# REAXYS

# **GETTING STARTED**

July 15, 2014



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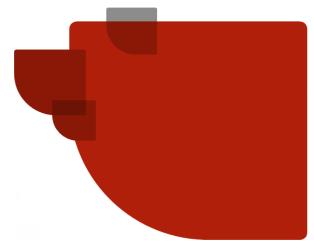
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# WELCOME TO REAXYS !

# YOU ARE SEARCHING MORE THAN:

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





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- <u>SUPPORT</u>
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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

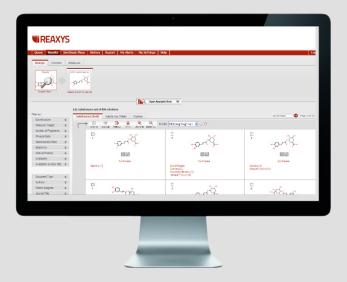
Data for those substances and reactions extracted and indexed into over 400 searchable fields

# eMolecules

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

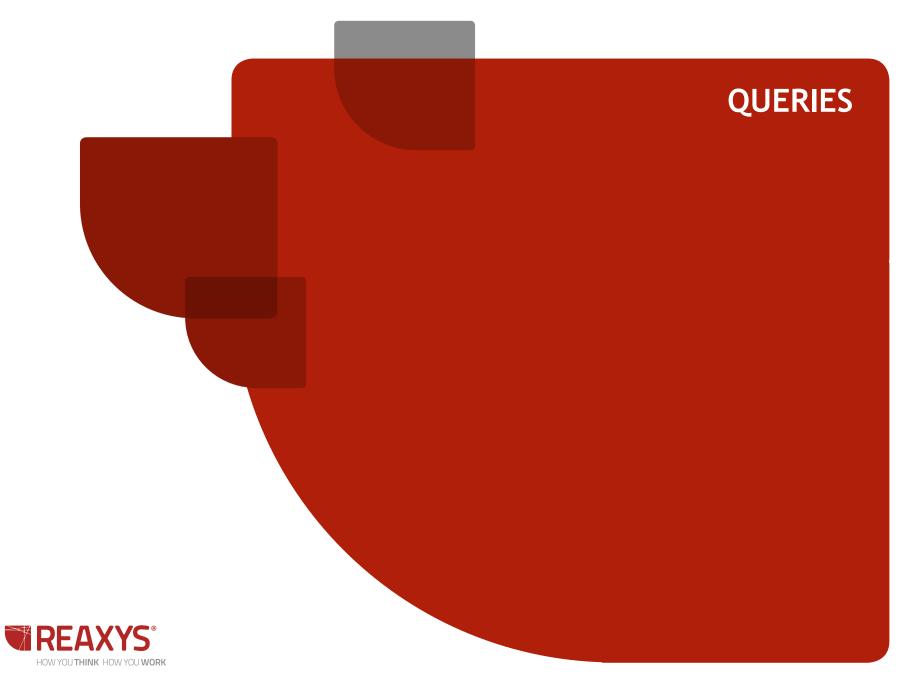
PubChem

Substances with links to additional data



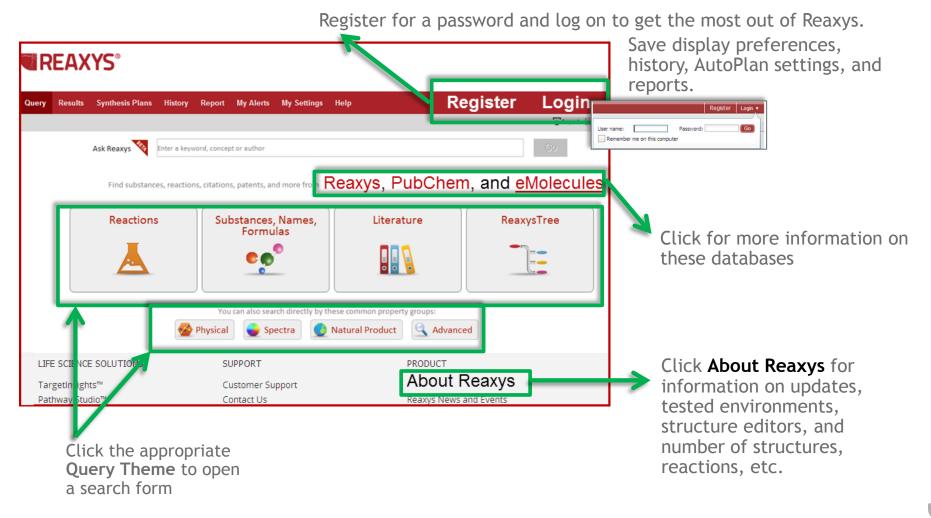


Additional content from books, conference proceedings, editorials, reviews, business articles. (>16,000 periodicals)





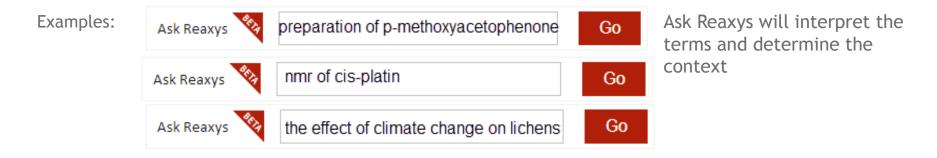
# THE START PAGE



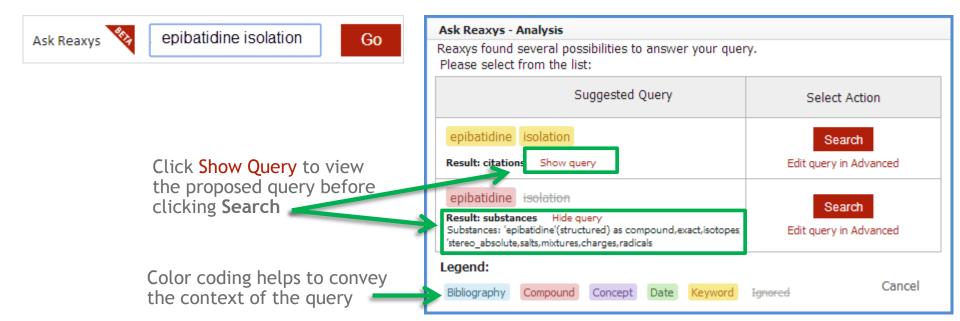


# **ASK REAXYS**

Type in a word or phrase and click "Go".

