

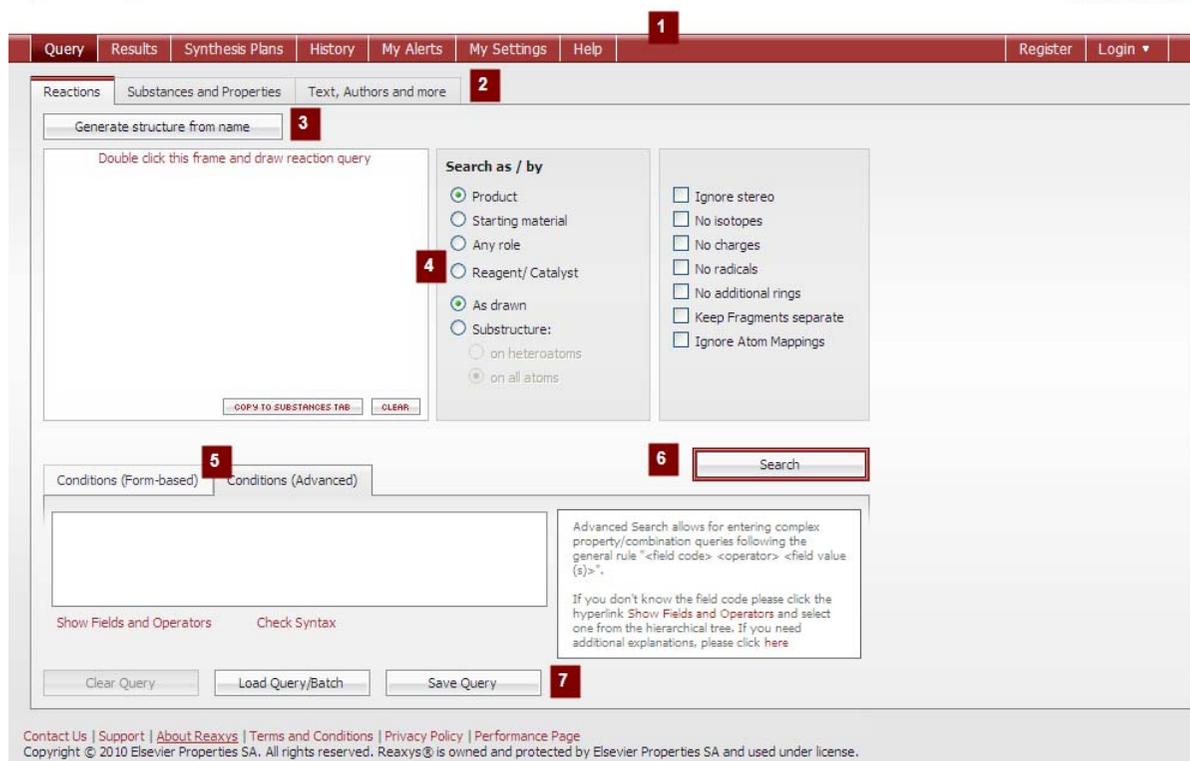


Reaxys Quick Reference Guide

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1	Homepage
2	My Settings
3	Generate a structure from a name
	Reactions
4	Query tab
5	Query tab – Conditions (Form-based)
6	Query tab – Conditions (Advanced)
7	Results – general overview
8	Results – reactions tab
9	Results– filter by
10	Synthesis Plans - Overview
11	Synthesis Plans
12	Output
13	History
14	My Alerts
	Substances and properties
15	Query tab
16	Query tab – Properties (Form-based)
17	Query tab – Properties (Advanced)
18	Results overview
19	Substances (Table) tab
20	Substances (Grid) tab
	Text, authors and more
21	Query tab – (Form-based)
22	Query tab – (Advanced)
23	Citations tab



1. Main Navigation: 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: Input field for chemical name

4. Structure/reaction window: Search as/by options (Product, Starting material, Any role, Reagent/Catalyst, As drawn, Substructure) and checkboxes (Ignore stereo, No isotopes, No charges, No radicals, No additional rings, Keep Fragments separate, Ignore Atom Mappings)

5. Add Reaction/Bibliographic data: Conditions (Form-based) and Conditions (Advanced) tabs

6. Search button: Search input field

7. Command buttons: Clear Query, Load Query/Batch, Save Query

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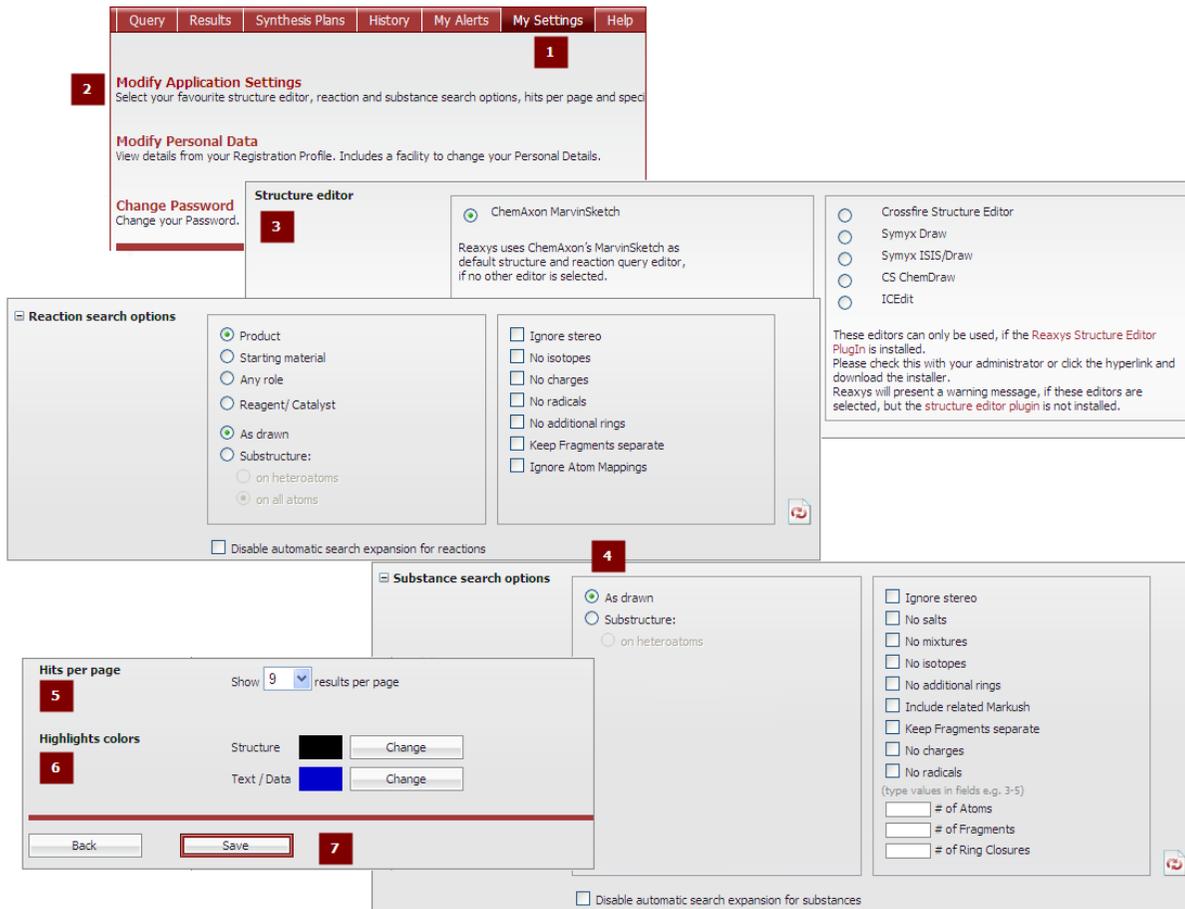
How to find the preparation of a compound?

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.

Generate a structure from name



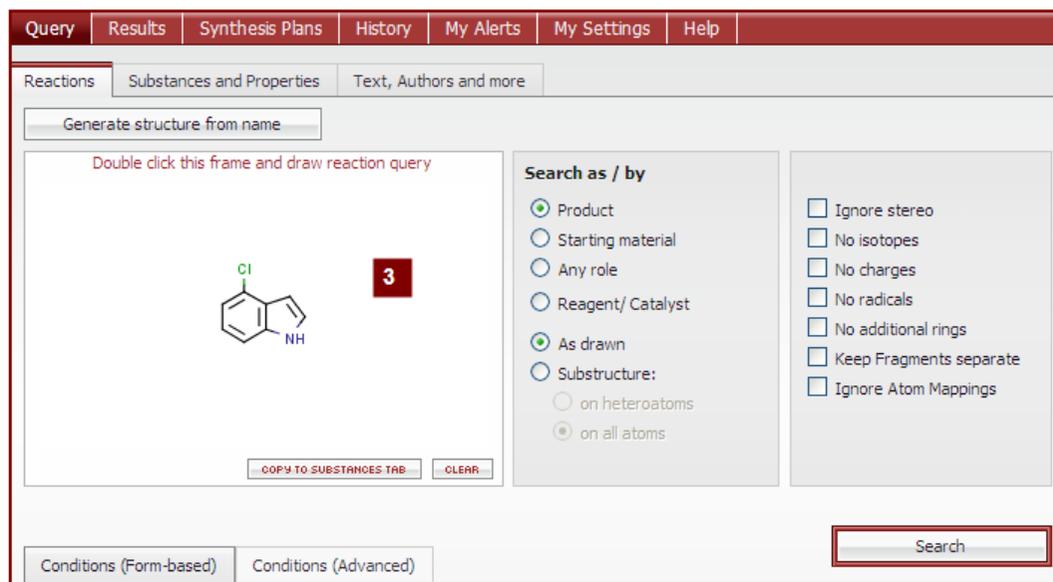
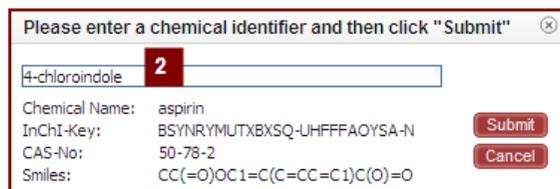
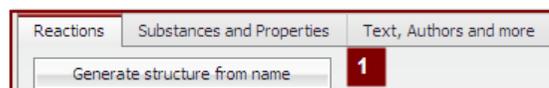
The screenshot shows the 'My Settings' page in the Reaxys interface. The page is divided into several sections:

