MDL® CrossFire Commander 7.0

Quick User Guide

03/2004

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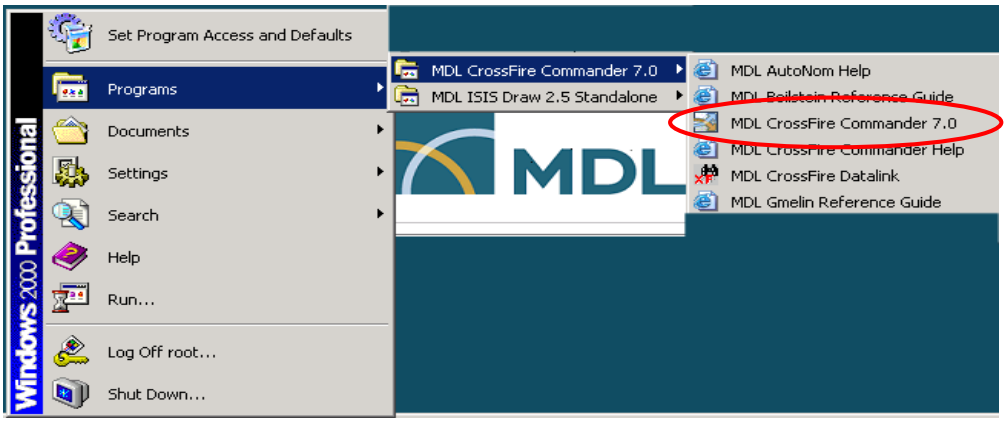
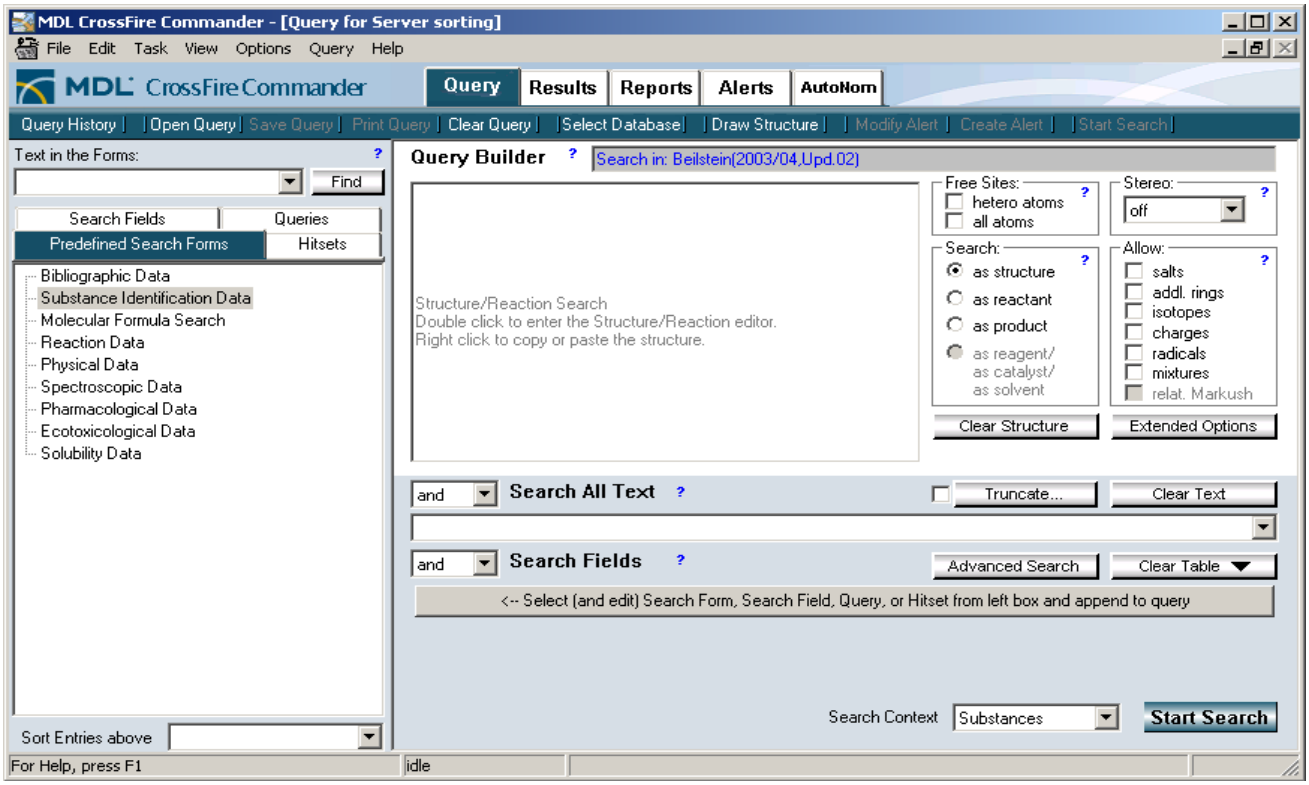
1 General

1.1 Starting MDL CrossFire Commander 7

- To start Commander from whichever platform you are using: double click the icon on your desktop or select in the Windows start menu "**Programs:MDL CrossFire Commander 7**"



1.2 Overview



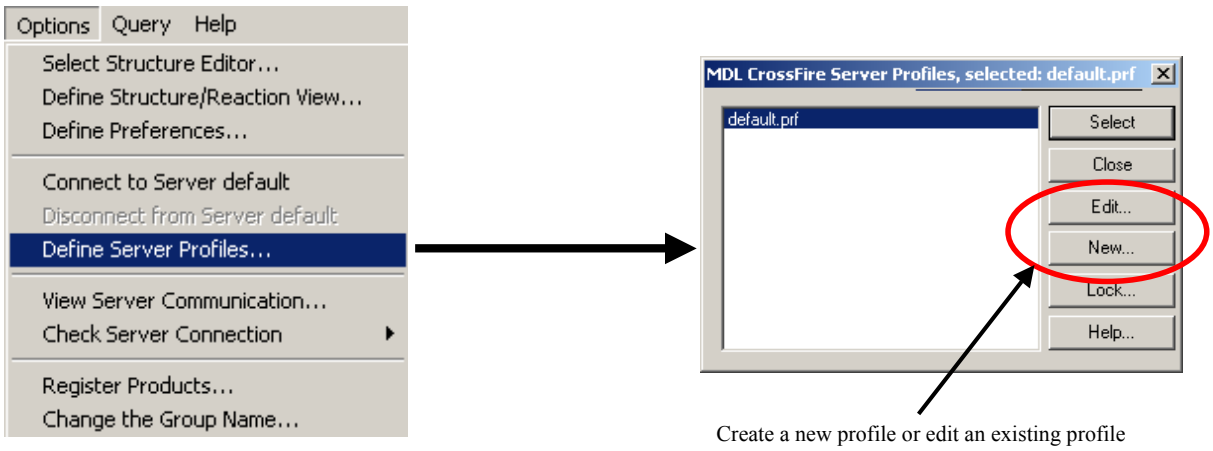
MDL CrossFire Commander 7.0

1.3 Connection

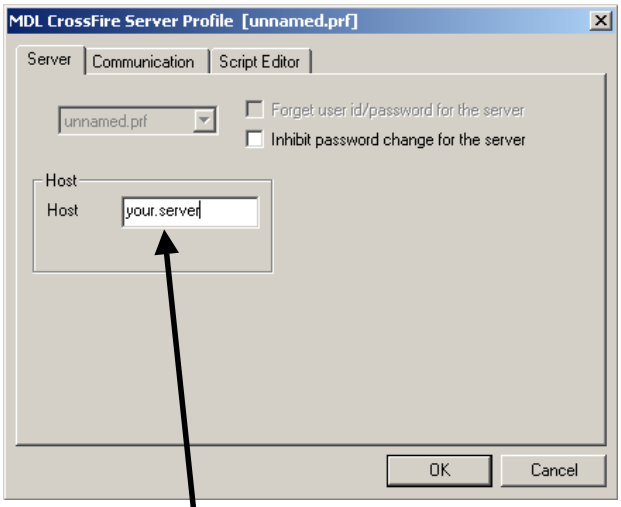
To access the CrossFire Server a profile has to be available which includes information about the Server, and a UserID/Password.

Note: these settings may have been automatically done already by your administrator!

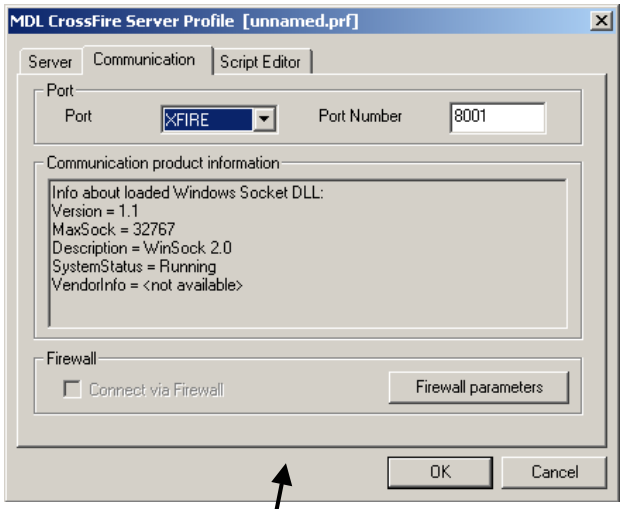
To create a profile select **Options:Define Server Profiles…**



Enter the server information (ask your administrator for details if needed).



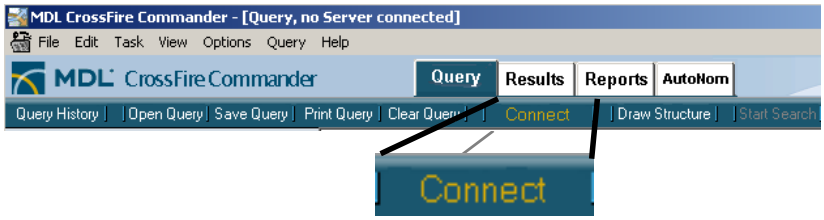
Server information

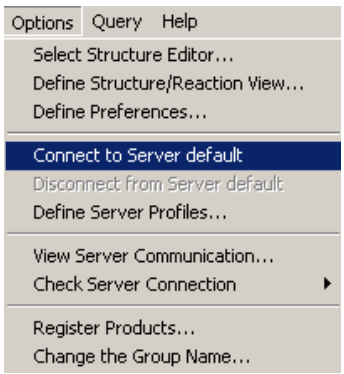


Communication parameter if needed

To connect to the CrossFire Server please choose "**Options:Connect to server <name of your profile>**"

You can also use the "Connect"-Button

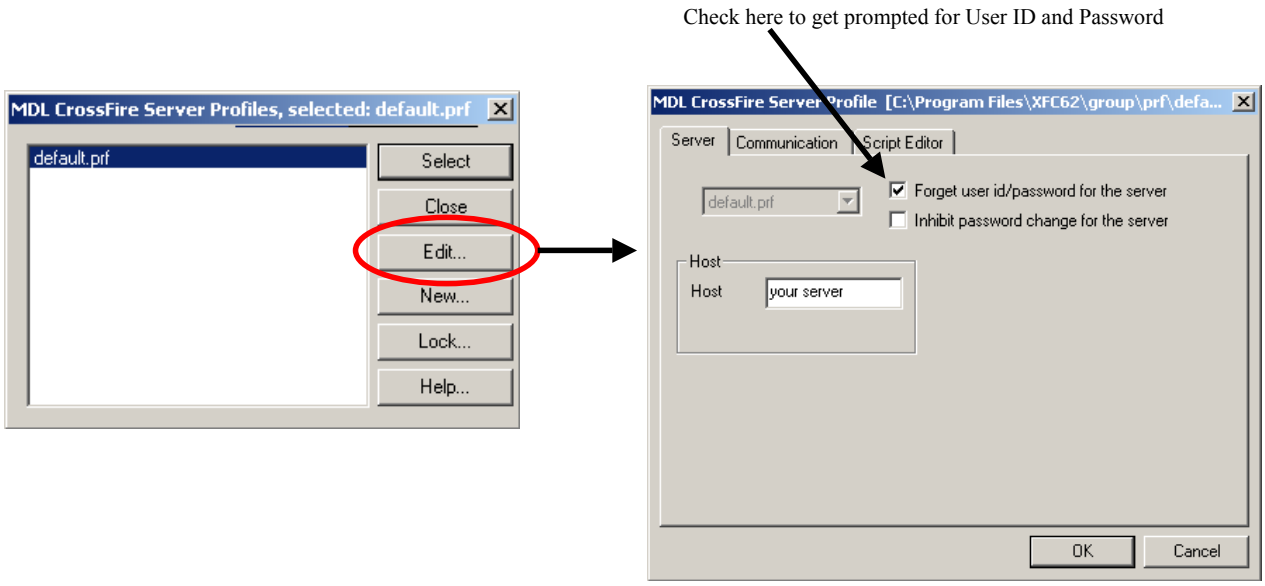




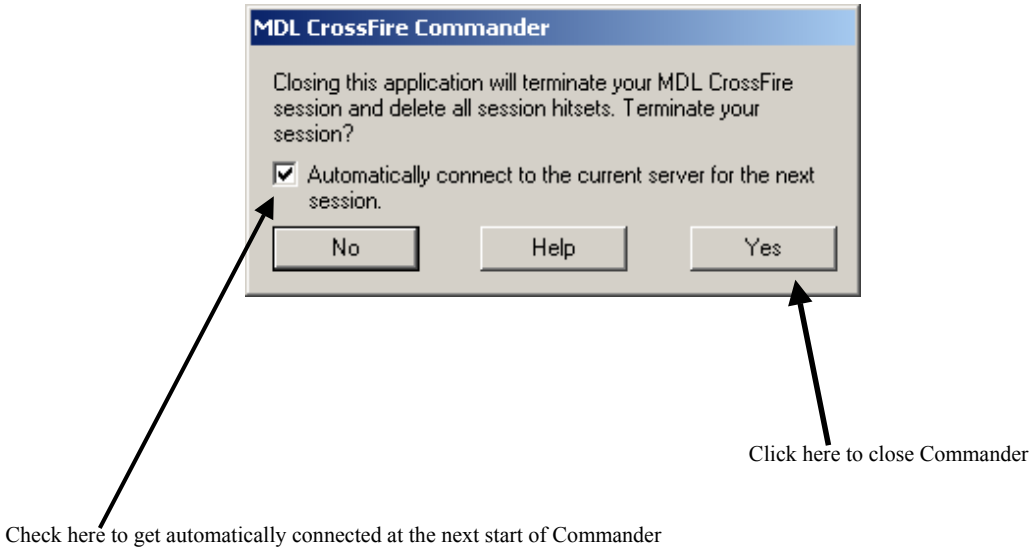
On first logon you will be prompted for your user ID and password

Check here to save your User ID / Password for automatic logon

If you want to change your saved User ID/password select “Options:Define Server Profiles…” and select the profile for which you want to change your credentials.