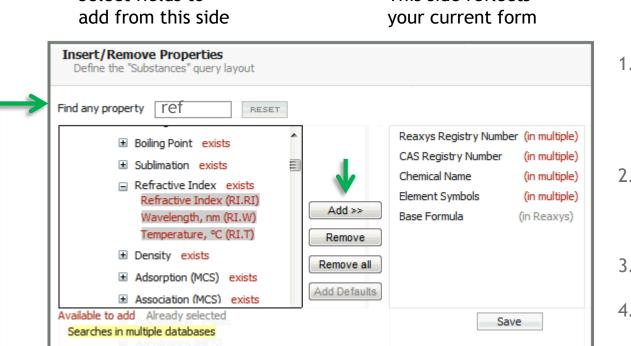


If more than one context is possible, Reaxys will present you with some choices



Substances		Reactions	SEARCH	FORMS	Literature	
tructure	As drawn     Include tautomers	Structure			Document Type	is 💌
	As drawn     Include rationers     Substructure     on heteroatoms     No isotopes		<ul> <li>As drawn</li> <li>Substructure</li> </ul>	Include tautomers Ignore stereo	Authors	is 💌
selected query editor:           Marvin Sketch           by chemAxon	on all atoms     No charges     Similarity     No radicals	selected query	O on beternatom	ns 🔲 No salts	Common Patent Number	is 💌
by o chemoton	No ring closures	Man	vinSketch Similarity	No mixtures	Patent Country Code	is
PASTE STRUCTURE EDITOR	Align results with que     Keep fragments     separate      toget	ry -		No charges	Journal Title	is 💌
Create Structure Template from Name	C oppinitio ( logo			No ring closures Align results with query	Publication Year	-
lease select role   Product  Starting material	Reagent / Catalyst	PASTE	STRUCTURE EDITOR	More options	DOI	is 💌
leaction Data			emplate from Name		Title	is 💌
Yield (numerical) = Solvent is		Identification			Abstract	is v
Reagent/Catalyst is		CAS Regis Chemical N	vame contains		Keywords	is V
Time (h) =		Molecular I			Citation Basic Index	15
Temperature (°C) = Pressure (Torr) =		Molecular	Weight =			
Reaction Type is Reaction Basic Index is	•	Show AND Buttons				
					Natural Product	- exists
Physical		Spe	ectra		Isolation from Natural Product	is 💌
Melting Point (°C)	=	NMR Sp	ectroscopy 🗌 exists		<b>-</b> ]	
Boiling Point (°C)	=	Nucleus	is		-	
Refractive Index	=	IR Spec	troscopy		ReaxysTree	
Density	exists	Descript				
Dissociation Exponent	exists	Mass Sp Descript	tion is		Find any term	SEARCH
Dynamic Viscosity (P)	=		Spectroscopy		Reset Select All Highlighted	Deselect All
		Descript				nsformations ion classification, chemical reaction classifications, ch
Optical Rotatory Power (deg)	=		ectroscopy			ion classification, chemical reaction classifications, ch mical analysis methods /sis, chemical analysis method, determination metho
log POW 5	=	Descript			Description: De	rsis, chemical analysis method, determination methor mical properties ical magnitude, physico chemical magnitudes, physi emical calculation methods mical calculation method, Quantum chemical calculat

# **CUSTOMIZE A SEARCH FORM**



This side reflects

Add/Remove Fields...

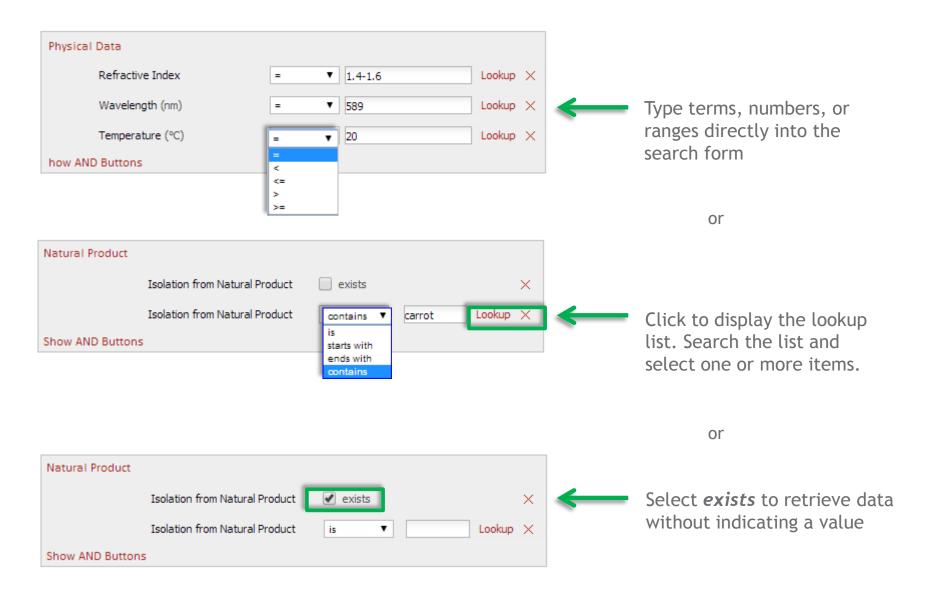
- Add fields to your query page by clicking the Add/Remove Fields hyperlink.
- 2. Select fields from the list on the left side of the window that appears
- 3. Click Add
- 4. Click Save

