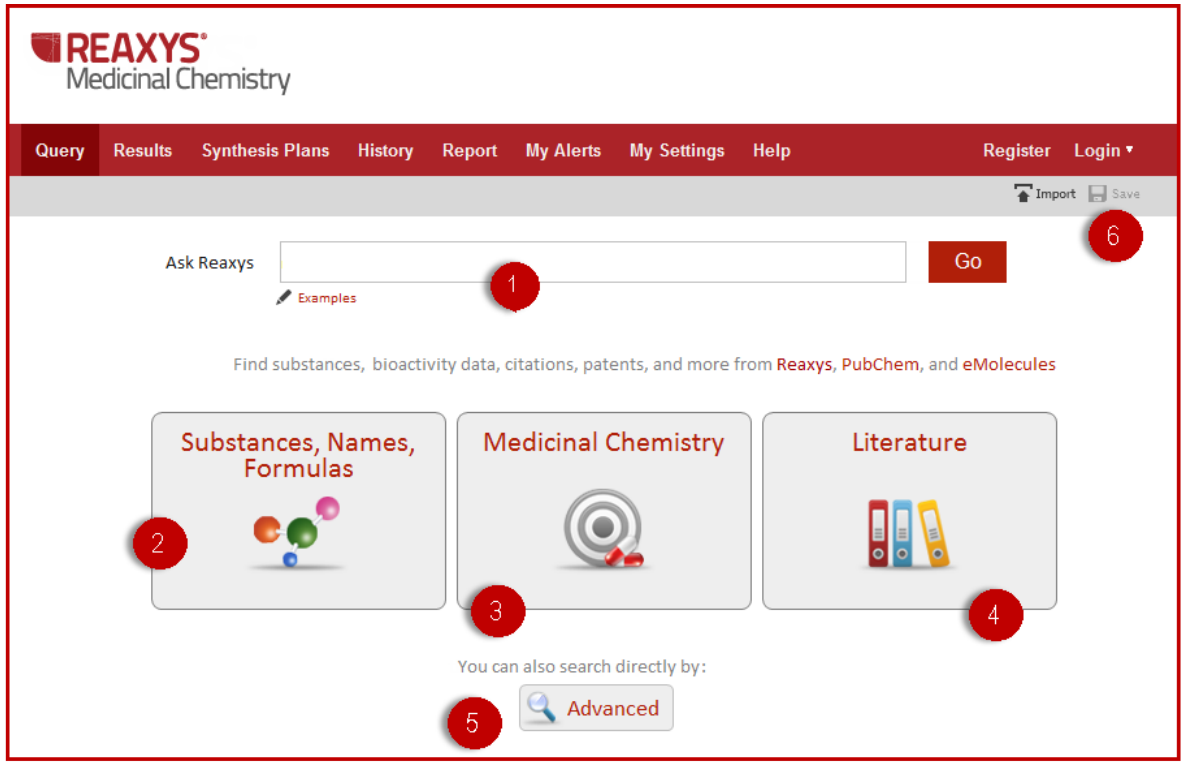
REAXYS® Medicinal Chemistry

Quick Reference Guide

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. **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.
3. **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.
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.

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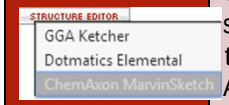
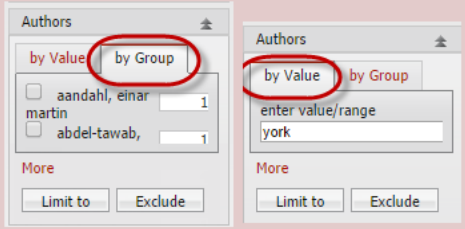
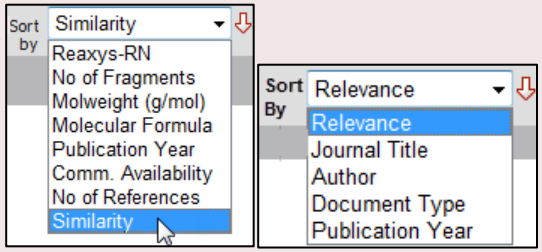
FEATURE	COMMENT
Ask Reaxys	Enter a name, property, bioactivity, target, etc. Ask Reaxys will interpret the query and determine the context. Several examples are given when you click on the ***Examples*** link under the **Ask Reaxys** box.
Create Structure Template from Name	Click the **Substances** query theme and then click the red link below the Structure box. Enter *Name, CAS#, etc.*
Search forms	Click the **Substances, Medicinal Chemistry, or Literature** query theme to open the form. Then 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. Click the Add/Remove fields link below the form to add more fields.
Structure Editors 	Click the **Substances** query theme. Click the **Structure Editors** button in the structure box and select one of the 3 options. Click the **Help** link for information about using ChemDraw, AccelrysDraw, ISISDraw, or ICEdit.
Add Structure to the Bioactivities Query	Click the **Structure** hyperlink below the Bioactivities form.

