Reaxys®

Quick Start Guide

1. Search

SUBSTANCES	
FEATURE	COMMENT
Quick search as text (See page 4)	Enter a substance name, molecular formula or CAS number in the **Search Reaxys** field and click **Search**. Examples: • Atenolol • Pt(PPh3)3 • 102625-70-7
Quick search with Structure or Reaction Drawing (See page 5)	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. The Structure drawing 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 6 & 7)	1. Click **Query builder** (See page 7). 2. For quick access to frequently used queries, click one of the Quick Querylets (Structure, Molecular Formula, CAS RN or Doc Index) in the menu bar under the search button. **OR** 2. **Drag & Drop from one of these options** a. **Fields**: drag & drop desired field onto the query screen or search fields using the **Find search fields and forms** box. b. **Forms:** use a Predefined Form such as **Physical Data**, **Reactions**, etc. or search for a form using the **Find search fields and forms** box. c. **History**: use a **Recent** or **Saved** search. 3. If you have multiple search fields, use the appropriate Boolean operator (see page 8). 4. Click **Search** at the top of the screen and select the desired content: e.g. **Substances**. **Note**: Click **Show fields** to enter specific search values.

REACTIONS	
FEATURE	COMMENT
Quick search as text (See page 4)	Enter a term(s) in the **Search Reaxys** field and click **Search**. Examples: • preparation of porphyrine • phosphorylation • Suzuki coupling • Adler phenol oxidation
Quick search with Structure or Reaction Drawing (See page 5)	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. The Structure drawing workflow. b. The Search for Reactions Workflow. c. View our Tips for using ChemAxon Marvin JS d. Visit the ChemAxon Marvin JS website which includes a MarvinJS User's Guide 3. Click **Transfer to query**, click **Search**.
Query builder (See page 6 & 7)	1. Click **Query builder** (See page 7). 2. For quick access to frequently used queries, click one of the Quick Querylets (Structure, Molecular Formula, CAS RN or Doc Index) in the menu bar under the search button. **OR** 2. **Drag & Drop from one of these options** a. **Fields**: drag & drop desired field onto the query screen or search fields using the **Find search fields and forms** box. b. **Forms:** use a Predefined Form such as **Physical Data**, **Reactions**, etc. or search for a form using the **Find search fields and forms** box. c. **History**: use a **Recent** or **Saved** search. 3. If you have multiple search fields, use the appropriate Boolean operator (see page 8). 4. Click **Search** at the top of the screen and select the desired content: e.g. **Reactions**. **Note**: Click **Show fields** to enter specific search values.

Search (continued)

LITERATURE	
FEATURE	COMMENT
Quick search (See page 4)	Enter a term(s) in the **Search Reaxys** field and click **Search**. Examples: • publications about quasicrystals • Tetrahedron, 2014, 70, 2343 • published by Schrock
Quick search with Structure or Reaction Drawing (See page 5)	**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 6 & 7)	1. Click **Query builder** (See page 7). 2. For quick access to frequently used queries, click one of the Quick Querylets (Structure, Molecular Formula, CAS RN or Doc Index) in the menu bar under the search button. **OR** 2. **Drag & Drop from one of these options** a. **Fields**: drag & drop desired field onto the query screen or search fields using the **Find search fields and forms** box. b. **Forms:** use a Predefined Form such as **Physical Data**, **Reactions**, etc. or search for a form using the **Find search fields and forms** box. c. **History**: use a **Recent** or **Saved** search. 3. If you have multiple search fields, use the appropriate Boolean operator (see page 8). 4. Click **Search** at the top of the screen and select the desired content: e.g. **Documents**. **Note**: Click **Show fields** to enter specific search values.

PROPERTIES	
FEATURE	COMMENT
Quick search (See page 4)	Enter terms in the **Search Reaxys** field and click **Search**. Examples: • boiling point of benzene • density of quinolone
Quick search with Structure or Reaction Drawing (See page 5)	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. The Structure drawing workflow. b. The Search for Substances Workflow. c. View our Tips for using ChemAxon Marvin JS d. 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 Reaxys** field. 5. Click **Search**.
Query builder (See page 6 & 6)	1. Click **Query builder** (See page 7). 2. For quick access to frequently used queries, click one of the Quick Querylets (Structure, Molecular Formula, CAS RN or Doc Index) in the menu bar under the search button. **OR** 2. **Drag & Drop from one of these options** a. **Fields**: drag & drop desired field onto the query screen or search fields using the **Find search fields and forms** box. b. **Forms:** use a Predefined Form such as **Physical Data**, **Reactions**, etc. or search for a form using the **Find search fields and forms** box. c. **History**: use a **Recent** or **Saved** search. 3. If you have multiple search fields, use the appropriate Boolean operator (see page 8). 4. Click **Search** at the top of the screen and select the desired content: e.g. **Documents**. **Note**: Click **Show fields** to enter specific search values.

Search (continued)

MEDICINAL CHEMISTRY	
FEATURE	COMMENT

Quick search
(See page 4)
	• Enter target names, gene names, Uniprot id, PDB id, cell lines, species, and substances action on target in the Search Reaxys field and click Search.
	• Examples:
	  • D(2) dopamine receptor
	  • ADORA1
	  • O75469
	  • 2pfr
	  • Caco-2
	  • 5-HT1a antagonist

Quick search with Structure or Reaction Drawing
(See page 5)
	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. The Structure drawing workflow.
	  b. The Search for Substances Workflow.
	  c. View our Tips for using ChemAxon Marvin JS
	  d. 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 Reaxys** field.
	5. Click **Search**.

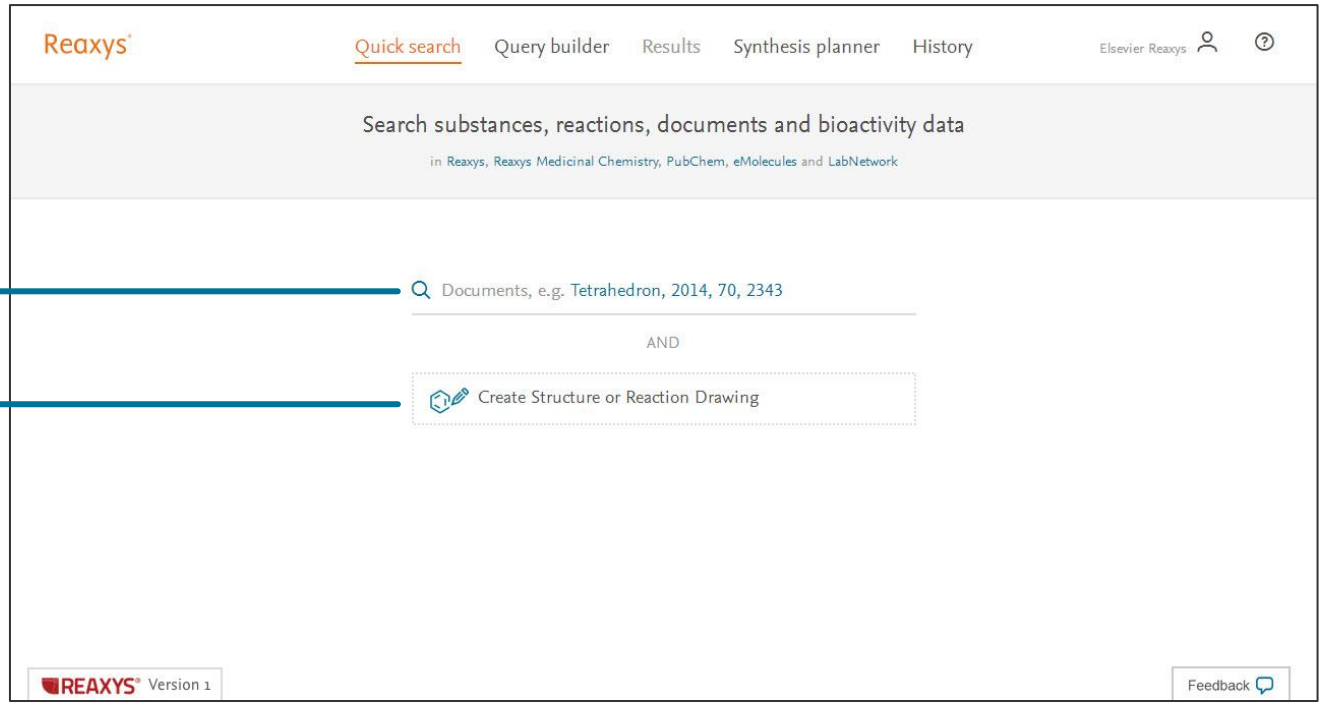
MEDICINAL CHEMISTRY	
FEATURE	COMMENT

Query builder
(See page 6 & 7)
	1. Click **Query builder** (See page 7).
	2. For quick access to frequently used queries click one of the Quick Querylets (Structure, Molecular Formula, CAS RN or Doc Index) in the menu bar under the search button.
	OR
	2. **Drag & Drop from one of these options**
	  a. **Fields:** and drag & drop desired field onto the query screen or search fields using the **Find search fields and forms** box.
	  b. **Forms:** use a Predefined Form such as **Affinity on target, Selectivity profile, Bioavailability**, etc. or search for a form using the **Find search fields and forms** box.
	  c. **History**: use a **Recent** or **Saved** search.
	3. Repeat for other properties as necessary.
	4. If you have multiple search fields, use the appropriate Boolean operator (see page 8).
	5. Click **Search** at the top of the screen and select the desired content: e.g. **Substances or Target**
	Note: Click **Show fields** to enter specific search values.

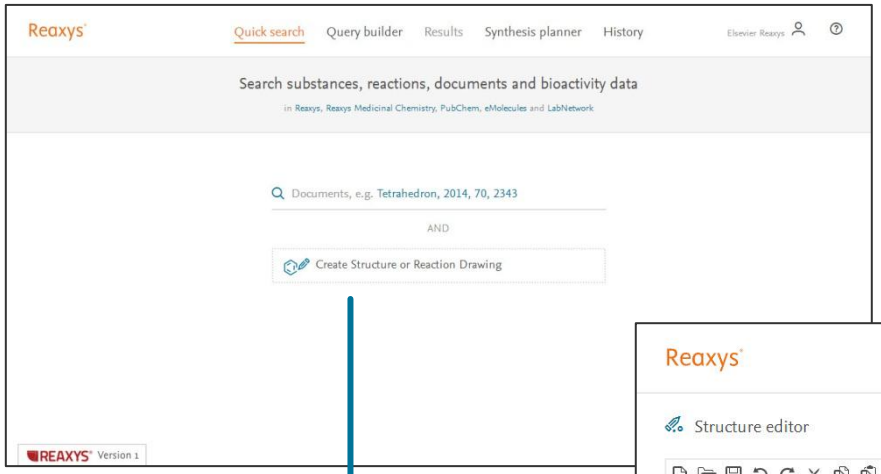
Quick search

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.

