

Reaxys Quick Reference Guide

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The basics Where to find what?

To **start Reaxys**, go to www.reaxys.com

To find **more user tips**, go to www.info.reaxys.com. Here you can find:

- Information on the coverage, usability and technical requirements of Reaxys
- 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

ninfo@reaxys.com

Americas

+1 888 615 4500

usinfo@reaxys.com

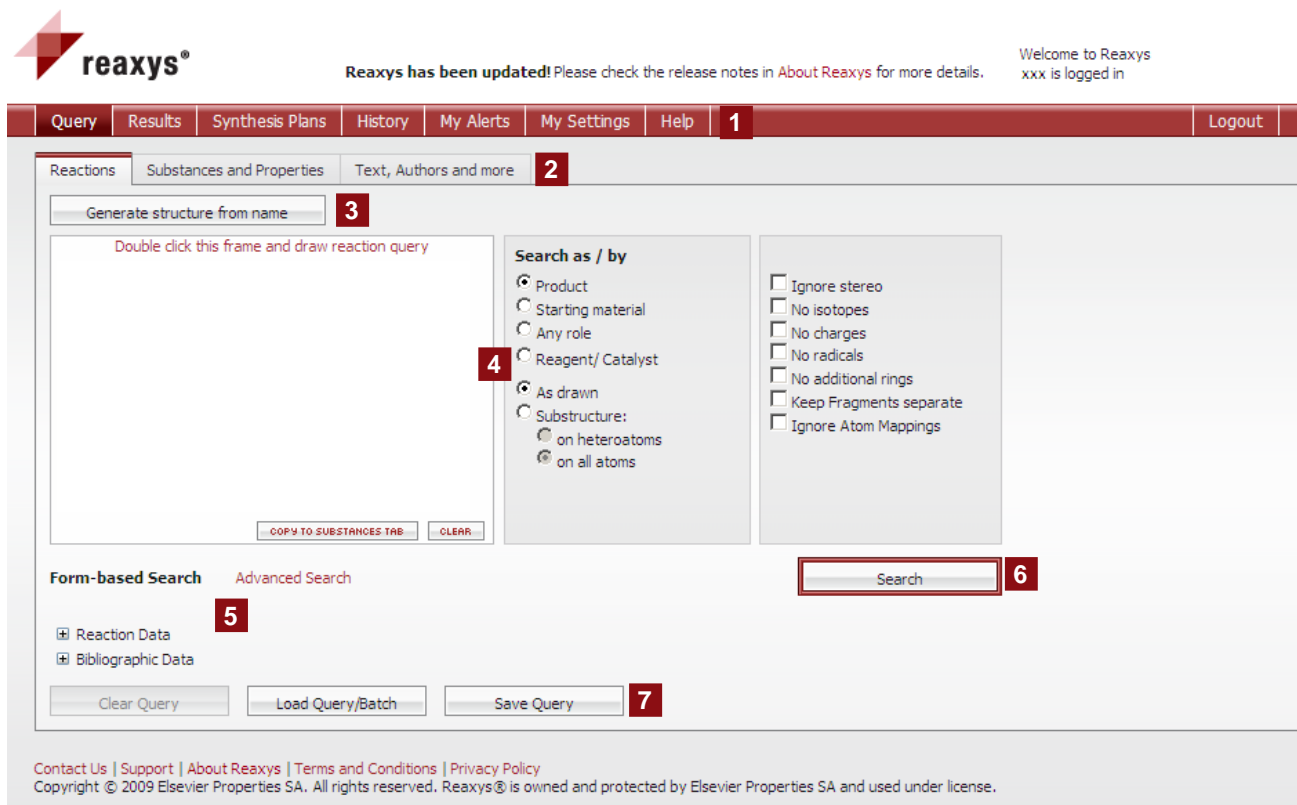
+1 212 462 1978 if calling outside USA & Canada

Japan

+81 3 5561 5034

jpinfo@reaxys.com

Homepage



The screenshot shows the Reaxys homepage interface. At the top left is the Reaxys logo. To its right, a message states "Reaxys has been updated! Please check the release notes in About Reaxys for more details." Further right, it says "Welcome to Reaxys xxx is logged in". A navigation bar contains tabs for Query, Results, Synthesis Plans, History, My Alerts, My Settings, Help, and Logout. Below this is a sub-navigation bar with tabs for Reactions, Substances and Properties, and Text, Authors and more. The main content area includes a "Generate structure from name" input field, a large drawing area with the instruction "Double click this frame and draw reaction query", a "Search as / by" section with radio buttons for Product, Starting material, Any role, and Reagent/ Catalyst, and checkboxes for search options like "Ignore stereo", "No isotopes", "No charges", "No radicals", "No additional rings", "Keep Fragments separate", and "Ignore Atom Mappings". Below the drawing area are "Form-based Search" and "Advanced Search" sections with expandable options for "Reaction Data" and "Bibliographic Data". At the bottom of the main area are buttons for "Clear Query", "Load Query/Batch", and "Save Query". A search button is located at the bottom right of the main area. The 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 & - Logout

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 *Form-based Search* and *Advanced Search* links allow entering further reaction or bibliographic data constraints.

6 Search button

Launch a search.

7 Command buttons

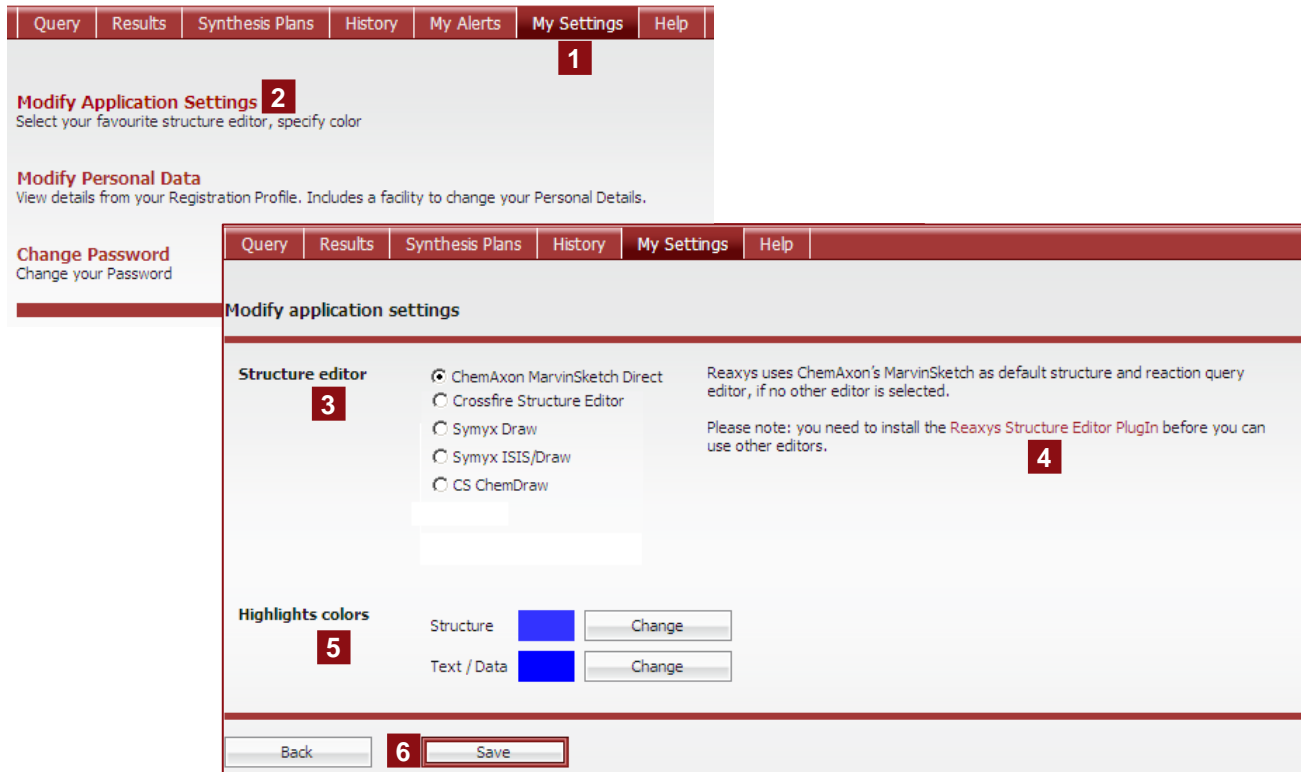
Clear, load or save a query. The Load feature also supports batch querying.

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 return to Reaxys by closing the editor
3. Click the search button and browse the result.

Note: the default settings are such that Reaxys immediately searches for compound preparations.

