REAXYS

GETTING STARTED

July 15, 2014

REAXYS®
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WELCOME TO REAXYS !

YOU ARE SEARCHING MORE THAN:

- 50 MILLION UNIQUE SUBSTANCES
- 36 MILLION REACTIONS
- 500 MILLION EXPERIMENTAL FACTS (PROPERTIES)

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TABLE OF CONTENTS

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CONTENT

Structures and Reactions from over **400 core org/inorg/organometal journals,** And **patents** from selected organic chemistry patent publications (1869 -1980), and selected English-language patent publications (WO, US, EP; 1976 -) including IPC's:

A01N Biocides, Agrochemicals
C09B Dyes
C07 Organic Chemistry
A61K Medicinal Preparations

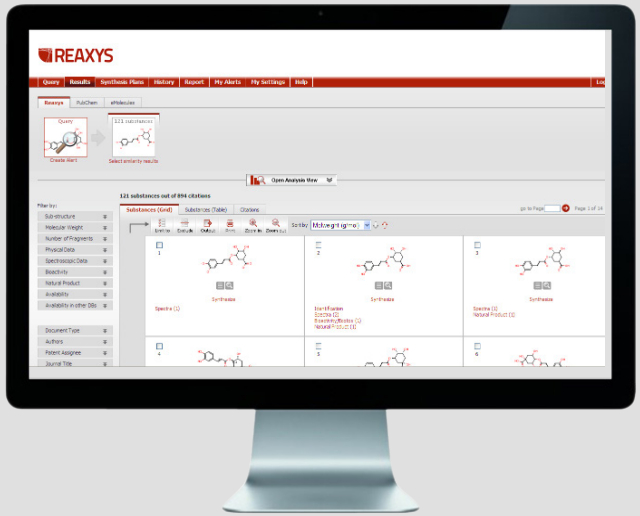
Data for those substances and reactions extracted and indexed into over 400 searchable fields

eMolecules

Supplier data including cost and availability, searchable and viewable from within Reaxys

PubChem

Substances with links to additional data



HEALTHINF
ADVANCES IN PHARMACOLOGY
C&EN CHEMICAL & ENGINEERING NEWS
The Oncology Report
NewScientist
THE Ocular Surface
A JOURNAL OF REVIEW LINKING LABORATORY SCIENCE, CLINICAL SCIENCE, AND CLINICAL PRACTICE

Additional content from books, conference proceedings, editorials, reviews, business articles. (>16,000 periodicals)

QUERIES

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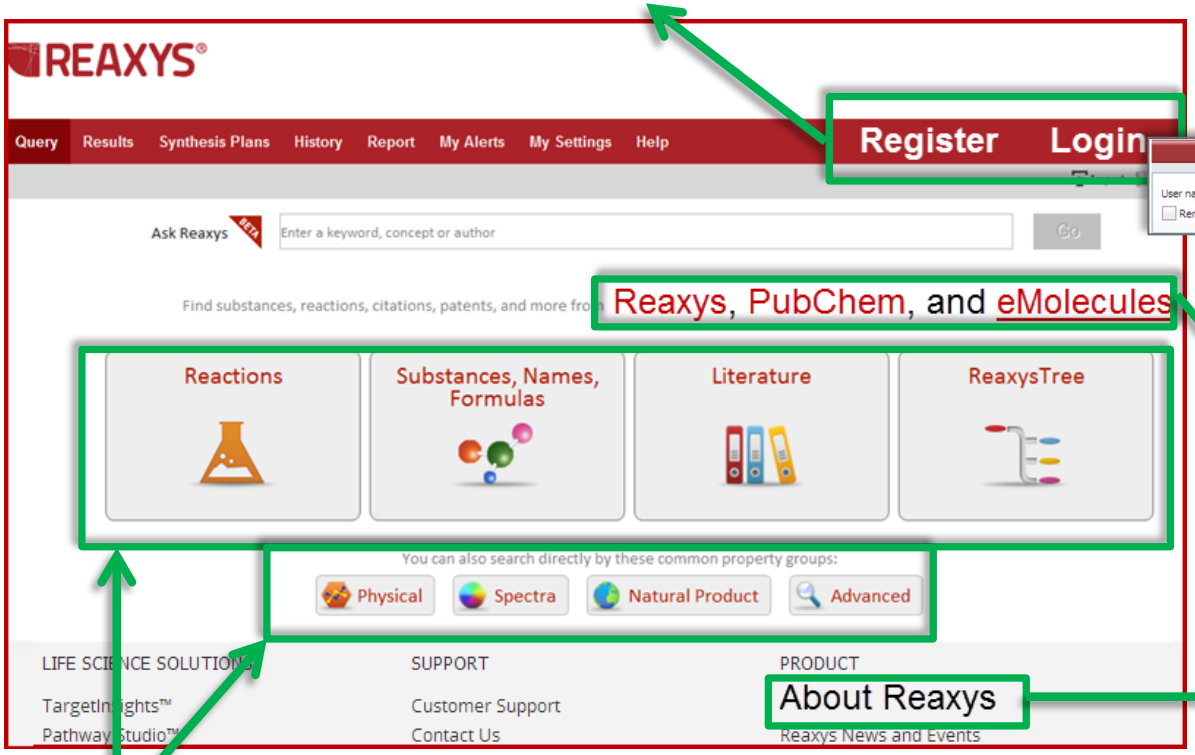
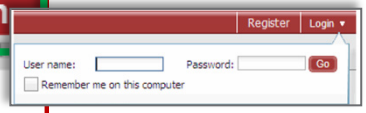
THE START PAGE

Register for a password and log on to get the most out of Reaxys.

Save display preferences, history, AutoPlan settings, and reports.





Click for more information on these databases

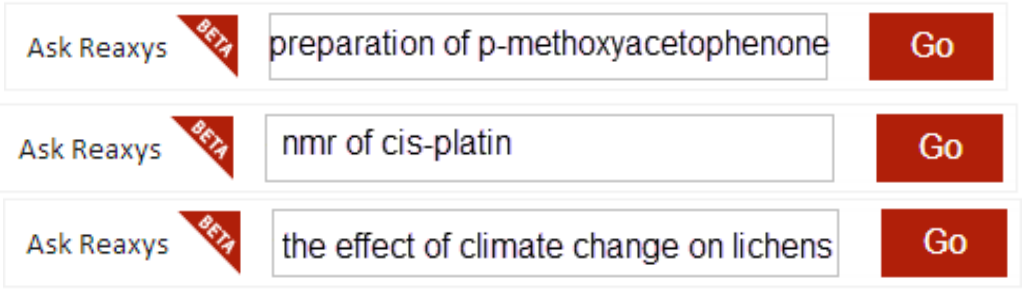
Click **About Reaxys** for information on updates, tested environments, structure editors, and number of structures, reactions, etc.

Click the appropriate **Query Theme** to open a search form

ASK REAXYS

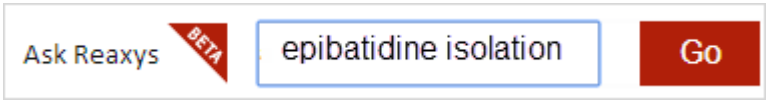
Type in a word or phrase and click “**Go**”.

Examples:



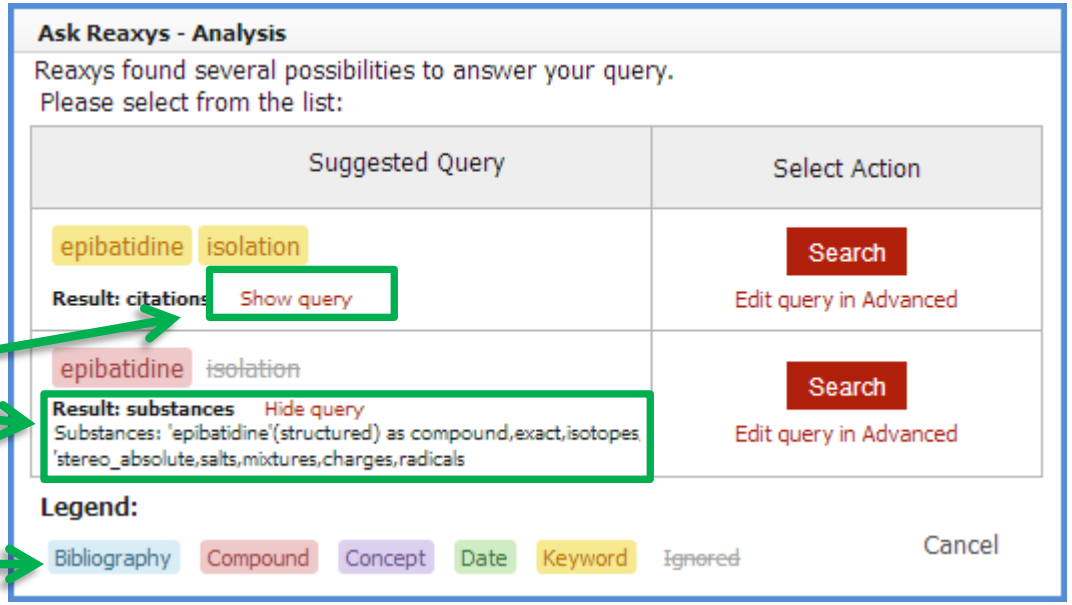
Ask Reaxys will interpret the terms and determine the context

