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Reaxys Quick Reference Guide

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Last revision: 2009-10-26

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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**	**nlinfo@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**

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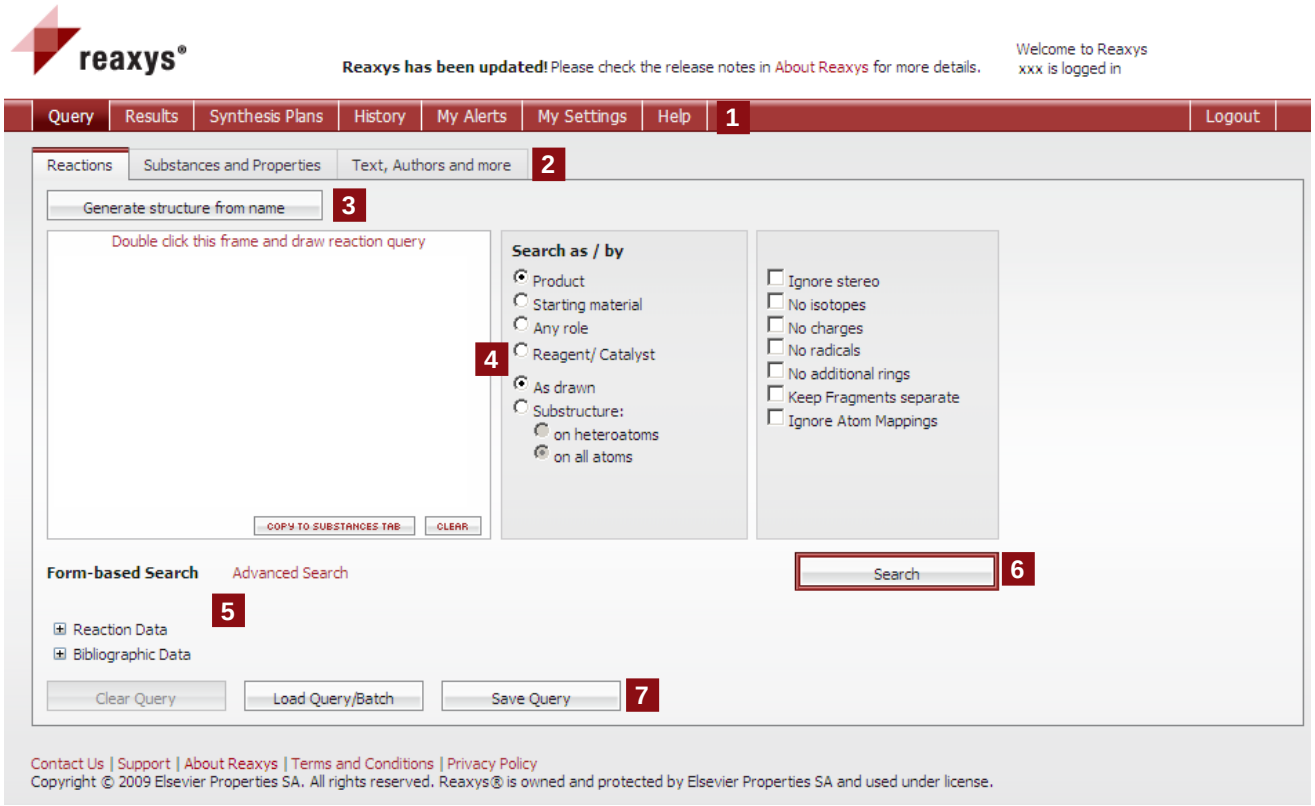
Homepage



How to find the preparation of a compound?

1. *Ensure the reaction tab is selected and double click the drawing pane*
2. *Draw the desired compound structure in your preferred editor and 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.

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.

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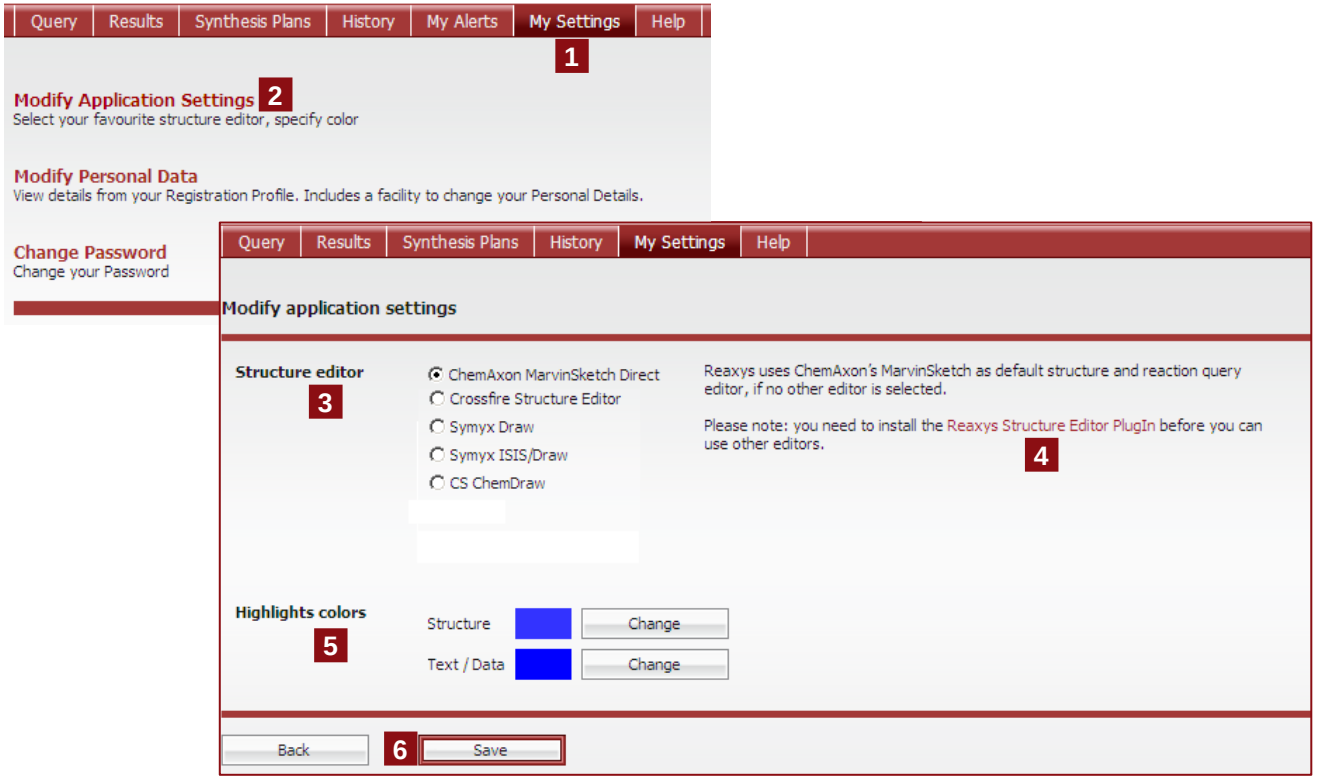
My settings



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.*

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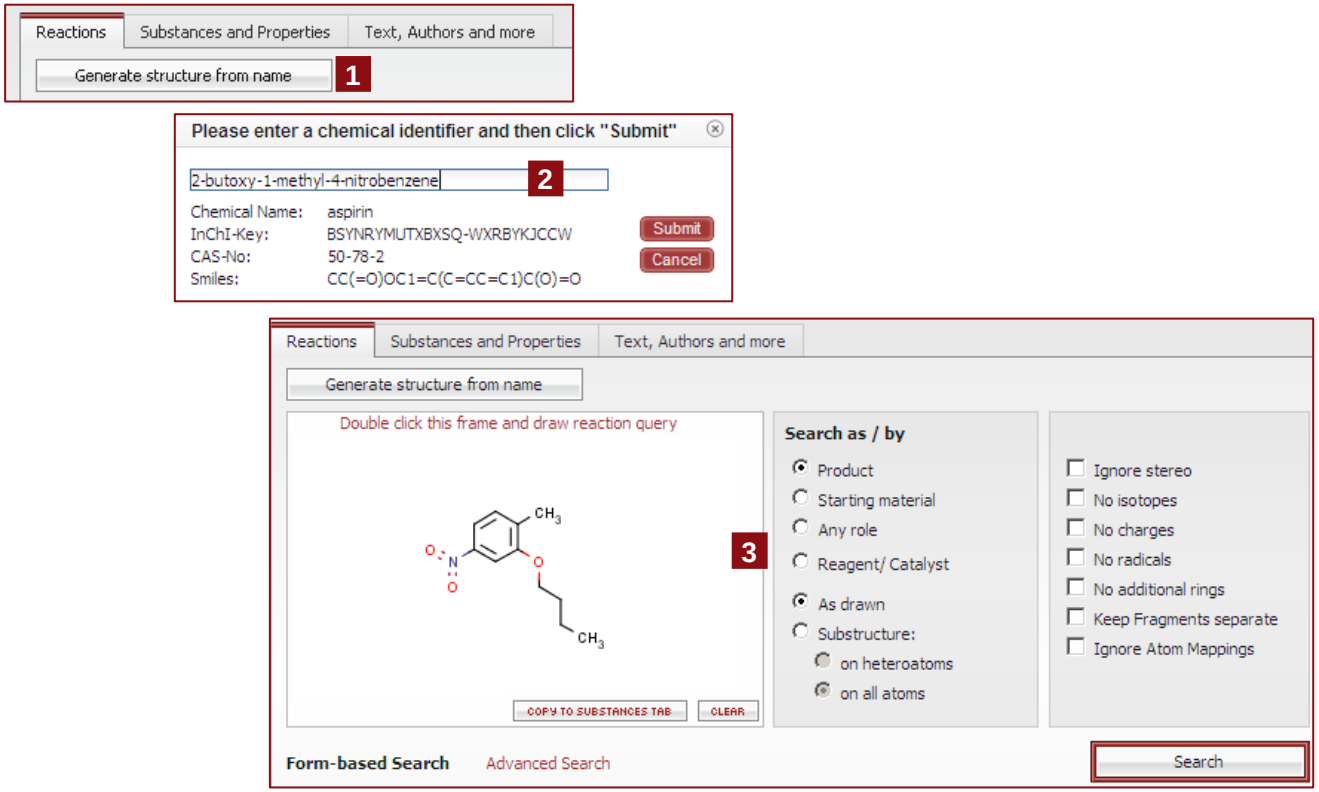
Generate a structure from name



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:

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.