My settings

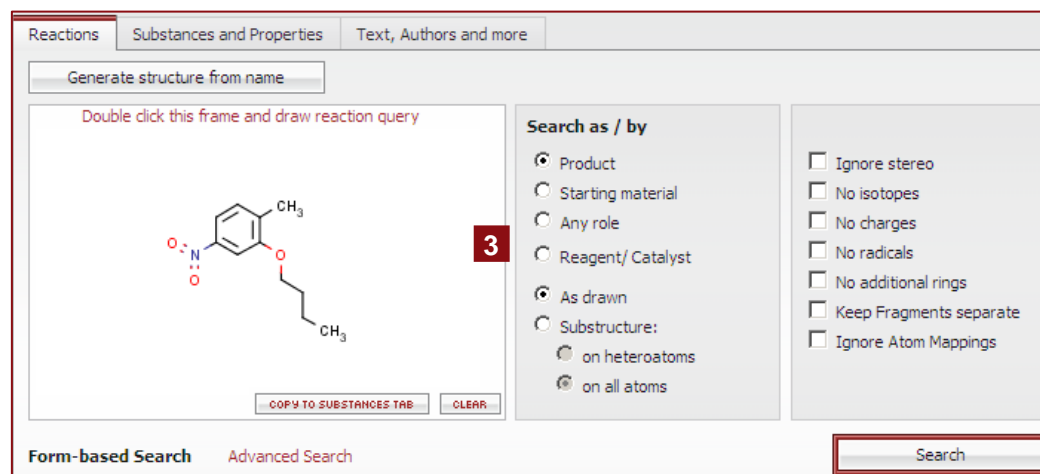
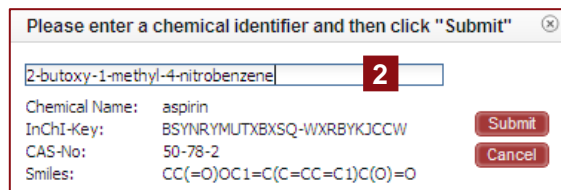
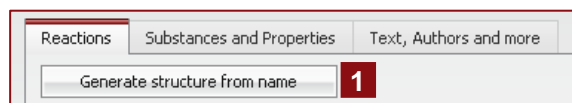


The screenshot shows the 'My Settings' page in the Reaxys interface. At the top, a navigation bar contains tabs for 'Query', 'Results', 'Synthesis Plans', 'History', 'My Alerts', 'My Settings', and 'Help'. The 'My Settings' tab is selected and highlighted with a red box labeled '1'. Below the navigation bar, there are three main sections: 'Modify Application Settings' (labeled '2'), 'Modify Personal Data', and 'Change Password'. The 'Modify Application Settings' section is expanded, showing the 'Modify application settings' form. This form has a sub-navigation bar with 'Query', 'Results', 'Synthesis Plans', 'History', 'My Settings', and 'Help'. The 'Structure editor' section (labeled '3') contains four radio button options: 'ChemAxon MarvinSketch Direct' (selected), 'Crossfire Structure Editor', 'Symyx Draw', and 'Symyx ISIS/Draw'. A note (labeled '4') states: 'Please note: you need to install the Reaxys Structure Editor PlugIn before you can use other editors.' Below this, there are two 'Highlights colors' sections (labeled '5'): 'Structure' with a blue color swatch and a 'Change' button, and 'Text / Data' with a blue color swatch and a 'Change' button. At the bottom of the form, there are 'Back' and 'Save' buttons (labeled '6').

- 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 and Highlights colors.
- 3 Structure Editor**
Choose your preferred editor.
- 4 Information**
Find information on the default settings used, and download the plugin required for its installation.
- 5 Highlights colors**
Select preferred colors to highlight the searched-for structure and/or the text/data.
- 6 Back & Save buttons**
Confirm new settings with **Save** or use **Back** to return to the item list.

Note: 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.

Generate a structure from name



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.

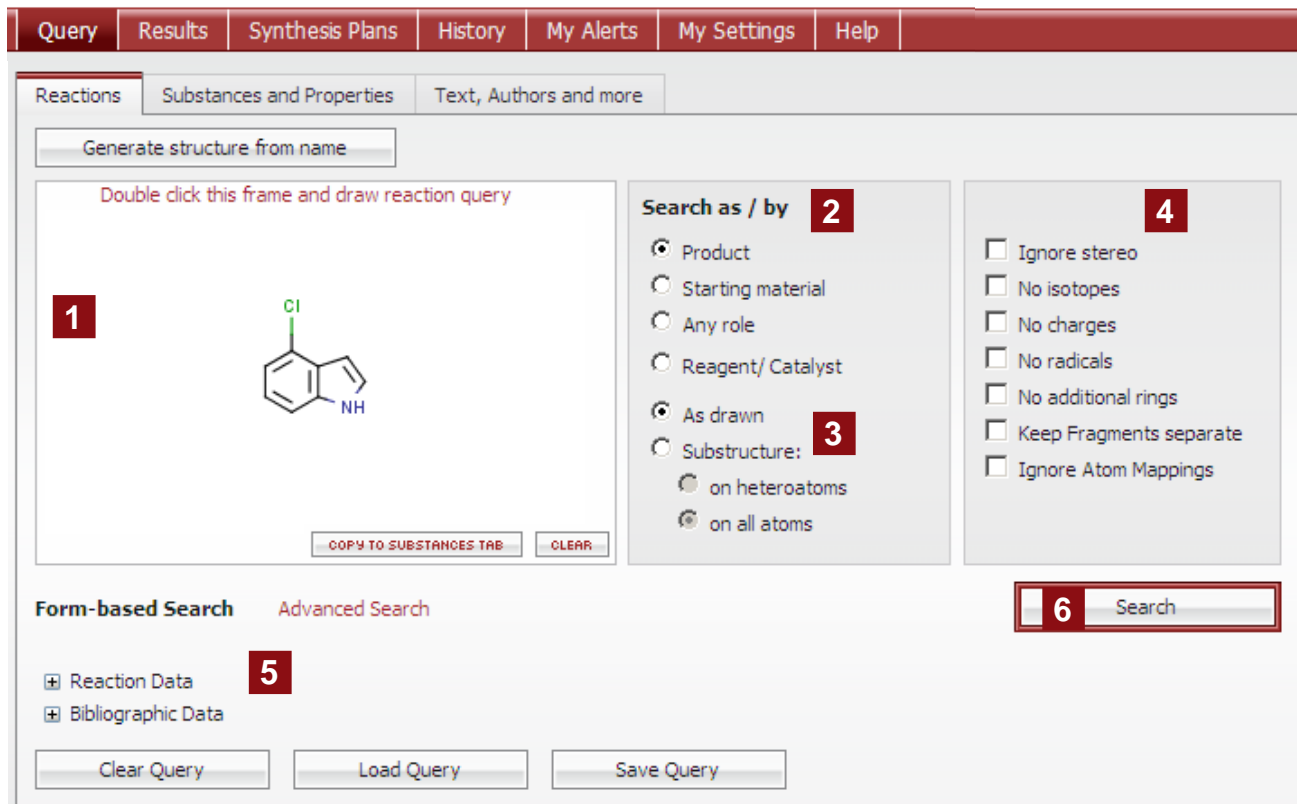
3 Structure/reaction window

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

- Start the search immediately.
- Edit the structure by double clicking the box (or by doing a right-click); modify it in the Structure editor.
- 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



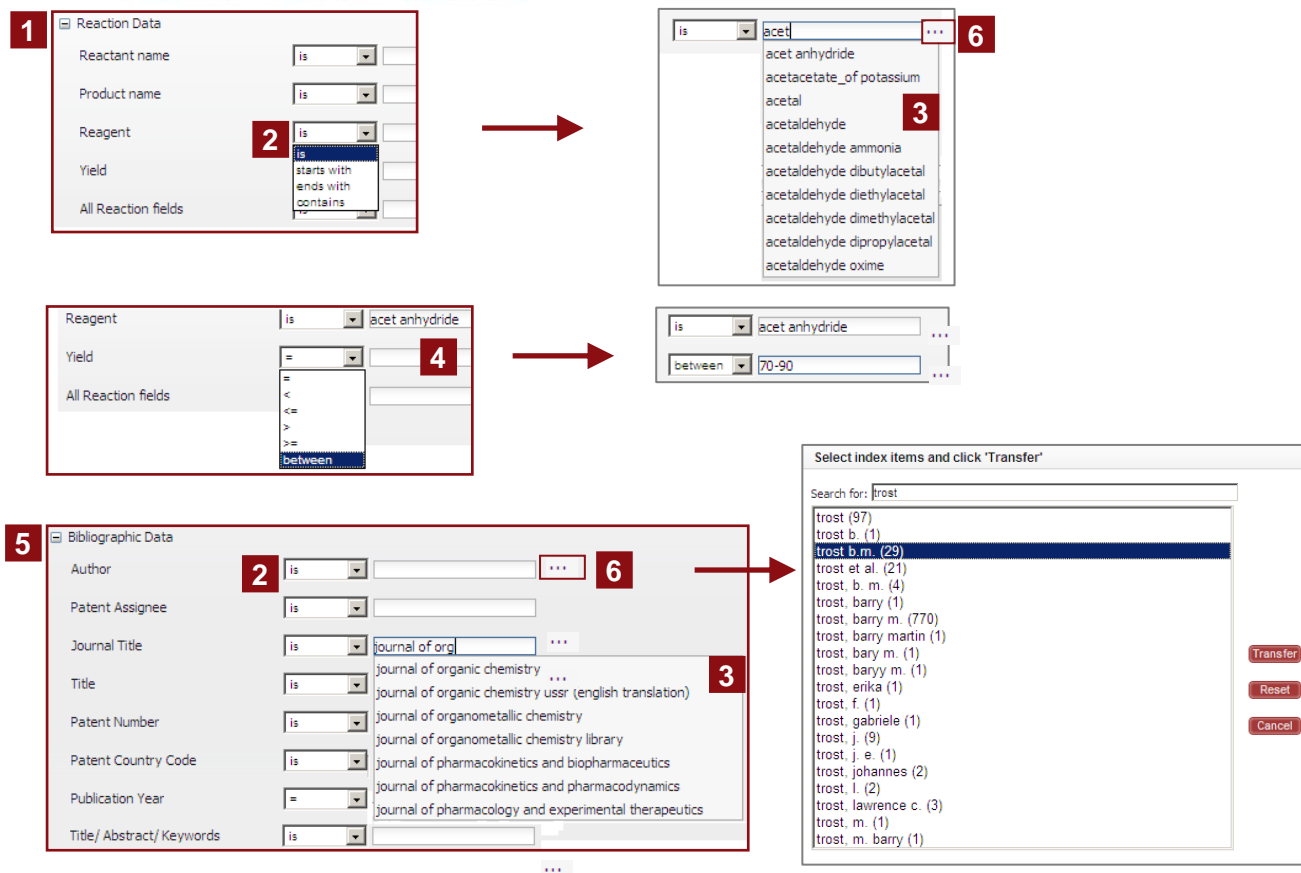
- 1 Structure/reaction box**
This window contains the requested structure or reaction, with additional query features. It is also possible to copy the structure to the Substances and Properties query tab.
- 2 Search as/by**
If needed, define the role of the substance.
- 3 Select the search type**
Select "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 *Form-based Search* or the *Advanced Search* 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 | C:\Documents and Settings\rypensc\Desktop\Reaxys\Cycle.xml | Browse... | Open