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



Select fields to

# ADD DATA TO A SEARCH FORM

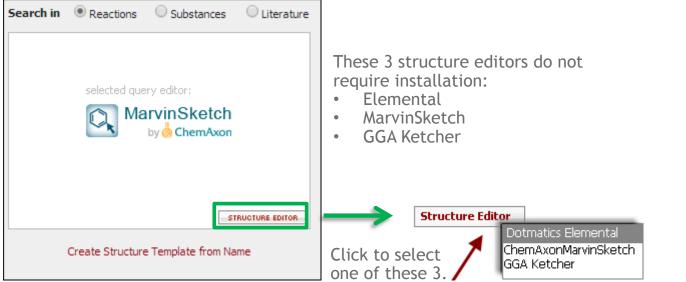




My Alerts

Report

# **STRUCTURE EDITORS**



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

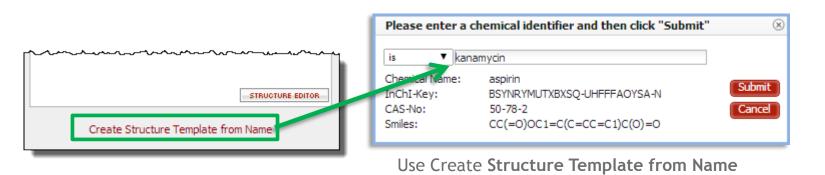
Editors that do not require a plugin to be installed:	The following editors can only be used, if the Reaxys Structure Editor PlugIn is installed:
<ul> <li>Dotmatics Elemental</li> <li>ChemAxon MarvinSketch (Note: requires Java to be installed)</li> <li>GGA Ketcher</li> </ul>	<ul> <li>Crossfire Structure Editor</li> <li>Accelrys Draw</li> <li>Accelrys ISIS/Draw</li> </ul>
Reaxys uses Dotmatic's Elemental as default structure and reaction query editor, if no other editor is selected	<ul> <li>CambridgeSoft ChemDraw</li> <li>ICEdit</li> </ul>
	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.