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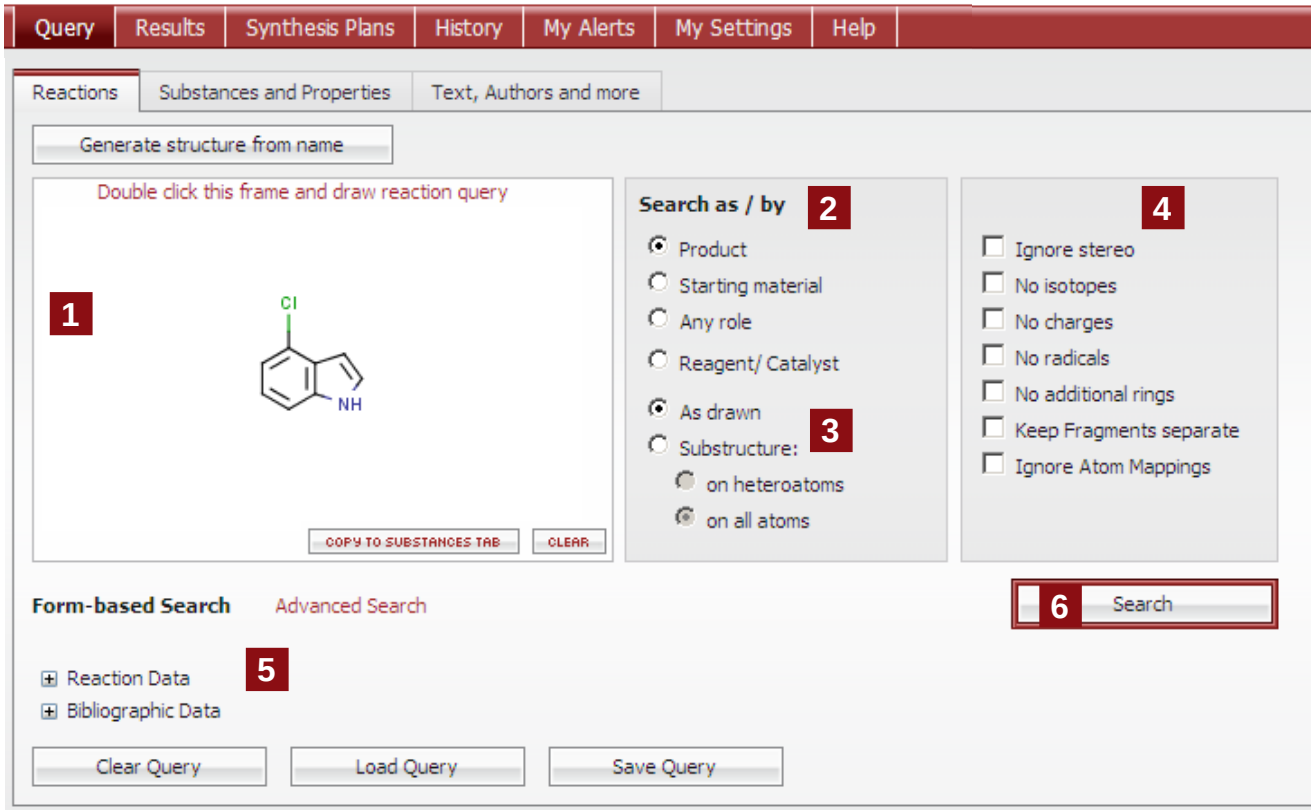
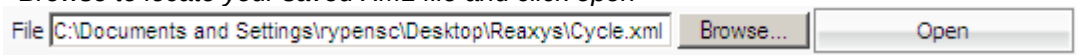
Reactions query tab



How to load a saved query?

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



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

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

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

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

5 Add further search conditions
Click the *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.

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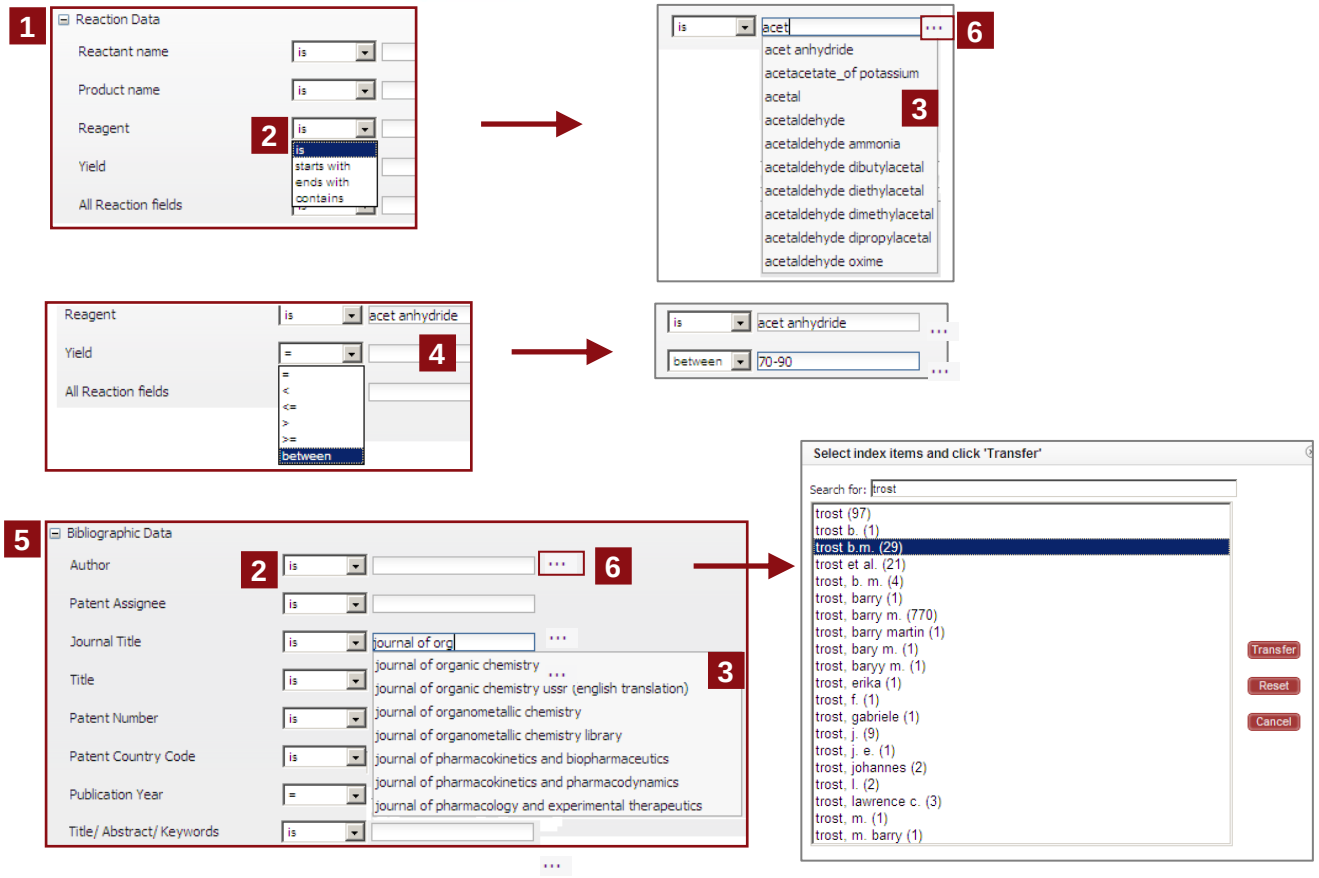
Reactions query tab
Form-based Search



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.