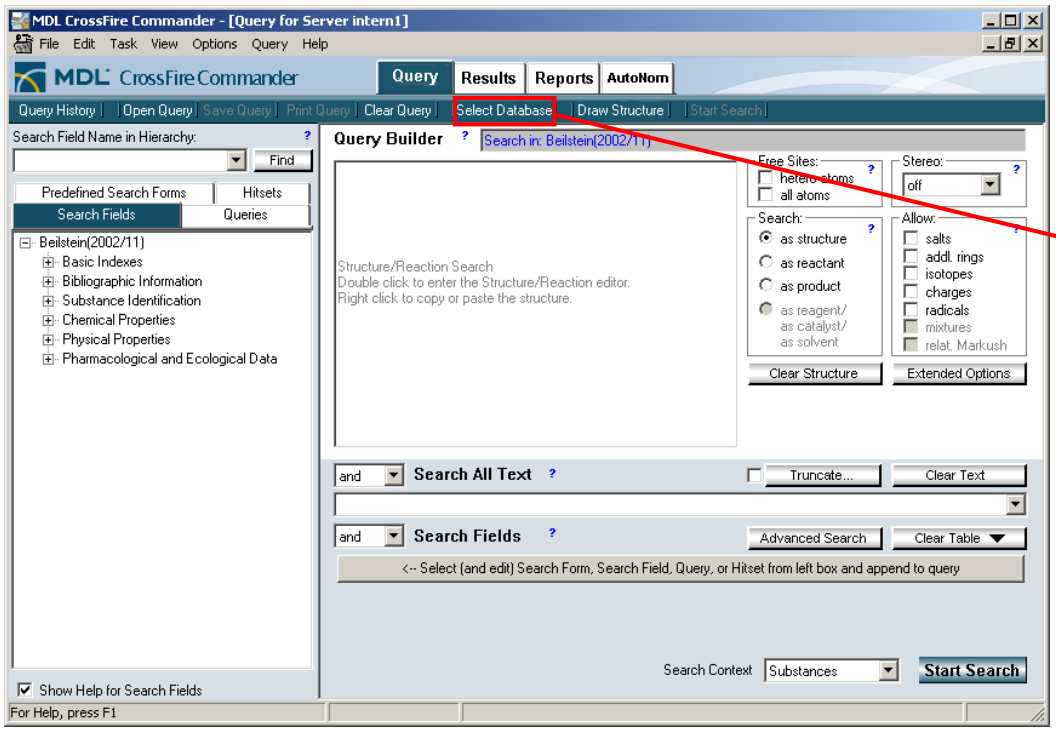


When Commander is closed it will offer to save the parameters of your current session for automatic setting :



2 Query

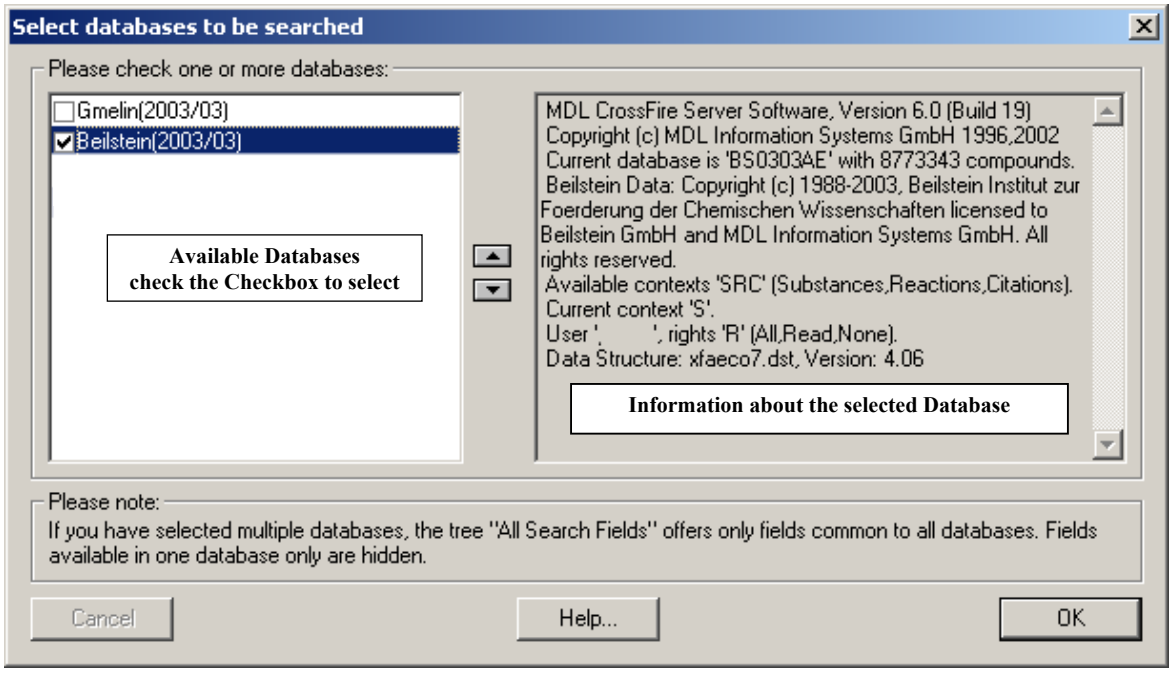
2.1 Select the Database



Click this button to select one or more databases for your search.
If you are not connected, this button will look like

Clicking this button will connect you and open the Database Selection

The Database Selection Window allows you to select one or more databases for your search

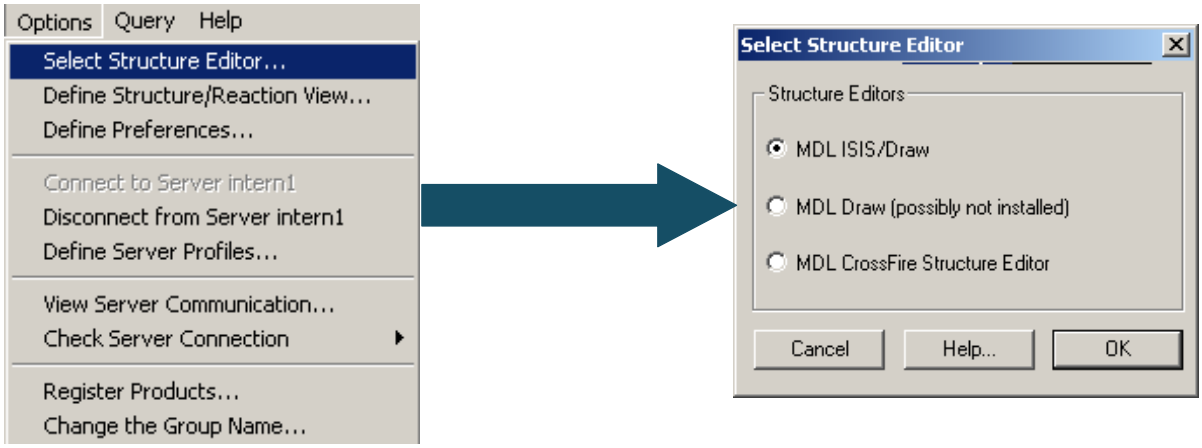


2.2 Working with the Query Pane

Structure Search

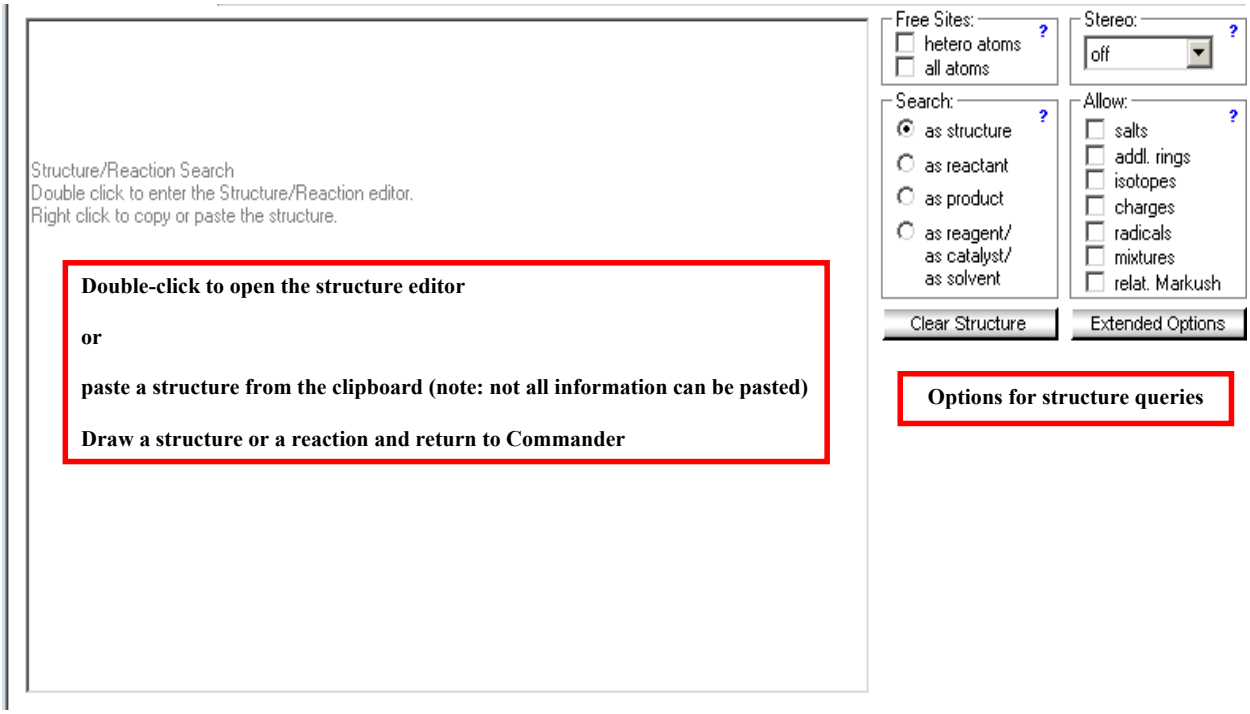
Three Structure Editors can be used to draw a structural query for use in MDL CrossFire Commander 7.0: The CrossFire Structure Editor, ISIS/Draw 2.5 and MDL Draw.

To select the Editor of your choice please use the menu **"Options:Select Structure Editor…"**

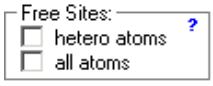


☞ **For individual guides to the structure editors please visit http://www.mdl.com**

2.2.1 The structure query formulation



A chemical structure can be searched with the following options:

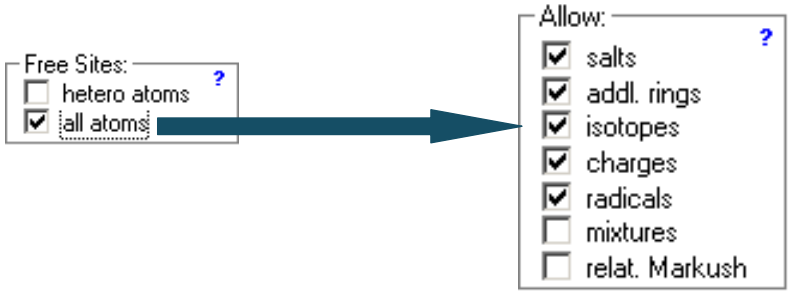


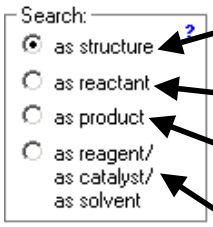
Use these options to set free sites on hetero atoms / on all atoms for the entire molecule

☞ **If AutoSearch is enabled these options will be set automatically during the search (see page 33)**

Note: free sites on individual atoms can be set in the structure editor!

Automatic settings: "Free Sites on all Atoms" is interpreted as a substructure search. To allow this the options "Allow: salts, additional rings, isotopes, charges and radicals" are set automatically. Each of them can be unchecked if not wanted





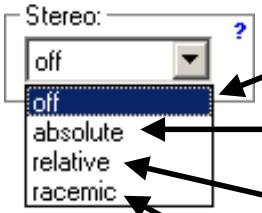
Search the drawn structure **as such** (recommended context: Substances)

Search the drawn structure **as reactant**, explore it's chemical reactivity (recommended context: Reactions)

Search the drawn structure **as product,** explore the preparations (recommended context: Reactions)

Search the drawn structure **as auxiliary** in a reaction (recommended context: Reactions)

Note: the option "search as reagent/as catalyst/as solvent" is not available for all databases!



