



# Reaxys Quick Reference Guide

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## The basics Where to find what?

To start Reaxys, go to [www.reaxys.com](http://www.reaxys.com)

To find **more user tips**, go to [www.info.reaxys.com](http://www.info.reaxys.com). Here you can find:

- Registration form for the Reaxys newsletter
- Training & Support information, with
  - Training Center giving access to various instructional materials (demos, videos, manuals)
  - Webinar schedule offering regular training sessions and registration form
  - Frequently Asked Questions
  - Downloads of software (plug-ins, structure editors) and of documentation (training materials)
  - Customer Care Contact details:

**Europe, Middle East, Asia and Africa**

**+49 69 5050 4268**

**[nlinfo@reaxys.com](mailto:nlinfo@reaxys.com)**

**Americas**

**+1 888 615 4500**

**[usinfo@reaxys.com](mailto:usinfo@reaxys.com)**

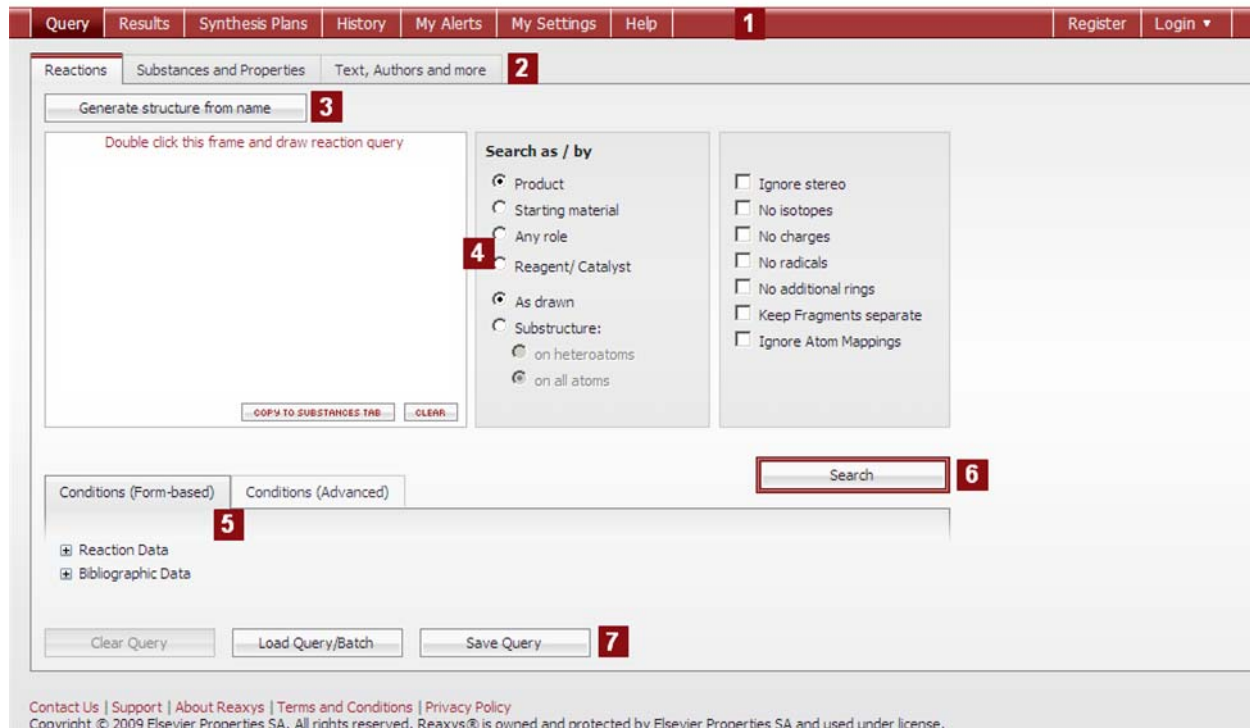
**+1 212 462 1978 if calling outside USA & Canada**

**Japan**

**+81 3 5561 5034**

**[jpinfo@reaxys.com](mailto:jpinfo@reaxys.com)**

## Homepage



The screenshot shows the Reaxys homepage interface. At the top is a navigation bar (1) with links: Query, Results, Synthesis Plans, History, My Alerts, My Settings, Help, Register, and Login. Below this is a sub-navigation bar (2) with tabs: Reactions, Substances and Properties, and Text, Authors and more. The main content area includes a 'Generate structure from name' input field (3) with a 'Double click this frame and draw reaction query' instruction. To the right is a 'Search as / by' section (4) with radio buttons for 'Product', 'Starting material', 'Any role', 'Reagent/ Catalyst', 'As drawn', and 'Substructure:'. The 'Substructure' section has options for 'on heteroatoms' and 'on all atoms'. To the right of these are checkboxes for 'Ignore stereo', 'No isotopes', 'No charges', 'No radicals', 'No additional rings', 'Keep Fragments separate', and 'Ignore Atom Mappings'. Below the search area is a 'Search' button (6). At the bottom are 'Conditions (Form-based)' and 'Conditions (Advanced)' tabs (5), with links for 'Reaction Data' and 'Bibliographic Data'. At the very bottom are 'Clear Query', 'Load Query/Batch', and 'Save Query' buttons (7). A footer contains contact information and copyright details.

- 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.

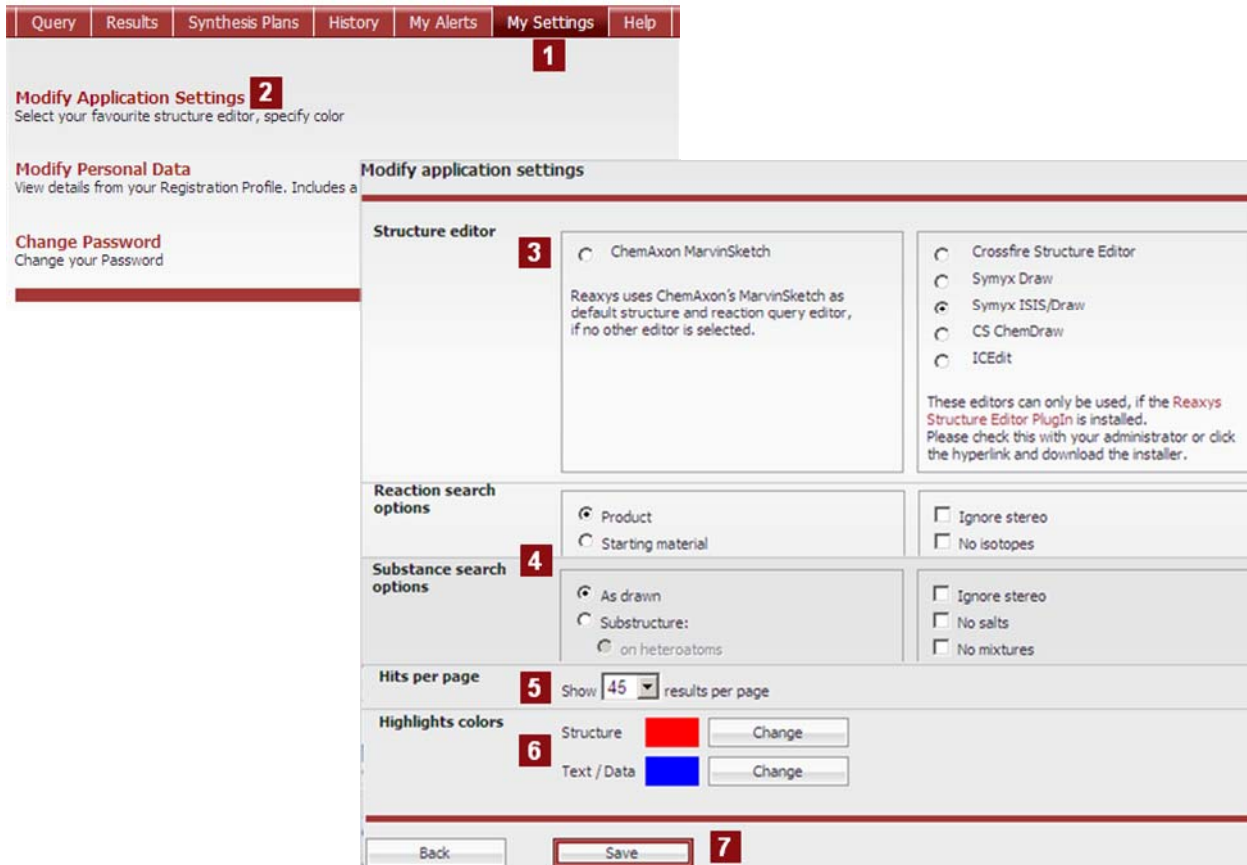
*How to find the preparation of a compound?*