- 1 My Settings:** The top navigation bar with 'My Settings' highlighted.
- 2 Modify Application Settings:** A section for selecting a structure editor, reaction and substance search options, hits per page, and highlights colors.
- 3 Structure editor:** A section for selecting a preferred editor (ChemAxon MarvinSketch, Crossfire Structure Editor, Symyx Draw, Symyx ISIS/Draw, CS ChemDraw, IEdit).
- 4 Reaction/Substance search options:** Two sections for defining default search options for reactions and substances, including checkboxes for 'Ignore stereo', 'No salts', 'No mixtures', 'No isotopes', 'No additional rings', 'Include related Markush', 'Keep Fragments separate', 'No charges', and 'No radicals'. There are also input fields for '# of Atoms', '# of Fragments', and '# of Ring Closures'.
- 5 Hits per page:** A section for selecting the preferred number of displayed hits (currently set to 9).
- 6 Highlights colors:** A section for selecting preferred colors to highlight the searched structure and/or text/data.
- 7 Back & Save buttons:** A section with 'Back' and 'Save' buttons.

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.

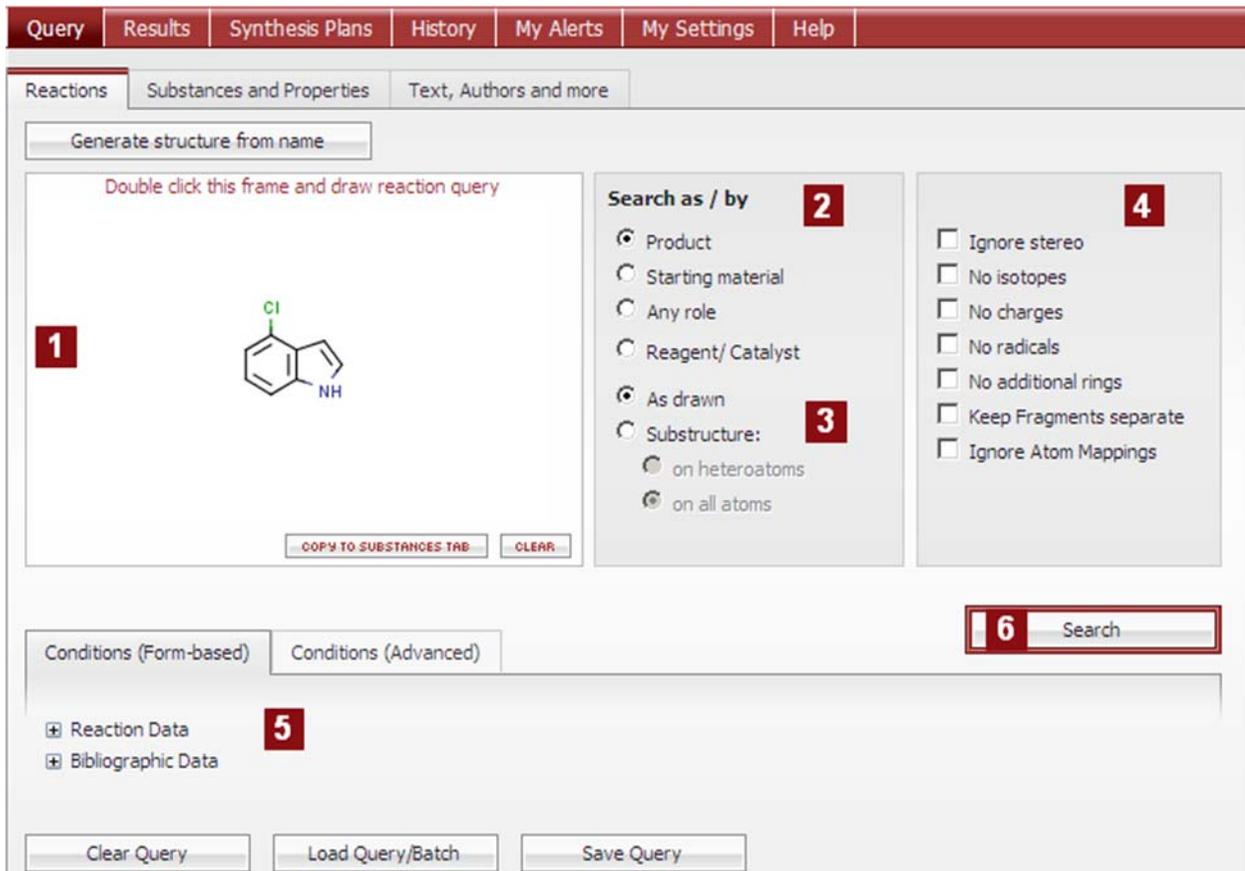
Generate a structure from name



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.



The screenshot shows the Reaxys interface with the following elements:

- 1**: A chemical structure of a chlorinated indole derivative is displayed in a frame labeled "Double click this frame and draw reaction query".
- 2**: The "Search as / by" section contains radio buttons for "Product", "Starting material", "Any role", "Reagent/ Catalyst", "As drawn", and "Substructure:". The "Substructure:" option is selected, with sub-options for "on heteroatoms" and "on all atoms".
- 3**: The "Substructure:" radio button is highlighted.
- 4**: A list of checkboxes for additional query options: "Ignore stereo", "No isotopes", "No charges", "No radicals", "No additional rings", "Keep Fragments separate", and "Ignore Atom Mappings".
- 5**: The "Conditions (Form-based)" and "Conditions (Advanced)" tabs are visible, with expandable sections for "Reaction Data" and "Bibliographic Data".
- 6**: A "Search" button is located at the bottom right of the main query area.

- 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.

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

File

Reactions query tab Conditions (Form-based)

Conditions (Form-based) Conditions (Advanced)

Reaction Data
 Bibliographic Data

1 Reaction Data

Reactant name is ...

Product name is ...

Reagent/Catalyst is acetald ...

2 **3**

- is
- starts with
- ends with
- contains

- acetaldehyde
- acetaldehyde acetals
- acetaldehyde ammonia
- acetaldehyde cyanohydrin
- acetaldehyde dibutylacetal
- acetaldehyde dipropylacetal

Yield

All Reaction fields

Yield **4** between 70-80 ...

All Reaction fields

Bibliographic Data

=

<

<=

>

>=

between

5 Bibliographic Data

Author is ...

Patent Assignee is ...

Journal Title is ...

Title is ...

Patent Number is ...

Patent Country Code is ...

Publication Year = ...

Title/ Abstract/ Keywords is ...

6 Select index items and click 'Transfer'

Search for: trost

trost (97)

trost b. (1)

trost b.m. (29)

trost et al. (21)

trost, andreas (1)

trost, b. m. (4)

trost, barry (1)

trost, barry m. (804)

trost, barry martin (1)

trost, barry, martin (1)

trost, bary m. (1)

Transfer

Reset

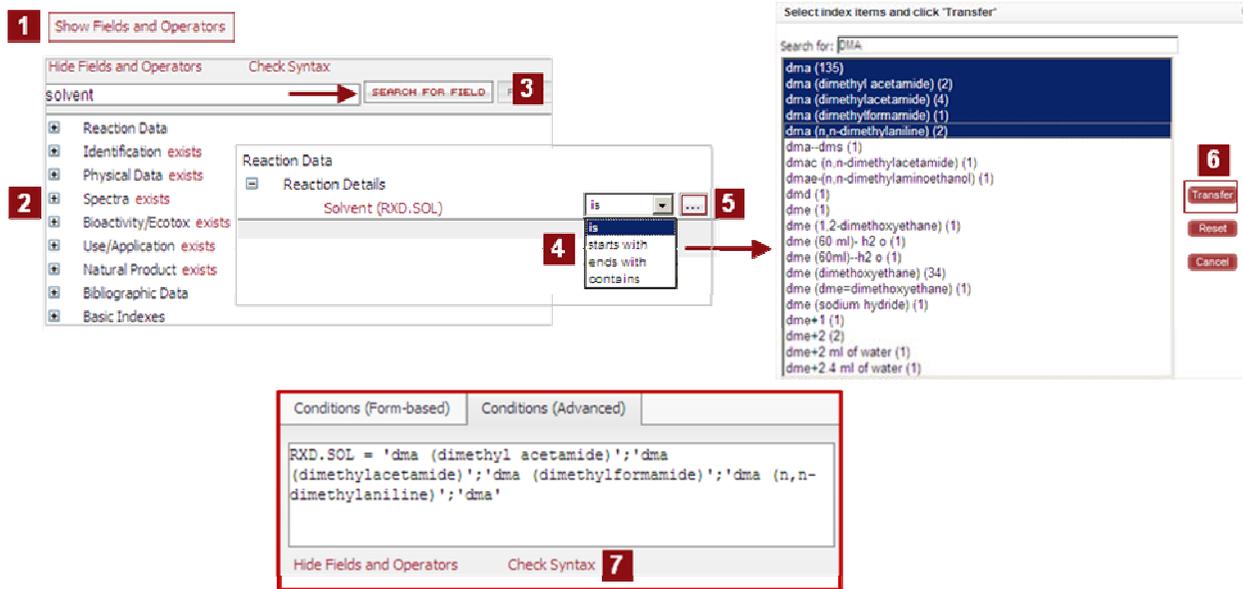
Cancel

Page 128171 of 143928

- 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.

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.