If more than one context is possible, Reaxys will present you with some choices



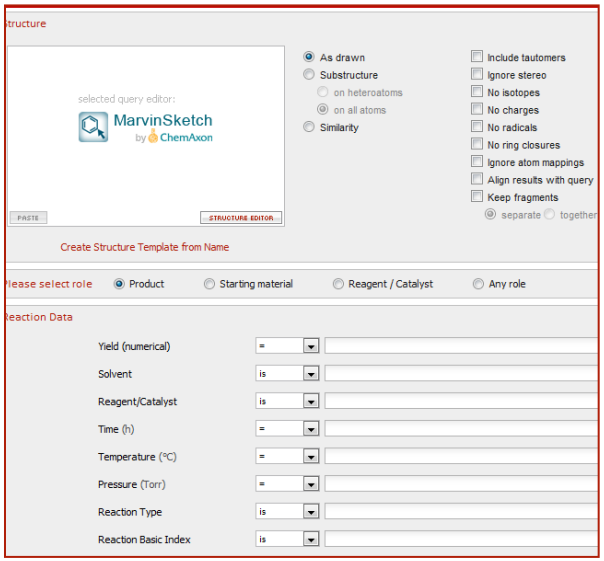
Click Show Query to view the proposed query before clicking **Search**

Color coding helps to convey the context of the query

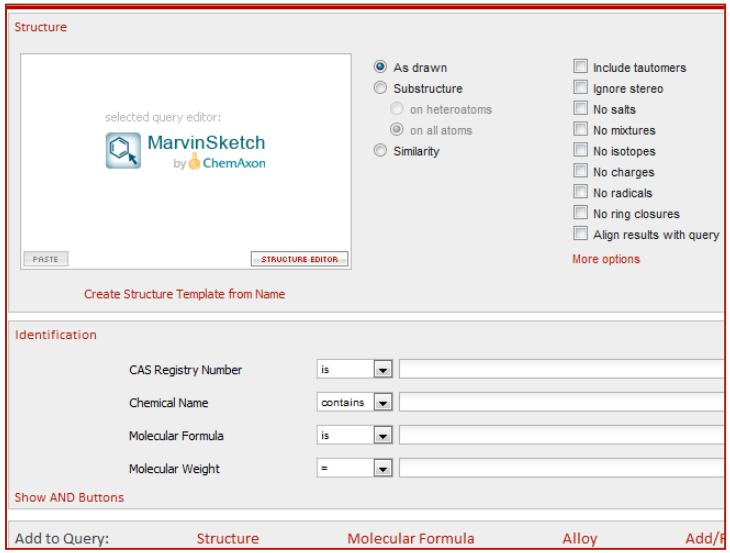


SEARCH FORMS

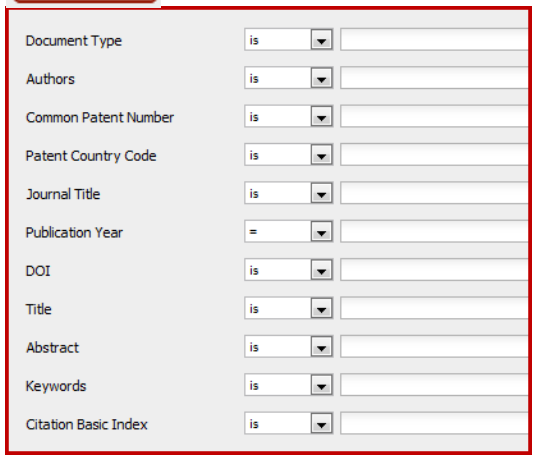
Substances



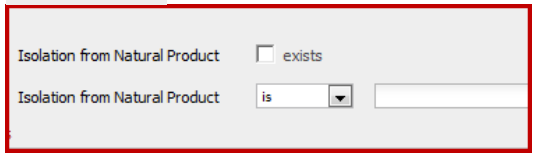
Reactions



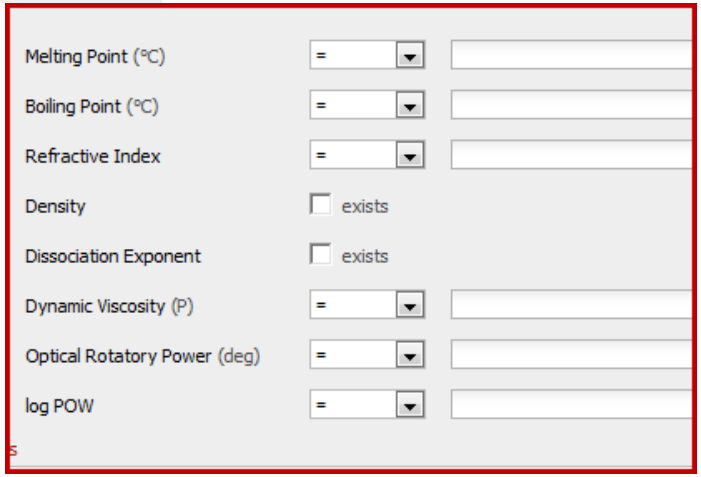
Literature



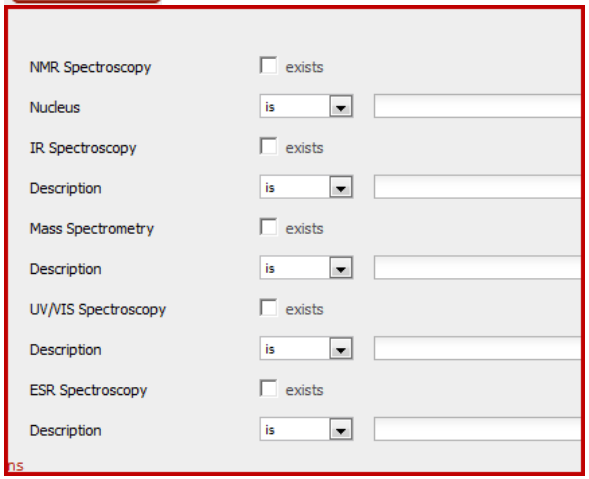
Natural Product



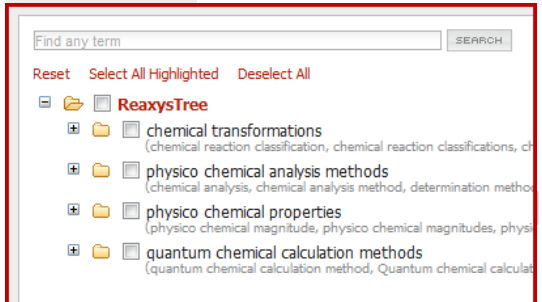
Physical



Spectra



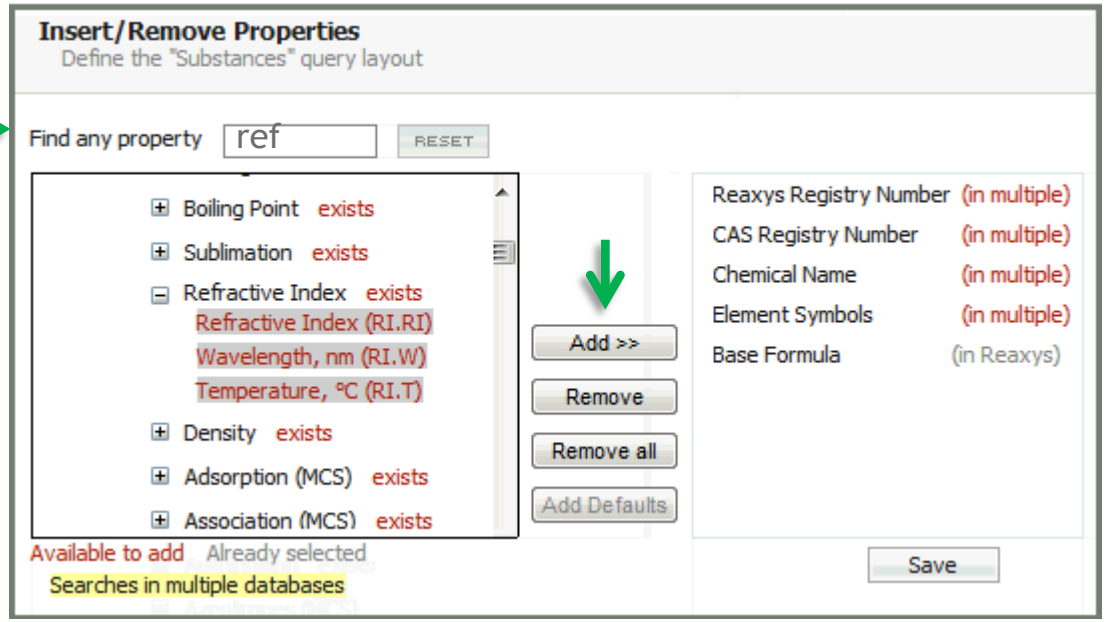
ReaxysTree



CUSTOMIZE A SEARCH FORM

Select fields to add from this side

This side reflects your current form



Locate a field by typing a portion of the field name into this box

Add/Remove Fields...