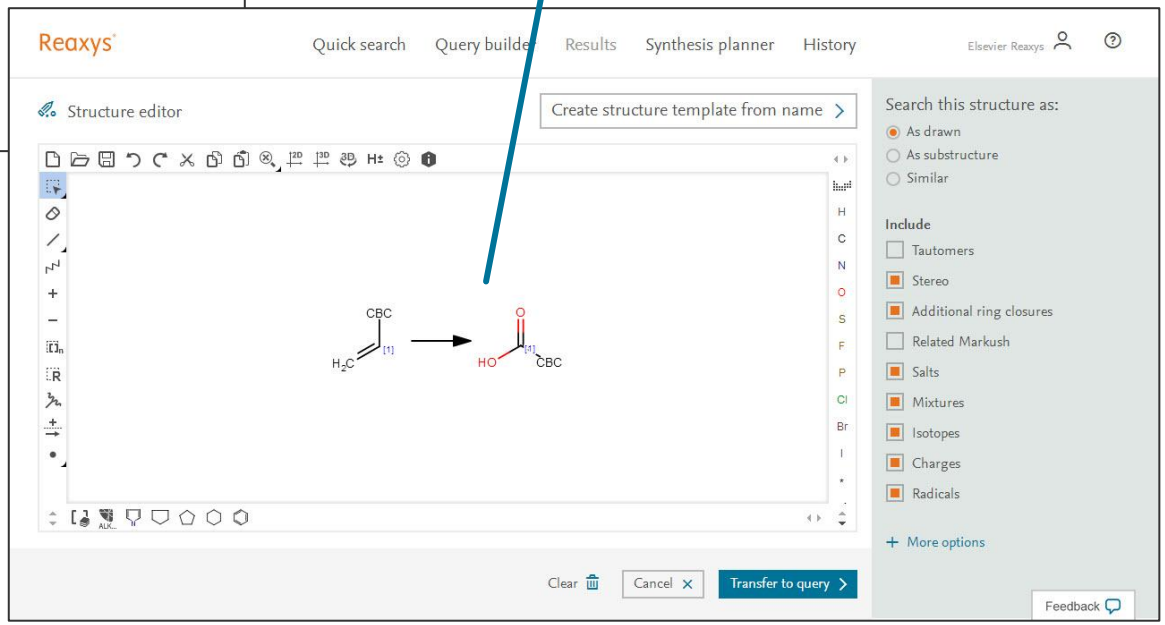


Quick search with Structure or Reaction Drawing



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

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



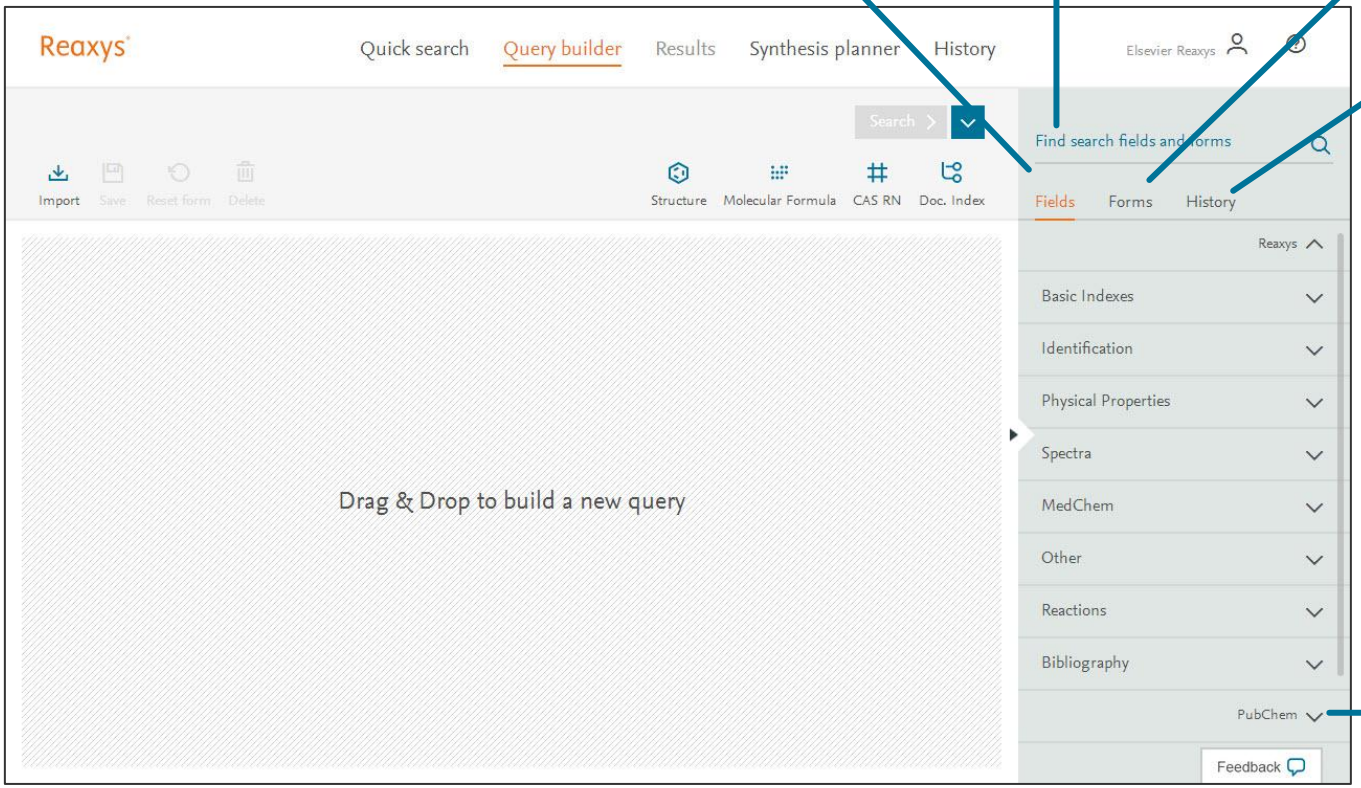
Query builder Fields, Forms & History Panel

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.

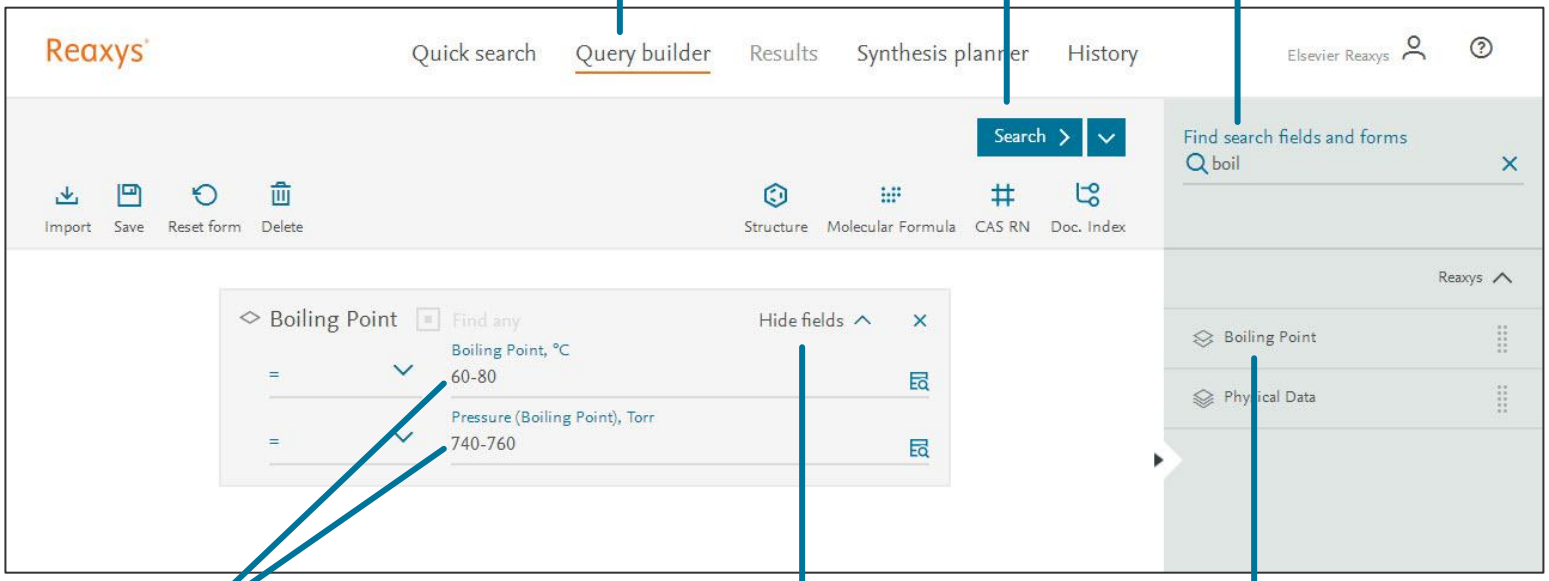
Click **History** to display **Recent** and **Saved** searches that can be dragged and dropped onto the Query builder.



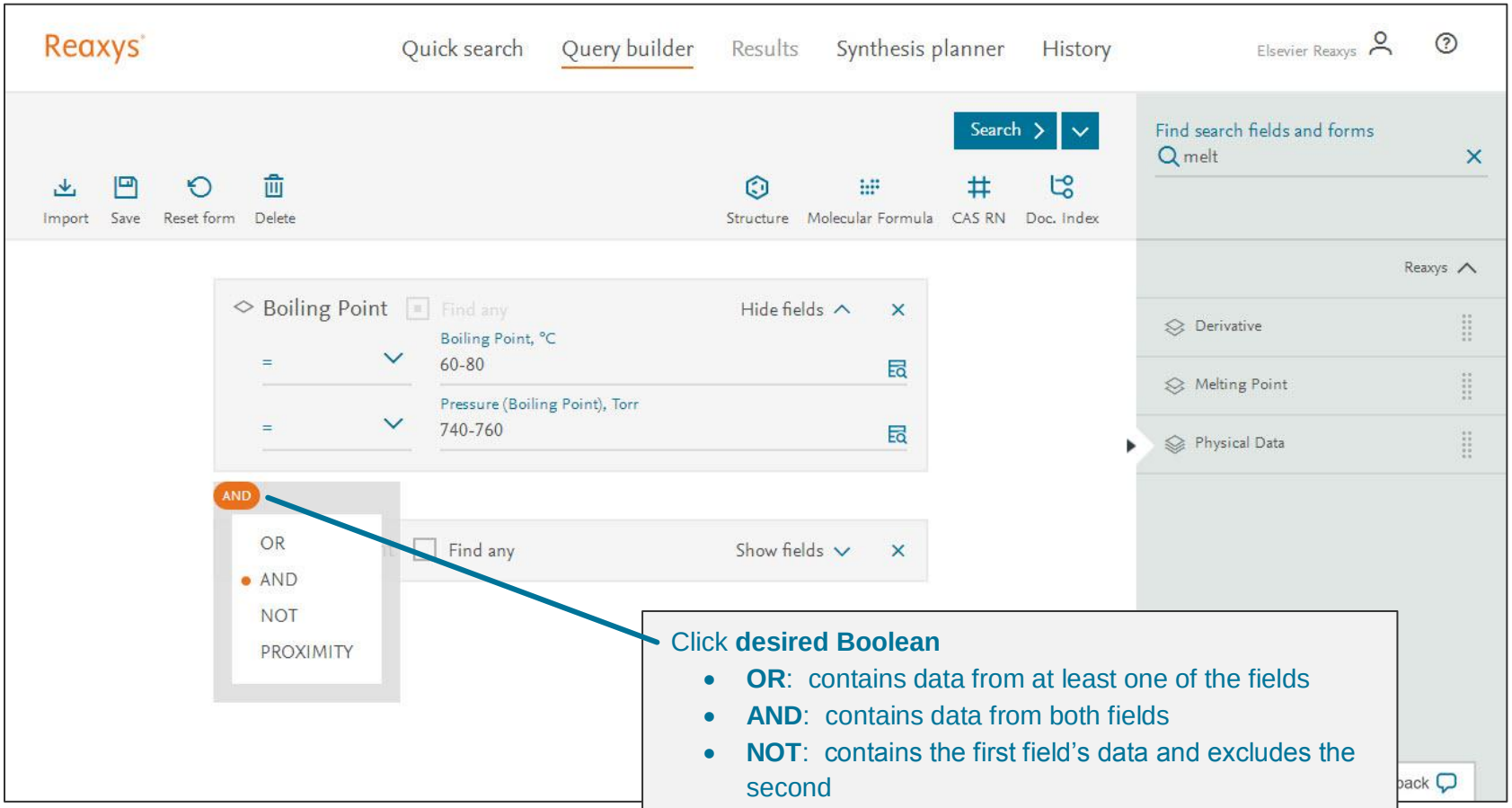
Click other Databases to view their available **Property fields**.