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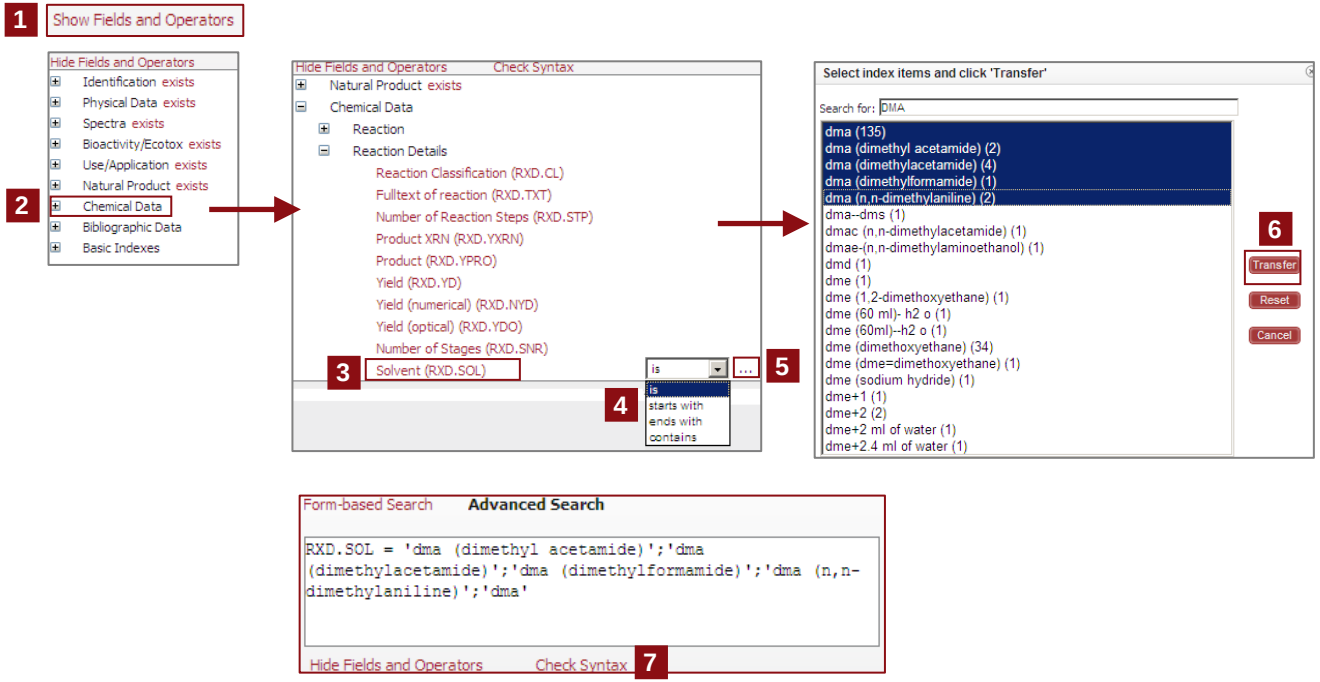
Reactions query tab
Advanced Search



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.*

1 Show Fields and Operators
Select the necessary field code form 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.

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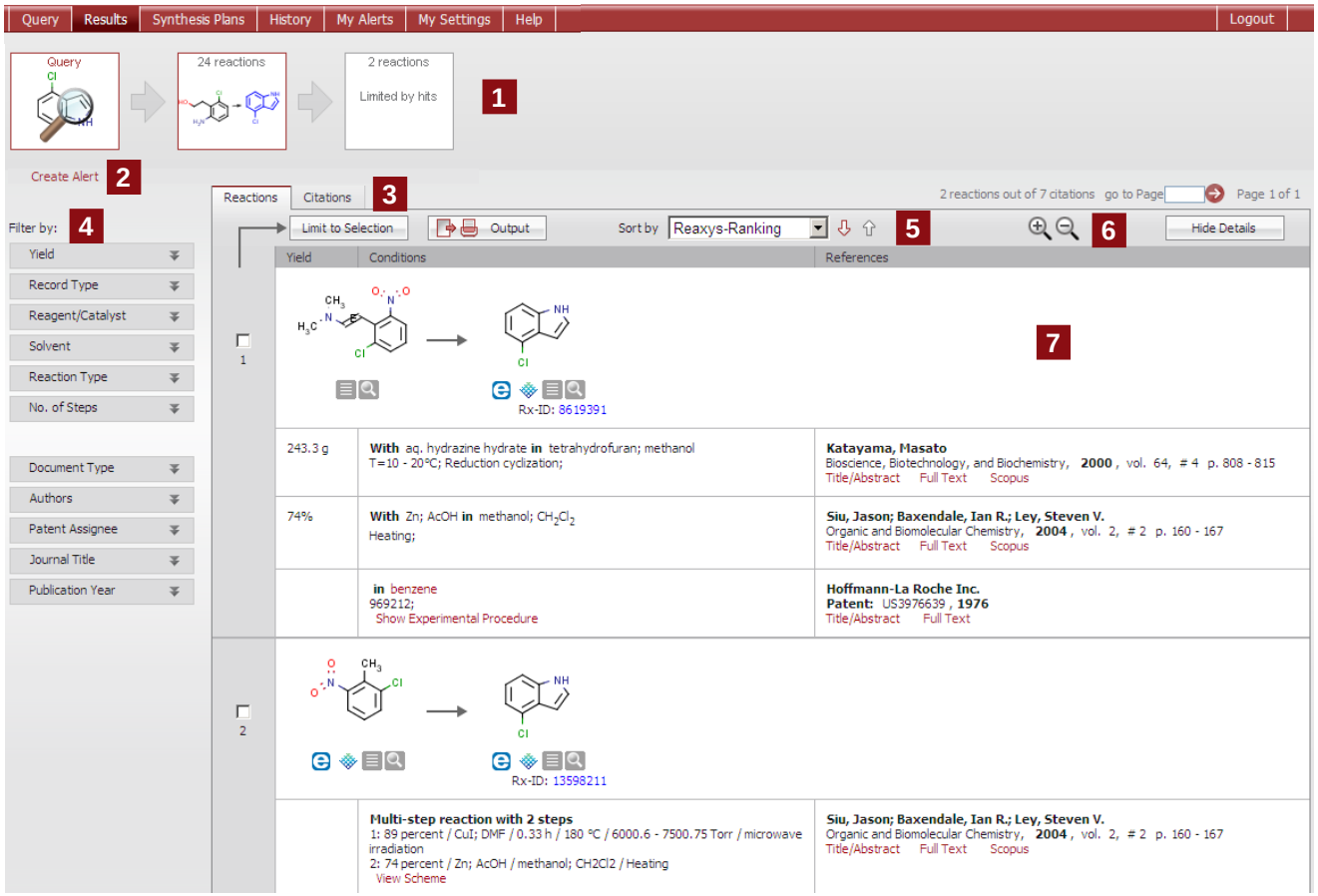
Reactions results
General overview



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.

1 Breadcrumbs
Graphical navigation helps keep track of your result 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.

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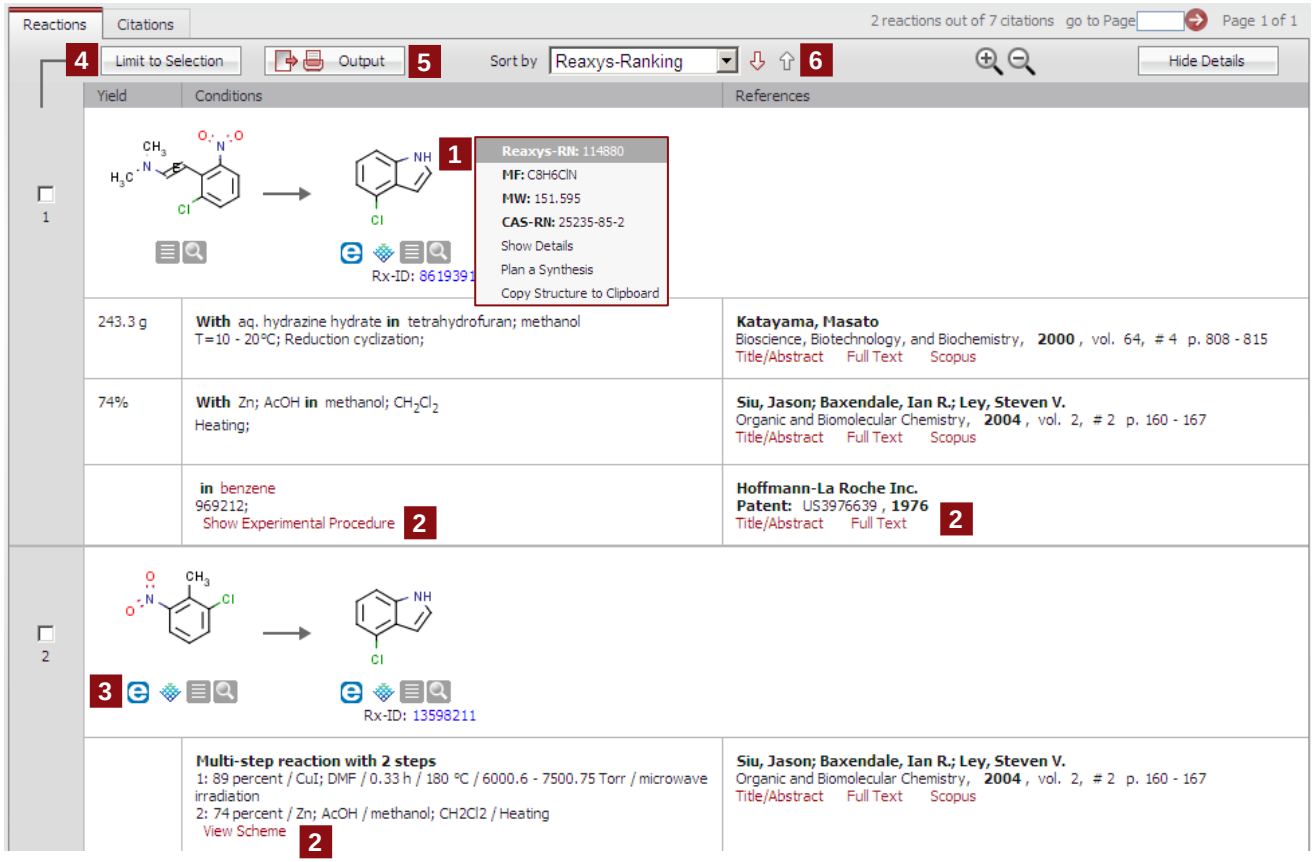
Reactions results
Reactions tab



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

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

1 **Display further options & Data**
Reaxys – RN (*Reaxys registry number*), MF (*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).

