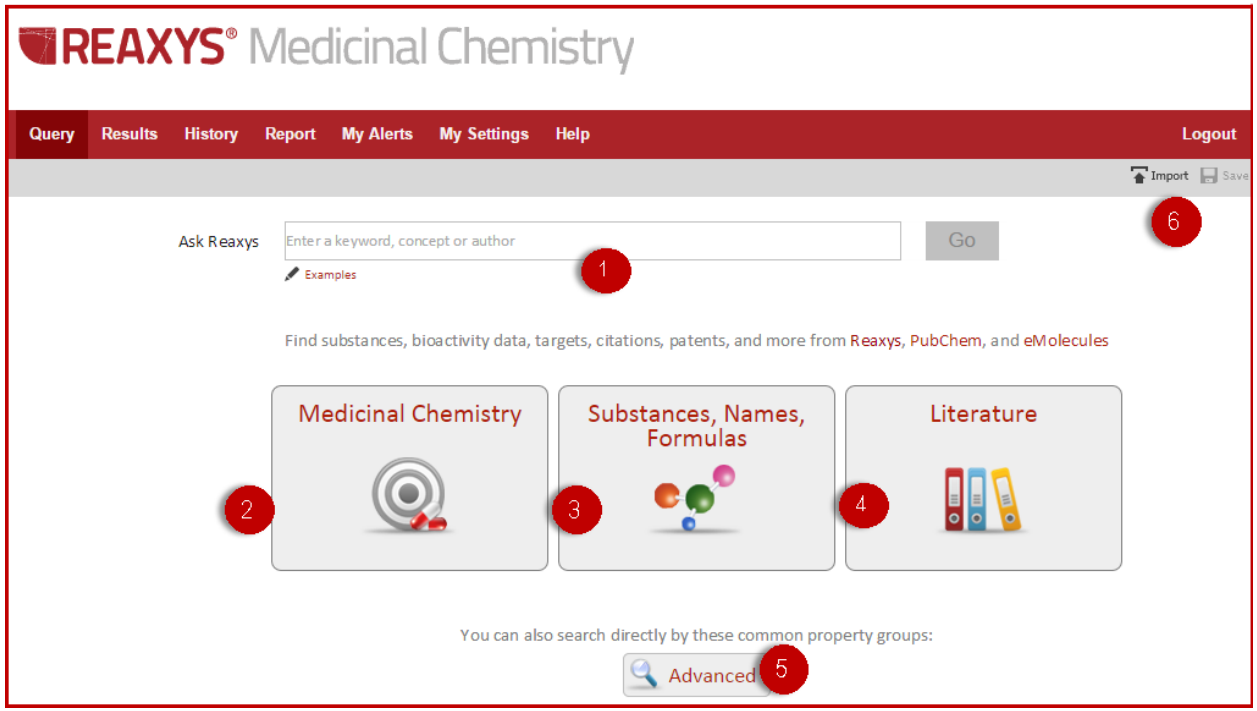
