Reaxys Quick Reference Guide

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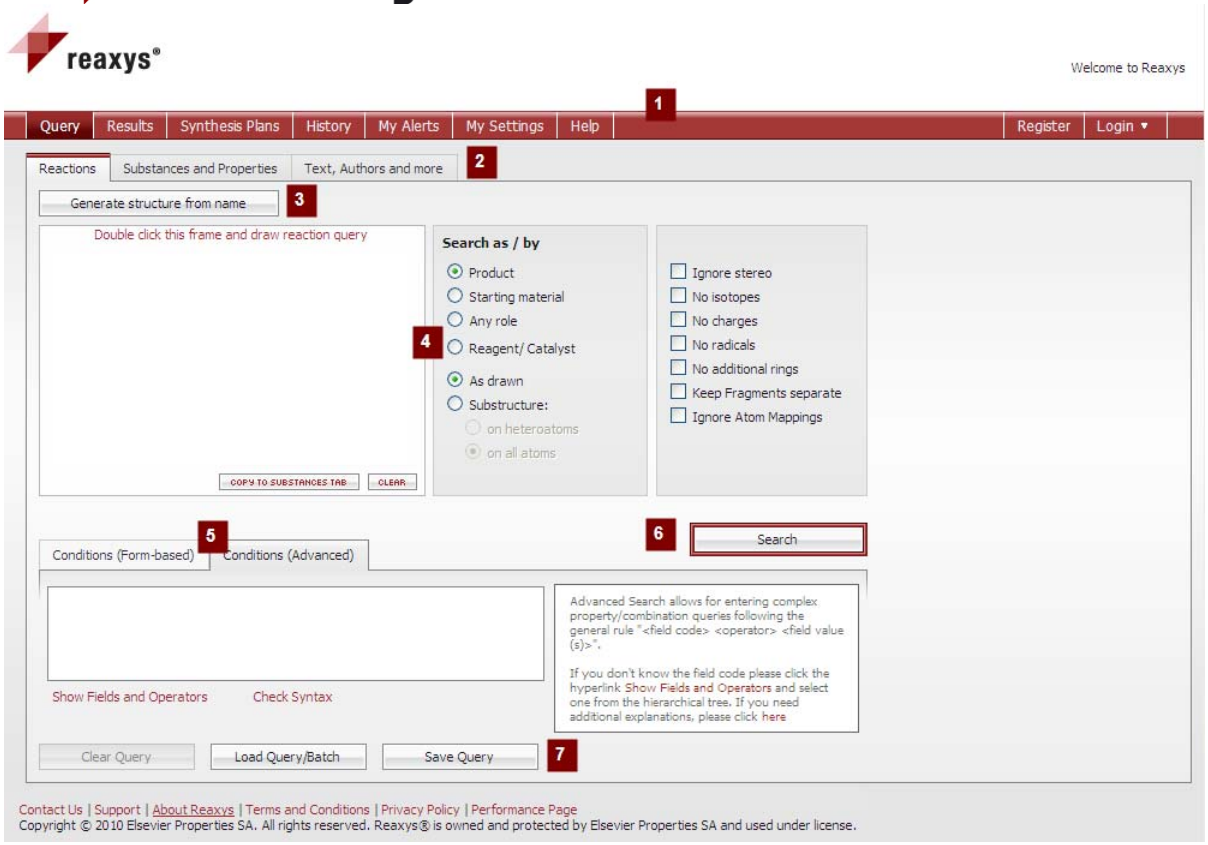
Homepage



How to find the preparation of a compound?

1. *Ensure the reaction tab is selected and double click the drawing pane*
2. *Draw the desired compound structure in your preferred editor and click "Transfer Query"*
3. *Click the search button and browse the result.*

Note: an Auto-Search algorithm starts if an "As Drawn" search has no hits; Reaxys performs a "substructure on heteroatoms" search, and then a "substructure on all atoms" (if no hits are found). When a structure/reaction query is combined with a factual query, this feature is turned off.

1 Main Navigation:
The following screens are available
- Query
- Results
- Synthesis Plans
- History
- My Alerts
- My Settings
- Help & Register, Login

2 Query tabs
- Reactions
- Substances and properties
- Text, authors and more

3 Generate structure from name
A chemical name will be translated into a structure.

4 Structure/reaction window
Window to add a structure or reaction with additional search possibilities.

5 Add Reaction/Bibliographic data
The *Conditions (Form-based)* and *Conditions (Advanced)* links allow entering further reaction or bibliographic data constraints.

6 Search button
Launch a search.

7 Command buttons
Clear, load or save a query. The Load feature also supports batch querying.

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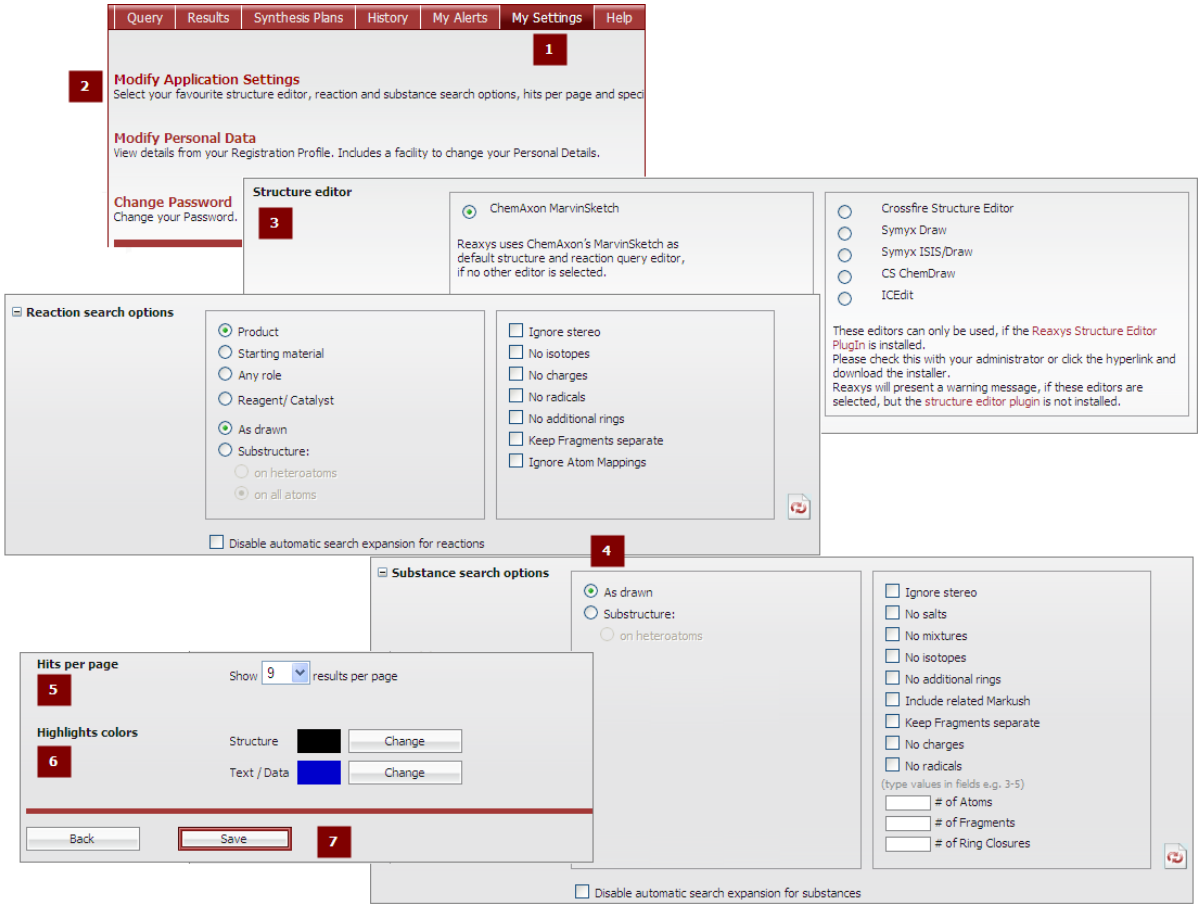
Generate a structure from name



Note: the default search settings can be changed through the My Settings menu. Click the **Save** *button and a confirmation that your settings have been updated is displayed. The new settings will be effective from the next time you login.*

1 My Settings
Select this tab to
- Modify application settings
- Modify personal data
- Change password

2 Modify Application Settings
Select this item to specify your preferred Structure editor, Reaction & Substance default search options, # of hits per page and Highlights colors.

3 Structure editor
Choose your preferred editor. Find information on download of the plugin required for the use of external structure editors.

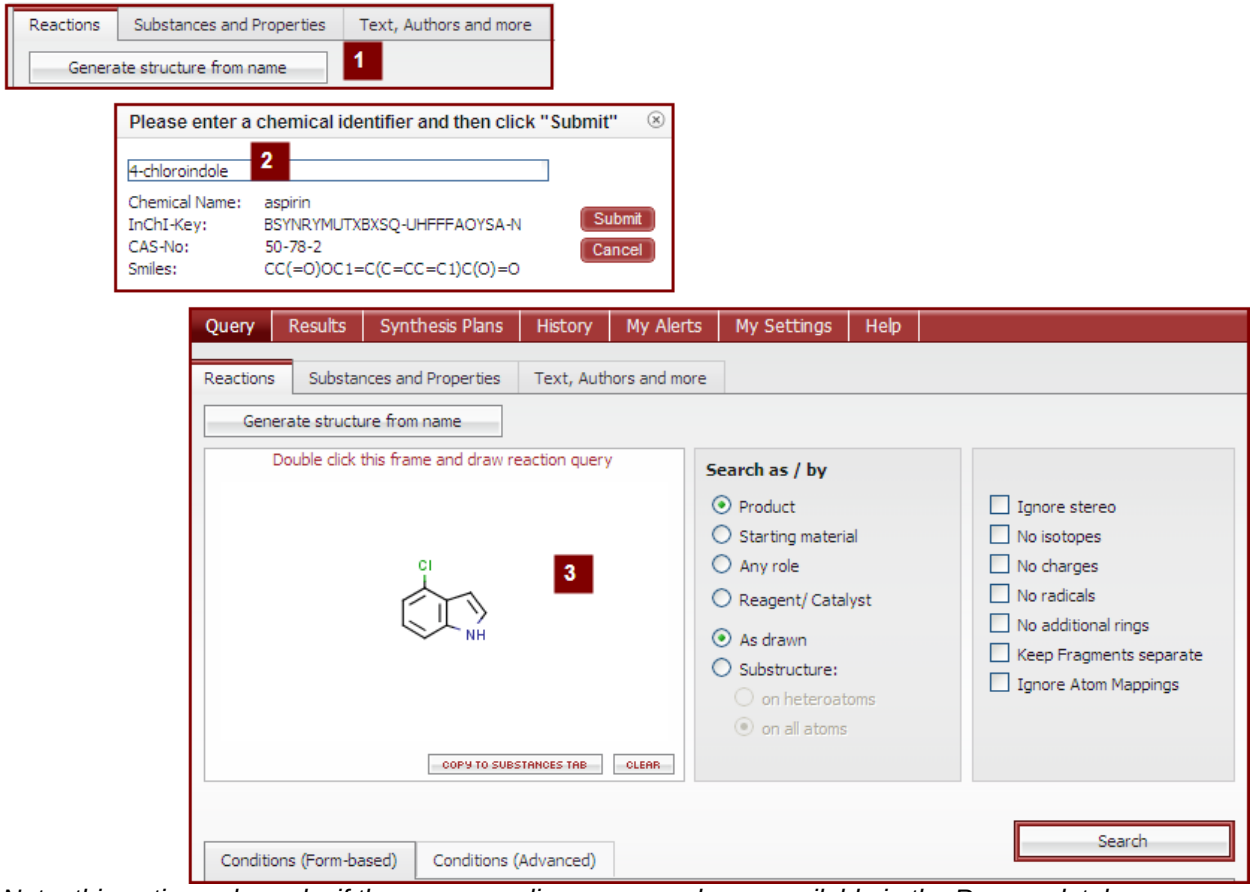
4 Reaction/Substance search options
Define the default search options for reactions and/or substances query. The circular arrows reset the options. The checkbox (bottom) disables auto searching when no hits are found.