Query builder Steps

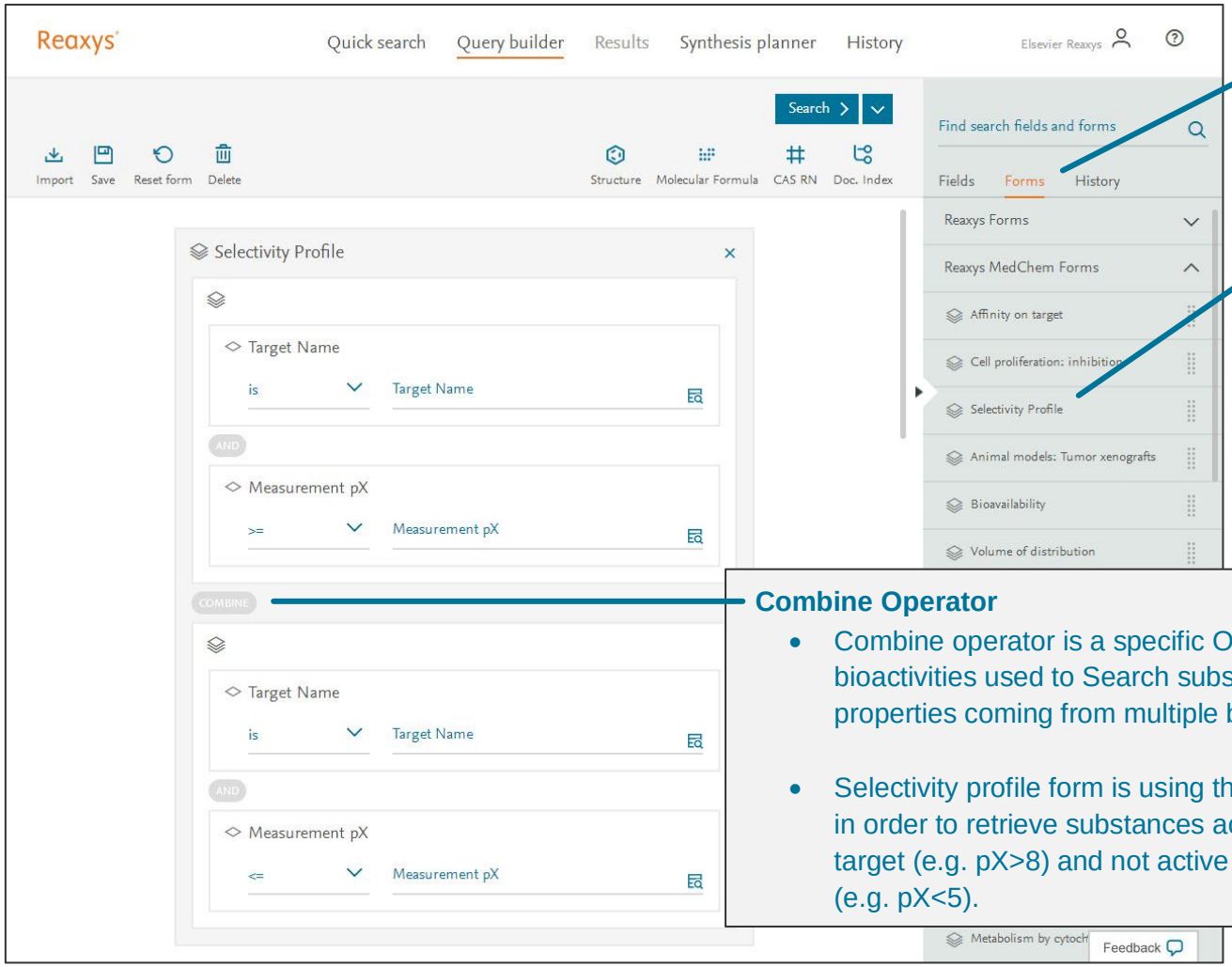
1. Click **Query builder**.
2. Start typing property name e.g. **boiling** in the **Find search fields and forms** box.
3. Drag & drop property onto the **Query builder**.
4. Click **Show fields**.
5. **Define specific Search Criteria**.
6. Click **Search** (Substances).



Query builder: Multiple Properties and Booleans



Query builder: Combine operator and Selectivity Profile form



1. Click **Forms**.

2. Drag & drop **Selectivity Profile** onto the **Query builder.**

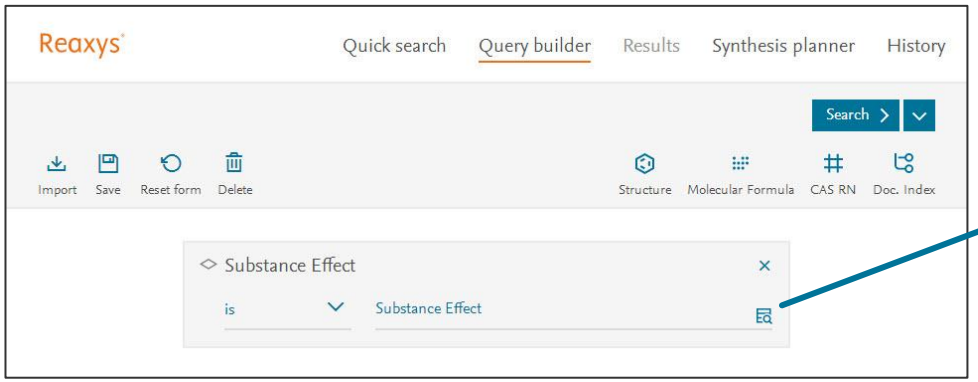
Combine Operator

- Combine operator is a specific Operator for bioactivities used to Search substance having properties coming from multiple bioassays.
- Selectivity profile form is using the combine operator in order to retrieve substances active on the first target (e.g. pX>8) and not active on the second one (e.g. pX<5).

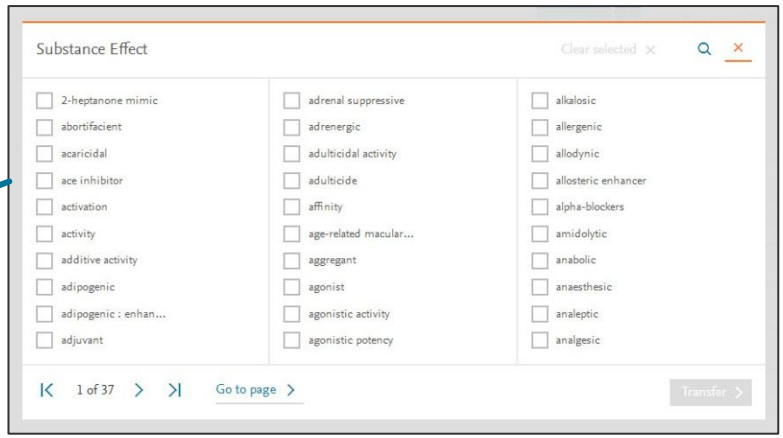
Query builder: Lookup Tool

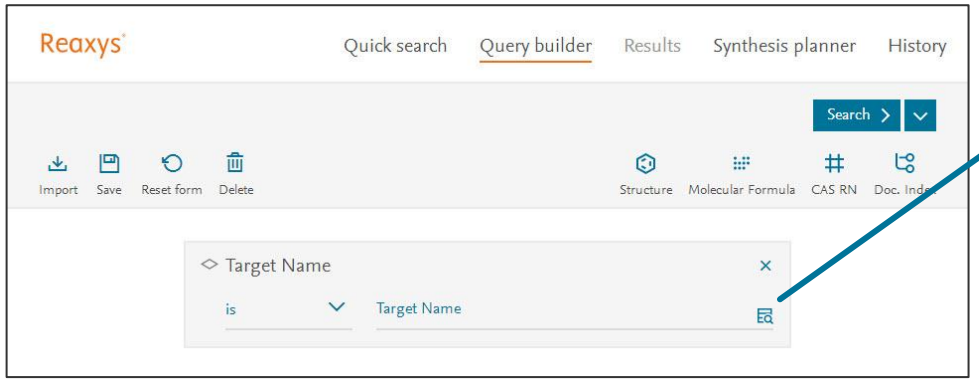
Clicking the **Lookup** tool in the query builder displays the content of the field in two modes:

- A *list view* for fields not based on Taxonomies
- A *tree view* for fields based on taxonomies (Target Name, Biological Species, Organs/tissues, Cells/Cell Lines, Administration route)

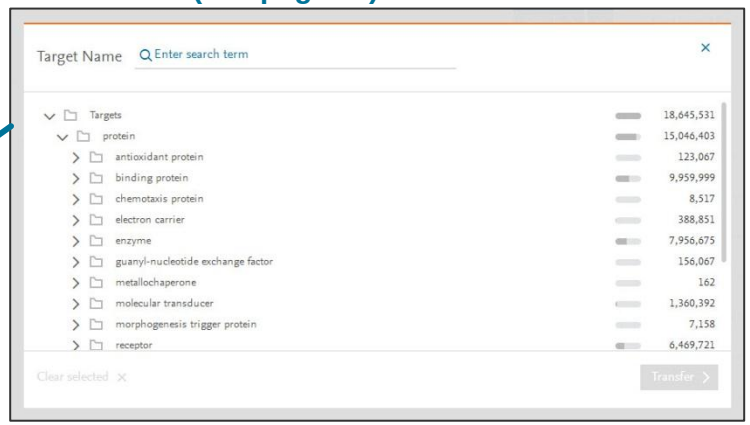


List View (see page 11)

