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 & 6)	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 & 6)	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)

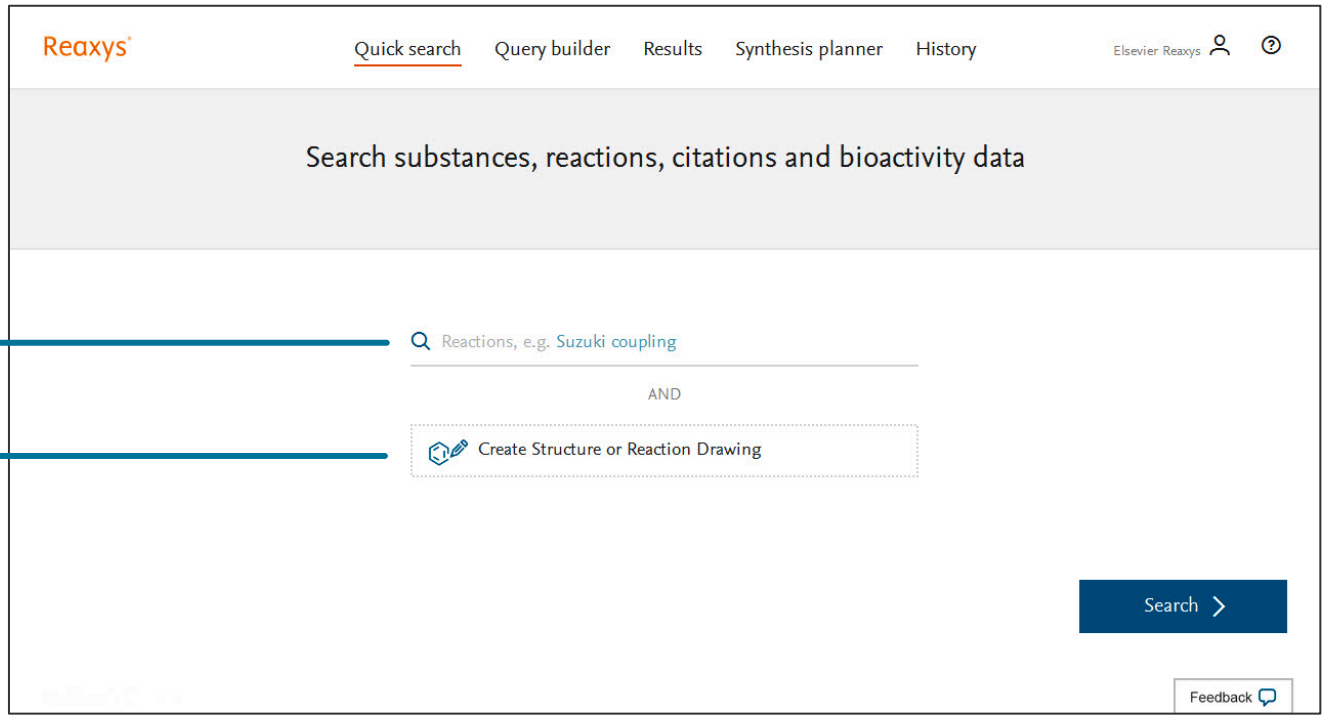
LITERATURE	
FEATURE	COMMENT
Quick search (See page 3)	Enter a term(s) in the search bar and click **Search**. Examples: • publications about quasicrystals • Tetrahedron, 2014, 70, 2343 • published by Schrock
Quick search with Structure or Reaction Drawing (See page 3 & 4)	**Note**: Any structure or reaction 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 & 6)	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. **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)	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**. 4. Enter property (e.g. boiling point) in the search bar. 5. Click **Search**.
Query builder (See page 5 & 6)	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. 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.

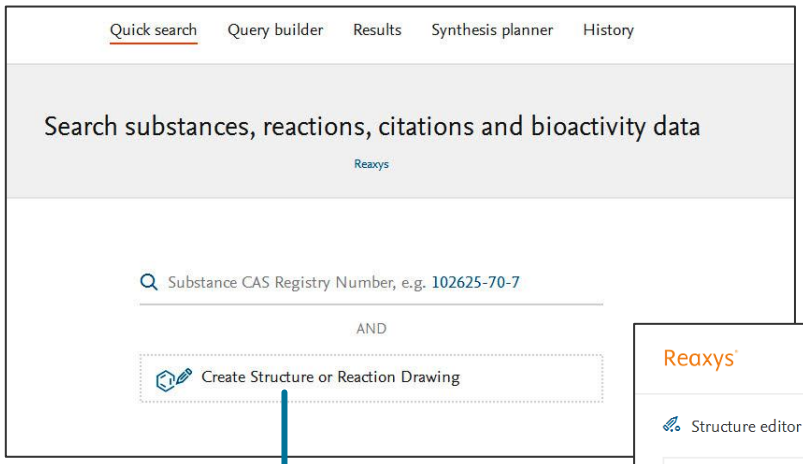
Quick search

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.