5 Hits per page
Select preferred number of displayed hits on the Results menu.

6 Highlights colors
Select preferred colors to highlight the searched structure and/or text/data.

7 Back & Save buttons
Confirm new settings with **Save** or use **Back** to return to the item list.

Generate a structure from name



Note: this option only works if the corresponding compounds are available in the Reaxys database.

Available on the Reactions and Substances & Properties query tabs.

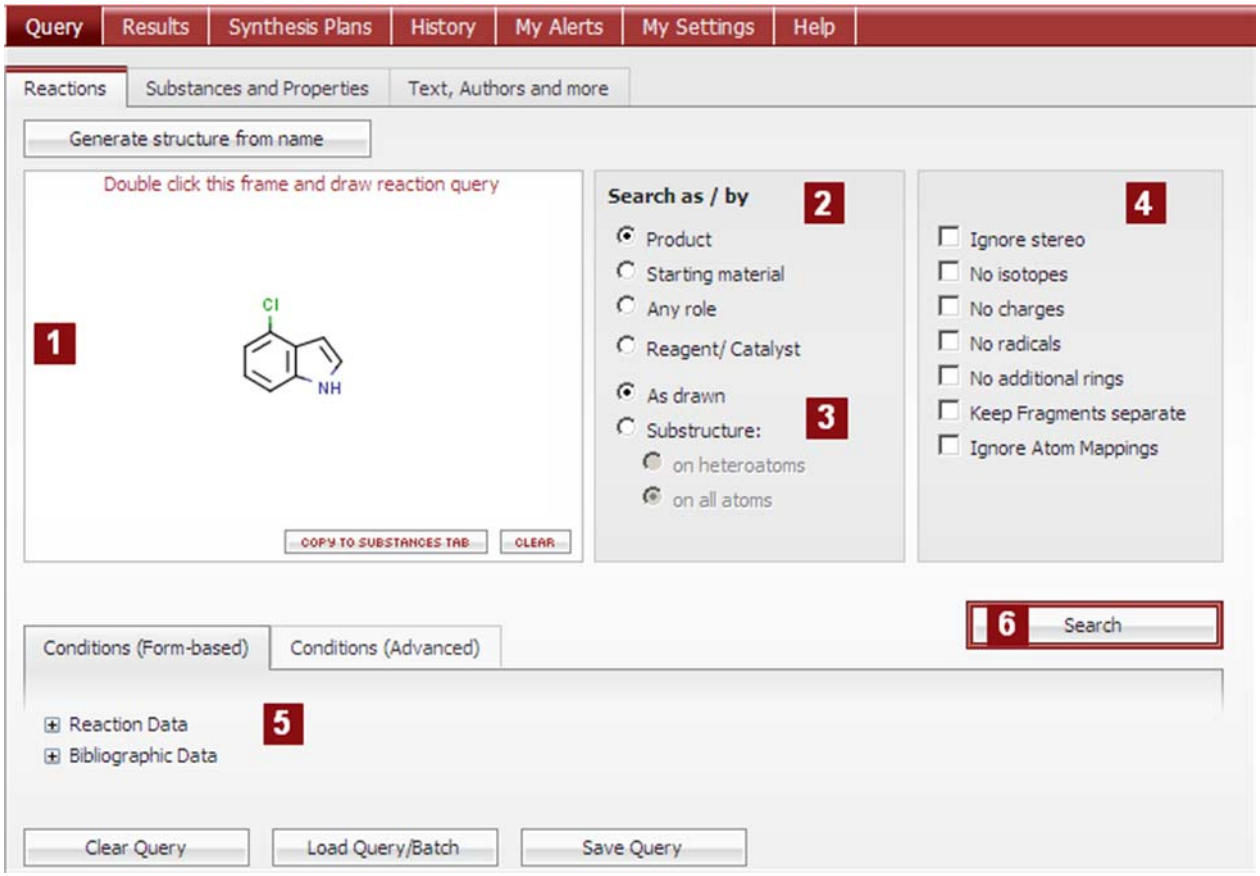
1 **Generate structure from name button**
Click this button to open an input field.

2 **Input field**
Enter a chemical name as systematic name or trivial name, an InChI key, a CAS Registry number or a SMILES string. Click **submit** to launch structure generation.

3 **Structure/reaction window**
The generated structure is displayed in the structure/reaction window, you can now:

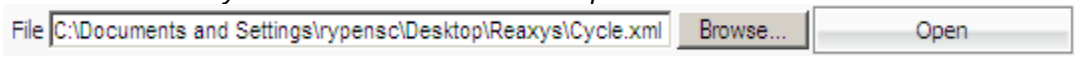
a) Start the search immediately.
b) Edit the structure by double clicking the box (or by doing a right-click); modify it in the Structure editor.
c) Define the search type, add further search conditions or/and select additional query options.

Reactions query tab



How to load a saved query?

1. *Ensure you are on the query tab and click the load query button*
2. *Browse to locate your saved XML file and click open*



1 Structure/reaction box
This window contains the requested structure or reaction, with additional query features. It is also possible to copy the structure to the Substances and Properties query tab.

2 Search as/by
If needed, define the role of the substance.

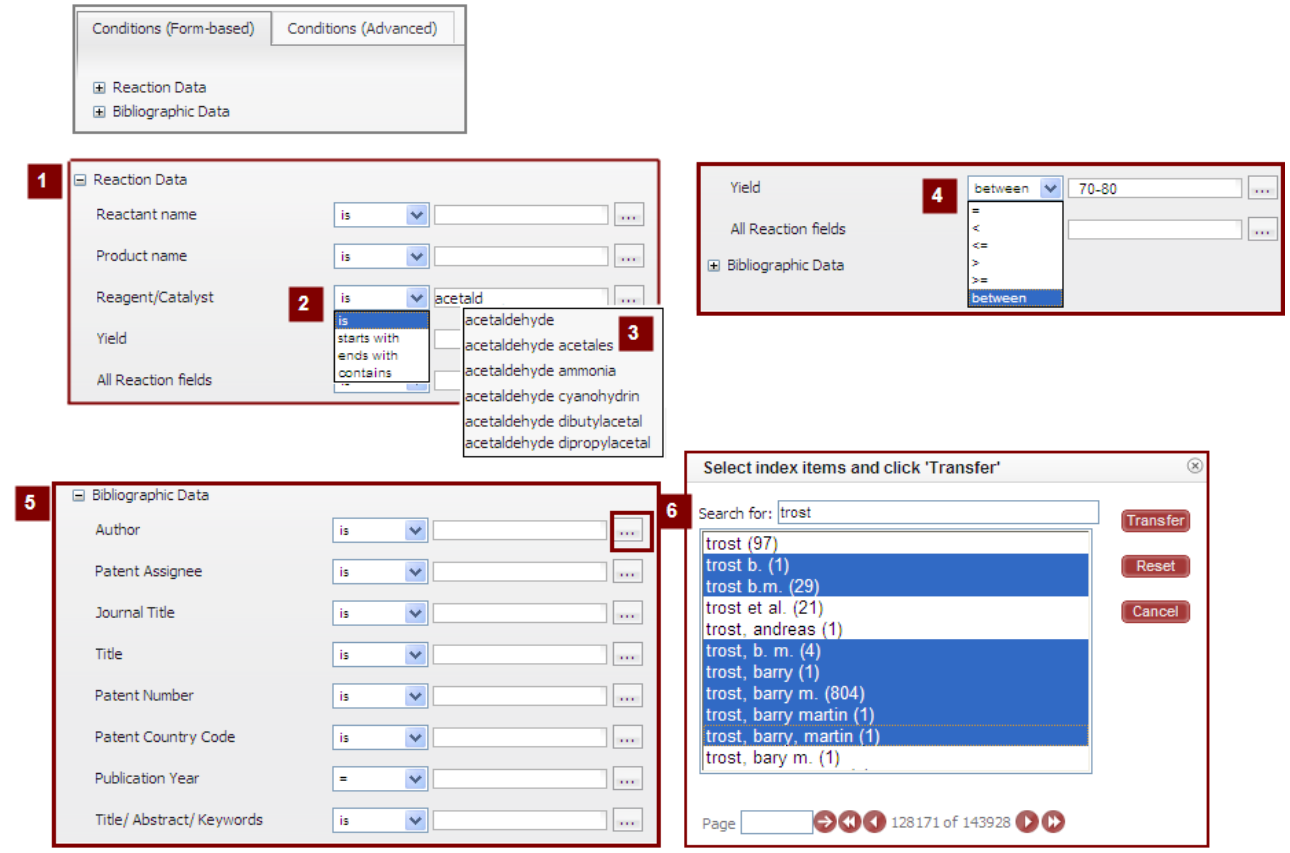
3 Select the search type
Select how the structure should be searched: *as drawn* (including possible query features added in your structure) or as *substructure search*. (In a substructure search the results include additional substituents).

4 Additional query options
Select additional options to refine your search.

5 Add further search conditions
Click the *Conditions (Form-based)* or the *Conditions (Advanced)* links to refine your search by adding further reaction or bibliographic data constraints (e.g. a yield or/and author constraint).

6 Search
Click this button to launch the search. A search progression box appears allowing you to cancel your research or to view your hits retrieved.

Reactions query tab
Conditions (Form-based)



Note: the Conditions (Form-based) link opens up forms containing commonly used fields for the given search form; they are grouped as either Reaction Data (such as yield or reagent name) or Bibliographic Data (such as journal title or patent assignee). The "All Reaction fields" and "Title/Abstract/Keywords" fields are text fields; use Boolean operators to search these fields.

1 Reaction data
Specify reactant name, product name, reagent, yield and/or all reaction fields.
Various selected fields are combined with the Boolean operator AND.

2 Operators
Select the appropriate operator from the drop-down menu.

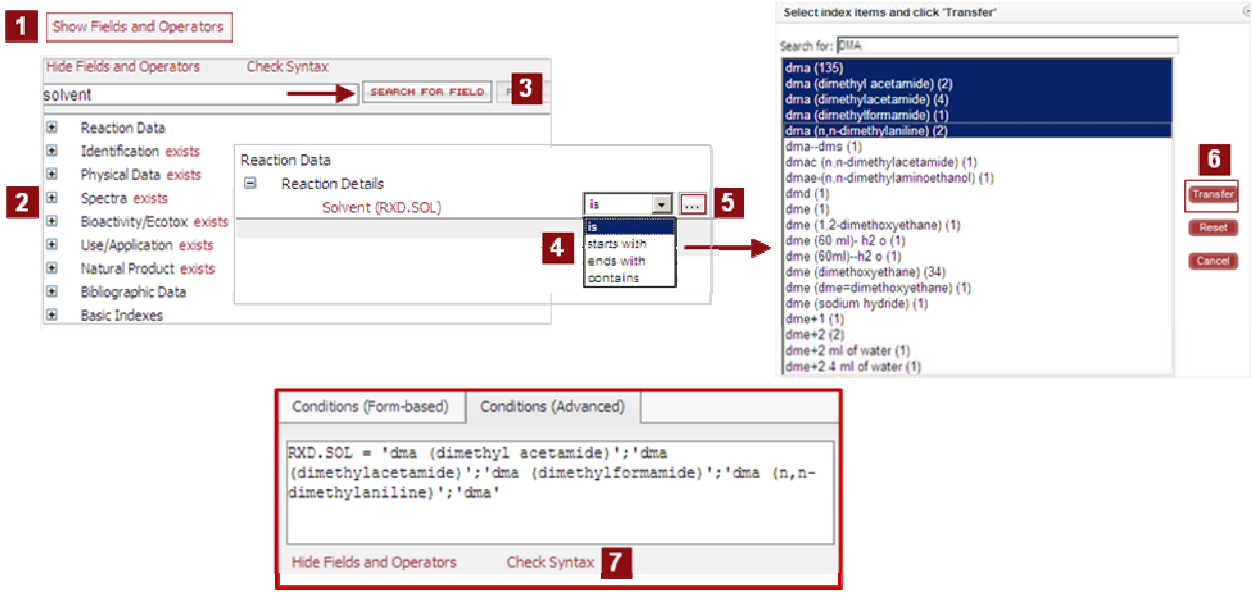
3 Selection list
Selection appears when typing entry.