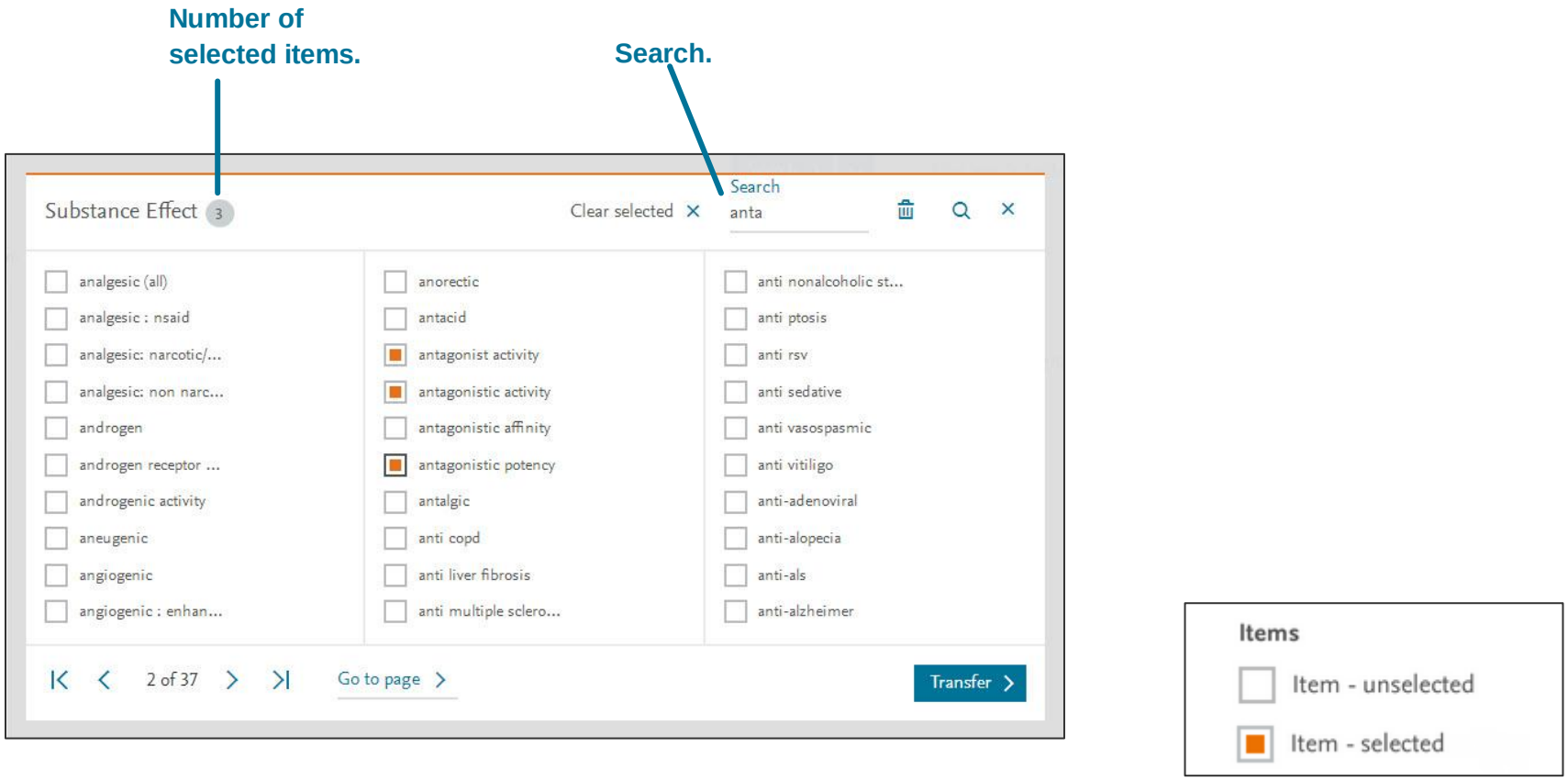




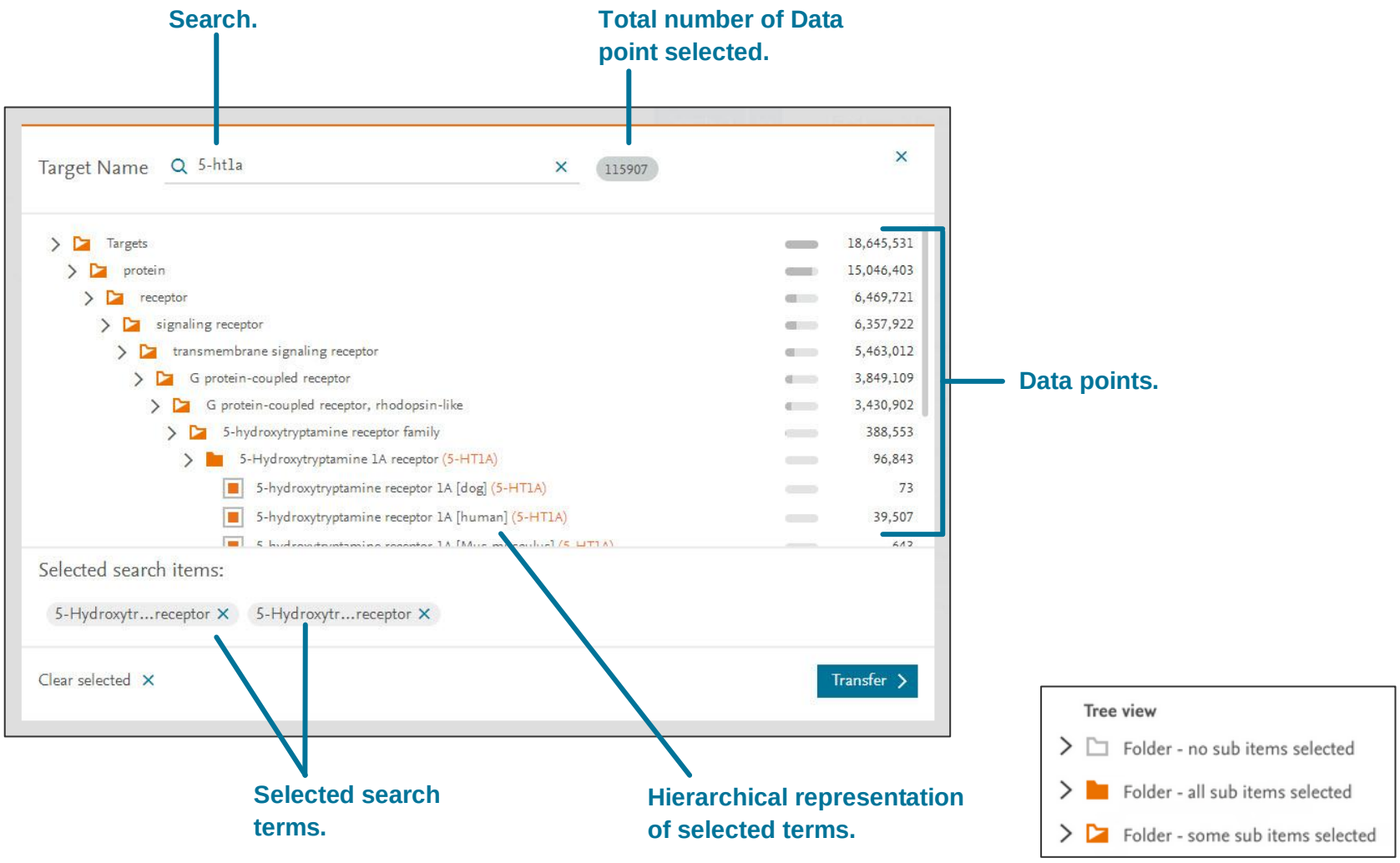
Tree View (see page 12)



Query builder: Lookup Tool: List View (continued)



Query builder: Lookup Tool: Tree View (continued)

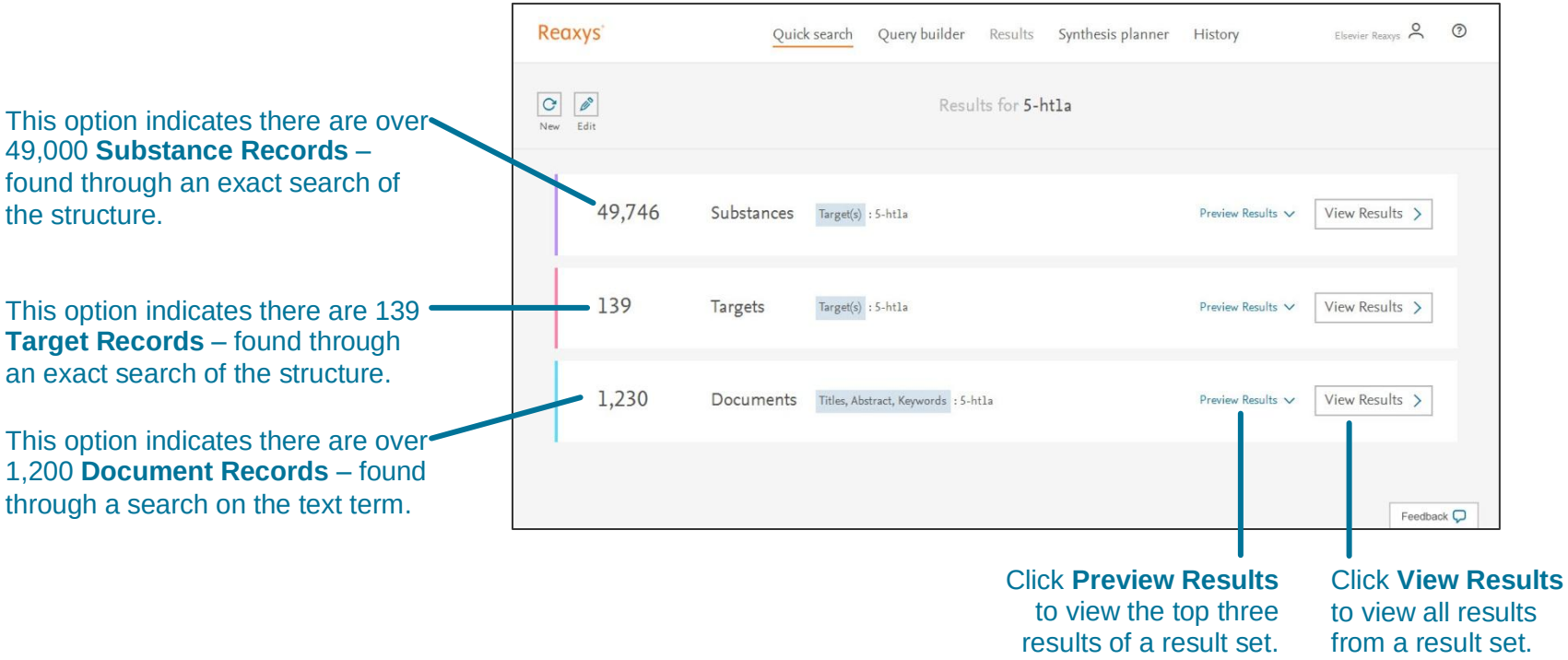


2. Results

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 name in Substance Records, Target Records and Document Records. 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

The **Back button** in your web browser is fully functional and will bring you back to the previous action or page.

Use **Filters and Analysis** to narrow your results.

Keep track of the session through the 'breadcrumbs'.

Sorting option is dependent on the selected Database.

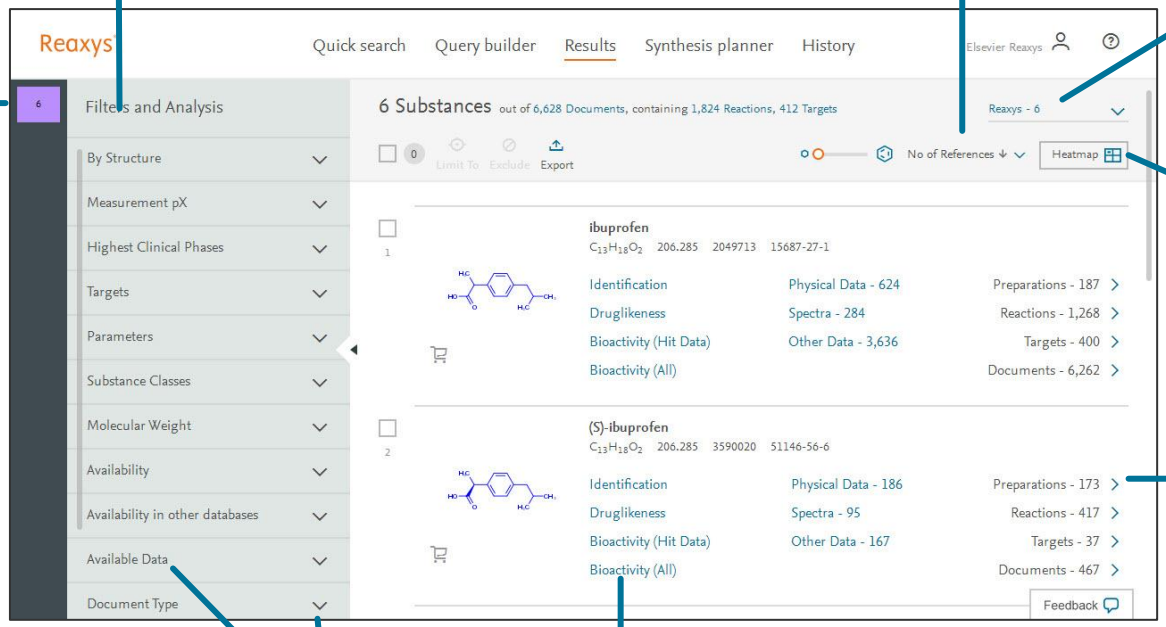
Click appropriate Database: **Reaxys**, eMolecules, LabNetwork, and PubChem.

Heatmap (available with RMC) provides a graphical and color coded display of structure activity relationships based on activity potency as pX.