Any stereochemical information in the drawn structure will be ignored

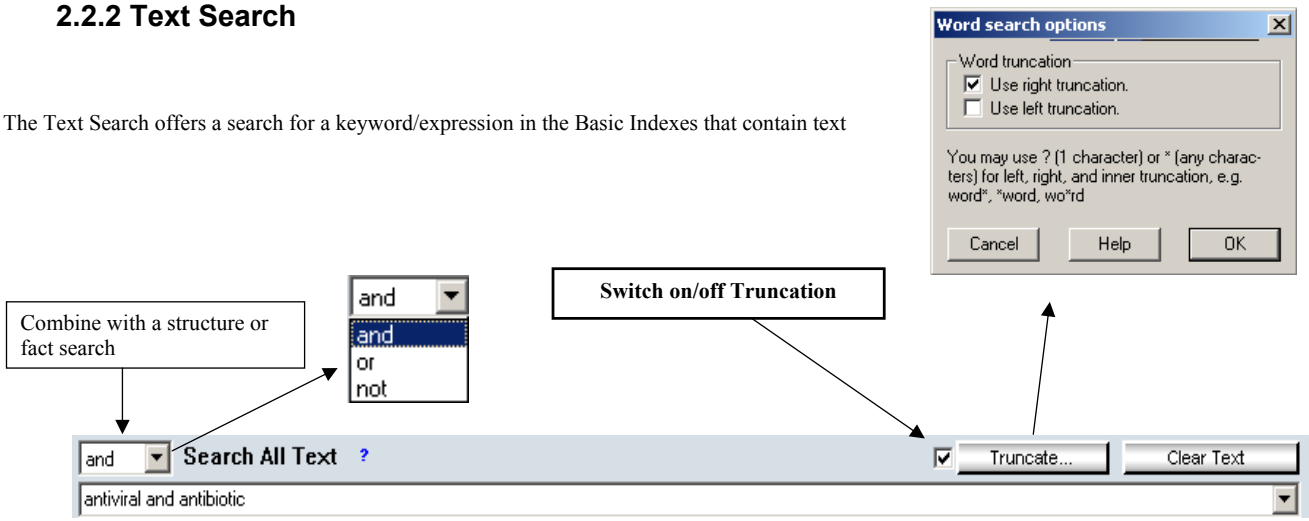
Any stereochemical information in the drawn structure will be searched exactly as drawn

Any stereochemical information in the drawn structure will be searched as relative stereochemical information

The racemic mixture is searched

2.2.2 Text Search

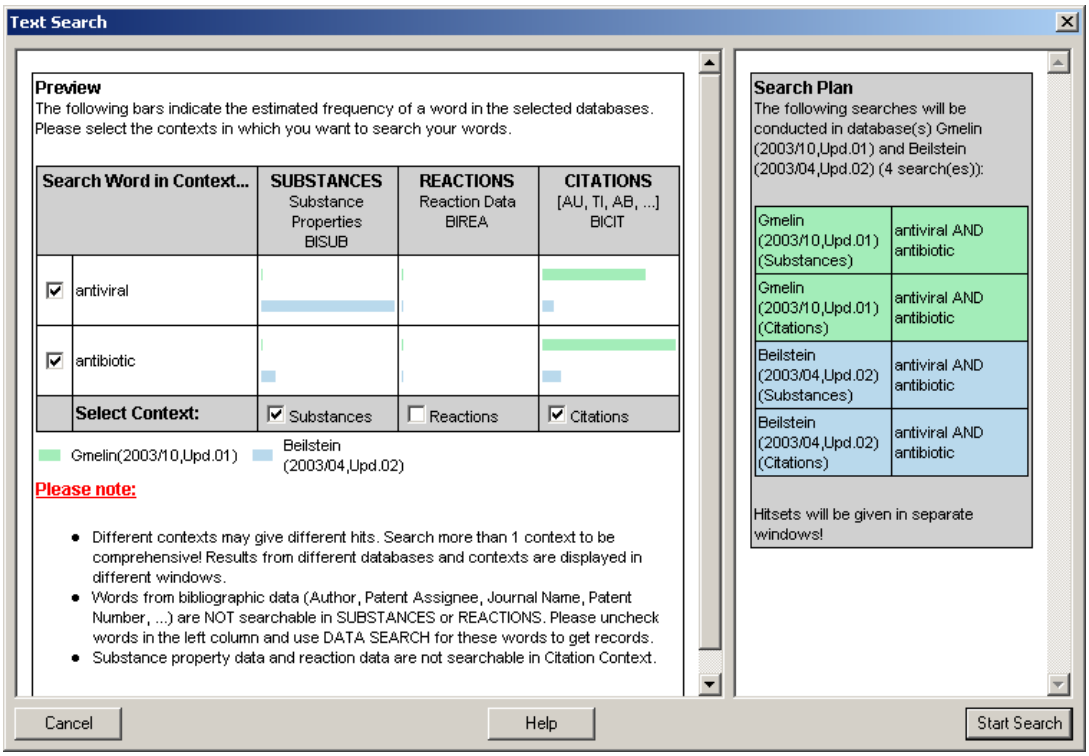
The Text Search offers a search for a keyword/expression in the Basic Indexes that contain text

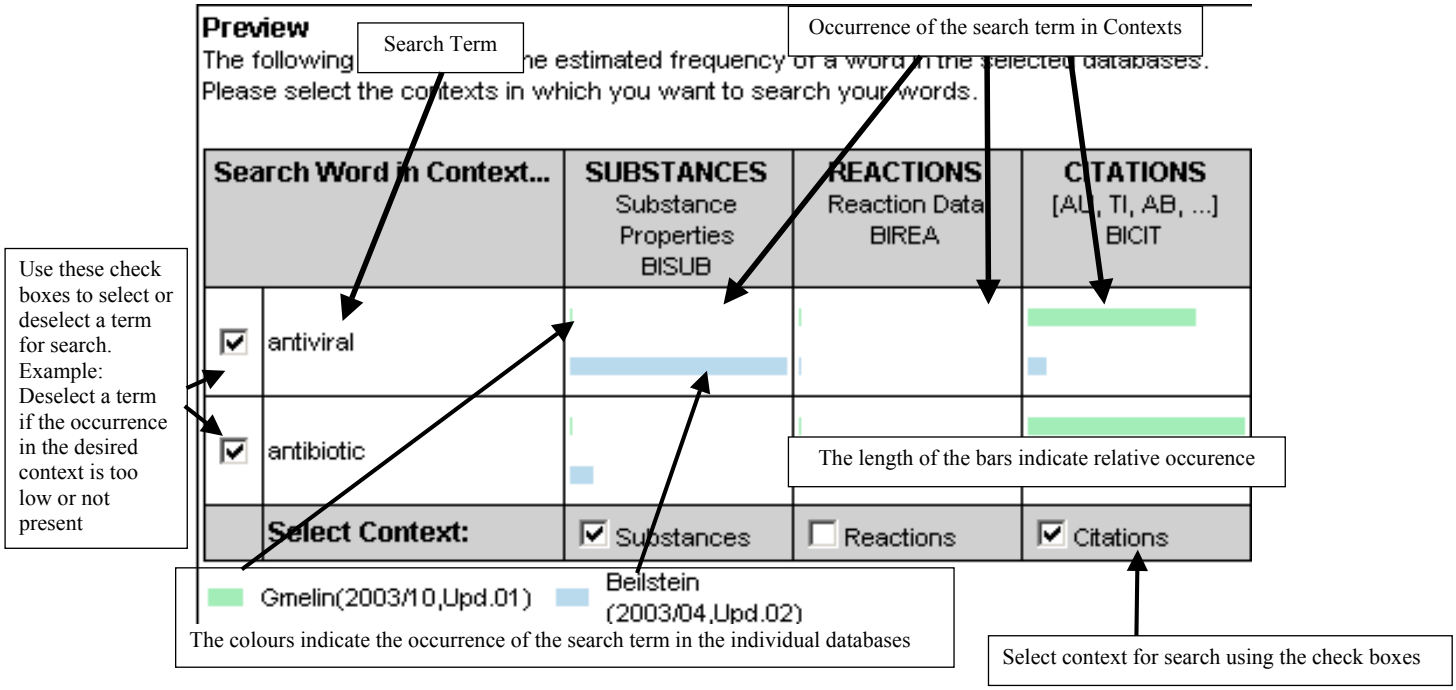


The Text Search will search your search term in the text -indexed Basic Indexes of the selected database(s).

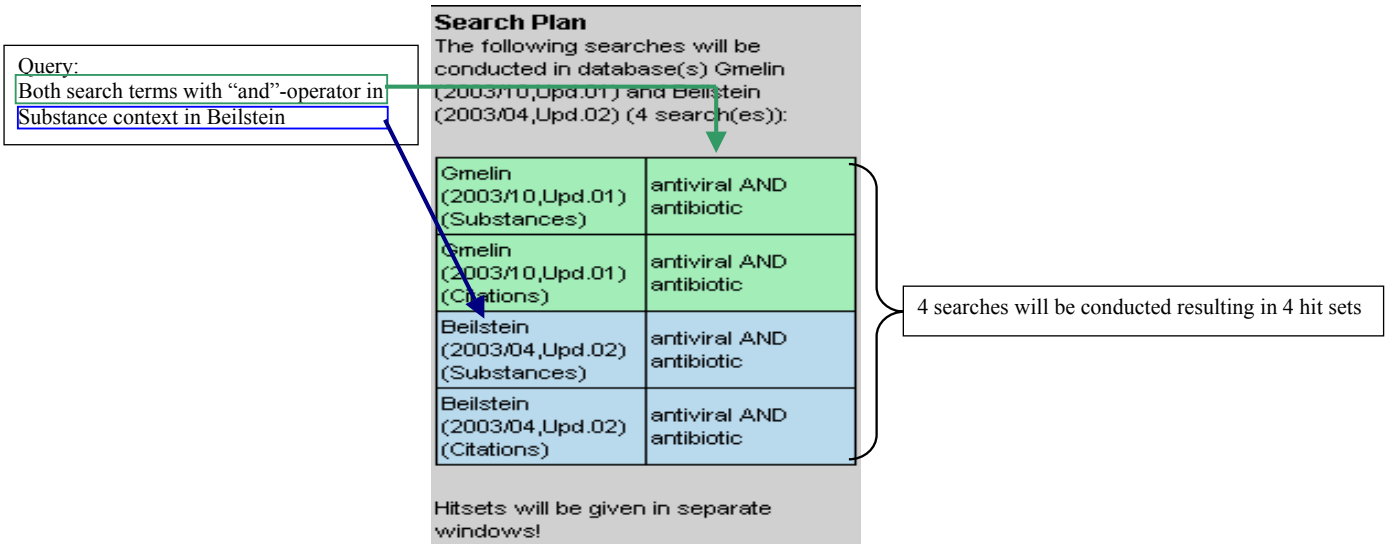
Operators “and”, “or”, “next”, “near”, “proximity“ can be used.

When a Text Search is started Commander displays a window to define your search:

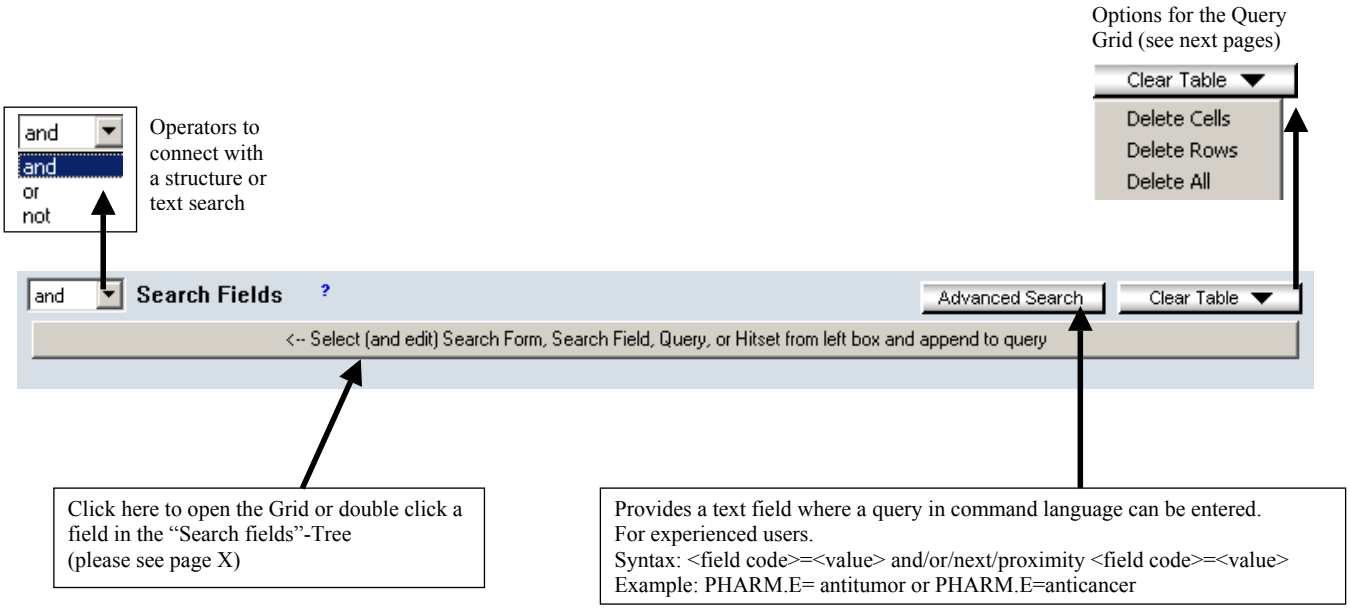




The selection of search term and context by using the checkboxes leads to a search plan, which is displayed at the right side for a convenient overview and to enable a preview or relevance check before starting the search:



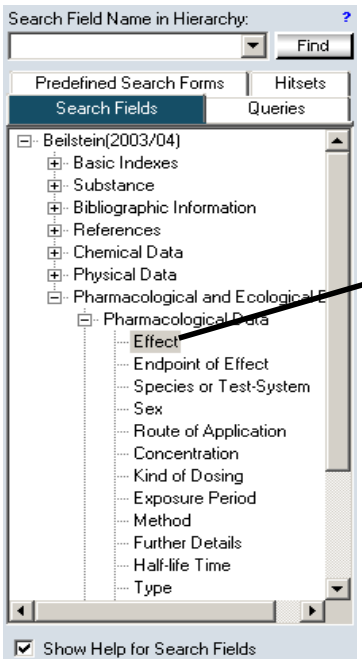
2.2.3 Search Fields



Search Field Selection

There are two ways to enter a field for search into the Grid:

Double click a field in the Datastructure tree

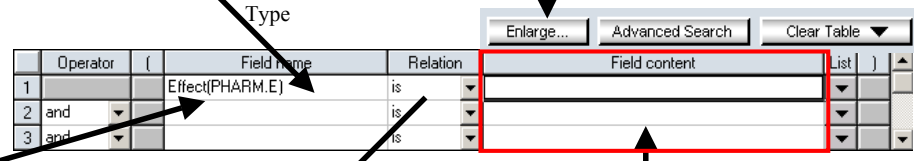


Type the field code directly into the grid (alternative to copy by double click in the tree)

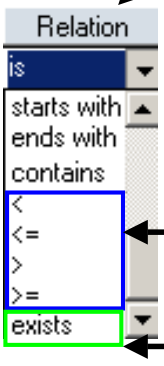
Type

Double click

New button: click to enlarge the grid to a full table



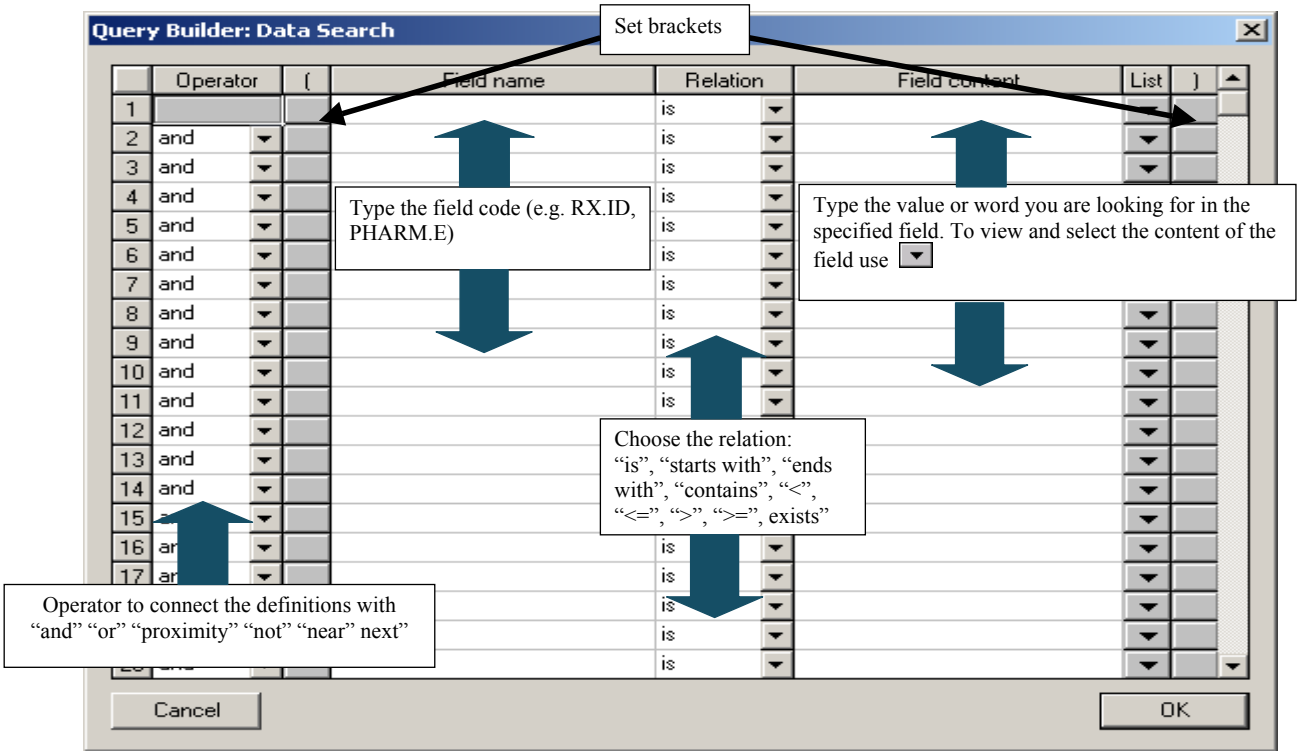
Type the value or word you are looking for in the specified field. To view and select the content of the field use



Use with numeric fields/values

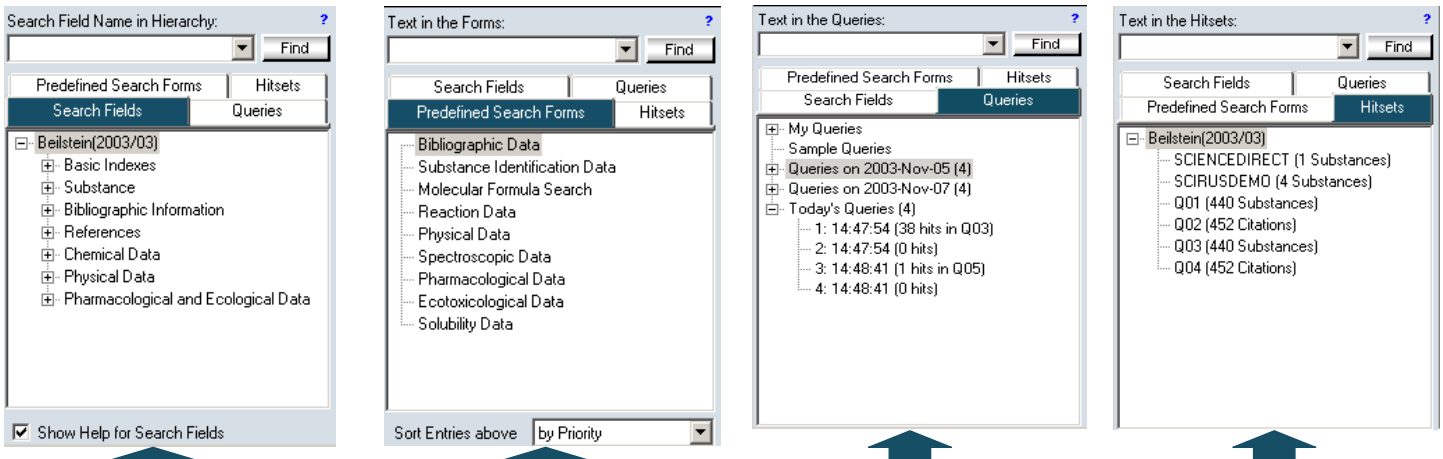
Operator to limit the search to records with entries in a certain field, e.g. "NMR must exist"
Note: not applicable for all fields!

The “Enlarge” Feature enables complex queries using multiple fileds from the Database.



2.2.4 Using the tree

The tree on the left side of this Window has multiple functions and offers various options to work with Commander



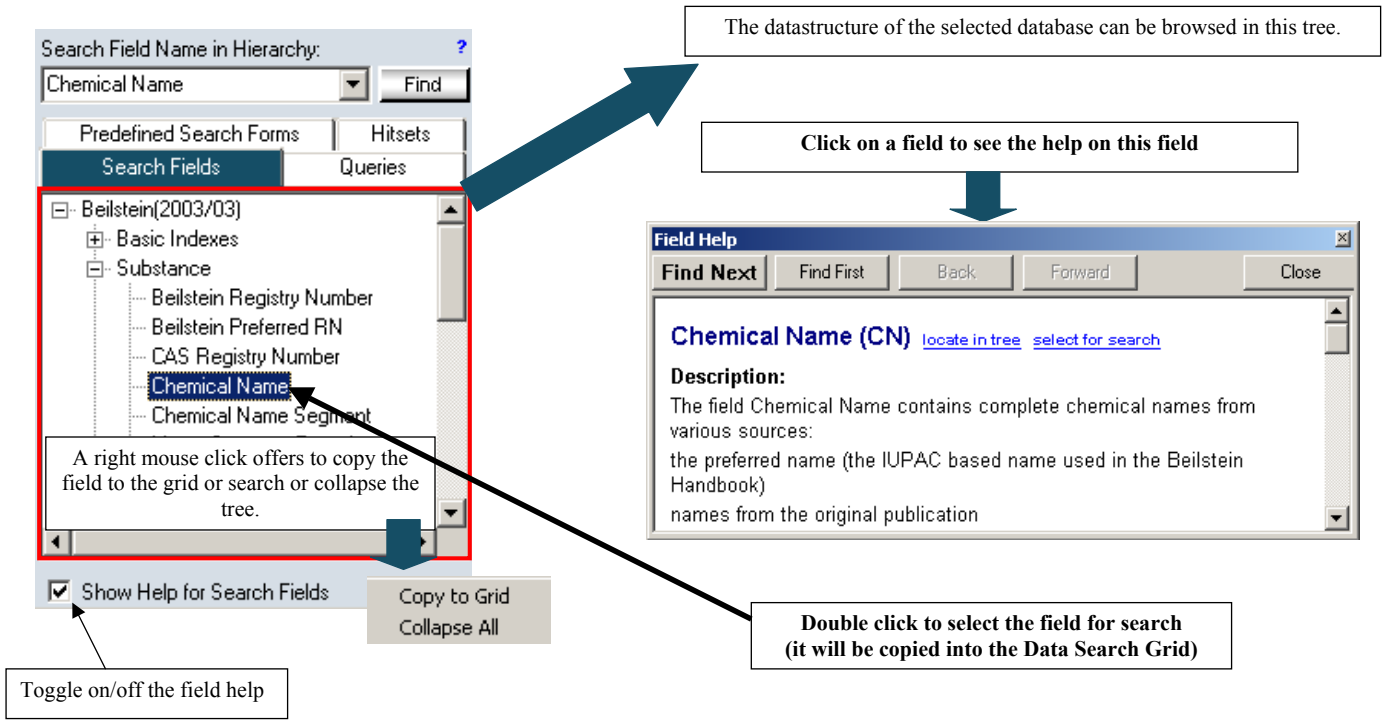
Browse and use the Database’s Datafields to formulate your query

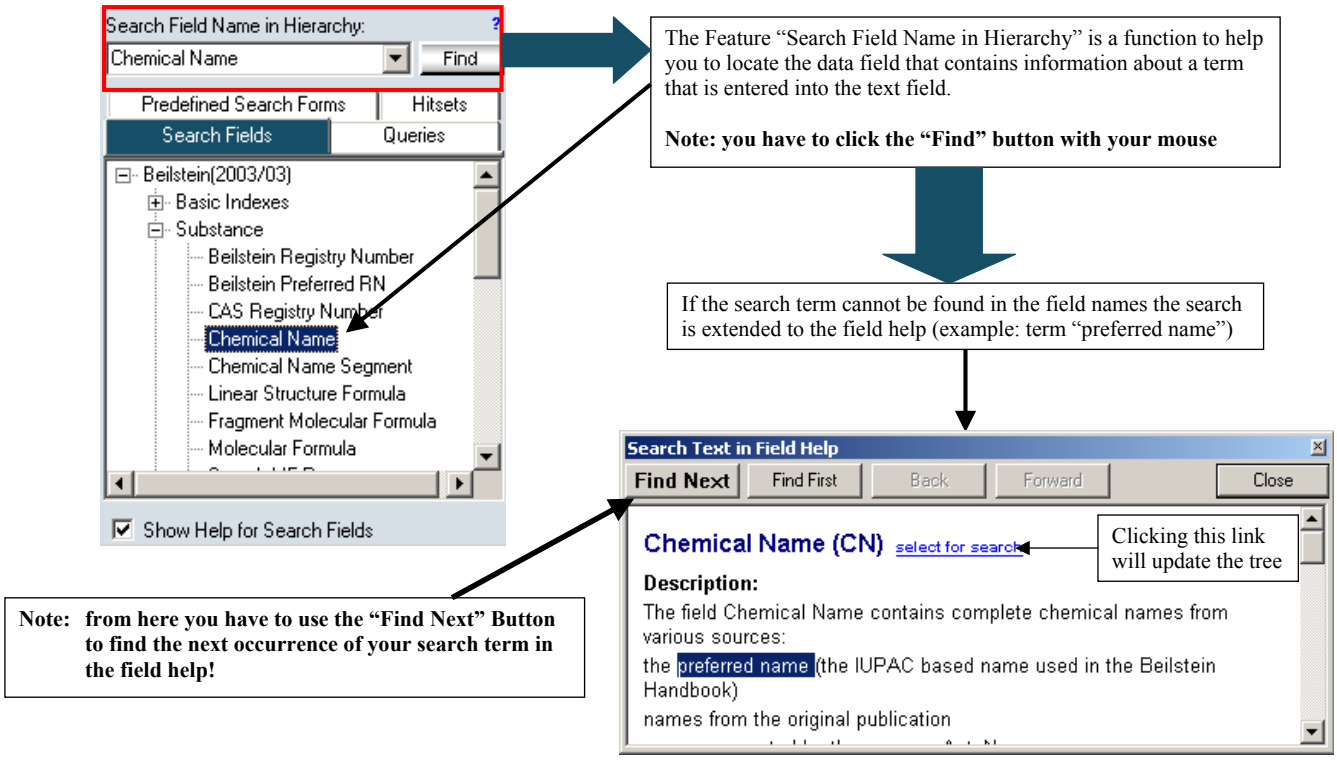
Use the Predefined Search Forms (PSF) to formulate your query

Browse and use queries from the last days

Browse and use Hitsets from the current session or saved Hitsets

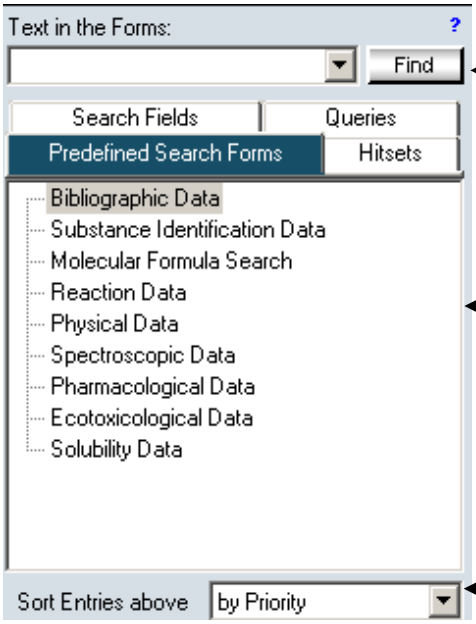
2.2.4.1 Search Fields:





2.2.4.2 Predefined Search Forms (PSF)

The Predefined Search Forms summarize the fields of a specific area of interest in an easy to use form.