4 Numeric Field
For a numeric field select the operator followed by entering the number or range in the text box.

5 Bibliographic data
Specify authors, patent assignee, journal title, title, patent number, patent country code, publication year and/or title/abstract/keywords.
Various selected fields are combined with the Boolean operator AND.

6 Expand Index feature (for all search fields)
The … box allows convenient index browsing and multiple entry selections. Click the **Transfer** button to add the selected data to the query.

Reactions query tab
Conditions (Advanced)



Note: the Conditions (Advanced) allows entry of complex and sophisticated property queries in combination with the structure or reaction queries following two ways:

1. *Type the query directly into the query box, with single quotes around the field data,*
2. *If the necessary field code is unknown, locate it using the Show fields and Operators hyperlink.*

1 Show Fields and Operators
Expand the fields list. Manually select the field code from the hierarchical list or use Search for Field button.

2 Fields Category
Click the + sign to expand the needed fields list.

3 Search for Field button
Type the name of the desired constraint, and click this button to locate the field.

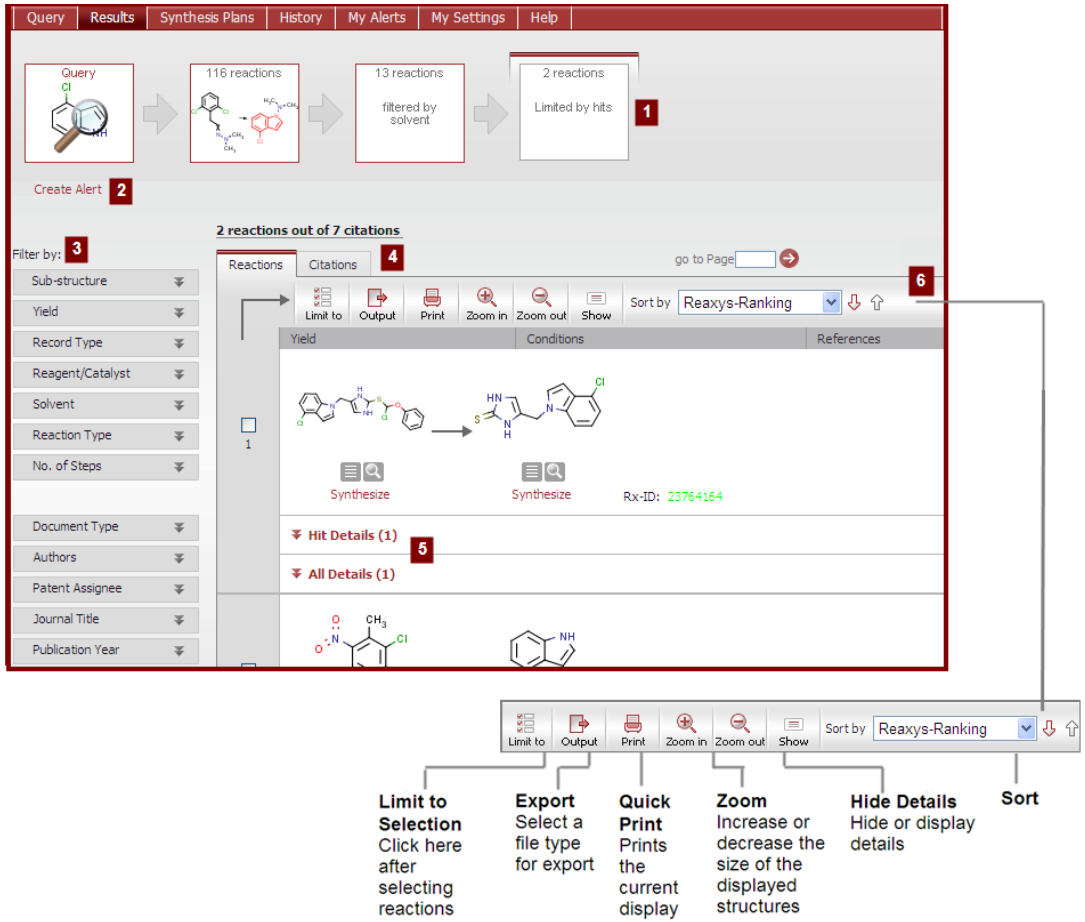
4 Operators
Select the appropriate operation from the drop-down menu.

5 Expand Index feature (for all search fields)
The ... box allows convenient index browsing and multiple entry selections.

6 Transfer the field data
Select the needed data entry(ies). Click the **Transfer** button to add the data to the query

7 Check Syntax
Allows query verification in case of manual entry.

Reactions results
General overview



The breadcrumbs at the top of the screen show the actions done on your initial hitset. Click one of the red-framed boxes to quickly jump to a previous set of data or initial query. The highlighted breadcrumb denotes the current hitset.

1 Breadcrumbs
Graphical navigation helps keep track of your results analysis.

2 Create Alert
Click this link to create an alert.

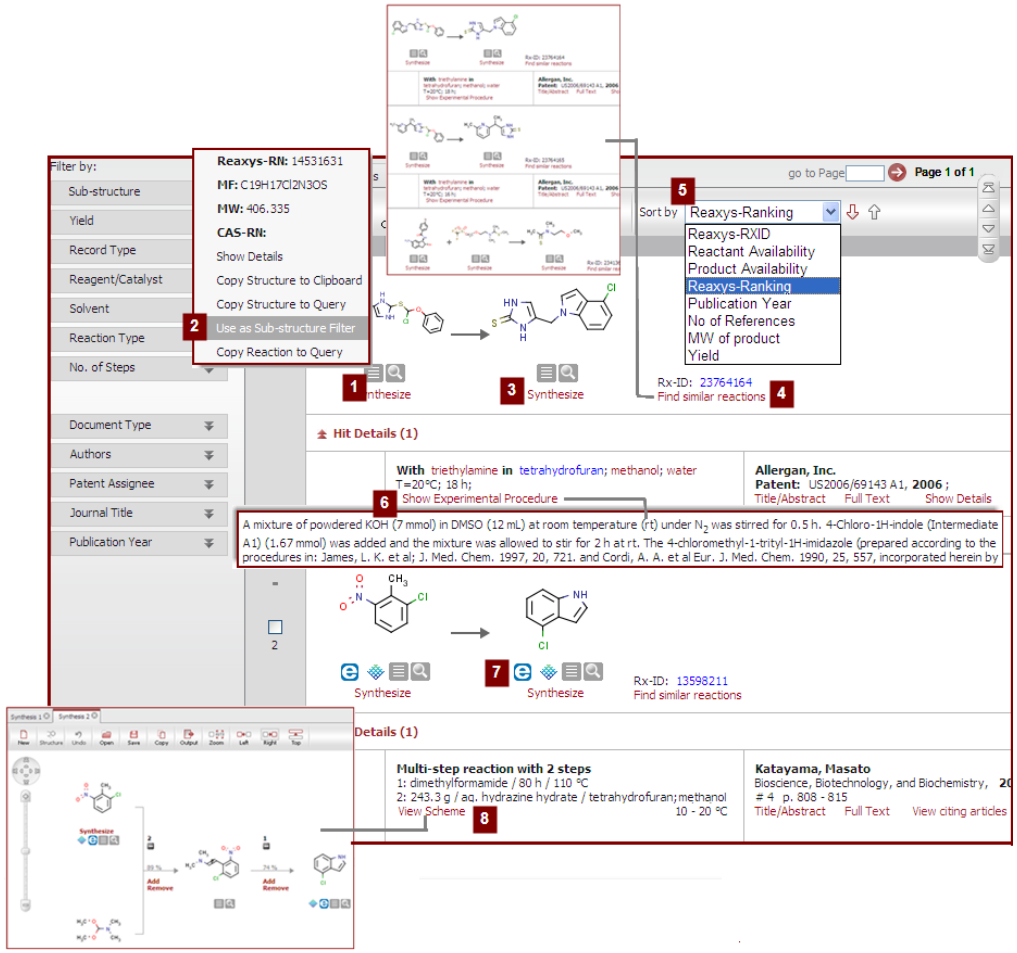
3 Filtered by
Refine results by applying filters linked to the reaction (yield, record type, reagent/catalyst, solvent, reaction type, no. of steps) or linked to bibliographic data (document type, authors, patent assignee, journal title and publication year).

4 Reactions/citations tab
Reactions tab is displayed by default, but you can switch to the citations tab.

5 Reaction results
Gives a quick overview of the results displayed with key data in a table. Display the title and the abstract, the original article or patent (Full Text) and access related information in Scopus (View citing articles).

6 Tool bar
Access Limit to Selection, Output, Quick Print, Zoom, Hide Details, and Sort by features.

Reactions results
Reactions tab



Note: Information on the Citations tab of Reaction Results can be Found on pg.24

The navigation tool to the right of the screen allows you to easily jump from one hit to another, or to the first/last hit, without need of scrolling down multiple times.

Click ☰ or a structure to get a pop-up menu with information or sub items.

1 Display further options & data
Reaxys – RN (*Reaxys registry number*), MF (*mol formula*), CAS-RN (*CAS registry number*), show details (*display information as physical-, spectral- data etc*), copy structure to Clipboard/Query screen, Copy Reaction to Query screen, View Related Markush, and use as Substructure Filter.

2 Use as Substructure Filter
This opens a query box allowing you to use the selected structure as Product, Reactant, or Any Role.

