

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: <ul style="list-style-type: none"> • Atenolol • Pt(PPh₃)₃ • 102625-70-7
Quick search with Structure or Reaction Drawing (See page 5)	<ol style="list-style-type: none"> 1. Click the Create Structure or Reaction Drawing box. 2. Create the substance structure drawing. For more information on using the Marvin JS structure editor see: <ol style="list-style-type: none"> a. 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)	<ol style="list-style-type: none"> 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 <ol style="list-style-type: none"> 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: <ul style="list-style-type: none"> • preparation of porphyrine • phosphorylation • Suzuki coupling • Adler phenol oxidation
Quick search with Structure or Reaction Drawing (See page 5)	<ol style="list-style-type: none"> 1. Click the Create Structure or Reaction Drawing box. 2. Create the reaction structure drawing. For more information on using the Marvin JS structure editor see: <ol style="list-style-type: none"> a. 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)	<ol style="list-style-type: none"> 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 <ol style="list-style-type: none"> 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: <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 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)	<ol style="list-style-type: none"> 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. <p>OR</p> <ol style="list-style-type: none"> 2. Drag & Drop from one of these options <ol style="list-style-type: none"> 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. <p>Note: Click Show fields to enter specific search values.</p>

PROPERTIES	
FEATURE	COMMENT
Quick search (See page 4)	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 5)	<ol style="list-style-type: none"> 1. Click the Create Structure or Reaction Drawing box. 2. Create the substance structure drawing. For more information on using the Marvin JS structure editor see: <ol style="list-style-type: none"> a. 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)	<ol style="list-style-type: none"> 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. <p>OR</p> <ol style="list-style-type: none"> 2. Drag & Drop from one of these options <ol style="list-style-type: none"> 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. <p>Note: Click Show fields to enter specific search values.</p>

Search (continued)

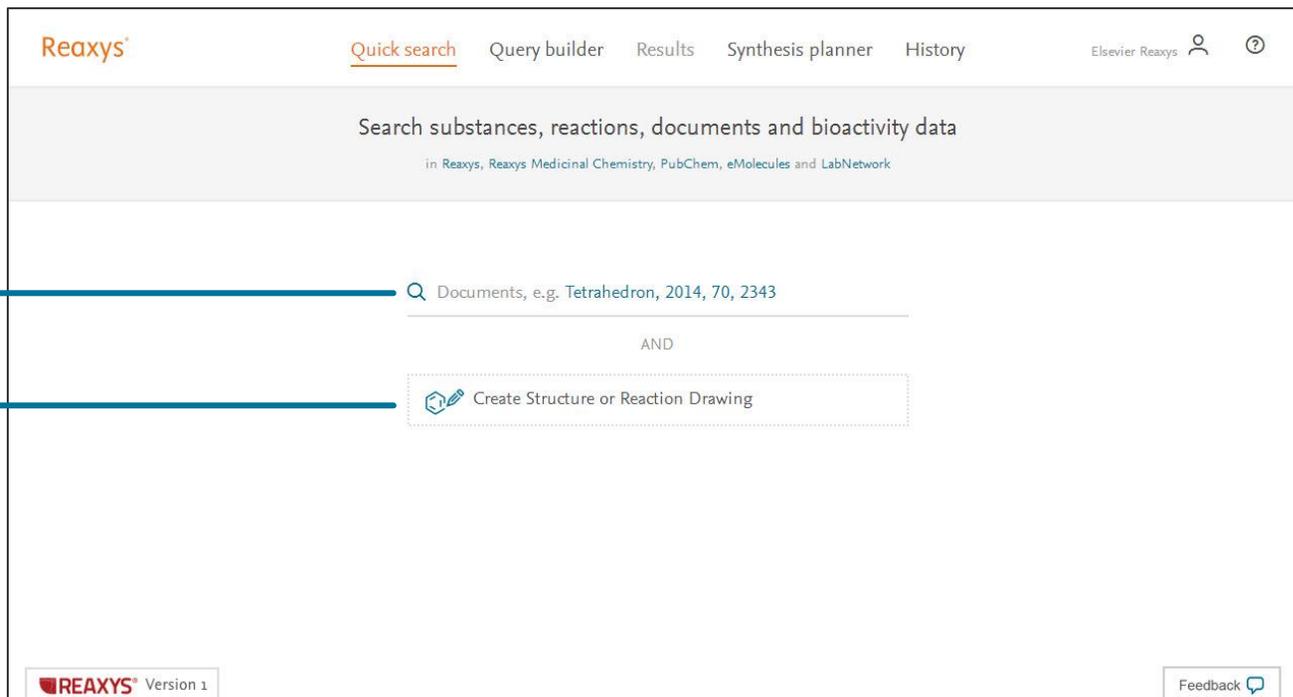
MEDICINAL CHEMISTRY	
FEATURE	COMMENT
Quick search (See page 4)	<ul style="list-style-type: none"> Enter target names, gene names, Uniprot id, PDB id, cell lines, species, and substances action on target in the Search Reaxys field and click Search. Examples: <ul style="list-style-type: none"> D(2) dopamine receptor ADORA1 O75469 2pfr Caco-2 5-HT1a antagonist
Quick search with Structure or Reaction Drawing (See page 5)	<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. 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.

MEDICINAL CHEMISTRY	
FEATURE	COMMENT
Query builder (See page 6 & 7)	<ol style="list-style-type: none"> Click Query builder (See page 7). 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 Drag & Drop from one of these options <ol style="list-style-type: none"> Fields: and drag & drop desired field onto the query screen or search fields using the Find search fields and forms box. 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. 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 8). 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.