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.*



## My Settings

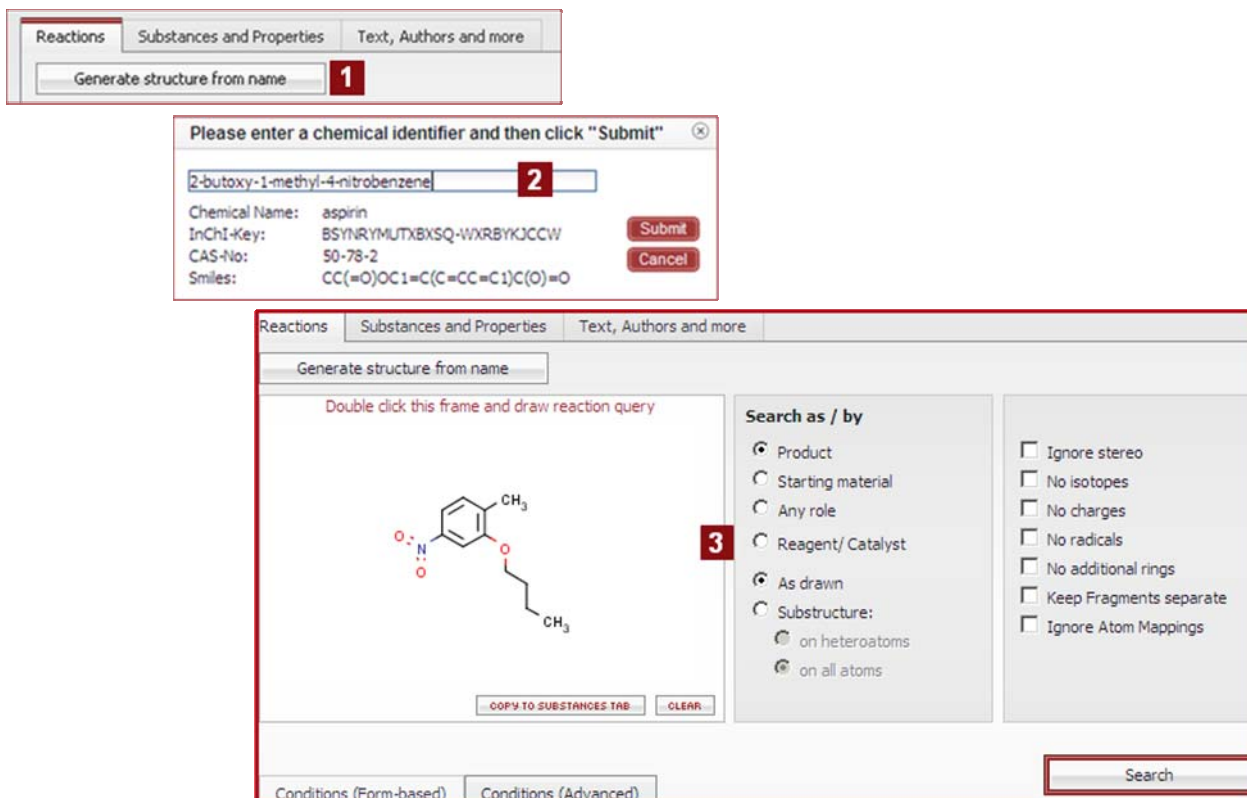


The screenshot shows the 'My Settings' page in the Reaxys interface. The top navigation bar includes 'Query', 'Results', 'Synthesis Plans', 'History', 'My Alerts', 'My Settings' (highlighted with a red box and number 1), and 'Help'. On the left sidebar, there are three main sections: 'Modify Application Settings' (with a red box and number 2), 'Modify Personal Data', and 'Change Password'. The main content area is titled 'Modify application settings' and contains several sections: 'Structure editor' (with a red box and number 3), 'Reaction search options', 'Substance search options' (with a red box and number 4), 'Hits per page' (with a red box and number 5), and 'Highlights colors' (with a red box and number 6). At the bottom, there are 'Back' and 'Save' buttons (with a red box and number 7).

*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, Nb 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.
- 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



Reactions Substances and Properties Text, Authors and more

Generate structure from name **1**

Please enter a chemical identifier and then click "Submit"

2-butoxy-1-methyl-4-nitrobenzene **2**

Chemical Name: aspirin  
InChI-Key: BSYNRYMUTXBXSQ-WXRBYKJCCW  
CAS-No: 50-78-2  
Smiles: CC(=O)OC1=C(C=CC=C1)C(O)=O

Submit Cancel

Reactions Substances and Properties Text, Authors and more

Generate structure from name

Double click this frame and draw reaction query

**3**

Search as / by

☒ Product  
☐ Starting material  
☐ Any role  
☐ Reagent/ Catalyst  
☒ As drawn  
☐ Substructure:  
☐ on heteroatoms  
☒ on all atoms

☐ Ignore stereo  
☐ No isotopes  
☐ No charges  
☐ No radicals  
☐ No additional rings  
☐ Keep Fragments separate  
☐ Ignore Atom Mappings

... COPY TO SUBSTANCES TAB ... CLEAR ...

Conditions (Form-based) Conditions (Advanced)

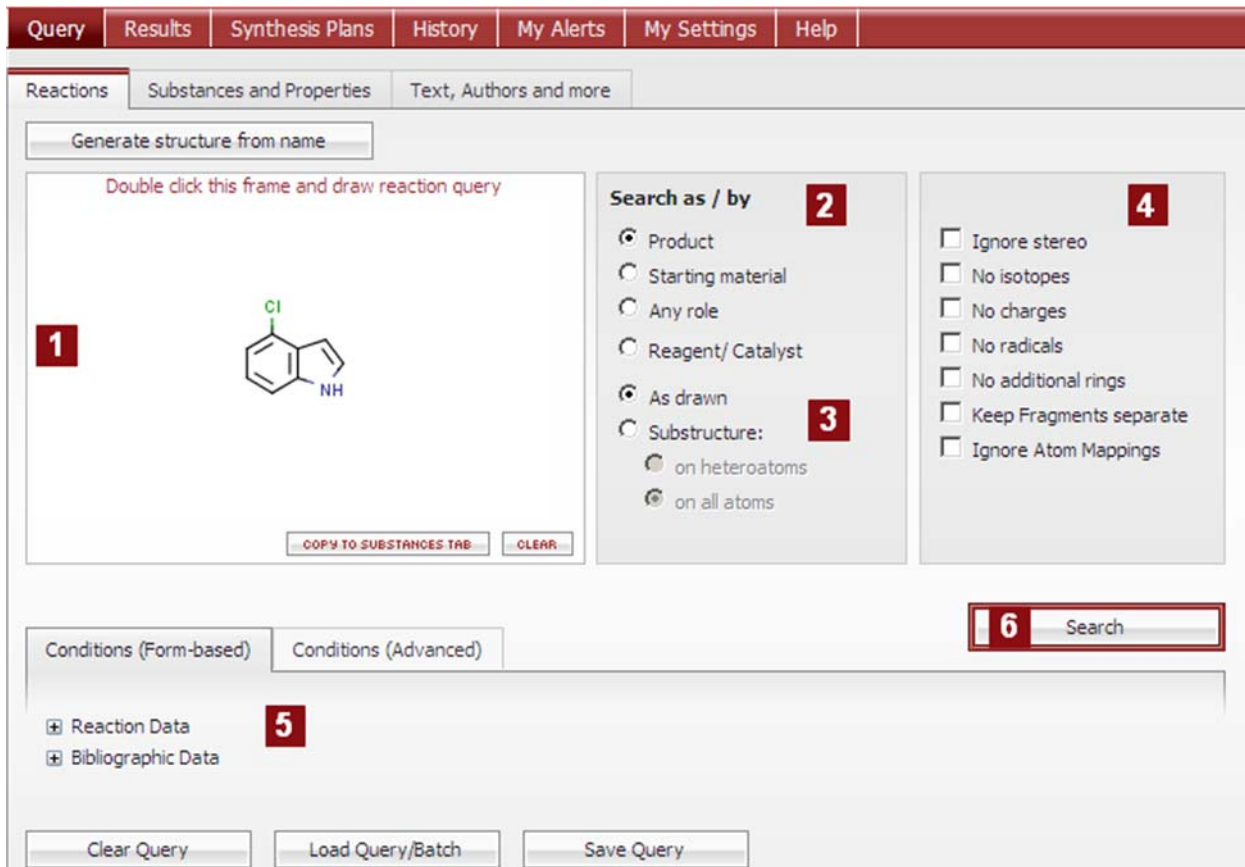
Search

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.

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

## Reactions query tab



The screenshot shows the Reaxys Reactions query tab interface. It includes a top navigation bar with tabs: Query, Results, Synthesis Plans, History, My Alerts, My Settings, and Help. Below this is a sub-navigation bar with tabs: Reactions, Substances and Properties, and Text, Authors and more. The main area contains a 'Generate structure from name' input field. A large central frame (1) displays a chemical structure of 2-chloro-1H-indole with the instruction 'Double click this frame and draw reaction query'. To the right of this frame is a 'Search as / by' section (2) with radio buttons for 'Product', 'Starting material', 'Any role', 'Reagent/ Catalyst', 'As drawn', and 'Substructure:'. The 'Substructure' option is selected, with sub-options 'on heteroatoms' and 'on all atoms' (3). To the right of the 'Search as / by' section is a list of checkboxes for additional query options (4): 'Ignore stereo', 'No isotopes', 'No charges', 'No radicals', 'No additional rings', 'Keep Fragments separate', and 'Ignore Atom Mappings'. At the bottom left, there are two tabs for 'Conditions (Form-based)' and 'Conditions (Advanced)', with the 'Form-based' tab selected (5). Below these tabs are checkboxes for 'Reaction Data' and 'Bibliographic Data'. At the bottom right, there is a 'Search' button (6). At the very bottom, there are buttons for 'Clear Query', 'Load Query/Batch', and 'Save Query'.

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 | C:\Documents and Settings\rypensc\Desktop\Reaxys\Cycle.xml | Browse... | 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.