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

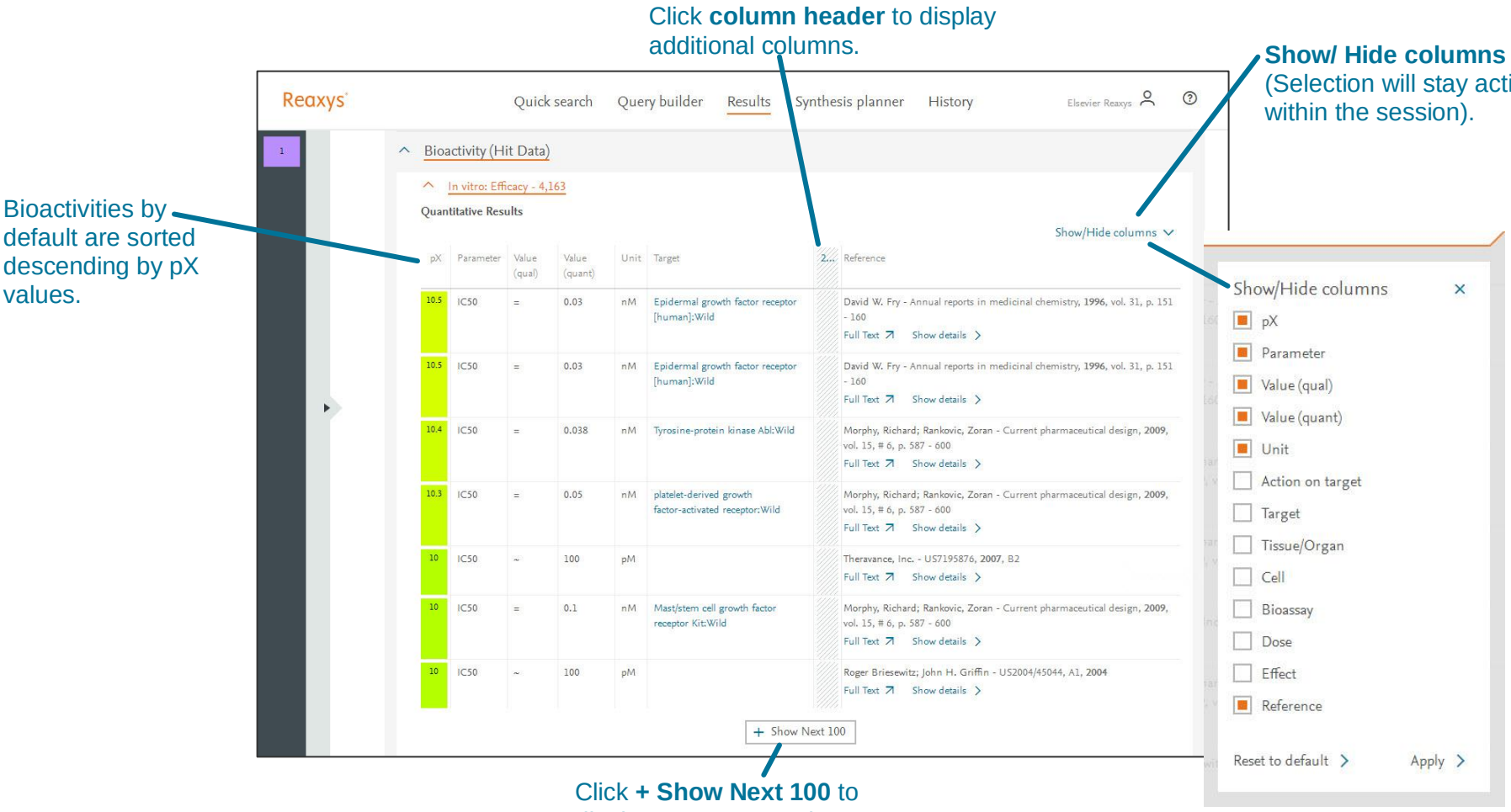
Click text or ⌄ to expand filters.

Click links to view specific information on the substance.



Quick search or Query builder Results – Substance Bioactivity

From the Substance's results page, click **Bioactivity (Hit Data)** to display bioactivity categories. Click category such as **In vitro: Efficacy**.



Quick search or Query builder Results – Reactions

Use **Filters and Analysis** to narrow your results.

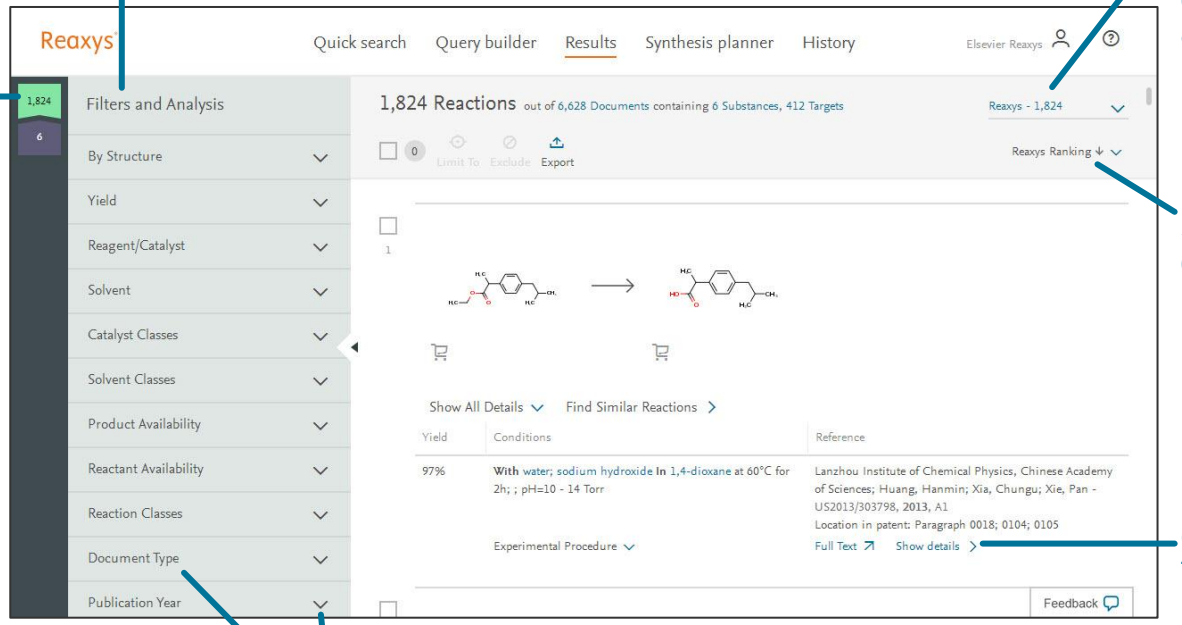
Keep track of the session through the 'breadcrumbs'.

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 **text** or ⌄ to expand filters.



Quick search or Query builder Results – Documents

The **Back button** in your web browser is fully functional and will bring you back to the previous action or page.

Use **Filters and Analysis** options to narrow your results.

Use Index Terms to narrow documents by topics.

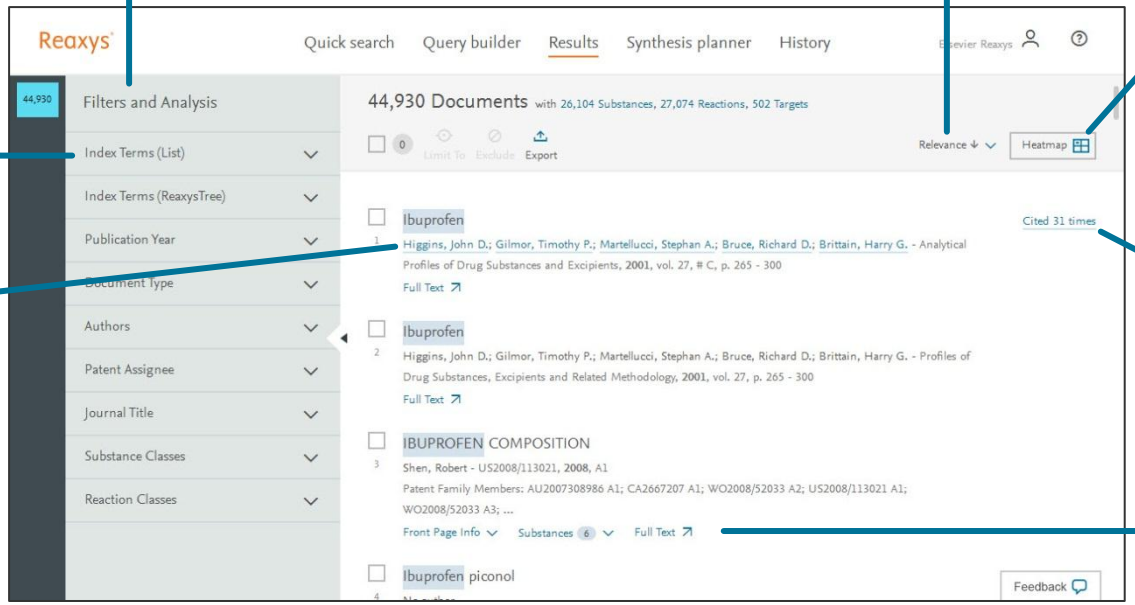
Click links for author(s) to explore details about their publications and additional analysis options in Scopus.

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

Heatmap (available with RMC) provides a graphical and color coded display of structure activity relationships based on activity potency as pX.

Click link to view citations in Scopus.

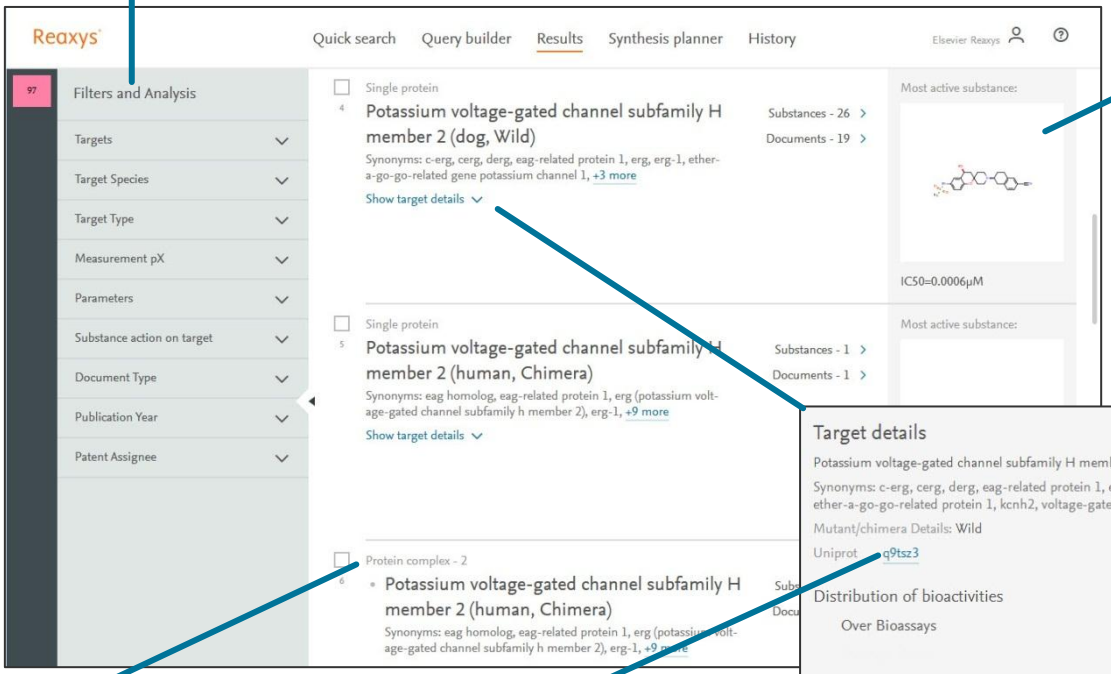
Click links to view Full Text, Front Page info (for patent records), Substances, Reactions, Abstract or Index Terms.



Quick search or Query builder Results – Target

The **Back button** in your web browser is fully functional and will bring you back to the previous action or page.

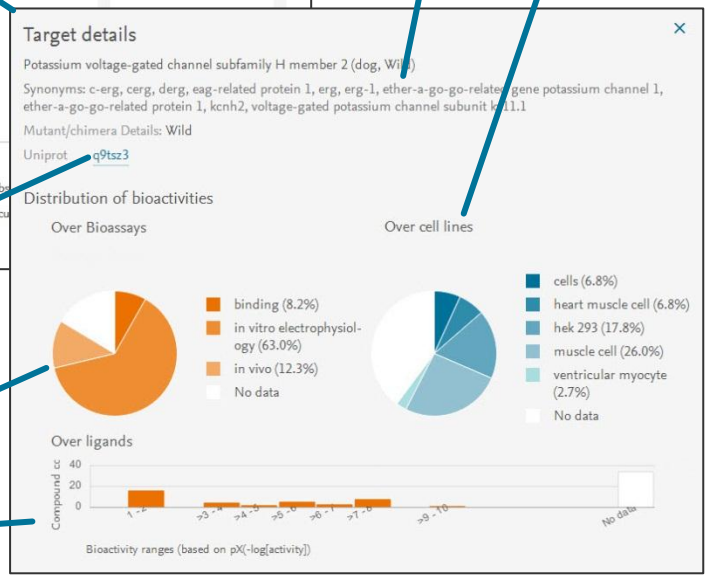
Use **Filters and Analysis** options to narrow your results.