3 Synthesize
Opens the Synthesis Planner

4 Find Similar Reactions
Opens a new list of reactions

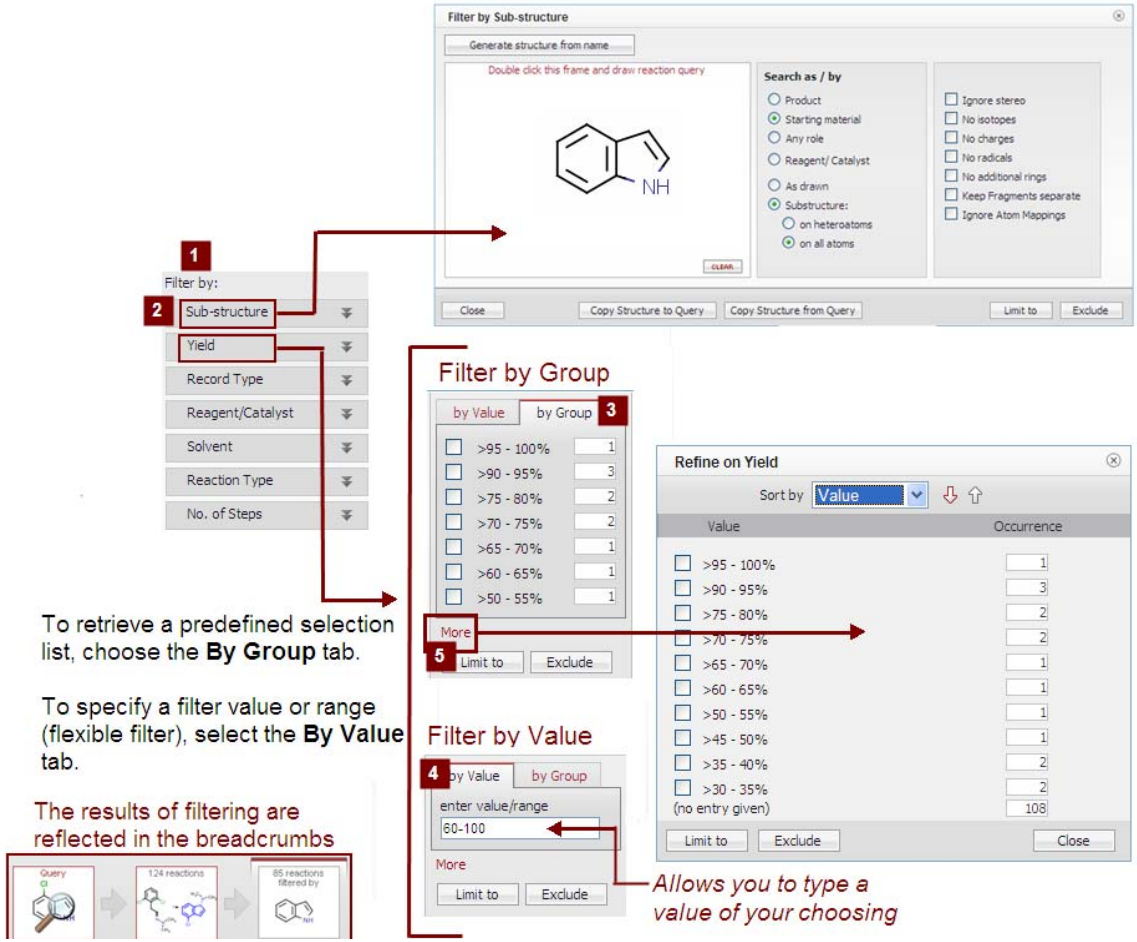
5 Sort by
Sort results in ascending ↑or descending ↓ order.

6 Show Experimental Procedure
Displays the experimental text from patents.

7 Commercial availability
Access the commercial availability of a substance and leads to appropriate companies (eMolecules/Symyx ACD).

8 View Scheme
Opens a separate window (Synthesis Planner) and displays the full scheme.

Reactions results tab
Filter by



The filter by feature allows you to refine your results. Click the double arrows to expand the list

1 Filter by

Reaction Specifications:
- Substructure - Yield
- Record type - Reagent/catalyst
- Solvent - Reaction type
- No. of steps

Bibliographic Specifications:
- Document type - Authors
- Patent assignee - Journal title

2 Filter by Substructure

This opens a query box and allows you to refine your list by drawing a structure or reaction and then clicking the **Limit to** or **Exclude** button.

3 By Group tab: pre-defined list

Check boxes to limit or exclude entries of the pre-defined selection.

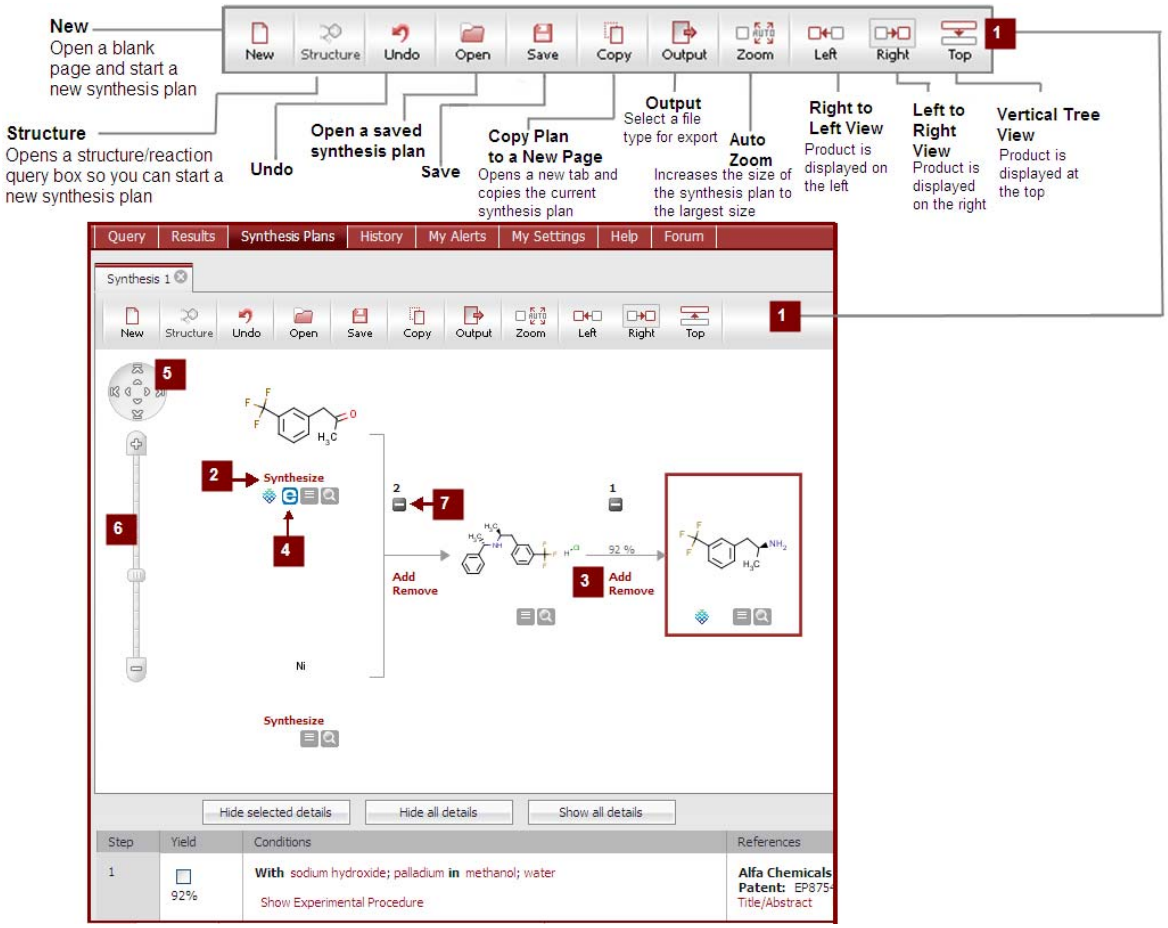
4 By Value tab: flexible filter

Enter a specific value or a range to refine result sets with more options.

5 Refine on Filter field

Click the **More** button to expand the scope of the selection. Sort the chosen data by **Value** or **Occurrence**.

Synthesis plans



Note: the overall scheme of multi-step reactions can be displayed in the synthesis plans page. A click on the View Scheme hyperlink opens the multi-step sequence as a new synthesis plan for a better overview.

Click Synthesize below any chemical structure in any of the results tabs to get the Synthesis Plans page.

1 Toolbar
Access new, undo, save, copy, and display features

2 Synthesize
Click the synthesize link to display various preparations for a compound. Click the add button of the selected step to incorporate it in your plan.

3 Add/Remove
Delete the current step or add another branch.

4 Commercial availability
Access the commercial availability of a substance and leads to appropriate companies (eMolecules/ACD).

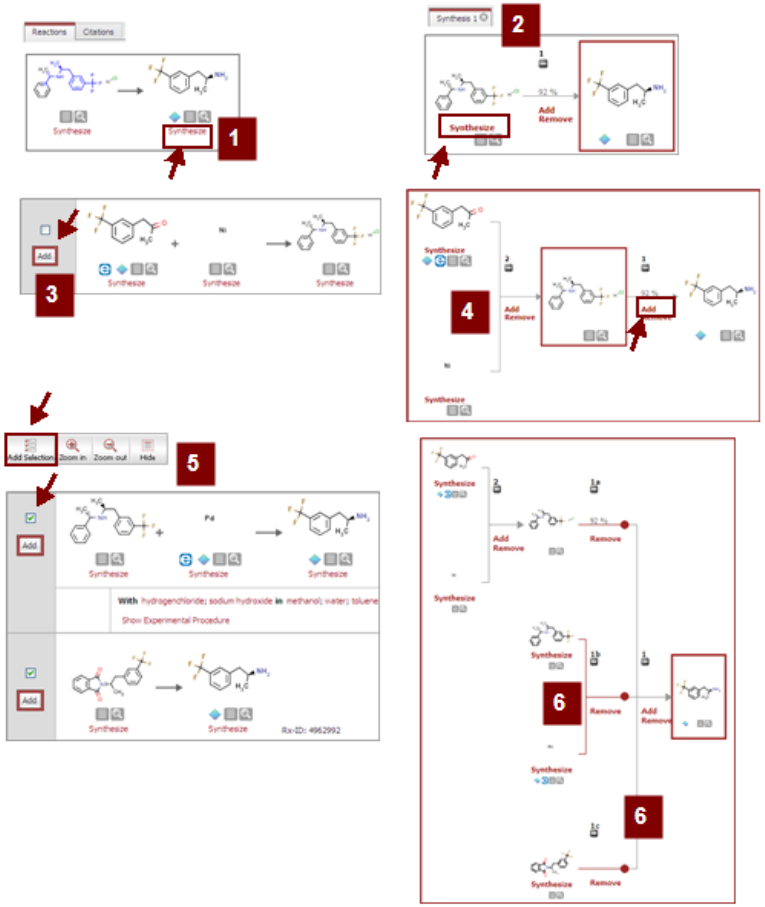
5 Navigation Tool
Adjusts the location of the synthesis plan on the page

6 Manual Zoom
Customize the size of the synthesis plan

7 Hide/Display
Hide or display parts of the synthesis plan

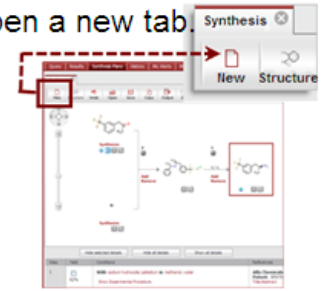
Synthesis plans

Start A Synthesis Plan:



To start a new plan from the Synthesis Planner:

Click the **New** button to open a new tab.



Click the **Structure** button to open a Query box.

