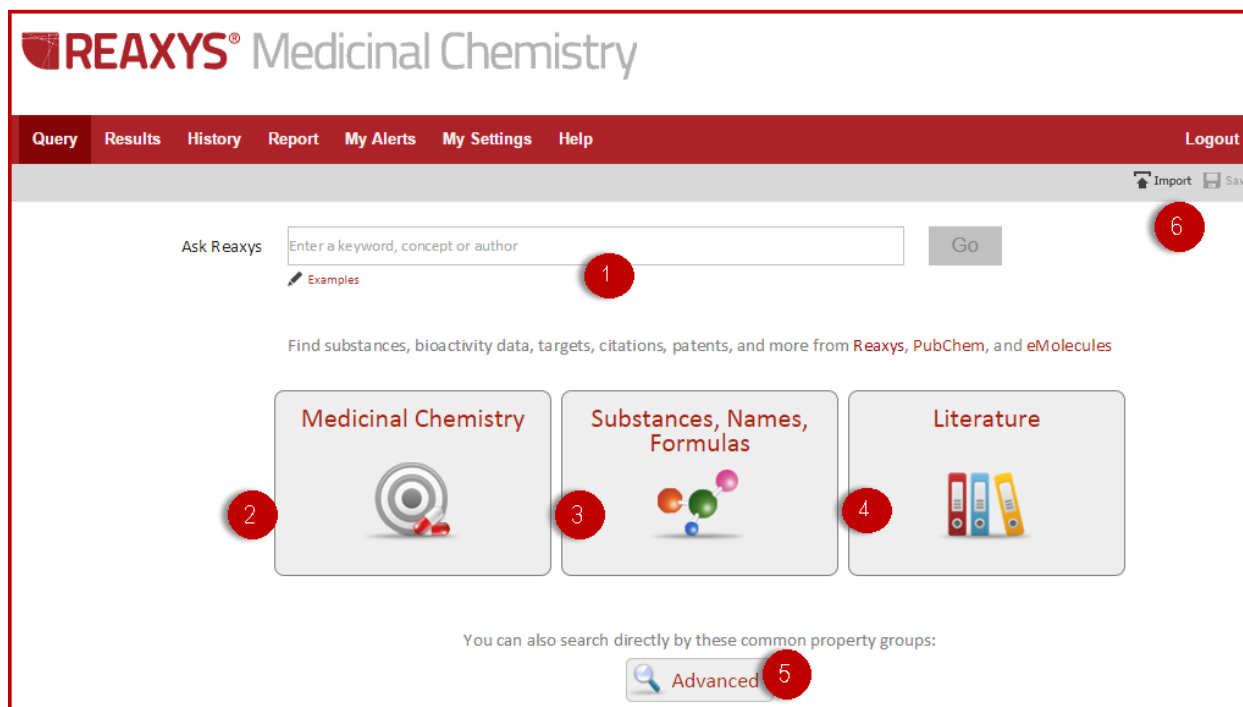


Quick Reference Guide

The Start Page - There are six ways to begin your search:



1. **Ask Reaxys** - Interprets search keywords written in natural language and retrieves the most relevant results.
2. **Medicinal Chemistry** - Clicking the **Medicinal Chemistry** query theme opens the Bioactivities form that contains searchable data fields such as, *Targets, Effect, Species, Bioassay Name, Cell, Tissue, Animal model, and Parameter*. These fields can be searched with or without a chemical structure.
3. **Substances** - Clicking the **Substances** query theme opens a form with a structure box and enables you to search with structures, data, or a combination of both. Structures can be drawn using Structure Editors, imported using the Import button in the upper right corner, or generated using the **Generate Structure Template from Name** button.
4. **Literature** - The **Literature** query theme will open a form containing fields such as *Authors, Patent Number, and Publication Year*.
5. **Advanced** - The **Advanced** query theme opens a form with access to the data structure where you can perform detailed bibliographic, data, and keyword searches (with or without structures).
6. **Import** - Save your query as an xml file by clicking **Save** in the upper right corner. Import your saved query using the **Import** button in the upper right corner. The Import feature also supports Batch querying.