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

Search substances, reactions, documents and bioactivity data
in Reaxys, Reaxys Medicinal Chemistry, PubChem, eMolecules and LabNetwork

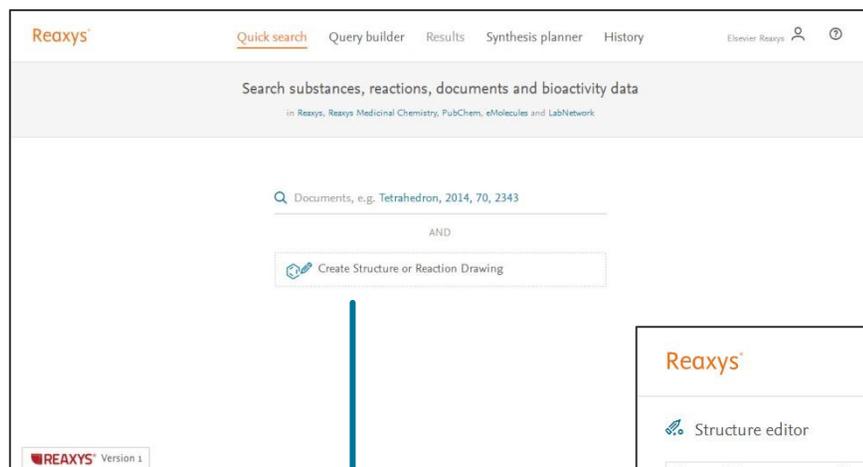
Q Documents, e.g. Tetrahedron, 2014, 70, 2343

AND

 Create Structure or Reaction Drawing

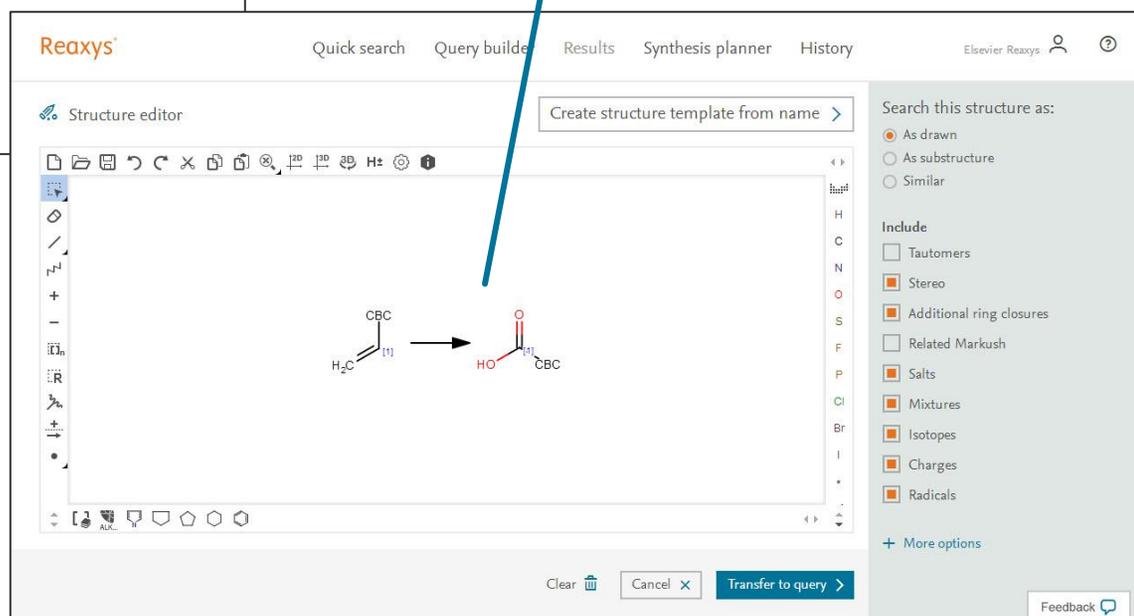
REAXYS[®] Version 1 Feedback 

Quick search with Structure or Reaction Drawing

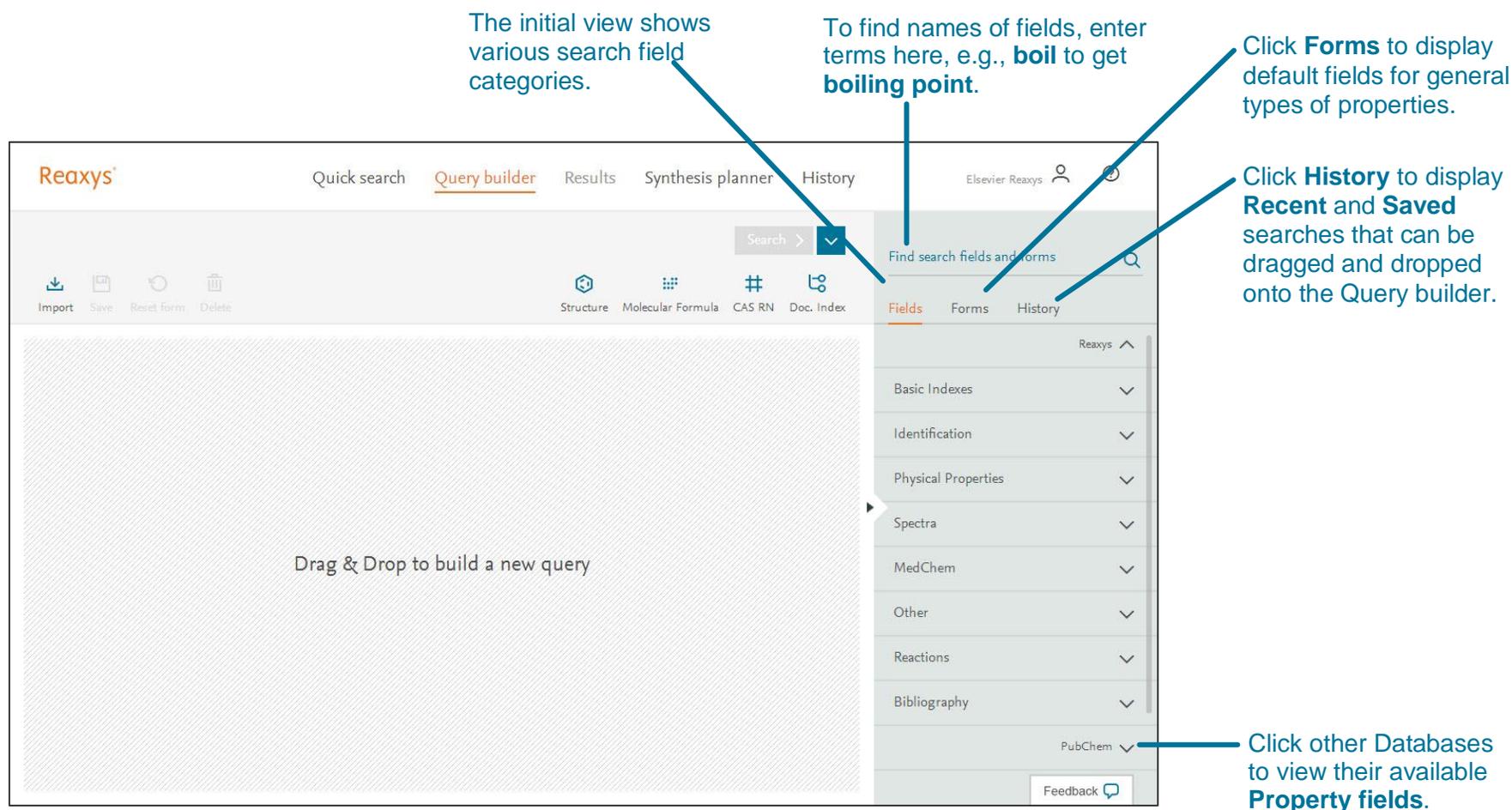


1. Click the **Create Structure or Reaction Drawing** box.

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



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**.