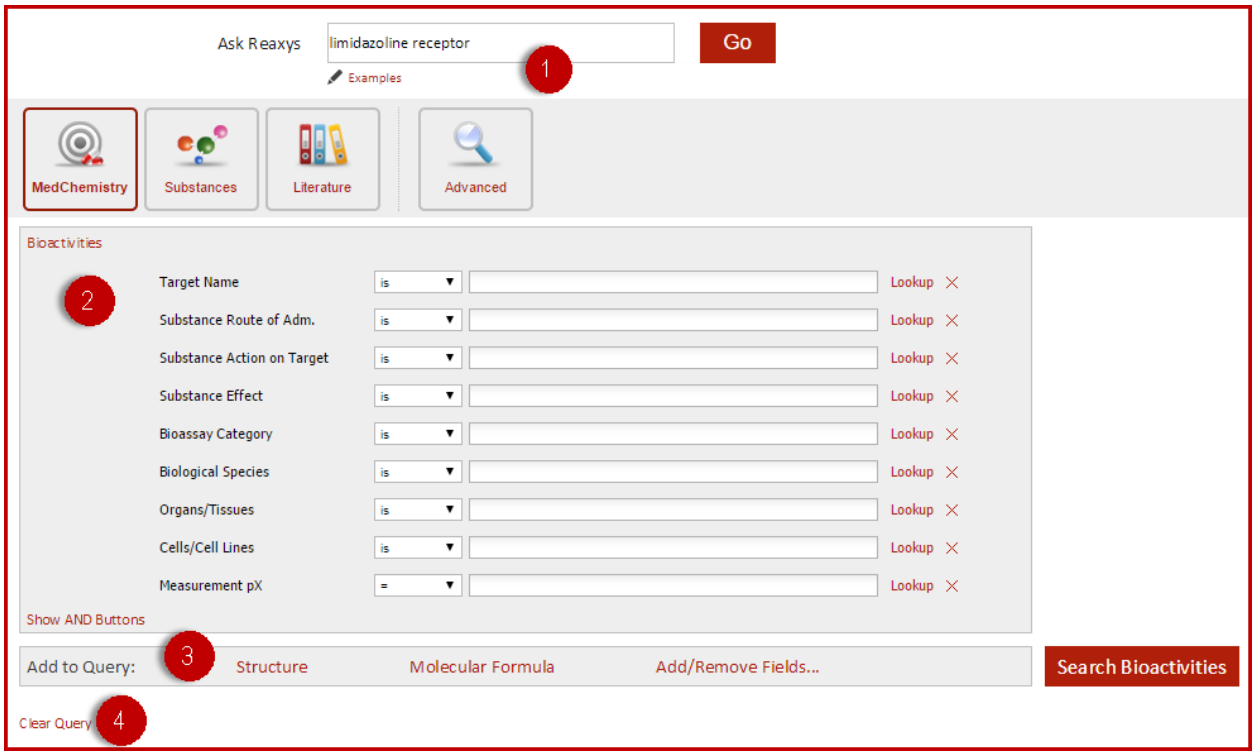
REAXYS® Medicinal Chemistry