Ask Reaxys

[Examples](#)

Bioactivities

Target Name
 Substance Route of Adm.
 Substance Action on Target
 Substance Effect
 Bioassay Category
 Biological Species
 Organs/Tissues
 Cells/Cell Lines
 Measurement pX

Show AND Buttons

Add to Query:

Clear Query

Medicinal Chemistry Search

1. **Ask Reaxys** - Enter a name, property, bioactivity, target, etc. Ask Reaxys will interpret the query and determine the context. The example shown on this page retrieves substances with *imidazoline receptor* activity data.

More examples:

- *Protease inhibitors and drug resistance* - retrieves citations with the terms in titles, abstracts, or keywords.
- *Lupeol* - The substance name will be translated into a structure and searched to retrieve a list of substances.

Several more examples are given when you click the **Examples** link under the Ask Reaxys box.

2. **Bioactivities form** - Type in the query or click the **Lookup** link to access the index. Click the + to browse categories or type in a search term to view the taxonomies. Then click the Transfer button.

3. **Add to Query bar** - Click the **Structure** link to add a structure search box. Click the **Molecular Formula** link to open the MF query builder. Click the **Add/Remove fields** link to customize the form with more, fewer, or different fields.

4. **Clear Query link** - Clears structure, text, property, and Ask Reaxys queries.

Reaxys

Enter search term:

Targets

Atrial natriuretic peptide (A)

Atrial natriuretic pep

Atrial natriuretic pep

Atrial natriuretic pep

Atrial natriuretic pep

Atrial natriuretic pep

Atrial natriuretic pep

Claudin (All)

Enzyme (All)

Browse the index

Reaxys

Enter search term:

Targets

Enzyme (All)

EC 2: Transferase (All)

Kinase (All)

Group 1: prot. S/T-Y-kinase/ Atypical protein kinase

Lipid kinase / ATP-grasp (All)

Protein S/T-Y kinase / Atypical kinase (All)

Protein S/T-Y kinase (All)

AGC (All)

AKT (All)

AKT

AKT [Human]

Substance Search

The screenshot shows the Substance Search interface with five numbered callouts:

- 1:** Points to the MarvinSketch logo in the Structure Editor window.
- 2:** Points to the 'STRUCTURE EDITOR' button in the Structure Editor window.
- 3:** Points to the 'Create Structure Template from Name' link in the Structure Editor window.
- 4:** Points to the 'Reaxys Registry Number' field in the Identification section.
- 5:** Points to the 'Add to Query' button in the bottom navigation bar.

The interface includes a top navigation bar with 'MedChemistry', 'Substances', 'Literature', and 'Advanced' tabs. The main area is divided into 'Structure' and 'Identification' sections. The 'Structure' section contains a 'selected query editor' (MarvinSketch), a 'PASTE' button, a 'STRUCTURE EDITOR' button, and a 'Create Structure Template from Name' link. The 'Identification' section contains five search fields: 'Reaxys Registry Number', 'CAS Registry Number', 'Chemical Name', 'Element Symbols', and 'Highest Clinical Phase', each with a dropdown menu and a 'Lookup' button. The bottom navigation bar includes 'Add to Query', 'Structure', 'Molecular Formula', 'Add/Remove Fields...', and a 'Search Substances' button.

1. **Structure box** - Click to open a structure editor.
2. **Structure Editor button** - Click to view and select SE options (MarvinSketch, GGA Ketcher, or Elemental). Click the **Help** link for information about using ChemDraw, AccelrysDraw, ISISDraw, or ICEdit.
3. **Create Structure Template from Name** - Click the **Create Structure Template from Name** link to enter a name, CAS number, InChI-key, or Smiles string to generate a structure.
4. **Identification form** - Enter your query in the fields provided or use the **Lookup** link to open the index for the field so that you can select terms for your query.
5. **Add to Query bar** - Click the **Structure** link to add a structure search box. Click the **Molecular Formula** link to open the MF query builder. Click the **Add/Remove fields** link to customize the form with more, fewer, or different fields.