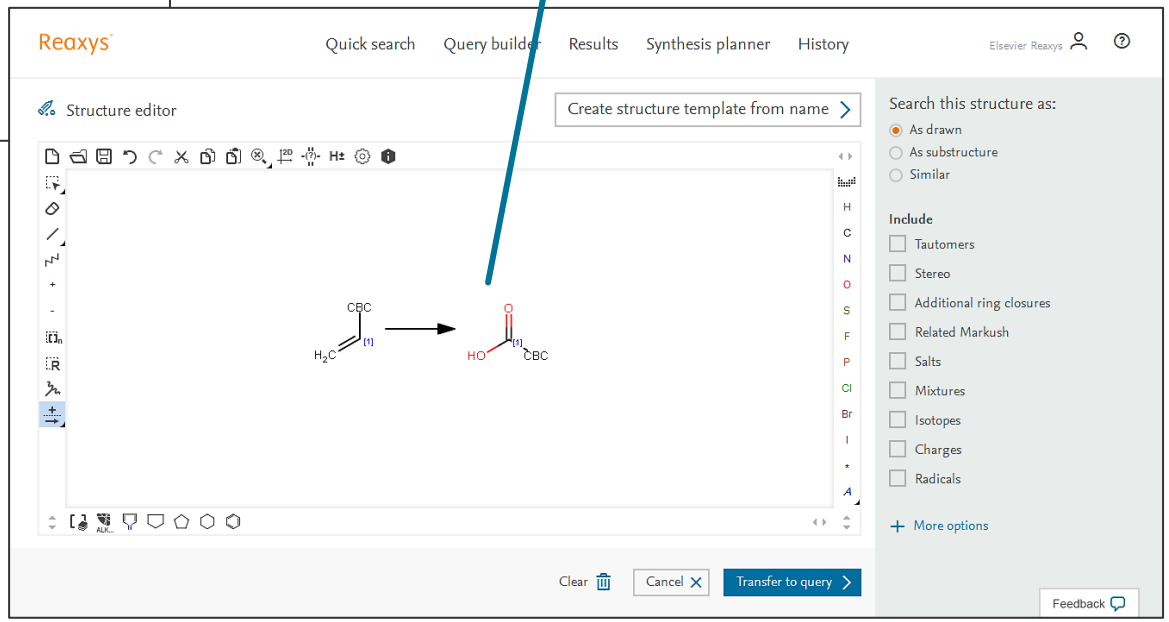


Quick search with Structure or Reaction Drawing

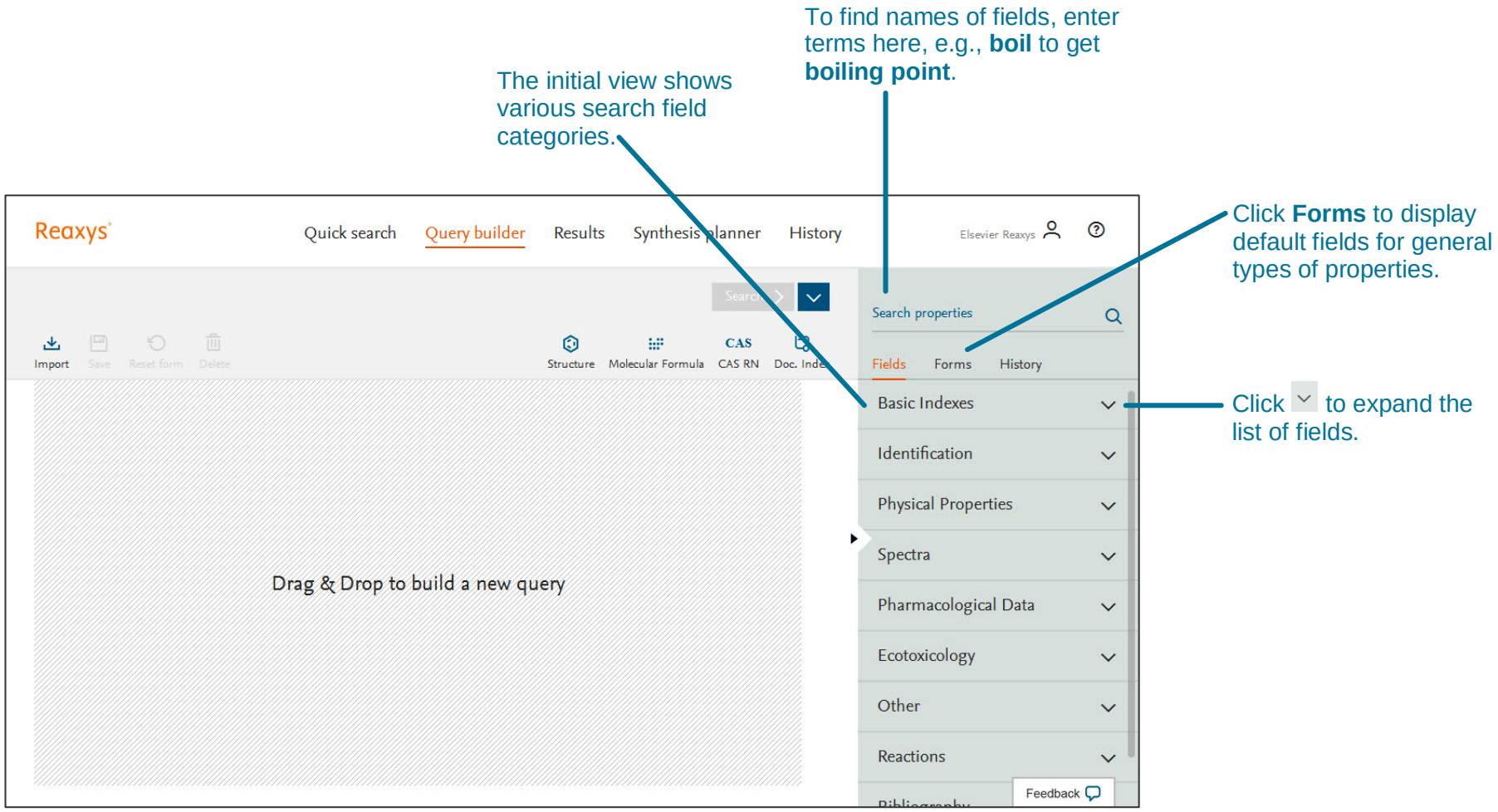