[illegible]

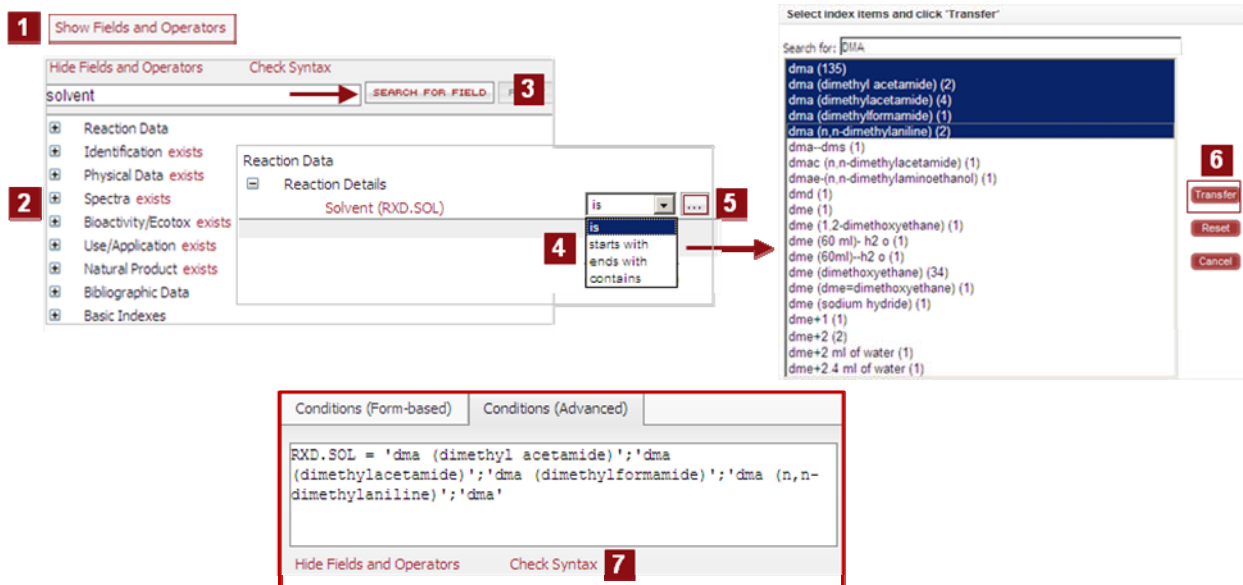
- 1 Reaction data**  
Specify reactant name, product name, reagent, yield and/or all reaction fields.  
*Various selected fields are combined with the Boolean operator AND.*
- 2 Operators**  
Select the appropriate operator from the drop-down menu.
- 3 Selection list**  
Selection appears when typing 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)**



ELSEVIER




## Reactions query tab Conditions (Advanced)

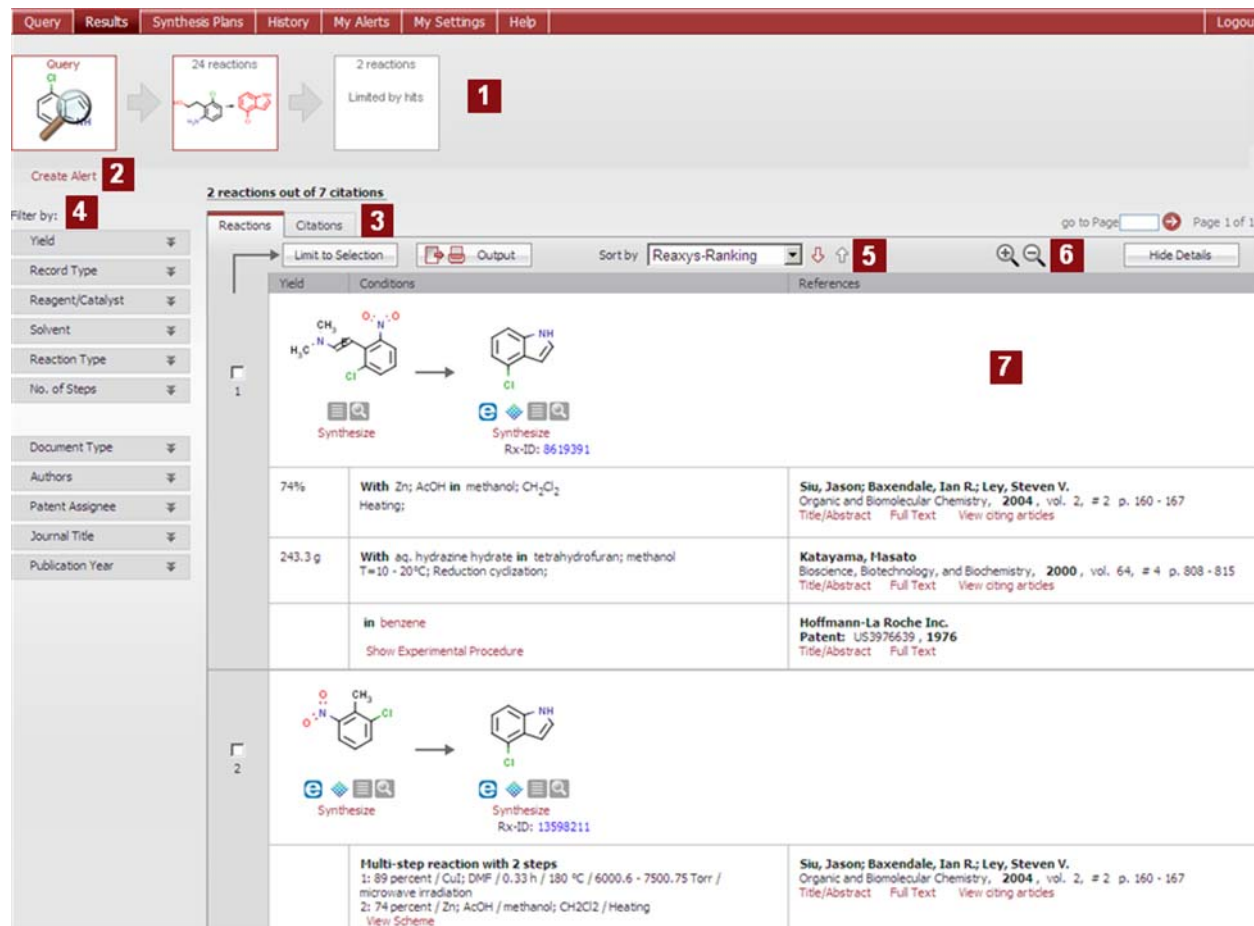


Note: the **Conditions (Advanced)** allows entry of complex and sophisticated property queries in combination with the structure or reaction queries following two ways:

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 screenshot displays the Reaxys interface with the following elements:

- 1 (Breadcrumbs):** A sequence of boxes at the top showing the navigation path: Query (24 reactions) → 2 reactions Limited by hits.
- 2 (Create Alert):** A button labeled "Create Alert" next to the first breadcrumb.
- 3 (Reactions/Citations tab):** The "Reactions" tab is selected, showing a list of reaction results.
- 4 (Filter by):** A sidebar on the left with various filters: Yield, Record Type, Reagent/Catalyst, Solvent, Reaction Type, No. of Steps, Document Type, Authors, Patent Assignee, Journal Title, and Publication Year.
- 5 (Tool bar):** A bar above the reaction list containing "Limit to Selection", "Output", and "Sort by" (set to Reaxys-Ranking).
- 6 (Maximizer/minimizer tool):** A magnifying glass icon used to zoom in or out of the displayed chemical structures.
- 7 (Reaction results):** The main content area showing two reaction schemes. Each scheme includes a chemical reaction diagram, a table of conditions and yields, and a list of references.

**Reaction 1 Details:**

Yield	Conditions	References
74%	With Zn; AcOH in methanol; CH <sub>2</sub> Cl <sub>2</sub> Heating;	Siu, Jason; Baxendale, Ian R.; Ley, Steven V. Organic and Biomolecular Chemistry, 2004, vol. 2, # 2, p. 160 - 167 <a href="#">Title/Abstract</a> <a href="#">Full Text</a> <a href="#">View citing articles</a>
243.3 g	With aq. hydrazine hydrate in tetrahydrofuran; methanol T=10 - 20°C; Reduction cyclization;	Katayama, Masato Bioscience, Biotechnology, and Biochemistry, 2000, vol. 64, # 4, p. 808 - 815 <a href="#">Title/Abstract</a> <a href="#">Full Text</a> <a href="#">View citing articles</a>
	in benzene <a href="#">Show Experimental Procedure</a>	Hoffmann-La Roche Inc. Patent: US3976639, 1976 <a href="#">Title/Abstract</a> <a href="#">Full Text</a>