1. Add fields to your query page by clicking the **Add/Remove Fields** hyperlink.
2. Select fields from the list on the left side of the window that appears
3. Click **Add**
4. Click **Save**

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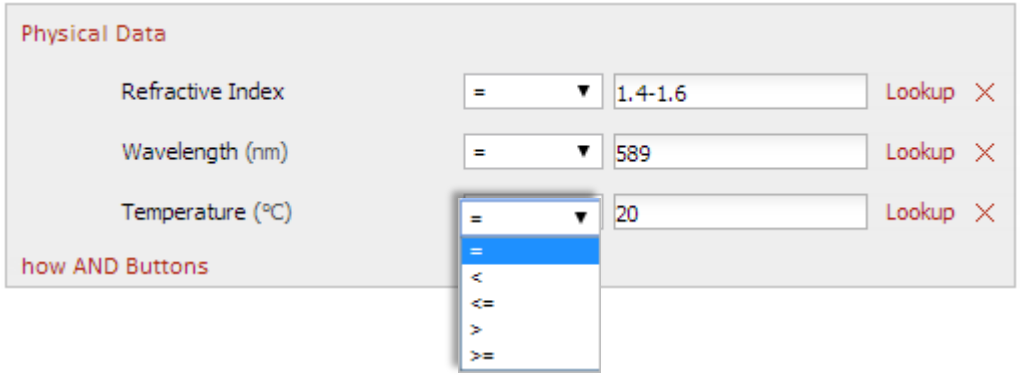
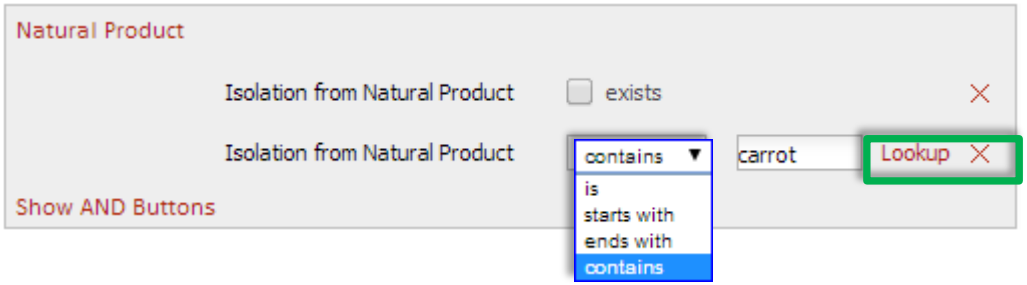
ADD DATA TO A SEARCH FORM



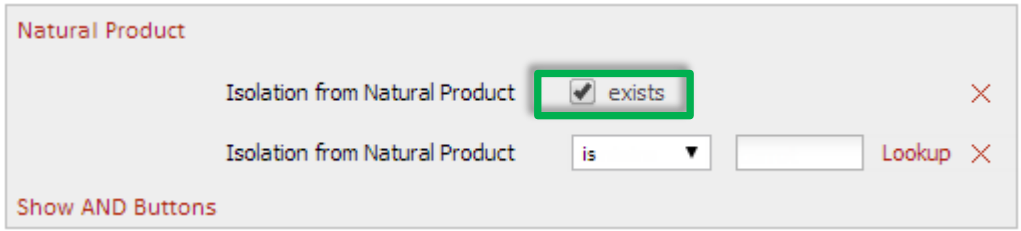
Type terms, numbers, or ranges directly into the search form

or



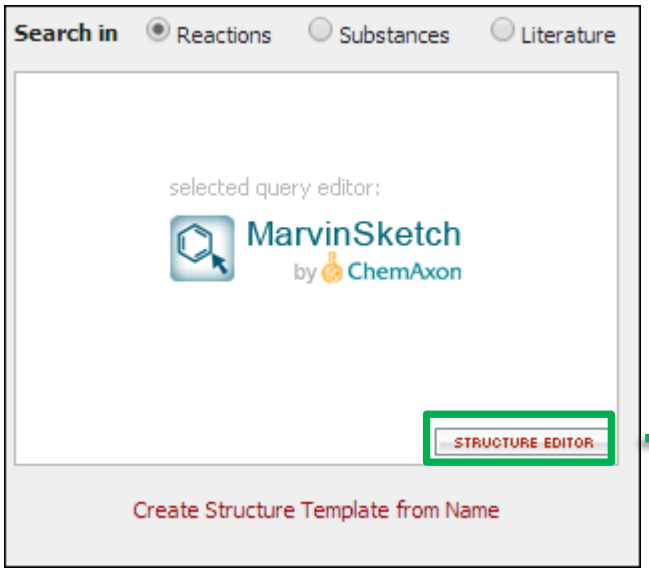
Click to display the lookup list. Search the list and select one or more items.

or



Select ***exists*** to retrieve data without indicating a value

STRUCTURE EDITORS



These 3 structure editors do not require installation:

- Elemental
- MarvinSketch
- GGA Ketcher

Click to select one of these 3.

Additional Structure Editors are available if you log in, select a structure editor from **My Settings**, and install the connection software.

Editors that do not require a plugin to be installed:

- Dotmatics Elemental
- ChemAxon MarvinSketch *(Note: requires Java to be installed)*
- GGA Ketcher

Reaxys uses Dotmatic's Elemental as default structure and reaction query editor, if no other editor is selected

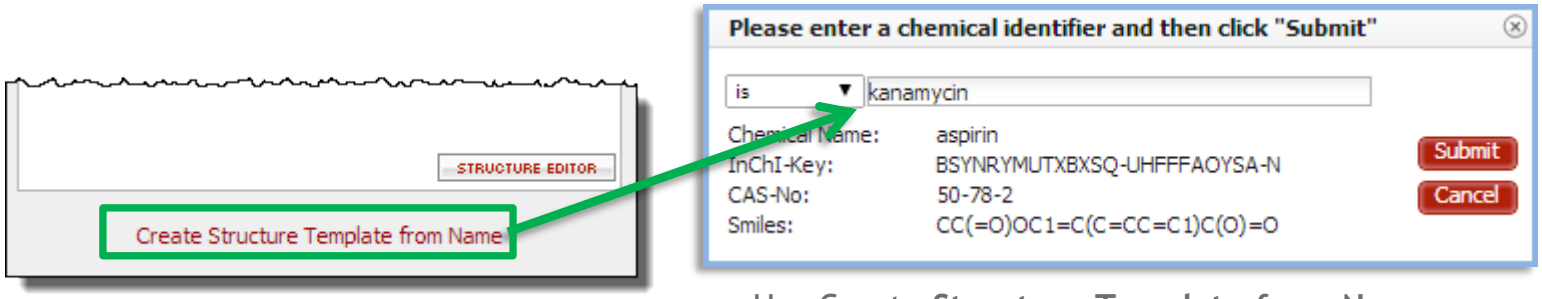
The following editors can only be used, if the Reaxys Structure Editor PlugIn is installed:

- Crossfire Structure Editor
- Accelrys Draw
- Accelrys ISIS/Draw
- CambridgeSoft ChemDraw
- ICEdit

Please check this with your administrator or click the hyperlink and download the installer.

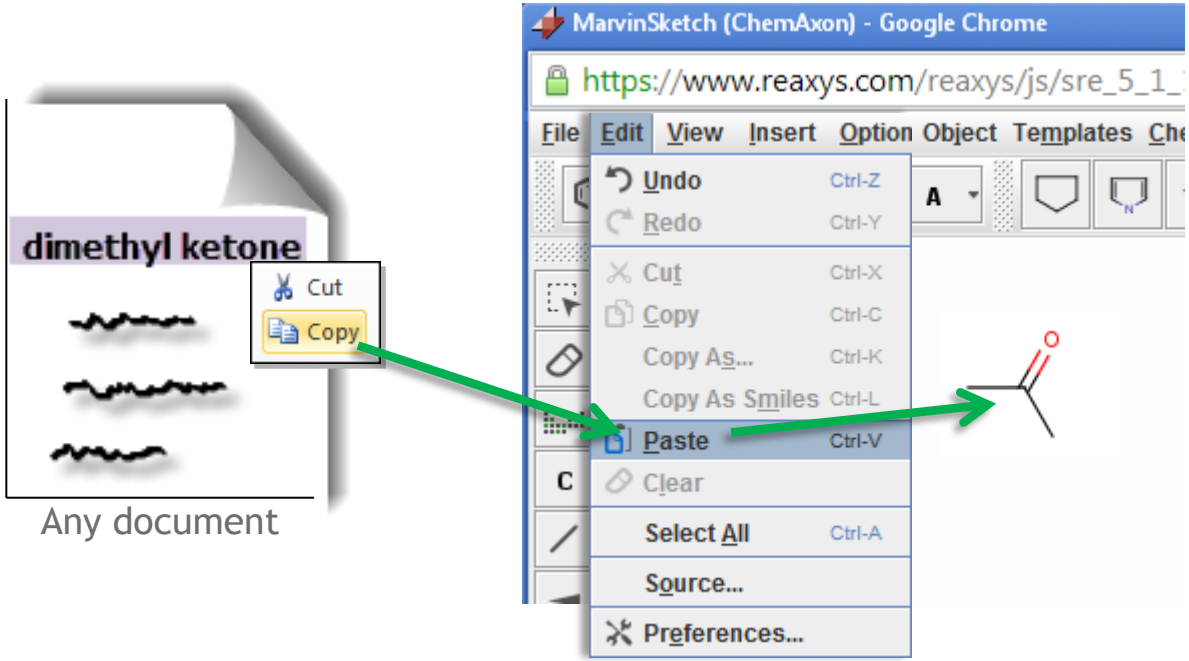
Reaxys will present a warning message, if these editors are selected, but the structure editor plugin is not installed.