FILTER AND SORT	
TASK	**COMMENT**
Filter	**Filter by** categories are displayed on the left side of the results page.
Filter by Value or by Group	Some filters offer a **by Value** tab that allows you to type in a term. 
Refine	Some filters offer a More link that allows you to filter using more details.
Sort 	

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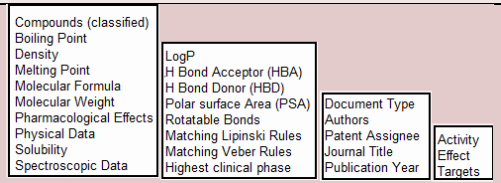
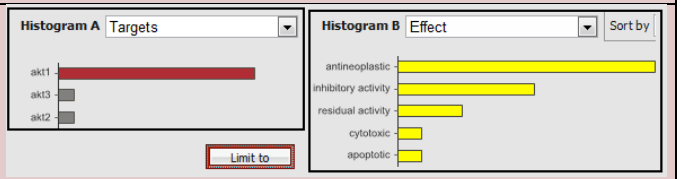
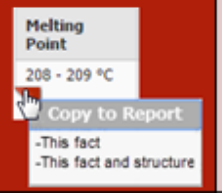
ANALYSIS VIEW

TASK	COMMENT
Open the Analysis View	Click the Analysis View button on the Results page (above the results list).
View Analysis Criteria	 **Analyze** results by any of these categories using histograms to see how one category may relate to another.
Select a category for Histogram A and Histogram B	 **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**).

SAVING, PRINTING, EXPORTING, AND REPORTING

FEATURE	COMMENT
Save a query 	Click **Save** in the upper right corner of the Query page.
Save a result list 	Click the **History** button. Click the Store link on the right side of the page.
Print the current page 	Click the **Print** button located on the button bar towards the left side.
Export results 	Click the **Export** button. Select options for format, range, and content.
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. Select data, substances, reactions, synthesis plans.
View a report 	Click Report button. Arrange items with the Show, Move up, Move down, Remove links. Add text using the Annotate link.
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.

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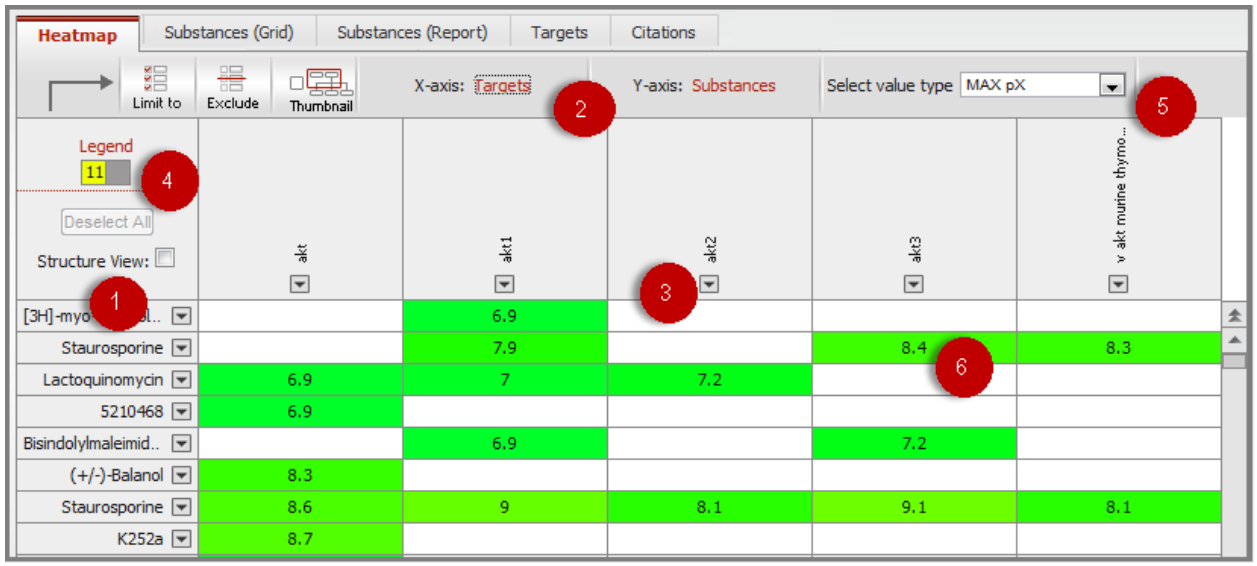
Heatmap



1. **Substances** – Click the **Structure View** box to display the structures. Click the dropdown menu for details about the substance and for copy options.

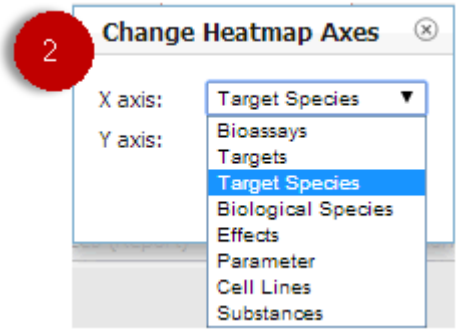
2. **X and Y Axis Display -** Substances are displayed on the **Y** axis and Targets are displayed on the **X** axis by default. You can change this by selecting different options in the dropdown menu.

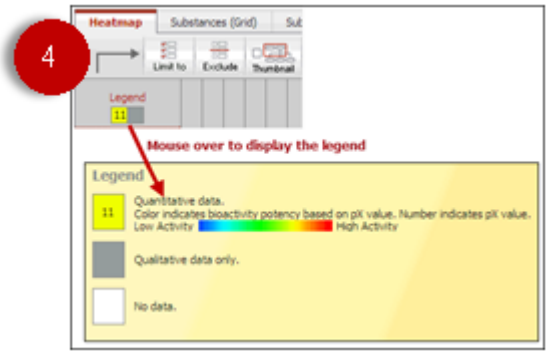
3. **Column Controls –** Click the dropdown arrow for deleting and sorting options.

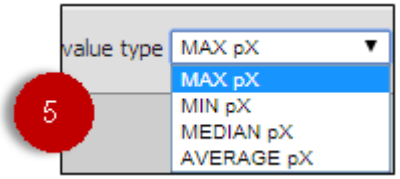
4. **Legend –** View color coding legend.

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.







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