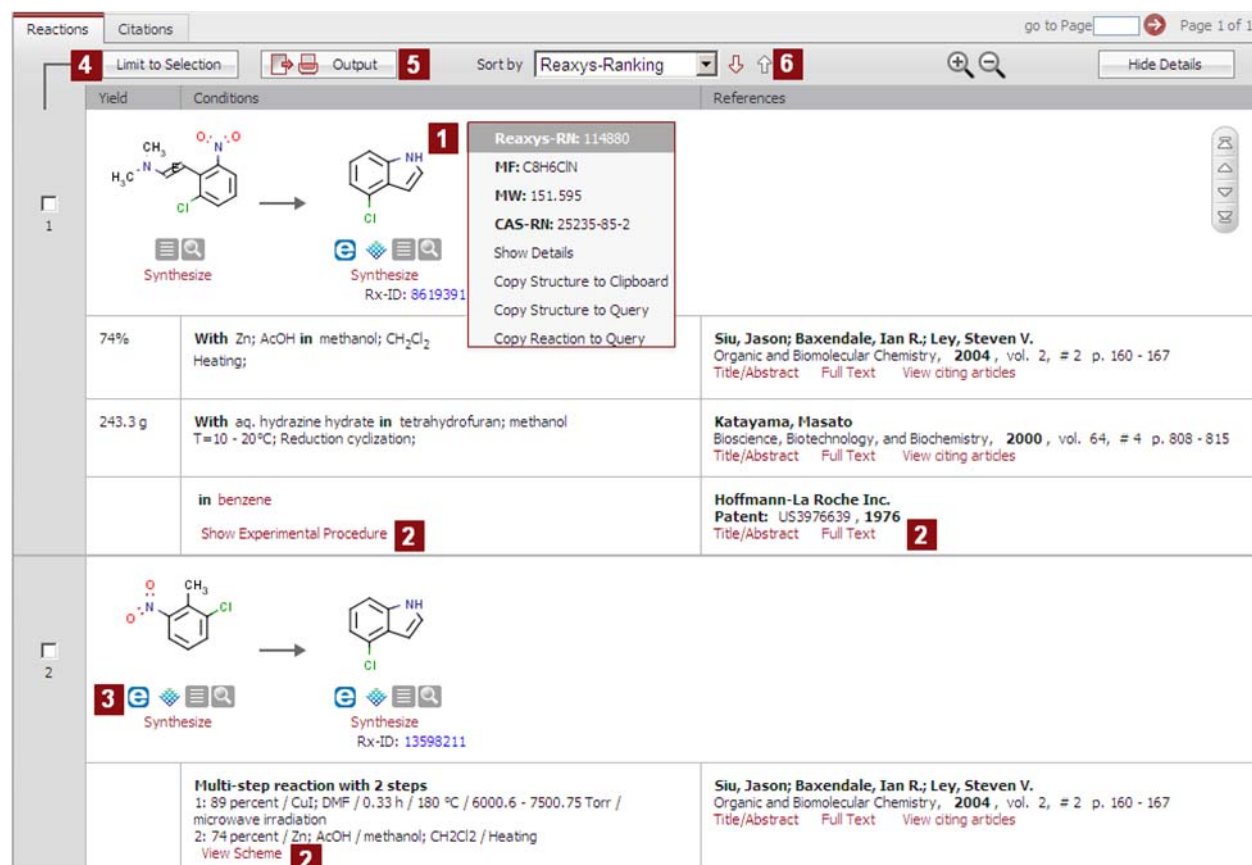
**Reaction 2 Details:**

Yield	Conditions	References
Multi-step reaction with 2 steps 1: 89 percent / CuI; DMF / 0.33 h / 180 °C / 6000.6 - 7500.75 Torr / microwave irradiation 2: 74 percent / Zn; AcOH / methanol; CH <sub>2</sub> Cl <sub>2</sub> / Heating <a href="#">View Scheme</a>		

Have a look at the breadcrumbs at the top of the screen; it shows 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.

- 1 Breadcrumbs**  
Graphical navigation helps keep track of your results analysis.
- 2 Create Alert**  
Click this link to create an alert.
- 3 Reactions/citations tab**  
Reactions tab is displayed by default, but you can switch to the citations tab.
- 4 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).
- 5 Tool bar**  
Access Limit to Selection, Output, and Sort by features.
- 6 Maximizer/minimizer tool**  
Increase or decrease the size of your displayed structures.
- 7 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](#)).


## Reactions results Reactions tab



The screenshot displays the Reaxys Reactions tab interface. At the top, there are tabs for 'Reactions', 'Citations', and 'References'. The 'Reactions' tab is active. The interface includes a navigation bar with buttons for 'Limit to Selection' (4), 'Output' (5), 'Sort by' (6), and 'Hide Details'. The main area shows a list of reaction results. The first reaction (highlighted with a red box and number 1) shows the synthesis of 2-chloro-1H-indole from 2-chloro-1H-indole-3-carbonitrile. The second reaction (highlighted with a red box and number 2) shows the synthesis of 2-chloro-1H-indole from 2-chloro-1H-indole-3-carbonitrile. The interface includes a navigation bar at the top with tabs for Reactions, Citations, and References. The main area is divided into columns for Yield, Conditions, and References. The bottom of the screen shows a multi-step reaction with 2 steps.

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.

Note: information on the citations tab of the reactions results window can be found on page 22.

- 1 **Display further options & data**  
Click  or a structure to get a pop-up menu with information or sub items.  
Reaxys – RN (Reaxys registry number), MF (molecular 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.
- 2 **Access bibliographic details**  
Display the title/abstract, the full text of your reference and view citing articles in Scopus. Show experimental procedure excerpted from patents. View scheme of multi-steps sequence as a synthesis plan.
- 3 **Commercial availability**  
Access the commercial availability of a substance and leads to appropriate companies (eMolecules/Symyx ACD).
- 4 **Limit to selection**  
Select the important hits and click this button to restrict your hitset.
- 5 **Output**  
Export data in the desired format.
- 6 **Sort by**  
Sort results ascending ↑ or descending ↓ by Reaxys-RxID, reactant & product availability, Nb of references, yield, MW of product or Reaxys ranking (default).

## Reactions results tab Filter by

**Filter by Value**

1 Yield

2 by Value by Group

3 enter value/range

4 Limit to Exclude

More

Record Type

Reagent/Catalyst

Solvent

Reaction Type

No. of Steps

**Filter by Group**

6 Document Type

by Value by Group

3 journal 18

4 patent 3

Limit to Exclude

Authors

Patent Assignee

Journal Title

Publication Year

**Refine on Yield**

5 Sort by Value Occ

Value Occ

Value

Occ

>275 - 280 1

>105 - 110 1

>100 - 105 1

>95 - 100 135

>90 - 95 148

>85 - 90 192

>80 - 85 190

>75 - 80 210

>70 - 75 182

>65 - 70 182

>60 - 65 170

>55 - 60 186

>50 - 55 121

>45 - 50 144

Limit to Exclude

**Effect of Filter by 'Yield' on Breadcrumbs**

Query

24 reactions

Query

24 reactions

1 reactions

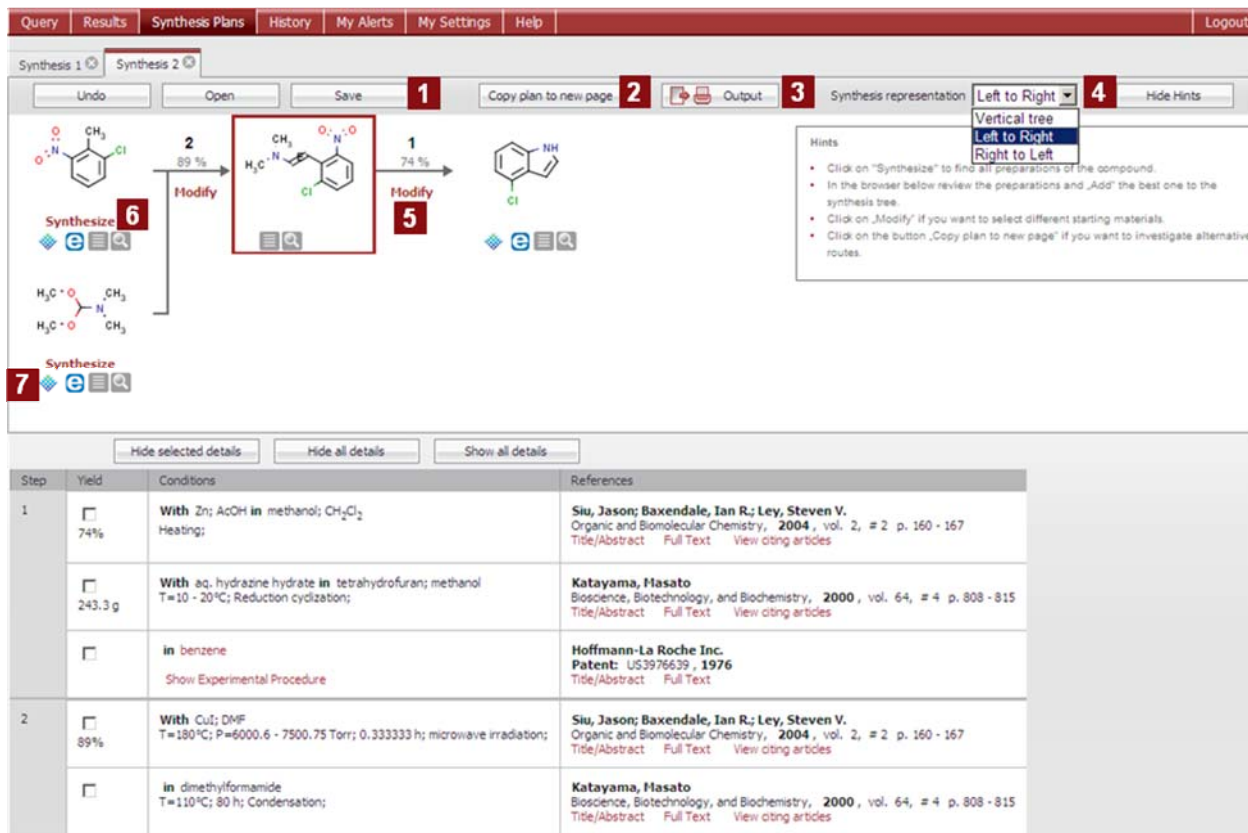
filtered by Yield

- Filter by**  
Select filter(s) linked to reaction specifications:  
- Yield  
- Record type  
- Reagent/catalyst  
- Solvent  
- Reaction type  
- No. of steps
- By Value tab: flexible filter**  
Enter a specific value or a range to refine result sets with more options.
- By Group tab: pre-defined list**  
Check boxes to limit or exclude entries of the pre-defined selection.
- Limit to/exclude buttons**  
Click the appropriate button.
- Refine on Filter field**  
Click the **More** button to expand the scope of the selection, and to further refine the filter by feature. Sort the chosen data by Value or by Occurrence.
- Filter by**  
Specify filter(s) linked to bibliographic data:  
- Document type  
- Authors  
- Patent assignee  
- Journal title  
- Publication year

Note: filter by feature allows for rapid and easy refinement of your results. Click the double arrows to expand the selection list. Two filter options are available for each reaction specification:

- To retrieve a pre-defined selection list, use the **by Group** tab.
- To specify a filter value or range (flexible filter), select the **by Value** tab.