1. Click the **Create Structure or Reaction Drawing** box.

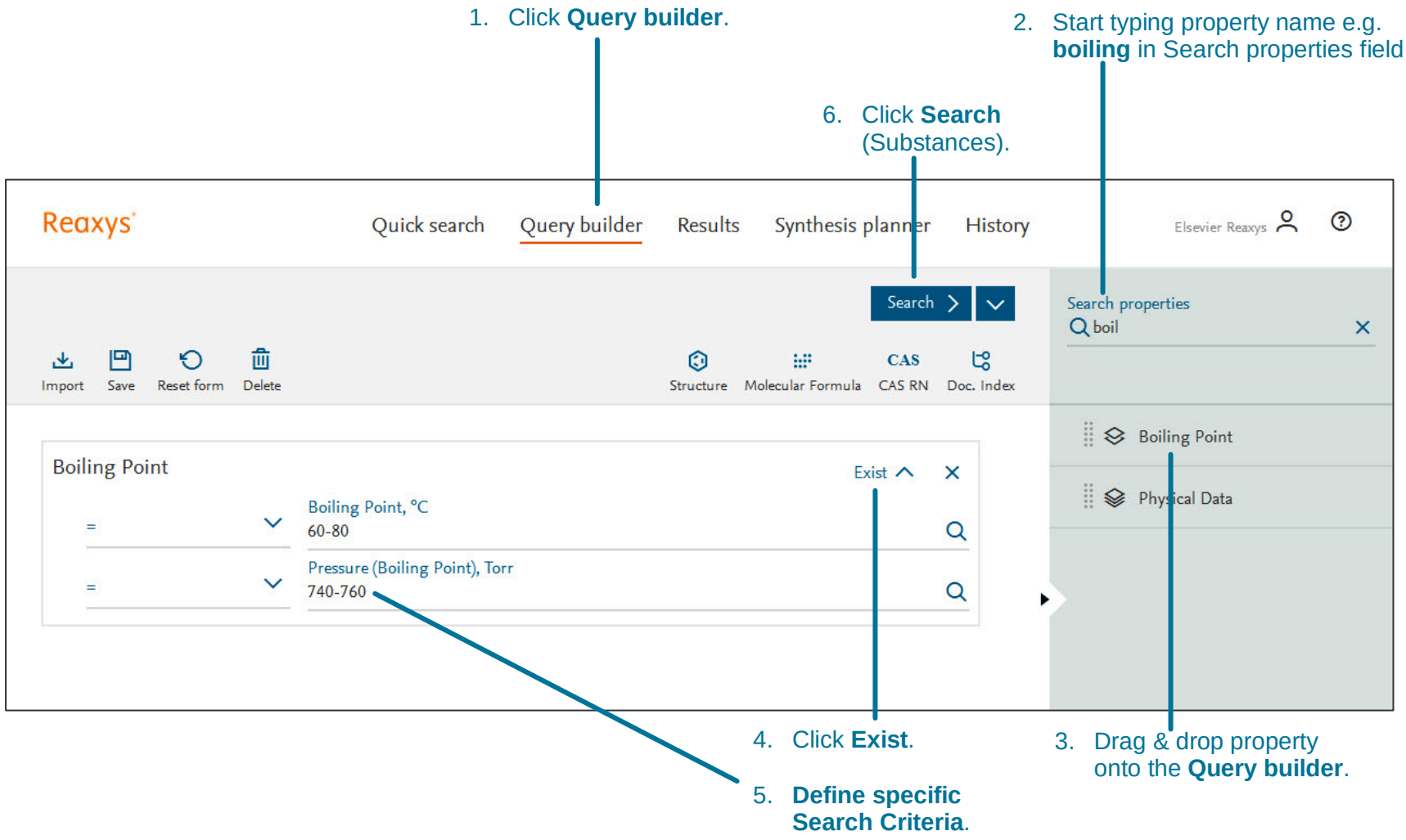
2. Use ChemAxon's Marvin JS tools to create a structure or reaction drawing.



