

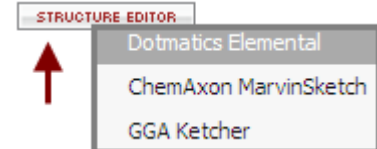

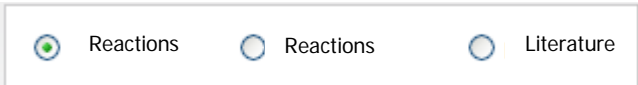



How do I.....	Instructions
Register for a password	 Click the Register button in the upper right part of the screen.
Change password	 Click the My Settings button. Then click the Change Password link
Find out about tested environments involving Windows, Mac, and Java	<div style="border: 1px solid gray; padding: 5px; margin: 10px auto; width: fit-content;"> <p>Tested Environments Please Note: Reaxys is a web-based application using Which support Java 1.5 or higher and JavaScript execut Windows PC Macintosh</p> </div> <div style="border: 1px solid gray; padding: 5px; margin: 10px auto; width: fit-content;"> <p>Contact Us Support About Reaxys Terms and Conditions</p> </div> <p style="text-align: center;">↑</p> <p>Click the About Reaxys link located at the bottom of the Query page.</p>
Find info about the databases included in a Reaxys search.	<div style="border: 1px solid gray; padding: 5px; margin: 10px auto; width: fit-content;"> <p>Sources: Reaxys, PubChem, eMolecules</p> </div> <p>Click on one of the hyperlinks towards the top of the Query page to display the info sites for those databases.</p>
Select a Structure Editor	 <p>Click the Structure Editor button located in the lower right side of the structure box on the Query page. Click the structure box to open the Structure Editor. If you are on the Start page, you will first have to click the box on the far left labeled Substances/Reactions to open the structure box.</p>
Use these external structure editors: -Accelrys ISIS/Draw - ChemDraw - Accelrys Draw - ICEdit -CrossFire SE	 <ol style="list-style-type: none"> 1. Install the external structure editor 2. Download the Reaxys Structure Editor Plug-in from http://www.reaxys.com/info/support_downloads and install it (Download ChemDraw/Reaxys Plug-in: http://scistore.cambridgesoft.com/ScistoreProductPage.aspx?ItemID=5943 and install.) (Download the ICEdit/Reaxys Plug-in from http://www.infochem.de/content/downloads/iceditinreaxys.pdf) 3. Click the My Settings button. Then click the Modify Application Settings link, select your structure editor and click Save.
Select Substances or Reactions as the type of search	 <p>Click the appropriate selection, Substances or Reactions, located above the structure box on the Standard and Advanced tab. If you are on the Start page, you will first have to click the box on the far left labeled Substances/Reactions to view the structure box.</p>
Create a structure from a name CAS#, InChIkey, or smiles string	 <p>Click the Create structure template from name link under the Structure box, type in the query and click Submit. (Use the operator dropdown menu, if needed). If several structures share the same name, a list of structures will appear with the most relevant first.</p>

Customize the settings for **reaction or substance search options**

My Settings

- Include tautomers
- Ignore stereo
- No salts
- No mixtures
- No isotopes
- No charges
- No radicals

Click the **My Settings** button. Then click the **Modify Application Settings** link and look for **Reaction or Structure Search Options**.

Customize the settings for **structure display options**

My Settings

Carbon Labels

- Always
- Never
- At straight angles and H atoms

Implicit Hydrogens

- On All
- On Hetero
- On Hetero and Terminal

(R)(S)

Numbers

Valence

Hydrogens

Click the **My Settings** button. Then click the **Modify Application Settings** link and look for **Structure Display Options**.

Display a form so that I can use **data** in my query.

Reaction Data
Physical
Spectra
Bio Activity
Natural Product

Reaction Data

Please select the fields you would like to add to your search by selecting the checkboxes. click OK.