Reactions query tab Conditions (Advanced)



1 Show Fields and Operators

2 Fields Category

3 Search for Field button

4 Operators

5 Expand Index feature (for all search fields)

6 Transfer the field data

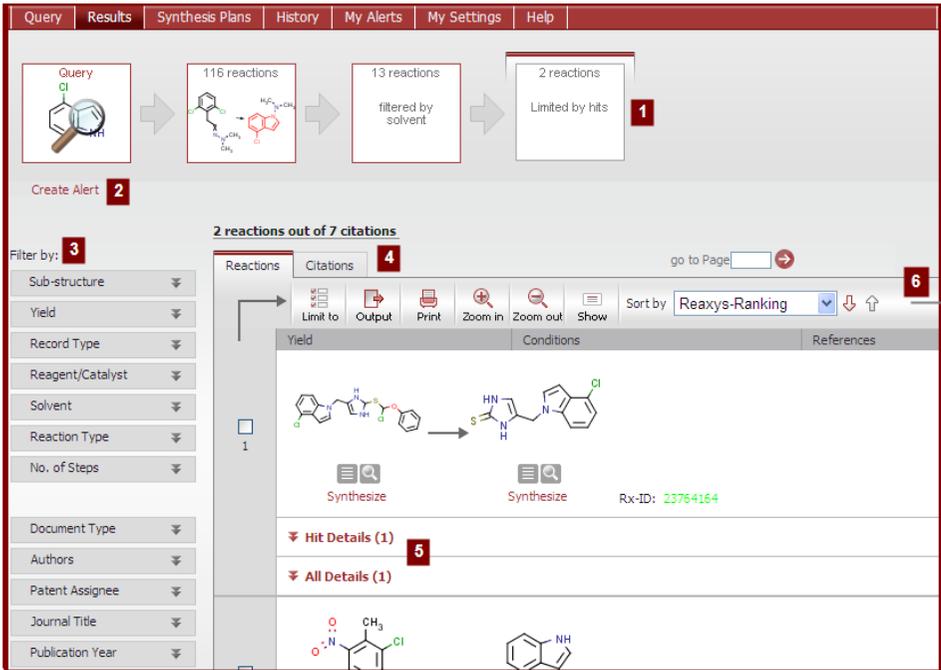
7 Check Syntax

- Show Fields and Operators**
Expand the fields list. Manually select the field code from the hierarchical list or use **Search for Field** button.
- Fields Category**
Click the + sign to expand the needed fields list.
- Search for Field button**
Type the name of the desired constraint, and click this button to locate the field.
- Operators**
Select the appropriate operation from the drop-down menu.
- Expand Index feature (for all search 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
- Check Syntax**
Allows query verification in case of manual entry.

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

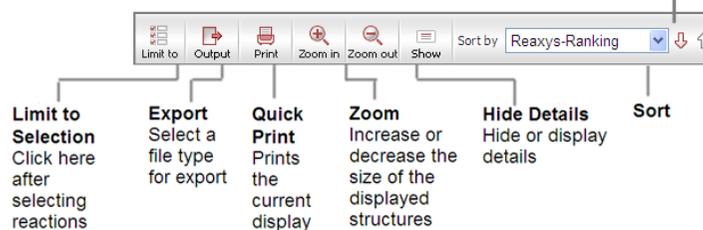
- Type the query directly into the query box, with single quotes around the field data,
- If the necessary field code is unknown, locate it using the **Show fields and Operators** hyperlink.

Reactions results General overview



The screenshot shows the Reaxys interface with the following elements:

- Query:** A search query for a benzimidazole derivative.
- Breadcrumbs:** A sequence of boxes showing the progression from 116 reactions to 13 reactions (filtered by solvent) to 2 reactions (limited by hits).
- Filter by:** A sidebar with various filters such as Sub-structure, Yield, Record Type, Reagent/Catalyst, Solvent, Reaction Type, No. of Steps, Document Type, Authors, Patent Assignee, Journal Title, and Publication Year.
- Reactions/Citations tab:** A tab showing 2 reactions out of 7 citations. The 'Reactions' tab is active, displaying a reaction scheme and its details (Rx-ID: 23764164).
- Tool bar:** A toolbar with icons for Limit to Selection, Output, Print, Zoom in, Zoom out, Show, and Sort by (Reaxys-Ranking).



The legend explains the icons in the tool bar:

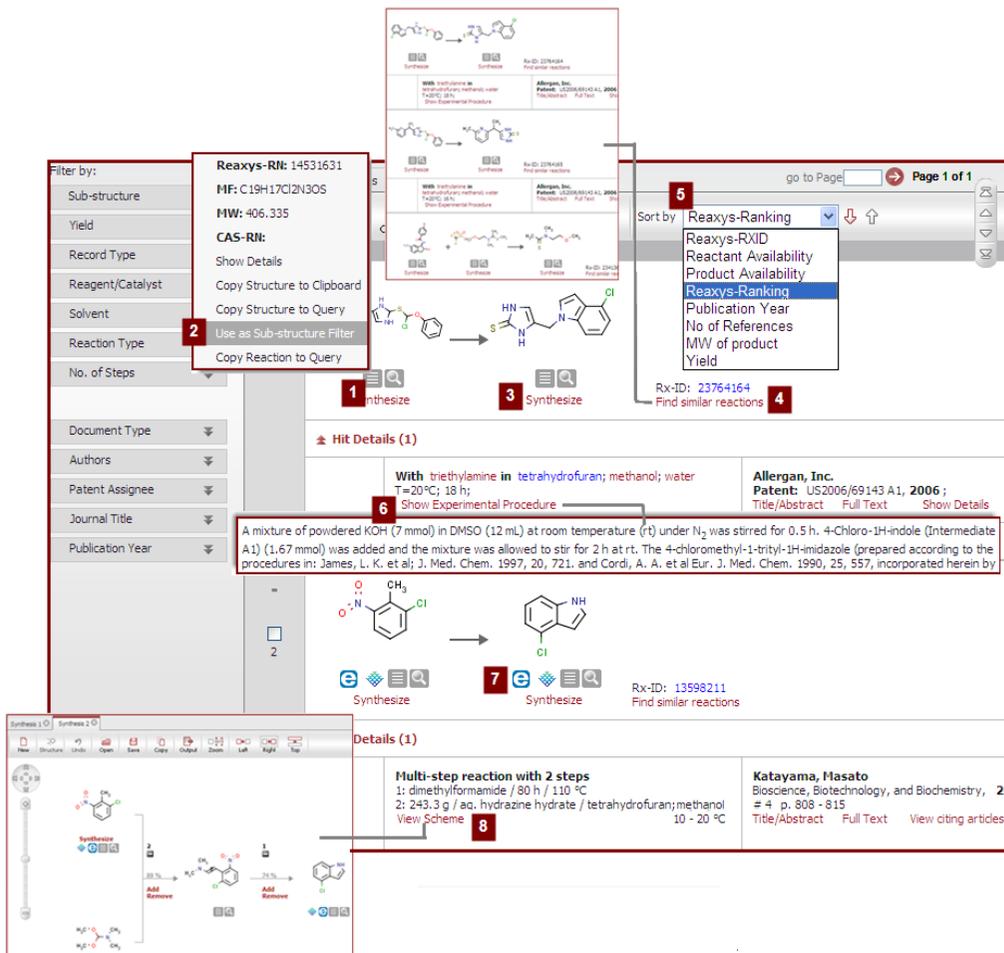
- Limit to Selection:** Click here after selecting reactions
- Export:** Select a file type for export
- Quick Print:** Prints the current display
- Zoom:** Increase or decrease the size of the displayed structures
- Hide Details:** Hide or display details
- Sort:** Sort by Reaxys-Ranking

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.

- Breadcrumbs**
Graphical navigation helps keep track of your results analysis.
- Create Alert**
Click this link to create an alert.
- 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).
- Reactions/citations tab**
Reactions tab is displayed by default, but you can switch to the citations tab.
- 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**).
- Tool bar**
Access Limit to Selection, Output, Quick Print, Zoom, Hide Details, and Sort by features.

Reactions results Reactions tab



The screenshot shows the Reaxys Reactions tab interface. On the left is a filter sidebar with options like Sub-structure, Yield, Record Type, Reagent/Catalyst, Solvent, Reaction Type, No. of Steps, Document Type, Authors, Patent Assignee, Journal Title, and Publication Year. A pop-up menu for a selected reaction (Reaxys-RN: 14531631) lists options: Show Details, Copy Structure to Clipboard, Copy Structure to Query, Use as Sub-structure Filter, and Copy Reaction to Query. A 'Sort by' dropdown menu is open, showing options: Reaxys-Ranking, Reaxys-RXID, Reactant Availability, Product Availability, Reaxys-Ranking, Publication Year, No of References, MW of product, and Yield. The main area displays a list of reaction hits. The first hit is selected, showing experimental details: 'With triethylamine in tetrahydrofuran; methanol; water; T=20°C; 18 h; Allergan, Inc. Patent: US2006/69143 A1; 2006;'. Below this is the experimental procedure text and a chemical reaction scheme. A 'Synthesize' button is visible. The second hit is also shown, labeled 'Multi-step reaction with 2 steps', with reagents and conditions listed, and a 'View Scheme' button. A navigation tool on the right side of the screen allows jumping between hits.