OBTAIN A STRUCTURE WITHOUT DRAWING



Use Create **Structure Template from Name**

Copy/past a chemical name into the MarvinSketch structure editor



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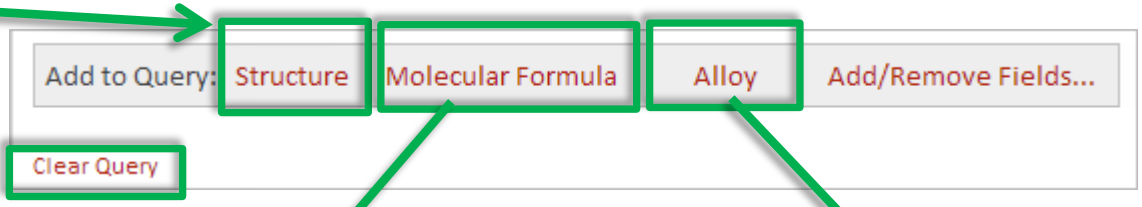
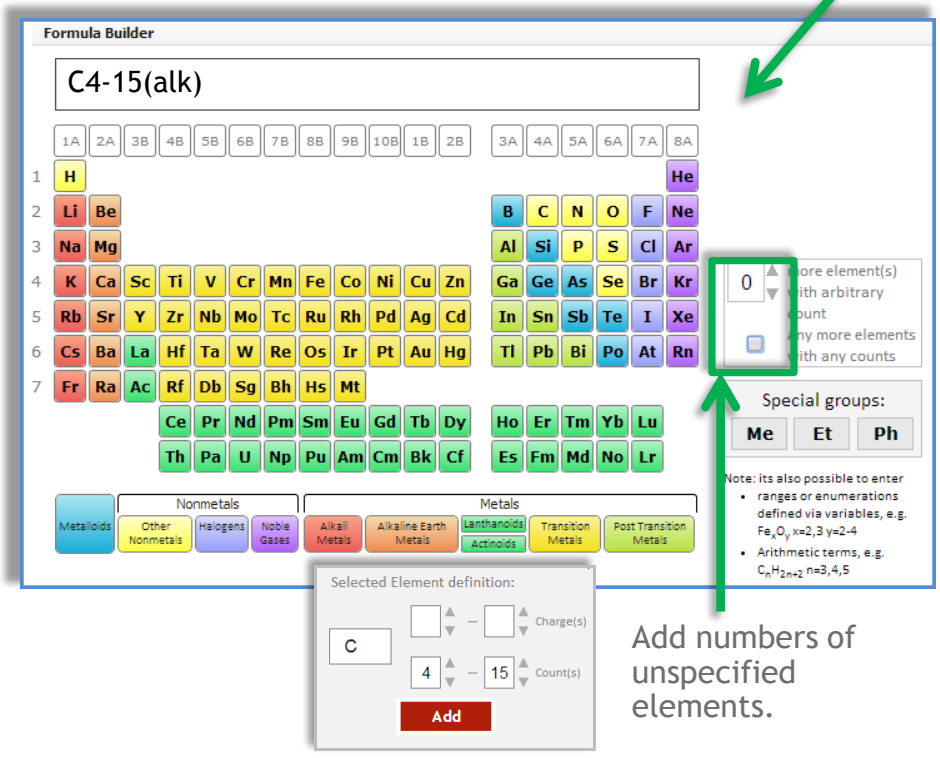
QUERY BUILDERS

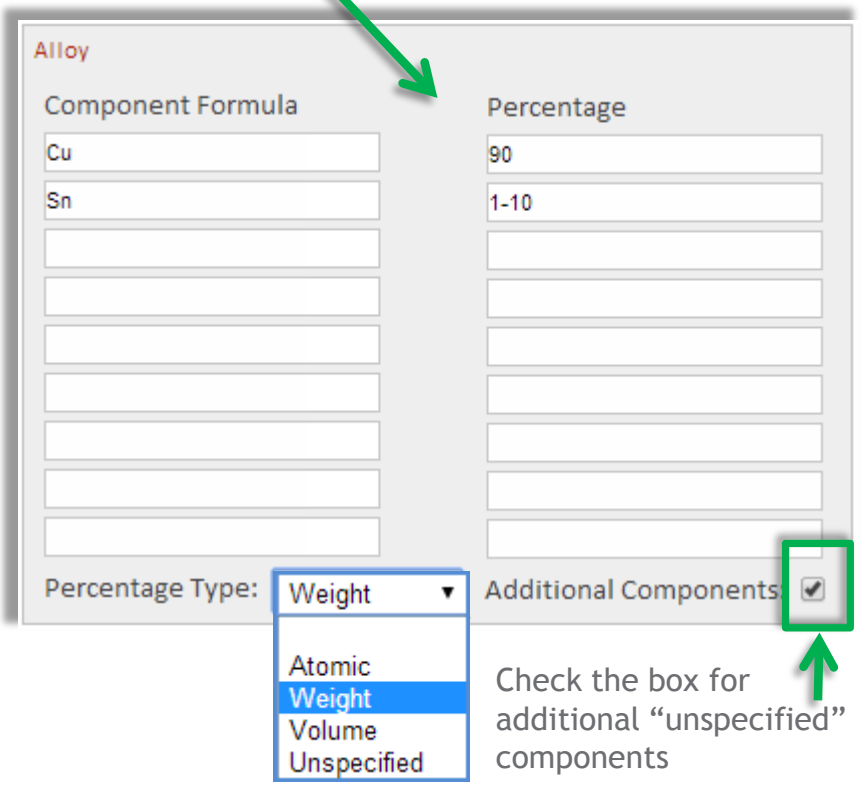
Click to display a structure search box on the page (if it isn't already displayed)



Clears all queries on the query page



Add numbers of unspecified elements.

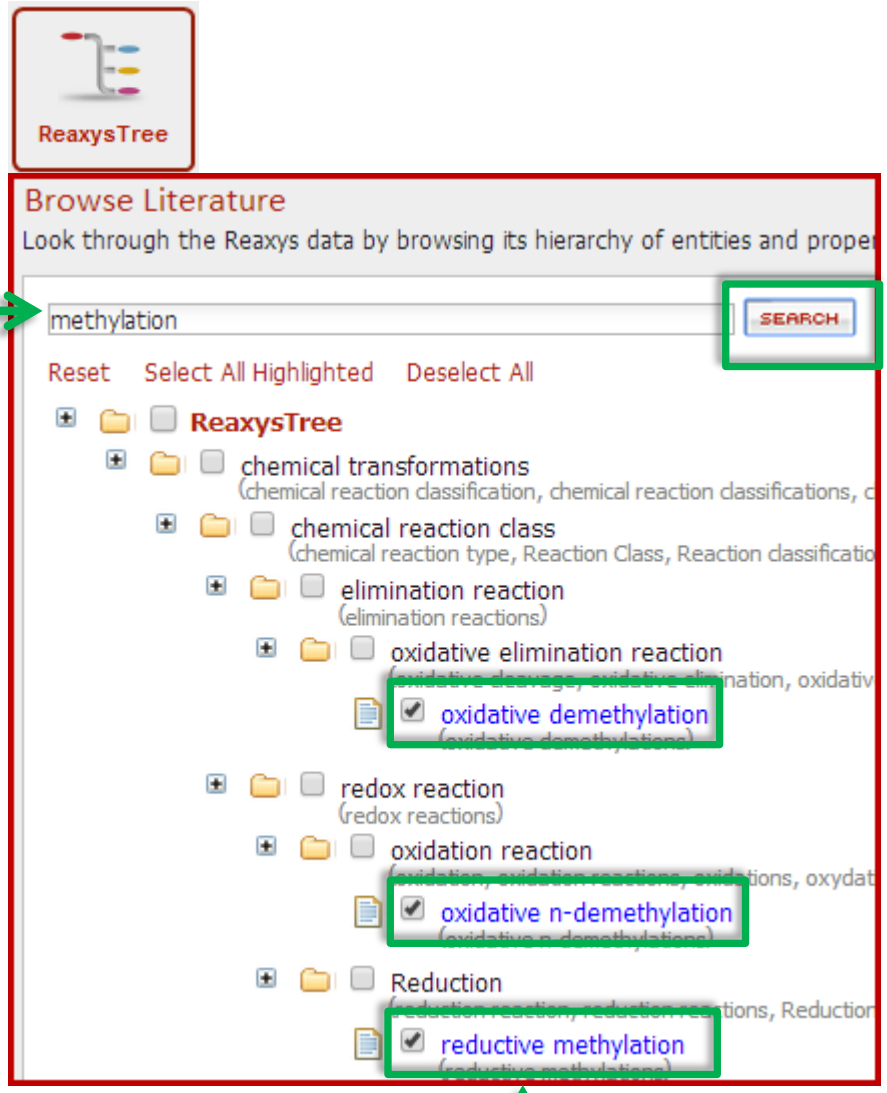


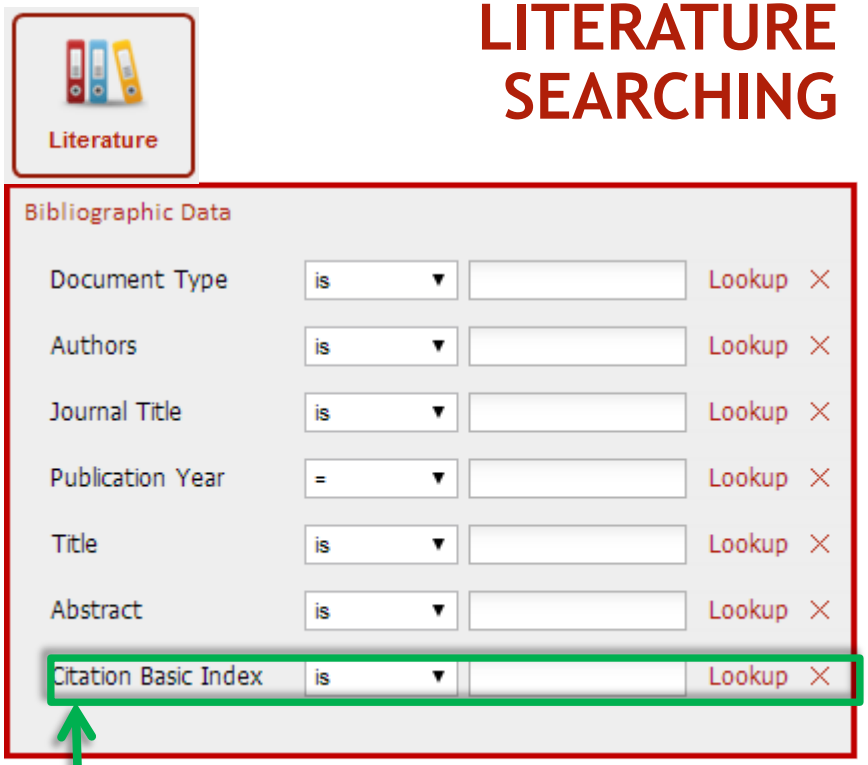
Check the box for additional "unspecified" components

Click an element and use the interactive boxes to add to the form using counts, charges, and ranges. Add groups from the periodic table, for example alkali metals.

