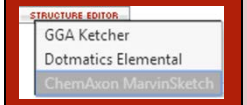
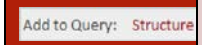
REAXYS®

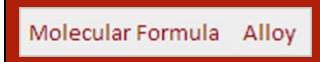
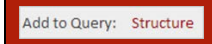
Quick Reference Guide

1. Select a query theme in Reaxys:

SUBSTANCES	
FEATURE	**COMMENT**
Ask Reaxys	Enter a name or CAS number. Examples: *quinolone, 91-22-5*
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** query theme and then use the **Identification** form below the structure box. Enter name, ID numbers, etc. Click Lookup to select a term. 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.

REACTIONS	
FEATURE	**COMMENT**
Ask Reaxys	Enter a term. Example: synthesis *of* p-phenylnitrobenzene, *Suzuki coupling, adler phenol oxidation.*
Create Structure Template from Name	Click the **Reactions** query theme and then click the red link below the Structure box. Enter *Name, CAS#,* or other identifier for a product, reactant, or catalyst.
Search forms	Click the **Reactions** query theme and then use the **Reaction Data** form below the structure box. Enter *Product Name, yield, Reaction Type, etc.* Click Lookup to select a term. Click the Add/Remove fields link below the form to add more fields.
Structure Editors	Click the **Reactions** query theme and then 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.

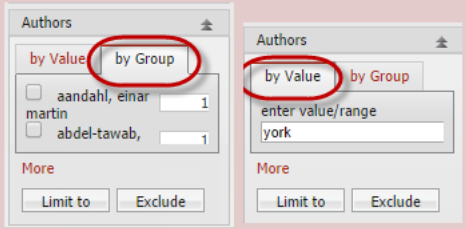
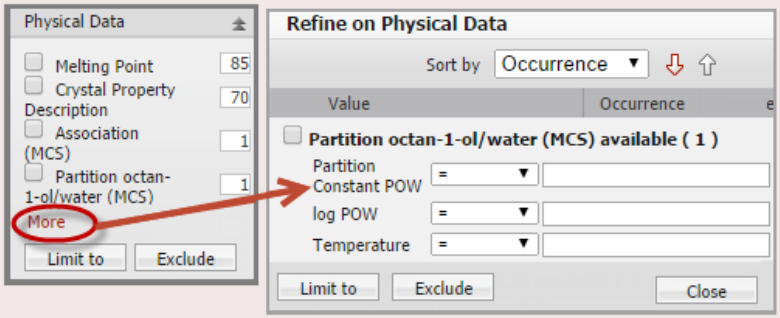
LITERATURE	
FEATURE	**COMMENT**
Ask Reaxys	Enter terms into the search box. Example: *cycloaddition of CO2 to epoxides, tropical deforestation, green solvents*
Reaxys Tree	Click the **Reaxys Tree** query theme. Open the folders to find a topic for searching the chemical literature, or type a term into the search box, click **Search** and uncheck boxes for unwanted topics. Click **Search Literature.**
Search forms	Click the **Literature** query theme and then use the **Bibliographic Data** form to enter a query for *Author, Document type, Journal Title,* etc. Click Lookup to select a term. Click the Add/Remove fields link below the form to add more fields.
Add a structure to the Literature query  	Click the Structure link below the query form to add a structure search box.

PROPERTIES	
FEATURE	**COMMENT**
Ask Reaxys	Enter a term. Examples: *boiling point of benzene*, *density of quinoline*
Molecular Formula and Alloy search 	Click the **Substances** Query theme. Click one of the links below the structure box. **MF**: Click an element, use arrows to add a range for the element count. Use displayed abbreviations to add groups from the P-table and other options shown on the right side of the MF query builder. **Alloy**: Select the percentage type from the dropdown menu. Add elements (they are case sensitive) in the columns on the left. Add percentages (or ranges) in the columns on the right. Check the box for **Additional Components** if needed.
Search forms	Click the **Physical** or **Spectra** query themes. Use the displayed fields in the forms or add more fields by clicking the Add/Remove fields link below the form. Click Lookup to select a term.
Add a structure to the properties query 	Click the Structure link below the query form to add a structure search box.

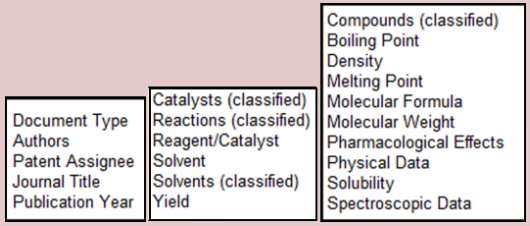
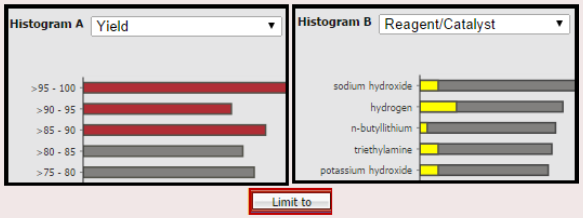
NATURAL PRODUCT	
FEATURE	**COMMENT**
Ask Reaxys	Enter a term. Examples: *isolation from olives* (retrieves citations), nmr of *luteolin* (retrieves a list of substances), *luteolin patents* (retrieves a list of patents that contain the structure for luteolin)
Search form (Natural Product)	Click the Natural Product query theme. Click Lookup to select a term.
Search form (Literature)	Click the **Literature** query theme. Use the **Citation Basic Index** field to perform a text search on titles, abstracts, and keywords.
Structure Editors	Draw the substance that was isolated from a natural product. 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.

2. Filter and Analyze

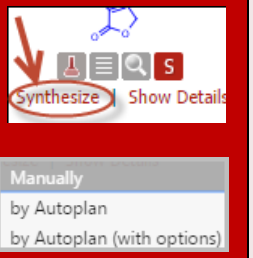
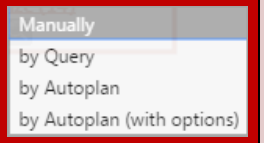
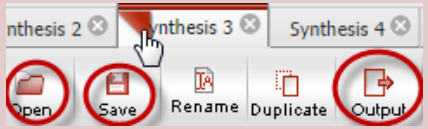
FILTER

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. 

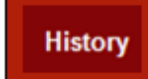
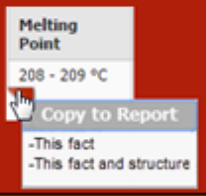
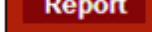
ANALYZE

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**). 

3. Synthesis Plans (Build a retrosynthetic pathway)

SYNTHESIS PLANS	
TASK	**COMMENT**
Start a plan from the Results screens 	Click the **Synthesize** link under a substance in either the *Reactions*, *Substances*, or *Citations* results. Then choose any of the following: **Manually** – You will select reactions from the bottom of the Synthesis Plans page. **AutoPlan** – Reaxys will automatically create up to 10 plans based on preselected options. **AutoPlan (with options)** - Reaxys will automatically create up to 10 plans based on options that will be presented to you.
Edit or add to your synthesis plan 	Click the **Synthesize** link under any of the substances in the plan. Select any of the 3 options mentioned above, or choose **by Query**, which will present you with a structure query form. Click the **Add** link to add and compare an alternate route. Click **Remove** to delete part of the plan.
	Click the **Details** link in the plan to display the reaction conditions. Click **Save** to save the plan as an xml file on your computer. Click **Output** to export the plan in various formats. Click the red triangle to save the plan to the **Report** page. 

4. Saving, Printing, Exporting, and Reporting

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 **Output** 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.