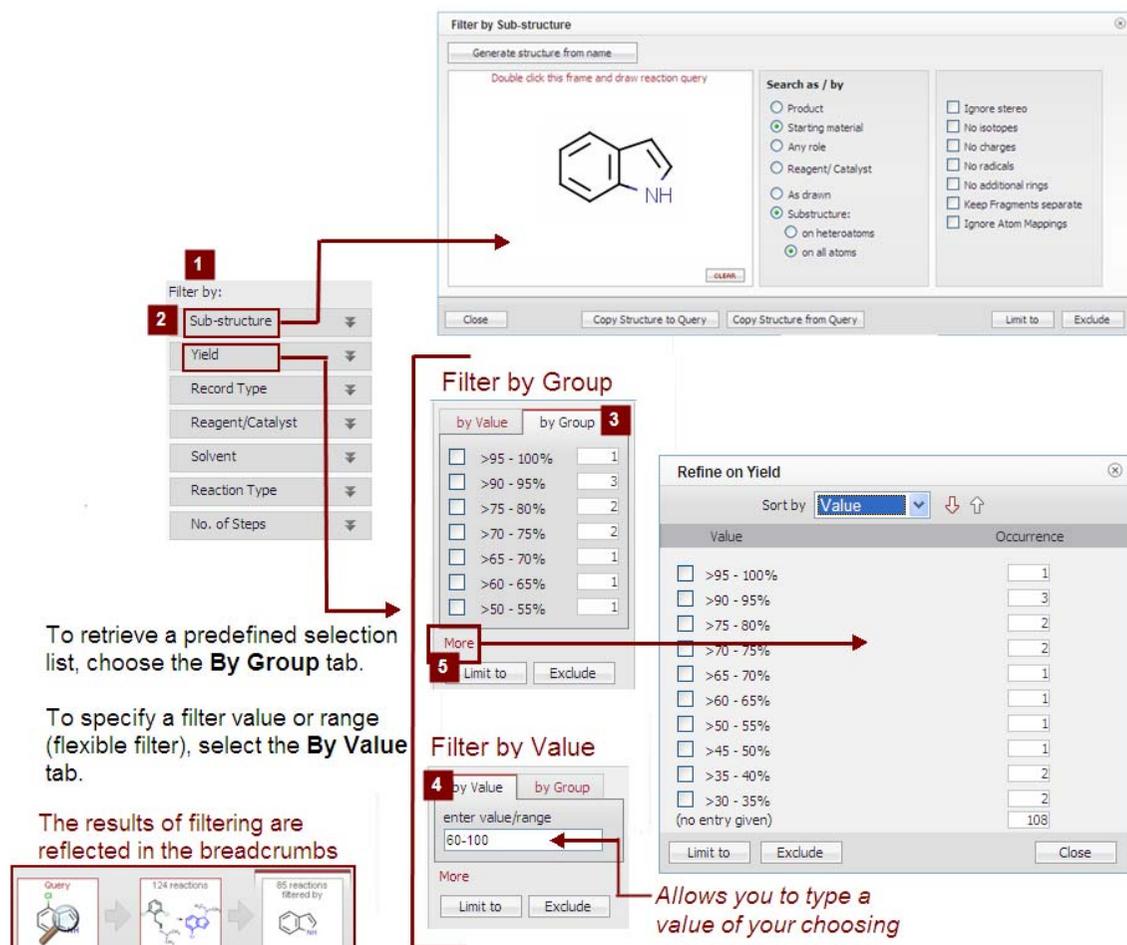
Note:
Information on
the Citations
tab of Reaction
Results can be
Found on pg.24

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.

- 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:

- 2** Sub-structure
- Yield
- Record Type
- Reagent/Catalyst
- Solvent
- Reaction Type
- No. of Steps

3 Filter by Group

by Value	by Group
<input type="checkbox"/> >95 - 100%	1
<input type="checkbox"/> >90 - 95%	3
<input type="checkbox"/> >75 - 80%	2
<input type="checkbox"/> >70 - 75%	2
<input type="checkbox"/> >65 - 70%	1
<input type="checkbox"/> >60 - 65%	1
<input type="checkbox"/> >50 - 55%	1

4 Filter by Value

enter value/range
60-100

5 More

Limit to Exclude

Refine on Yield

Sort by Value

Value	Occurrence
<input type="checkbox"/> >95 - 100%	1
<input type="checkbox"/> >90 - 95%	3
<input type="checkbox"/> >75 - 80%	2
<input type="checkbox"/> >70 - 75%	2
<input type="checkbox"/> >65 - 70%	1
<input type="checkbox"/> >60 - 65%	1
<input type="checkbox"/> >50 - 55%	1
<input type="checkbox"/> >45 - 50%	1
<input type="checkbox"/> >35 - 40%	2
<input type="checkbox"/> >30 - 35%	2
(no entry given)	108

Limit to Exclude Close

To retrieve a predefined selection list, choose the **By Group** tab.

To specify a filter value or range (flexible filter), select the **By Value** tab.

The results of filtering are reflected in the breadcrumbs

Allows you to type a value of your choosing

- 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**.

New
Open a blank page and start a new synthesis plan

Structure
Opens a structure/reaction query box so you can start a new synthesis plan

Undo
Open a saved synthesis plan

Save
Copy Plan to a New Page
Opens a new tab and copies the current synthesis plan

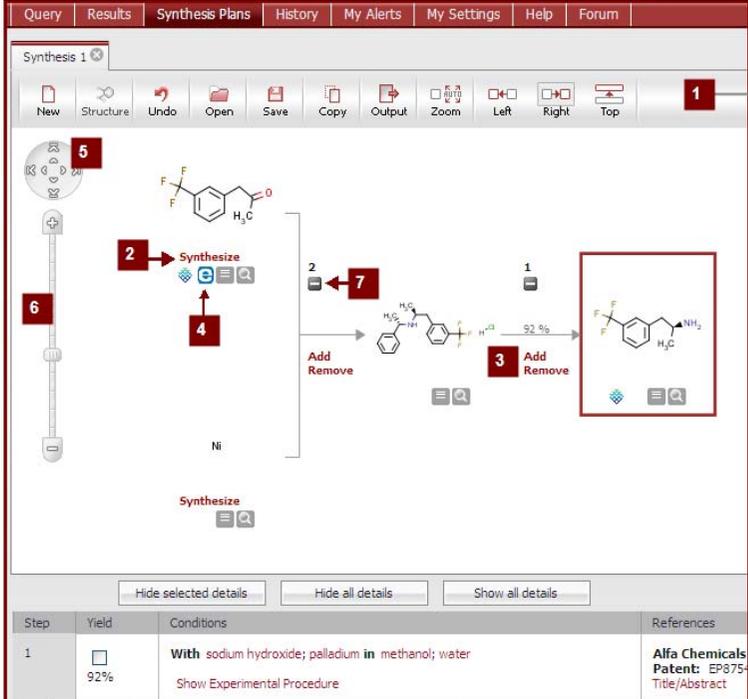
Output
Select a file type for export

Auto Zoom
Increases the size of the synthesis plan to the largest size

Right to Left View
Product is displayed on the left

Left to Right View
Product is displayed on the right

Vertical Tree View
Product is displayed at the top



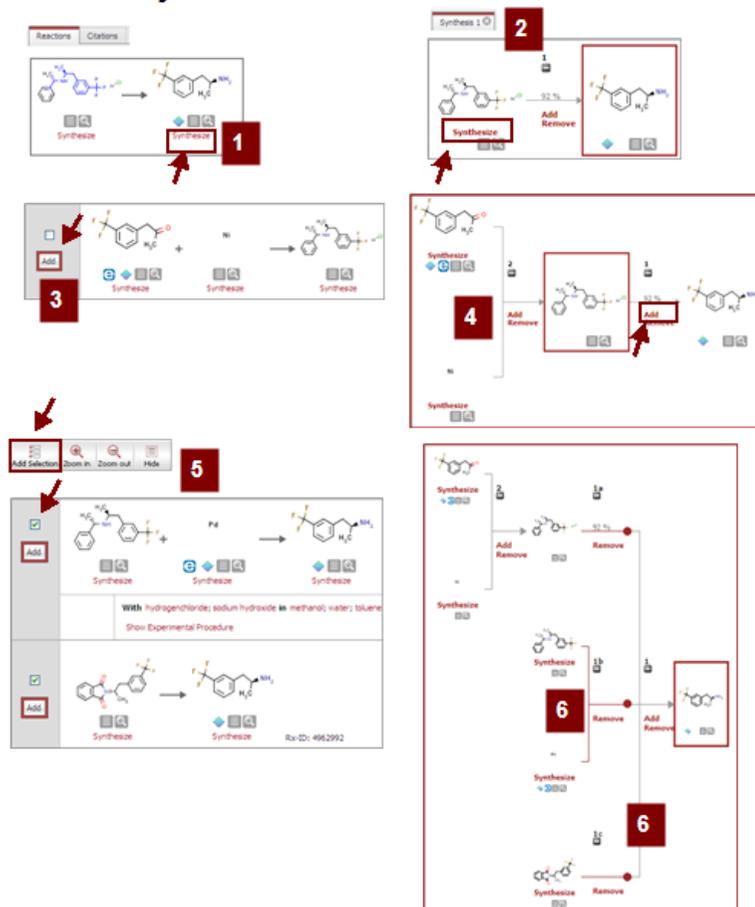
Step	Yield	Conditions	References
1	92%	With sodium hydroxide; palladium in methanol; water Show Experimental Procedure	Alfa Chemicals Patent: EP875- Title/Abstract

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

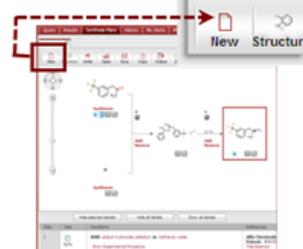
Note: the overall scheme of multi-step reactions can be displayed in the synthesis plans page. A click on the **View Scheme** hyperlink opens the multi-step sequence as a new synthesis plan for a better overview.

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

Output

Select file type:

Output Substance Results

1 Output Substance Grid Substance Details Table Substance Citations Table

2 to PDF/Print XML Microsoft Word Literature Management Systems (e.g. ReferenceManager, EndNote etc.) RD File SD/Molfile Microsoft Excel Smiles

Output Reaction Results

Output Reactions Table Reactions Citation Table

to PDF/Print XML Microsoft Word Literature Management Systems (e.g. ReferenceManager, EndNote etc.) RD File Microsoft Excel

Output Citation Results

Output Citations Table Citation Reactions Table Citation Substances Grid Citation Substances Table

to PDF/Print XML Microsoft Word Literature Management Systems (e.g. ReferenceManager, EndNote etc.) RD File Microsoft Excel

Select range:

Include the following headline **3**

Output range All Hits Range: **4**
e.g. 1, 2-5, 10

5 Output Contains:

Citations

include Abstracts

include Structures

include Reactions

include Front page Information

All available data

Reactions

include Structures

include Experimental Procedure

All available data

Identification data only

Hit data only

Substances

include Structures

All available data

Identification data only

Hit data only

Select data

Select All

Please select the facts you want to export from the list below.