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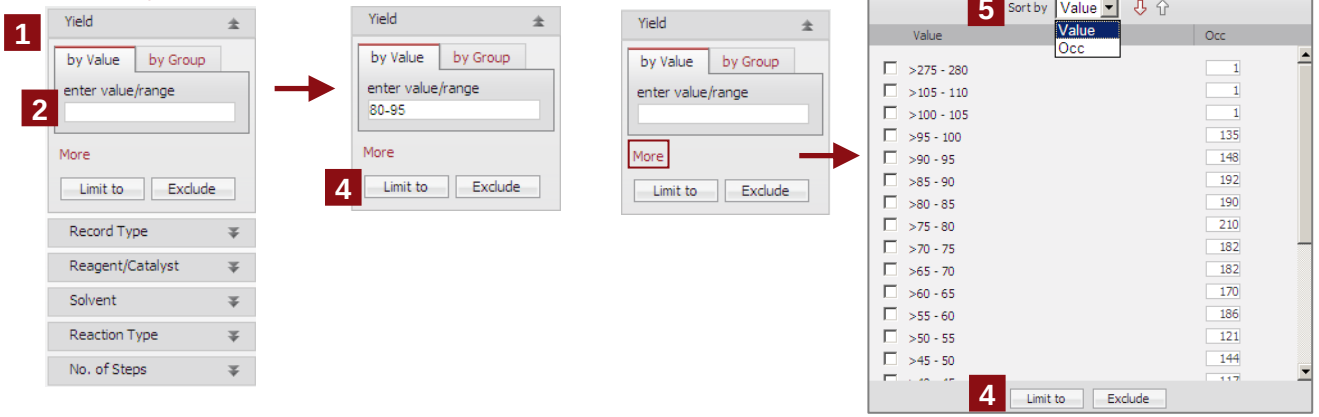
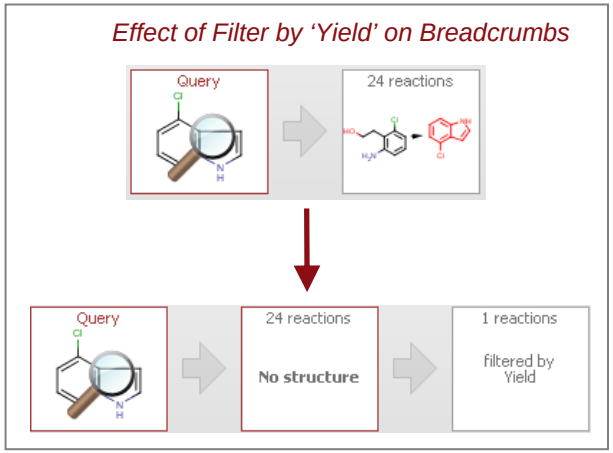
Reactions results tab
Filter by

Filter by Value



Filter by Group

Effect of Filter by 'Yield' on Breadcrumbs



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

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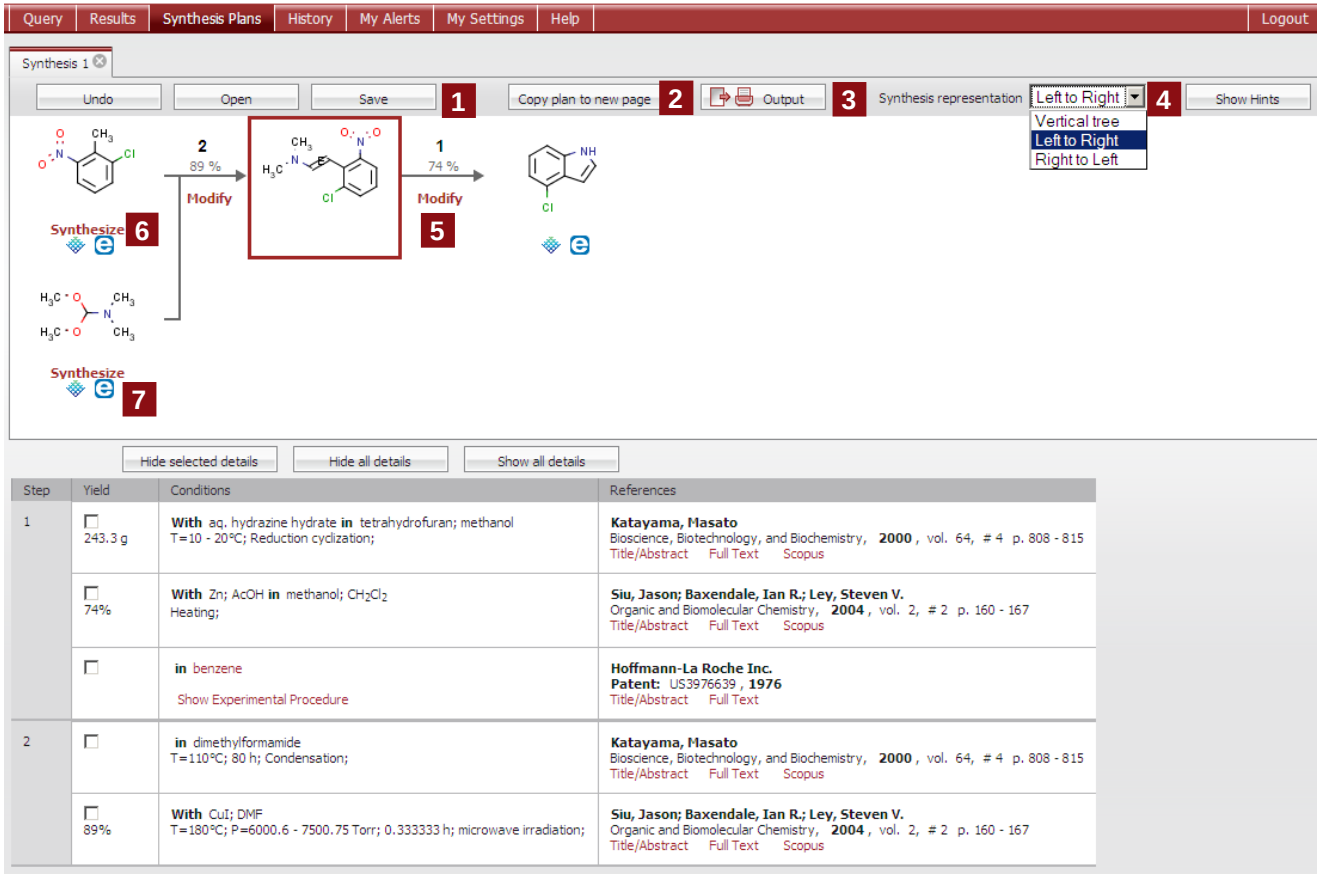
Synthesis plans



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

Click 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 uncessary 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).

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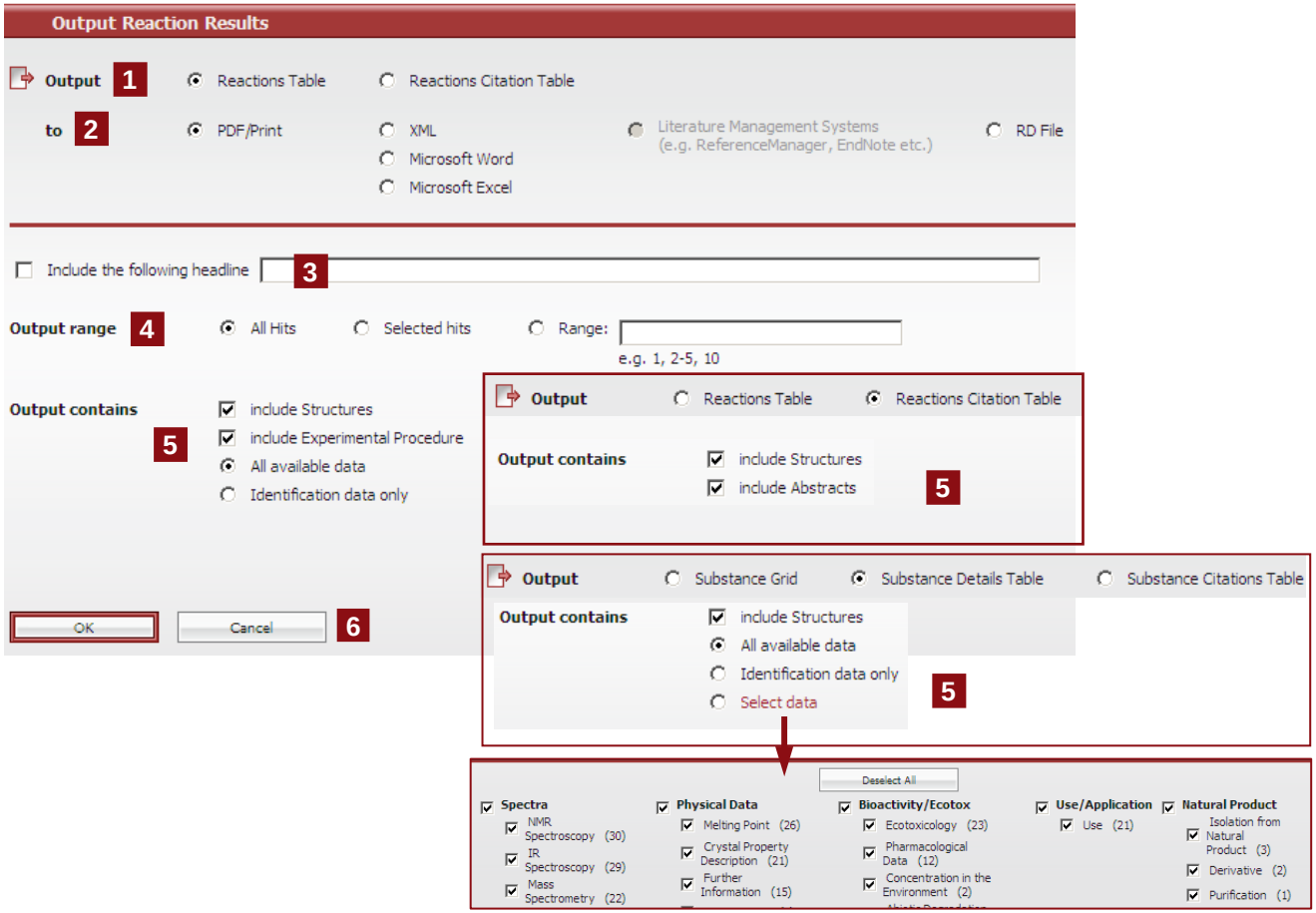
Output