<input type="checkbox"/>	Reactant	is	<input type="text"/>	Lookup
<input type="checkbox"/>	Product	is	<input type="text"/>	Lookup
<input type="checkbox"/>	Reagent/Catalyst	is	<input type="text"/>	Lookup

View more fields

Cancel
OK

Select a category and click to display the corresponding form. Type in a query or use the **Lookup** table to select an entry. If you'd like to add more fields to the form, click the **View more fields** link. Click in the checkboxes near the fields that you want to add to the query page. Searching the **Literature** fields together with a structure or reaction will retrieve a list of all substances and all reactions from documents that fit the bibliographic search criteria. If, instead, you wish to do a **Literature search** you can find information [here](#).

Use the **Lookup** tables in the **Data** forms.

Reaxys Search Form

Reaction Data Properties

Reactant	is	<input type="text"/>	Lookup
Product	is	<input type="text"/>	Lookup
Reagent/Catalyst	is	<input type="text"/>	Lookup
Yield (numerical)	=	<input type="text"/>	Lookup

Select index items and click 'Transfer'

Search for:

- tetraacetyl diborate (141)
- tetraacetyl riboflavin (17)**
- tetraacetylriboflavin (35)**
- tetraalkoxydiboron (1) (1)
- tetraalkoxysilane (1)
- tetraalkoxytellurane (6)
- tetraalkyl ammonium perchlorates (1)
- tetraalkyl-gem-dialuminohexane (1)
- tetraalkylammonium bromide (7)

Page of 10000

Transfer
Reset
Cancel

Click the appropriate **Lookup** link to open the index to select specific data. In the index, type in your data. Click to select your data from the list. Use the **Shift** and **Control** keys to make multiple selections. Then click the **Transfer** button to add the data to your form. Check the boxes for the datafields you want to add to the **Query** page. Click **OK**.

Customize a **Data** form.

