

Quick User Guide

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How do I	Example	Instructions
Register for a password	Register	Click the Register button in the upper right part of the screen.
Change password	My Settings	Click the My Settings button. Then click the Change Password link.
Set/change reaction/substance search options	My Settings	Click the My Settings button. Then click the Modify Application Settings link.
Change structure display options	My Settings	Click the My Settings button. Then click the Modify Application Settings link.
Set the number of hits per page	My Settings	Click the My Settings button. Then click the Modify Application Settings link.
Change the structure and text highlight colors	My Settings	Click the My Settings button. Then click the Modify Application Settings link.
Use these external structure editors: ISIS/Draw ChemDraw SymyxDraw ICEdit	My Settings	 Install the external structure editor Download the Reaxys Structure Editor Plug-in from http://www.reaxys.com/info/support_downloads and install. Download the ChemDraw/Reaxys Plug-in from 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 Click the My Settings button. Then click the Modify Application Settings link, select your structure editor and click Save.
Generate structure from name CAS#, InChlkey, smiles string	Generate structure from name	Click the Generate Structure From Name button, type in the query and click Submit. (Use the operator drop down menu, if needed). If several structures share the same name, a list of structures will appear with the most relevant first.
Add a keyword or data to a Substance or Reaction query using the Form-based tab	Properties (Form-based) Conditions (Form-based)	Click the appropriate Form-based tab on either the Reactions or Substances query page. The keyword field for Substances is the Search text in all facts field . The keyword field for Reactions is the All reaction fields field. The other Substance or Reactions fields are data-specific and the query can be typed in directly or selected from the index (see below for more info). Searching the bibliographic fields on these query pages will retrieve a list of all substances or all reactions from documents that fit the bibliographic search criteria.
Add a keyword or data to a Substance or Reaction query using the Advanced tab (offers more fields)	Properties (Advanced) Conditions (Advanced) Search for Field	Click the appropriate Advanced tab on either the Reactions or Substances query page. Find the appropriate field by typing a partial field name into the box next to the Search for Field button and then click this button. 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 small grey box 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
Perform Bibliographic Searching	Text, Authors and more	While the Substances and Reactions tabs allow for bibliographic searching , the results will be structure or reaction lists with their associated citations and most likely will include additional citations that were not in your query. To find a list of specific citations with their associated substances and reactions, use the Text, Authors, and more tab .
Perform Form-based searching from the Text , Authors & more tab	Form-based	Use the Quick Search box 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). The fields for Author, Patent Number, etc. can be used as previously described for the Reactions and Substances (Form-based) search section.
Perform Advanced searching from the Text, Authors, & more tab	Advanced Search for Field	The technique described in the Properties (Advanced) tab section also applies to this section. Just remember that if you search a substance or reaction field from the Text , Authors , and more tab, you will receive a list of citations that contain substances or reactions with the properties that you searched for. The associated lists of substances and reactions will contain all of the substances and reactions from those citations (not just the ones with the properties in your query).



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How do I	Example	Instructions
Save Query	Save Query	Click the Save Query button at the bottom of the Query page.
Change the size of substances/reactions	Zoom in Zoom out	Use the zoom buttons on the toolbar on the results page.
Show/Hide reaction details	Show Hide	Click the appropriate button on the tool bar on the results page.
Generate a list of associated reactions from a list of substances	N of preparations All Preps All Reactions	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).
Limit results to specific hits	Limit to	Click the check-boxes (left side of hit) to select the hits, and then click the Limit to Selection button.
Limit results to hits with specific properties	Filter by:	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 .
Limit results to a specific author	By Value entre value/range	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 button 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).
View compound supplier availability and pricing info	()	Click the blue icon (shown here on the far left) under a substance to link to eMolecules, a free website. Click the dark blue icon under a substance to link to Accelrys ACD database (requires a license).
Create an Alert	Create Alert	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. If a query gave no results, a Create Alert link will be displayed in a pop-up box.
Save Results	History	Click the History button in the button bar. Then click the Store link on the right side of the screen.
Copy a substance or reaction from the Results screen		Click the Options Menu 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.
Export	Cutput	Click the Output button and select from several options.
Start a Synthesis Plan	Synthesize Synthesis Plans	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 .
Link to external docs		Links to Title/Abstract , Full Text , and View Citing Articles appear with each reference.





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