## Synthesis plans



Step	Yield	Conditions	References
1	<input type="checkbox"/> 74%	With Zn; AcOH in methanol; CH <sub>2</sub> Cl <sub>2</sub> Heating;	Siu, Jason; Baxendale, Ian R.; Ley, Steven V. Organic and Biomolecular Chemistry, 2004, vol. 2, # 2 p. 160 - 167 Title/Abstract Full Text View citing articles
	<input type="checkbox"/> 243.3 g	With aq. hydrazine hydrate in tetrahydrofuran; methanol T=10 - 20°C; Reduction cyclization;	Katayama, Masato Bioscience, Biotechnology, and Biochemistry, 2000, vol. 64, # 4 p. 808 - 815 Title/Abstract Full Text View citing articles
	<input type="checkbox"/>	in benzene Show Experimental Procedure	Hoffmann-La Roche Inc. Patent: US3976639, 1976 Title/Abstract Full Text
2	<input type="checkbox"/> 89%	With CuI; DMF T=180°C; P=6000.6 - 7500.75 Torr; 0.333333 h; microwave irradiation;	Siu, Jason; Baxendale, Ian R.; Ley, Steven V. Organic and Biomolecular Chemistry, 2004, vol. 2, # 2 p. 160 - 167 Title/Abstract Full Text View citing articles
	<input type="checkbox"/>	in dimethylformamide T=110°C; 80 h; Condensation;	Katayama, Masato Bioscience, Biotechnology, and Biochemistry, 2000, vol. 64, # 4 p. 808 - 815 Title/Abstract Full Text View citing articles

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 Undo, open and save buttons**  
To undo last action, open or save synthesis plans. Click on the X of the tab to delete an unnecessary plan.
- 2 Copy plan to new page**  
Opens a new tab of your current synthesis plan, where you can develop another retrosynthesis.
- 3 Output**  
Export Synthesis plan
- 4 Synthesis plans representation**  
Choose horizontal tree or vertical tree for the display of your plan.
- 5 Modify**  
Modify discards the already defined synthetic step and proposes other preparations for the compound.
- 6 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.
- 7 Commercial availability**  
Access the commercial availability of a substance and leads to appropriate companies (eMolecules/ACD).



## Output

**Output Reaction Results**

**Output** 1 ☒ Reactions Table ☐ Reactions Citation Table

**to** 2 ☒ PDF/Print ☐ XML ☐ Literature Management Systems (e.g. ReferenceManager, EndNote etc.) ☐ RD File ☐ Microsoft Word ☐ Microsoft Excel

☐ Include the following headline 3

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

**Output contains** 5 ☒ include Structures ☒ include Experimental Procedure ☒ All available data ☐ Identification data only

**Output** ☐ Reactions Table ☒ Reactions Citation Table

**Output contains** ☒ include Structures ☒ include Abstracts 5

**Output** ☐ Substance Grid ☒ Substance Details Table ☐ Substance Citations Table

**Output contains** ☒ include Structures ☒ All available data ☐ Identification data only ☐ Select data 5

**OK** **Cancel** 6

**Spectra** ☒ NMR Spectroscopy (30) ☒ IR Spectroscopy (29) ☒ Mass Spectrometry (22)

**Physical Data** ☒ Melting Point (26) ☒ Crystal Property Description (21) ☒ Further Information (15)

**Bioactivity/Ecotox** ☒ Ecotoxicology (23) ☒ Pharmacological Data (12) ☒ Concentration in the Environment (2)

**Use/Application** ☒ Use (21)

**Natural Product** ☒ Isolation from Natural Product (3) ☒ Derivative (2) ☒ Purification (1)

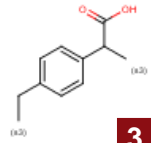
*Note: output function is available on each of the results screens; it allows the export of any type of hitset (reactions, substances and bibliographic data) in any desired format. In the substance details table, click **select data** to choose the type of property you want to export.*

- 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
- 6 **OK button**  
Click the OK button to launch your export. Click cancel to stop this action.

## History

Query Results Synthesis Plans History My Alerts My Settings Help Logout

Combine hitsets 5 Select at least two hitsets for combining

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

Combine hitsets 5

Select how you want to combine the hitsets

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

If 2 hits selected

Select how you want to combine the hitsets

Merge all Overlap all

If >2 hits selected

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

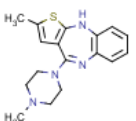
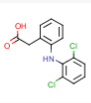
*Note: the history table displays all current-session hitsets resulting from queries or from any analysis of your results; the most recent hitsets are shown at the top of the list. Here you can also graphically combine hitsets.*



## My Alerts

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

Modify alert **2** View results

**3** Modify alert **4** Save

**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 (Name of Alert, Copy to, Comment/Description, Frequency and Email format). Click the Save button.