Search for alloys, glasses, ceramics by typing in an element or formula. Select a percentage type from the dropdown menu.

LITERATURE SEARCHING





Use this field to do a text search over titles, abstracts, and keywords

Search for a term in the tree and click **Search**

Uncheck unwanted terms, then click **Search Literature**

RESULTS

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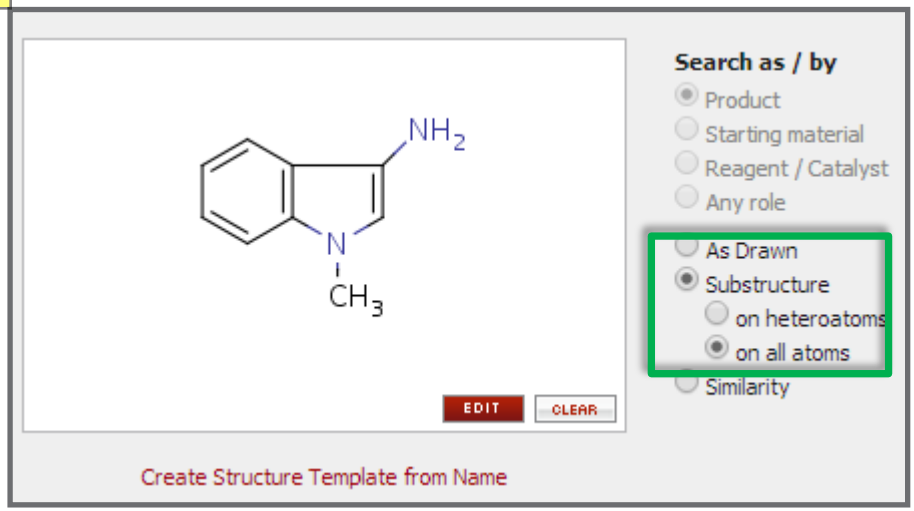
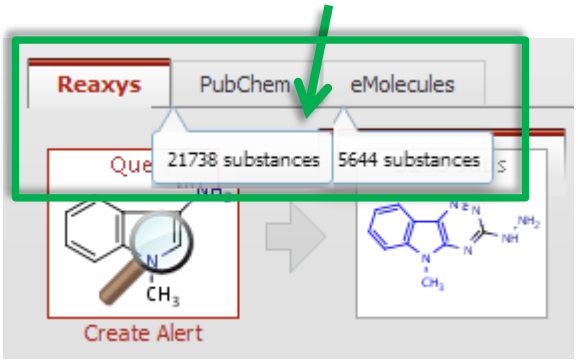


RESULTS FROM 3 DATABASES

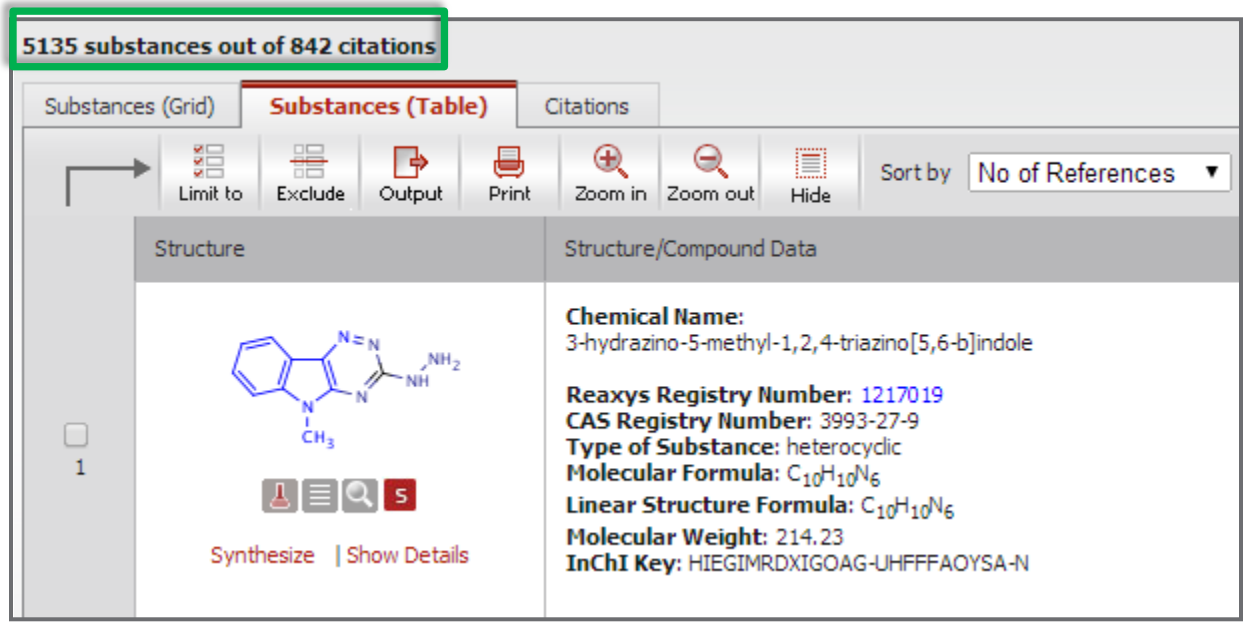
Query

Reaxys PubChem eMolecules

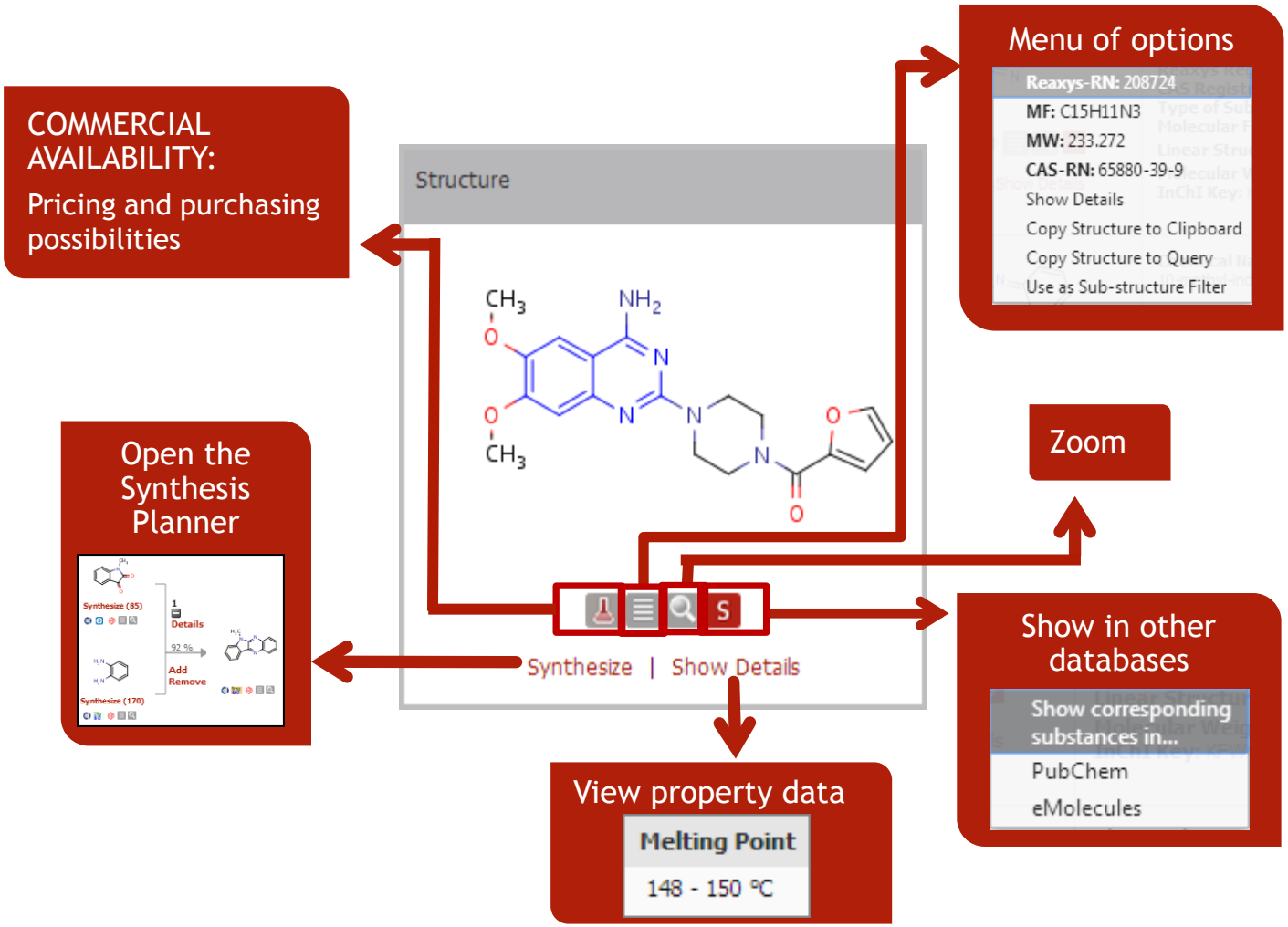
Mouse over the tabs to see the number of hits in each of the other databases