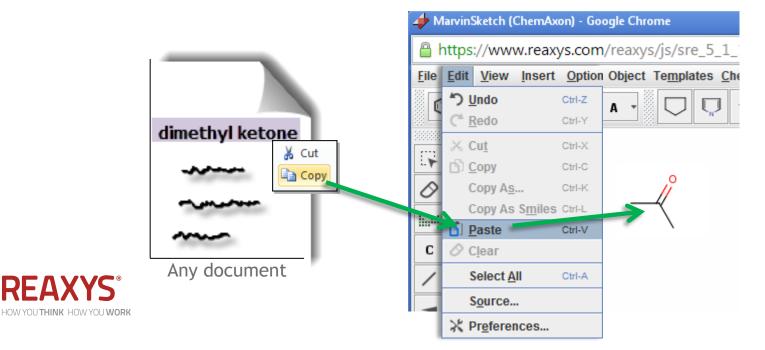
REA

# **OBTAIN A STRUCTURE WITHOUT DRAWING**

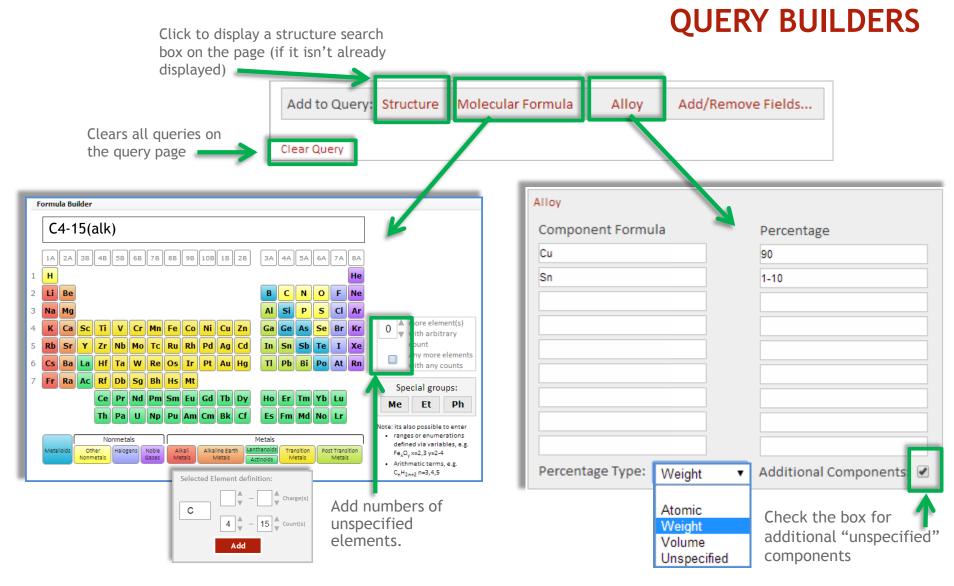
12



Copy/past a chemical name into the MarvinSketch structure editor

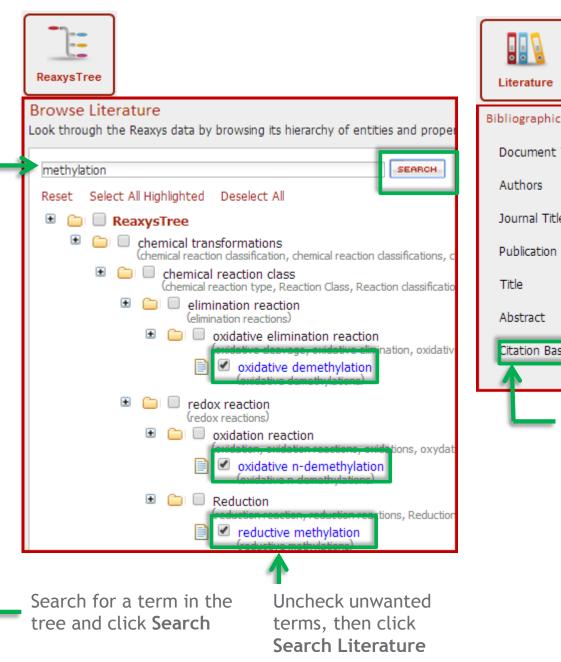






Click an element and use the interactive boxes to add to the form using counts, charges, and ranges. Add groups from the periodic table, for example alkali metals.

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



# LITERATURE SEARCHING

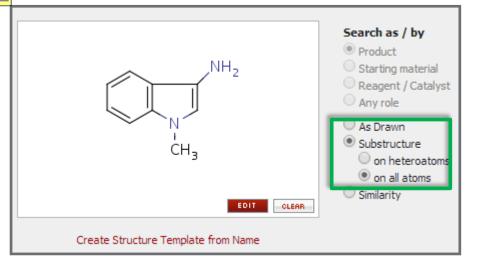
libliographic Data		
Document Type	is 🔻	Lookup $ imes$
Authors	is v	Lookup $ imes$
Journal Title	is v	Lookup $ imes$
Publication Year	= •	Lookup $ imes$
Title	is v	Lookup $ imes$
Abstract	is 🔻	Lookup $ imes$
Citation Basic Index	is 🔻	Lookup $ imes$
1		