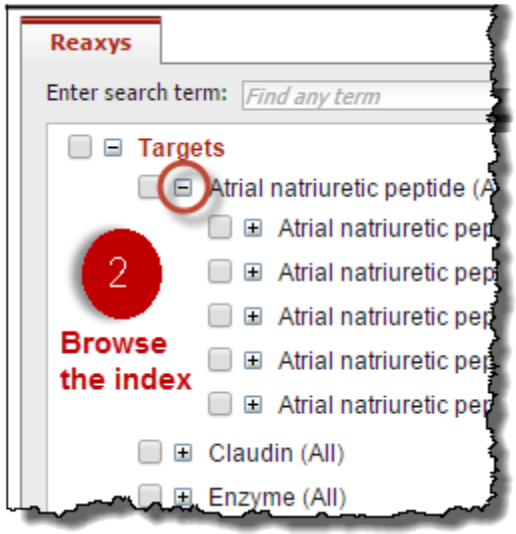
# Quick Reference Guide

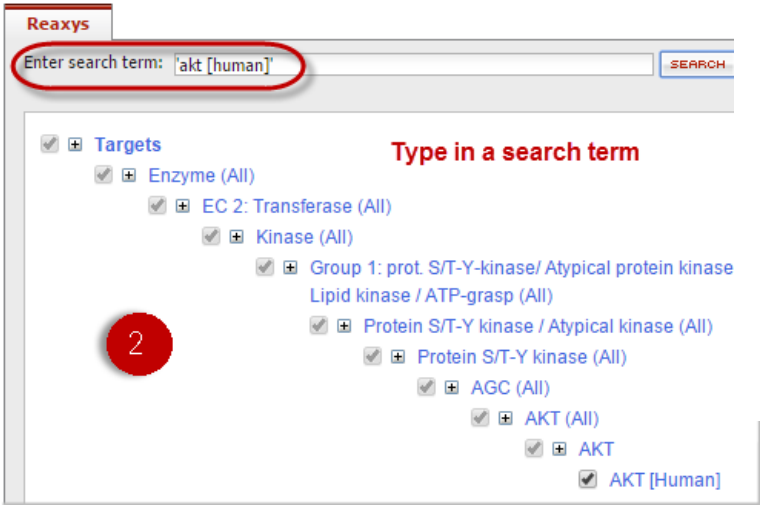



**The Start Page** - There are six ways to begin your search:

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.




## 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.

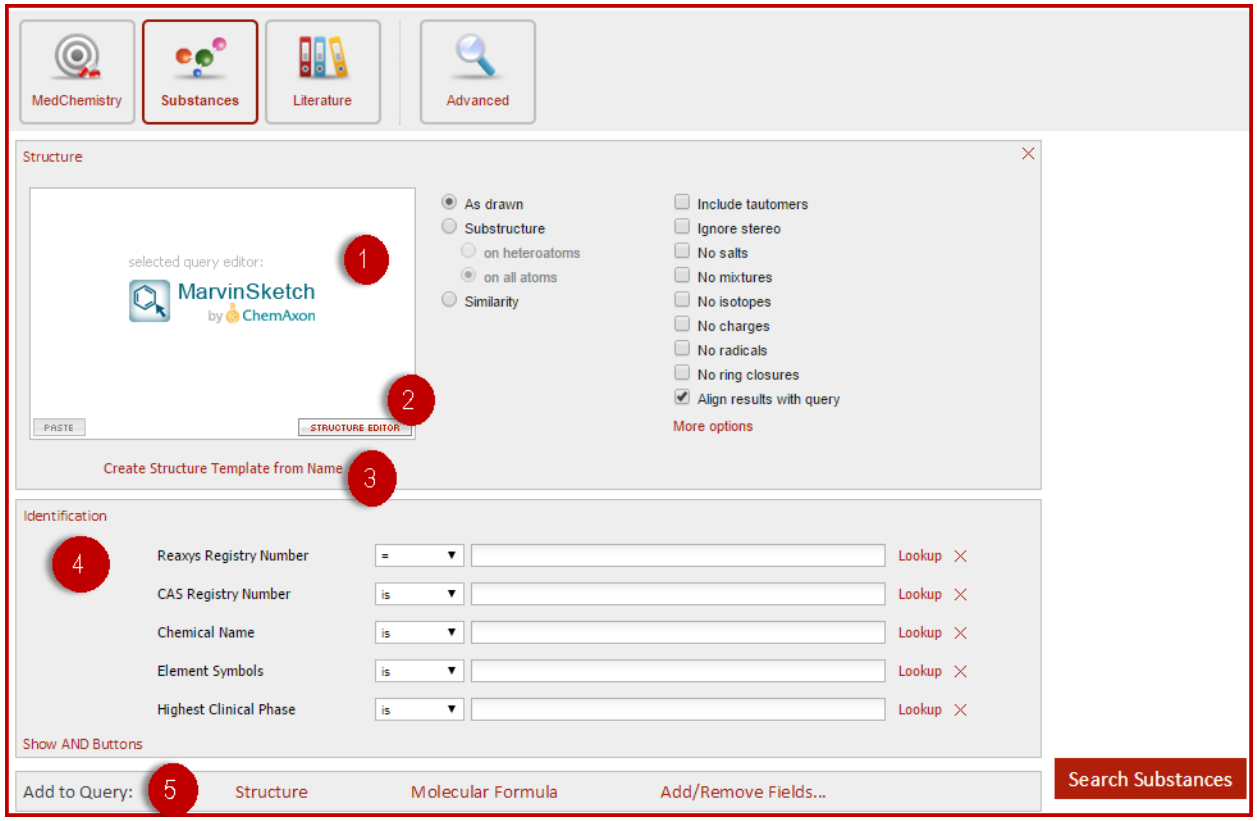
   Several more examples are given when you click the Examples link under the **Ask Reaxys** box.