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.

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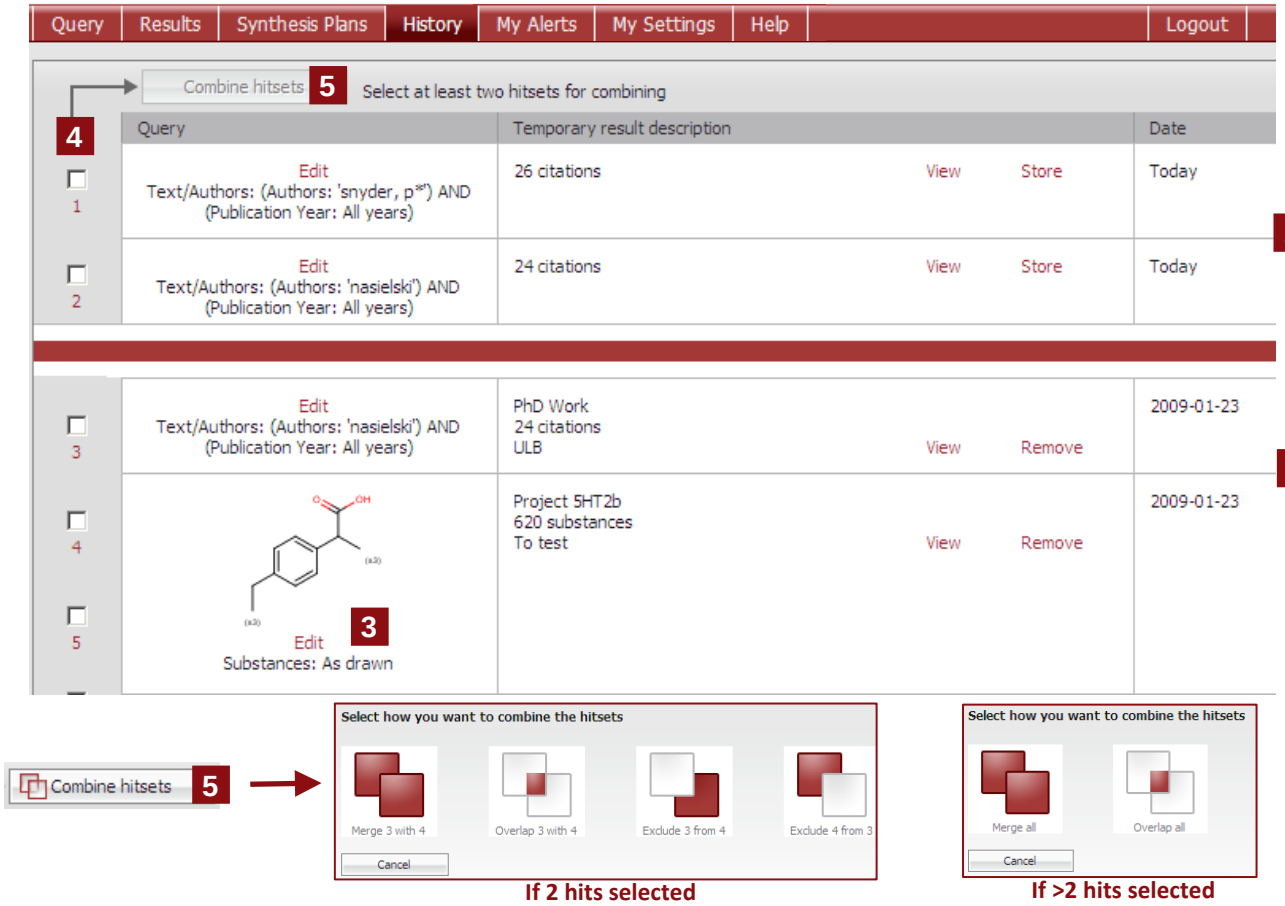
History



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

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

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

4 Combine hitsets
5 Select two or more lists by checking the box 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.

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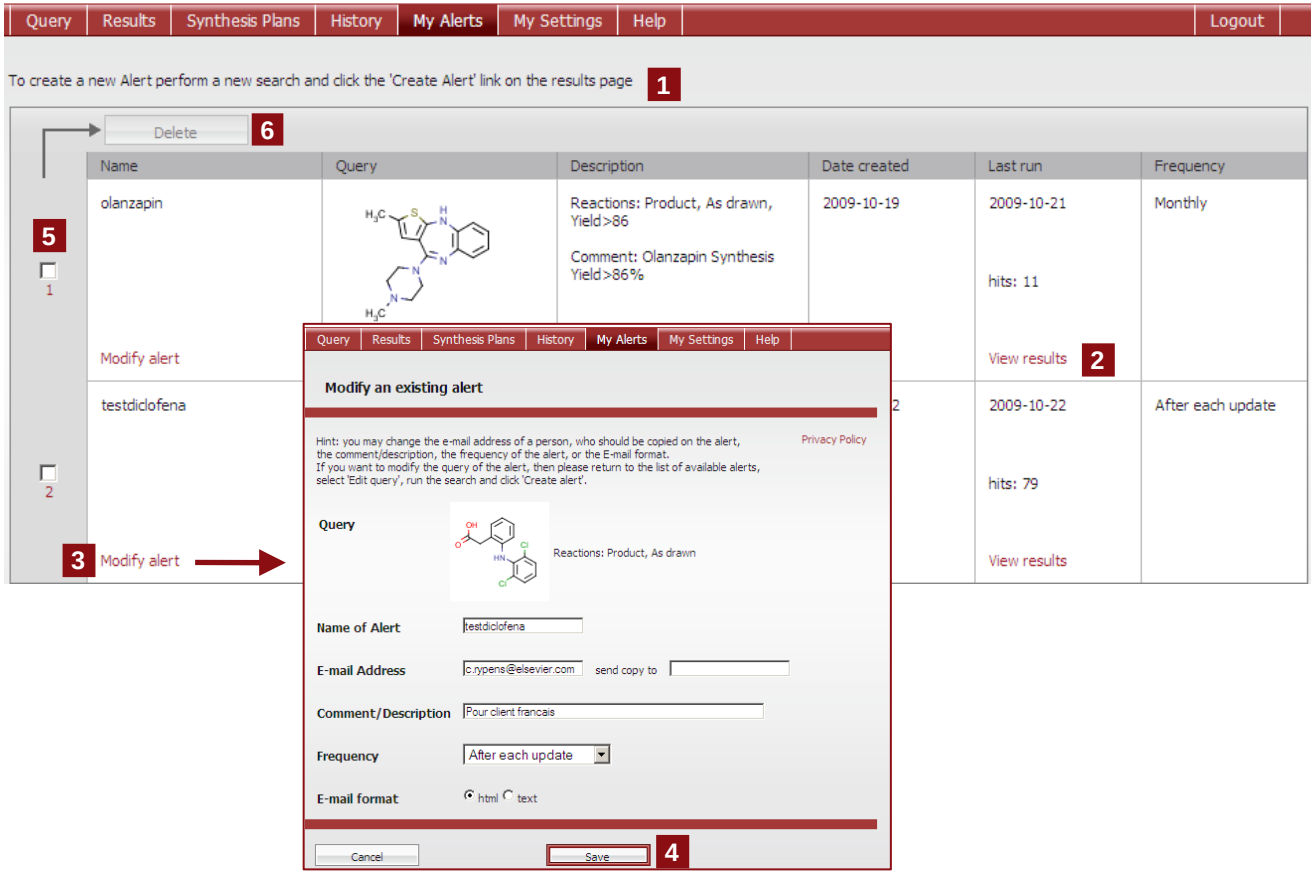
My Alerts



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.