Reactions query tab Form-based Search



1 Reaction Data

Reactant name is

Product name is

Reagent is

Yield is

All Reaction fields

2

starts with

ends with

contains

3

is acet

acet anhydride

acetacetate_of potassium

acetal

acetaldehyde

acetaldehyde ammonia

acetaldehyde dibutylacetal

acetaldehyde diethylacetal

acetaldehyde dimethylacetal

acetaldehyde dipropylacetal

acetaldehyde oxime

4

Reagent is acet anhydride

Yield is

All Reaction fields

between

5 Bibliographic Data

Author is

Patent Assignee is

Journal Title is journal of org.

Title is journal of organic chemistry

Patent Number is

Patent Country Code is

Publication Year is

Title/ Abstract/ Keywords is

6

trost (97)

trost b. (1)

trost b.m. (29)

trost et al. (21)

trost. b. m. (4)

trost. barry (1)

trost. barry m. (770)

trost. barry martin (1)

trost. bary m. (1)

trost. bary m. (1)

trost. erika (1)

trost. f. (1)

trost. gabriele (1)

trost. j. (9)

trost. j. e. (1)

trost. johannes (2)

trost. l. (2)

trost. lawrence c. (3)

trost. m. (1)

trost. m. barry (1)

Transfer

Reset

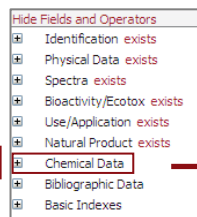
Cancel

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

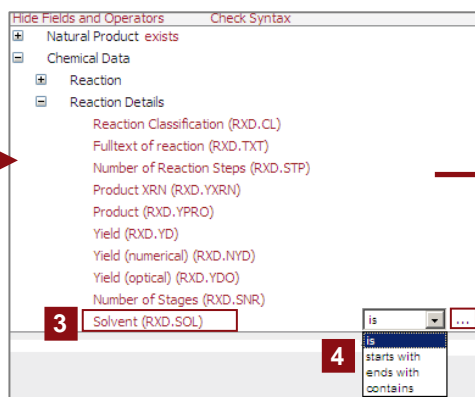
- 1 Reaction data**
Specify Reactant name, Product name, Reagent, Yield and/or All Reaction fields.
Various selected fields are combined with the Boolean operator AND.
- 2 Operators**
Select the appropriate operator from the drop-down menu.
- 3 Selection list**
Selection appears when typing entry.
- 4 Numeric Field**
For a numeric field select the operator followed by entering the number or range in the text box.
- 5 Bibliographic data**
Specify Authors, Patent Assignee, Journal Title, Title, Patent Number, Patent Country Code, Publication Year and/or Title/Abstract/Keywords.
Various selected fields are combined with the Boolean operator AND.
- 6 Expand Index feature (for all search fields)**
The **...** box allows convenient index browsing and multiple entry selections. Click the **Transfer** button to add the selected data to the query.

Reactions query tab Advanced Search

1 Show Fields and Operators



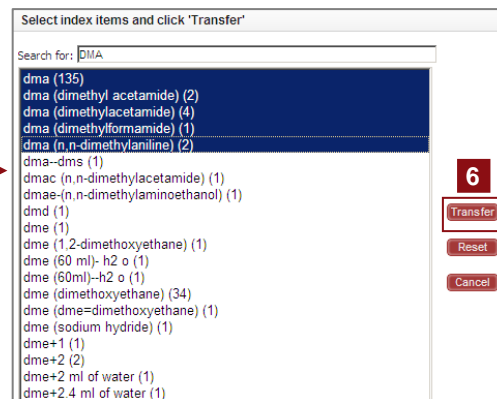
2



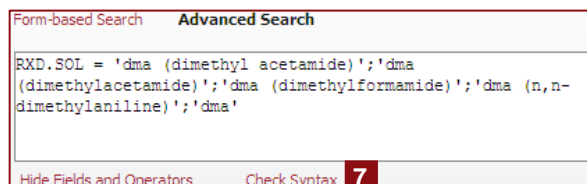
3

4

5



6



7

1 Show Fields and Operators

Select the necessary field code from a hierarchical list (field list navigator) available with the **Show fields and operators** hyperlink.

2 Fields Category

Click the + sign to expand the needed fields list.

3 Needed field

Click the needed 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

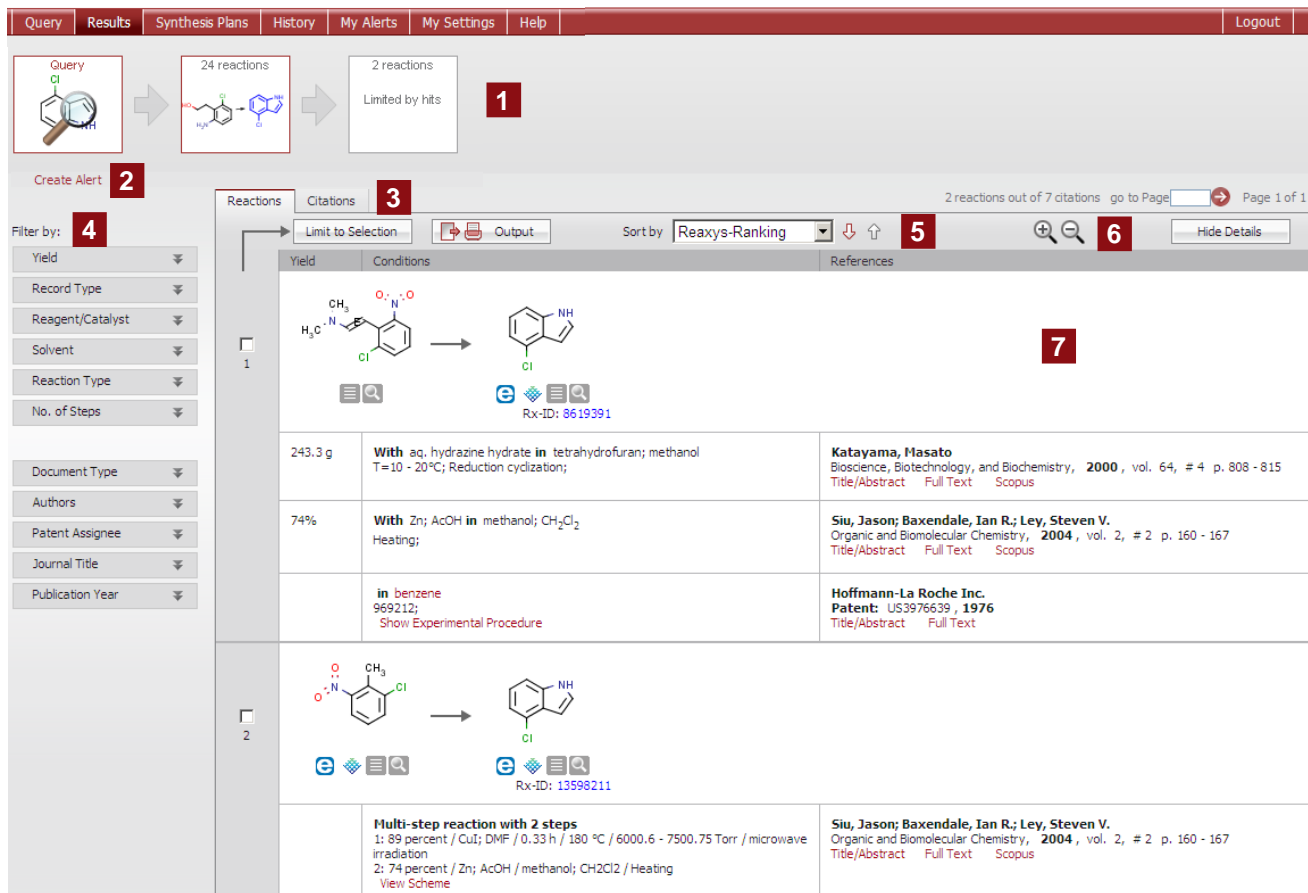
7 Check Syntax

In case of manual entry of the query into the Advanced Search box, verify your query by clicking the **Check Syntax** hyperlink.

*Note: the **Advanced Search** 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.*

Reactions results General overview



The screenshot displays the Reaxys interface with the following elements:

- 1**: Breadcrumbs at the top showing the navigation path: Query (24 reactions) → 24 reactions → 2 reactions (Limited by hits).
- 2**: "Create Alert" button.
- 3**: "Reactions" and "Citations" tabs.
- 4**: Filter sidebar on the left with categories: Yield, Record Type, Reagent/Catalyst, Solvent, Reaction Type, No. of Steps, Document Type, Authors, Patent Assignee, Journal Title, and Publication Year.
- 5**: "Limit to Selection", "Output", and "Sort by" (set to Reaxys-Ranking) controls.
- 6**: Magnifying glass icon for search.
- 7**: Reaction results table with columns for Yield, Conditions, and References.