Most active substance on the target based on highest pX. When pX is not available for substances tested on the target, a substance is displayed randomly.

Target synonyms and Genes name.

Cell lines used for testing the target.



Heteromeric target that consists of multiple proteins (subunits).

Link to Uniprot.

Link to PDB is provided when available.

Type of bioassays where the target was involved.

Potency Of substances tested on the aforementioned target.

3. Analyze and Filter

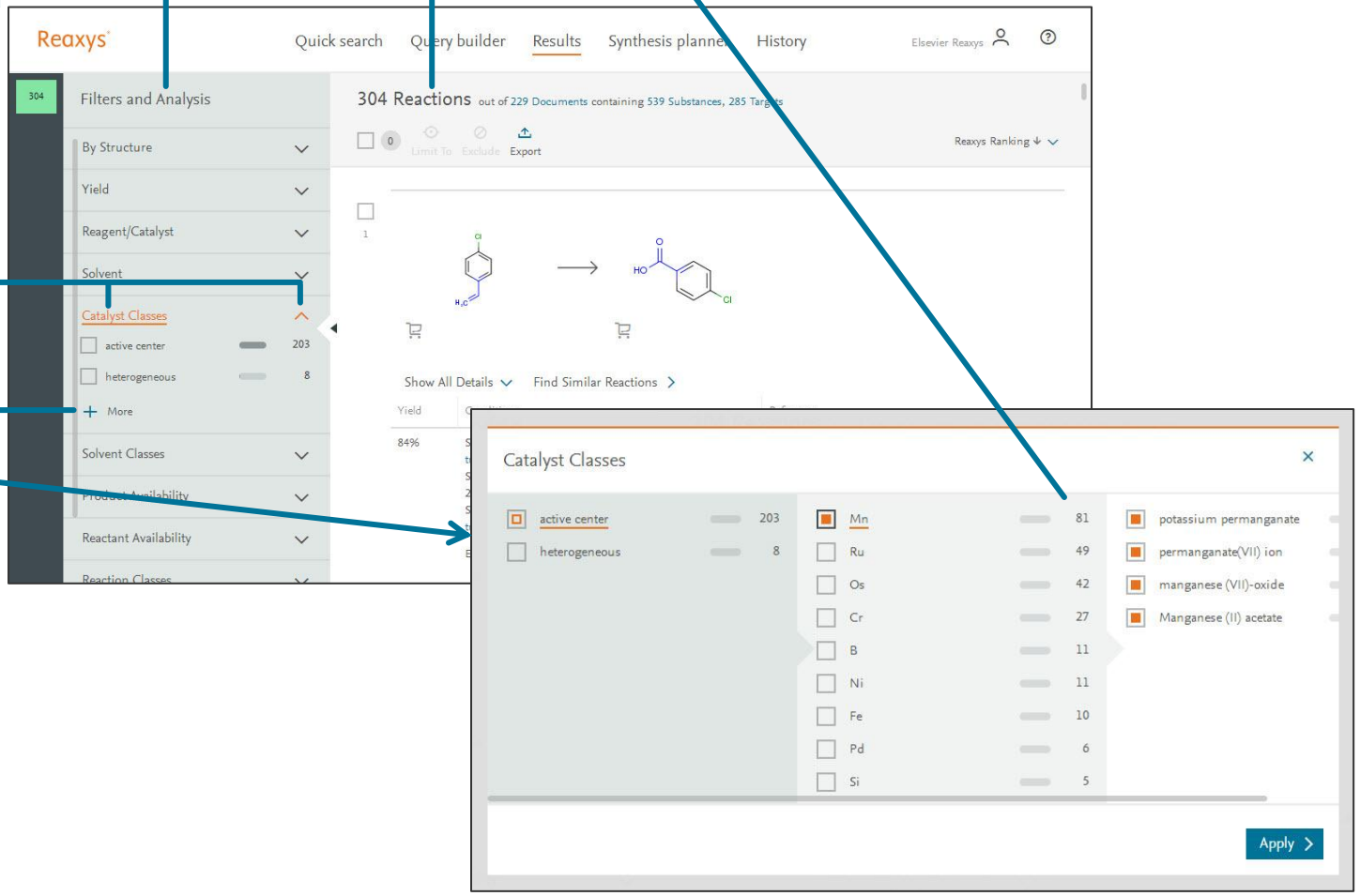
Use the **Filter & Analysis panel** to narrow your results:

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 304 Reactions to 81.

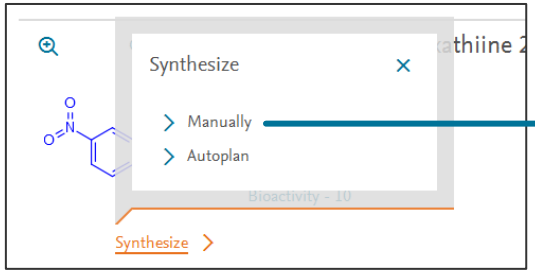
1. Click **text** or ⌄ to expand the Catalyst Classes Filter.

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



4. Synthesis planner – Manually

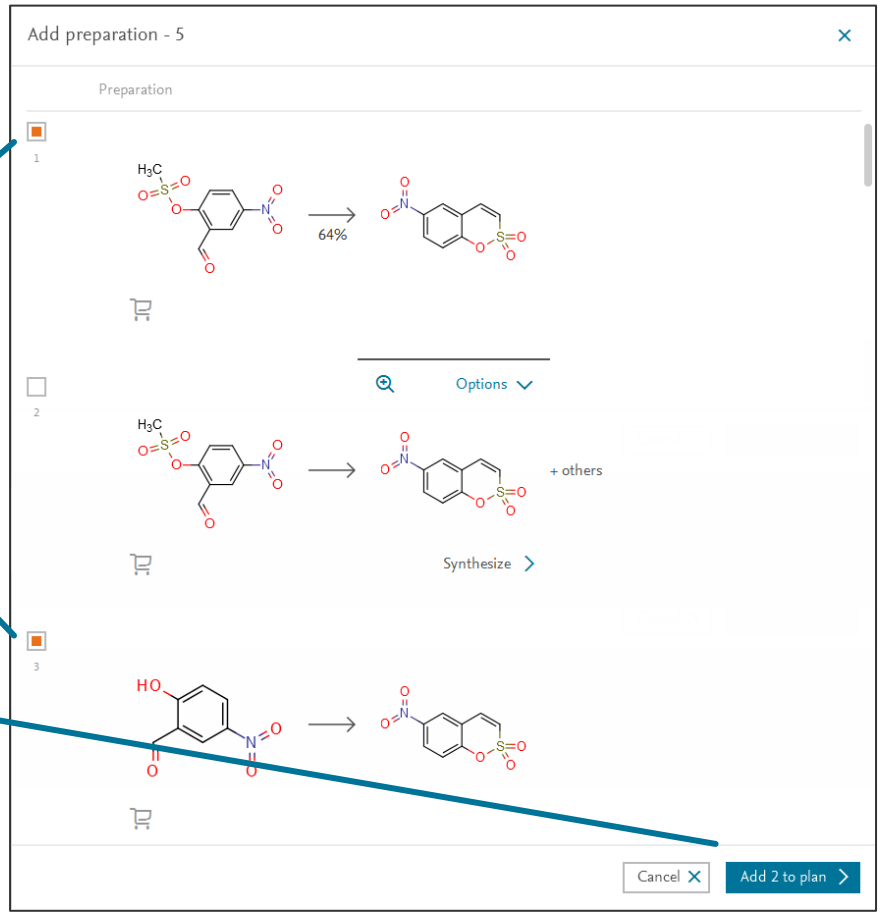
Build a synthesis pathway manually or let Reaxys do it automatically (see page 15). To begin, from a results page click **Synthesize** below a structure.



1. Click **Manually.**

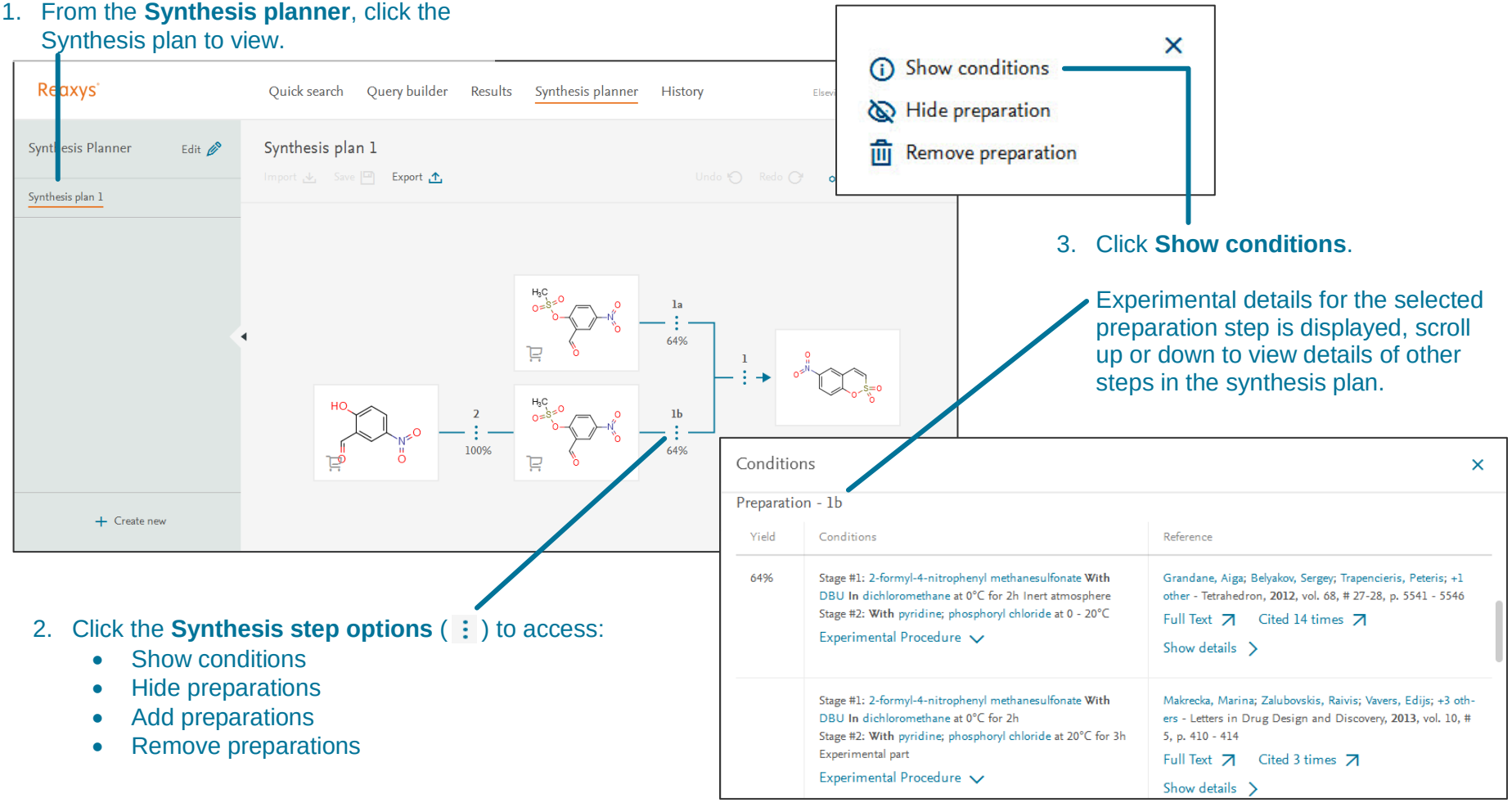
2. In the **Add preparation** window, select reactions to add to your plan.
   Note: the product structure is not shown because it is the same as the starting structure.