Drag & Drop to build a new query

Reaxys

Quick search Query builder Results Synthesis planner History

Elsevier Reaxys

Search >

Find search fields and forms

Fields Forms History

Reaxys

Basic Indexes

Identification

Physical Properties

Spectra

MedChem

Other

Reactions

Bibliography

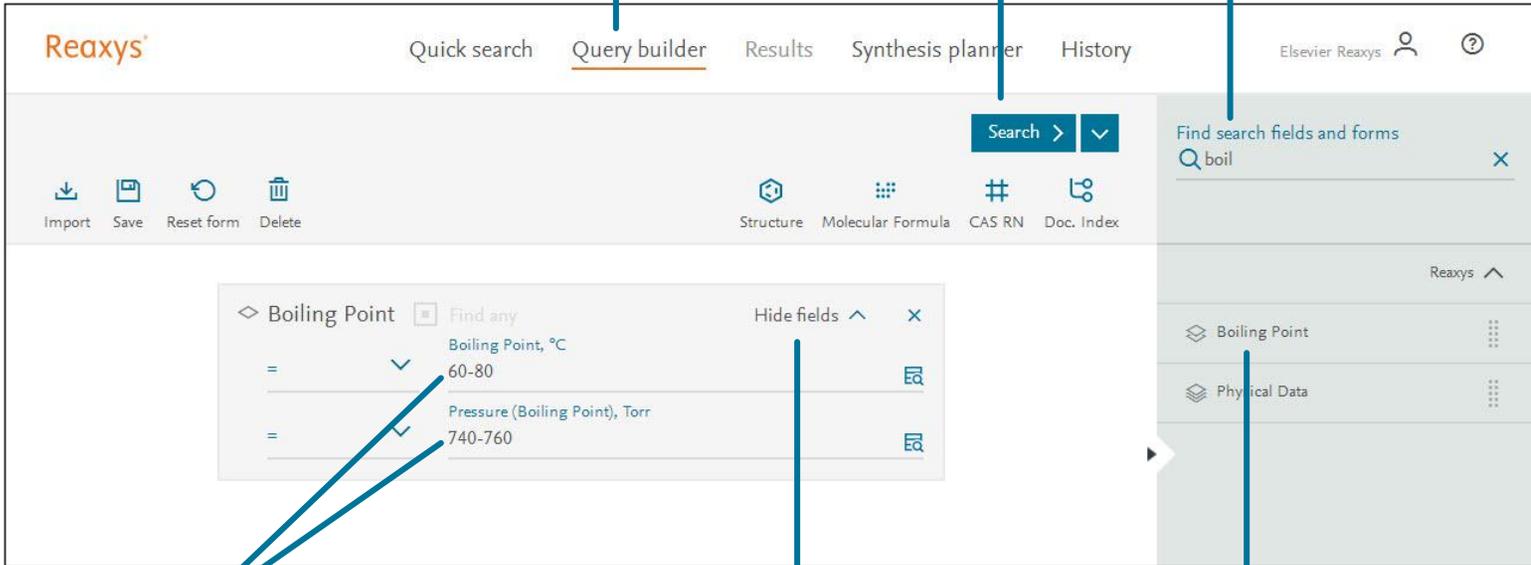
PubChem

Feedback

Import Save Reset form Delete

Structure Molecular Formula CAS RN Doc. Index

Query builder Steps



1. Click **Query builder**.

2. Start typing property name e.g. **boiling** in 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)**.

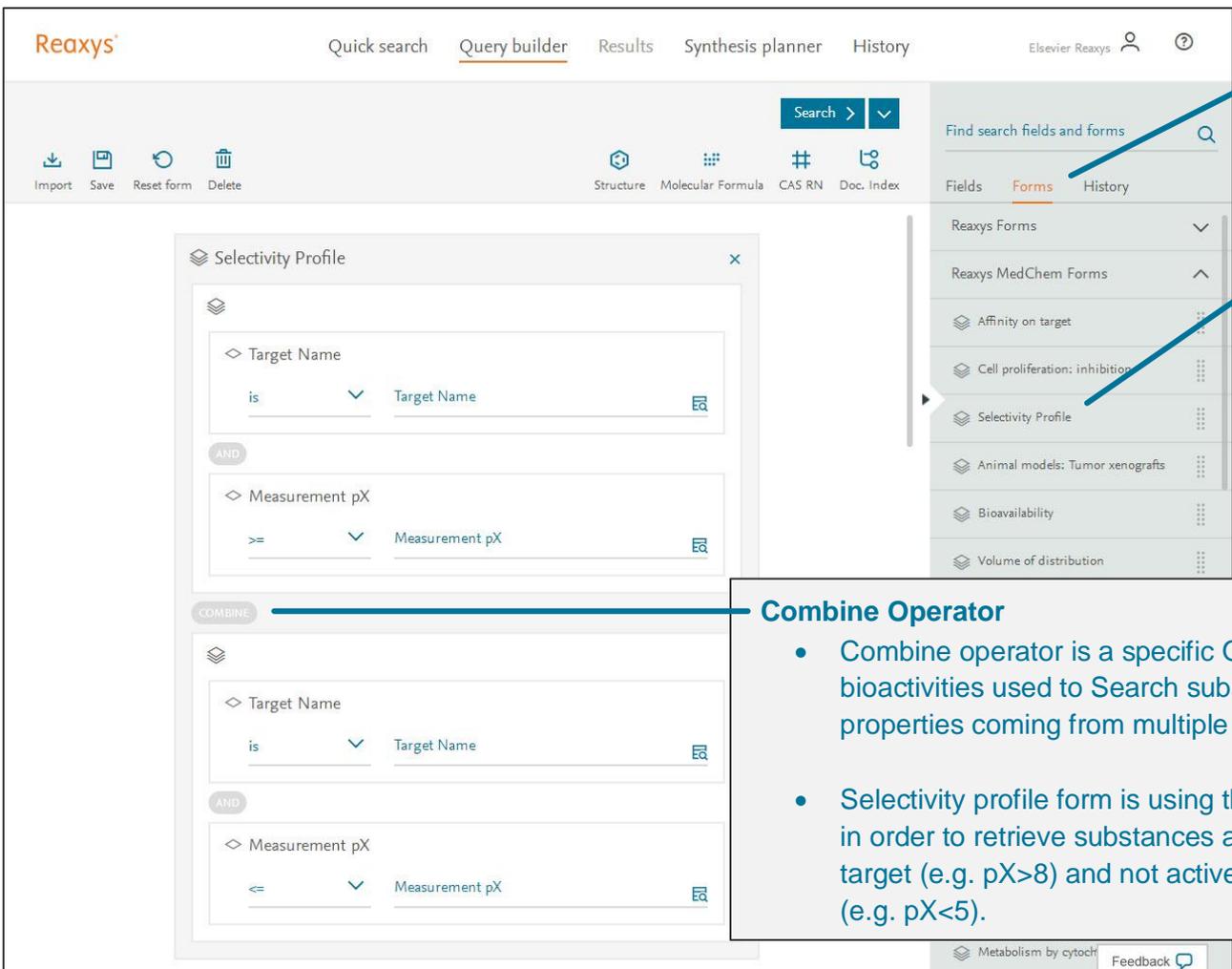
Query builder: Multiple Properties and Booleans