Physical Data Use/Application

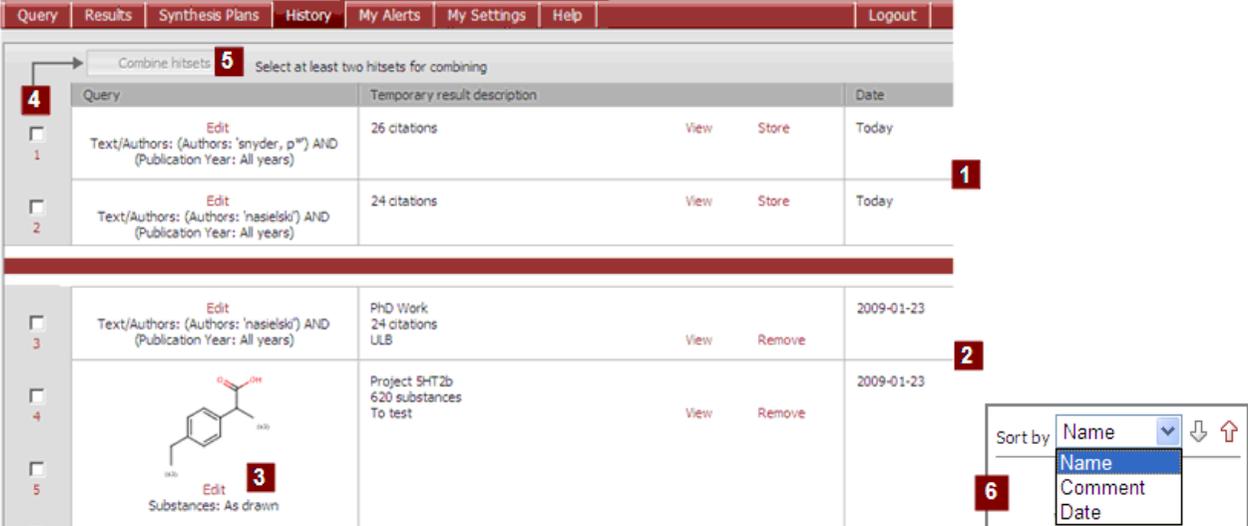
Liquid/Solid Systems (HCS) (2) Use (4)

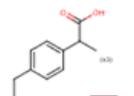
Boiling Point (2) Spectra

Melting Point (2) NMR Spectroscopy (4)

- 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.



Query	Temporary result description	Date
1 Text/Authors: (Authors: 'snyder, p*') AND (Publication Year: All years)	26 citations View Store	Today
2 Text/Authors: (Authors: 'nasielski') AND (Publication Year: All years)	24 citations View Store	Today
3 Text/Authors: (Authors: 'nasielski') AND (Publication Year: All years)	PHD Work 24 citations ULB View Remove	2009-01-23
4  Substances: As drawn	Project 5HT2b 620 substances To test View Remove	2009-01-23

Select how you want to combine the hitsets

Combine hitsets 5

If 2 hits are selected

Merge 3 with 4, Overlap 3 with 4, Exclude 3 from 4, Exclude 4 from 3

Select how you want to combine the hitsets

If >2 hits are selected

Merge all, Overlap all

Sort by: Name

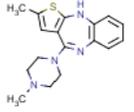
- Name
- Comment
- Date

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**
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.
- 5 **Combine hitsets**
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.

Query Results Synthesis Plans History **My Alerts** My Settings Help Logout

To create a new Alert perform a new search and click the 'Create Alert' link on the results page **1**

Name	Query	Description	Date created	Last run	Frequency
olanzapin		Reactions: Product, As drawn, Yield>86 Comment: Olanzapin Synthesis Yield>86%	2009-10-19	2009-10-21 hits: 11	Monthly
testdiclofena		Reactions: Product, As drawn	2009-10-22	2009-10-22 hits: 79	After each update

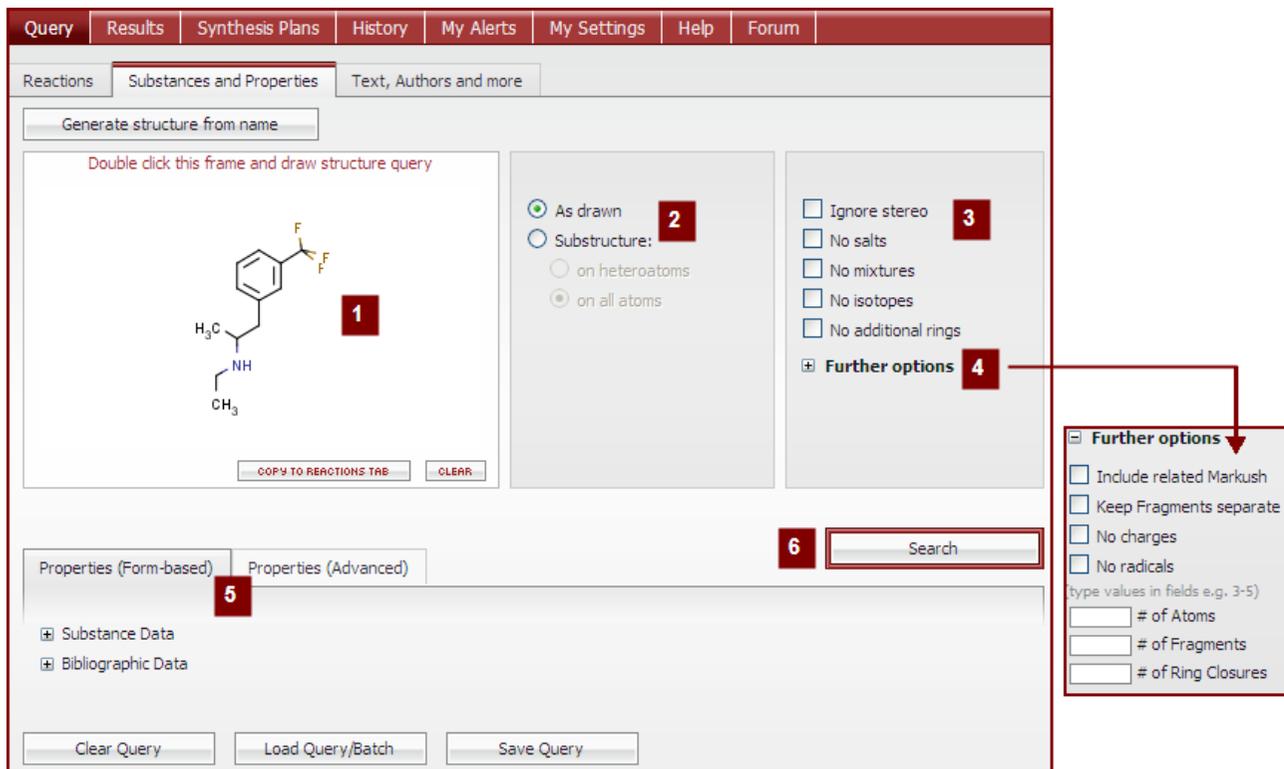
5 1 **6** Delete **2** View results **3** Modify alert **4** Save

7 Info: Reaxys didn't find a result that matched your query. Please consider a reformulation with less constraints and search again. [Create Alert](#) from this query... Show technical details... Close

- My Alerts menu displays the list of available alerts together with the given result sets.*
- 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.
 - View results button**
Click this link to jump to the Results menu and access the hits linked to your alert.
 - Modify alert**
Modify the options of your alert (*Name of Alert, Copy to, Comment/Description, Frequency and Email format*). Click the Save button.
 - Delete**
Check the box close to the alert name column; the delete button becomes available and will discard the concerned alert.
 - What if there are no hits?**
Reaxys will display a message box with a *Create Alert* link.

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.