Yield	Conditions	References
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 Scopus
74%	With Zn; AcOH in methanol; CH ₂ Cl ₂ Heating;	Siu, Jason; Baxendale, Ian R.; Ley, Steven V. Organic and Biomolecular Chemistry, 2004 , vol. 2, # 2 p. 160 - 167 Title/Abstract Full Text Scopus
	in benzene 969212; Show Experimental Procedure	Hoffmann-La Roche Inc. Patent: US3976639, 1976 Title/Abstract Full Text
	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 ₂ Cl ₂ / Heating View Scheme	Siu, Jason; Baxendale, Ian R.; Ley, Steven V. Organic and Biomolecular Chemistry, 2004 , vol. 2, # 2 p. 160 - 167 Title/Abstract Full Text Scopus

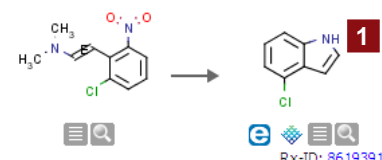
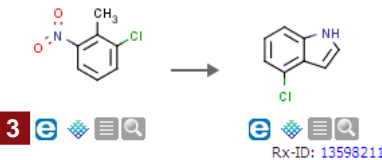
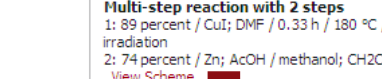
Have a look at the breadcrumbs at the top of the screen; it shows the actions done on your initial hitset. Click one of the red-framed boxes to quickly jump to a previous set of data or the query.


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

Reactions results Reactions tab

Reactions Citations 2 reactions out of 7 citations go to Page Page 1 of 1

4 Limit to Selection Output 5 Sort by Reaxys-Ranking 6

Yield	Conditions	References
 Rx-ID: 8619391	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 Scopus
74%	With Zn; AcOH in methanol; CH ₂ Cl ₂ Heating;	Siu, Jason; Baxendale, Ian R.; Ley, Steven V. Organic and Biomolecular Chemistry, 2004 , vol. 2, # 2 p. 160 - 167 Title/Abstract Full Text Scopus
 Rx-ID: 13598211	in benzene 969212; Show Experimental Procedure	Hoffmann-La Roche Inc. Patent: US3976639, 1976 Title/Abstract Full Text
 Rx-ID: 13598211	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 ₂ Cl ₂ / Heating View Scheme	Siu, Jason; Baxendale, Ian R.; Ley, Steven V. Organic and Biomolecular Chemistry, 2004 , vol. 2, # 2 p. 160 - 167 Title/Abstract Full Text Scopus

- 1 Click  or a structure to get a pop-up menu with information or sub items.
Display further options & Data
 Reaxys – RN (Reaxys registry number), MF (molecular formula), CAS-RN (CAS registry number), show details (display information as physical-, spectral- data etc), plan a synthesis (create a retrosynthesis), copy structure to clipboard
- 2 **Access bibliographic details**
 Display the title/abstract, the full text of your reference and access 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 lead to appropriate companys (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).

Note: information on the citations tab of the reactions results window can be found on page 21.

Reactions results tab Filter by

Filter by Value

1 Yield

2 by Value by Group

enter value/range

80-95

More

Limit to Exclude

Record Type

Reagent/Catalyst

Solvent

Reaction Type

No. of Steps

Yield

by Value by Group

enter value/range

80-95

More

Limit to Exclude

5 Refine on Yield

Sort by Value Value Occ

Value	Occ
<input type="checkbox"/> >275 - 280	1
<input type="checkbox"/> >105 - 110	1
<input type="checkbox"/> >100 - 105	1
<input type="checkbox"/> >95 - 100	135
<input type="checkbox"/> >90 - 95	148
<input type="checkbox"/> >85 - 90	192
<input type="checkbox"/> >80 - 85	190
<input type="checkbox"/> >75 - 80	210
<input type="checkbox"/> >70 - 75	182
<input type="checkbox"/> >65 - 70	182
<input type="checkbox"/> >60 - 65	170
<input type="checkbox"/> >55 - 60	186
<input type="checkbox"/> >50 - 55	121
<input type="checkbox"/> >45 - 50	144
<input type="checkbox"/> >40 - 45	117

4 Limit to Exclude

Filter by Group

6 Document Type

by Value by Group

journal 18

patent 3

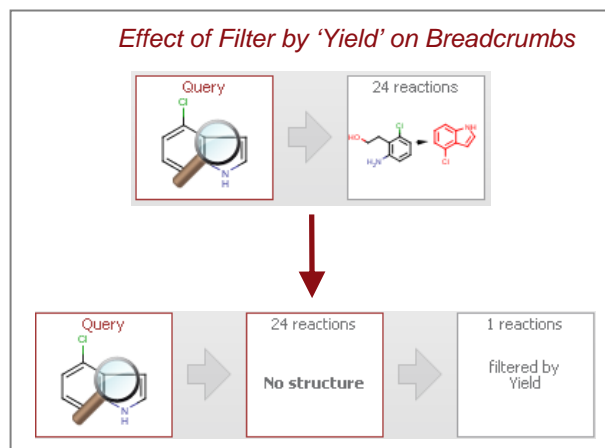
Limit to Exclude

Authors

Patent Assignee

Journal Title

Publication Year

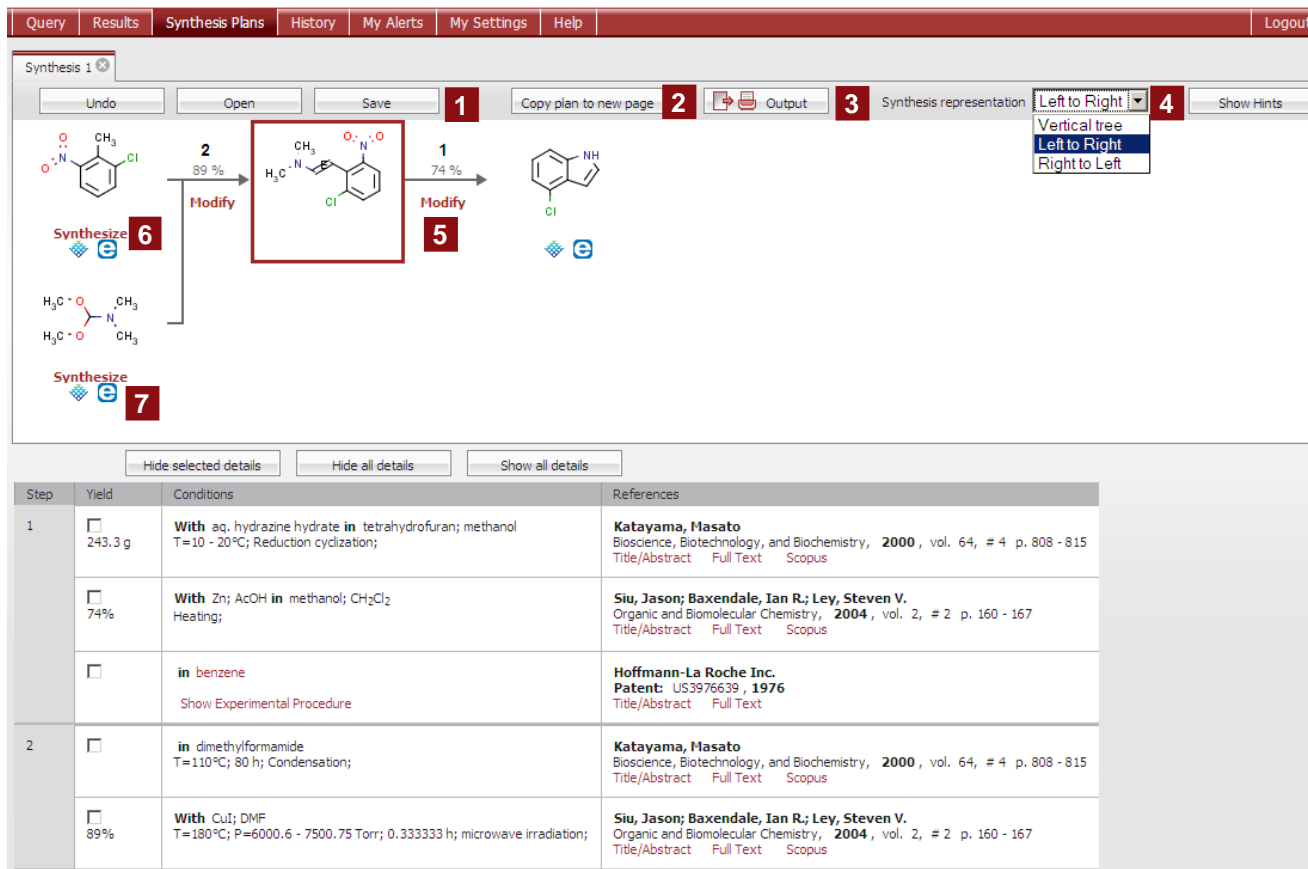


Note: filter by feature allows for rapid and easy refinement of your results. Click the double arrows to expand the selection list. Two filter options are available for each reaction specification:

1. To retrieve a predefined selection list, use the **by Group** tab.
2. To specify a filter value or range (flexible filter), select the **by Value** tab.