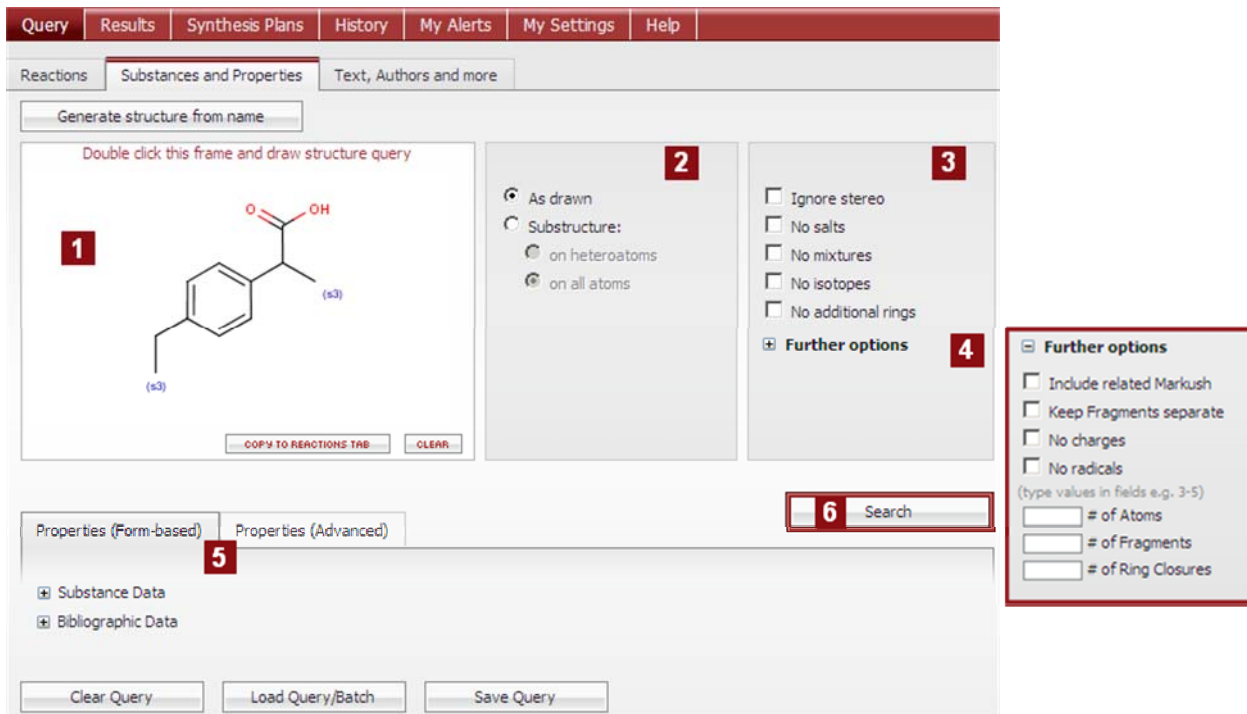
**4** Save

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

**6** Delete

*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



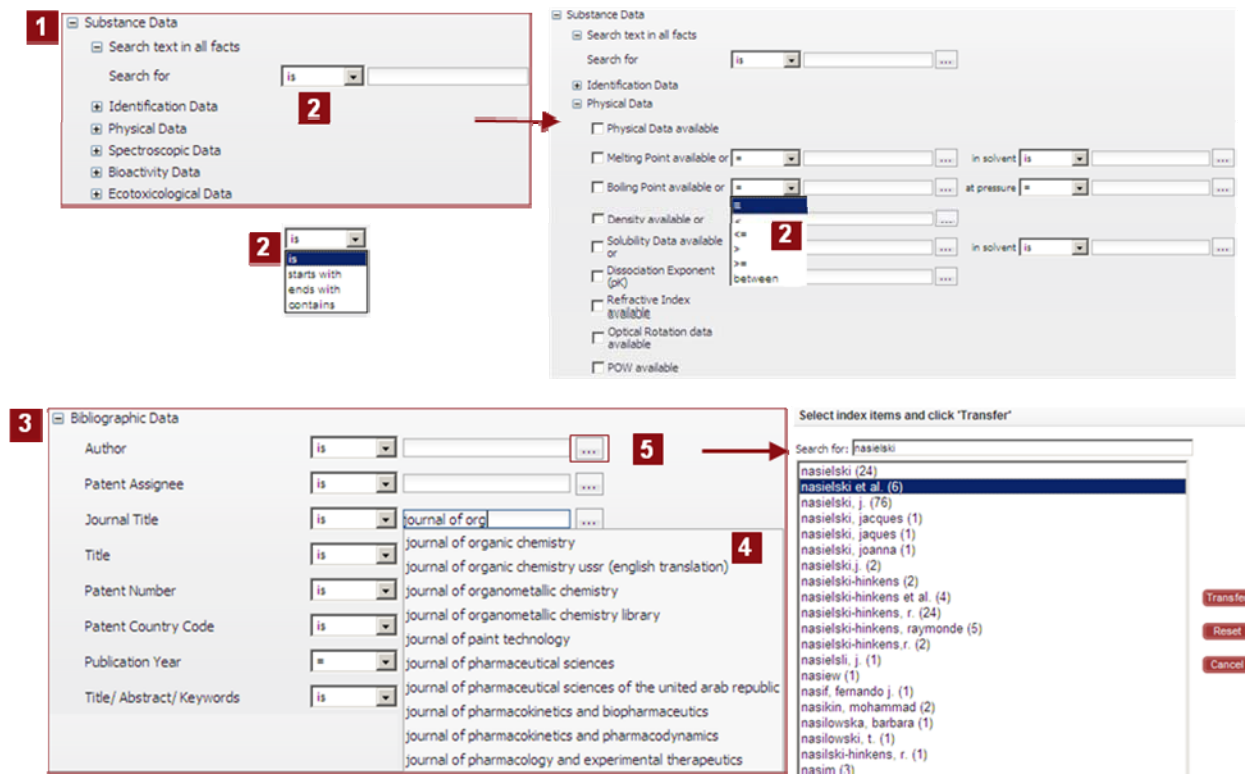
- 1 Structure/reaction box**  
This window contains the needed structure, with additional query features. Two buttons enable the structure to be copied to the reactions query tab, and also to delete it.
- 2 Search as**  
Define the type of structure search: as *drawn* (including possible query features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

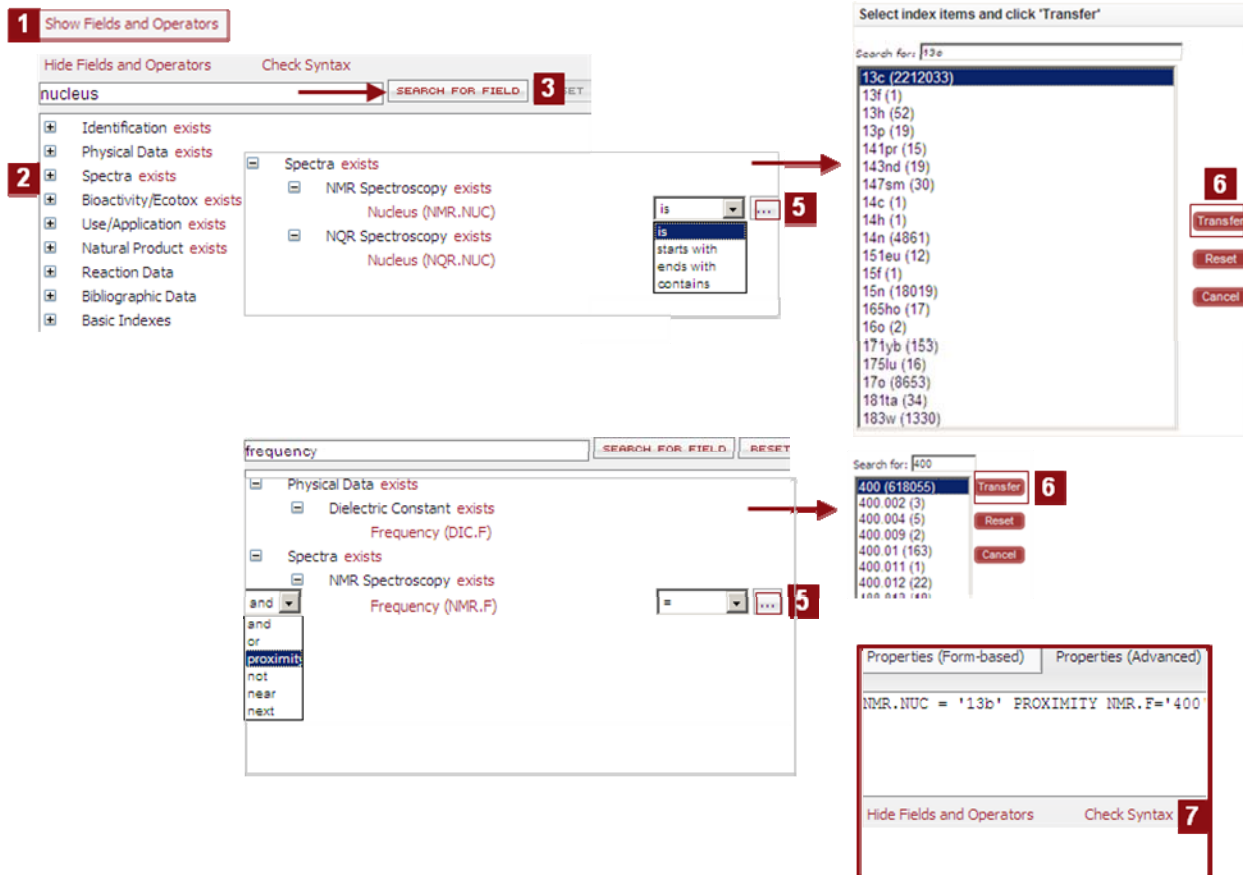
## Substances query tab Properties (Form-based)



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.

## Substances query tab Properties (Advanced)



1 Show Fields and Operators

2 Fields Category

3 Search for Field button

4 Operators

5 Expand Index feature (for all fields)

6 Transfer the field data

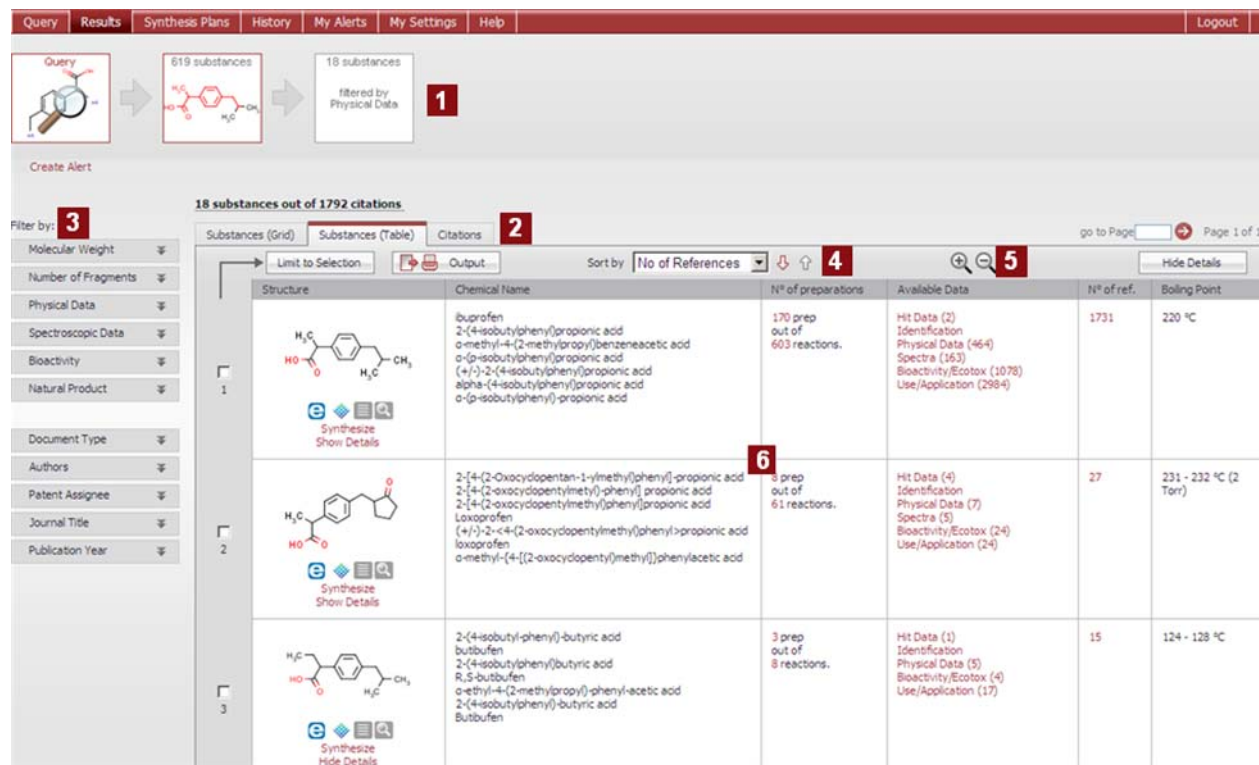
7 Check Syntax

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.