Draw a structure, select the role of the structure in the reaction, and click the **Add** button

1 **Click the Synthesis link**
Below a substance on the results page

2 **Synthesis Planner Opens**
Your reaction is displayed. Click another Synthesize link to view a list of reactions

3 **Click Add Button**
Select a reaction to add to the retrosynthesis

4 **Add Branches**
Click the Add link at the appropriate step in the scheme

5 **Select Several Reactions**
Check the boxes near your selections and click the **Add Selections** button

6 **View Display**
The 2 selected reactions are added. The scheme now shows 3 routes leading to the synthesis of the product

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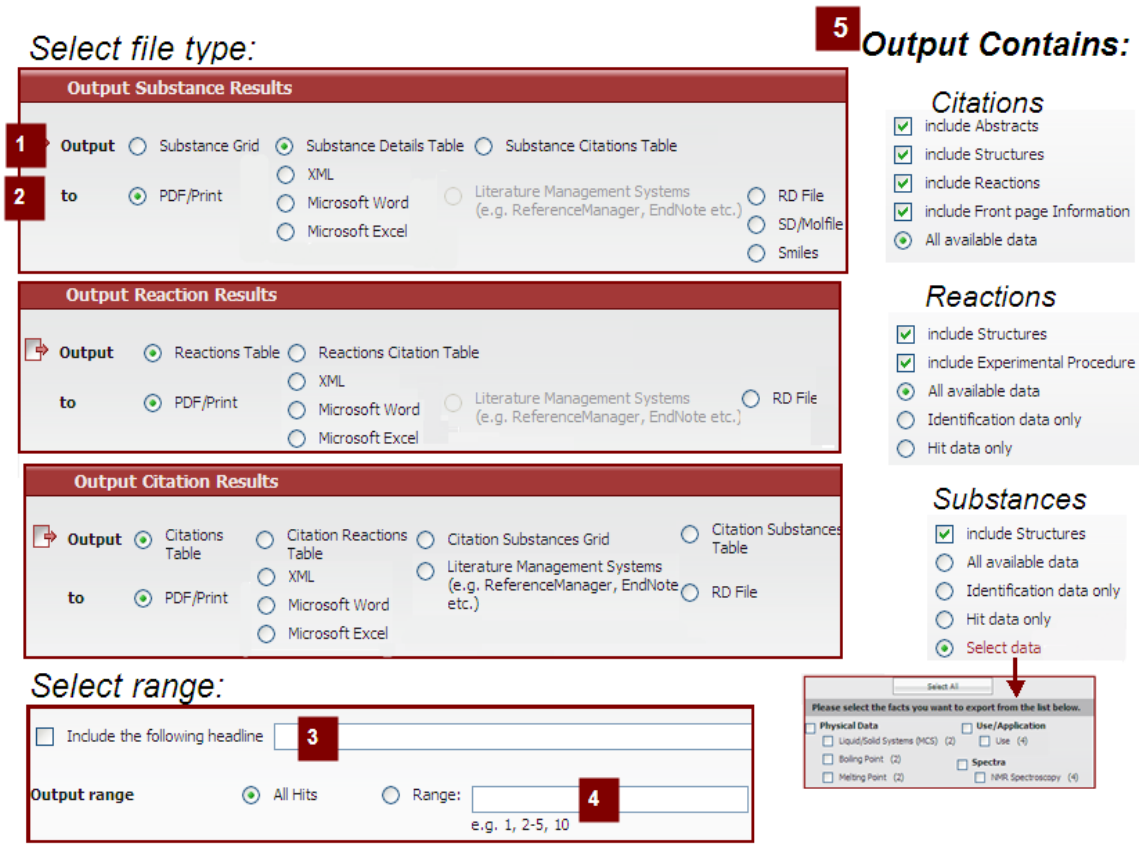
Output



1 Output
Choose the type of results to export:

2 to
Define the format of exported file: PDF/Print, XML, Microsoft Word or Excel, TXT for Literature Management Systems, or RD File.

3 Include the following headline
Check the box and enter a headline that will be shown on each page of the document.

4 Output range
Define the hits to export: all hits, selected hits (select it before clicking the output button), or a range (enter it in the box).

5 Output contains
Define the type of data to export.
Reactions output: include structures and/or experimental procedure, all available data or identification data only.
Substances output: include structures and all available data or identification data only or select data.
Citations output: include structures and/or abstracts

Note: output function is available on each of the results screens; it allows the export of any type of hitset (reactions, substances and bibliographic data) in any desired format. In the substance details table, click select data to choose the type of property you want to export.

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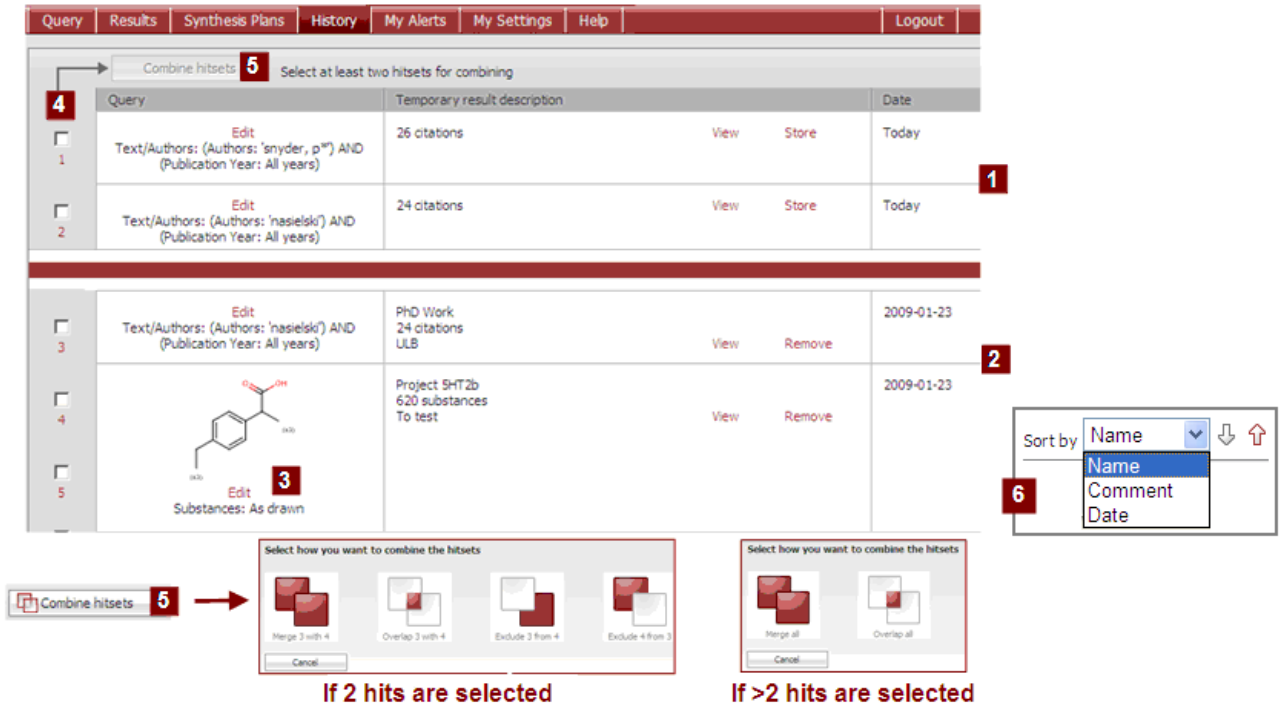
History



Note: the history table displays all current-session hitsets resulting from queries or from any analysis of your results; the most recent hitsets are shown at the top of the list. Here you can also graphically combine hitsets.

1 Temporary lists
The upper part of the table shows all hitsets from the current session.
Click View to display a list as active hitsets in the results page.
Click Store (enter a filename and comment) to save a list.

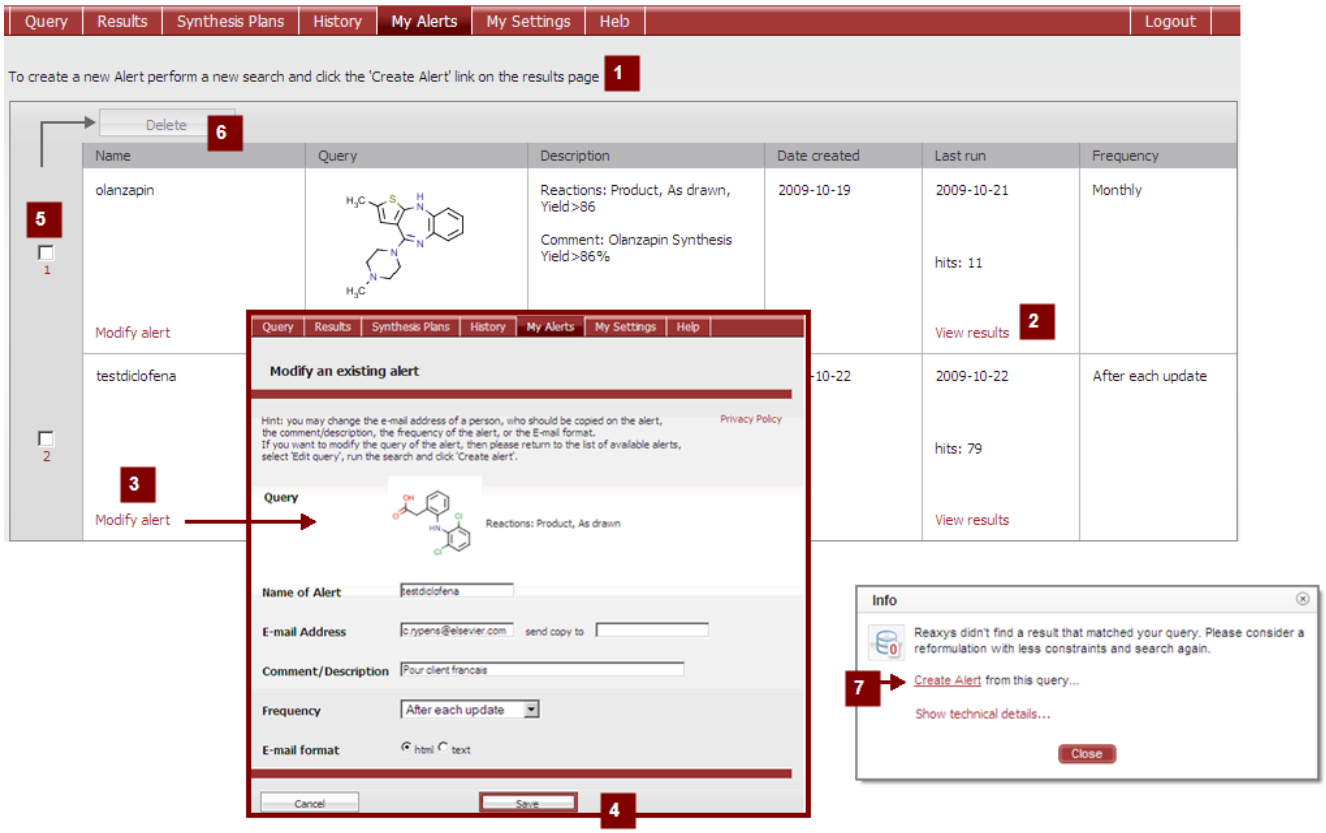
2 Saved lists
The lower part of the table shows the hitsets stored by the user. All saved hitsets are displayed if the user is logged in to Reaxys.
Click remove to delete a saved list.

3 Query column
Click Edit to display the query associated with the hitset in the query page
Note that hitsets resulting from filtering will not display the query in this column

4 Combine hitsets
5 Select two or more lists by checking the box close to the query column; the combine hitsets button becomes available and will provide graphical tools to combine the selected hitsets in various ways.

6 Sort
Sort saved and session hitsets by Name, Comment, or Date.

My Alerts



Note: alerts are user-defined search queries stored on the Reaxys server, so that they can be accessed and retrieved any time you log-in to Reaxys. You can choose to run it either monthly or each time the database is updated. You will receive an alert notification by email with a link to Reaxys allowing you to access the Alert results. Alerts are by default sorted by their Name.

My Alerts menu displays the list of available alerts together with the given result sets.

1 **How to create an alert?**
Create and run a query. On the results menu, click the *Create Alert* link located just below the Query breadcrumb. Fill in the Alert form and click the Save button.

