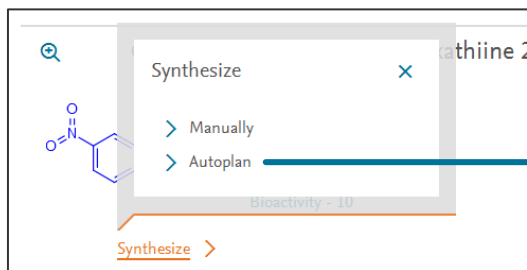
Conditions

Preparation - 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 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

☐ Yes
 ☒ No

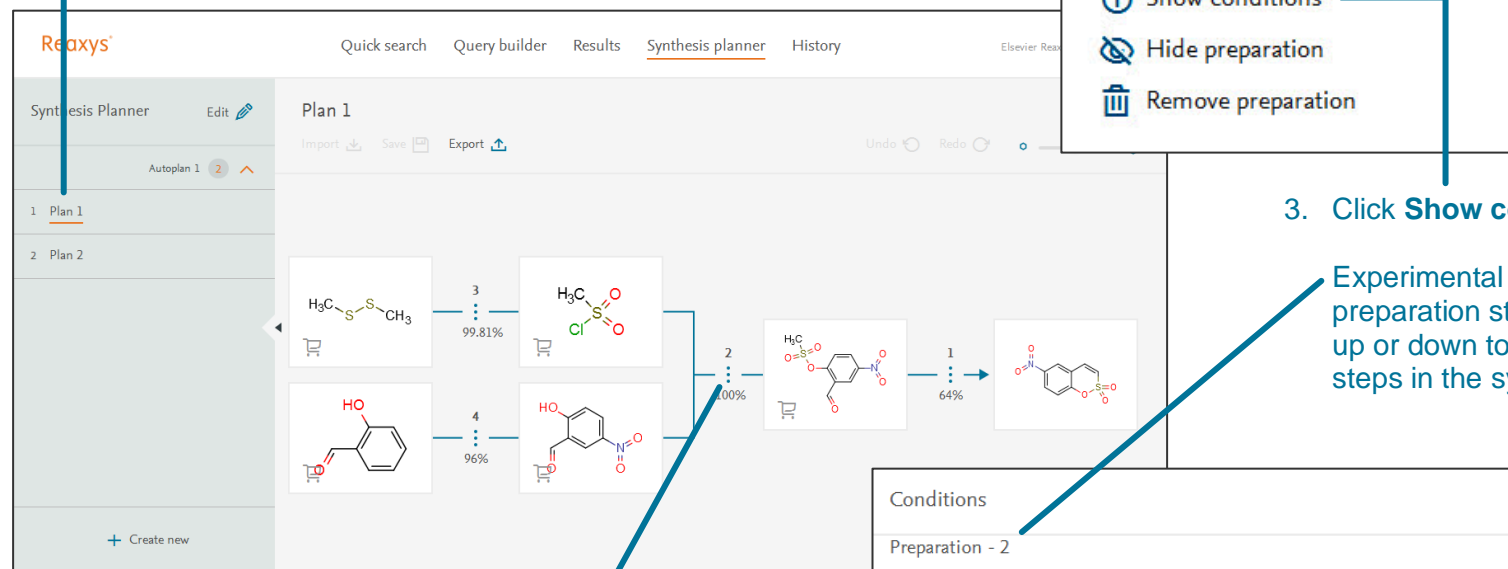
Default yield for reactions without a given yield

☐ Always show screen before creating autoplan

Create Plans >

Synthesis planner – Autoplan (continued)

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



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 - 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 6 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 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	Click Save <ul style="list-style-type: none"> The query is saved to a .json file.
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"> If necessary, click Options, then Export. Define Format, Range, Export data and Additional options. Click Export. The progress of the download is displayed 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. The progress of the download is displayed in the lower right corner of the screen. <ul style="list-style-type: none"> When the export is complete, click Download.