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

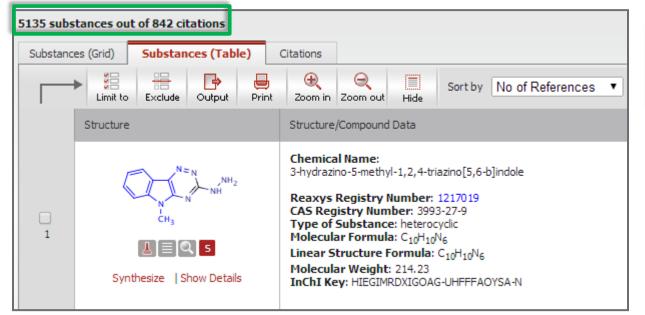


HOW YOU THINK HOW YOU WORK

15



### Results appear in the Reaxys database by default

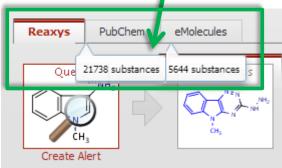


# **RESULTS FROM 3 DATABASES**

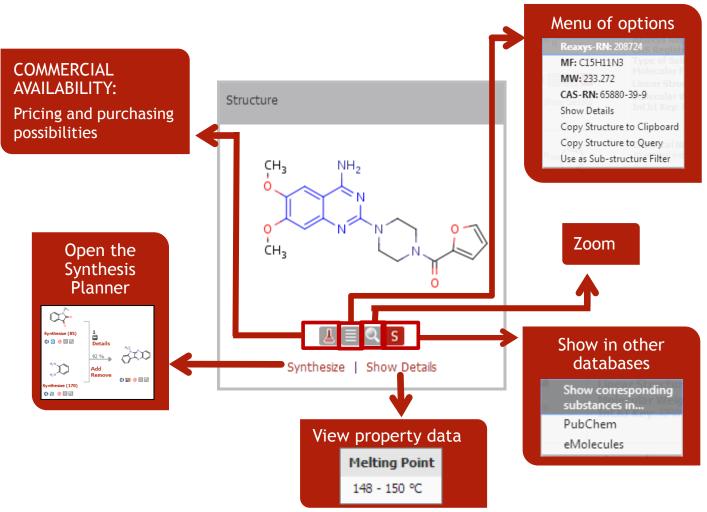
Query

### Reaxys PubChem eMolecules

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



# **SUBSTANCE ICONS**





Filter by:		Available Filte	rc	FILTERS	Authors	\$	
Sub-structure	¥		1.5		by Value by	Group	Authors 🔶 🖈
Molecular Weight	¥	Yield	¥		enter value/rand	e	by Value by Group
Number of Fragments	s ¥	Record Type	¥		burda*		biniecki 1
Physical Data	¥	Reagent/Catalyst	¥		More		🕑 burda, 👘 👔
Spectroscopic Data	¥	Solvent	¥		Limit to	Exclude	whittney n fleeman, renee 1
Bioactivity	¥	Reaction Type	¥	Document Type 🛛 🐺			font, maria <u>1</u>
Ecological Data	¥	No. of Steps	¥	Authors ¥	by Val		gonzalez,
Natural Product	¥	Product Availability	¥	Patent Assignee 🛛 🐺	by Gro	bup	alvaro
Availability	¥	Reactant Availability	Ŧ	Journal Title 🛛 🔻			igfarbenind 2
Availability in other D	Bs ∓	Availability in other DBs	¥	Publication Year 🛛 🐺			More
							Limit to Exclude
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Open the full list 🔶	Potentia More			ctrochemical Behaviour available scription is	( 51 ) Close		18

18



categories ι	ults by any of Ising histogran Legory may rel	Compounds (classified) Boiling Point Density Melting Point	1	
to another.	Document Type Authors Patent Assignee Journal Title Publication Year	Catalysts (classified) Reactions (classified) Reagent/Catalyst Solvent Solvents (classified) Yield	Molecular Formula Molecular Weight Pharmacological Effects Physical Data Solubility Spectroscopic Data	

# **ANALYSIS VIEW**





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

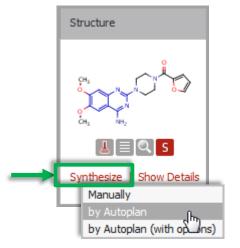


# SYNTHESIS PLANNER





# SYNTHESIS PLANNER

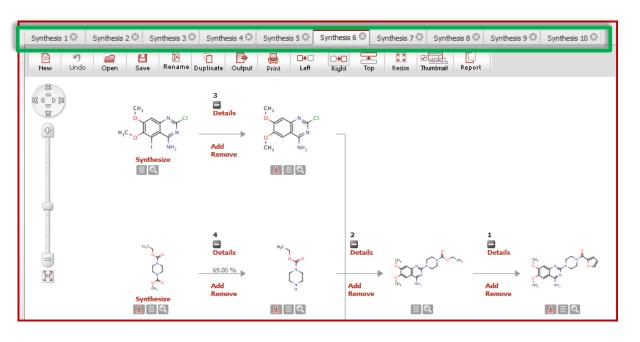


Click the <u>Synthesize</u> link below a structure. Then choose one of the 3 options.



**AutoPlan** - Reaxys automatically generates up to 10 synthesis plans.

**By AutoPlan (with options)** - You select options upon clicking the <u>Synthesize</u> link.



My Settings	No of plans to create 10  Max. alternative branches 5
Preselect options	Max. steps 5 ▼ ✓ All starting materials commercially available Default yield for reactions without a given yield: 50 ▼ %
from the <b>Settings</b> page	<ul> <li>On click offer option to select between simple search and AutoPlan</li> <li>On click only search for the reactions of the given compound as product</li> <li>On click start AutoPlan with the given compound</li> </ul>