- 1 Filter by**
Select filter(s) linked to reaction specifications:
 - Yield,
 - Record Type
 - Reagent/Catalyst
 - Solvent
 - Reaction Type
 - No. of Steps
- 2 By Value tab: flexible filter**
Enter a specific value or a range to refine result sets with more options.
- 3 By Group tab: predefined list**
Check boxes to limit or exclude entries of the predefined selection.
- 4 Limit to/exclude buttons**
Click the appropriate button.
- 5 Refine on Filter field**
Click the **More** button to expand the scope of the selection, and to refine further the filter by feature. Sort the chosen data by Value or by Occurrence.
- 6 Filter by**
Specify filter(s) linked to bibliographic data:
 - Document Type
 - Authors
 - Patent Assignee
 - Journal Title
 - Publication Year

Synthesis plans



Step	Yield	Conditions	References
1	<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 Scopus
	<input type="checkbox"/> 74%	With Zn; AcOH in methanol; CH ₂ Cl ₂ Heating;	Siu, Jason; Baxendale, Ian R.; Ley, Steven V. Organic and Biomolecular Chemistry, 2004 , vol. 2, # 2 p. 160 - 167 Title/Abstract Full Text Scopus
	<input type="checkbox"/>	in benzene Show Experimental Procedure	Hoffmann-La Roche Inc. Patent: US3976639, 1976 Title/Abstract Full Text
2	<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 Scopus
	<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 Scopus

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  or a structure in any of the results tab, choose "Plan Synthesis" 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 lead to appropriate companys (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

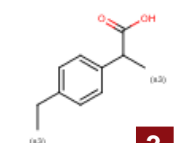
6

<input checked="" type="checkbox"/> Spectra	<input checked="" type="checkbox"/> Physical Data	<input checked="" type="checkbox"/> Bioactivity/Ecotox	<input checked="" type="checkbox"/> Use/Application	<input checked="" type="checkbox"/> Natural Product
<input checked="" type="checkbox"/> NMR Spectroscopy (30)	<input checked="" type="checkbox"/> Melting Point (26)	<input checked="" type="checkbox"/> Ecotoxicology (23)	<input checked="" type="checkbox"/> Use (21)	<input checked="" type="checkbox"/> Isolation from Natural Product (3)
<input checked="" type="checkbox"/> IR Spectroscopy (29)	<input checked="" type="checkbox"/> Crystal Property Description (21)	<input checked="" type="checkbox"/> Pharmacological Data (12)		<input checked="" type="checkbox"/> Derivative (2)
<input checked="" type="checkbox"/> Mass Spectrometry (22)	<input checked="" type="checkbox"/> Further Information (15)	<input checked="" type="checkbox"/> Concentration in the Environment (2)		<input checked="" type="checkbox"/> 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.

- Output**
Choose the type of results to export:
- to**
Define the format of exported file: PDF/Print, XML, Microsoft Word or Excel, TXT for Literature Management Systems, or RD File.
- Include the following headline**
Check the box and enter a headline that will be shown on each page of the document.
- 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).
- 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
- 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							
4	<input type="checkbox"/>	1	1	1	1	1	1
Query	Temporary result description						
<input type="checkbox"/>	1 Text/Authors: (Authors: 'snyder, p*') AND (Publication Year: All years)	26 citations	View	Store			Today
<input type="checkbox"/>	2 Text/Authors: (Authors: 'nasielski') AND (Publication Year: All years)	24 citations	View	Store			Today
<input type="checkbox"/>	3 Text/Authors: (Authors: 'nasielski') AND (Publication Year: All years)	PhD Work 24 citations ULB	View	Remove			2009-01-23
<input type="checkbox"/>	4  Substances: As drawn	Project 5HT2b 620 substances To test	View	Remove			2009-01-23
<input type="checkbox"/>	5						

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

Cancel

If 2 hits selected

Select how you want to combine the hitsets

Merge all

Overlap all

Cancel

If >2 hits selected

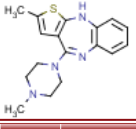

- 1 Temporary lists**
The upper part of the table shows all hitsets from the current session. Click **View** to display a list as active hitsets in the results page. Click **Store** (enter a filename and comment) to save a list.
- 2 Saved lists**
The lower part of the table shows the hitsets stored by 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 closed to the query column; the combine hitsets button becomes available and will provide graphical tools to combine the selected hitsets in various ways.
- 5**

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** Delete **6**

Modify alert **2** View results

3 Modify alert **4** Save

Modify an existing alert

Hint: you may change the e-mail address of a person, who should be copied on the alert, the comment/description, the frequency of the alert, or the E-mail format. Privacy Policy
If you want to modify the query of the alert, then please return to the list of available alerts, select 'Edit query', run the search and click 'Create alert'.

Query  Reactions: Product, As drawn

Name of Alert

E-mail Address send copy to

Comment/Description

Frequency

E-mail format html text

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

- 1 How to create an alert?**
Create and run a query. On the results menu, click the *Create Alert* link located just below the Query breadcrumb. Fill in the Alert form and click the Save button.
- 2 View results button**
Click this link to jump to the Results menu and access the hits linked to your alert.
- 3 Modify alert**
Modify the options of your alert (*Name of Alert, Copy to, Comment/Description, Frequency and Email format*). Click the Save button.
- 5 Delete**
Check the box closed to the alert name column; the delete button becomes available and will discard the concerned alert.
- 6**

Note: alerts are user-defined search query 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 email notification with a link into Reaxys allowing you to access the Alert results.

Substances and properties Query tab

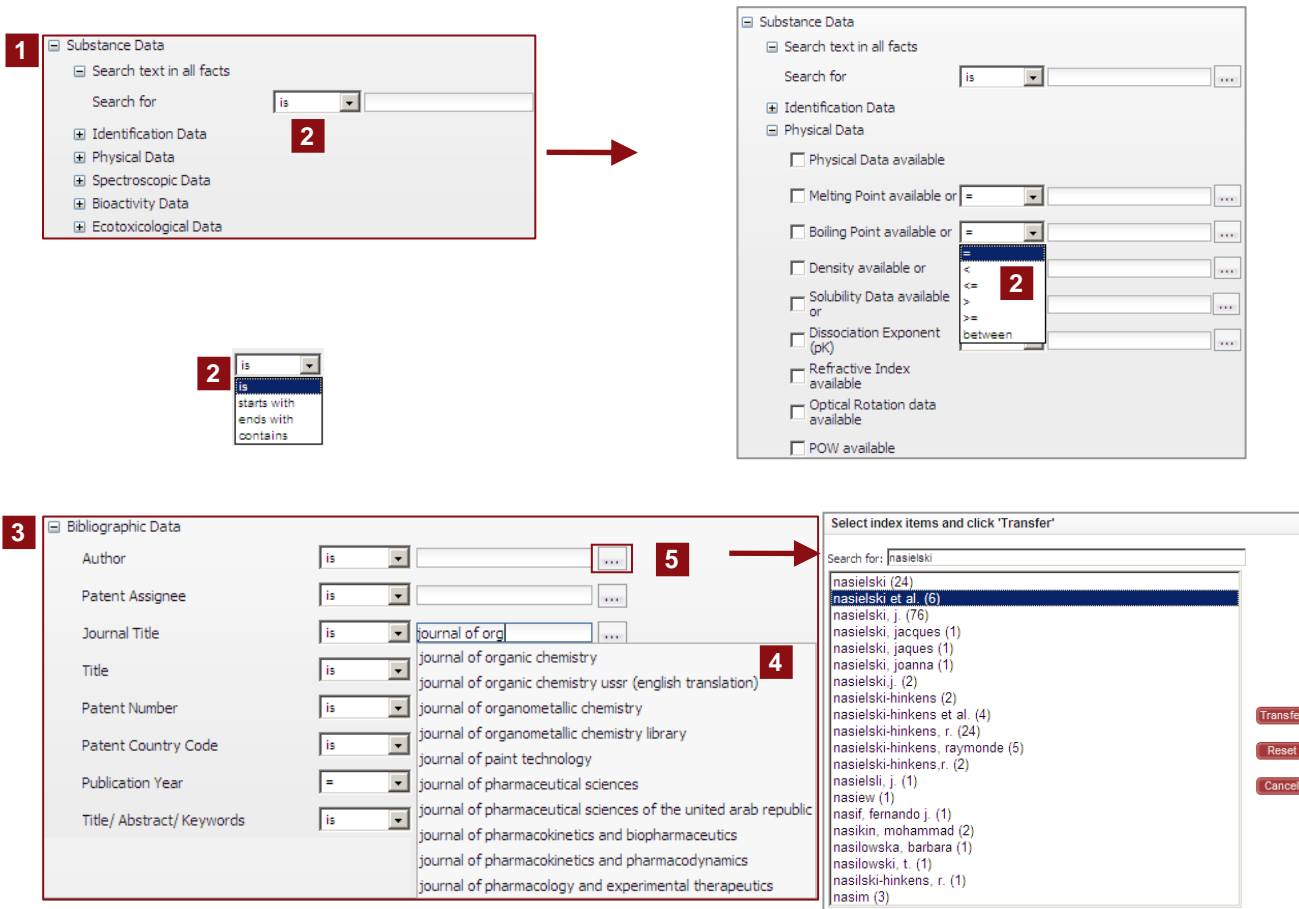
- 1 Structure/reaction box**
This window contains the needed structure, with additional query features. Two buttons allow to copy the structure to the Reactions query tab, and also to delete it.
- 2 Search as**
Define the type of structure search: *as drawn* (including possible query features added on 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 *Form-based Search* or the *Advanced Search* 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 closing the editor
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 Form-based Search



1 Substance Data

- Search text in all facts
- Search for: is
- Identification Data
- Physical Data
- Spectroscopic Data
- Bioactivity Data
- Ecotoxicological Data