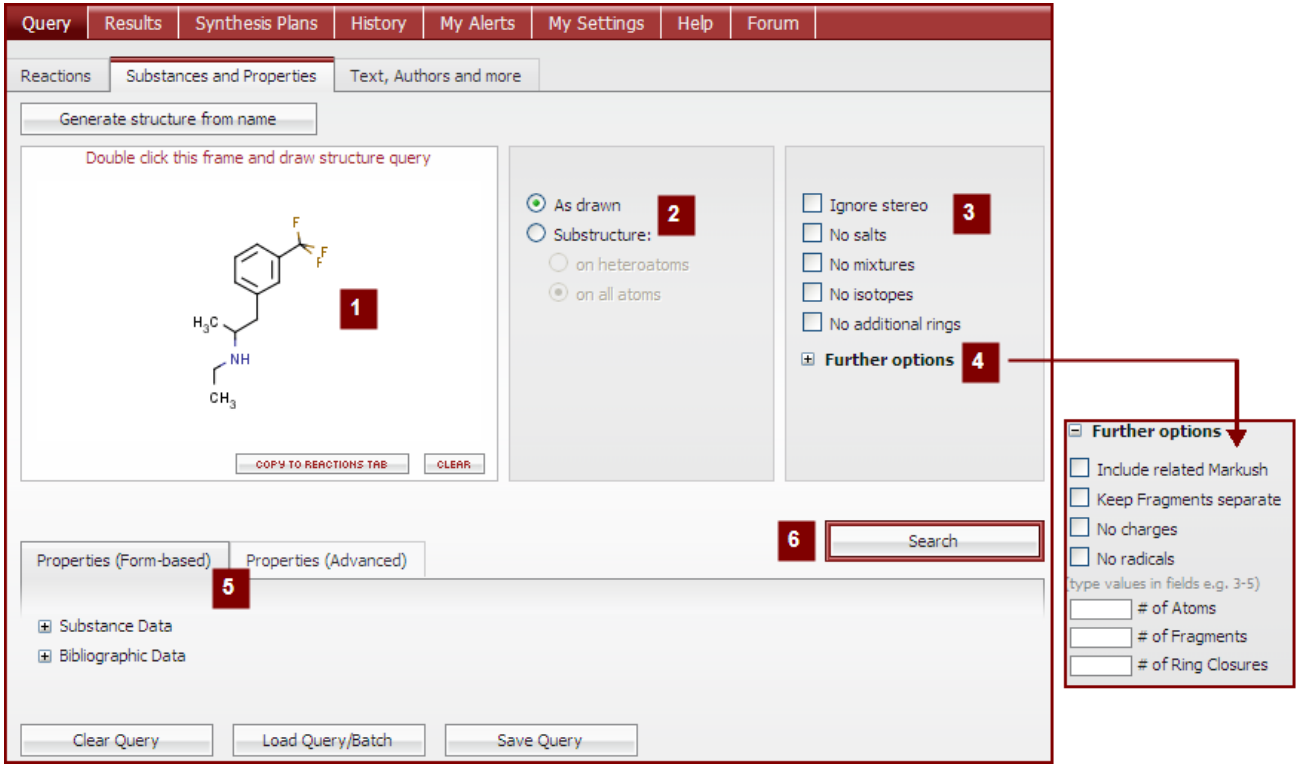
2 **View results button**
Click this link to jump to the Results menu and access the hits linked to your alert.

3 **Modify alert**
Modify the options of your alert
4 (*Name of Alert, Copy to, Comment/Description, Frequency* and *Email format*). Click the Save button.

5 **Delete**
Check the box close to the alert
6 name column; the delete button becomes available and will discard the concerned alert.

7 **What if there are no hits?**
Reaxys will display a message box with a Create Alert link .

Substances and properties
Query tab



1 **Structure/reaction box**
This window contains the needed structure, with additional query features. Two buttons enable the structure to be copied to the reactions query tab, and also to delete it.

2 **Search as**
Define the type of structure search: *as drawn* (including possible query features added on your structure), or *Substructure search*.

3 **Additional query options**
Select additional options to refine the search.

4 **Further options**
If needed, add further options, such as Include related Markush or Number of Ring Closures …

5 **Add further search conditions**
Click the *Properties (Form-based)* or the *Properties (Advanced)* links to enter further substance or bibliographic data constraints.

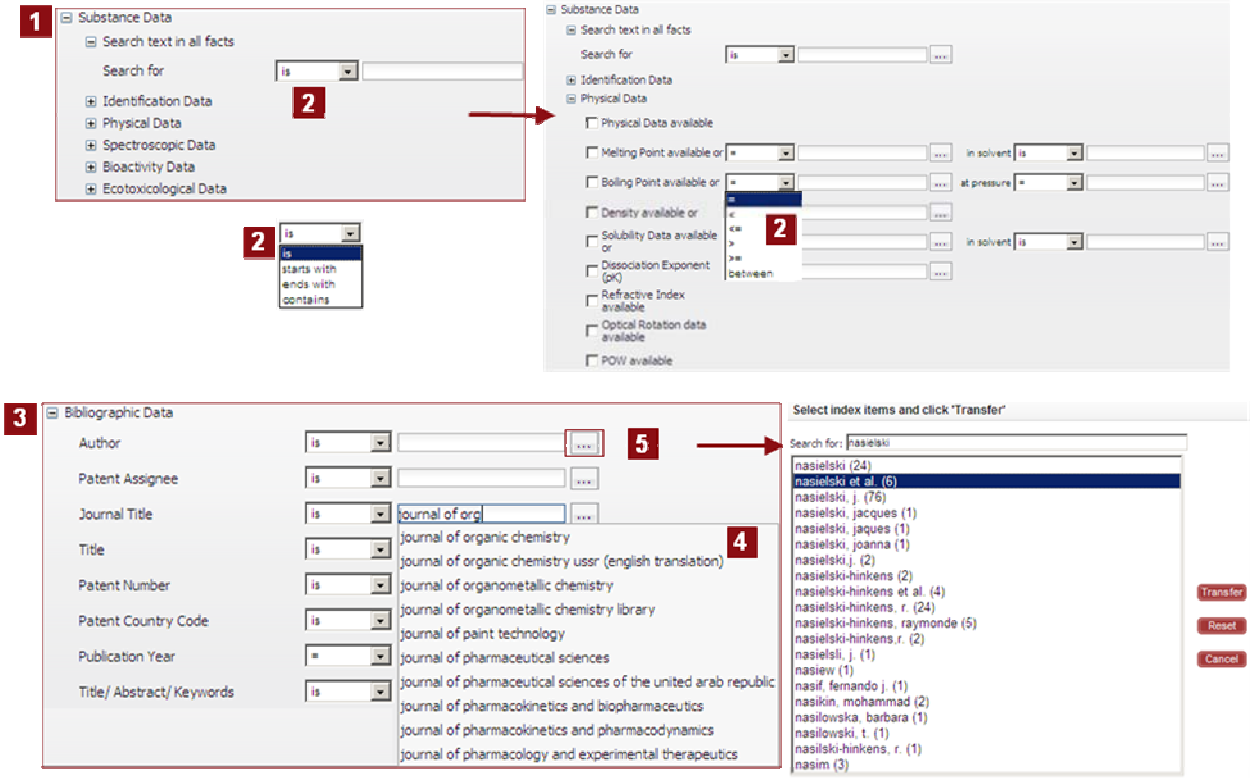
6 **Search**
Click this button to start searching

How to find information on specific compounds?

1. *Ensure the substances & properties tab is selected and double click the drawing pane*
2. *Draw the desired compound structure in your preferred editor and return to Reaxys by clicking the transfer button*
3. *Click the search button and browse the result.*

Note: Reaxys remembers the last query form used, and will reopen it in the next session; the substances and properties query tab can then become an entry form.

Substances query tab
Properties (Form-based)



Note: the Properties (Form-based) link opens up forms containing commonly used fields for the given search form; they are grouped as either Substance Data (such as spectra or solubility data) or Bibliographic Data (such as journal title or patent assignee). The "Search text in all facts" and "Title/Abstract/Keywords" fields are text fields; use Boolean operators to search these fields.

1 Substance data

Specify Search text in all facts/ Search for (*to add several terms in this text box, separate them with a ";"; they will be combined with the Boolean operator OR*), Identification Data, Physical Data, Spectroscopic Data, Bioactivity Data and/or Ecotoxicological Data.
Various selected fields are combined with the Boolean operator AND.

2 Operators

Select the appropriate operation from the drop-down menu; for a numeric field enter the number or range in the text box.

3 Bibliographic data

Specify authors, patent assignee, journal title, title, patent number, patent country code, publication year and/ or title/abstract/keywords
Various selected fields are combined with the Boolean operator AND.

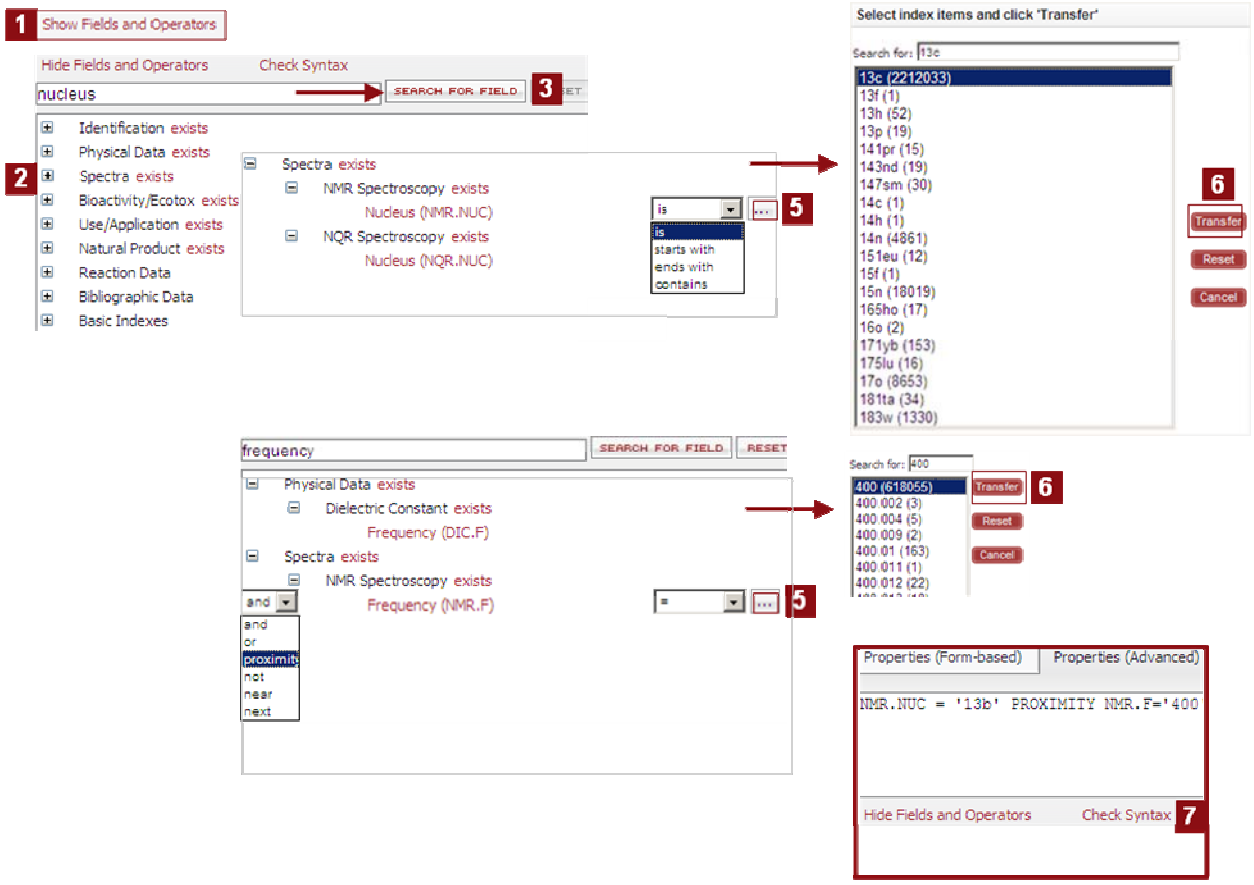
4 Selection list

Selection appears when typing entry.

5 Expand Index feature

The ... box allows convenient index browsing and multiple entry selections. Click the **Transfer** button to add the selected data to the query.

Substances query tab
Properties (Advanced)



1 **Show Fields and Operators**
Expand the fields list. Manually select the field code from the hierarchical list or use Search for Field button.

2 **Fields Category**
Click the + sign to expand the needed fields list.

3 **Search for Field button**
Type the name of the desired constraint, and click this button to locate the needed field.

4 **Operators**
Select the appropriate operation from the drop-down menu.

5 **Expand Index feature (for all fields)**
The ... box allows convenient index browsing and multiple entry selections.