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.

## Substance Search



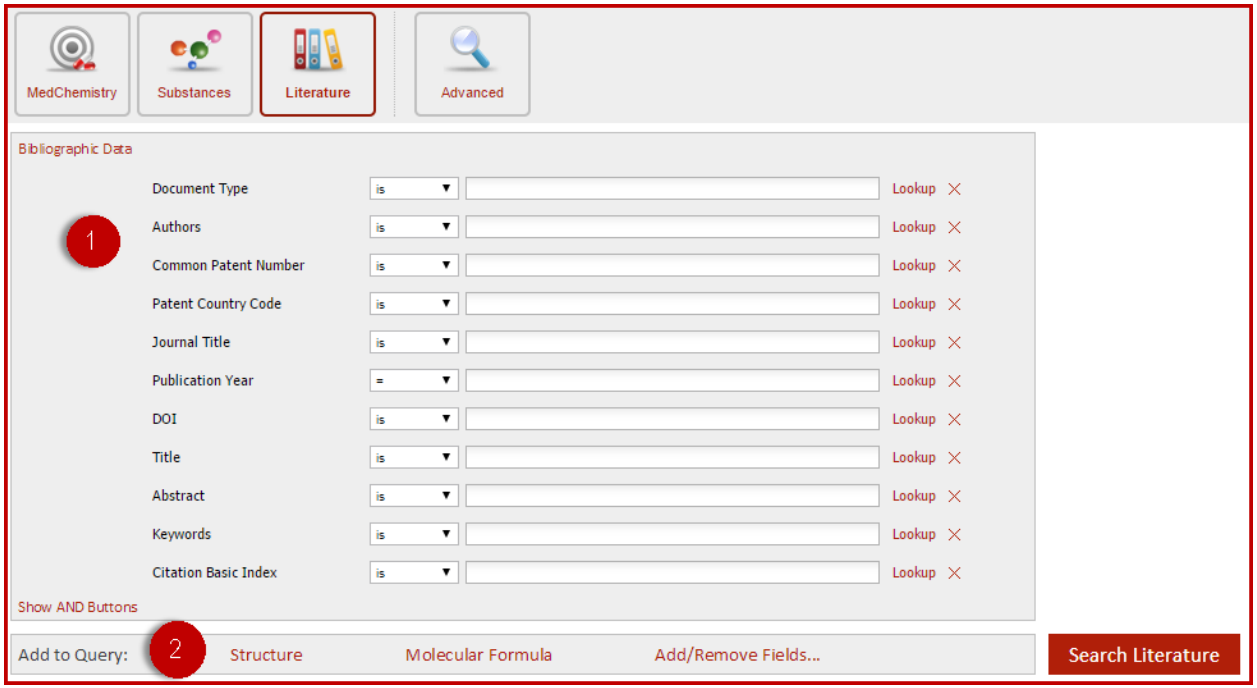

1. **Structure box** - Click to open a structure editor.

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.