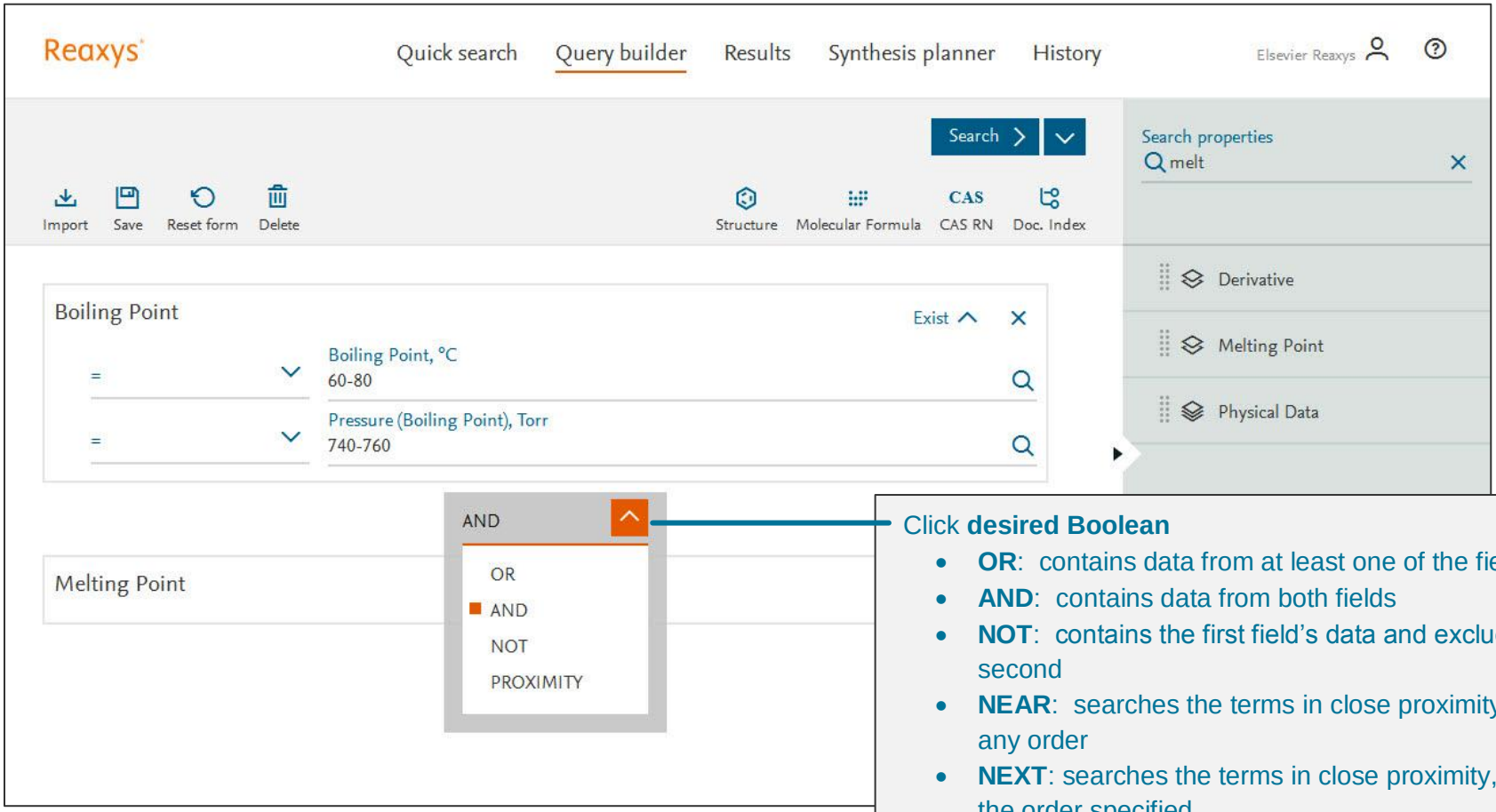
Query builder Fields & Forms Panel



Query builder Steps



Query builder: Multiple Properties and Booleans



Click **desired Boolean**

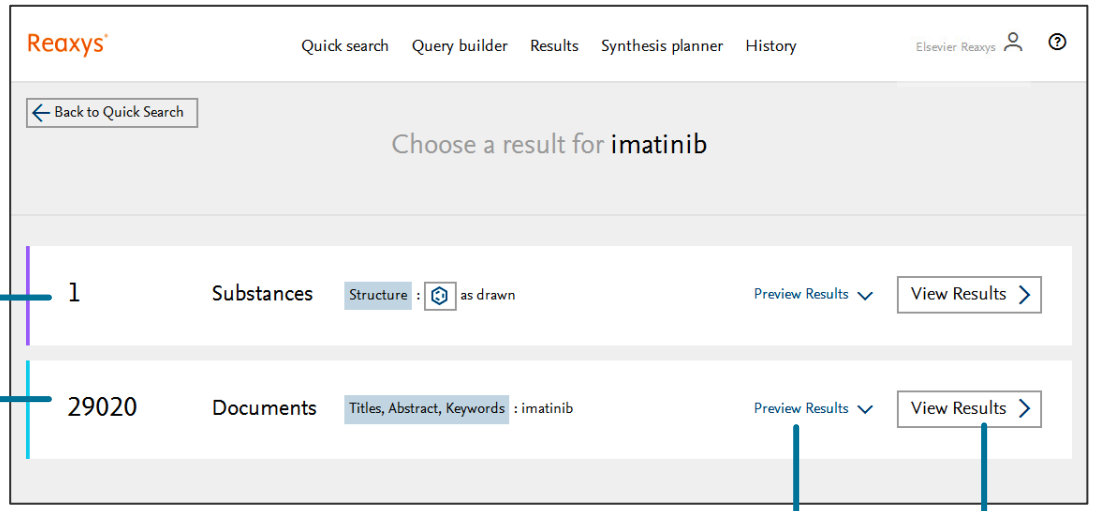
- **OR**: contains data from at least one of the fields
- **AND**: contains data from both fields
- **NOT**: contains the first field's data and excludes the second
- **NEAR**: searches the terms in close proximity, but in any order
- **NEXT**: searches the terms in close proximity, and in the order 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.

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

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

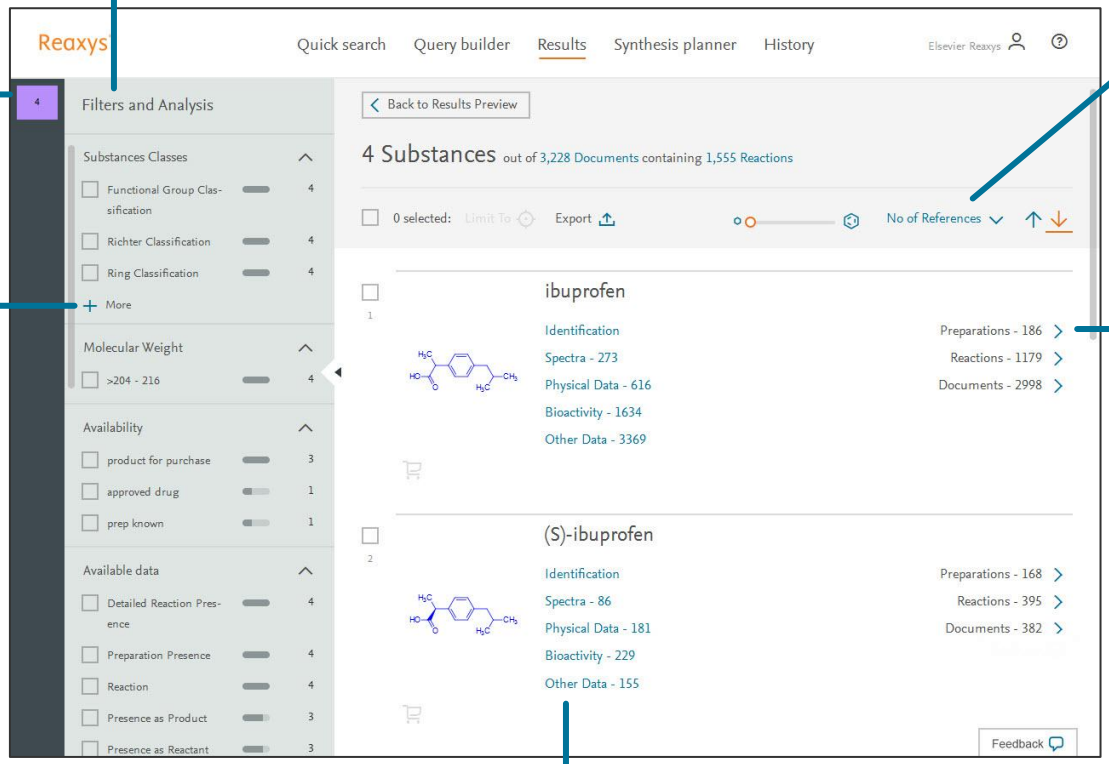
In other cases, **Search Reaxys** may give options that display **Reaction Records** or **Document Records** with different combinations of search terms entered.