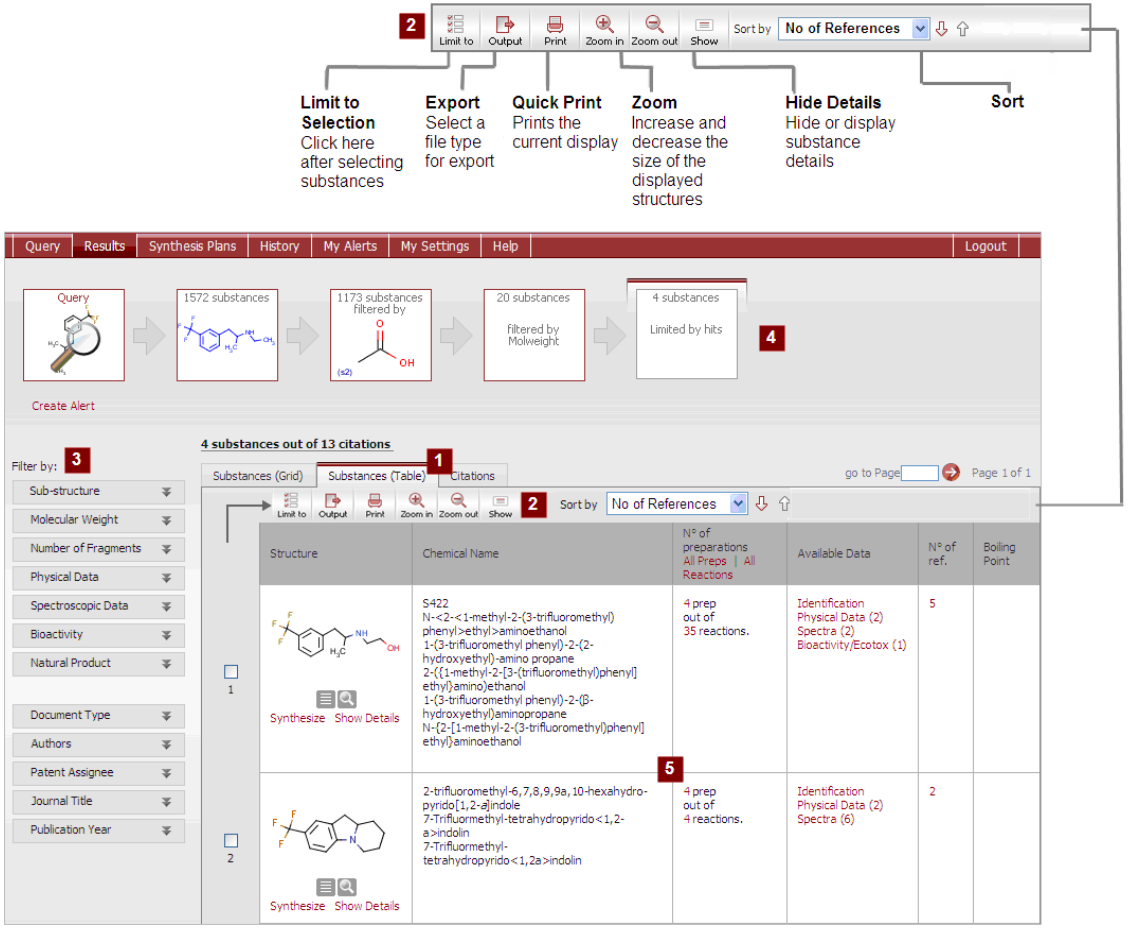
6 **Transfer the field data**
Select the needed data entry(ies). Click the **Transfer** button to add the data to the query.

7 **Check Syntax**
If you type the query directly into the Advanced Search box, you can use the Check Syntax link to ensure proper syntax.

Note: The Properties (Advanced) allows entry of complex and sophisticated property queries in combination with the structure queries following two ways:

1. *Type the query directly into the query box, with single quotes around the field data,*
2. *If the necessary field code is unknown, locate it using the Show fields and Operators hyperlink.*

Substances and properties
Results overview



Note: information on the citations tab of the substances results window can be found on page 24.

1 Substances (grid)/substances (table)/citations tab
The substances (table) tab is displayed by default, but you can switch to the substances (grid) or citations tab.

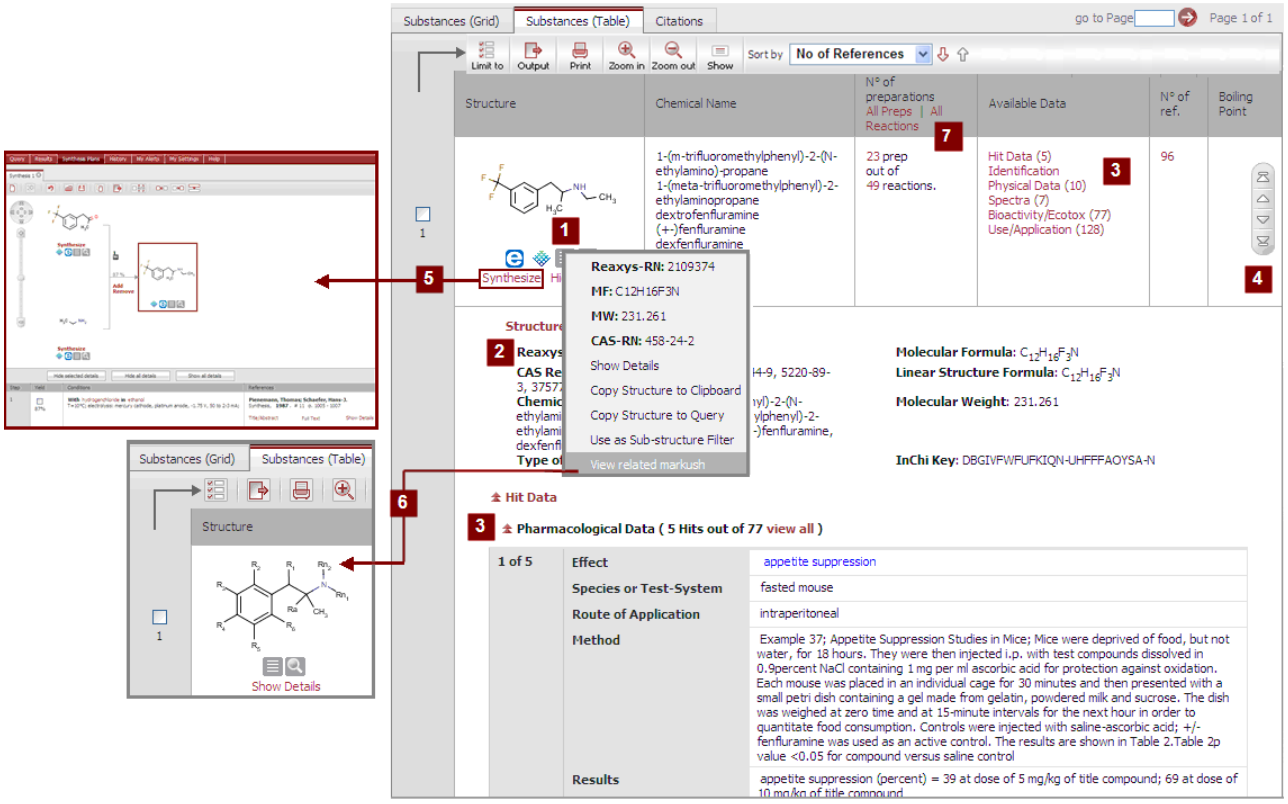
2 Tool bar
Access limit to selection, output, display, and sort by features.

3 Filtered by
Apply filters for substance (substructure, mol weight, number of fragments, physical data, spectroscopic data, bioactivity and natural product) or bibliographic data (document type, authors, patent assignee, journal title and publication year).

4 Breadcrumbs
Graphical navigation keeps track of your result analysis. The highlighted breadcrumb denotes the current result display.

5 Substances and properties results
Gives an overview of the results displayed with key data in a table. Show details & data hyperlinks allow displaying properties for each hit.

Substances and properties
Substances (Table) tab



Click a specific link in the available data column to only expand the needed data.

Click ☰ *or a structure to get a pop-up menu with information or sub items.*

1 Additional information / sub items
Reaxys –RN (*Reaxys registry number),* MF (*mol formula),* MW (*mol weight*), CAS-RN (*CAS registry number*), Show details (*displays Structure/compound data*), Copy Structure to Clipboard/ Query screen, Use as Substructure Filter, and View related Markush.

2 Structure/compound data
Display structure/ compound details.

3 Available data
Links to Hit Data and to All Available Data (from organic, inorganic & organometallic sources). Data excerpted from Gmelin has a from Gmelin flag.

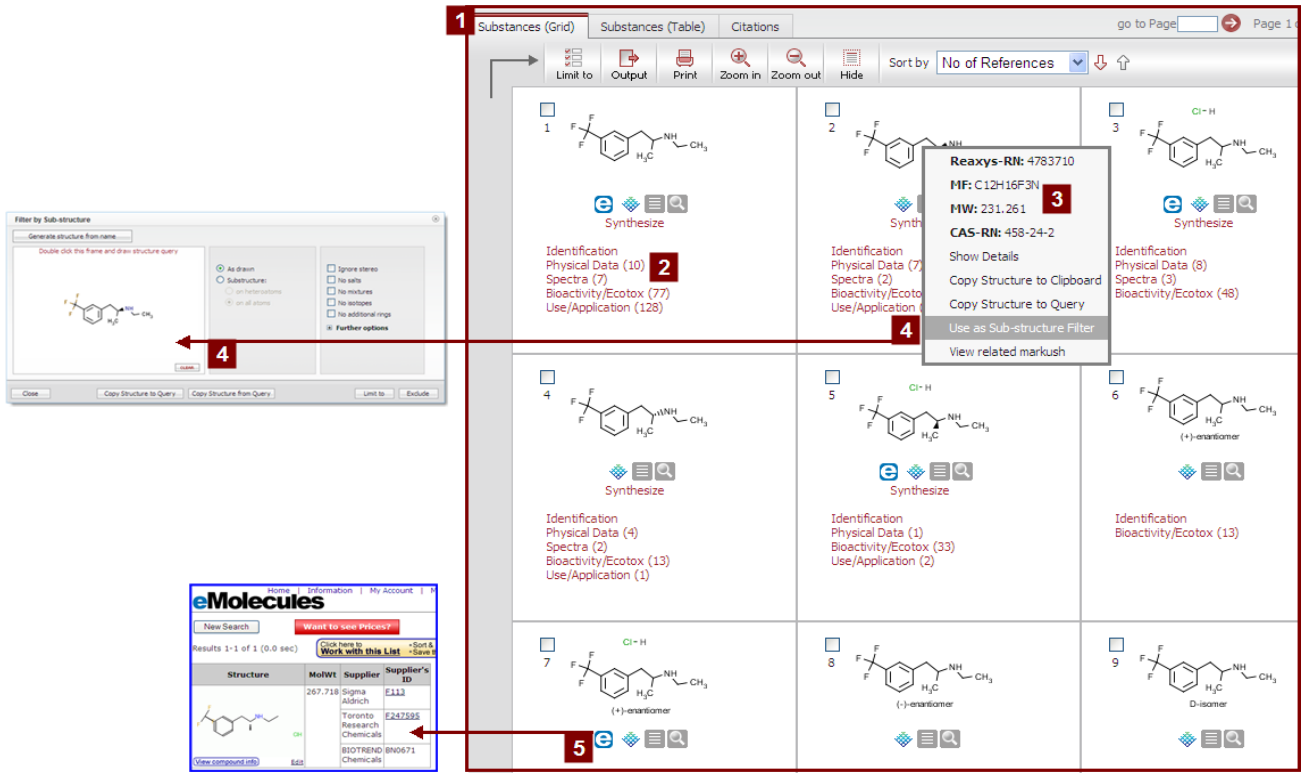
4 Navagation Bar
Navigation throughout the page.