Select fields to add to your form from this side

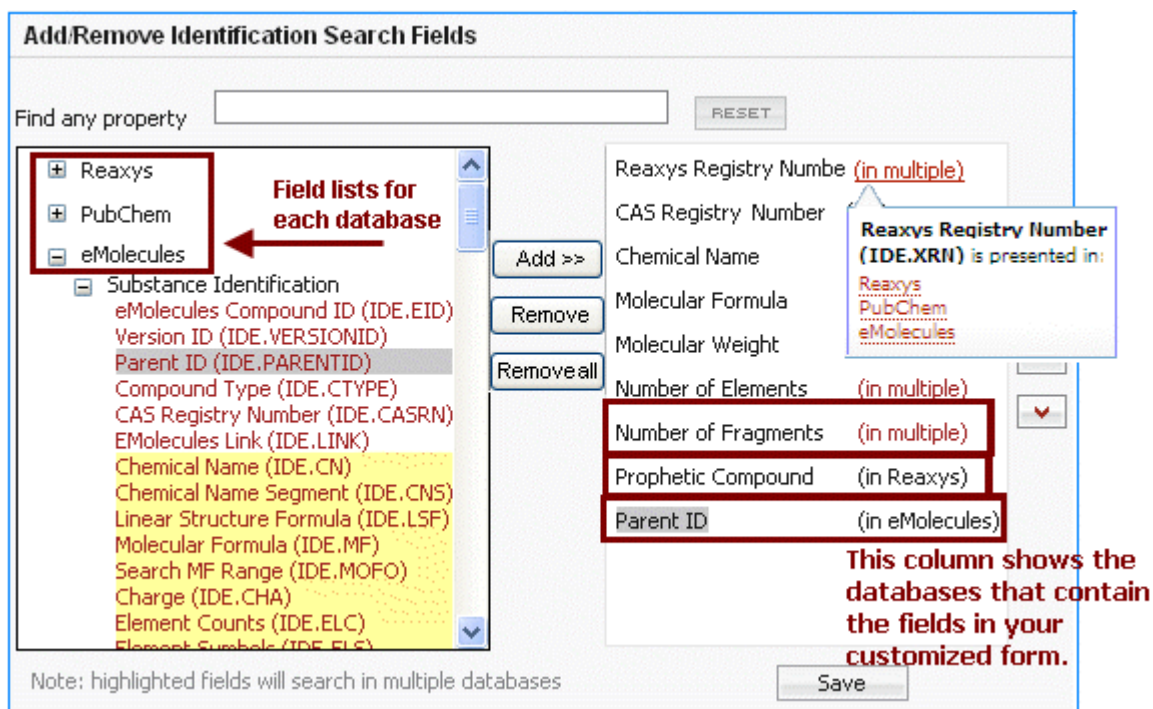
This side reflects your current form

Add/Remove Physical Search Fields

Find any property

<ul style="list-style-type: none"> [-] Reaxys <ul style="list-style-type: none"> [-] Melting Point <ul style="list-style-type: none"> Melting Point, °C (MP.MP) Solvent (MP.SOL) [-] Boiling Point <ul style="list-style-type: none"> Boiling Point, °C (BP.BP) Pressure, Torr (BP.P) [+] Sublimation [-] Refractive Index <ul style="list-style-type: none"> Refractive Index (RI.RI) Wavelength, nm (RI.W) Temperature, °C (RI.T) [-] Density <ul style="list-style-type: none"> Density, gcm⁻³ (DEN.DEN) Reference Temperature, °C Measurement Temperature [+] Adsorption (MCS) 	<input type="button" value="Add >>"/> <input type="button" value="Remove"/> <input type="button" value="Remove all"/>	<ul style="list-style-type: none"> Boiling Point (in Reaxys) Boiling Point (in Reaxys) Density (in Reaxys) Density (in Reaxys) Solubility (MCS) (in Reaxys) Dissociation Exponent (in Reaxys) Refractive Index (in Reaxys) Optical Rotatory Power (in Reaxys) Partition octan-1-ol/water (MCS) (in Reaxys)
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Select a form from the buttons labeled *Reaction*, *Physical*, etc. and click to open it. Then click the **View more fields** link at the bottom of the form. The **Add/Remove** box is displayed with all of the available fields shown on the left and the fields chosen in your current form on the right. Select a field from the left (use the **Shift** or **Ctrl** keys for multiple selections) and then click the **Add** button (between the left and right columns) to move your selection to the right. (Adjust the placement of the fields in your new list by clicking the arrows on the far right). Click the **Save** button. The new fields will now appear on your form. Fields can be removed in a similar way: click **View more fields** and select the fields you want to remove from the right column, click the **Remove** button, and then click **Save**. Please note: If you cannot find the field you need on the left, begin typing part of the field name into the entry box at the top of the form and the relevant fields will be displayed at the top of the list.



Add/Remove Identification Search Fields

Find any property

Field lists for each database

- Reaxys
- PubChem
- eMolecules
 - Substance Identification
 - eMolecules Compound ID (IDE.EID)
 - Version ID (IDE.VERSIONID)
 - Parent ID (IDE.PARENTID)
 - Compound Type (IDE.CTYPE)
 - CAS Registry Number (IDE.CASRN)
 - eMolecules Link (IDE.LINK)
 - Chemical Name (IDE.CN)
 - Chemical Name Segment (IDE.CNS)
 - Linear Structure Formula (IDE.LSF)
 - Molecular Formula (IDE.MF)
 - Search MF Range (IDE.MOFO)
 - Charge (IDE.CHA)
 - Element Counts (IDE.ELC)
 - Element Symbols (IDE.ELS)

Buttons: Add >>, Remove, Remove all

Selected fields on the right:

- Reaxys Registry Number (in multiple)
- CAS Registry Number
- Chemical Name
- Molecular Formula
- Molecular Weight
- Number of Elements (in multiple)
- Number of Fragments (in multiple)
- Prophetic Compound (in Reaxys)
- Parent ID (in eMolecules)

Tooltip for Reaxys Registry Number (IDE.XRN):
 Reaxys Registry Number (IDE.XRN) is presented in:
 Reaxys
 PubChem
 eMolecules

Note: highlighted fields will search in multiple databases

Many fields in **Reaxys** have been mapped to fields in **PubChem** and **eMolecules** and those results appear automatically when you do a substance search. There are also many fields that are unique to **PubChem** and **eMolecules** that can be searched from within **Reaxys**. For example eMolecules has a unique field for the parent compound identification. This field can be added to your customized form. Notice that in the example above you can hover over a hyperlink on the right side to see which databases contain that field. When the field appears in only one database, the name of the database is shown.