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).

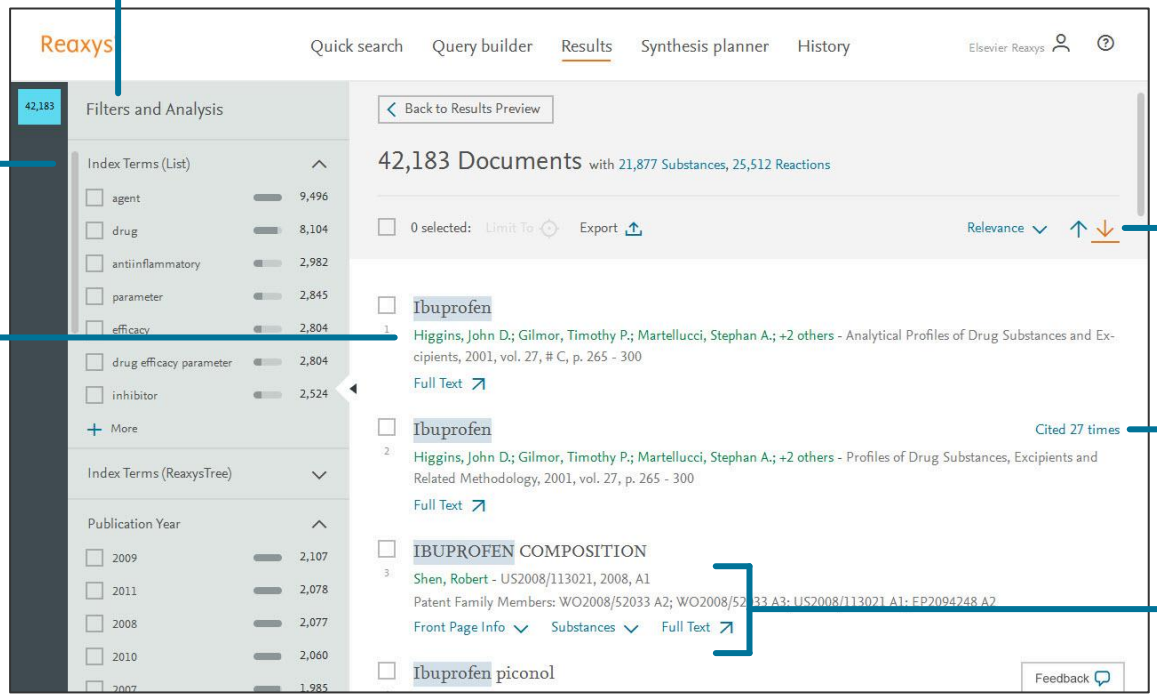
Click links to see specific information on the substance.

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.



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.

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3. Analyze and Filter

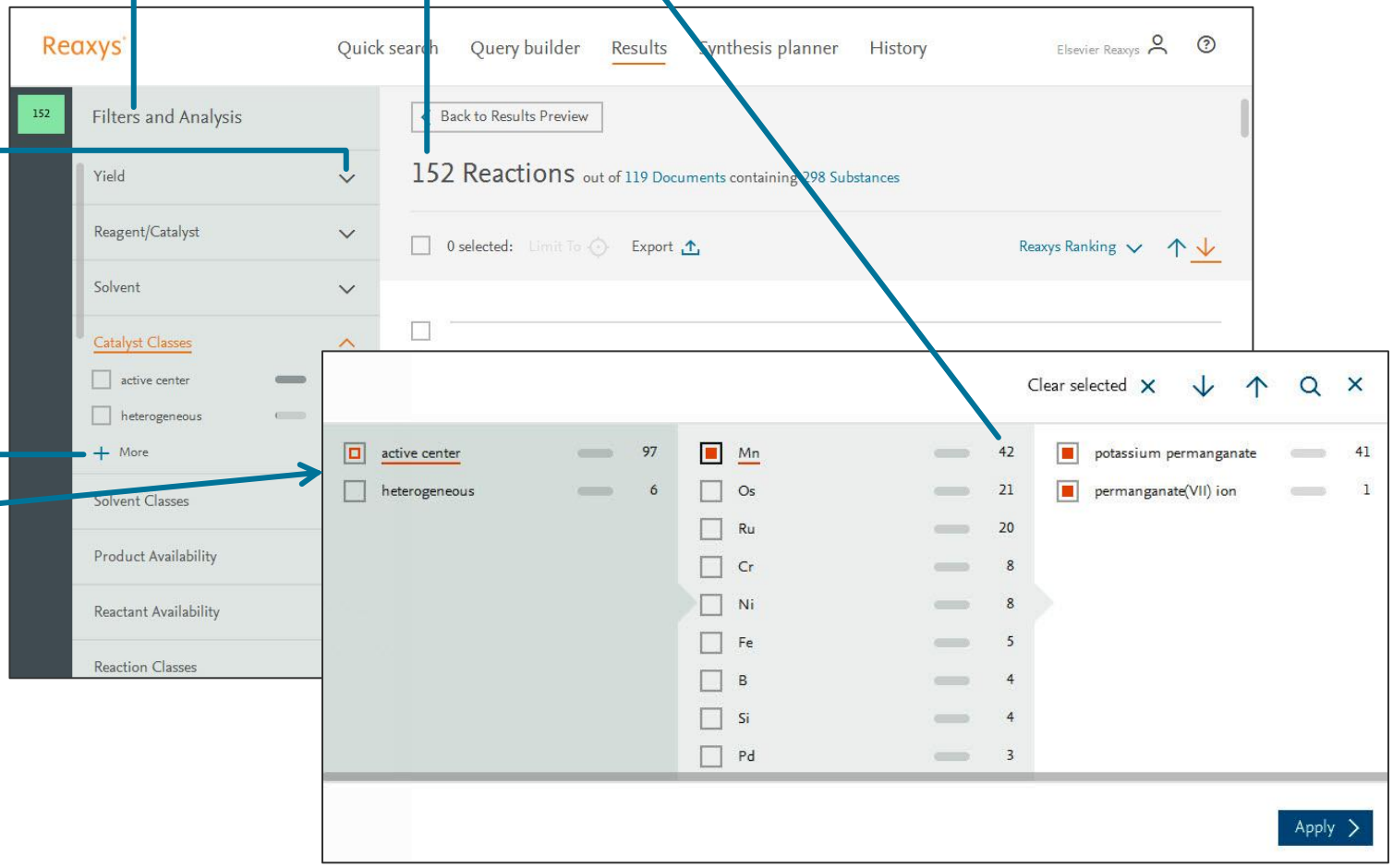
Use the **Filter & Analysis panel** to narrow your results:

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.

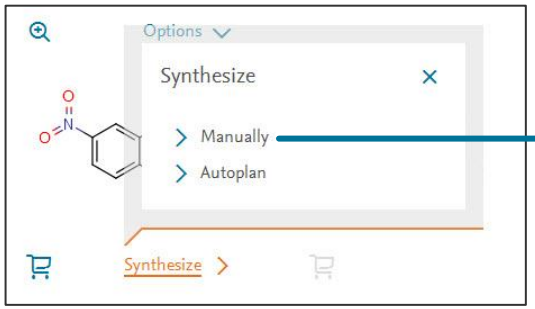
2. Click **More** to display additional filter options.

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



4. Synthesis planner - Manually

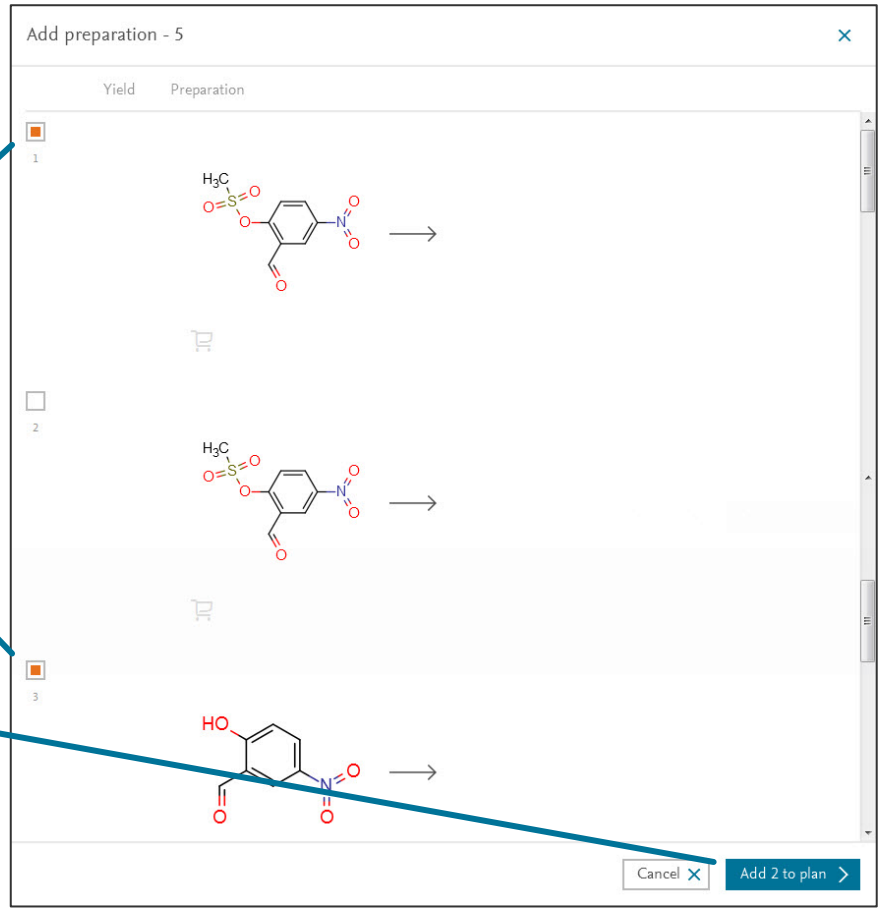
Build a synthesis pathway manually or let Reaxys do it automatically (see page 14). To begin, click **Synthesize** below a structure.