2 is

- is
- starts with
- ends with
- contains

2 Substance Data

- Search text in all facts
- Search for: is
- Identification Data
- Physical Data
 - Physical Data available
 - Melting Point available or =
 - Boiling Point available or =
 - Density available or < <= > >= between
 - Solubility Data available or
 - Dissociation Exponent (pK)
 - Refractive Index available
 - Optical Rotation data available
 - POW available

3 Bibliographic Data

- Author: is
- Patent Assignee: is
- Journal Title: is journal of org
- Title: is journal of organic chemistry
- Patent Number: is journal of organometallic chemistry
- Patent Country Code: is journal of organometallic chemistry library
- Publication Year: = journal of paint technology
- Title/ Abstract/ Keywords: is journal of pharmaceutical sciences

4 journal of organic chemistry

5 journal of pharmaceutical sciences

Select index items and click 'Transfer'

Search for: nasielski

- nasielski (24)
- nasielski et al. (6)
- nasielski, j. (76)
- nasielski, jacques (1)
- nasielski, jacques (1)
- nasielski, joanna (1)
- nasielski, j. (2)
- nasielski-hinkens (2)
- nasielski-hinkens et al. (4)
- nasielski-hinkens, r. (24)
- nasielski-hinkens, raymonde (5)
- nasielski-hinkens, r. (2)
- nasielski, j. (1)
- nasiew (1)
- nasif, fernando j. (1)
- nasikin, mohammad (2)
- nasilowska, barbara (1)
- nasilowski, t. (1)
- nasilowski, r. (1)
- nasim (3)

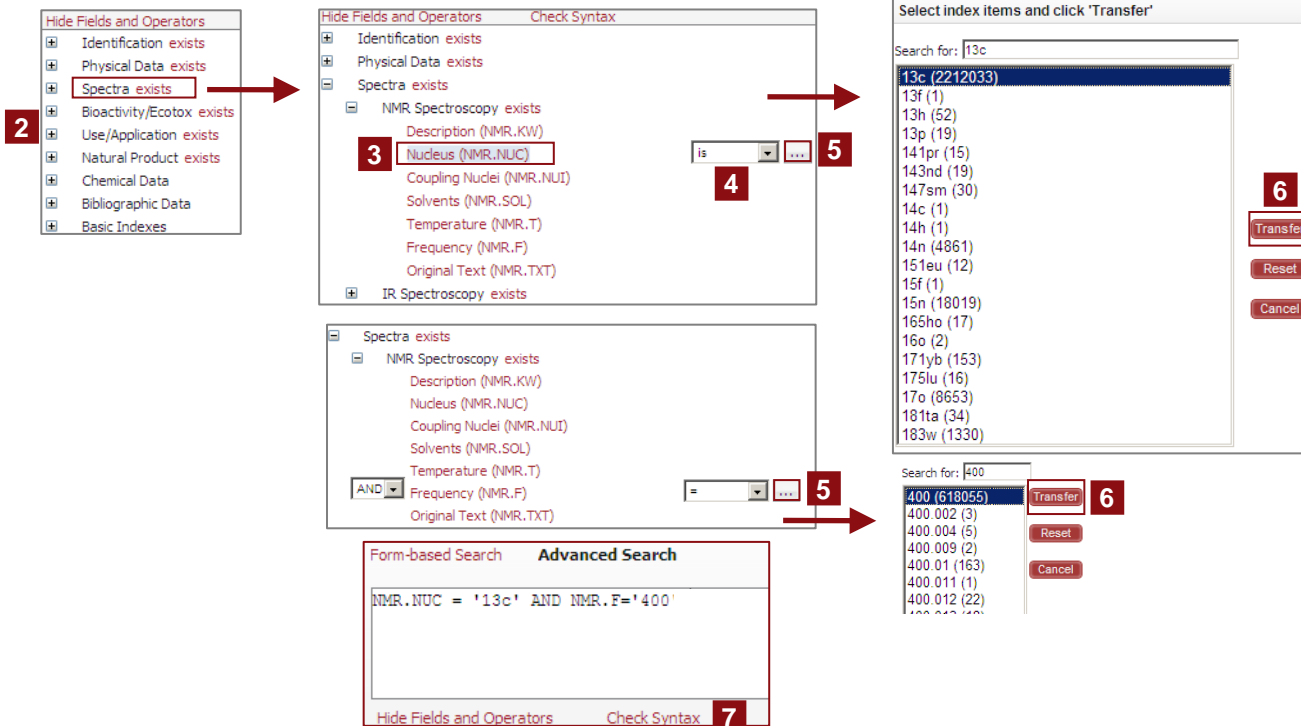
Transfer
Reset
Cancel

Note: the **Form-based Search** 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.

- 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.
- Operators**
Select the appropriate operation from the drop-down menu; for a numeric field enter the number or range in the text box.
- 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.
- Selection list**
Selection appears when typing entry.
- 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 Advanced Search

1 Show Fields and Operators



2 Fields Category

3 Needed field

4 Operators

5 Expand Index feature (for all fields)

6 Transfer the field data

7 Check Syntax

Form-based Search **Advanced Search**

NMR.NUC = '13c' AND NMR.F='400'

Note: The **Advanced Search** 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

Select the necessary field code from a hierarchical list (field list navigator) available through the **Show fields and Operators** hyperlink.

2 Fields Category

Click the + sign to expand the needed fields list.

3 Needed field

Click 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.

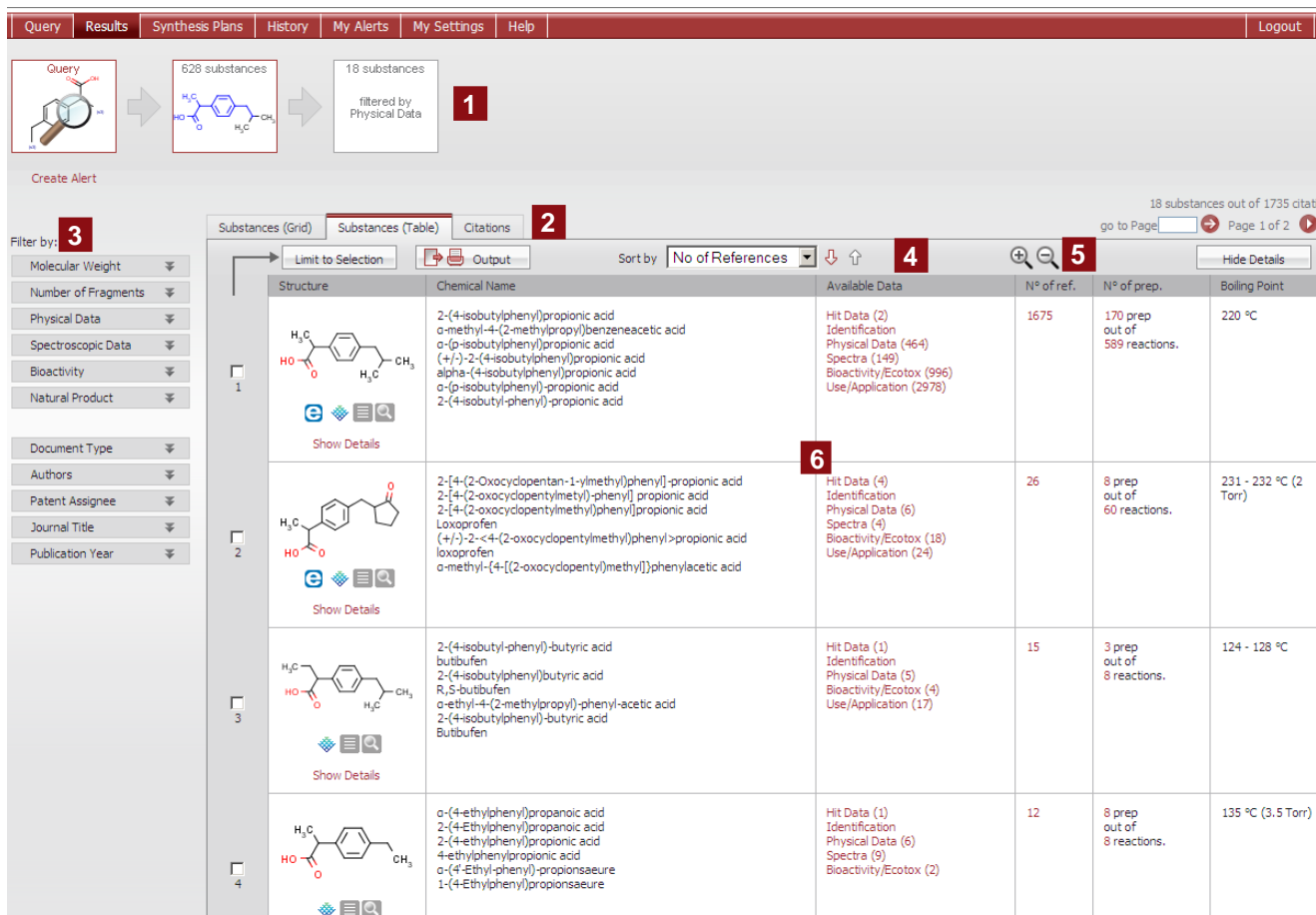
6 Transfer the field data

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

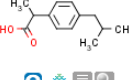
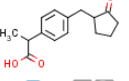
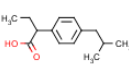
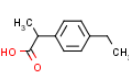