Substances and properties Query tab



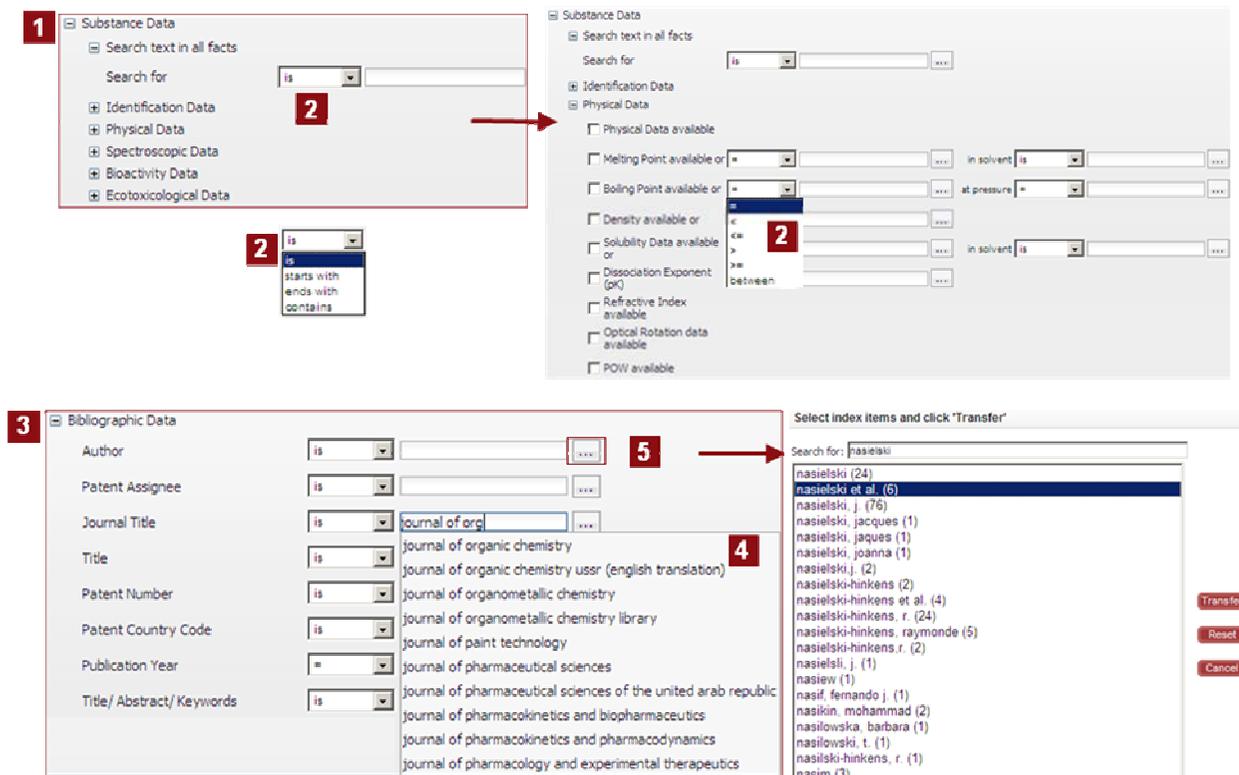
- 1 Structure/reaction box**
This window contains the needed structure, with additional query features. Two buttons enable the structure to be copied to the reactions query tab, and also to delete it.
- 2 Search as**
Define the type of structure search: as *drawn* (including possible query features added 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.

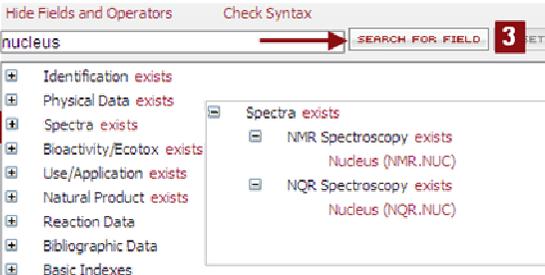
Note: Reaxys remembers the last query form used, and will reopen it in the next session; the substances and properties query tab can then become an entry form.

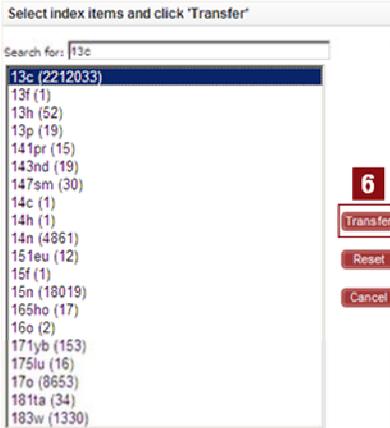
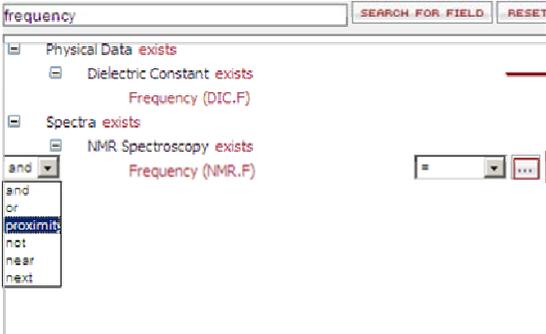
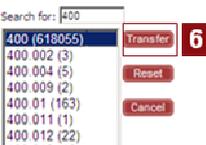
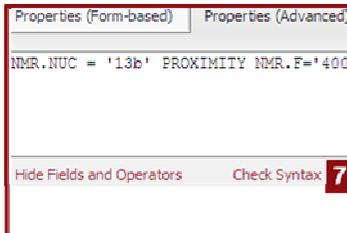
Substances query tab Properties (Form-based)



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.

1 Show Fields and Operators

2

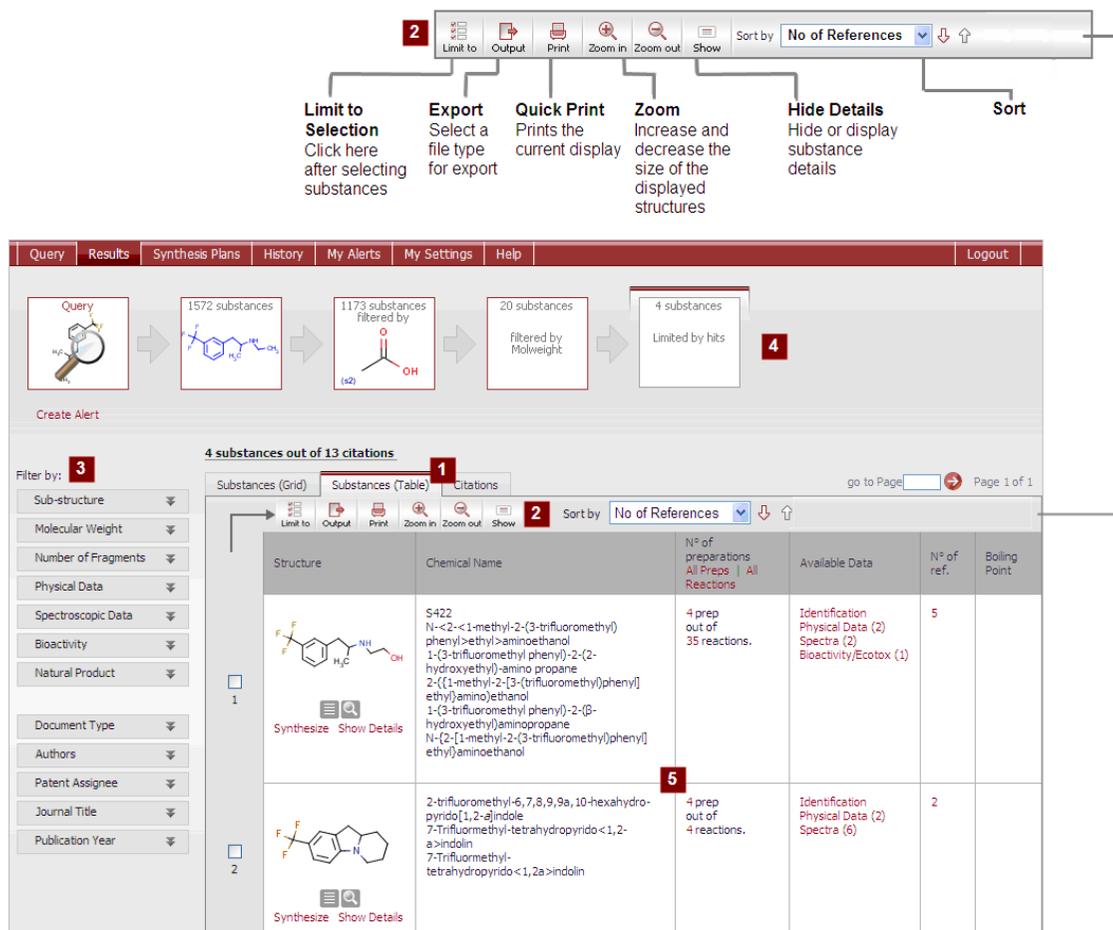





- 1 Show Fields and Operators**
Expand the fields list. Manually select the field code from the hierarchical list or use **Search for Field** button.
- 2 Fields Category**
Click the + sign to expand the needed fields list.
- 3 Search for Field button**
Type the name of the desired constraint, and click 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



2 Limit to Selection: Click here after selecting substances

2 Export: Select a file type for export

2 Quick Print: Prints the current display

2 Zoom: Increase and decrease the size of the displayed structures

2 Hide Details: Hide or display substance details

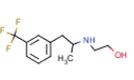
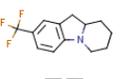
2 Sort: Sort by No of References

3 Filtered by: Sub-structure, Molecular Weight, Number of Fragments, Physical Data, Spectroscopic Data, Bioactivity, Natural Product, Document Type, Authors, Patent Assignee, Journal Title, Publication Year

4 Breadcrumbs: 1572 substances → 1173 substances filtered by → 20 substances filtered by Molweight → 4 substances Limited by hits

1 Substances (Grid) | Substances (Table) | Citations

5 Substances and properties results table:

Structure	Chemical Name	N° of preparations All Preps All Reactions	Available Data	N° of ref.	Boiling Point
	S-422 N-<2-<1-methyl-2-(3-trifluoromethyl)phenyl>ethyl>aminoethanol 1-(3-trifluoromethyl phenyl)-2-(2-hydroxyethyl)-amino propane 2-((1-methyl-2-[3-(trifluoromethyl)phenyl]ethyl)amino)ethanol	4 prep out of 35 reactions.	Identification Physical Data (2) Spectra (2) Bioactivity/ECotox (1)	5	
	2-trifluoromethyl-6,7,8,9,9a,10-hexahydro-pyrido[1,2-a]indole 7-Trifluoromethyl-tetrahydropyrido<1,2-a>indolin 7-Trifluoromethyl-tetrahydropyrido<1,2a>indolin	4 prep out of 4 reactions.	Identification Physical Data (2) Spectra (6)	2	