The screenshot shows the Reaxys Query Builder interface. The top navigation bar includes "Quick search", "Query builder" (selected), "Results", "Synthesis planner", and "History". The user is logged in as "Elsevier Reaxys". The main area displays a query for "Boiling Point" and "Pressure (Boiling Point), Torr". A dropdown menu is open, showing the Boolean operator "AND" selected. A callout box provides a legend for the Boolean operators:

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
- **PROXIMITY**: typically used with parameter fields, ensuring the content of both fields relate to each other (e.g. melting point and solvent)

Query builder: Combine operator and Selectivity Profile form



The screenshot shows the Reaxys Query Builder interface. At the top, there are navigation tabs: Quick search, **Query builder**, Results, Synthesis planner, and History. Below the navigation is a toolbar with icons for Import, Save, Reset form, and Delete. A search bar is also present. The main area is divided into two panels. On the left, the 'Selectivity Profile' form is open, showing two conditions: 'Target Name is Target Name' and 'Measurement pX >= Measurement pX'. Below these is a 'COMBINE' button. On the right, the 'Forms' panel is visible, listing various search fields and forms, including 'Reaxys Forms', 'Reaxys MedChem Forms', 'Affinity on target', 'Cell proliferation: inhibition', 'Selectivity Profile', 'Animal models: Tumor xenografts', 'Bioavailability', and 'Volume of distribution'. A blue arrow points from the 'Selectivity Profile' form to the 'COMBINE' button, and another blue arrow points from the 'Selectivity Profile' form to the 'Selectivity Profile' entry in the 'Forms' panel.

1. Click **Forms**.

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

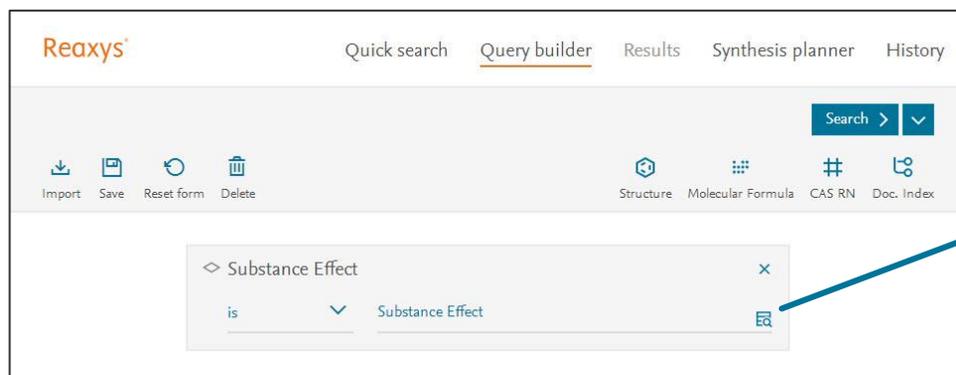
Combine Operator

- 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. $pX < 5$).

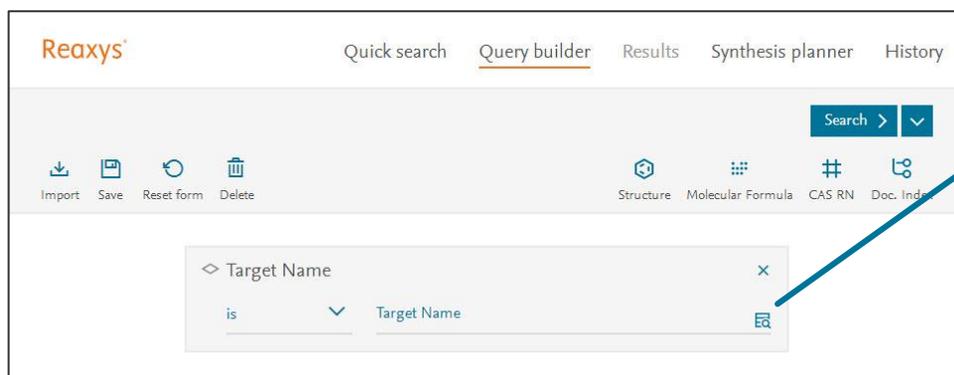
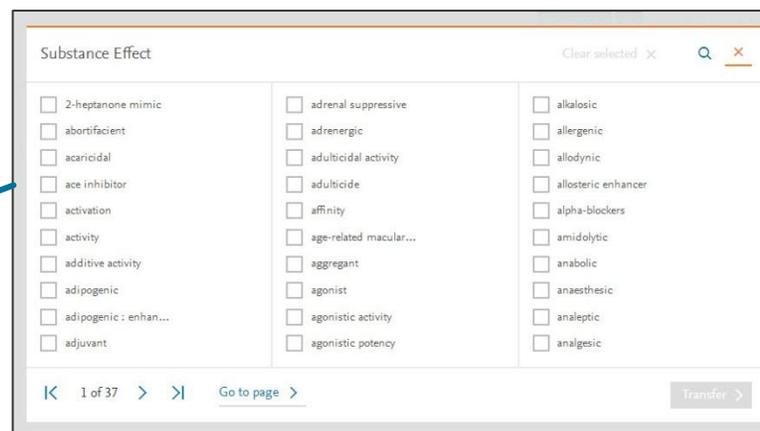
Query builder: Lookup Tool