1. Click **Manually.**

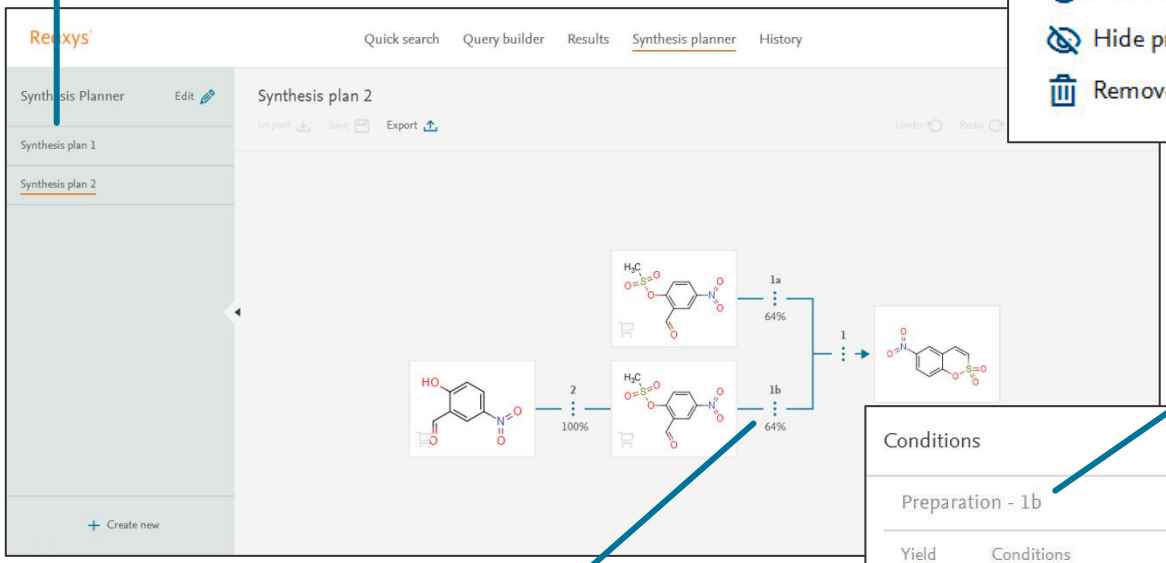
2. In the **Add preparation** window, select reactions to add to your plan. Note: the product structure is not shown because it is the same as the starting structure.

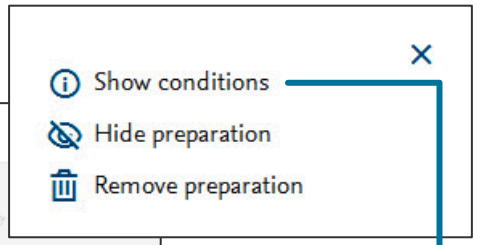
3. Click **Add # to plan.**



Synthesis planner – Manually (continued)

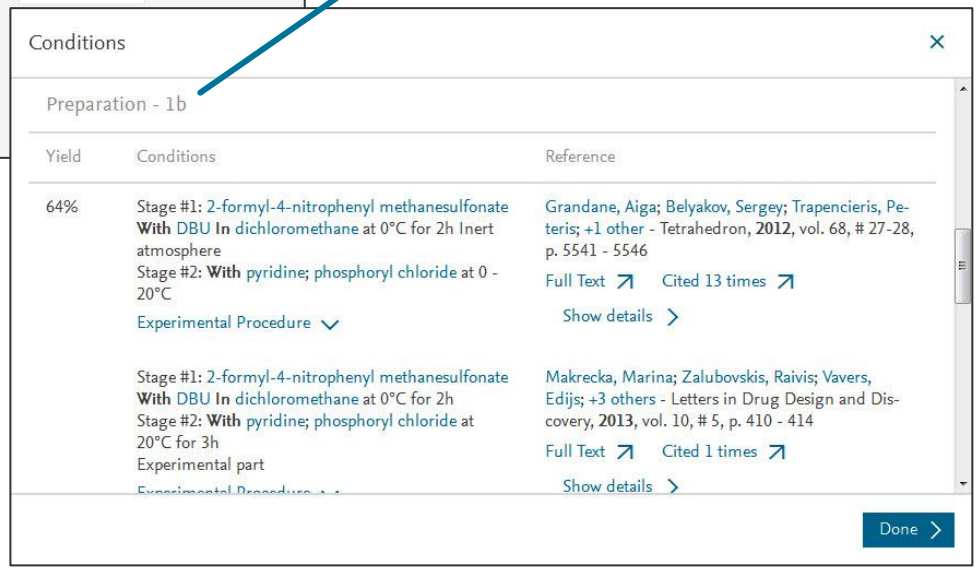
1. From the **Synthesis planner**, click the Synthesis plan to view.





3. Click **Show conditions**.

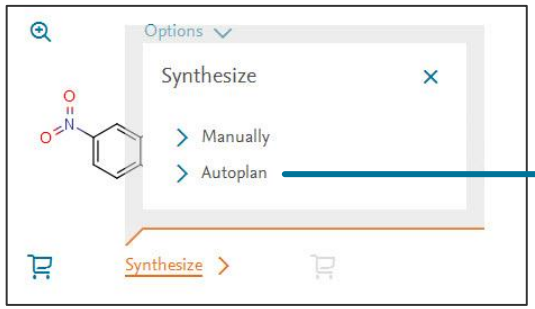
Experimental details for the selected preparation step is displayed, scroll up or down to view details of other steps in the synthesis plan.



2. Click the **Synthesis step options** (⋮) to access:
   - Show conditions
   - Hide preparations
   - Add preparations
   - Remove preparations

Synthesis planner - Autoplan

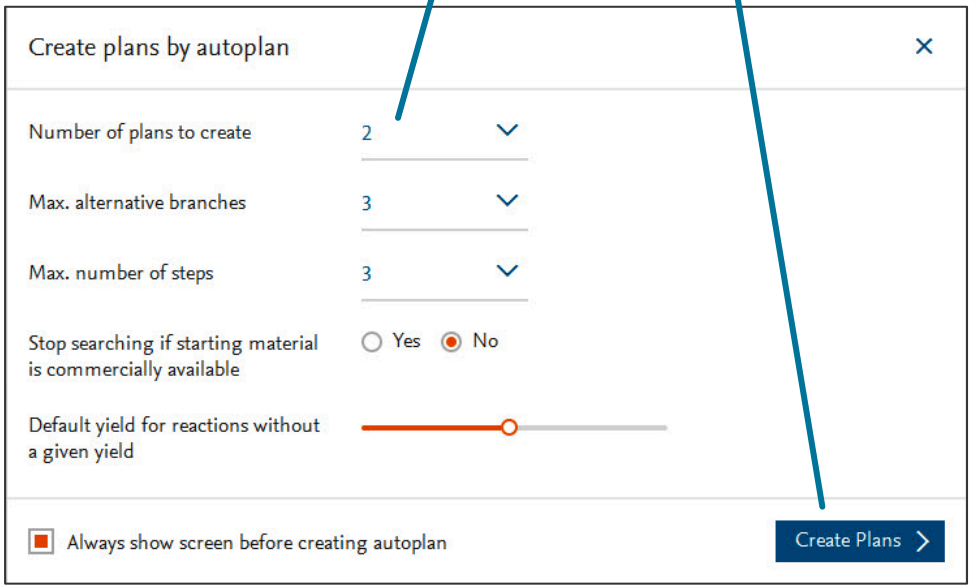
Let Reaxys build a synthesis pathway automatically. To begin, click **Synthesize** below a structure.