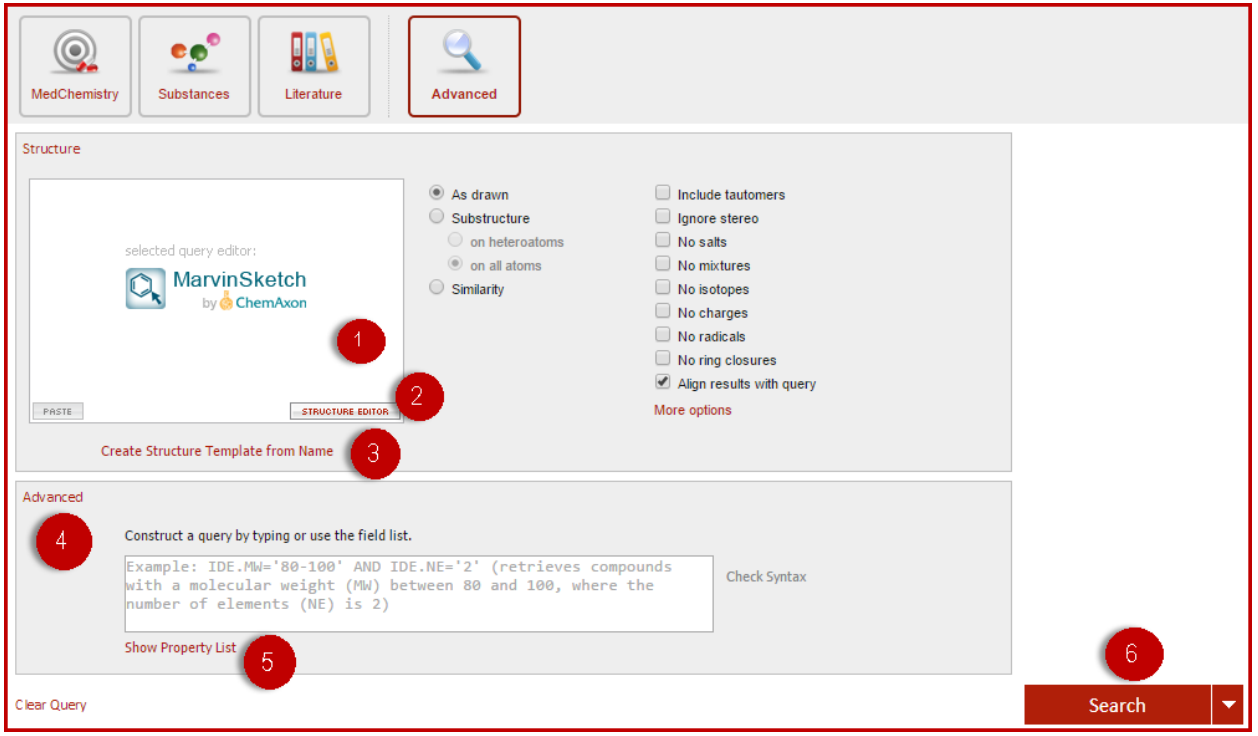
5. **Add to Query** bar – Click the Structure link to add a structure search box. Click the Molecular Formula link to open the MF query builder. Click the Add/Remove fields link to customize the form with more, fewer, or different fields.

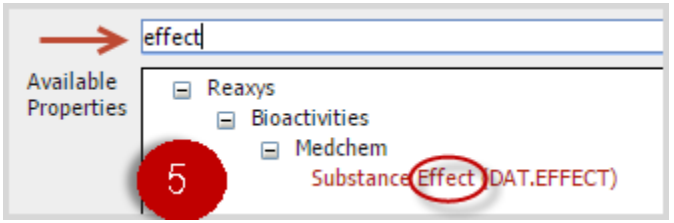



## Literature Search

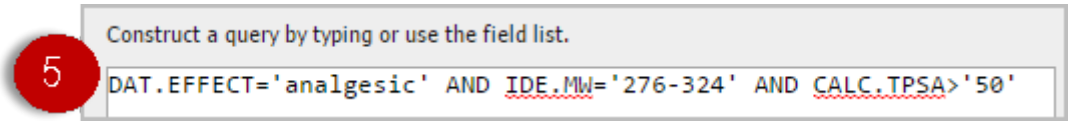
1. **Bibliographic Data form** - Enter your query in the fields provided or use the Lookup link to open the index for the field so that you can select terms for your query.

2. **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

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 ti 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.

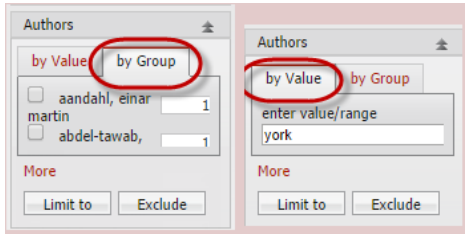
## Filter, Sort, and Analyze

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.