Save a **Data Form** for future use

Select the appropriate radio button (Reactions, Substances, Literature). Select the desired fields by clicking any of the buttons on the bottom of the **Standard** tab and then clicking the appropriate checkboxes near each field. If a field you need does not already appear on the form, click **View more fields** (see above), and then select the needed fields. Click OK. You can mix fields from any of the categories (*Physical, Identification, etc.*). Then click the **Save** button in the top right corner to save the form to your computer. Retrieve the form by clicking the **Import** button (next to the **Save** button.)

Add a **keyword** or **data** to your query using the **Advanced** form

Search for the field name here

Click to open the index and select data

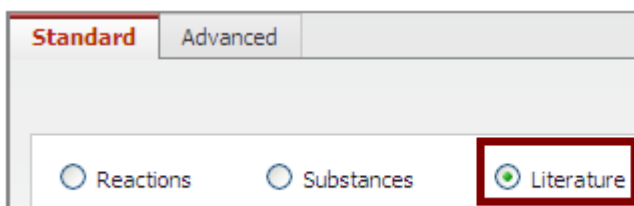
The **Advanced** form gives you access to the data structure so that you can create complex queries using different fields and data operators. Click the **Advanced** tab. Then click the **Show Searchable Fields** link towards the bottom of the page. Find the appropriate field by typing a partial field name into the box under the words **If you don't know the field code search for a topic here**. Relevant field names will appear as you type. Select the field from the list that appears. Select **exists** for a general search of that field, or click the field name and then click the **Lookup** link to open the index to select specific data. In the index, type in your data. Click to select your data from the list. Use the **Shift** and **Control** keys to make multiple selections. Then click the **Transfer** button. Please note: If several subfields are listed under a field name, e. g., *boiling point* and *b.p. pressure*, you can use the operator **Proximity** when building your query with these fields. This will ensure that your results are aligned.

The Basic Index fields are for keyword searching. The other fields are for data searching.

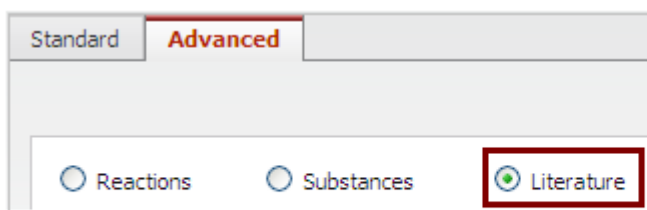
Perform Literature Searching



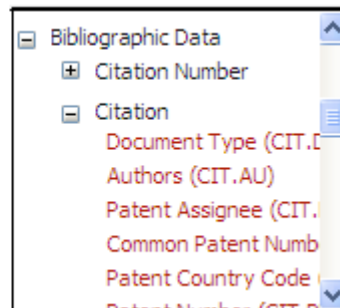
From Start page



From the Standard tab



From the Advanced tab



To find a list of specific citations *with their associated substances and reactions (if any)*, do any of the following:

- Click the **Literature** picture on the **Start** page to open the **default Literature form**.
- Click the **Literature** radio button on the **Standard tab** and then click the **Literature button** at the bottom to open the **default Literature form**.
- Click the **Literature** radio button on the **Advanced tab** and then click the **Show Searchable Fields** link at the bottom of the page. Scroll to **bibliographic Data**.

Use the **field at the top of the page** on the **default Literature form** to find keywords or phrases that may be contained in titles, abstracts, or author names. Use wildcards (*) and operators like *and*, *or*, *near* (within a few words), and *next* (adjacent words). Use the **Lookup** link next to each field to search the index.