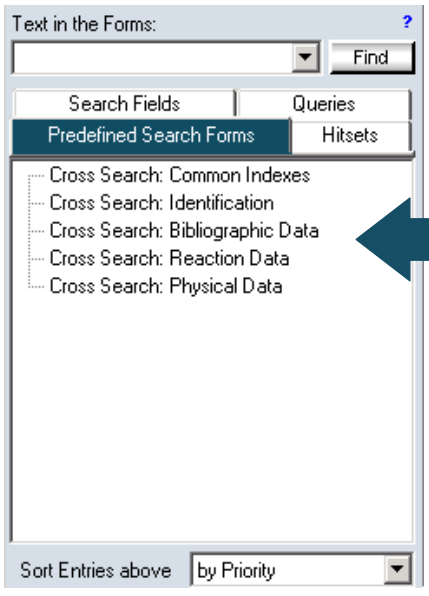


Use the search feature to locate a specific topic in the forms

Double click an entry to open the form

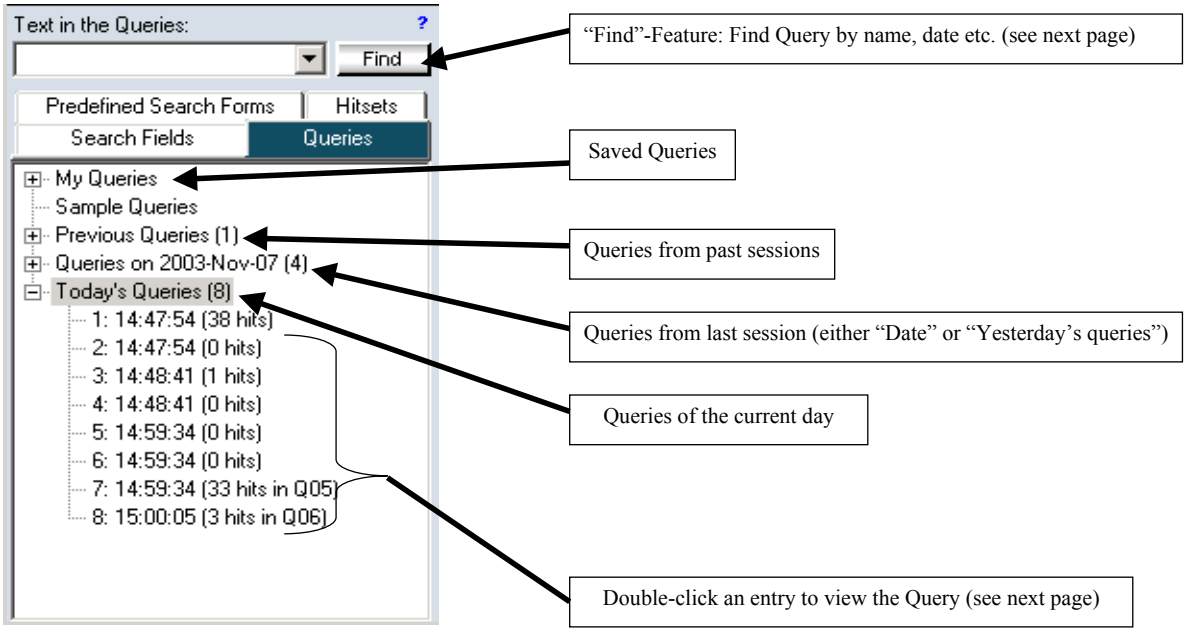
Sort the Search Forms in alphabetical order or by priority

If more than one database is selected the search forms are replaced by the Predefined Search Forms for Cross Searches. These summarize the fields that are available for simultaneous search over multiple CrossFire databases in an easy-to-use form.



Predefined Search Forms for simultaneous searches over multiple databases

2.2.4.3 Query History



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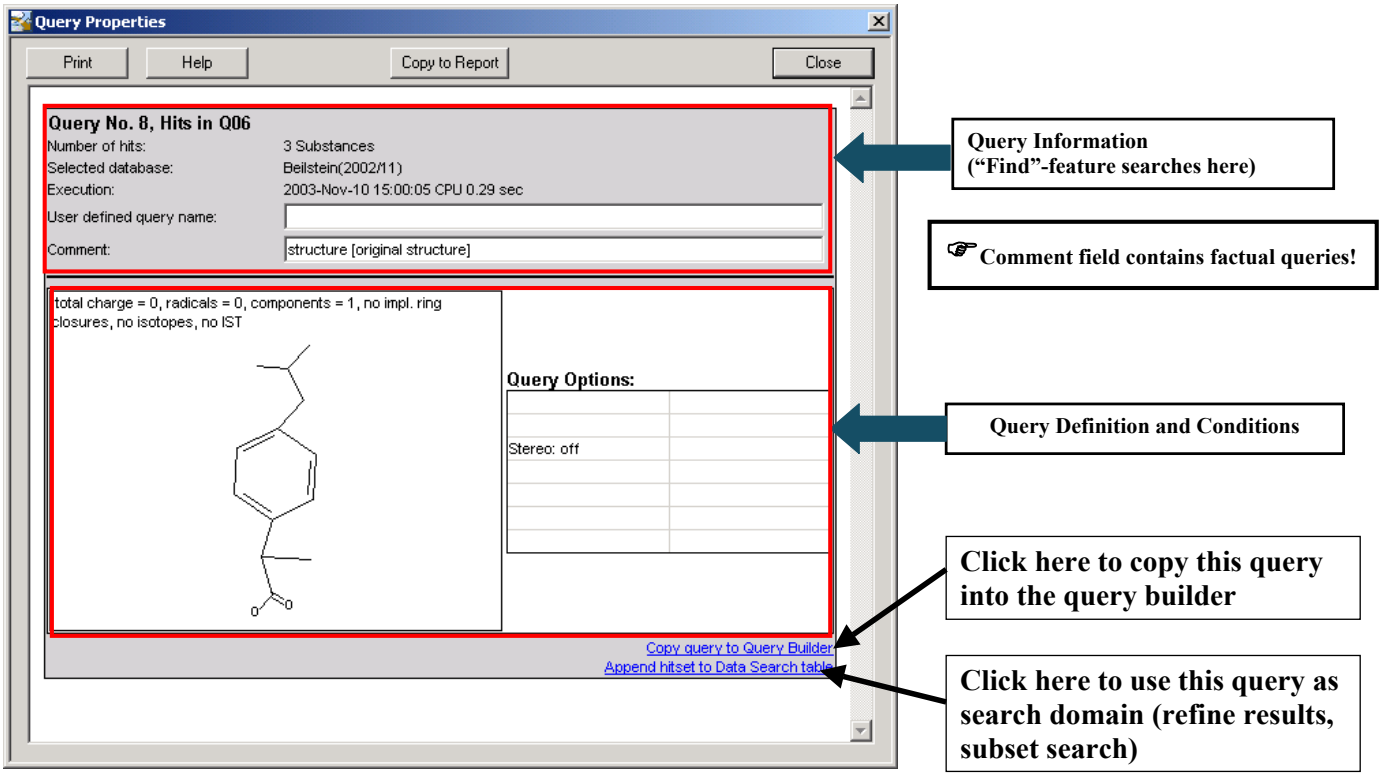
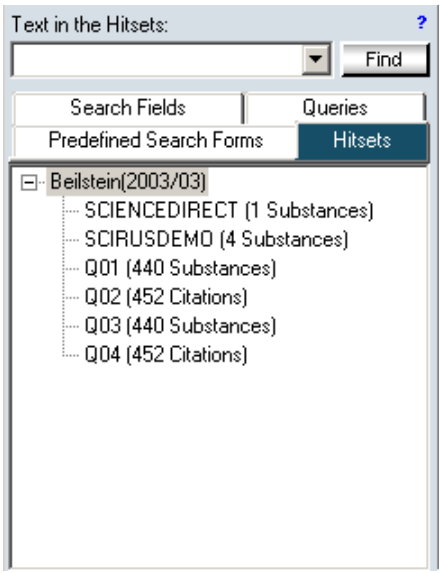


2.2.4.4 Hitset History

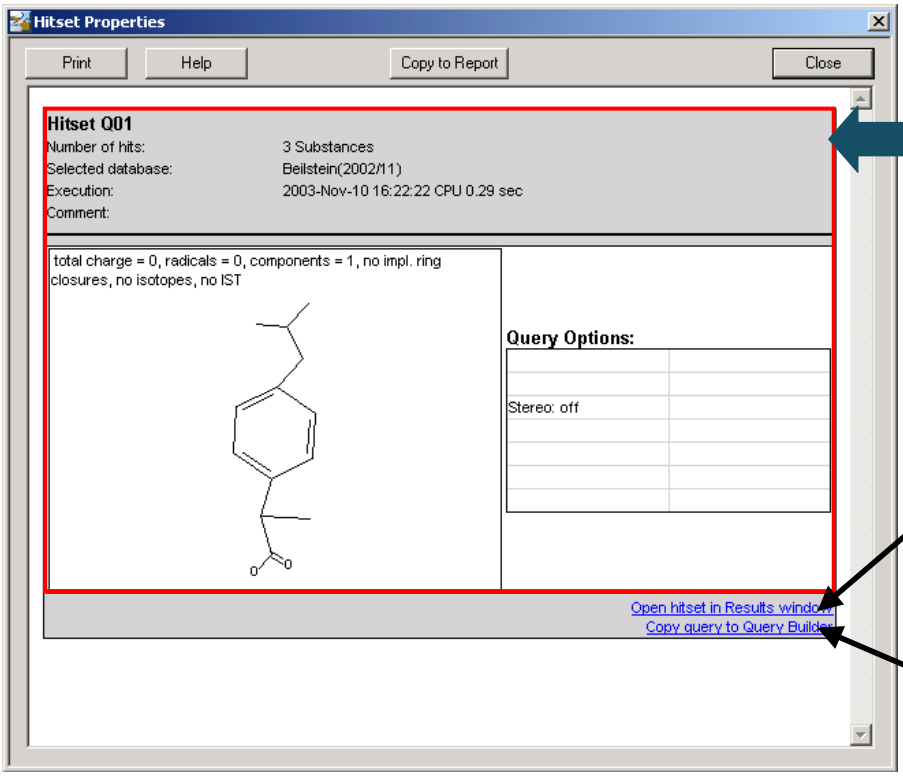


Double-click an entry to use as search domain (refine results, subset search)

Right-click to

- view the properties (see next page)
- open the hitset in the results window
- collapse the tree (if there are hitsets from more than one database present)

Hitset Properties:



Information about the hitset's corresponding query

Click here to open the hitset in the results window

Click here to copy this query to the query builder

3 Search

3.1 Start a search

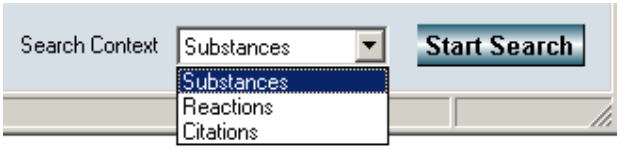
Before a search is started it is critical to select the context of your search. A search in CrossFire Commander 7.0 can be done in one of three contexts :

Choose this context if you have drawn a structure or if you are looking for data or properties of a compound

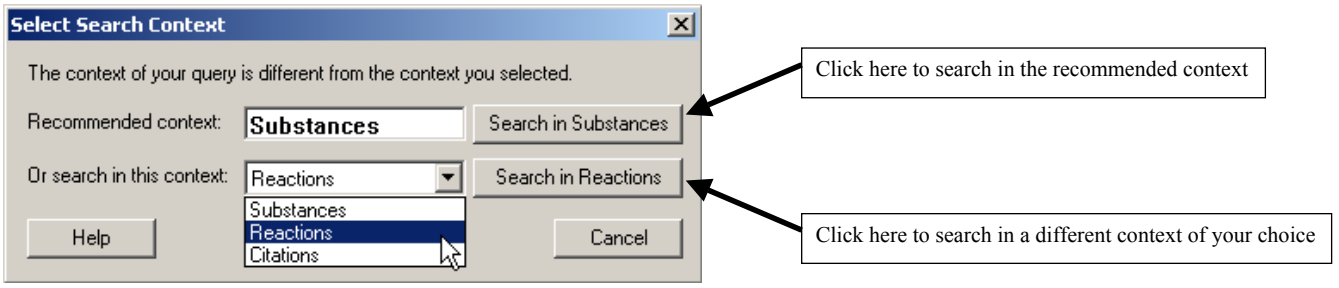
Choose this context if you have drawn a structure and selected “as product” or “as reactant”, if you have drawn a reaction or if you are looking for data and properties of a reaction