1

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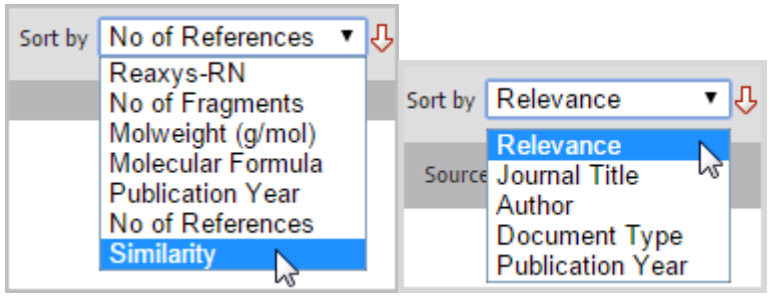


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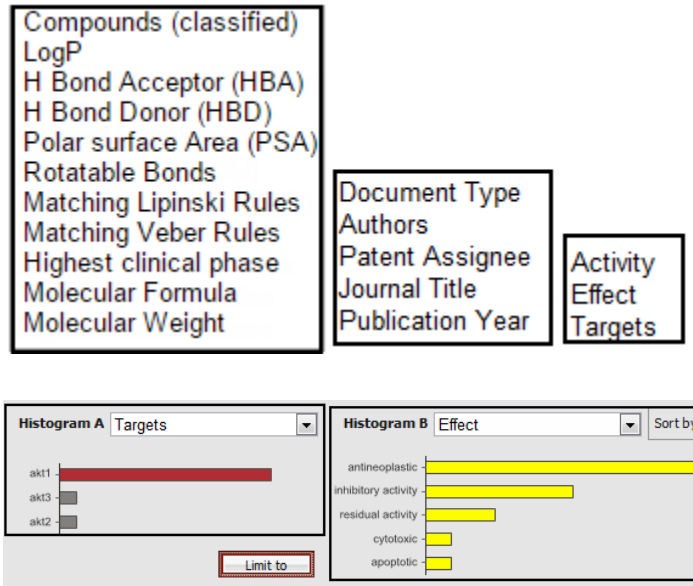
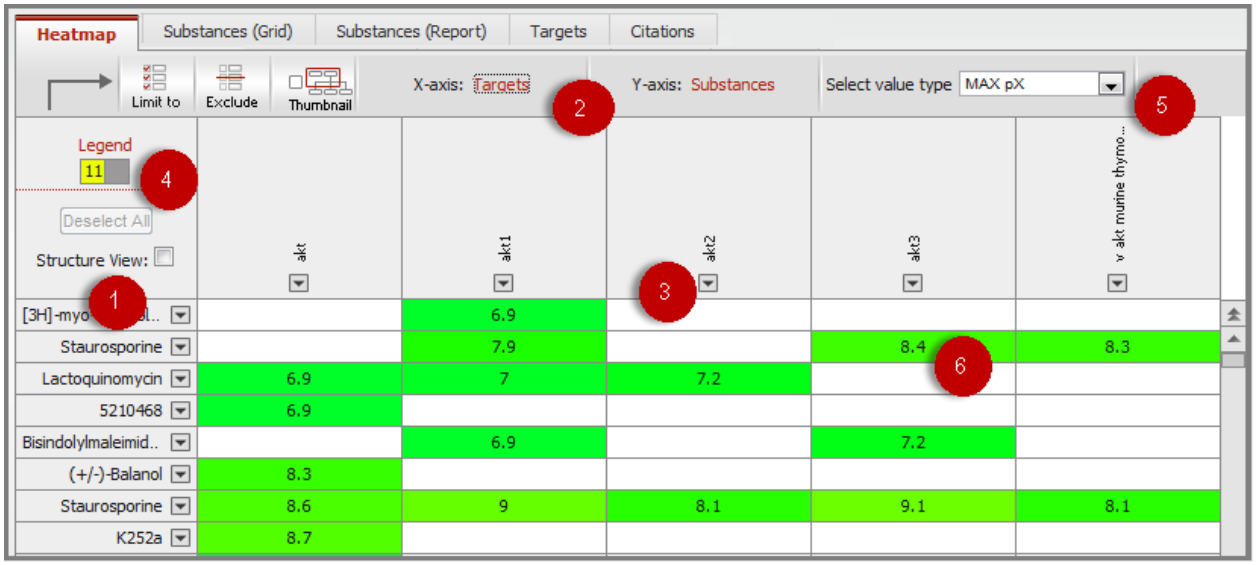