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

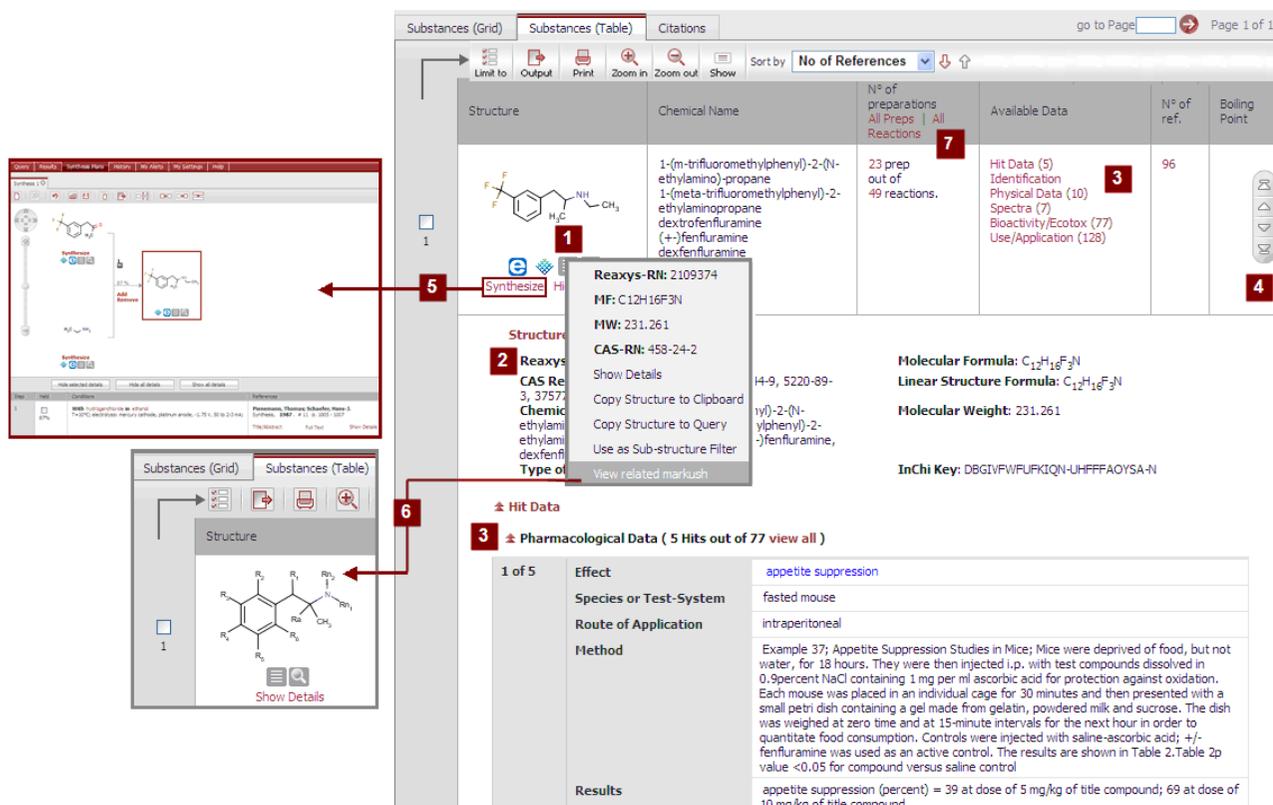
Graphical navigation keeps track of your result analysis. The highlighted breadcrumb denotes the current result display.

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.

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

Substances and properties Substances (Table) tab



The screenshot shows the Reaxys interface with the 'Substances (Table)' tab selected. The table lists substances with columns for Structure, Chemical Name, N° of preparations, Available Data, N° of ref., and Boiling Point. Callouts 1-7 highlight specific features:

- 1**: Points to the chemical name and structure of dextrofenfluramine.
- 2**: Points to the 'Structure' link in the available data column.
- 3**: Points to the 'Available Data' column, which lists various data types like Hit Data, Physical Data, Spectra, etc.
- 4**: Points to the navigation bar on the right side of the table.
- 5**: Points to the 'Synthesize' link in the available data column.
- 6**: Points to the 'View Related Markush' link in the available data column.
- 7**: Points to the 'All Preps / All Reactions' link in the available data column.

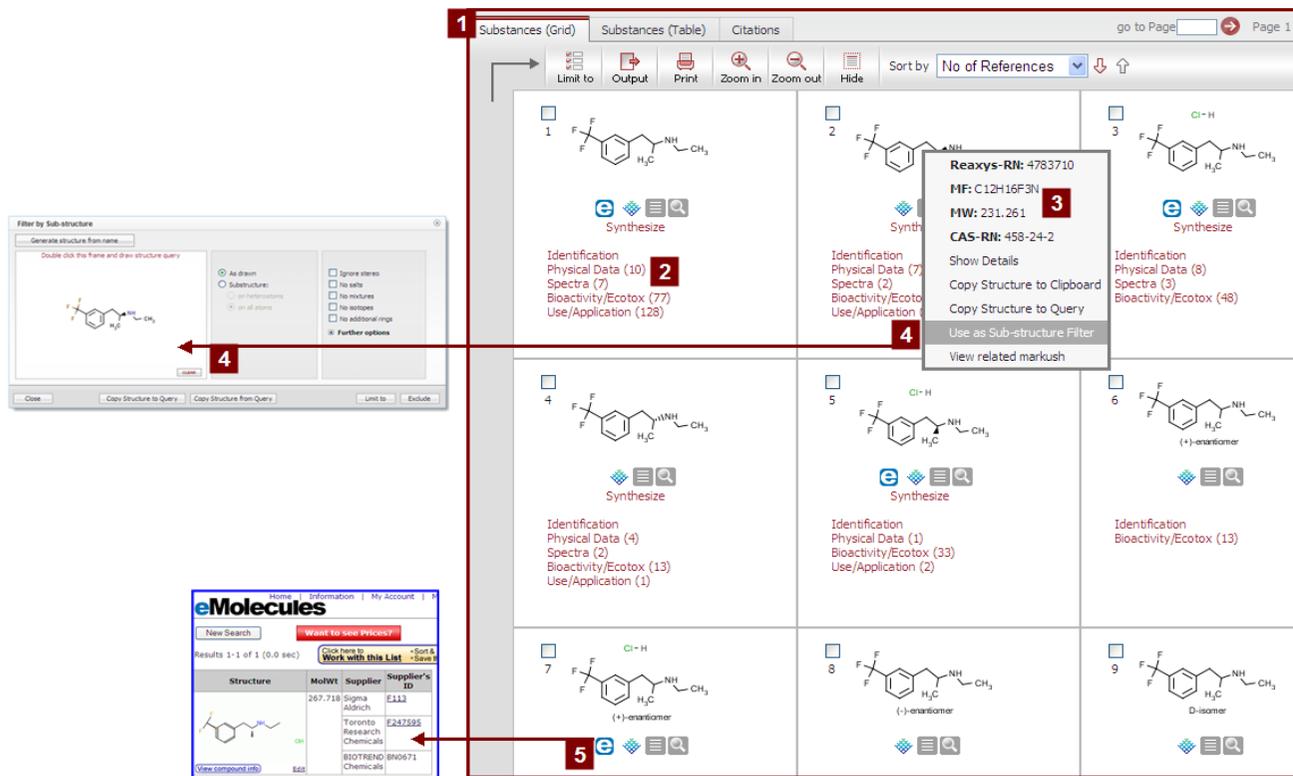
Below the table, a 'Hit Data' section is visible, showing pharmacological data for the selected substance, including effect (appetite suppression), species (fasted mouse), and route of application (intraperitoneal).

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 Navigation 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.

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

Substances and properties Substances (Grid) tab



The screenshot shows the Reaxys interface with the 'Substances (Grid)' tab selected. The grid contains several chemical structures, each with a 'Synthesize' button and a list of available data. A red box highlights the 'Substances (Grid)' tab. A red box highlights the 'Synthesize' button for the first structure. A red box highlights the 'Reaxys-RN: 4783710' link in the pop-up menu. A red box highlights the 'Use as Sub-structure Filter' link in the pop-up menu. A red box highlights the 'eMolecules' link in the bottom left corner. A red box highlights the 'Structure' column in the eMolecules table.

1 Substances (Grid) Substances (Table) Citations go to Page Page 1

Limit to Output Print Zoom in Zoom out Hide Sort by No of References

1 2 3

4 5

Filter by Sub-structure
Generate structure from name
Double click the frame and draw structure query

As drawn
Substructure:
No stereo
on all atoms
Ignore stereo
No wets
No residues
No isotopes
No additional rings
Further options

Close Copy Structure to Query Copy Structure from Query Limit to Exclude

eMolecules
Home Information My Account
New Search Want to see prices?
Click here to Work with this List Sort & Save

Structure	MolWt	Supplier	Supplier's ID
	267.718	Sigma Aldrich	E113
		Toronto Research Chemicals	E247595
		BIOTREND	BN0671 Chemicals

View compound (8)

View related markush

Reaxys-RN: 4783710
MF: C₁₂H₁₆F₃N
MW: 231.261
CAS-RN: 458-24-2

Show Details
Copy Structure to Clipboard
Copy Structure to Query
Use as Sub-structure Filter
View related markush

Identification
Physical Data (10)
Spectra (7)
Bioactivity/ECotox (77)
Use/Application (128)

Identification
Physical Data (7)
Spectra (2)
Bioactivity/ECotox (48)
Use/Application (1)

Identification
Physical Data (8)
Spectra (3)
Bioactivity/ECotox (48)

Identification
Physical Data (4)
Spectra (2)
Bioactivity/ECotox (13)
Use/Application (1)

Identification
Physical Data (1)
Spectra (2)
Bioactivity/ECotox (33)
Use/Application (2)

Identification
Bioactivity/ECotox (13)

Identification
Physical Data (1)
Spectra (2)
Bioactivity/ECotox (33)
Use/Application (2)

Identification
Bioactivity/ECotox (13)

Identification
Physical Data (1)
Spectra (2)
Bioactivity/ECotox (33)
Use/Application (2)