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

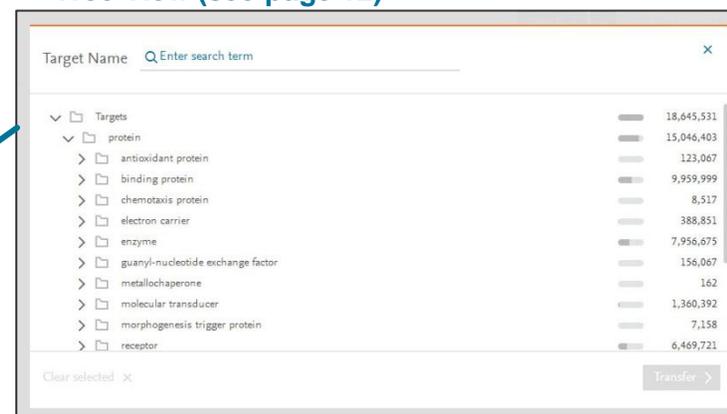
- A *list view* for fields not based on Taxonomies
- A *tree view* for fields based on taxonomies (Target Name, Biological Species, Organs/tissues, Cells/Cell Lines, Administration route)



List View (see page 11)



Tree View (see page 12)



Query builder: Lookup Tool: List View (continued)

Number of selected items.

Search.

The screenshot shows the 'Substance Effect' list view in the Reaxys Query Builder. At the top left, the title 'Substance Effect' is followed by a circle containing the number '3', indicating the count of selected items. To the right is a search bar with the text 'anta' and a 'Search' button. Below the search bar are three columns of checkboxes, each with a corresponding label. Three items are selected: 'antagonist activity', 'antagonistic activity', and 'antagonistic potency'. At the bottom of the list, there are navigation controls including '2 of 37' and a 'Transfer' button.

Items

- Item - unselected
- Item - selected

Query builder: Lookup Tool: Tree View (continued)

Search.

Total number of Data point selected.

Data points.

Selected search terms.

Hierarchical representation of selected terms.

Tree view

- > Folder - no sub items selected
- > Folder - all sub items selected
- > Folder - some sub items selected

Target Name	Total number of Data point selected
Targets	18,645,531
protein	15,046,403
receptor	6,469,721
signaling receptor	6,357,922
transmembrane signaling receptor	5,463,012
G protein-coupled receptor	3,849,109
G protein-coupled receptor, rhodopsin-like	3,430,902
5-hydroxytryptamine receptor family	388,553
5-Hydroxytryptamine 1A receptor (5-HT1A)	96,843
5-hydroxytryptamine receptor 1A [dog] (5-HT1A)	73
5-hydroxytryptamine receptor 1A [human] (5-HT1A)	39,507
5-hydroxytryptamine receptor 1A [Mus musculus] (5-HT1A)	642

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.

This option indicates there are over 49,000 **Substance Records** – found through an exact search of the structure.

This option indicates there are 139 **Target Records** – found through an exact search of the structure.

This option indicates there are over 1,200 **Document Records** – found through a search on the text term.

The screenshot displays the Reaxys interface for a quick search of '5-ht1a'. The top navigation bar includes 'Quick search', 'Query builder', 'Results', 'Synthesis planner', and 'History'. The user is identified as 'Elsevier Reaxys'. The main content area shows 'Results for 5-ht1a' with three categories: Substances (49,746 records), Targets (139 records), and Documents (1,230 records). Each category has a 'Preview Results' dropdown and a 'View Results' button. The 'View Results' button for the Substances category is highlighted with a red box. A 'Feedback' button is located at the bottom right.

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

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

Quick search or Query builder Results – Substances

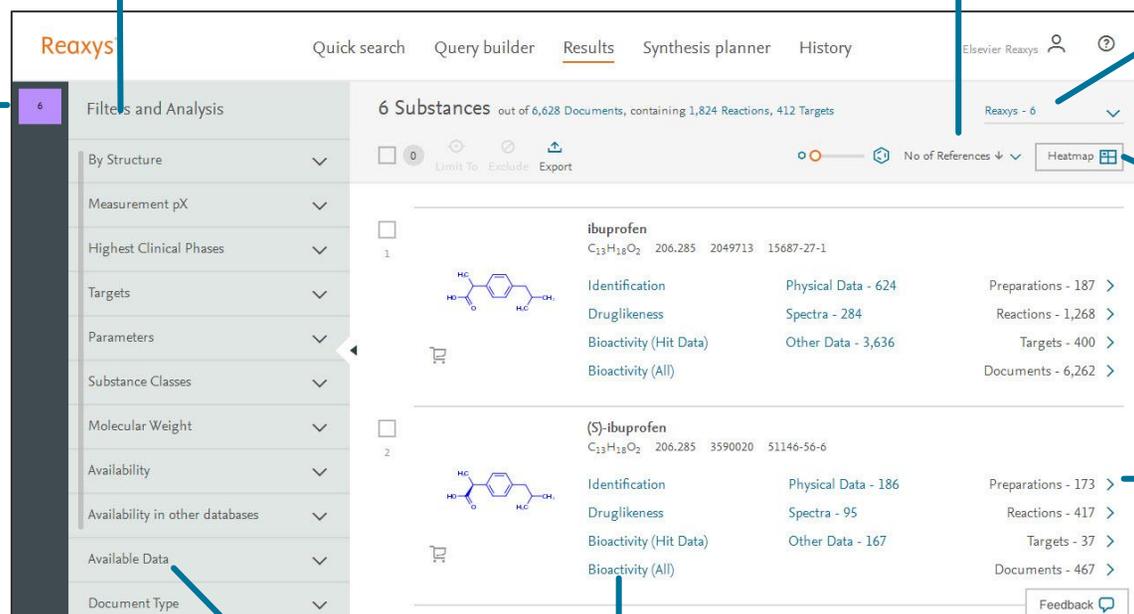
The **Back button** in your web browser is fully functional and will bring you back to the previous action or page.