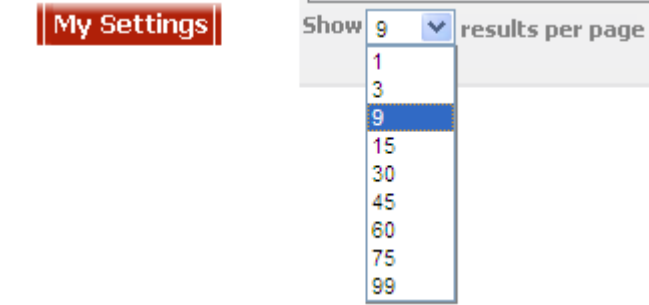



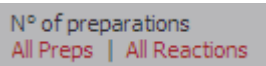
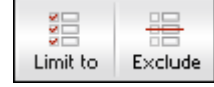
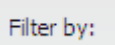
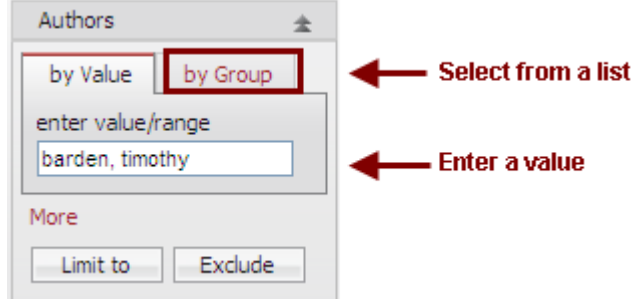
Click [here](#) for information on using the **Advanced tab**.

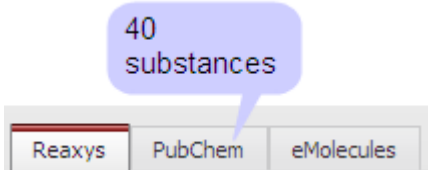
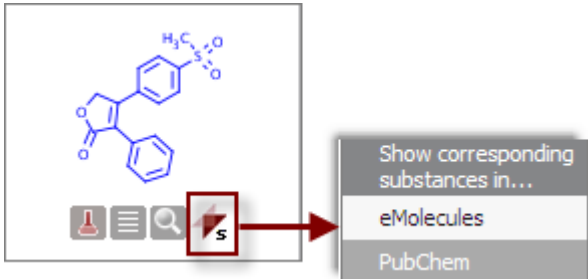

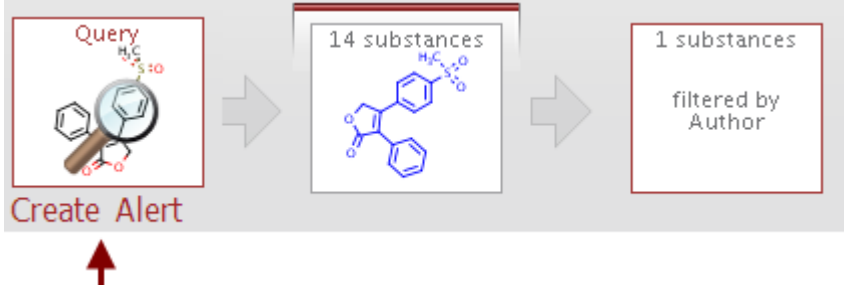

Please Note: Clicking the **Substances** or **Reactions** radio button will allow for **bibliographic searching**, but the results will be structure/ reaction lists *with their associated citations* and most likely will include additional citations that were not in your query.

Save a query


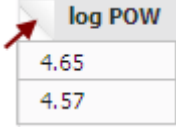

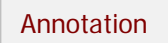




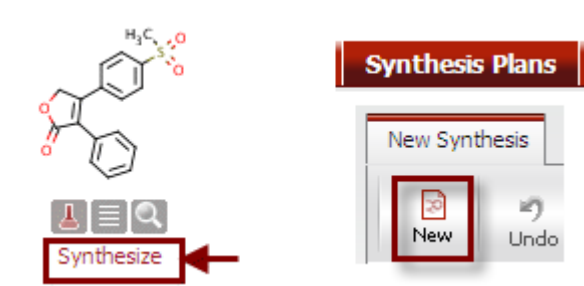


Click the **Save** button in the upper right corner of the **Query** tab.