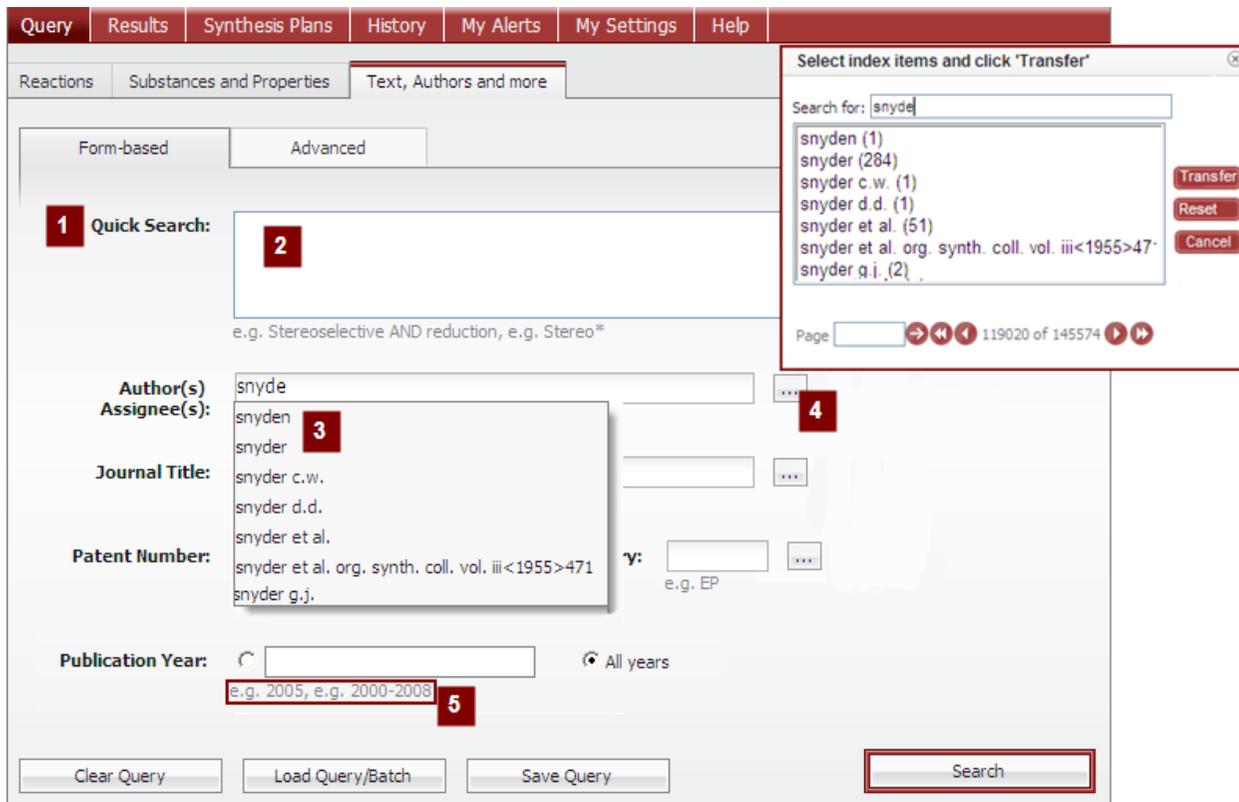
Identification
Bioactivity/ECotox (13)

Identification
Physical Data (1)
Spectra (2)
Bioactivity/ECotox (33)
Use/Application (2)

Identification
Bioactivity/ECotox (13)

- Grid view**
For a quick overview results are displayed in a grid.
- Available data for this substance**
Various red hyperlinks display the information available by substance.
- 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
- Use as Substructure Filter**
Opens a separate query box with the structure in it.
- 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.

Text, authors and more Query tab (Advanced)

1 Show Fields and Operators

- 2 Bibliographic Data
- 2 Identification exists
- 2 Physical Data exists
- 2 Spectra exists
- 2 Bioactivity/Ecotox exists
- 2 Use/Application exists
- 2 Natural Product exists
- 2 Quantum Chemical Data exists
- 2 Reaction Data
- 2 Basic Indexes

Select index items and click 'Transfer'

Search for: tetra

- tetrahedon lettes (1)
- tetrahedom letters (1)
- tetrahedron (37230)**
- tetrahedron letters (80841)
- tetrahedron, (1)
- tetrahedron, supplement (146)
- tetrahedron. letters (1)
- tetrahedron: asymmetry (8633)
- tetrahedron letters (1)

Transfer Reset Cancel

Page: 777 of 918

The final query looks like this:

Form-based Advanced

```
CIT.JT = 'tetrahedron' AND CIT.PY>'2007'
```

3

Hide Fields and Operators Check Syntax **6**

title SEARCH FOR FIELD RESET

- Bibliographic Data
 - Citation
 - Journal Title (CIT.JT)**
 - Journal Title (Short) (CIT.JTS)
 - Abstract
 - Title (AB.TI)

4

is

is

starts with

ends with

contains

5

Select index items and click 'Transfer'

Search for: 2007

- 2007 (132427)**
- 2008 (125956)
- 2009 (109306)
- 2010 (38960)
- 2011 (1)
- 2021 (1)
- 19036 (1)
- 20008 (1)
- 20100 (1)

Transfer Reset Cancel

Add more parameters

year SEARCH FOR FIELD RESET

- Bibliographic Data
 - Citation
 - Patent Year (CIT.PPY)
 - Publication Year (CIT.PY)**

and

=

<

<=

>

>=

between

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.

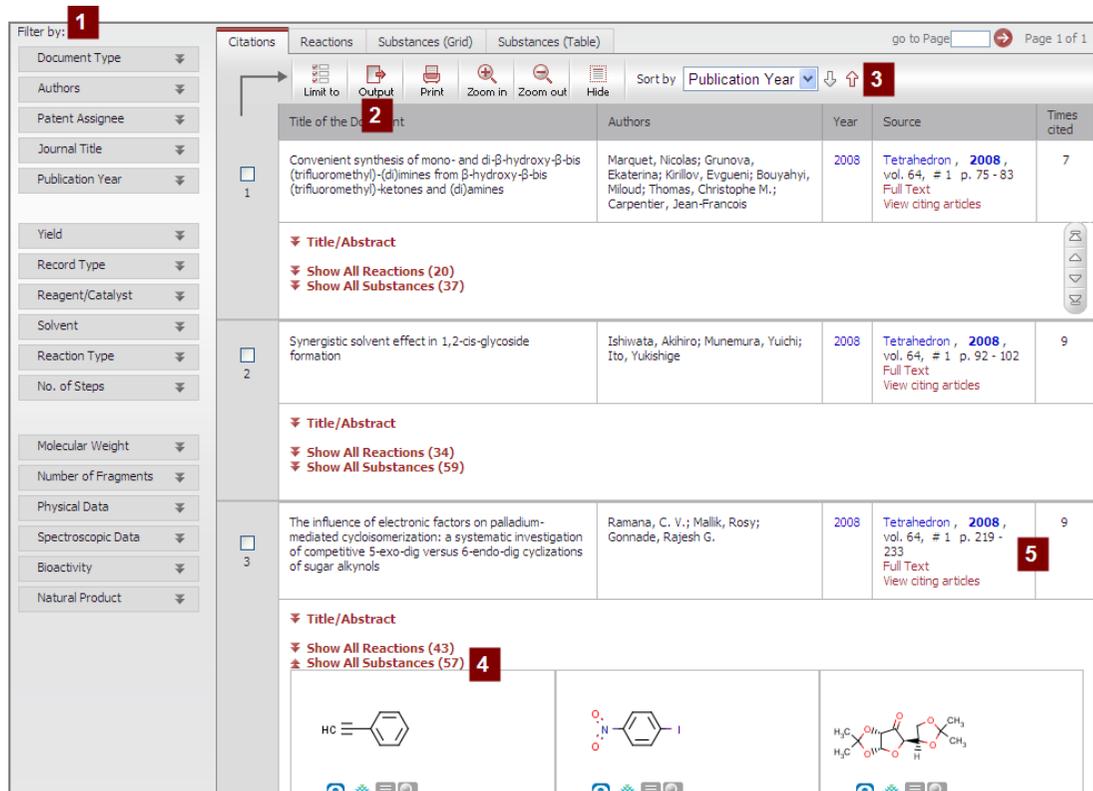
3 Search for Field button
Type the name of the desired constraint, and click this button to locate the needed field.

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.





The screenshot shows the Reaxys Citations tab interface. On the left, a 'Filter by:' sidebar (1) contains various filters such as Document Type, Authors, Patent Assignee, Journal Title, Publication Year, Yield, Record Type, Reagent/Catalyst, Solvent, Reaction Type, No. of Steps, Molecular Weight, Number of Fragments, Physical Data, Spectroscopic Data, Bioactivity, and Natural Product. The main area displays a table of citations. The table has columns for Title of the Document (2), Authors, Year, Source, and Times cited (3). Three entries are visible:

Title of the Document	Authors	Year	Source	Times cited
Convenient synthesis of mono- and di-β-hydroxy-β-bis (trifluoromethyl)-(d)imines from β-hydroxy-β-bis (trifluoromethyl)-ketones and (d)amines	Marquet, Nicolas; Grunova, Ekaterina; Kirillov, Evguenii; Bouyahyi, Miloud; Thomas, Christophe M.; Carpentier, Jean-Francois	2008	Tetrahedron , 2008 , vol. 64, # 1 p. 75 - 83 Full Text View citing articles	7
Synergistic solvent effect in 1,2-dis-glycoside formation	Ishiwata, Akshiro; Munemura, Yuichi; Ito, Yukishige	2008	Tetrahedron , 2008 , vol. 64, # 1 p. 92 - 102 Full Text View citing articles	9
The influence of electronic factors on palladium-mediated cycloisomerization: a systematic investigation of competitive 5-exo-dig versus 6-endo-dig cyclizations of sugar alkynols	Ramana, C. V.; Mallik, Rosy; Gonnade, Rajesh G.	2008	Tetrahedron , 2008 , vol. 64, # 1 p. 219 - 233 Full Text View citing articles	9

Below the table, there are expandable sections for 'Title/Abstract' (4) and links to 'Show All Reactions' and 'Show All Substances'. The third entry also includes chemical structures (5).

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.