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

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

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

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

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

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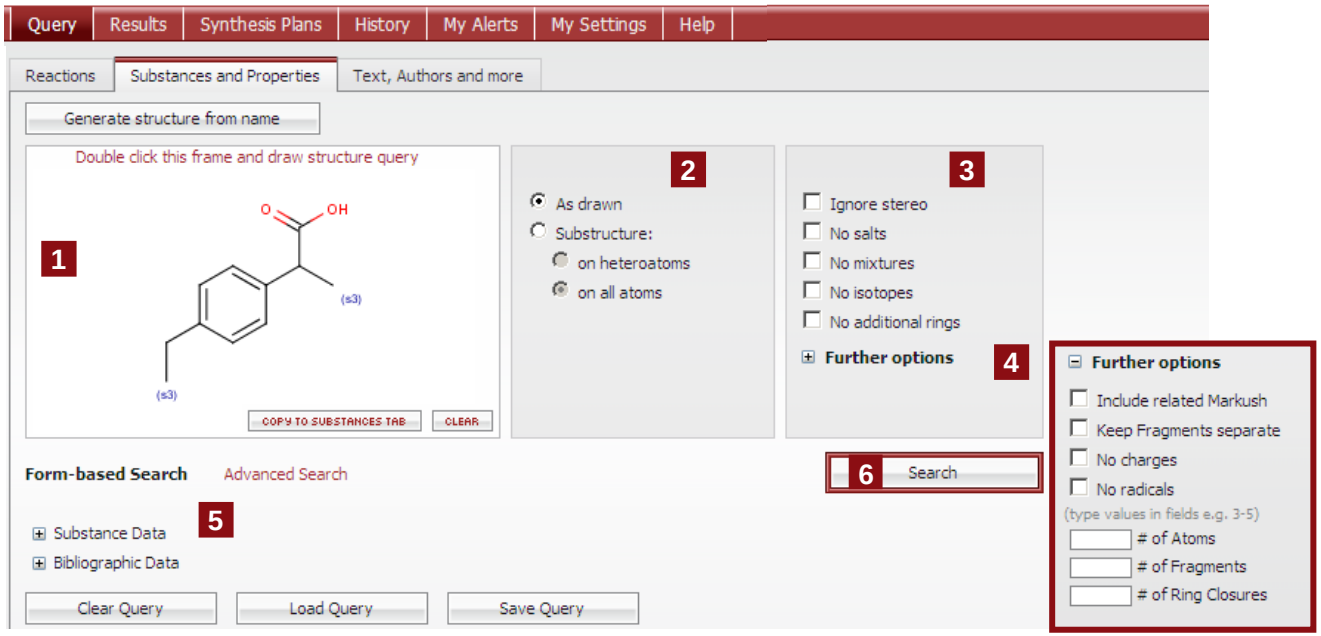
Substances and properties Query tab



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.

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

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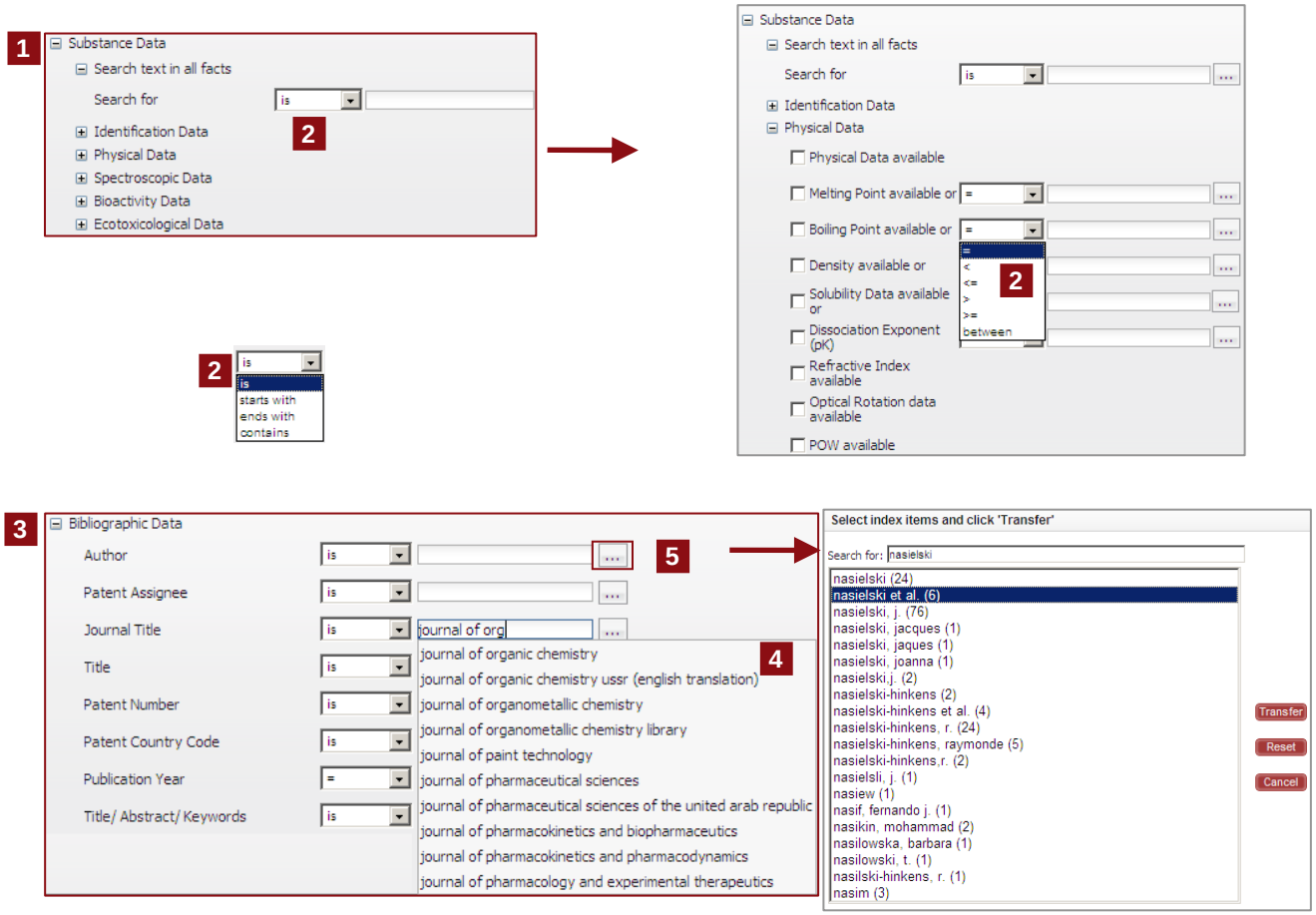
Substances query tab
Form-based Search



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.

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.

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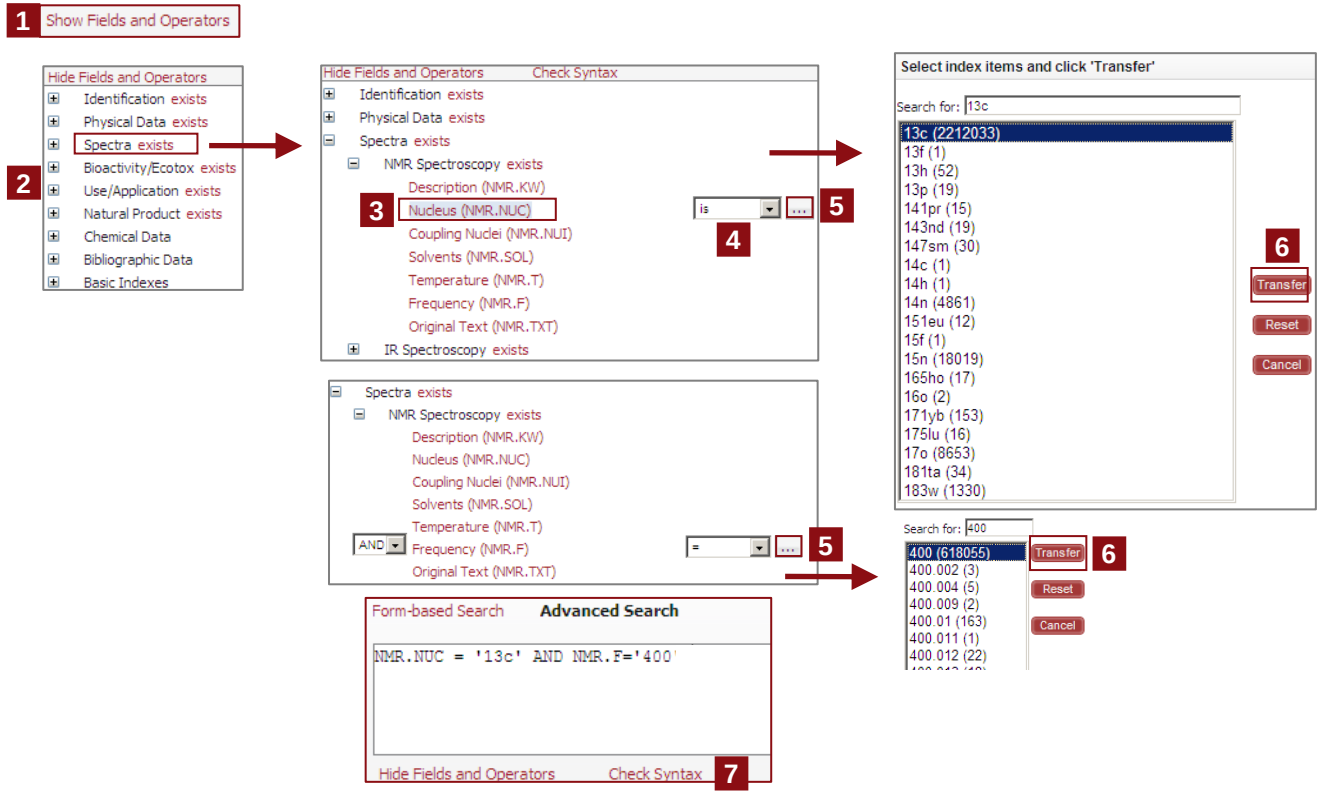
Substances query tab
Advanced Search



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 trough 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.