<p>Set the number of hits per page</p>	 <p>Click the My Settings button. Then click the Modify Application Settings link. To temporarily change the number of hits per page, select the appropriate number from the drop-down menu in the lower left side of the Results page.</p>
<p>Change the structure and text highlight colors</p>	 <p>Click the My Settings button. Then click the Modify Application Settings link.</p>
<p>Change the size of substances or reactions</p>	 <p>Use the zoom buttons on the toolbar on the results page.</p>
<p>Show/ Hide reaction or Substance details</p>	 <p>Click the appropriate button on the tool bar on the results page.</p>
<p>Generate a list of associated reactions from a substance list</p>	 <p>From the Substances (Table) results tab, select the link for All Preps (substances in the list are products in the reactions) or All Reactions (substances in the list can be products or reactants).</p>
<p>Limit results to specific hits</p>	 <p>Click the check-boxes (left side of hit) to select the hits, and then click the Limit to Selection button.</p>
<p>Limit results to hits with specific properties</p>	 <p>Find the appropriate filter on the left side of the results screen, select properties and click the Limit to button. If the word more appears at the bottom of the filter, click the more link and specify property data in the pop-up box. After filtering, the available data for the hit will include a link called Hit Data.</p>
<p>Limit results to a specific author</p>	 <p>Some filters give you the choice of entering the value or selecting the value from a list. For example, to filter by author, find the appropriate filter on the left side of the results screen, click to select author(s). If the list is very long, clicking the more link will not display the complete list. In this case, click the By Value tab in the filter and type in the name (wildcards can be used).</p>

<p>View the results from different databases.</p>	 <p>By default, the Reaxys results will be displayed on the Results page. You can hover over the tab for other databases to see the number of results and then click the tab to view the results from within Reaxys. If no results were found in Reaxys, the tab for the database with the largest number of hits will automatically be selected.</p>
<p>View a single substance in multiple databases</p>	 <p>Click the Reaxys logo under a structure and select a database.</p>
<p>View supplier availability and pricing info</p>	 <p>eMolecules pricing and availability information is displayed by clicking the eMolecules tab. Click the flask icon under a substance to find options for linking to eMolecules, a free website, Accelrys ACD database (requires a license), and CambridgeSoft's ACX (requires a license).</p>
<p>Create an Alert</p>	 <p>Click the Create Alert link under the first breadcrumb in the upper left corner of the results screen or click the History button and then click the Create Alert link under the query.</p>
<p>Save Results</p>	 <p>Click the History button from the Results page. Then click the Store link on the right side of the screen.</p>

<p>Copy a substance or reaction from the Results screen</p>	<p>Copy Reaction to Clipboard Copy Reaction to Query Copy Reaction to Synthesis Planner</p> <p>Reaxys-RN: 8269007 MF: C17H14O4S MW: 314.362 CAS-RN: 162011-90-7 Show Details Copy Structure to Clipboard Copy Structure to Query Use as Sub-structure Filter Copy Reaction to Query View related Markush</p> <p>Display the Options Menu by clicking the grey box below a substance (or below any substance in a reaction), or click directly on a substance, and select the appropriate option. You can also click the arrow in the reaction and then select an option.</p>
<p>Start an AutoPlan</p>	<p>Synthesize</p> <p>Manually by AutoPlan by AutoPlan (with options)</p> <p>Click the Synthesize link under a structure in the results or in the Synthesis Planner and select by AutoPlan.</p>
<p>Select the settings for AutoPlan</p>	<p>My Settings + AutoPlan options</p> <p>From the My Settings page, click Modify Application Settings>AutoPlan options.</p>
<p>Close tabs in the Synthesis Planner</p>	<p>Synthesis 3 Synthesis 4 Synthesis 5</p> <p>Close: - This Tab - All Tabs - Other Tabs - Left Tabs - Right Tabs</p> <p>Click the Close X to reveal the options.</p>
<p>Copy a synthesis plan to the Reaxys Report</p>	<p>Report Synthesis 1</p> <p>Click the Report button on the Synthesis Planner tool bar or click the page curl on one of the tabs.</p>
<p>Filter using histograms</p>	<p>Open Analysis View</p> <p>From the Results page, select the Open Analysis View button. Select a category from the dropdown menu of Histogram A and then click the desired bins. Analyze the data by comparing it to other categories and bins in Histogram B.</p>