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

## Substances and properties Results overview



Query Results Synthesis Plans History My Alerts My Settings Help Logout

Query 619 substances 18 substances filtered by Physical Data 1

Create Alert

18 substances out of 1792 citations

Filter by: 3

Molecular Weight  
Number of Fragments  
Physical Data  
Spectroscopic Data  
Bioactivity  
Natural Product

Document Type  
Authors  
Patent Assignee  
Journal Title  
Publication Year

Substances (Grid) Substances (Table) Citations 2

Limit to Selection Output Sort by No of References 4

go to Page Page 1 of 1

Structure	Chemical Name	N° of preparations	Available Data	N° of ref.	Boiling Point
1	ibuprofen 2-(4-isobutylphenyl)propionic acid o-methyl-4-(2-methylpropyl)benzeneacetic acid o-(p-isobutylphenyl)propionic acid (+/-)-2-(4-isobutylphenyl)propionic acid alpha-(4-isobutylphenyl)propionic acid o-(p-isobutylphenyl)propionic acid	170 prep out of 603 reactions.	Hit Data (2) Identification Physical Data (464) Spectra (163) Bioactivity/Ecotox (1078) Use/Application (2984)	1731	220 °C
2	2-[4-(2-oxocyclopentylmethyl)phenyl]propionic acid 2-[4-(2-oxocyclopentylmethyl)phenyl]propionic acid 2-[4-(2-oxocyclopentylmethyl)phenyl]propionic acid loxoprofen (+/-)-2-(4-(2-oxocyclopentylmethyl)phenyl)propionic acid loxoprofen o-methyl-4-[(2-oxocyclopentyl)methyl]phenylacetic acid	6 prep out of 61 reactions.	Hit Data (4) Identification Physical Data (7) Spectra (5) Bioactivity/Ecotox (24) Use/Application (24)	27	231 - 232 °C (2 Torr)
3	2-(4-isobutylphenyl)butyric acid butufen 2-(4-isobutylphenyl)butyric acid R,S-butufen o-methyl-4-(2-methylpropyl)phenyl-acetic acid 2-(4-isobutylphenyl)butyric acid Butufen	3 prep out of 8 reactions.	Hit Data (1) Identification Physical Data (5) Bioactivity/Ecotox (4) Use/Application (17)	15	124 - 128 °C

Note: information on the citations tab of the substances results window can be found on page 22.

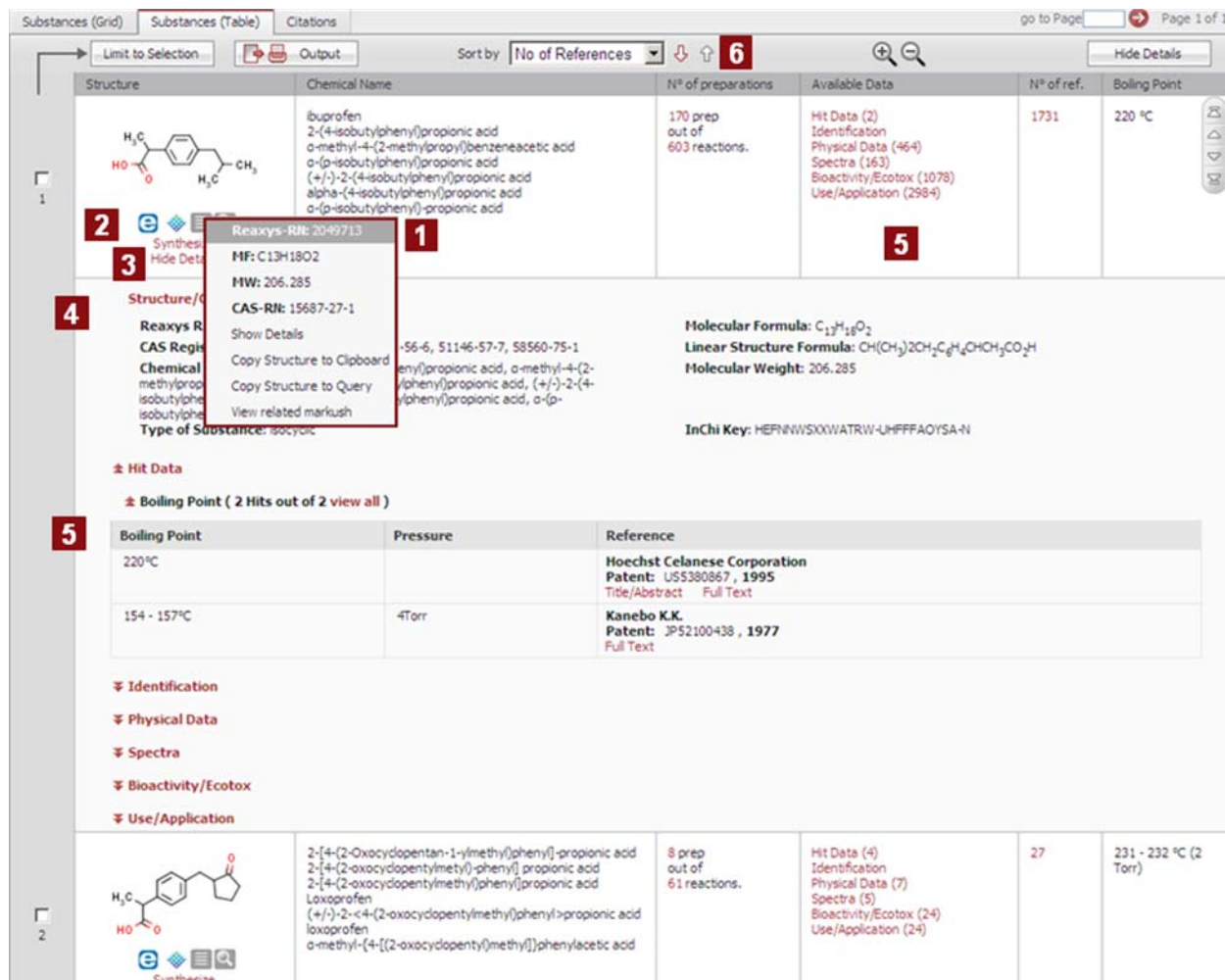
- Breadcrumbs**  
Graphical navigation helps keeping track of your result analysis.
- Substances (grid)/substances (table)/citations tab**  
The substances (table) tab is displayed by default, but you can switch to the substances (grid) or citations tab.
- Filtered by**  
Refine results by applying filters linked to the substance (molecular weight, number of fragments, physical data, spectroscopic data, bioactivity and natural product) or linked to bibliographic data (document type, authors, patent assignee, journal title and publication year).
- Tool bar**  
Access limit to selection, output, sort by features.
- Maximizer/minimizer tool**  
Increase or decrease the size of displayed structures.
- 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.



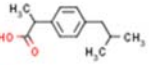
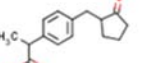
## Substances and properties

### Substances (Table) tab

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



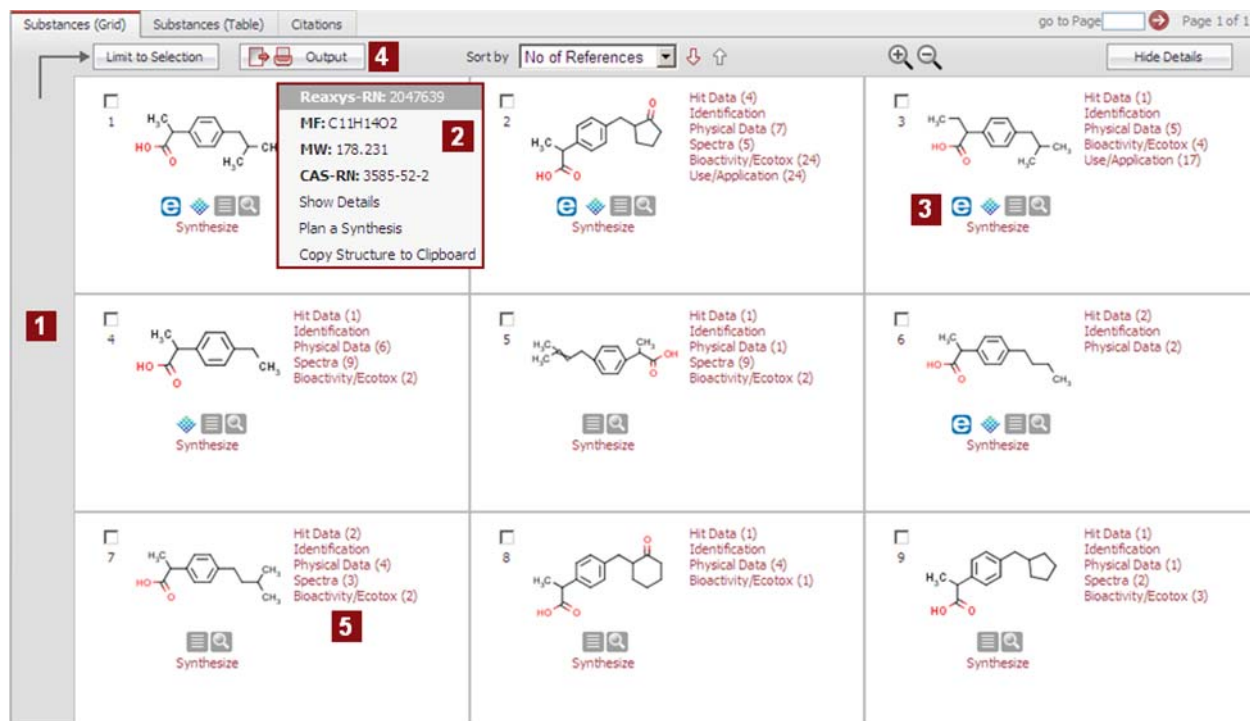
The screenshot displays the Reaxys Substances (Table) tab. The table lists chemical substances with columns for Structure, Chemical Name, N° of preparations, Available Data, N° of ref., and Boiling Point. The first entry is ibuprofen, with its chemical structure shown. A pop-up menu is visible over the first entry, showing options like 'Reaxys-RN: 2049713', 'MF: C<sub>13</sub>H<sub>18</sub>O<sub>2</sub>', 'MW: 206.285', 'CAS-RN: 15687-27-1', and 'Show Details'. The table also includes a section for 'Hit Data' and 'Boiling Point' with a table of values. The second entry is a complex molecule with a chemical structure shown. The table is sorted by 'No of References' in descending order.