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

Sorting option is dependent on the selected Database.

Keep track of the session through the 'breadcrumbs'.

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**.

Click **column header** to display additional columns.

Show/ Hide columns
(Selection will stay active within the session).

Bioactivities by default are sorted descending by pX values.

The screenshot shows the Reaxys interface with the 'Bioactivity (Hit Data)' section expanded. The 'In vitro: Efficacy' category is selected, showing 4,163 results. The 'Quantitative Results' table is displayed, sorted by pX values in descending order. A 'Show/Hide columns' dialog box is open on the right, showing a list of columns with checkboxes. The 'pX' column is checked, while others are unchecked. A '+ Show Next 100' button is visible at the bottom of the table.

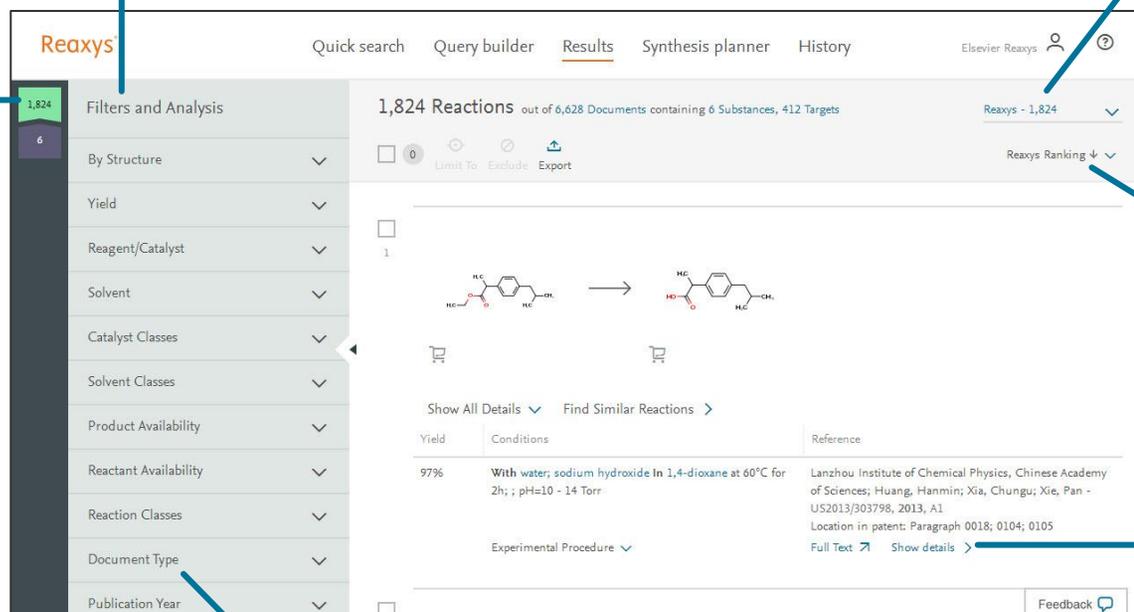
pX	Parameter	Value (qual)	Value (quant)	Unit	Target	Reference
10.5	IC50	=	0.03	nM	Epidermal growth factor receptor [human]:Wild	David W. Fry - Annual reports in medicinal chemistry, 1996, vol. 31, p. 151 - 160 Full Text ↗ Show details >
10.5	IC50	=	0.03	nM	Epidermal growth factor receptor [human]:Wild	David W. Fry - Annual reports in medicinal chemistry, 1996, vol. 31, p. 151 - 160 Full Text ↗ Show details >
10.4	IC50	=	0.038	nM	Tyrosine-protein kinase Abl:Wild	Morphy, Richard; Rankovic, Zoran - Current pharmaceutical design, 2009, vol. 15, # 6, p. 587 - 600 Full Text ↗ Show details >
10.3	IC50	=	0.05	nM	platelet-derived growth factor-activated receptor:Wild	Morphy, Richard; Rankovic, Zoran - Current pharmaceutical design, 2009, vol. 15, # 6, p. 587 - 600 Full Text ↗ Show details >
10	IC50	~	100	pM		Theravance, Inc. - US7195876, 2007, B2 Full Text ↗ Show details >
10	IC50	=	0.1	nM	Mast/stem cell growth factor receptor Kit:Wild	Morphy, Richard; Rankovic, Zoran - Current pharmaceutical design, 2009, vol. 15, # 6, p. 587 - 600 Full Text ↗ Show details >
10	IC50	~	100	pM		Roger Briesewitz; John H. Griffin - US2004/45044, A1, 2004 Full Text ↗ Show details >

Click **+ Show Next 100** to display next 100 results.

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.

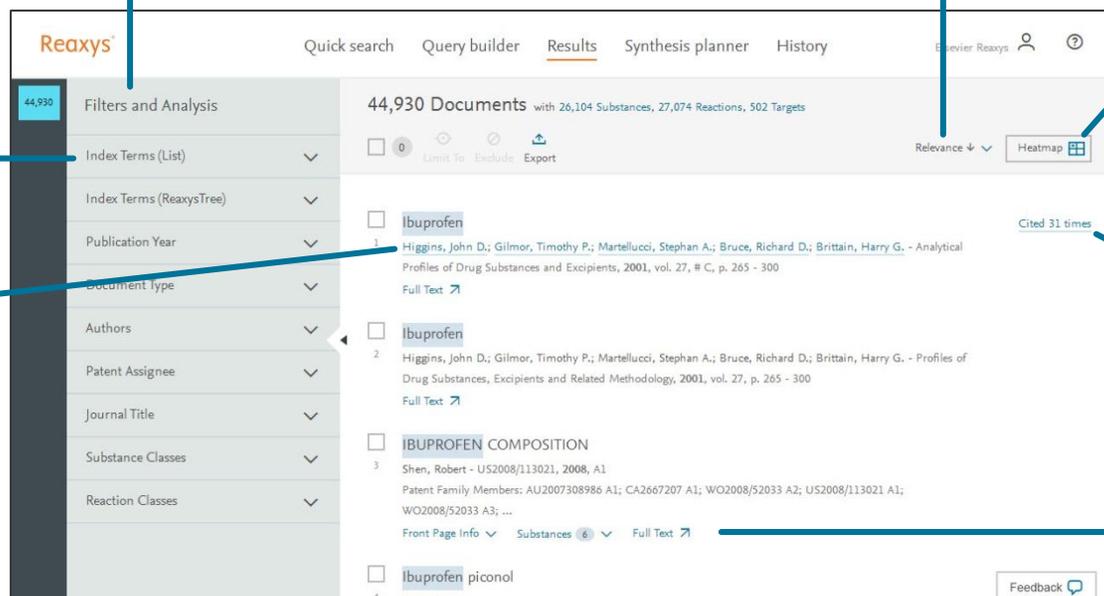
Click links for author(s) to explore details about their publications and additional analysis options in Scopus.