Choose this context if you are looking for an Author, a publication or any other publication related topic

The context has to be defined on the query formulation page:



At each start of a search MDL CrossFire Commander 7.0 compares the query with the selected context. If the query is unusual for the chosen context Commander will prompt you to verify or change the context:



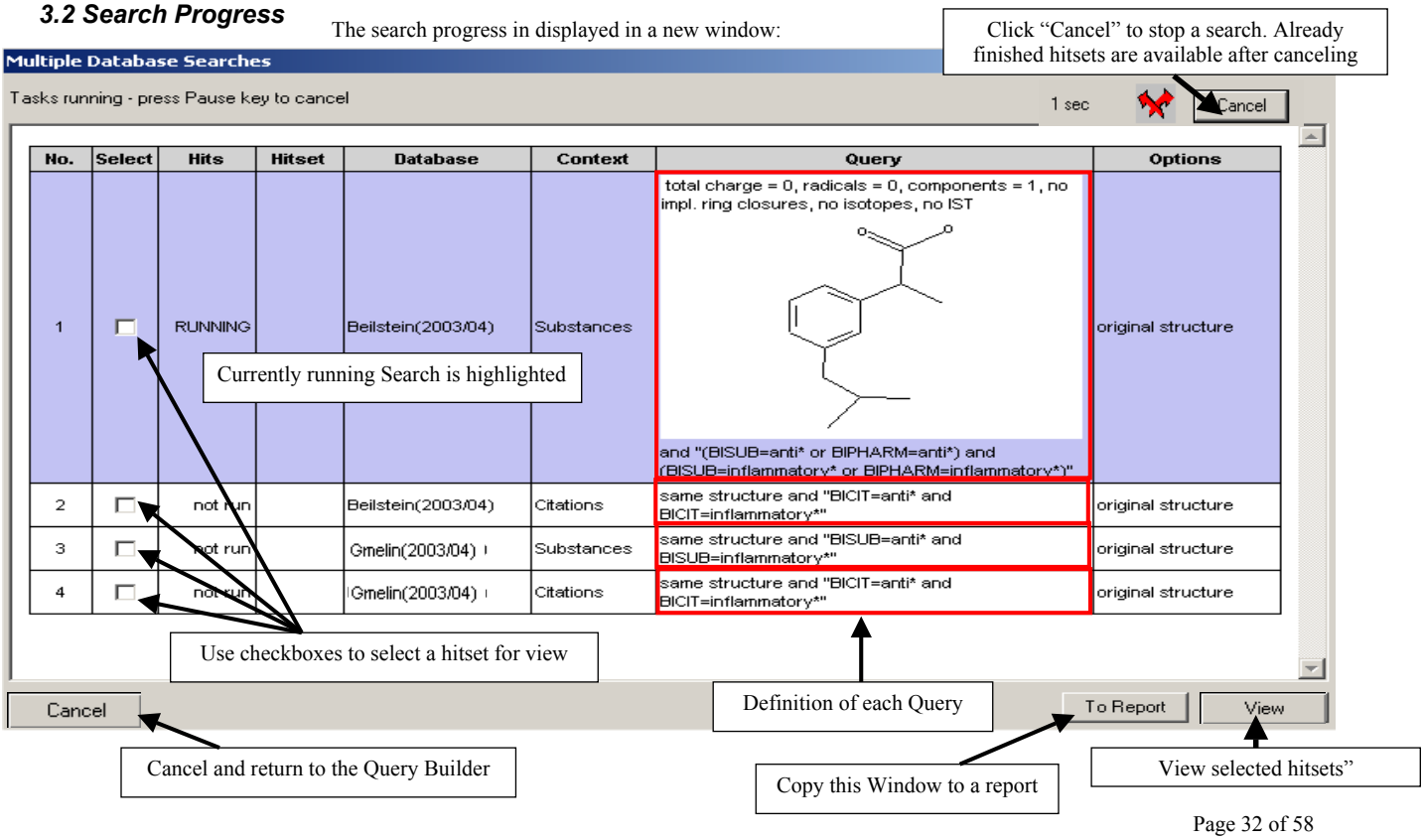
Each search can be started in two ways: Press “F7” 

or click the “Start Search Button” 

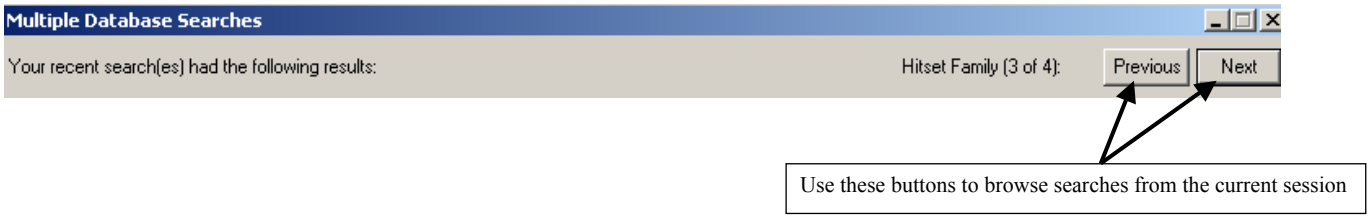
Note: you can not start a search using the Return/Enter Key!

3.2 Search Progress

The search progress in displayed in a new window:

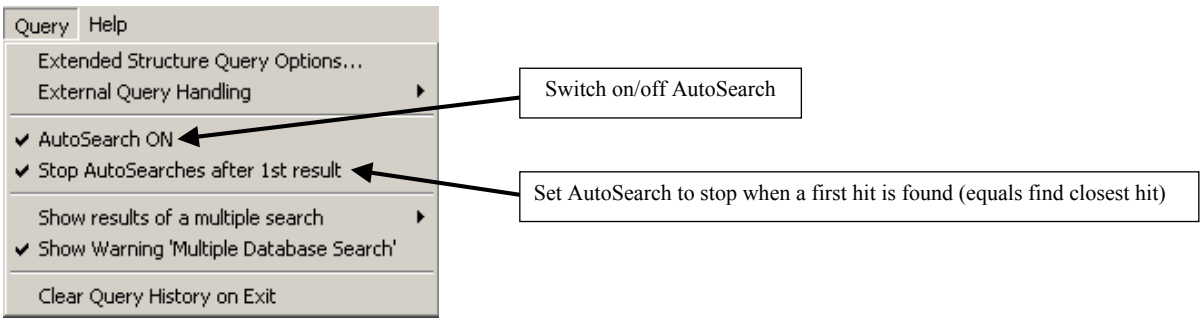


When a search is finished the top of the Search Progress Window changes to allow browsing of the sessions's searches:



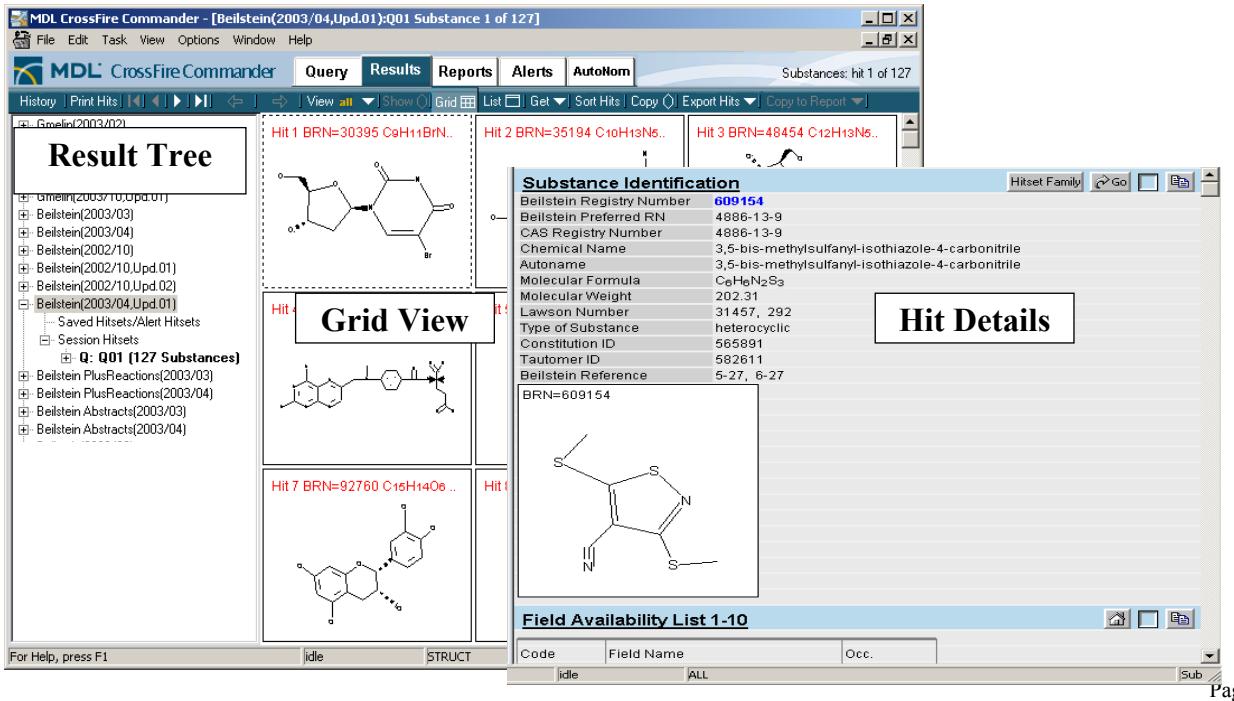
AutoSearch

If "AutoSearch" is enabled Commander will refine a structure step by step to find the closest hit. "AutoSearch" can be enabled/disabled in the Menu "**Query**".



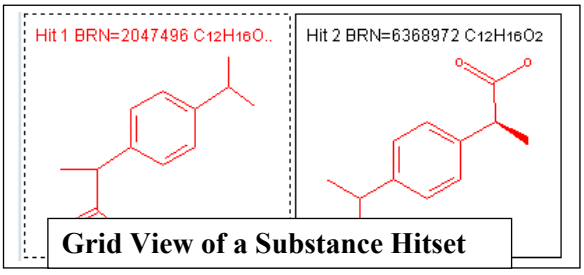
4 Results

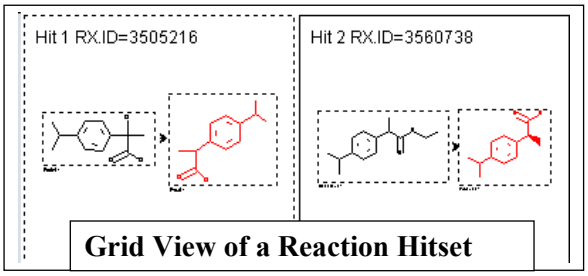
4.1 Overview

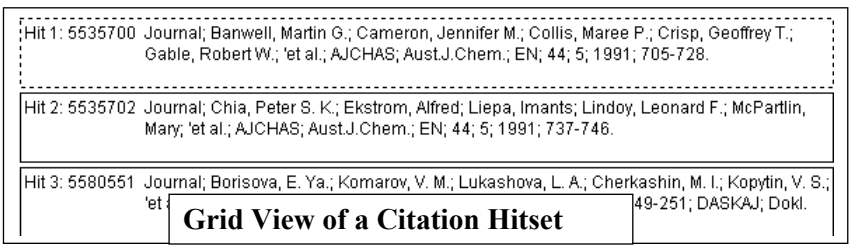


4.2 Grid View

The Grid View provides an overview over the structures, reactions or citations of a hitset