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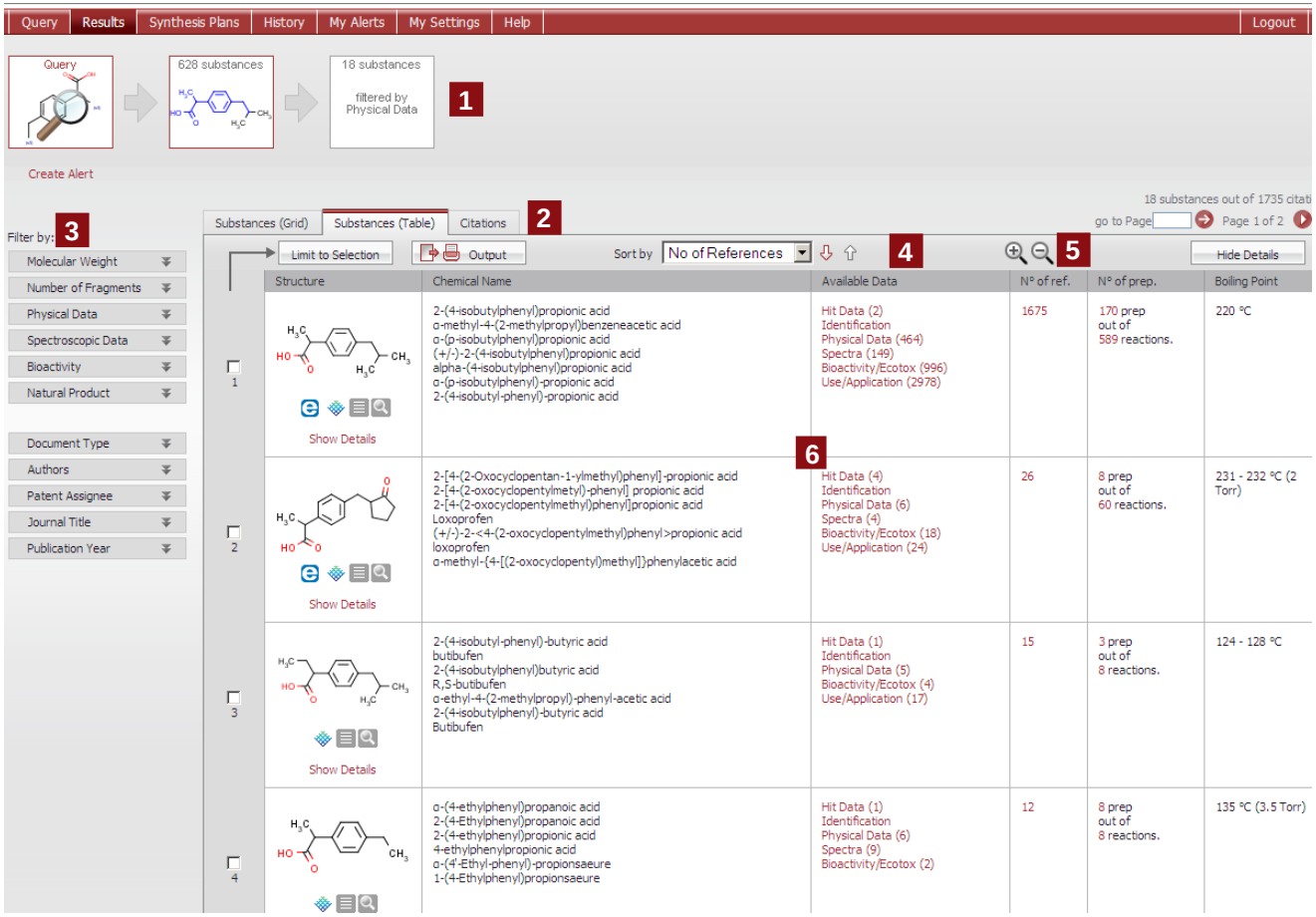
Substances and properties Results overview



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.

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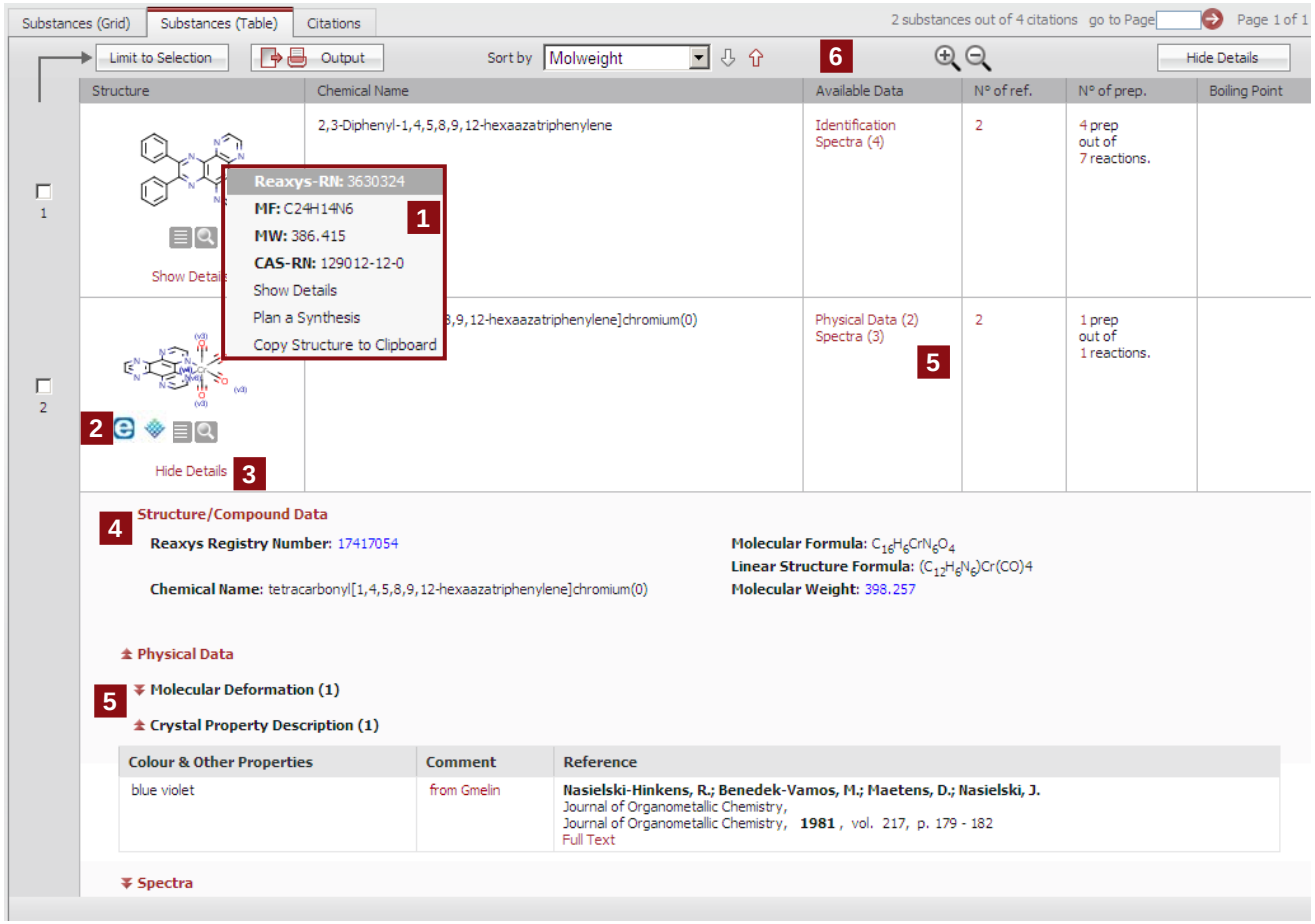
Substances and properties
Substances (table) tab



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.

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

1 Additional information / sub items
Reaxys –RN (*Reaxys registry number),* MF (*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

2 Commercial availability
Access the commercial availability of a substance and lead to appropriate company's (eMolecules/ACD).

3 Show/hide details button

4 Structure/compound data
Find details about structure/ compound.

5 Available data
Links to all available data (from organic, inorganic & organometallic sources). Data excerpted from Gmelin has a from Gmelin flag.

6 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).