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.



The screenshot displays the Reaxys search results page. On the left, a sidebar titled 'Filters and Analysis' shows 44,930 results and various filter categories like Index Terms, Publication Year, and Authors. The main content area shows a list of documents, with the first three entries for 'Ibuprofen' highlighted. Each entry includes the title, authors, and a 'Full Text' link. A 'Heatmap' button is visible in the top right of the results area. A 'Cited 31 times' link is also present next to the first document entry. The interface includes navigation tabs for 'Quick search', 'Query builder', 'Results', 'Synthesis planner', and 'History'.

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.

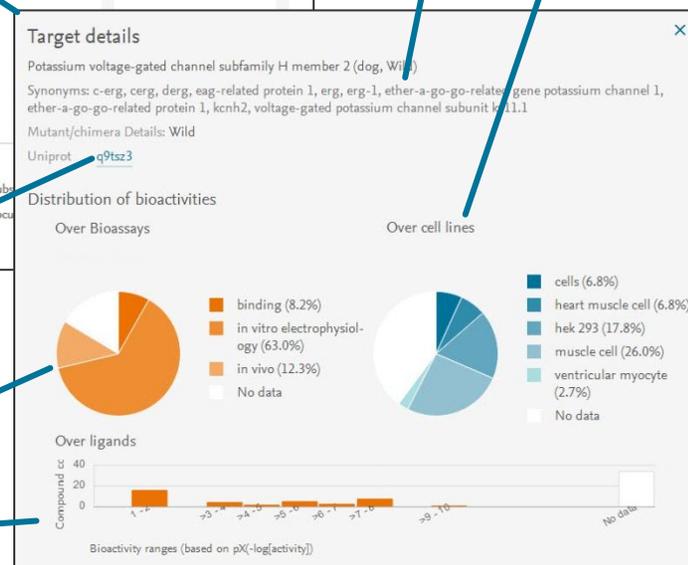
Heteromeric target that consists of multiple proteins (subunits).

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.

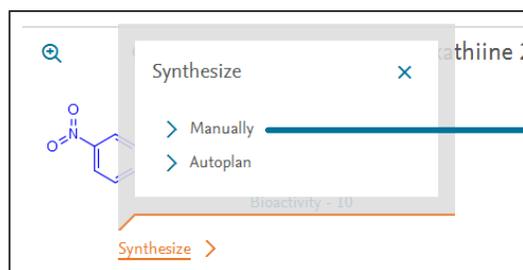
2. Click **More** to display additional filter options.

The screenshot displays the Reaxys interface with the 'Filters and Analysis' panel on the left and a 'Catalyst Classes' modal window open. The main panel shows 304 reactions. The modal window shows a list of catalyst classes with 'Mn' selected, resulting in 81 reactions.

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, 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.

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.

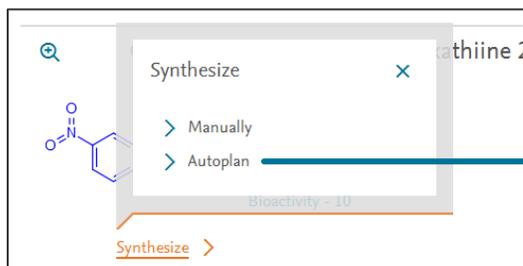
2. Click the **Synthesis step options** () to access:

- 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 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, from a results page click **Synthesize** below a structure.



2. Define parameters for automatically generating synthetic pathways.

3. Click **Create Plans**.

Create plans by autoplan ×

Number of plans to create 2 ▼

Max. alternative branches 3 ▼

Max. number of steps 3 ▼

Stop searching if starting material is commercially available Yes No

Default yield for reactions without a given yield

Always show screen before creating autoplan **Create Plans** >

Synthesis planner – Autoplan (continued)

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

The screenshot shows the Reaxys Synthesis Planner interface. On the left, there is a sidebar with 'Plan 1' selected. The main area displays a reaction scheme with four steps. Step 3 is highlighted with a blue arrow pointing to its options menu. The reaction scheme shows the synthesis of a sulfonamide derivative from dimethyl sulfide, a chlorosulfonamide, and a hydroxybenzaldehyde derivative.

A close-up of the options menu for a synthesis step. The menu items are: 'Show conditions' (with an information icon), 'Hide preparation' (with a hide icon), and 'Remove preparation' (with a trash icon). A blue arrow points from the 'Show conditions' option to the 'Conditions' window shown below.

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

The 'Conditions' window displays experimental details for 'Preparation - 2'. It includes a table with columns for Yield, Conditions, and Reference.

Yield	Conditions	Reference
100%	With triethylamine In dichloromethane at 0 - 20°C for 2h Experimental part	Grandane, Aiga; Tanc, Muhammet; Di Cesare Mannelli, Lorenzo; +4 others - Journal of Medicinal Chemistry, 2015, vol. 58, # 9, p. 3975 - 3983 Full Text Cited 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. 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.).