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



Synthesis planner – Manually (continued)

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



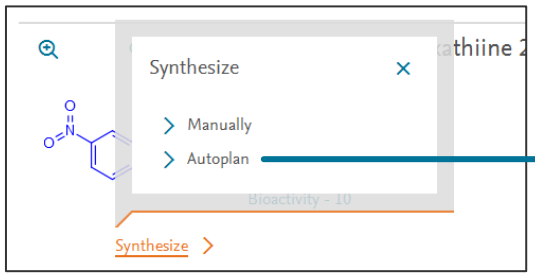
2. Click the **Synthesis step options** (⋮) to access:
   - Show conditions
   - Hide preparations
   - Add preparations
   - Remove preparations

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.

Synthesis planner - Autoplan

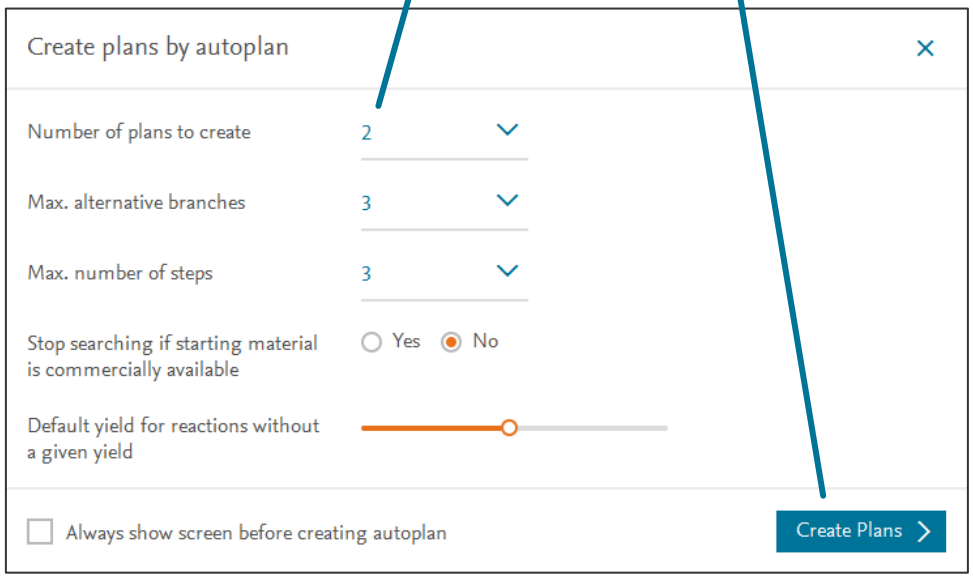
Let Reaxys build a synthesis pathway automatically. To begin, from a results page click **Synthesize** below a structure.



1. Click **Autoplan**.

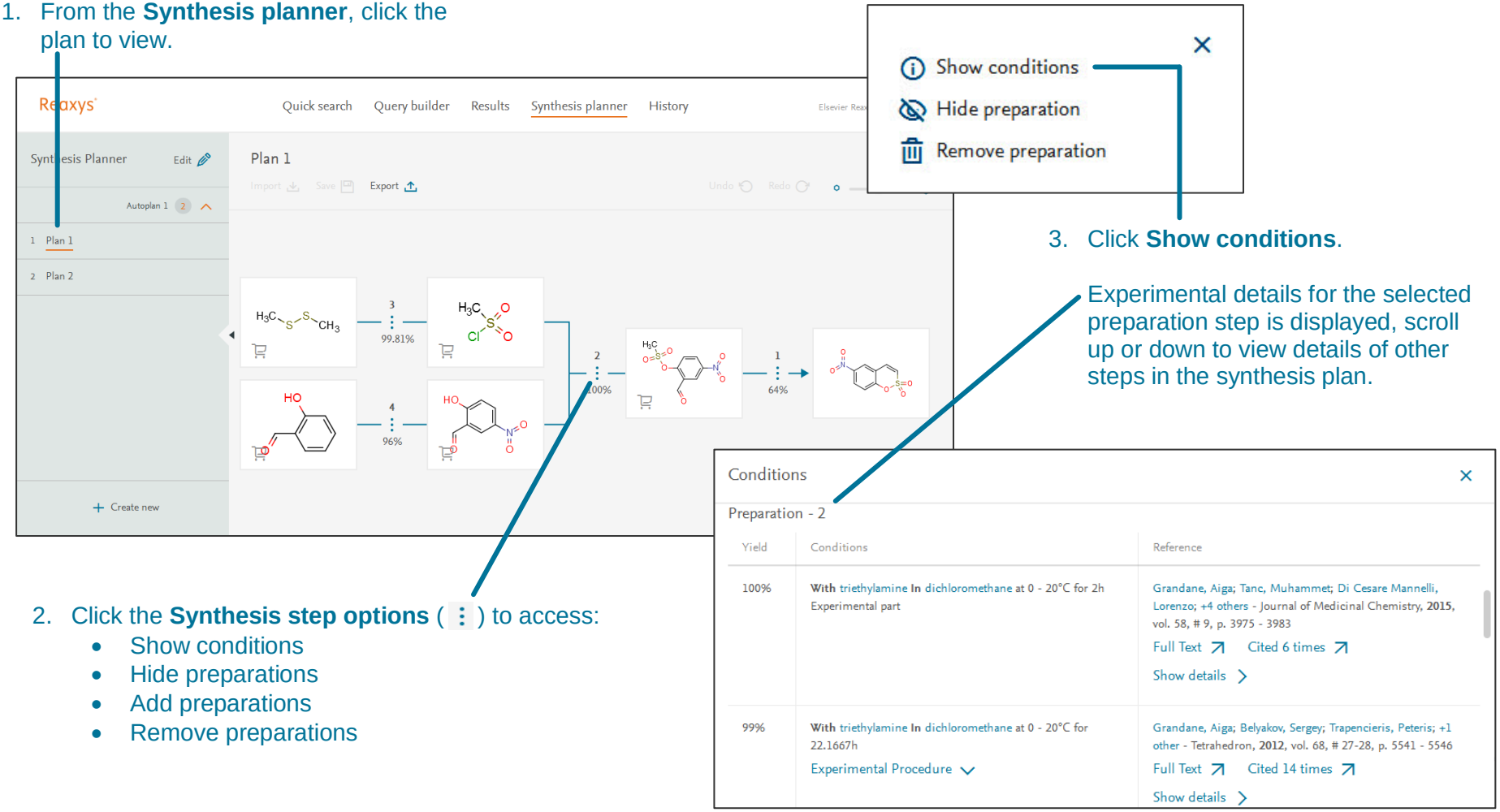
2. Define parameters for automatically generating synthetic pathways.

3. Click **Create Plans.**



Synthesis planner – Autoplan (continued)

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



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

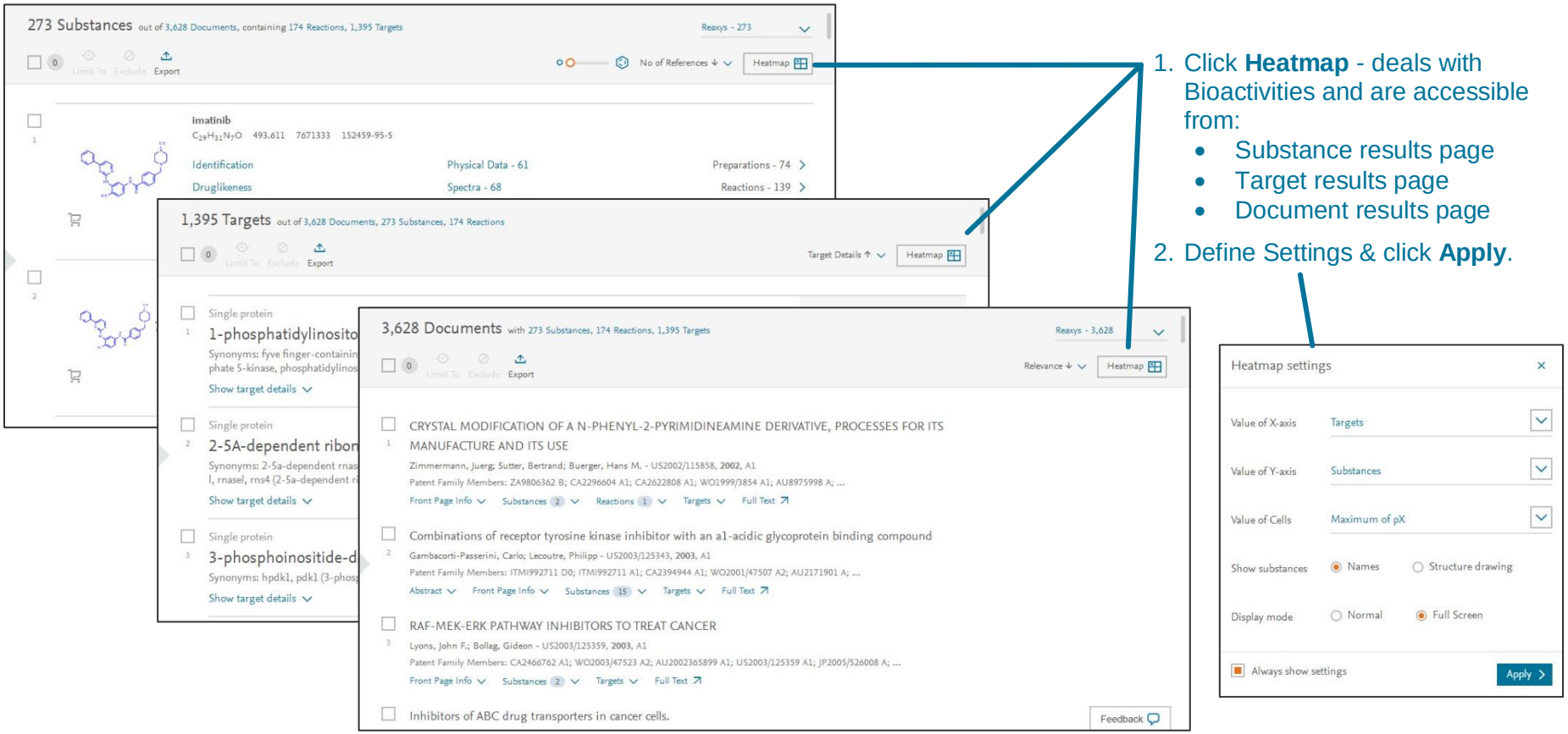
3. Click **Show conditions**.

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

5. Heatmap

Heatmaps in **Reaxys Medicinal Chemistry** display normalized and standardized data affinity measures (pX) for various compound (on the x-axis) and target (on the y-axis) pairings. The user can filter the affinity values (pX) to narrow in on values relevant to a specific research question or experimental condition. Its parameter settings are flexible: changing them reveals new relationships between compounds and protein targets or cell lines.

The pX value is a systematic conversion of affinity measures to a standardized parameter via compound concentration. All measures of affinity that are concentration dependent can be transformed into pX values, regardless of whether they are expressed on a logarithmic scale (pIC50, pEC50, pED50, pLD50, etc.) or a normal scale (LC50, ED50, Ki, etc.), and regardless of the units used (µM, nM, mM, g/l, etc.).