18 substances out of 1735 citations
go to Page Page 1 of 2

Filter by: **3**

Substances (Grid) Substances (Table) Citations **2**

Limit to Selection Output Sort by No of References **4** **5** Hide Details

Structure	Chemical Name	Available Data	N° of ref.	N° of prep.	Boiling Point
	2-(4-isobutylphenyl)propionic acid o-methyl-4-(2-methylpropyl)benzeneacetic acid o-(p-isobutylphenyl)propionic acid (+)-2-(4-isobutylphenyl)propionic acid alpha-4-(4-isobutylphenyl)propionic acid o-(p-isobutylphenyl)-propionic acid 2-(4-isobutyl-phenyl)-propionic acid	Hit Data (2) Identification Physical Data (464) Spectra (149) Bioactivity/ECotox (996) Use/Application (2978)	1675	170 prep out of 589 reactions.	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- α -(2-oxocyclopentylmethyl)phenyl>propionic acid loxoprofen o-methyl-4-[[2-oxocyclopentyl]methyl]phenylacetic acid	Hit Data (4) Identification Physical Data (6) Spectra (4) Bioactivity/ECotox (18) Use/Application (24)	26	8 prep out of 60 reactions.	231 - 232 °C (2 Torr)
	2-(4-isobutyl-phenyl)-butyric acid butbufen 2-(4-isobutylphenyl)butyric acid R,S-butbufen o-ethyl-4-(2-methylpropyl)-phenyl-acetic acid 2-(4-isobutylphenyl)-butyric acid Butbufen	Hit Data (1) Identification Physical Data (5) Bioactivity/ECotox (4) Use/Application (17)	15	3 prep out of 8 reactions.	124 - 128 °C
	o-(4-ethylphenyl)propanoic acid 2-(4-Ethylphenyl)propanoic acid 2-(4-ethylphenyl)propionic acid 4-ethylphenylpropionic acid o-(4'-Ethyl-phenyl)-propionsaeure 1-(4-Ethylphenyl)propionsaeure	Hit Data (1) Identification Physical Data (6) Spectra (9) Bioactivity/ECotox (2)	12	8 prep out of 8 reactions.	135 °C (3.5 Torr)

6 Show Details

1 Breadcrumbs
Graphical navigation helps keeping track of your result analysis.

2 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.

3 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).

4 Tool bar
Access limit to selection, output, sort by features.

5 Maximizer/minimizer tool

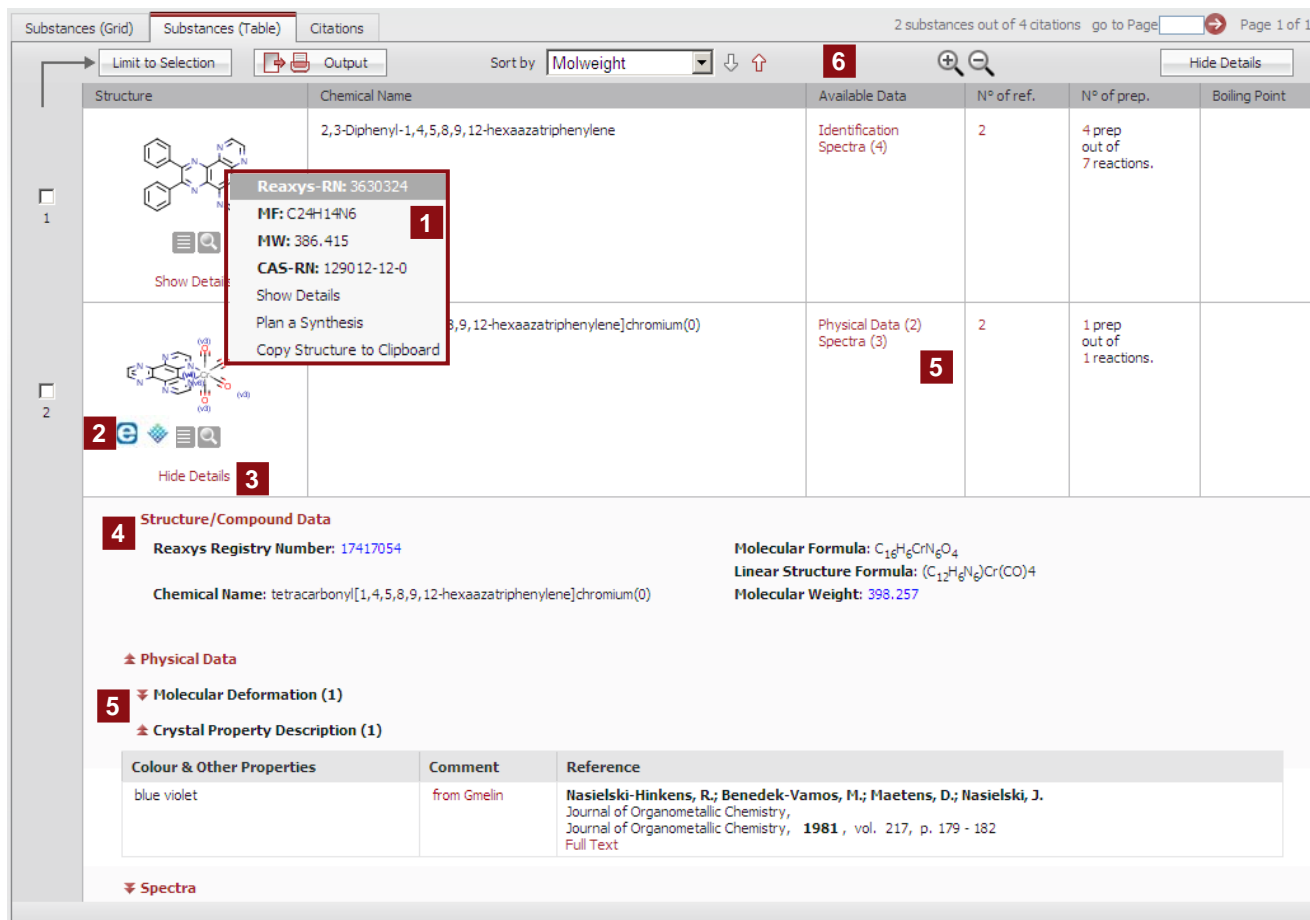
Increase or decrease the size of displayed structures.

6 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.

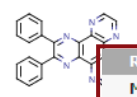

Note: information on the citations tab of the substances results window can be found on page 21.

Substances and properties Substances (table) tab



Substances (Grid) Substances (Table) Citations 2 substances out of 4 citations go to Page 1 of 1

Limit to Selection... Output Sort by Molweight 6 Hide Details

Structure	Chemical Name	Available Data	N° of ref.	N° of prep.	Boiling Point
	2,3-Diphenyl-1,4,5,8,9,12-hexaazatriphenylene	Identification Spectra (4)	2	4 prep out of 7 reactions.	
	8,9,12-hexaazatriphenylene]chromium(0)	Physical Data (2) Spectra (3)	2	1 prep out of 1 reactions.	

1 Reaxys-RN: 3630324
MF: C₂₄H₁₄N₆
MW: 386.415
CAS-RN: 129012-12-0
Show Details
Plan a Synthesis
Copy Structure to Clipboard


2 **3** **4** **5**

4 Structure/Compound Data
Reaxys Registry Number: 17417054
Molecular Formula: C₁₈H₈CrN₆O₄
Linear Structure Formula: (C₁₂H₈N₆)Cr(CO)₄
Molecular Weight: 398.257
Chemical Name: tetracarbonyl[1,4,5,8,9,12-hexaazatriphenylene]chromium(0)

5 **Physical Data**
Molecular Deformation (1)
Crystal Property Description (1)

Colour & Other Properties	Comment	Reference
blue violet	from Gmelin	Nasielski-Hinkens, R.; Benedek-Vamos, M.; Maetens, D.; Nasielski, J. Journal of Organometallic Chemistry, Journal of Organometallic Chemistry, 1981 , vol. 217, p. 179 - 182 Full Text

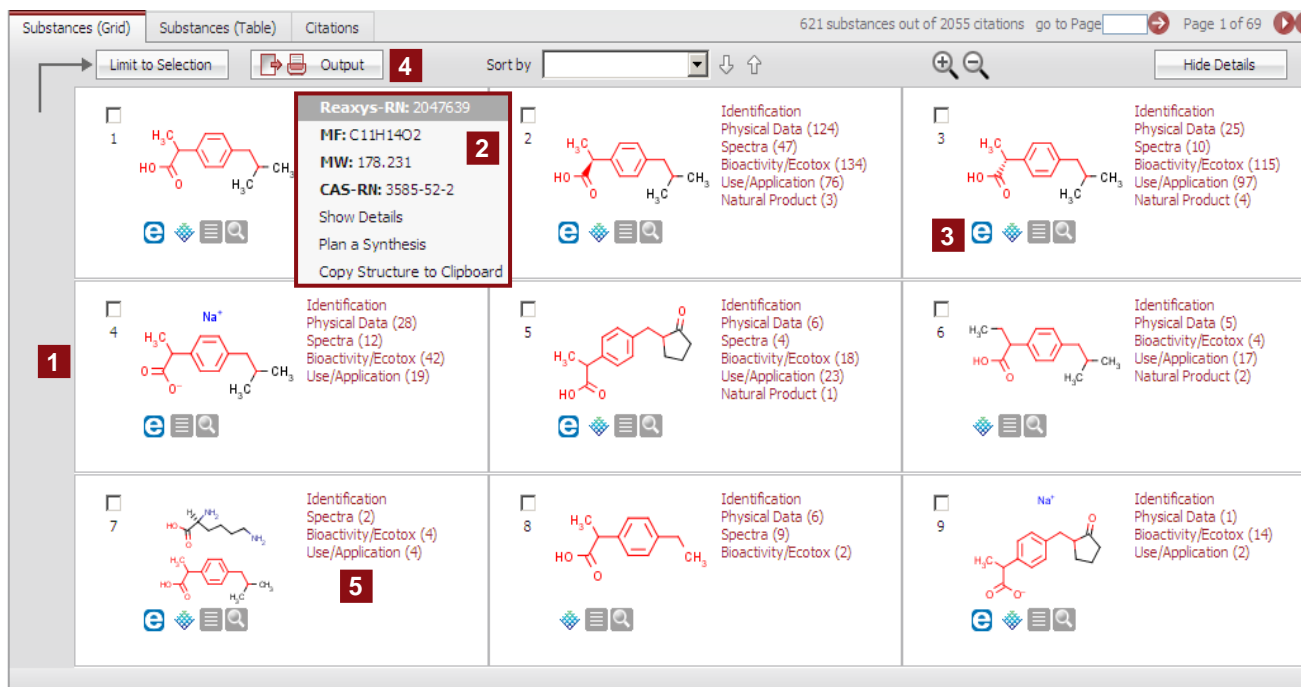
Spectra

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

- 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), Plan a synthesis (create your retrosynthesis), Copy structure to clipboard
- Commercial availability**
Access the commercial availability of a substance and lead to appropriate company's (eMolecules/ACD).
- Show/hide details button**
- Structure/compound data**
Find details about structure/compound.
- Available data**
Links 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).