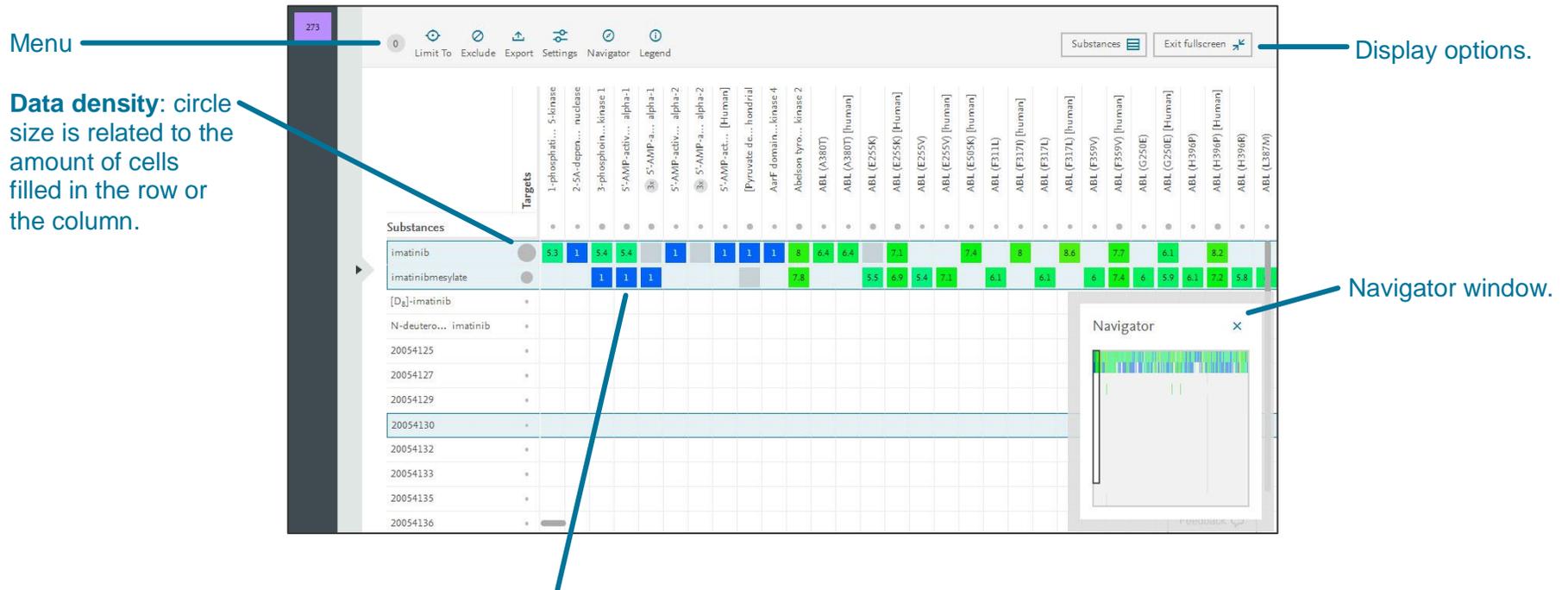
The screenshot illustrates the Heatmap feature in Reaxys across three different views: Substance, Target, and Document. Each view includes a 'Heatmap' button in the top right corner. A blue callout box with arrows points to these buttons and contains the following instructions:

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

The 'Heatmap settings' dialog box is shown in the bottom right, with the following configuration:

- Value of X-axis: Targets
- Value of Y-axis: Substances
- Value of Cells: Maximum of pX
- Show substances: Names Structure drawing
- Display mode: Normal Full Screen
- Always show settings
- Apply button

Heatmap Overview (Full Screen Mode)



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.

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

Click header to select the column or row.

The screenshot shows the heatmap interface with several callouts:

- Legend:** A color scale from High (red) to Low (blue) for quantitative data, and a grey box for qualitative data. It includes the text "n = px value" and "Colour indicates bioactivity potency based on pX value".
- Row options:** A dropdown menu with options: Sort by activity, Limit to selected row(s), Exclude selected row(s), Copy structure to, and All substance details.
- Navigator:** A small heatmap view at the bottom with a vertical line indicating the current column position.

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

This screenshot shows a detailed tooltip for the 'imatinib' column. The tooltip includes:

- Chemical structure:** A chemical structure of imatinib.
- Reaxys ID:** 7671333
- CAS Registry Number:** 152459-95-5
- Molecular Formula:** C₂₉H₃₁N₇O
- Molecular Weight:** 493.611

Heatmap Cell Click

Click cell to display Bioactivity details.

Click header to select the column or row.

The heatmap shows bioactivities (pX values) for substances like imatinib, imatinibmesylate, and [D₂]-imatinib across targets such as 1-phosphatidylinositol-3-phosphate 5-kinase, 2-5k-depen... kinase, 3-phosphoin... kinase 1, 5'-AMP-acti... alpha-1, 5'-AMP-a... alpha-1, 5'-AMP-acti... alpha-2, 5'-AMP-a... alpha-2, 5'-AMP-act... [Human], [Pyruvate de... isondrial], AarF domain... kinase 4, Ablason tyr... kinase, ABL (A380T), and ABL (E75K).

Bioactivity detail for imatinib:

- Targets: 1-phosphatidylinositol-3-phosphate 5-kinase
- Substances: imatinib
- Active substances: imatinib (Maximum pX Value: 5.3)
- Chemical structure: C1=NC2=C(N1)C(=C(C=C2)N)C3=CC=CC=C3C4=CC=CC=C4C5=CC=CC=C5C6=CC=CC=C6C7=CC=CC=C7C8=CC=CC=C8C9=CC=CC=C9C10=CC=CC=C10
- Identification: C₂₉H₃₁N₇O, 493.611, 7671333, 152459-95-5
- Druglikeness: In vitro: Efficacy - 1
- Quantitative Results:

pX	Parameter	Value (qual)	Value (quant)	Unit	Reference
5.38	IC50	=	4.2	µM	Patricelli, Matthew P.; Nomanbhoy, Tysoon K.; Wu, Jjiangyue; Brown, Heidi; Zhou, David; Zhang, Jianming; Jagannathan, Subadhra; (...) Gray, Nathanael S.; Kozarich, John W. - Chemistry and Biology, 2011, vol. 18, # 6, p. 699 - 710

- 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. <ul style="list-style-type: none"> 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 <ul style="list-style-type: none"> 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 . <ul style="list-style-type: none"> 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. <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. <p>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.</p> <p>Excel export is the format of choice to retrieve chemical structure of substances (smile), targets, bioassays details and bioactivity results (datapoints).</p>
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.

Saving and Exporting (continued)

Exporting (continued)	
From the Results Heatmap :	<p>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.</p> <ul style="list-style-type: none"> • 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. <ul style="list-style-type: none"> ○ When the export is complete, click Download. <p>Note: - Excel export is the format of choice to retrieve chemical structure of substances (smile), targets , bioassays details and bioactivity results (data points).</p> <p>The same export (content) of bioactivities is available from the Heatmap view or from the substances or targets list view.</p>