Results appear in the Reaxys database by default



SUBSTANCE ICONS



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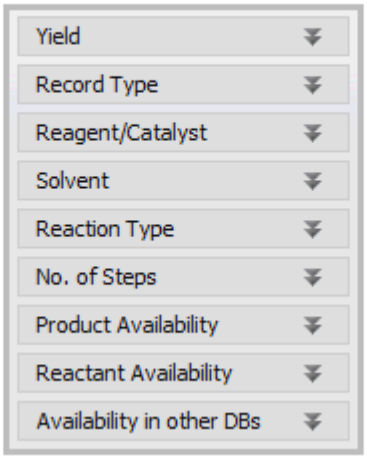
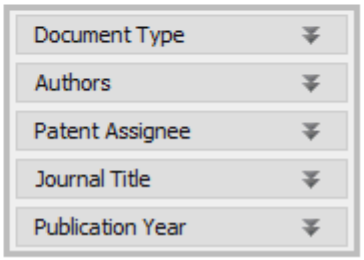
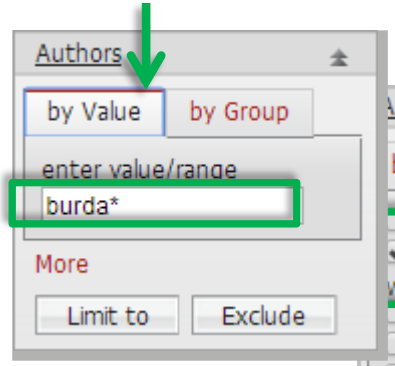
FILTERS

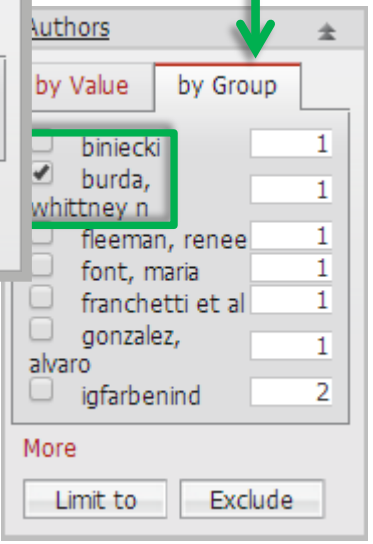
Available Filters

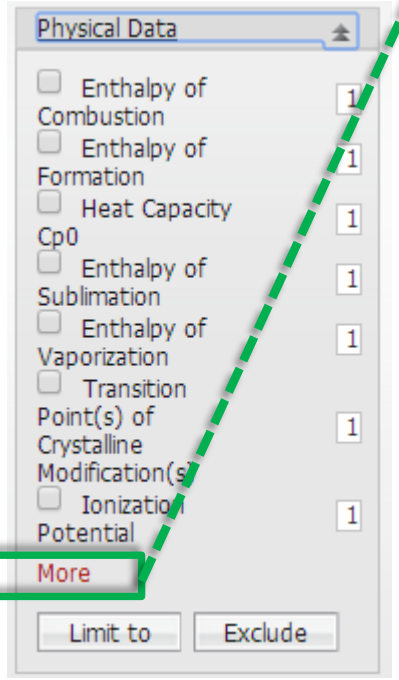




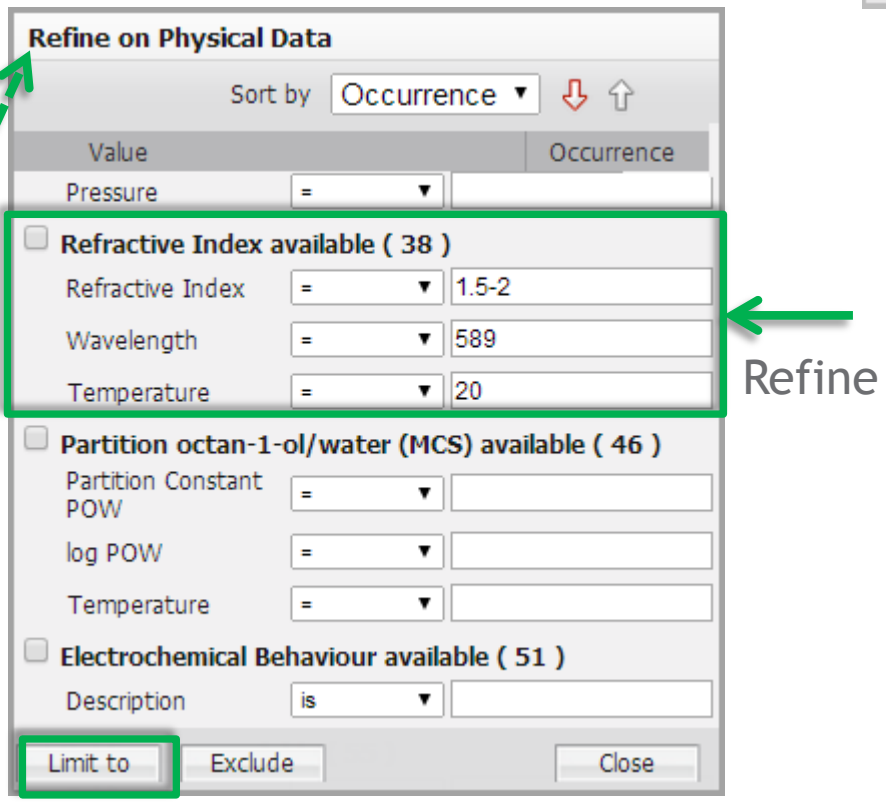


by Value or by Group





Open the full list



Refine

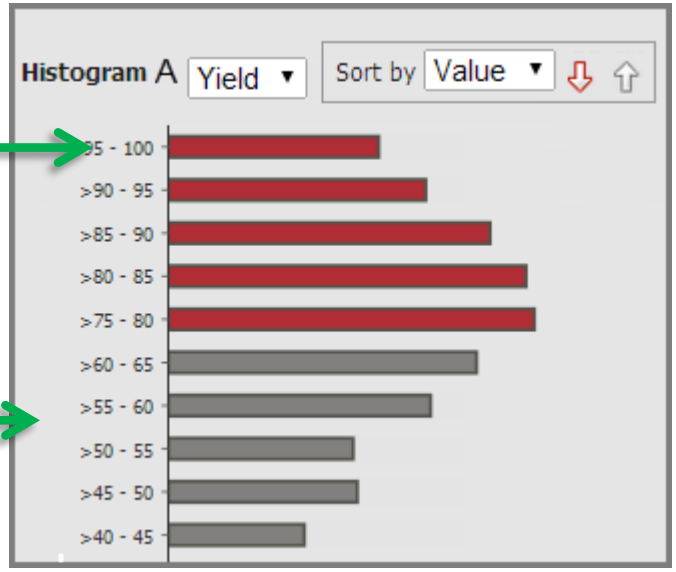
ANALYSIS VIEW

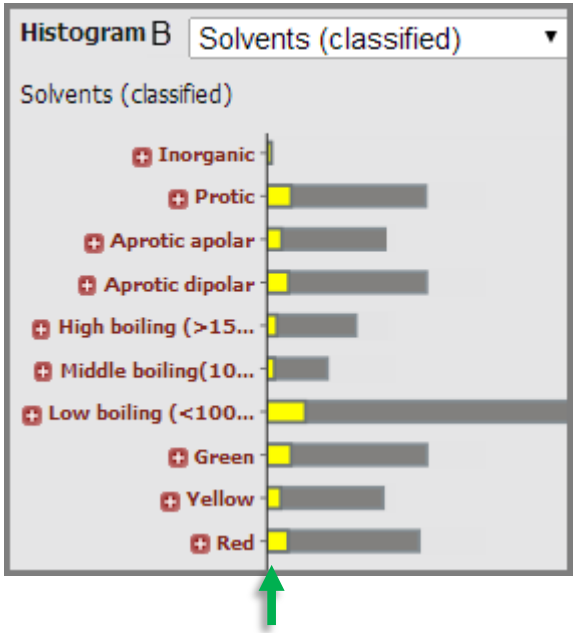
Analyze results by any of these categories using histograms to see how one category may relate to another.

Document Type	Catalysts (classified)	Compounds (classified)
Authors	Reactions (classified)	Boiling Point
Patent Assignee	Reagent/Catalyst	Density
Journal Title	Solvent	Melting Point
Publication Year	Solvents (classified)	Molecular Formula
	Yield	Molecular Weight
		Pharmacological Effects
		Physical Data
		Solubility
		Spectroscopic Data

The red bars correspond to your selections.

Grey bars give you an over-view of the items in your list.





Yellow bars show the numbers of hits per category in your result list that are a subset of the **Histogram A** list.

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SYNTHESIS PLANNER

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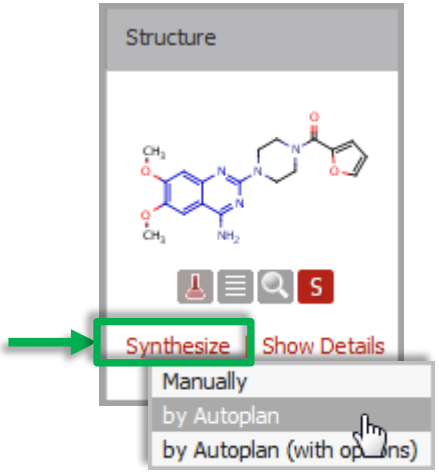
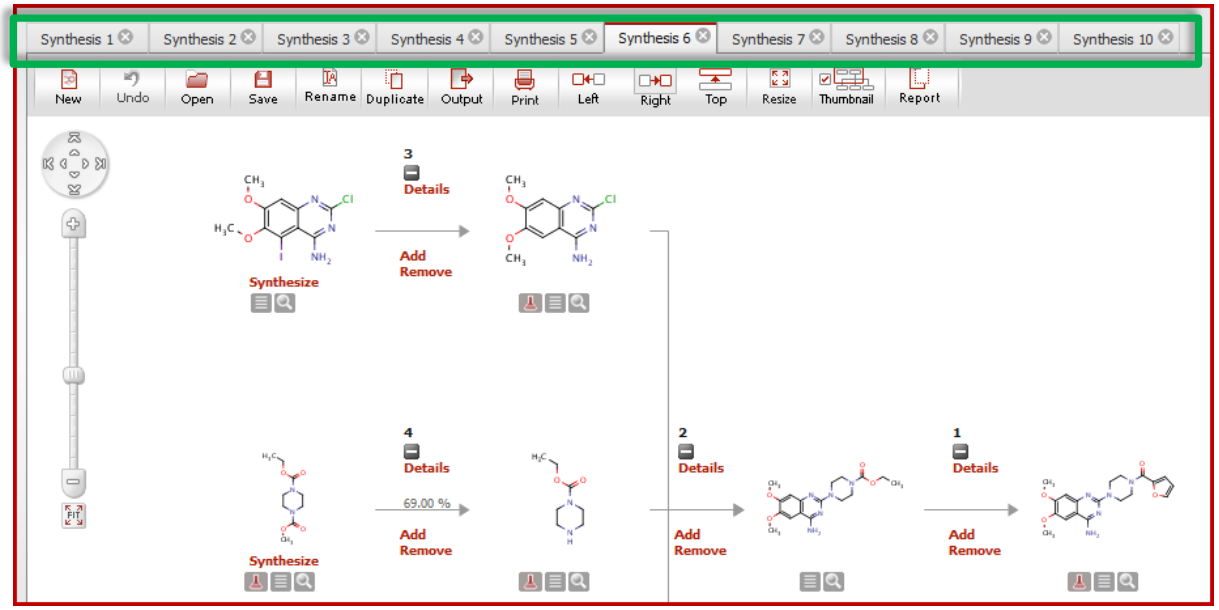
SYNTHESIS PLANNER