1. Click **Autoplan**.

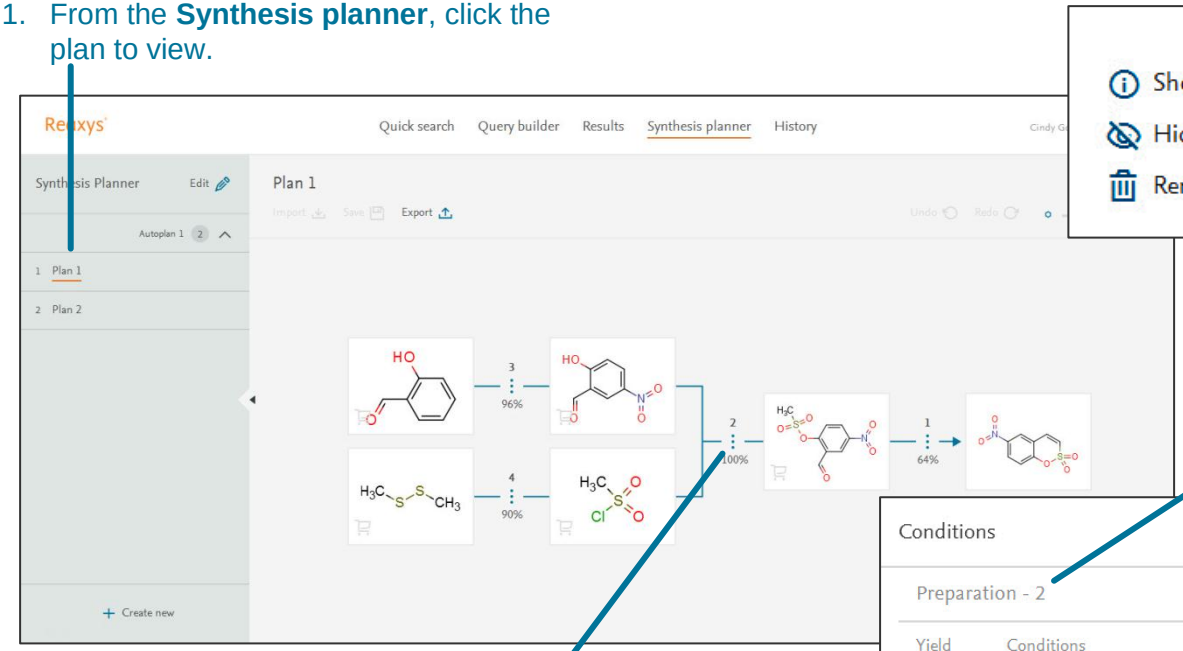
2. Define parameters for automatically generating synthetic pathways.

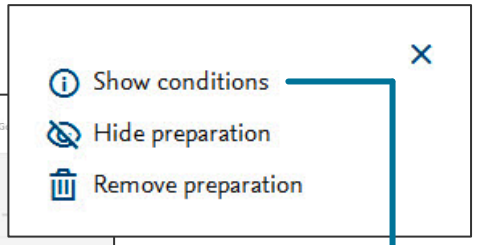
3. Click **Create Plans.**



Synthesis planner – Autoplan (continued)

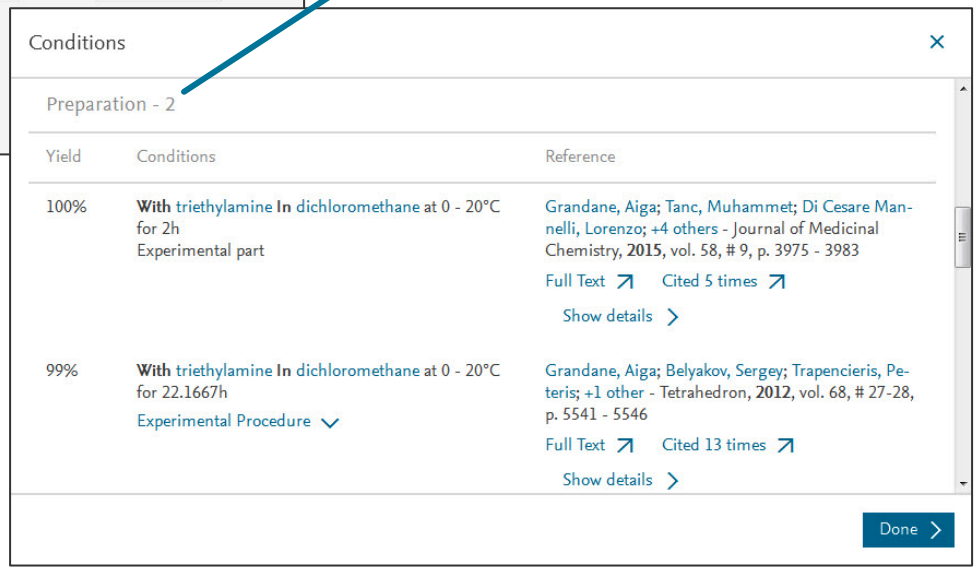
1. From the **Synthesis planner**, click the plan to view.





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

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**.