Settings>Modify Application Settings>AutoPlan Options<sup>21</sup>

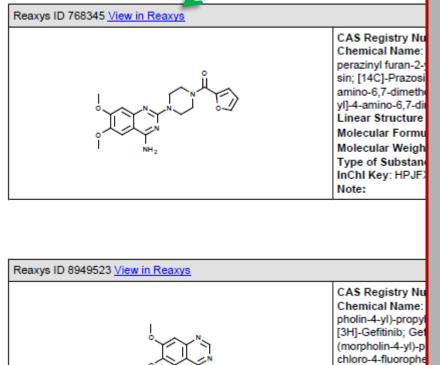
# PRINT, EXPORT, REPORT, AND SAVE





### **Export PRINT AND EXPORT** 9 ۲ $\Rightarrow$ Output Print Zoom in Zoom out Print Print the Select format, page that is range, and output currently 7 contents displayed Output Print Zoom in Zoom out Reavys: Output Substance Results - Output Substances Details Table 💿 Substances Reactions Table Substances Citations Substances Grid ۲ XML Microsoft Word Literature Management Systems (e.g. ReferenceManager, EndNote etc.) RD File SD/Molfile PDF/Print REAXYS Microsoft Excel Electronic Lab Notebook Smiles Include the following headline Output range All hits Range: e.g. 1, 2-5, 10 Reaxys ID 768345 View in Reaxys Output contains Include structures All available data Identification data only CAS Registry Nu Hit data only Select data Chemical Name: perazinyl furan-2sin; [14C]-Prazosi Cancel amino-6,7-dimeth yl]-4-amino-6,7-di Linear Structure

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



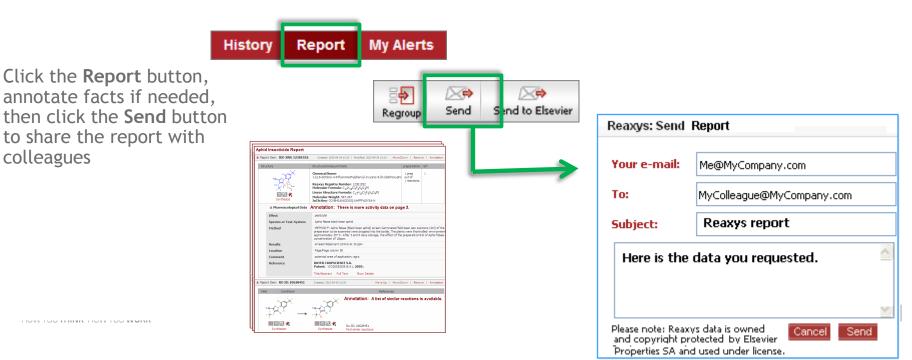


# REPORT

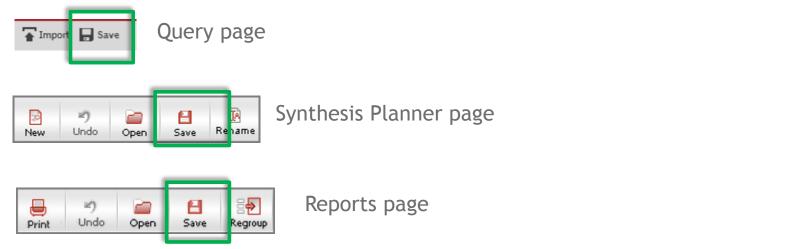
Mouse over details in any of the results screens (Structures, Reactions, Synthesis Planner, Citations, and Breadcrumbs).

Click the red page curl and select an option.

Enthalpy of Combustion (	(1)		
Enthalpy of Combustion	Temperature	Pressure	Reference
-4.172E+06 Jmol <sup>-1</sup>	25 °C	750.06 Torr	Silva, Manuel A Journal of the Ch Title/Abstract
Copy to Reaxys Report: - This fact - This fact and the structure - This fact, the structure and			