**Step 1 –** Select a category for **Histogram A** from the dropdown menu(the bar will be displayed in red and shows the number of relevant hits in your result list).
**Step 2 –**Select a category for **Histogram B** (the bars will be displayed in yellow and show the numbers of hits per category in your 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.

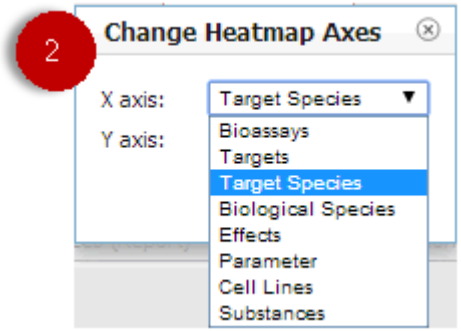
3. **Column Controls –** Click the dropdown arrow for deleting and sorting options.

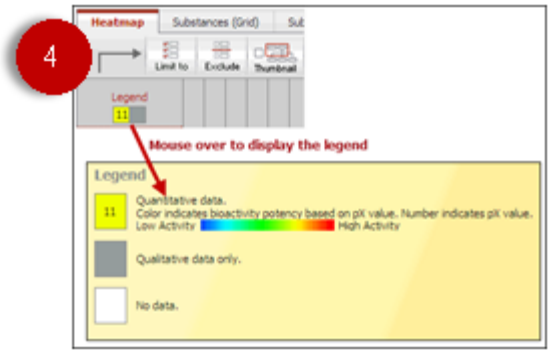
4. **Legend –** View color coding legend.

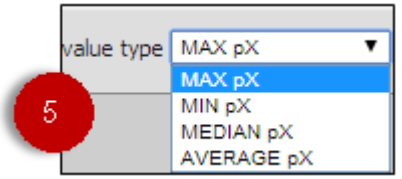
5. **Value Type** – Px values are calculated from data points. If multiple data points are available for an assay/target you can select Max, Min, Median, or Average.

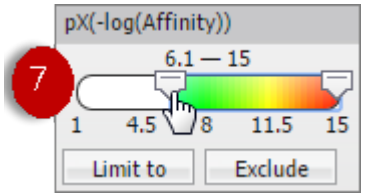
6. **Px value** – A value calculated from experimental data points. This allows you to compare data from different sources, different assays, or with different parameters. The Px value is hyperlinked to the real data.

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.



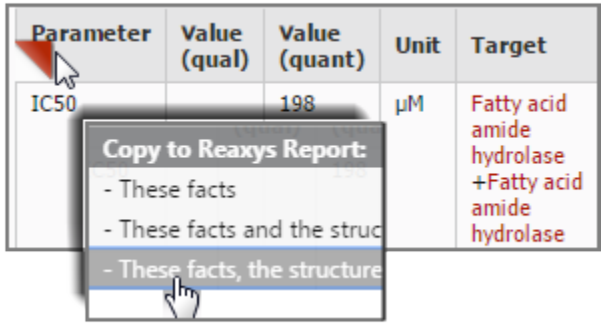



## Saving, Printing, Exporting, and Reporting










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.