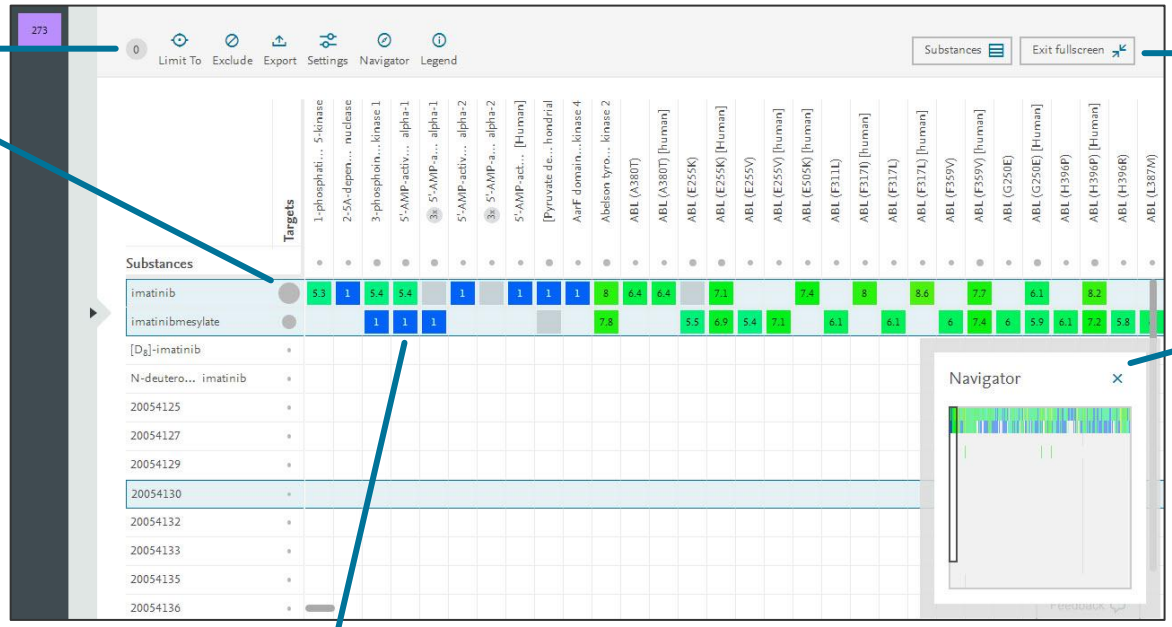


1. Click **Heatmap** - deals with Bioactivities and are accessible from:
   - Substance results page
   - Target results page
   - Document results page
2. Define Settings & click **Apply**.

Heatmap Overview (Full Screen Mode)

Menu

Data density: circle size is related to the amount of cells filled in the row or the column.



Display options.

Navigator window.

Heatmap colors:

- Green: High activity
- Blue: Low activity
- White: No data
- Gray: Qualitative data only (pX not available)
- Number: pX Value

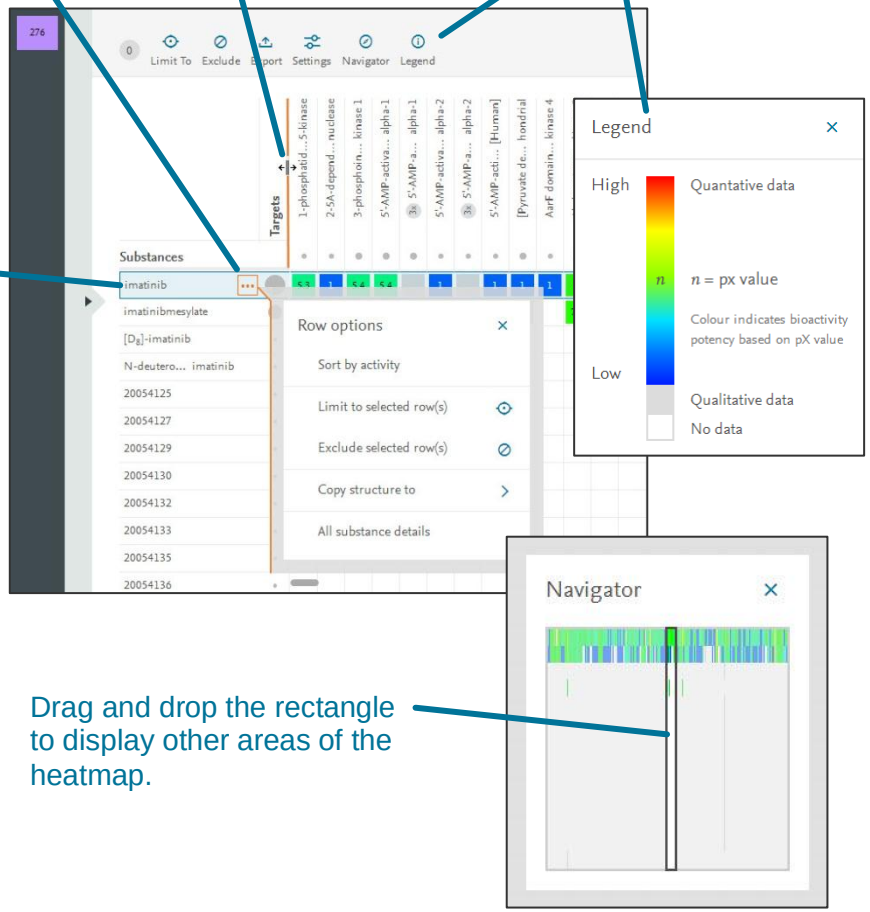
Heatmap Columns and Rows Management

Click the 3 dots to display options (columns or rows).

Drag to increase header size (columns or rows).

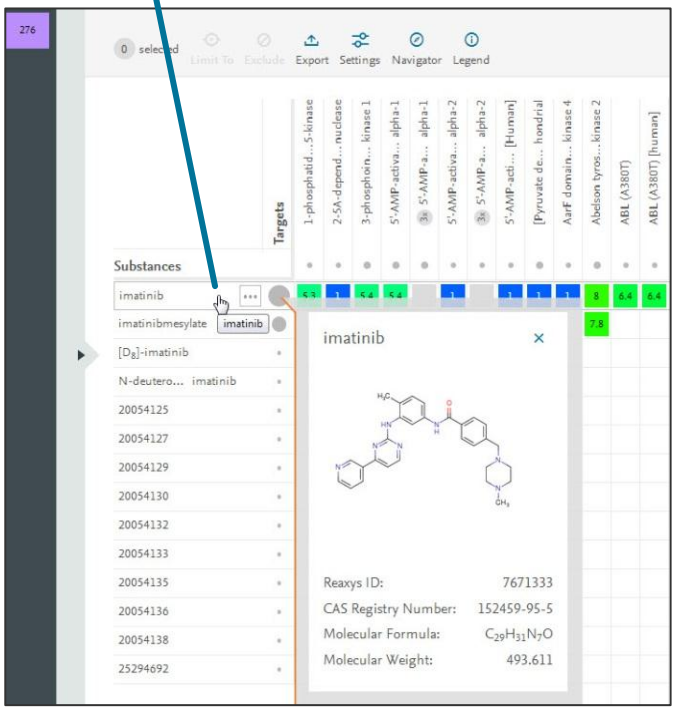
Displays Legend.

Click header to select the column or row.



Drag and drop the rectangle to display other areas of the heatmap.

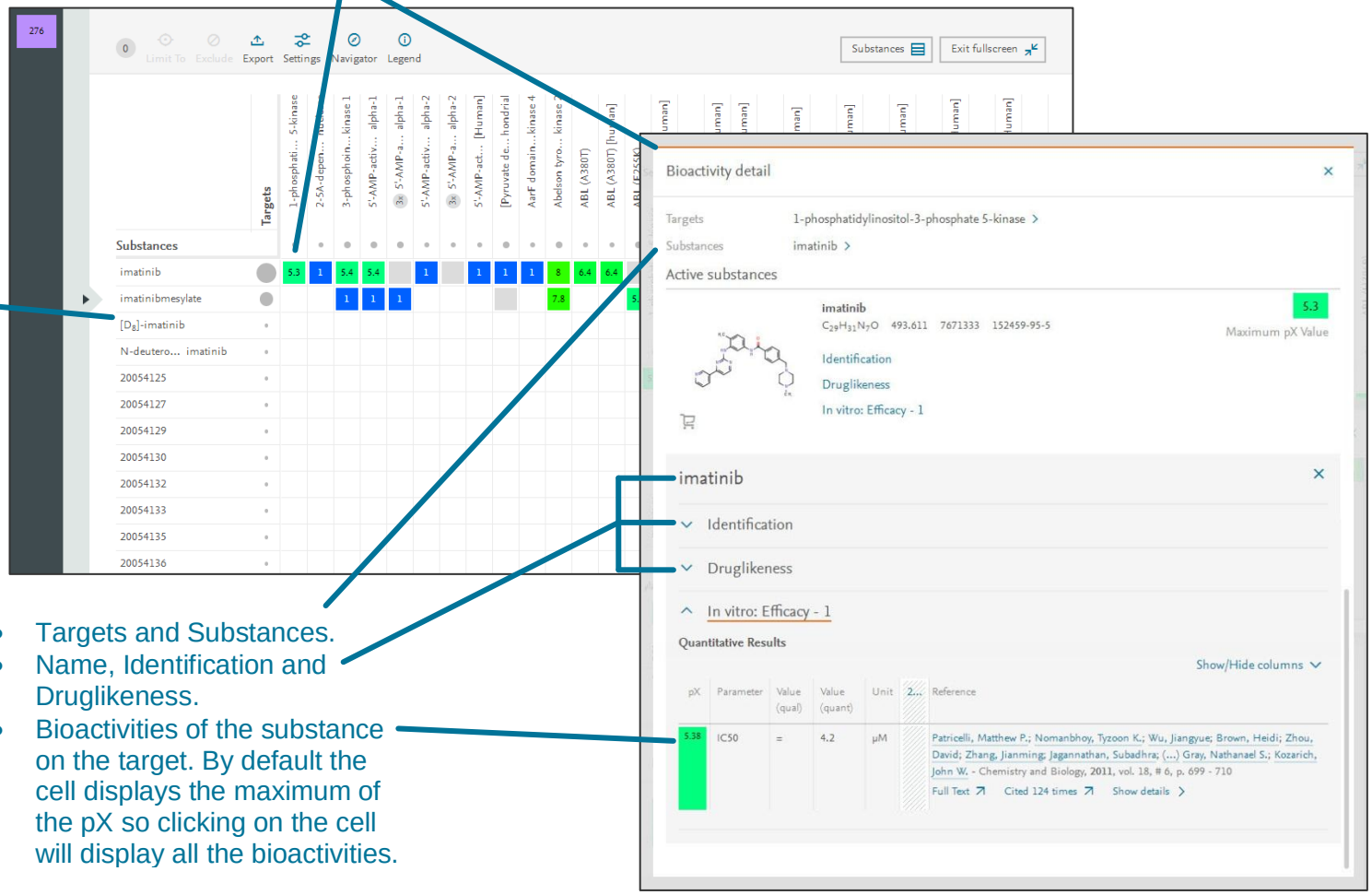
Hover over the column or row header to display more details such as chemical structure, target full name and synonyms.



Heatmap Cell Click

Click cell to display Bioactivity details.

Click header to select the column or row.



- Targets and Substances.
- Name, Identification and Druglikeness.
- Bioactivities of the substance on the target. By default the cell displays the maximum of the pX so clicking on the cell will display all the bioactivities.

6. 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 on your hard drive or elsewhere. This file can be then imported by clicking on the import button.
From the **Synthesis planner**	Click **Save** • The query is saved to a .json file on your hard drive or elsewhere. This file can be then imported by clicking on the import button.
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 item(s) you would like to export by ticking the boxes above the number of the search result and then clicking on limit to. • 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. ○ When the export is complete, click **Download**. **Note** : Exporting in Excel, SD or XML with an RMC License from Substances or Target results page will provide Bioactivities results as well as chemical structures such as smile, targets, and bioassays details. Excel export is the format of choice to retrieve chemical structure of substances (smile), targets, bioassays details and bioactivity results (datapoints).
From the **Synthesis planner**:	Click **Export**. • 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. ○ When the export is complete, click **Download**.

Saving and Exporting (continued)

Exporting (continued)	
From the **Results Heatmap**:	Use the export button in the Heatmap to retrieve raw data like substances (Names, Smiles etc.), targets (Names, Species, mutations etc.), cell lines, Bioassays and bioactivities (pX, IC50, Ki etc.) that are used to construct and display the heatmap to excel, SD file or XML but not the heatmap itself as a picture or in excel. • Click **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. ○ When the export is complete, click **Download**. **Note**: - Excel export is the format of choice to retrieve chemical structure of substances (smile), targets , bioassays details and bioactivity results (data points). The same export (content) of bioactivities is available from the Heatmap view or from the substances or targets list view.