<p>Select specific details to copy to the Reaxys Report</p>	 <p>To select a detail, look for a page curl image as you hover over details. Click the page curl to see the options specific to that detail and click to select.</p>
<p>Select a whole list of details to copy to the Reaxys Report</p>	 <p>A whole list of facts can be copied by clicking the header on the list of facts.</p>
<p>View your selected facts in the Report</p>	 <p>After making your selections, click the Report button on the button bar to open your Reaxys Report.</p>
<p>Add notes to selected facts in the Report</p>	 <p>Click the Annotation link on the upper right side of an item to add notes to the selected fact.</p>
<p>Display the structure for a selected fact in the Report</p>	 <p>Click the Show Substance link to display the substance that goes with the selected fact. The substance will display even though it was not selected with the fact on the results page.</p>
<p>Regroup selected facts in the Reaxys Report</p>	 <p>Click the Regroup button to reconstruct your report by collecting individual items that were derived from the same record and combining them into one item.</p>
<p>Email the selected facts to a colleague</p>	 <p>Click the Send button to email your comments to colleagues along with your Reaxys Report as an attachment to an email.</p>
<p>Export</p>	 <p>Click the Output button and select from several options.</p>
<p>Start a Synthesis Plan</p>	 <p>Click the Synthesize link below a substance to start a plan using that substance. Alternatively, you can click the Synthesis Plans button from the button bar and then click the New button in the upper left side of the screen to begin a search from within the Synthesis Planner.</p>
<p>Link to external docs</p>	<p>Title/Abstract Full Text View citing articles Show Details Links to Title/Abstract, Full Text, and View Citing Articles appear with references when available.</p>

Topic	Page
Register for a password	1
Change password	1
Find out about tested environments involving Windows, Mac, and Java	1
Find information about the databases included in a Reaxys search.	1
Select a Structure Editor	1
Use these external structure editors: - Accelrys ISIS/Draw - ChemDraw - Accelrys Draw - ICEdit - CrossFire SE	1
Select Substances or Reactions as the type of search	1
Create a structure from a name CAS#, InChIkey, or smiles string	1
Customize the settings for reaction or substance search options	2
Customize the settings for structure display options	2
Display a form so that I can use keywords or data in my query.	2
Use the Lookup tables in the Data forms .	3
Customize a Data form .	3
Save a Data Form for future use	5
Add a keyword or data to your query using the Advanced form	5
Perform Literature Searching	6
Save a query	6
Set the number of hits per page	7
Change the structure and text highlight colors	7
Change the size of substances or reactions	7
Show/ Hide reaction or Substance details	7
Generate a list of associated reactions from a substance list	7
Limit results to specific hits	7
Limit results to hits with specific properties	7
Limit results to a specific author	7
View the results from different databases.	8
View a single substance in multiple data-bases	8
View supplier availability and pricing info	8
Create an Alert	8

Save Results	8
Copy a substance or reaction from the Results screen	9
Start an AutoPlan	9
Select the settings for Autoplan	9
Close tabs in the Synthesis Planner	9
Copy a synthesis plan to the Reaxys Report	9
Filter using histograms	9
Select specific details to copy to the Reaxys Report	10
Select a whole list of details to copy to the Reaxys Report	10
View your selected facts in the Report	10
Add notes to selected facts in the Report	10
Display the structure for a selected fact in the Report	10
Regroup selected facts in the Reaxys Report	10
Email the selected facts to a colleague	10
Export	10
Start a Synthesis Plan	10
Link to external docs	10



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