Click **Show Details** to expand the list of all the types of data available for a compound.
Click a specific link in the available data column to only expand the needed data.

Substances and properties Substances (grid) tab



Substances (Grid) | Substances (Table) | Citations | 621 substances out of 2055 citations | go to Page | Page 1 of 69

Limit to Selection | Output | 4 | Sort by | Hide Details

1 | **2** | **3** | **4** | **5**

Reaxys-RN: 20-47639
MF: C₁₁H₁₄O₂
MW: 178.231
CAS-RN: 3585-52-2
Show Details
Plan a Synthesis
Copy Structure to Clipboard

Identification
Physical Data (124)
Spectra (47)
Bioactivity/ECotox (134)
Use/Application (76)
Natural Product (3)

Identification
Physical Data (25)
Spectra (10)
Bioactivity/ECotox (115)
Use/Application (97)
Natural Product (4)

Identification
Physical Data (28)
Spectra (12)
Bioactivity/ECotox (42)
Use/Application (19)

Identification
Physical Data (6)
Spectra (4)
Bioactivity/ECotox (18)
Use/Application (23)
Natural Product (1)

Identification
Physical Data (5)
Bioactivity/ECotox (4)
Use/Application (17)
Natural Product (2)

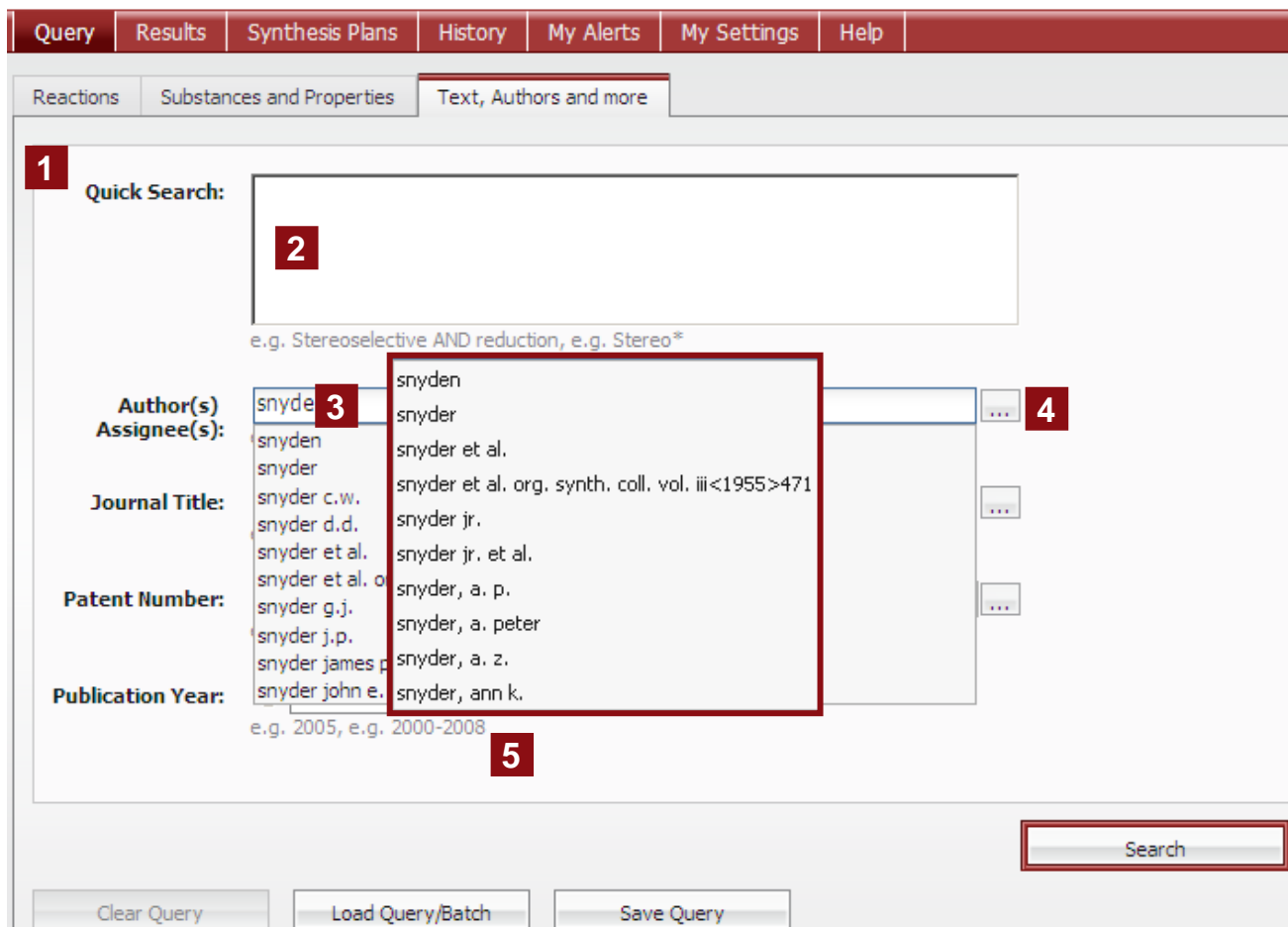
Identification
Spectra (2)
Bioactivity/ECotox (4)
Use/Application (4)

Identification
Physical Data (6)
Spectra (9)
Bioactivity/ECotox (2)

Identification
Physical Data (1)
Bioactivity/ECotox (14)
Use/Application (2)

- 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 lead to appropriate company's (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



1 Quick Search:

e.g. Stereoselective AND reduction, e.g. Stereo*

2

3 Author(s) Assignee(s):

4

5

Search

Clear Query Load Query/Batch Save Query

- 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.

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

Text, authors and more Citations tab

26 citations go to Page Page 1 of 3

Filter by: **1**

- Document Type
- Authors
- Patent Assignee
- Journal Title
- Publication Year

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

	Title of the Document	Authors	Year	Source	Times cited
<input type="checkbox"/> 1	Biocatalytic Microcontact Printing	Snyder, Phillo W.; Johannes, Matthew S.; Vogen, Briana N.; Clark, Robert L.; Toone, Eric J.	2007	Journal of Organic Chemistry, 2007, vol. 72, # 19 p. 7459 - 7461 Full Text Scopus	
	Title/Abstract Show All Reactions (13) 4 Show All Substances (11)				
<input type="checkbox"/> 2	Nucleic acid molecules, polypeptides and uses therefor, including diagnosis and treatment of Alzheimer's disease	Durham, L. Kathryn; Friedman, David L.; Herath, Herath Mudiyansele Athula Chandrasiri; Kimmel, Lida H.; Parekh, Rajesh Bhikhu; Potter, David M.; Rohlf, Christian; Silber, B. Michael; Snyder, Peter Jeffrey; Soares, Holly Dana; Stiger, Thomas R.; Sunderland, P. Trey; Townsend, Robert Reid; White, W. Frost; Williams, Stephen A.	2005	Patent: US2005/163789; A9 Full Text	
	Title/Abstract				
<input type="checkbox"/> 3	Nucleic acid molecules, polypeptides and uses therefor, including diagnosis and treatment of Alzheimer's disease	Durham, L. Kathryn; Friedman, David L.; Herath, Herath Mudiyansele Athula Chandrasiri; Kimmel, Lida H.; Parekh, Rajesh Bhikhu; Potter, David M.; Rohlf, Christian; Silber, B. Michael; Snyder, Peter Jeffrey; Soares, Holly Dana; Stiger, Thomas R.; Sunderland, P. Trey; Townsend, Robert Reid; White, W. Frost; Williams, Stephen A.	2004	Patent: US2004/22794; A1 Full Text	
	Title/Abstract				
<input type="checkbox"/> 4	Ethylene. Experimental Evidence for New Assignments of Electronic Transitions in the n - >n* Energy Region. Absorption and Magnetic Circular Dichroism Measurements with Synchrotron Radiation	Snyder, Patricia Ann; Atanasova, Sylvia; Hansen, Roger W. C.	2004	Journal of Physical Chemistry A: Molecules, Spectroscopy, Kinetics, Environment, & General Theory, 2004, vol. 108, # 19 p. 4194 - 4201 Full Text Scopus 5	
	Title/Abstract				

- Filter by**
Refine search results by applying filters (document type, authors, patent assignee, journal title and publication year).
- 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 in Scopus.

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