Click the **Synthesize** link below a structure. Then choose one of the 3 options.



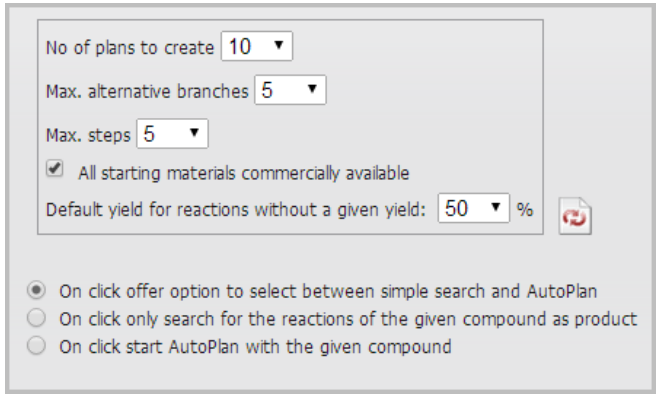
Manually – You pick the reactions and build a retrosynthetic pathway.

AutoPlan – Reaxys automatically generates up to 10 synthesis plans.

By AutoPlan (with options) – You select options upon clicking the Synthesize link.

My Settings

Preselect options from the **Settings** page



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Settings>Modify Application Settings>AutoPlan Options

PRINT, EXPORT, REPORT, AND SAVE

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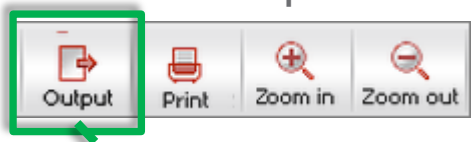
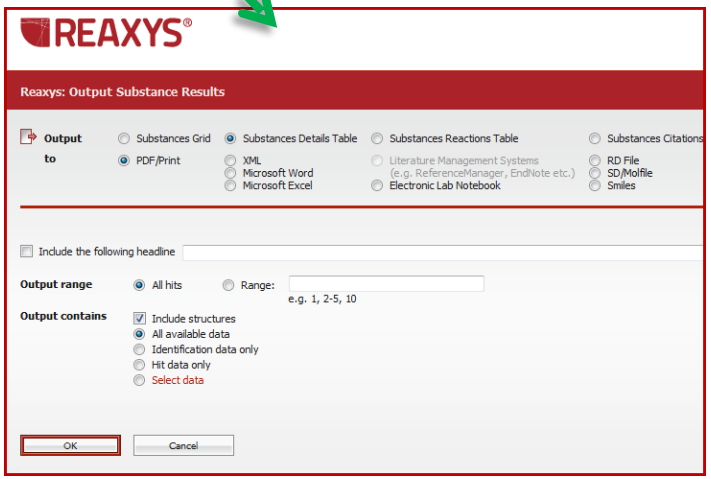
PRINT AND EXPORT

Export



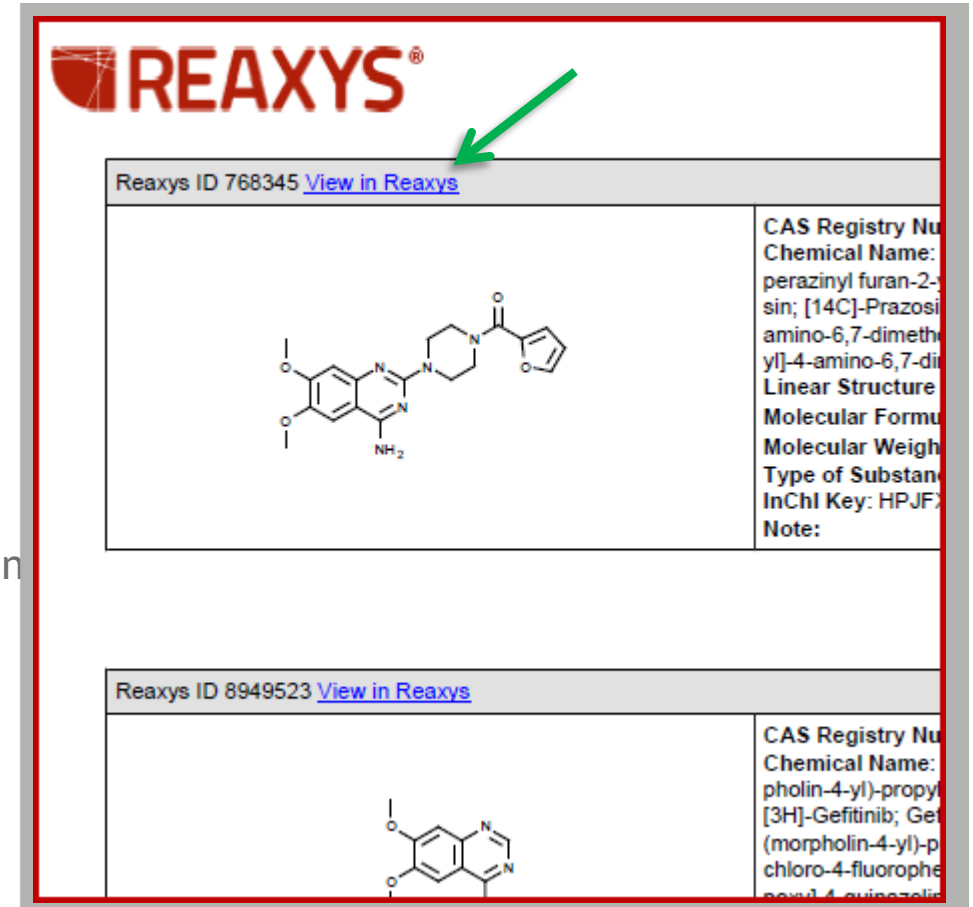
Select format, range, and output contents



Print

Print the page that is currently displayed

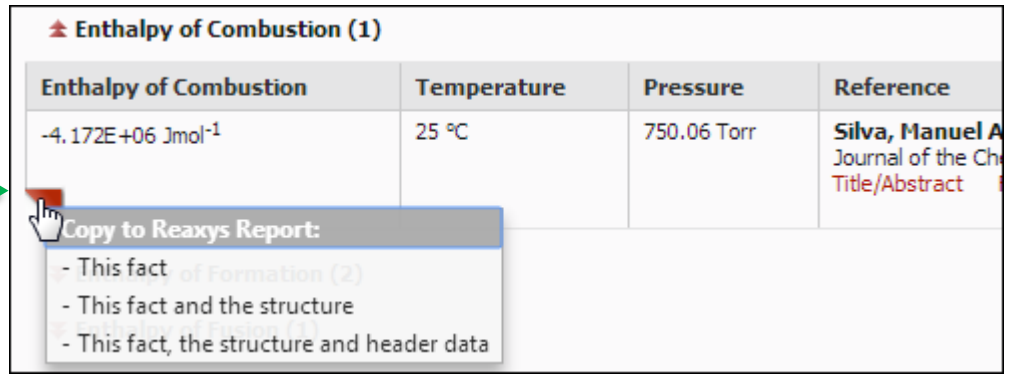
Exported documents contain the hyperlinked phrase **View in Reaxys.** Clicking the link will automatically open Reaxys and begin a search.



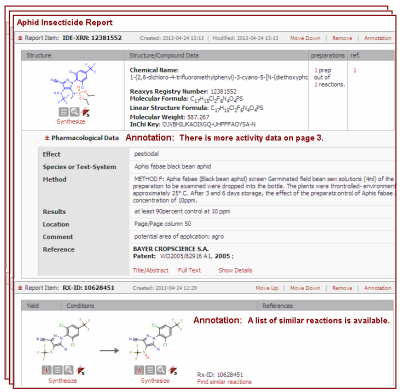
REPORT

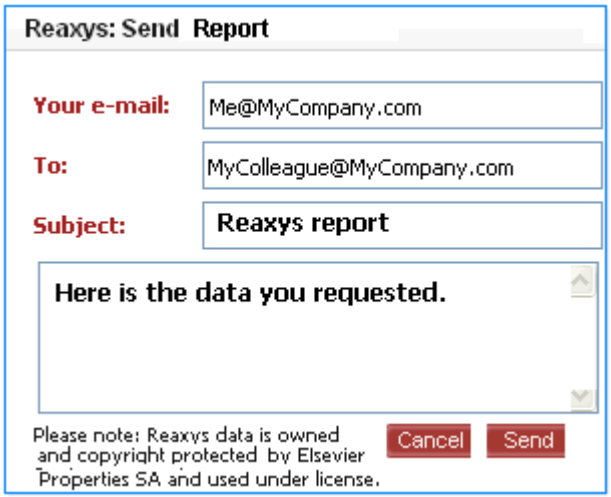
Mouse over details in any of the results screens (Structures, Reactions, Synthesis Planner, Citations, and Breadcrumbs).