### Saved as xml on your computer:



## Saved in Reaxys:

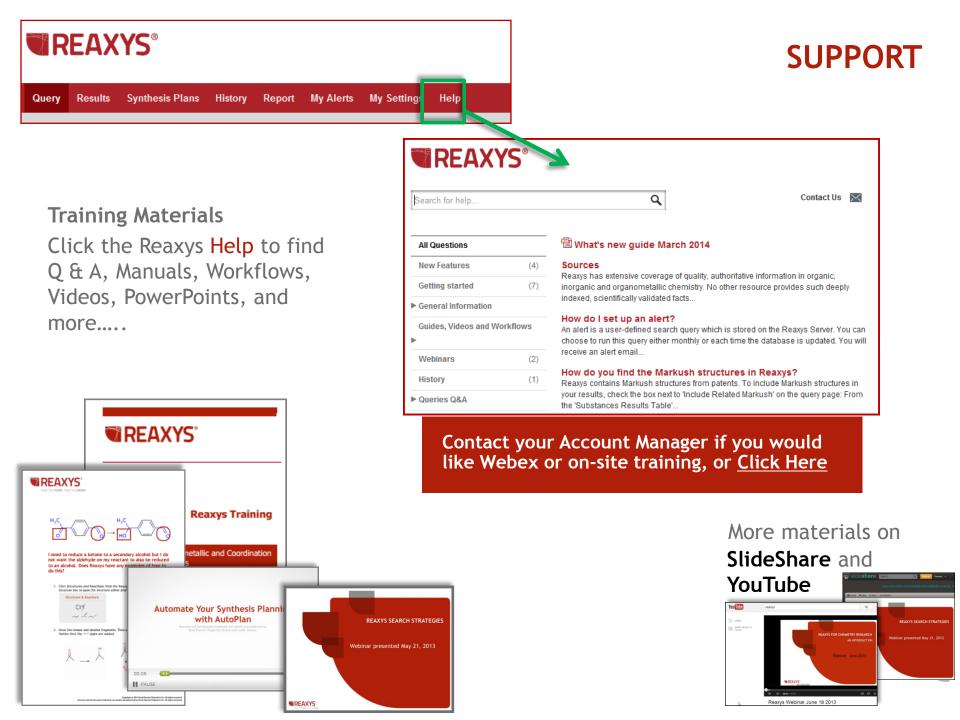
Query	Results Synthesis Plans Histo	ory Report My Alerts My Settings H	lelp		History pag
Reaxys	PubChem eMolecules				
	Combine hitsets Select at least tv	o hitsets for combining			
1	Query	Temporary result description			
6		102338 substances Substances: Substructure: on all atoms	View	Store	
5		122567 reactions	View	Store	
<b>1</b>	Edit Create Alert Substances: Substructure: on all atoms	10194 citations	View	Store	

25

**SAVE** 

# SUPPORT AND PROFESSIONAL SERVICES



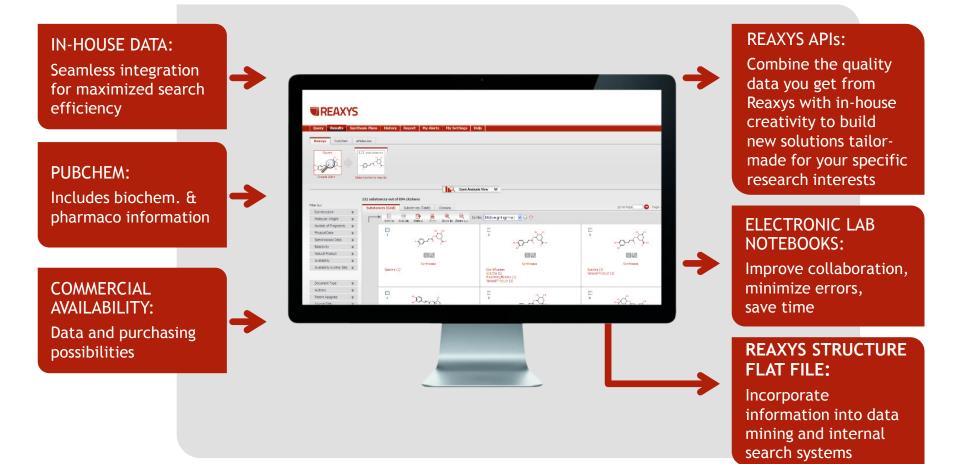




# **PROFESSIONAL SERVICES**

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**.









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