5 Synthesize Link
Opens Synthesis Planner page.

6 View Related Markush
Opens a separate page with a link to Markush Details.

7 All Preps/All Reactions
Opens a list of reactions that are associated with the substances in the hitset.

Substances and properties
Substances (Grid) tab



1 Grid view
For a quick overview results are displayed in a grid.

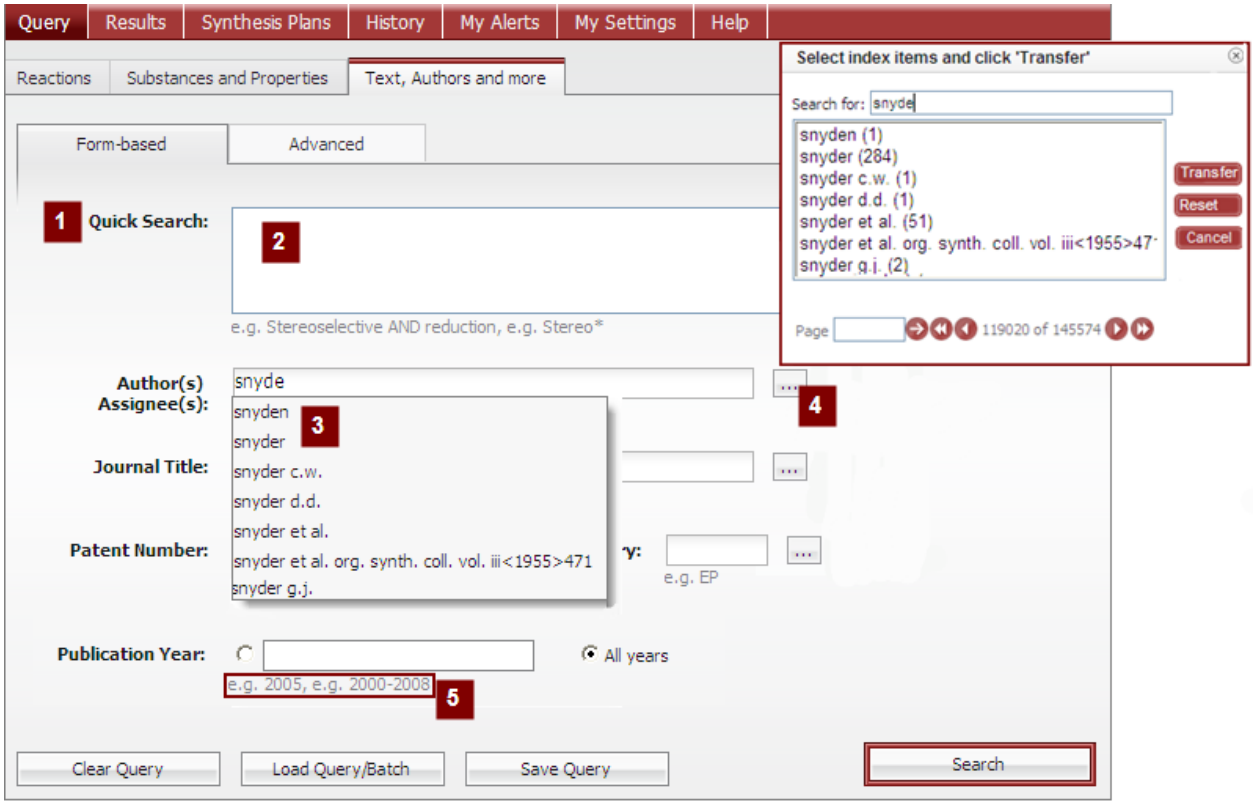
2 Available data for this substance
Various red hyperlinks display the information available by substance.

3 Additional Information/sub items
Click a structure to get a pop-up menu leading to additional information or sub items.
Reaxys –RN: *Reaxys registry number*
MF: *molecular formula*
MW*: molecular weight*
CAS-RN: *CAS registry number*
Show Details: *display information as Structure/compound data*
Copy structure to clipboard: *copies as a mol file*
Copy Structure to Query: *opens the query page with that structure*
Use as Substructure Filter: *see below*

4 Use as Substructure Filter
Opens a separate query box with the structure in it.

5 Commercial availability
Access the commercial availability of a substance and leads to appropriate companies (eMolecules/ACD).

Text, Authors and more
Query tab (Form-based)



Note: in the Quick Search box you can use and enter the following Boolean operators: AND, OR, PROXIMITY, NEAR and NEXT.

1 Search page
Enter Quick Search, author(s)/assignee(s), journal title, patent number, patent country, and/or publication year.

Different specified fields are combined with the Boolean operator AND.

2 Quick Search
Enter free text and combine it with the Boolean operators of your choice.
If needed use truncations.
Truncation:
*"***** " = any number of characters*
*"**?**" = one character*

3 Text field/selection list
Selection appears when typing entry.

4 Expand Index feature
The ... box allows convenient index browsing and multiple entry selections.(Use the Shift or ctrl key)
If several terms are chosen in one field, they are combined with the Boolean operator OR (;).

5 Entry example
Hints on how to enter your search term are displayed below each of the field data boxes.

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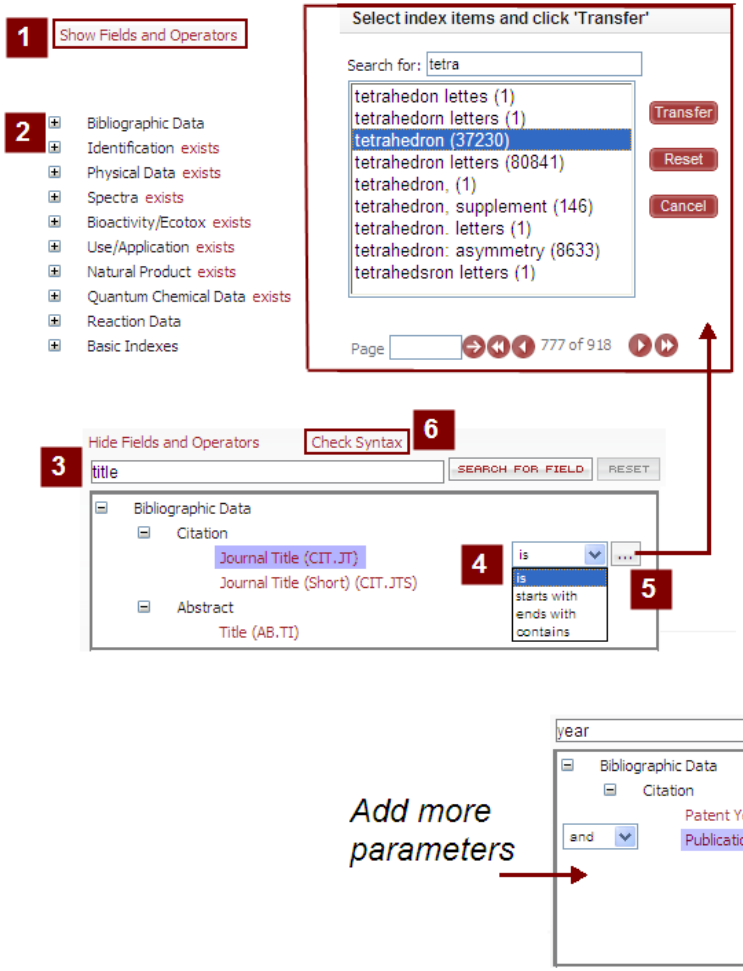
Text, authors and more
Query tab (Advanced)



1 Show Fields and Operators
Expand the fields list. Manually select the field code from the hierarchical list or use Search for Field button.

2 Fields Category
Click the + sign to expand the needed fields list.

3 Search for Field button
Type the name of the desired constraint, and click this button to locate the needed field.

4 Operators
Select the appropriate operation from the drop-down menu.

5 Expand Index feature (for all fields)
The ... box allows convenient index browsing and multiple entry selections.**Transfer the field data**
Select the needed data entry(ies). Click the Transfer button to add the data to the query.

6 Check Syntax
In case of manual entry of the query into the Advanced search box, check the used syntax by using the Check Syntax hyperlink.

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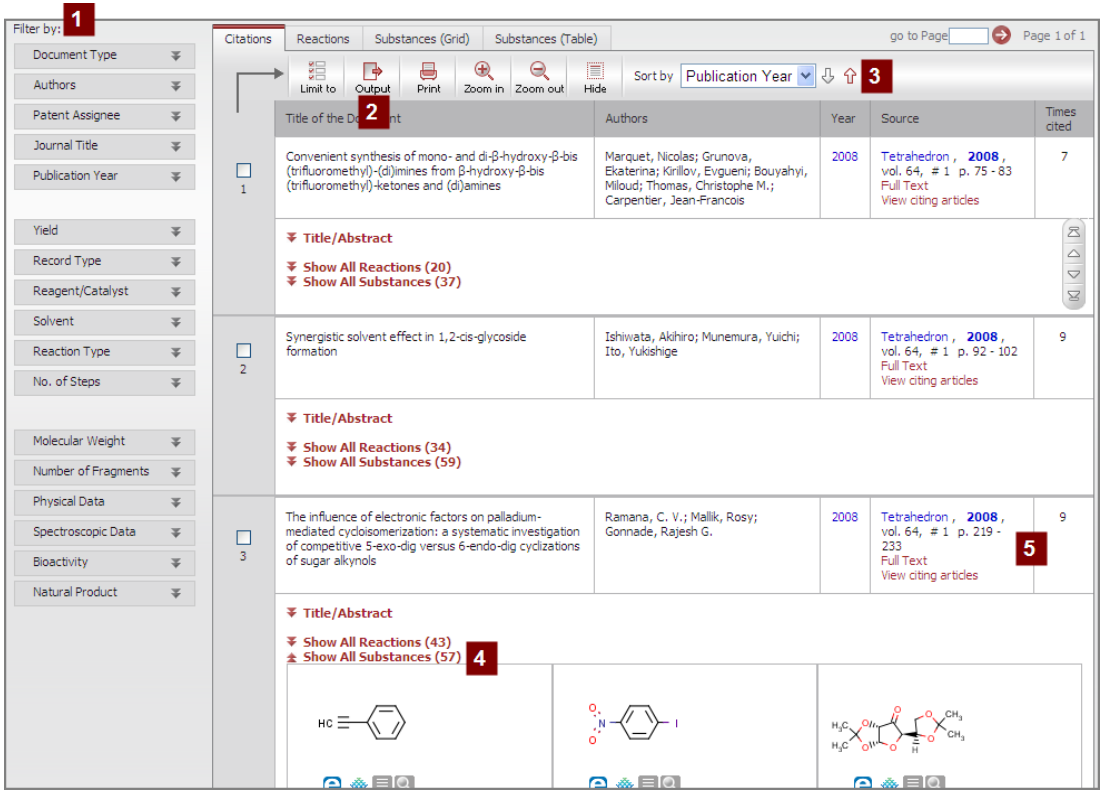
Citations tab
Results Overview



Reactions *and* ***Substances & Properties*** *citations tabs have almost the same layout and content as the bibliographic citations tab. The only differences are the presence of one additional link on each of those tabs and additional filters:*

- *Reactions results/citations tab: presence of Hit Reactions in this article (# out of total #) link*
- *Substances & properties results/citations tab: presence of Hit Substances in article (# out* of total *#) link*

1 Filter by
Refine search results by applying bibliographic (document type, authors, patent assignee, journal title and publication year), reaction or substance filters.

2 Output
Export results in an appropriate format.

3 Sort by
Sort results ascending or descending by Document Type, Authors, Journal Title or Publication Year (default).

4 Abstract/Reactions/Substances
Display the abstract, and show all reactions or show all substances which are related to the article.

5 Source
Find here the literature reference. Display the original text with the Full Text link and access related information from Scopus with the View citing articles link.
The Times cited column displays the number of articles from Scopus citing a specific reference.