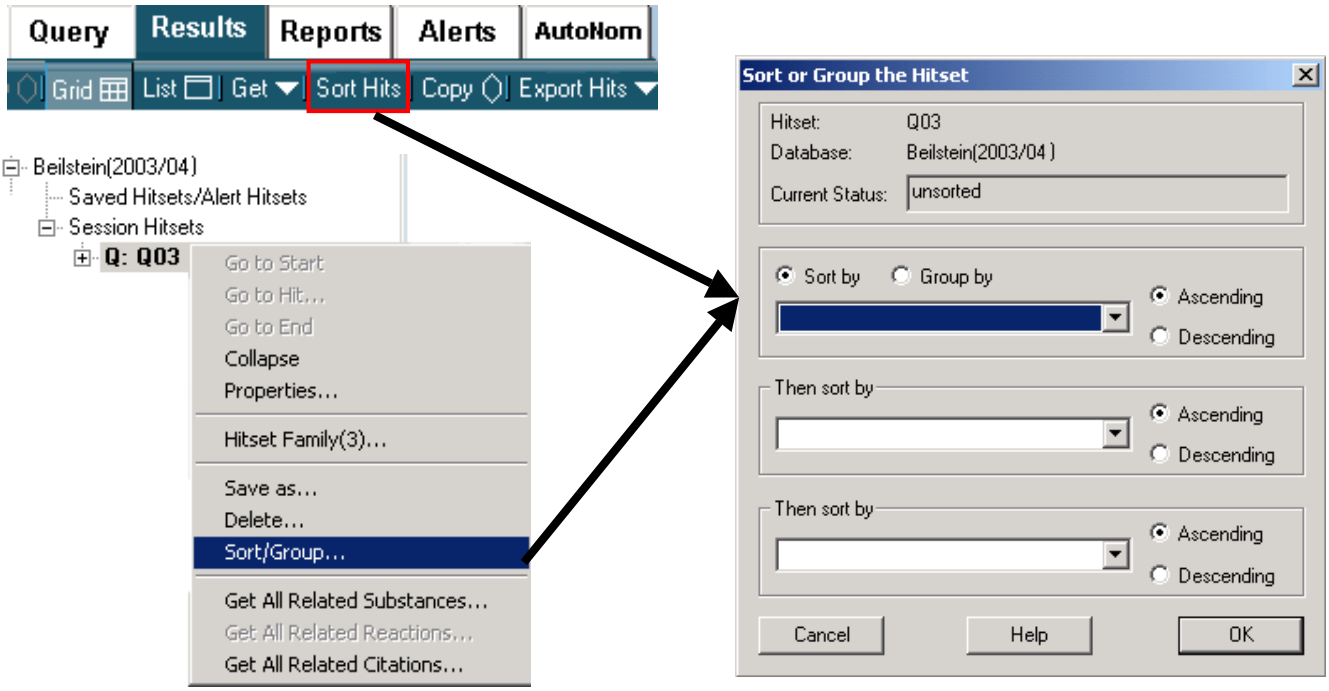


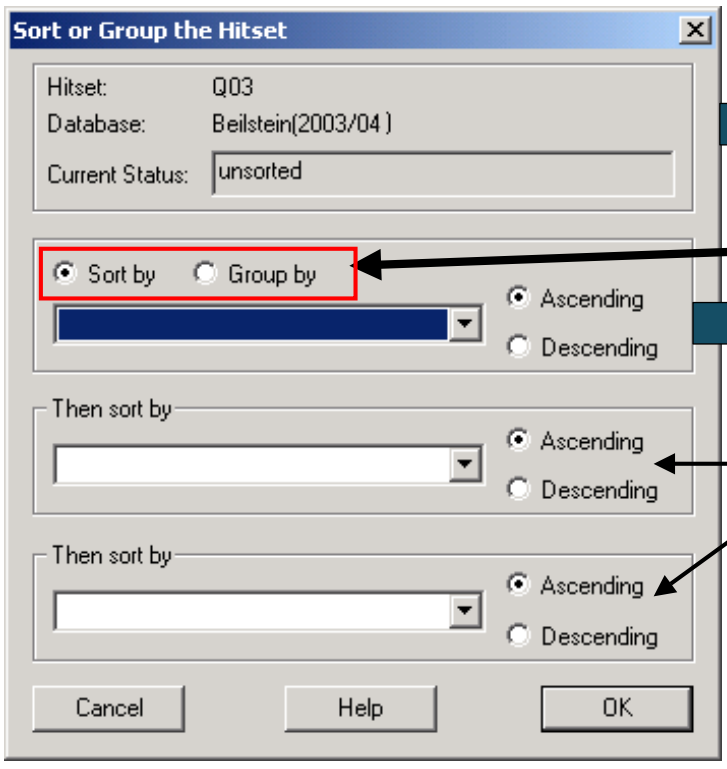


Double Click an Item in the Grid to see the hit details or use the buttons “Grid” and “List” Grid List to switch between the Grid and the Hit Details

4.3 Grouping and Sorting

A Hitset can be sorted and grouped by the values of selected fields. Select the Hitset in the tree and click the "Sort Hits" Button or right-click the hitset and select "Sort/Group"





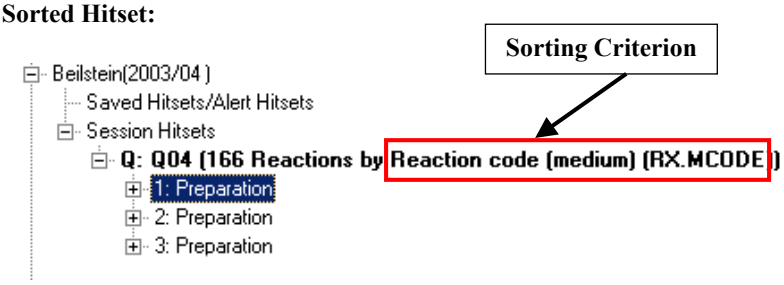
Display of current status: Hitset, Database and current status:
"Unsorted", "sorted", "sorted,grouped"

Click here to select the action for the top level: "Sort by" or "Group by"

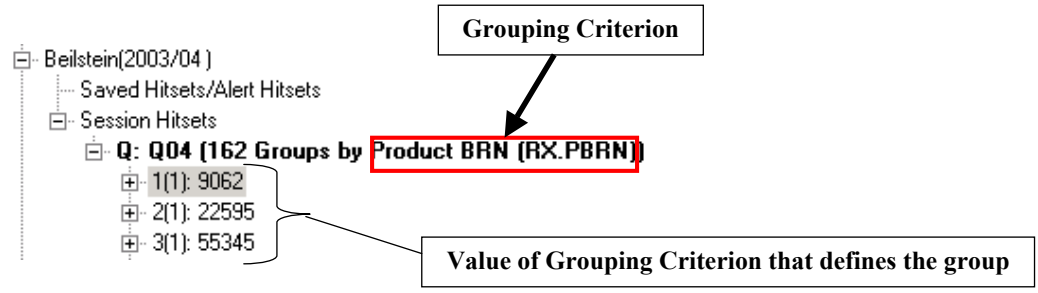
Grouping is available on 1st level only, subgrouping is not possible.

A grouped hitset can be sorted.

Sorted Hitset:

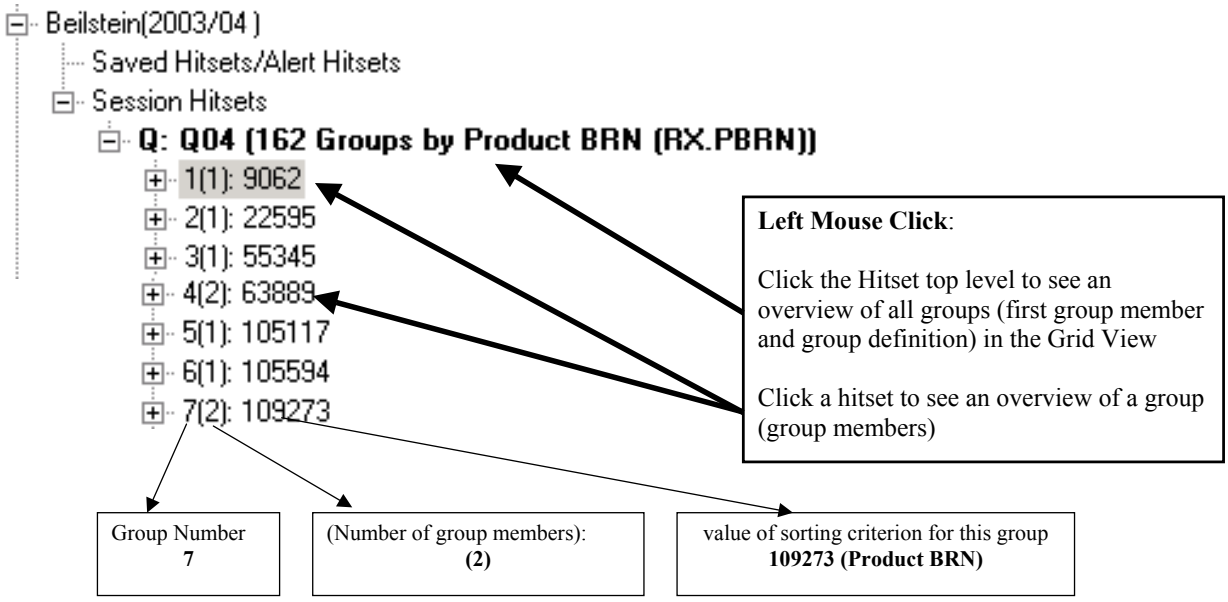


Grouped Hitset:

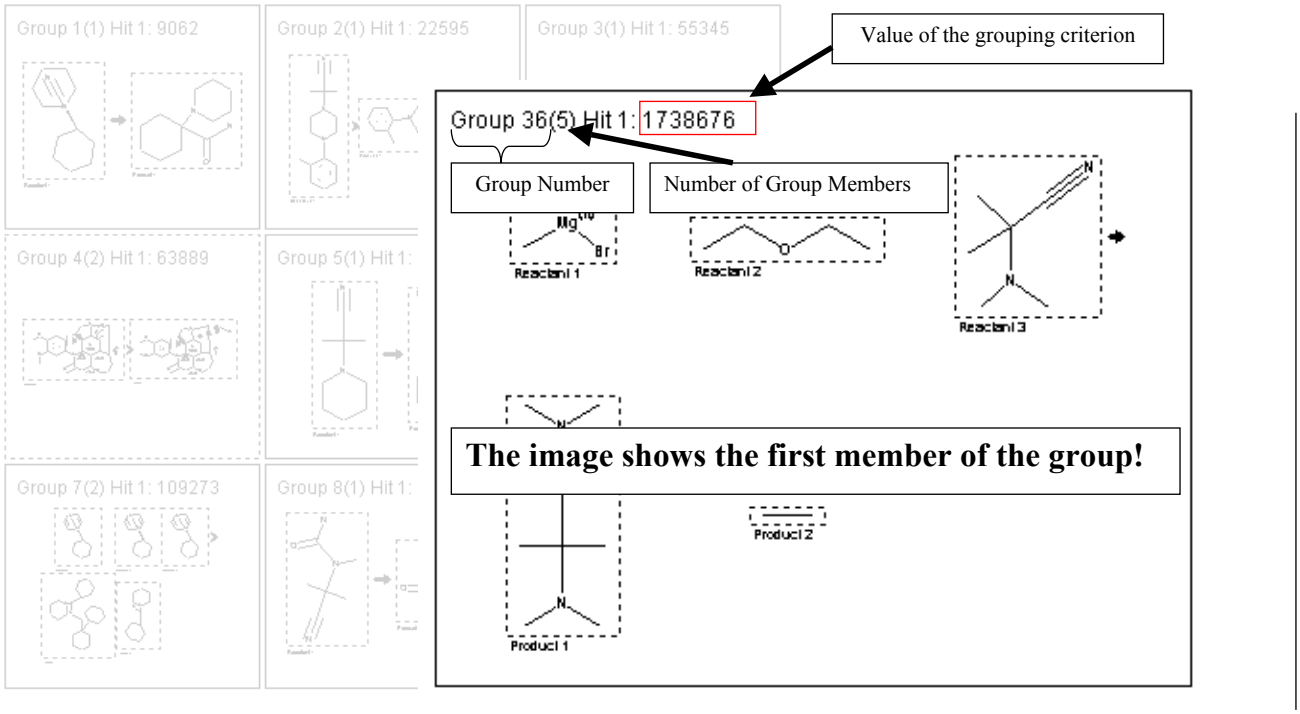


4.3.1 Working with a grouped hitset

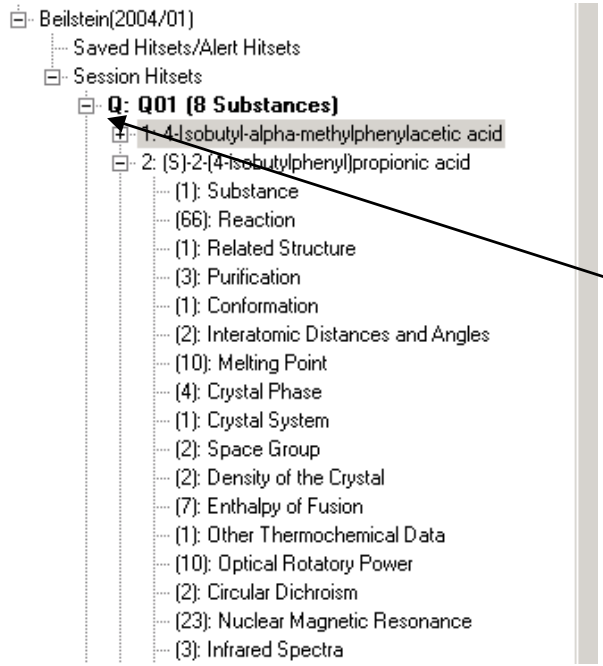
- In the tree:



- in the grid view:



4.4 Tree View



On the left side of the screen the tree view provides fast navigation through saved Hitsets and Session Hitsets.

Select the Hitset you want to see and the main screen switches to Short Display.

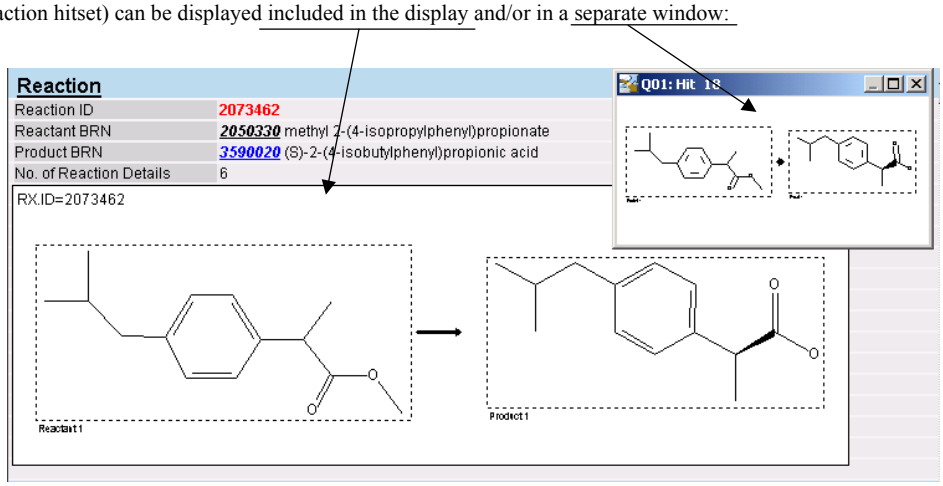
Click on ⊞ to drill down to details, ultimately to field level.

Click on these details to display them in the main screen.

4.5 Detail View

The detail view contains all data about a compound, citation or reaction that are available in the database.