Structure	Chemical Name	N° of preparations	Available Data	N° of ref.	Boiling Point
	ibuprofen 2-(4-isobutylphenyl)propionic acid o-methyl-4-(2-methylpropyl)benzeneacetic acid o-(p-isobutylphenyl)propionic acid (+/-)-2-(4-isobutylphenyl)propionic acid alpha-(4-isobutylphenyl)propionic acid o-(p-isobutylphenyl)propionic acid	170 prep out of 603 reactions.	Hit Data (2) Identification Physical Data (464) Spectra (163) Bioactivity/ECotox (1078) Use/Application (2984)	1731	220 °C
	2-[4-(2-Oxocyclopentan-1-ylmethyl)phenyl]propionic acid 2-[4-(2-oxocyclopentylmethyl)phenyl]propionic acid 2-[4-(2-oxocyclopentylmethyl)phenyl]propionic acid loxoprofen (+/-)-2-(4-(2-oxocyclopentylmethyl)phenyl)propionic acid loxoprofen o-methyl-4-[[[2-oxocyclopentyl]methyl]]phenylacetic acid	8 prep out of 61 reactions.	Hit Data (4) Identification Physical Data (7) Spectra (5) Bioactivity/ECotox (24) Use/Application (24)	27	231 - 232 °C (2 Torr)

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

- Additional information / 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/Query screen, View related Markush.
- Commercial availability**  
Access the commercial availability of a substance and leads to appropriate companies (eMolecules/ACD).
- Show/Hide details button**
- Structure/compound data**  
Find details about structure/compound.
- 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.
- Sort by**  
Sort results ascending ↑ or descending ↓ by Reaxys-RN, Comm Availability, Molec Formula, Nb Fragments, Publication Year, Mol Weight and Nb of References (default).

## Substances and properties Substances (Grid) tab



The screenshot displays the Reaxys Substances (Grid) tab. The interface includes a search bar, a 'Limit to Selection' button, and a 'Sort by' dropdown menu set to 'No of References'. A grid of chemical structures is shown, each with a 'Synthesize' button and a list of available data. A pop-up menu for the first structure (1) shows the following details:

- Reaxys-RN: 2047639
- MF: C<sub>11</sub>H<sub>14</sub>O<sub>2</sub>
- MW: 178.231
- CAS-RN: 3585-52-2
- Show Details
- Plan a Synthesis
- Copy Structure to Clipboard

Numbered callouts highlight specific features:

- Grid view**: The main grid of chemical structures.
- Additional information/sub items**: The pop-up menu for a specific structure.
- Commercial availability**: The 'Synthesize' button.
- Output**: The 'Output' button.
- Available data for this substance**: The list of available data for a specific structure.

### 1 Grid view

For a quick overview results are displayed in a grid.

### 2 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

Plan a synthesis: develop your retrosynthesis

Copy structure to clipboard

### 3 Commercial availability

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

### 4 Output

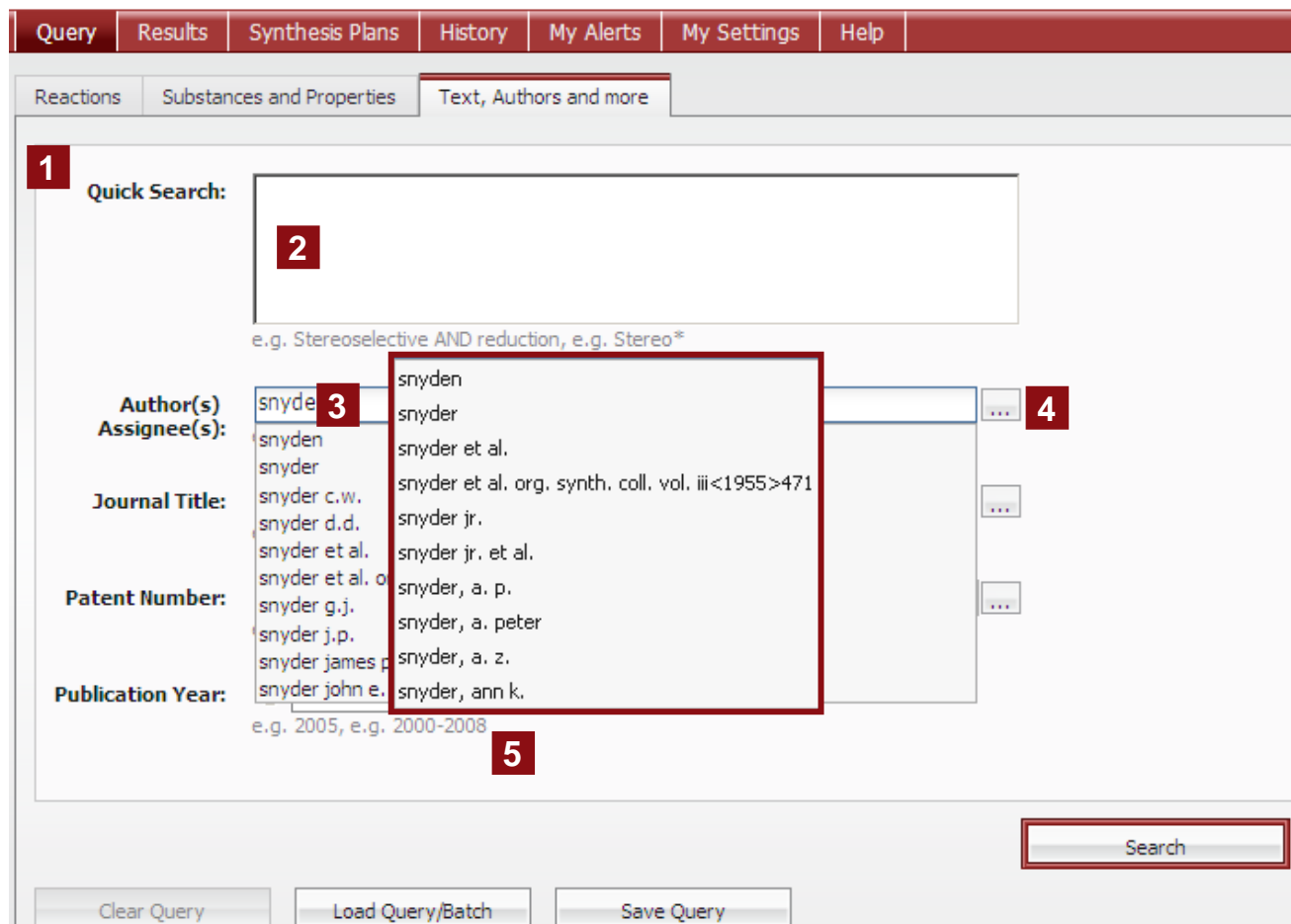
Export results in the desired format.

### 5 Available data for this substance


Various red hyperlinks display the information available by substance.



## Text, Authors and more Query tab



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.  
*If several terms are chosen in one field, they are combined with the Boolean operator OR (;).*
- 5 Entry example**  
Hints how to enter your search term are displayed below each of the field data boxes.

## Text, authors and more Citations tab

Filter by: **1**

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 ▾  
Natural Product ▾

Citations Reactions Substances (Grid) Substances (Table)

Limit to Selection **2** Output **2** Sort by Publication Year **3** **3** Hide Details

	Title of the Document	Authors	Year	Source	Times cited
<b>1</b>	MULTINUCLEAR COMPLEX AND CONDENSATION PRODUCT THEREOF	Sugahara, Yoshiyuki; Ishiyama, Takeshi; Higashimura, Hideyuki	2009	Patent: US2009/36687; A1 Full Text	
	<b>4</b> Title/Abstract Show All Reactions (11) Show All Substances (22)				
<b>2</b>	Hydrogenation of various organic substrates using polystyrene anchored orthometallated ruthenium (II) complex as catalyst	Islam, S. M.; Tuhina, K.; Mubarak, M.; Mondal, P.	2009	Journal of Molecular Catalysis A: Chemical, 2009, vol. 297, p. 18 - 25 Full Text View citing articles	1
	<b>4</b> Title/Abstract Show All Substances (1)				
<b>3</b>	Metallopeptides	Maayan, Galia; Ward, Michael D.; Kirshenbaum, Kent	2009	Chemical Communications (Cambridge, United Kingdom), 2009, p. 56 - 58 Full Text View citing articles <b>5</b>	3
	<b>4</b> Title/Abstract Show All Reactions (4) Show All Substances (8)				
<b>4</b>	Epoxidation of olefins with H <sub>2</sub> O <sub>2</sub> catalyzed by new symmetrical acetylacetonate-based Schiff bases/Mn(II) homogeneous systems: A catalytic and EPR study	Stamatis, Ag.; Dousti, P.; Vartzouma, Ch.; Christoforidis, K. C.; Deligiannakis, Y.; Louloudi, M.	2009	Journal of Molecular Catalysis A: Chemical, 2009, vol. 297, p. 44 - 53 Full Text View citing articles	2
	<b>4</b> Title/Abstract Show All Substances (2)				

- Filter by**  
Refine search results by applying bibliographic (document type, authors, patent assignee, journal title and publication year), reaction or substance filters.
- Output**  
Export results in an appropriate format.
- Sort by**  
Sort results ascending ↑ or descending ↓ by Document Type, Authors, Journal Title or Publication Year (default).
- Abstract/Reactions/Substances**  
Display the abstract, and show all reactions or show all substances which are related to the article.
- 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.

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 this article (# out of total #)** link