MedChemistry Substances **Literature** Advanced

Bibliographic Data

Document Type	is	<input type="text"/>	Lookup X
Authors	is	<input type="text"/>	Lookup X
Common Patent Number	is	<input type="text"/>	Lookup X
Patent Country Code	is	<input type="text"/>	Lookup X
Journal Title	is	<input type="text"/>	Lookup X
Publication Year	=	<input type="text"/>	Lookup X
DOI	is	<input type="text"/>	Lookup X
Title	is	<input type="text"/>	Lookup X
Abstract	is	<input type="text"/>	Lookup X
Keywords	is	<input type="text"/>	Lookup X
Citation Basic Index	is	<input type="text"/>	Lookup X

Show AND Buttons

Add to Query: **2** Structure Molecular Formula Add/Remove Fields... Search Literature

Literature Search

- Bibliographic Data form** - Enter your query in the fields provided or use the **Lookup** link to open the index for the field so that you can select terms for your query.
- Add to Query bar** - Click the **Structure** link to add a structure search box. Click the **Molecular Formula** link to open the MF query builder. Click the **Add/Remove fields** link to customize the form with more, fewer, or different fields.

Advanced Search

The screenshot shows the 'Advanced' search tab selected. It features a 'Structure' section with a 'MarvinSketch' query editor (1), a 'STRUCTURE EDITOR' button (2), and a 'Create Structure Template from Name' link (3). The 'Advanced' section contains a text input field (4) with an example query, a 'Check Syntax' button, and a 'Show Property List' link (5). A 'Search' button (6) is located at the bottom right.

1. **Structure box** - Click to open a structure editor.
2. **Structure Editor button** - Click to view and select SE options (MarvinSketch, GGA Ketcher, or Elemental). Click the **Help** link for information about using ChemDraw, AccelrysDraw, ISISDraw, or ICEdit.
3. **Create Structure Template from Name** - Click the **Create Structure Template from Name** link to enter a name, CAS number, InChI-key, or Smiles string to generate a structure.
4. **Advanced form** - Enter your query in the box provided if you are familiar with Reaxys field names and data operators.
5. **Show Property List** - Click the **Show Property List** link to build your query. Use the search box to find your field(s). Use data operators to string your query together.
For Example, the following query retrieves substances tested for analgesic effects with a Mol. Wt. between 276-324 that have a PSA value above 50:
DAT.EFFECT='analgesic' AND IDE.MW='276-324' AND CALC.TPSA>'50'
6. **Search button** - Select the desired context for your search.

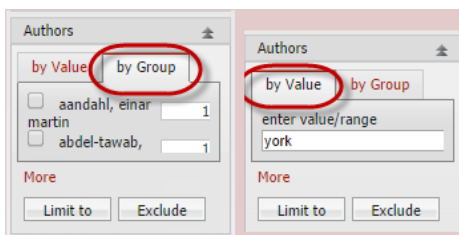
The 'Available Properties' dropdown menu is open, showing a search for 'effect'. The 'Effect' property is circled in red, and its full name 'Substance Effect (DAT.EFFECT)' is visible below it.

The 'Search' dropdown menu is open, showing options: 'Search Bioactivities', 'Search Substances', and 'Search Literature'. The 'Search' button is highlighted with a red circle and a mouse cursor.

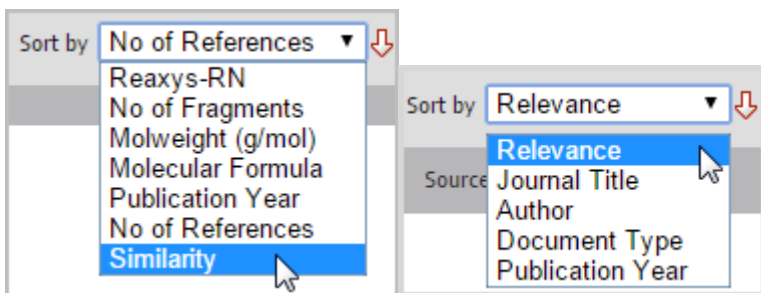
The query construction field contains the following query: `DAT.EFFECT='analgesic' AND IDE.MW='276-324' AND CALC.TPSA>'50'`