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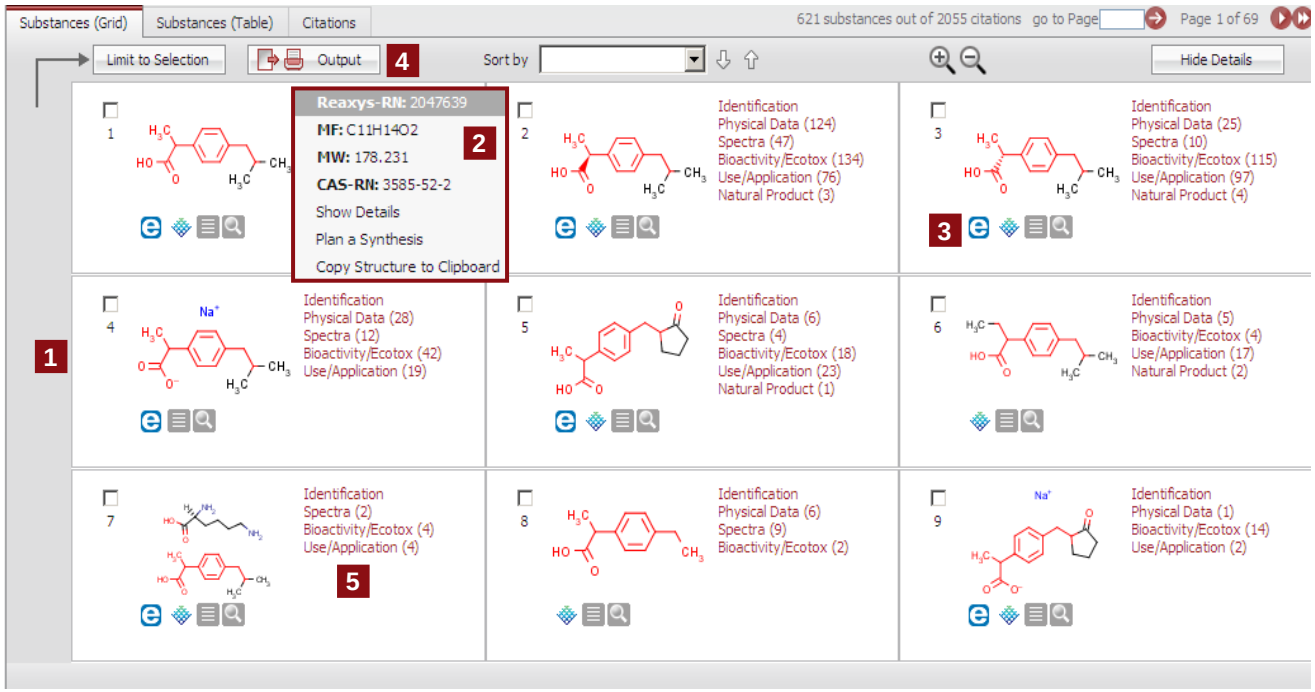
Substances and properties
Substances (grid) tab



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.

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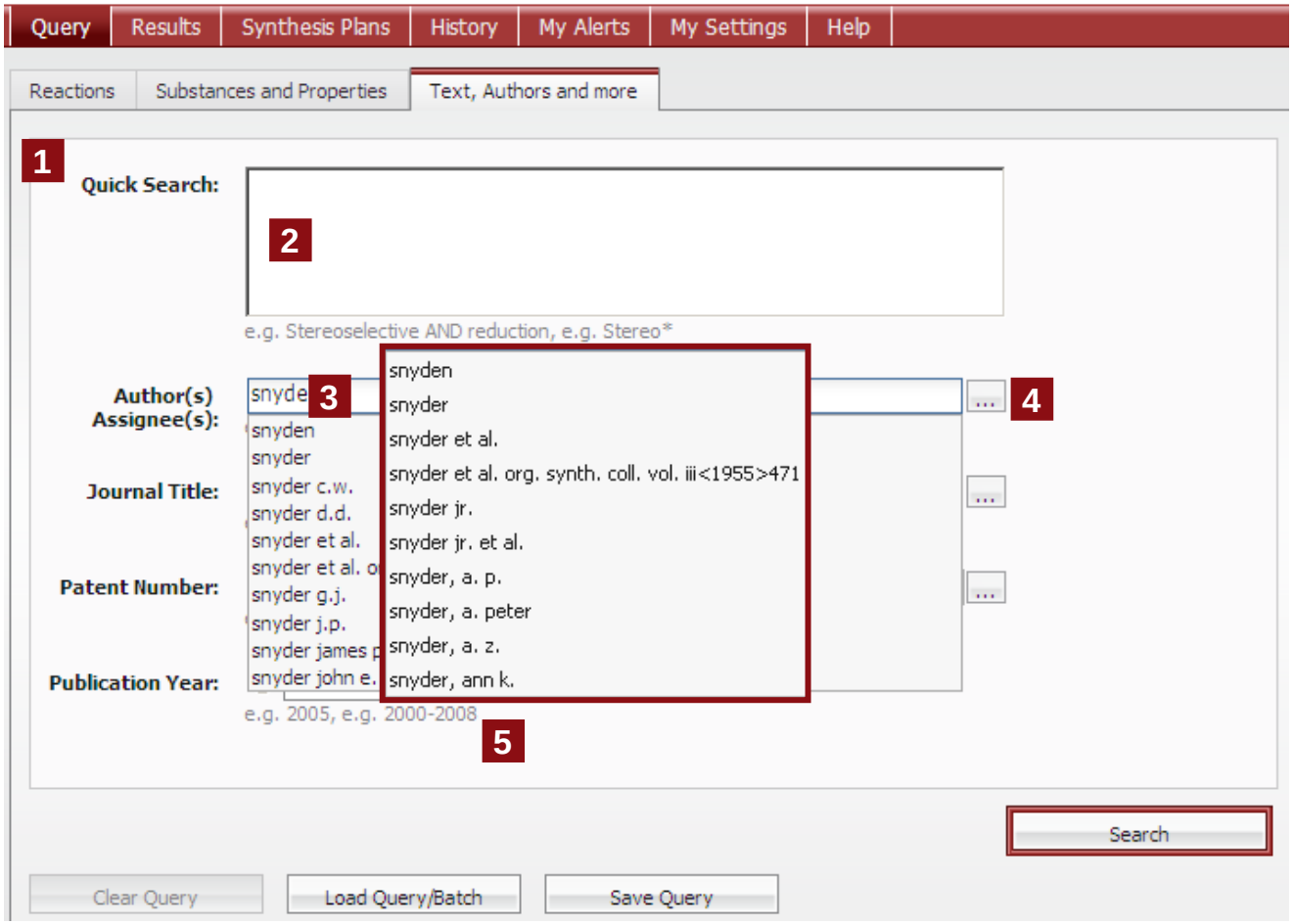
Text, authors and more
Query tab



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.

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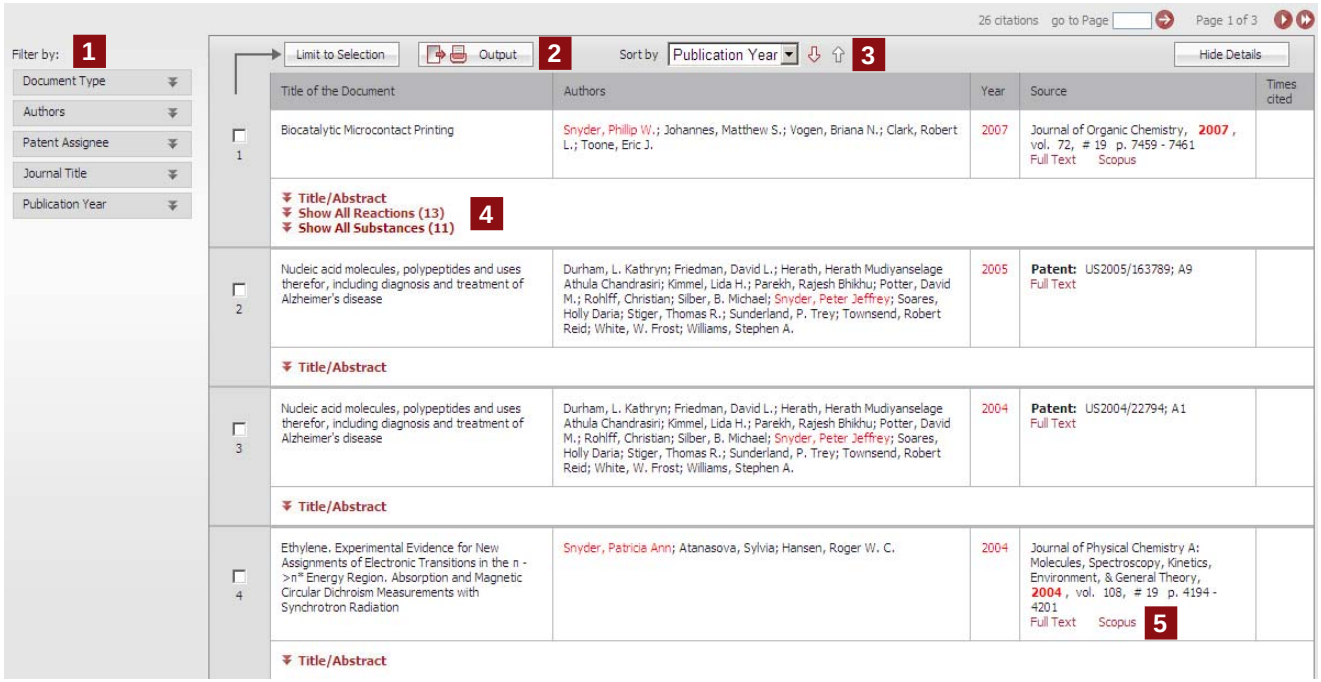
Text, authors and more
Citations tab



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

2 Output
Export results in an appropriate format.

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

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

5 Source
Find here the literature reference. Display the original text with the full text link and access related information 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*

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