Click the red page curl and select an option.



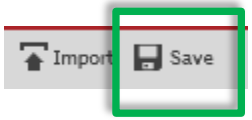
Click the **Report** button, annotate facts if needed, then click the **Send** button to share the report with colleagues





SAVE

Saved as xml on your computer:

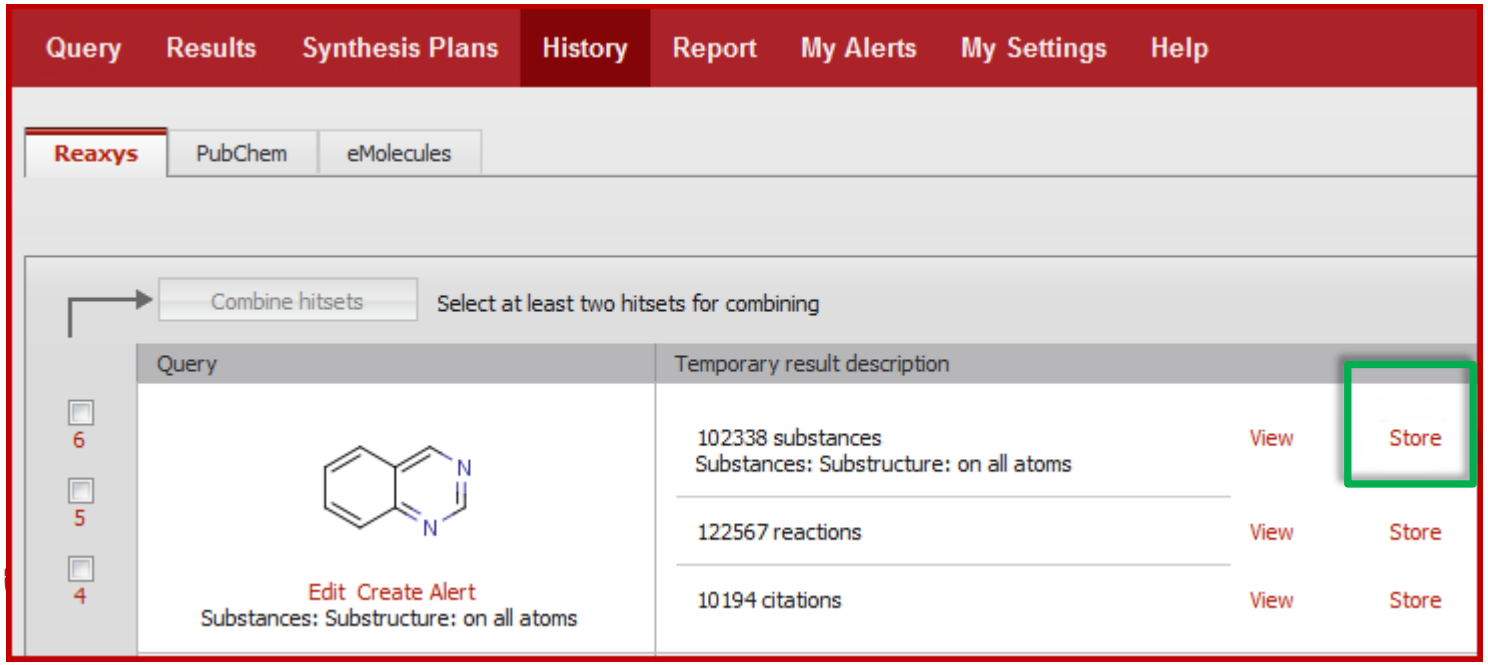


Query page

Synthesis Planner page

Reports page

Saved in Reaxys:

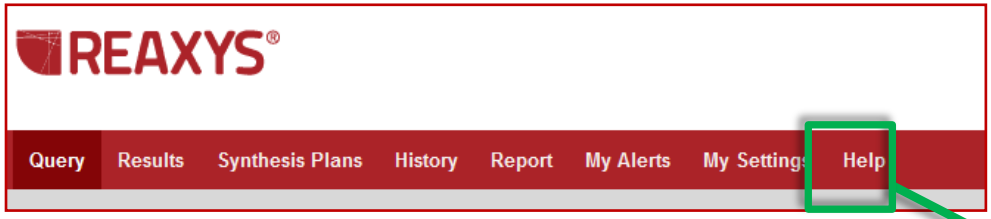


History page

SUPPORT AND PROFESSIONAL SERVICES

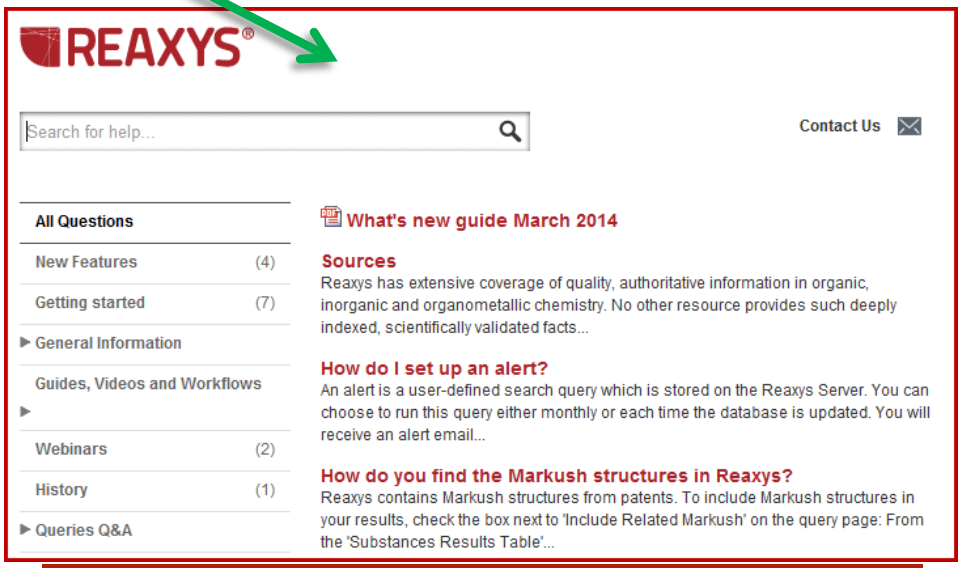
REAXYS®
HOW YOU THINK HOW YOU WORK

SUPPORT



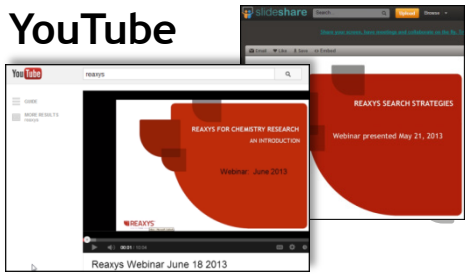
Training Materials

Click the Reaxys Help to find Q & A, Manuals, Workflows, Videos, PowerPoints, and more…..



Contact your Account Manager if you would like Webex or on-site training, or Click Here

More materials on **SlideShare** and **YouTube**



PROFESSIONAL SERVICES

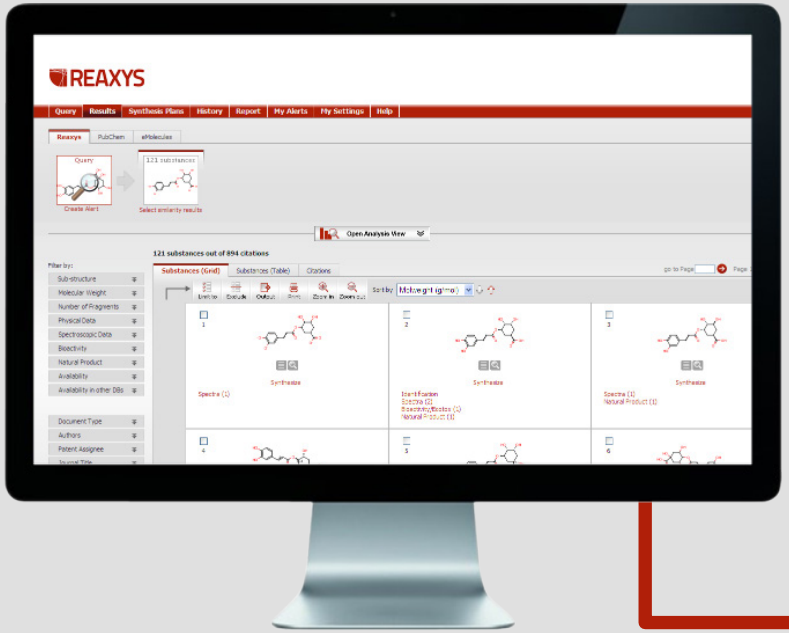
Our team works in close partnership with you to develop and deploy solutions that are customized to your specific information needs

Contact your Reaxys Account Manager or Click Here.

IN-HOUSE DATA:
Seamless integration for maximized search efficiency

PUBCHEM:
Includes biochem. & pharmaco information

COMMERCIAL AVAILABILITY:
Data and purchasing possibilities



REAXYS APIs:
Combine the quality data you get from Reaxys with in-house creativity to build new solutions tailor-made for your specific research interests

ELECTRONIC LAB NOTEBOOKS:
Improve collaboration, minimize errors, save time

REAXYS STRUCTURE FLAT FILE:
Incorporate information into data mining and internal search systems

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THANK YOU

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