Filter, Sort, and Analyze

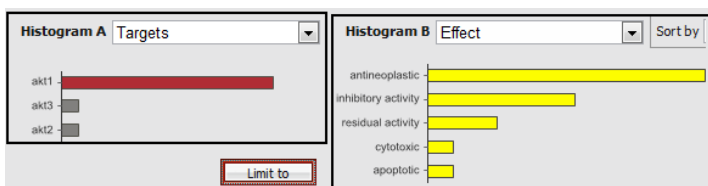
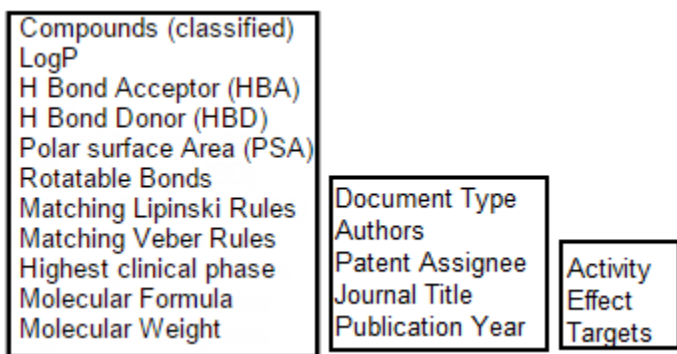
1



2



3



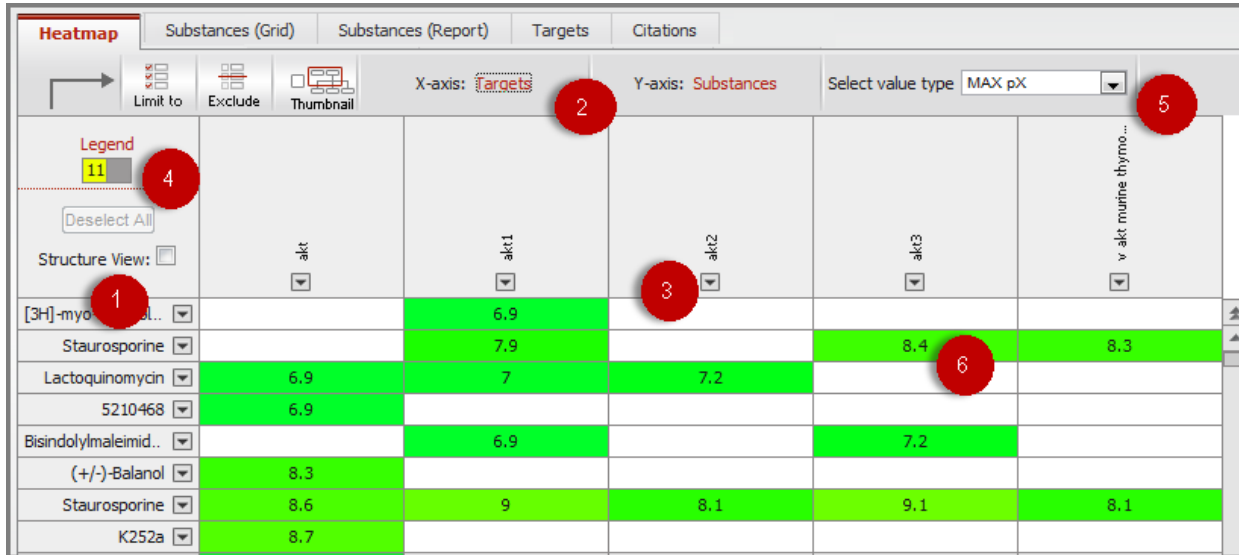
1. **Filter** - Filter by categories are displayed on the left side of the results page. Some filters offer a **By Value** tab that allows you to type in a term. Some filters offer a **More** link that allows you to refine using more details.
2. **Sort** - Click to view and select sorting options.
3. **Analysis View** - Click the **Analysis View** button on the **Results** page (above the results list). **Analyze** results by any of the categories shown using histograms to see how one category may relate to another.

Step 1 – Select a category for **Histogram A** from the dropdown menu (the bar will be displayed in red and shows the number of relevant hits in your result list).

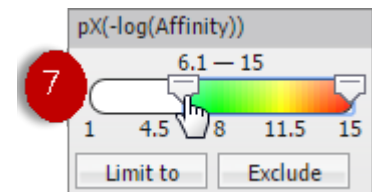
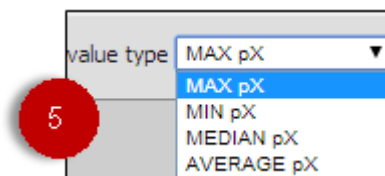
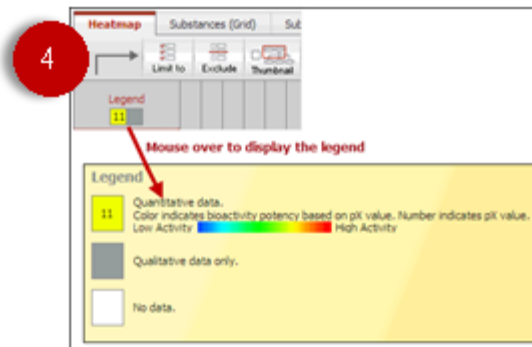
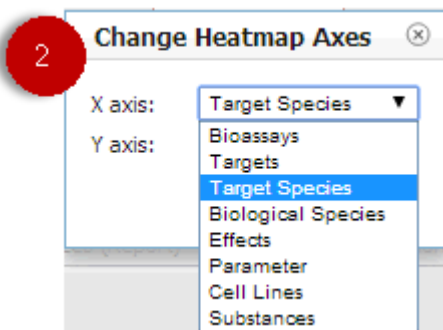
Step 2 – Select a category for **Histogram B** (the bars will be displayed in yellow and show the numbers of hits per category in your result list that are a subset of the **Histogram A** list).

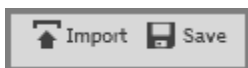
Step 3 - After analyzing various combinations, click **Limit to** (or **Exclude**).

Heatmap



1. **Substances** - Click the **Structure View** box to display the structures. Click the dropdown menu for details about the substance and for copy options.
2. **X and Y Axis Display** - Substances are displayed on the Y axis and Targets are displayed on the X axis by default. You can change this by selecting different options in the dropdown menu.
3. **Column Controls** - Click the dropdown arrow for deleting and sorting options.
4. **Legend** - View color coding legend.
5. **Value Type** - Px values are calculated from data points. If multiple data points are available for an assay/target you can select Max, Min, Median, or Average.
6. **Px value** - A value calculated from experimental data points. This allows you to compare data from different sources, different assays, or with different parameters. The Px value is hyperlinked to the real data.
7. **Filter by Px value** - Use the filter on the left side of the Results page. Use the slider on the filter to limit results to a particular Px range.





History



Parameter	Value (qual)	Value (quant)	Unit	Target
IC50		198	µM	Fatty acid amide hydrolase +Fatty acid amide hydrolase

Copy to Reaxys Report:

- These facts
- These facts and the structure
- These facts, the structure and the target

Report



Saving, Printing, Exporting, and Reporting

1. **Save a Query** - Click Save in the upper right corner of the Query page.
2. **Save a Result list** - Click the History button. Click the Store link on the right side of the page.
3. **Print the current page** - Click the Print button located on the button bar towards the left side.
4. **Export Results** - Click the Export button. Select options for format, range, and content. Available formats are xml, SD file, and Excel.
5. **Add Data to a Report** - Mouse over results. Click the red triangle that appears near individual data points and structures. Select from the options that appear.
6. **View a Report** - Click the Report button. Arrange items with the Show, Move up, Move Down, Remove links. Add text using the Annotate link.
7. **Send Report through email** - Click the Send button on the Report page and fill in the form. The report will be sent as a zipped html attachment