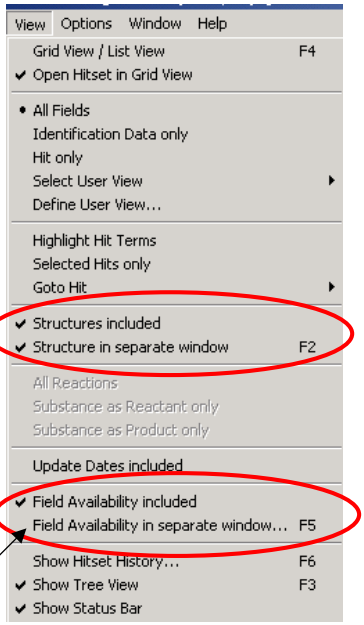
The structures contained in a substance or reaction hitset (the structure of the title compound in a substance hitset, the graphical display of the reaction in a reaction hitset) can be displayed included in the display and/or in a separate window:



The display in a separate window can be toggled on/off by pressing the function key F2 on the keyboard, by pressing the "Show()"-Button in the button bar

or using the menu **"View:Structure in separate Window"**

To include structures in the display use the menu **"View:Structures included"**



The structures of all substances and reactions described in a citation can be viewed as included structures.

The **Field Availability** provides information how much entries for which field are present in the record for the selected substance, reaction or citation and links to get directly to these data:

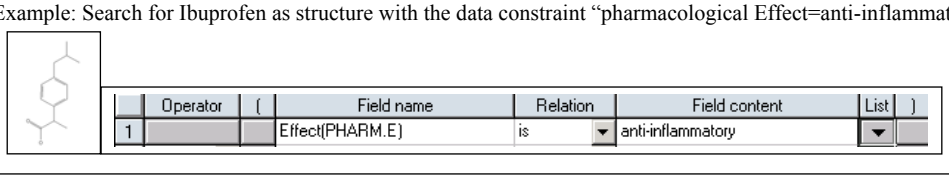
Field Availability List 1-10 of 30

Code	Field Name	Occ.
PHARM	Bioactivity: Pharmacological Data	54
BIOD	Ecological Data: Biodegradation	3
RX	Reaction	65
RSTR	Related Structure	1
PUR	Purification	3
CNF	Conformation	1
IDA	Interatomic Distances and Angles	2
MP	Melting Point	10
CRYPH	Crystal Phase	4
CSYS	Crystal System	1

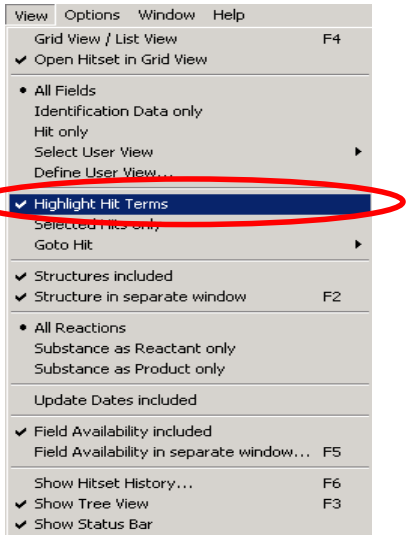
It can be viewed included in the text or in a separate window. Use the menu "View:Field Availability included" to include it in the text. Press the function key F5 on the keyboard or select "View:Field Availability in separate window…" to toggle on/off the setting of your choice.

When conducting a factual search or a text search (combined with a structure or without) the findings for the search term in the hit can be used for better overview in two ways:

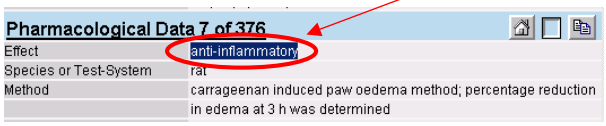
Example: Search for Ibuprofen as structure with the data constraint “pharmacological Effect=anti-inflammatory”



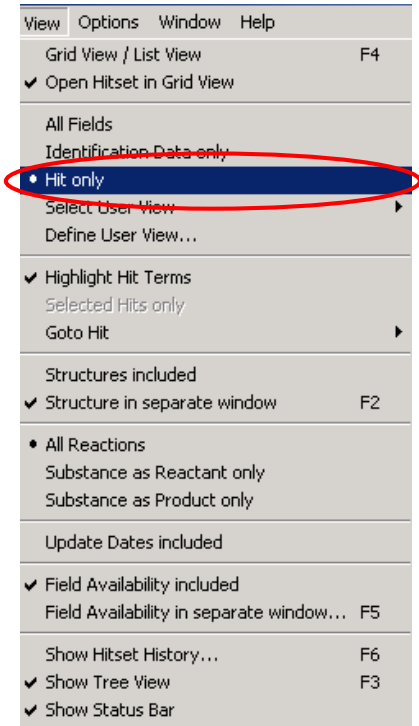
The term can be highlighted using **“View:Highlight Hit terms”**

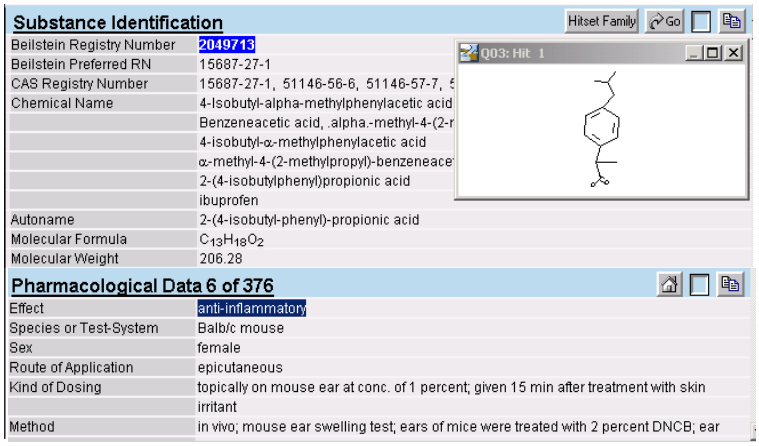


Search Term highlighted in text

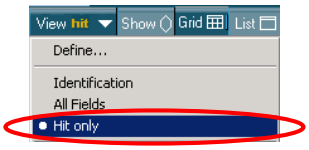


The display can be reduced to show the substance or reaction identification data and the fact that includes the search term only using **“View:Hit only”.**

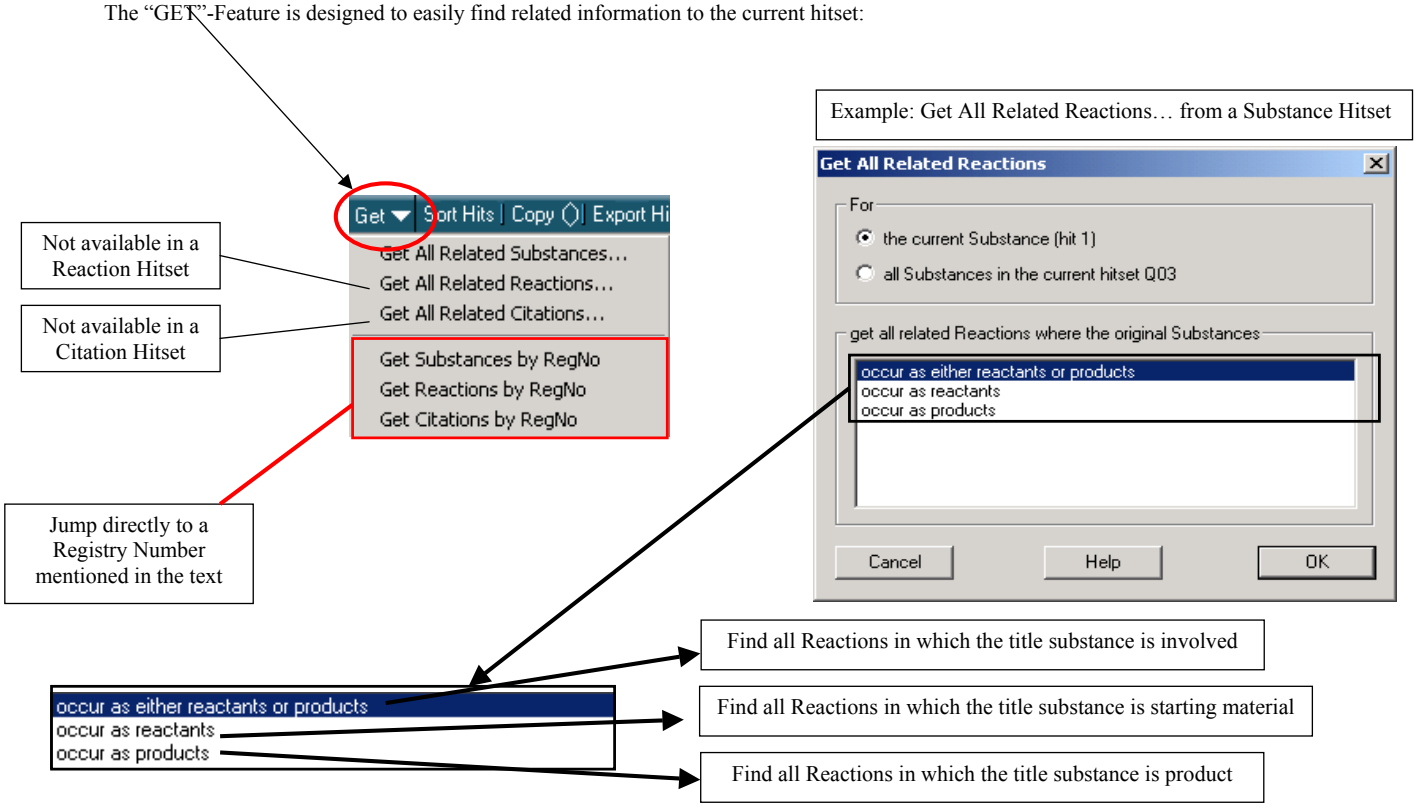




This View can be achieved as well using the “View”-Button in the Button-Bar:



The "GET"-Feature is designed to easily find related information to the current hitset:



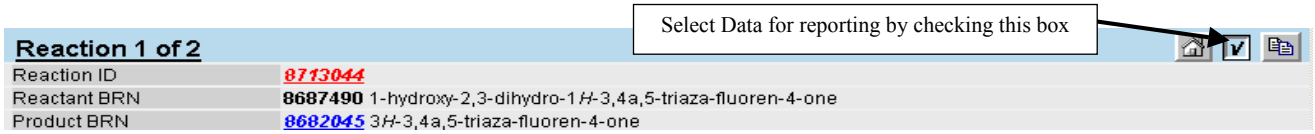
5 Reporting and Exporting

5.1 Reports

The reporting of selected information into a simple web-like form has been extended in CrossFire Commander 7. The items that can be reported are selected information from a hit display, Queries and Information about search results and progress.

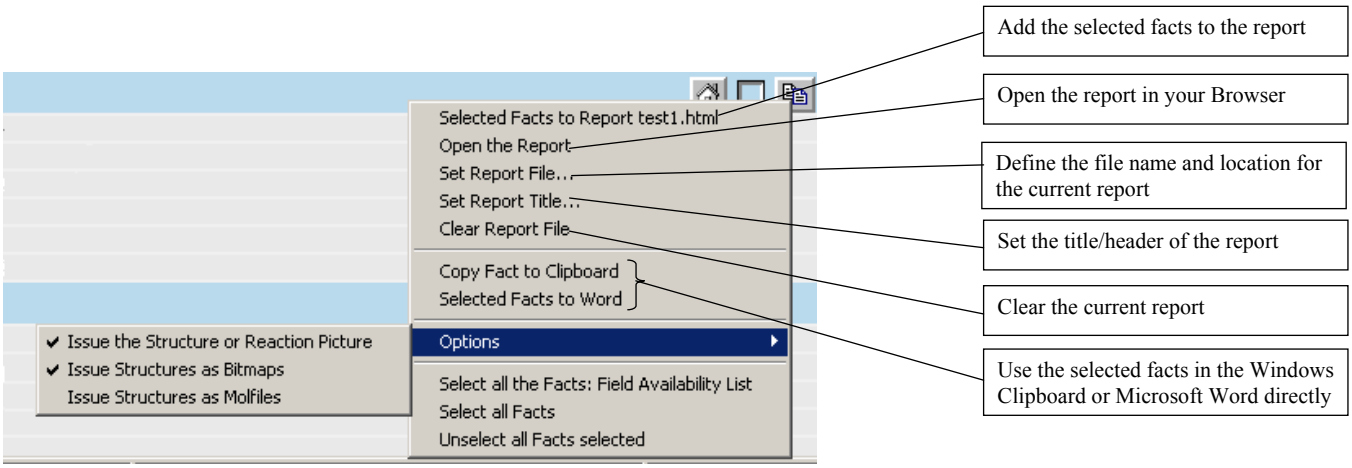
Reporting selected Facts

In the Full Display view, each field is equipped with a Title Bar on top that is used to select factual data



Several facts can be selected separately and reported in one step, additional facts can be appended to an existing report as well.

Clicking on the  button or a right mouse click anywhere inside the fact opens a menu:



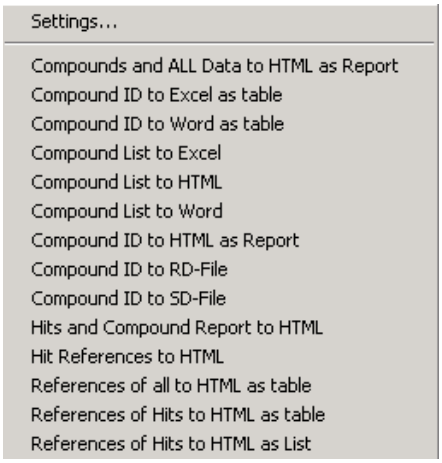
The reports are available inside the Commander:

Furthermore Queries, Search Status Information and other information can be reported. Look for the button 

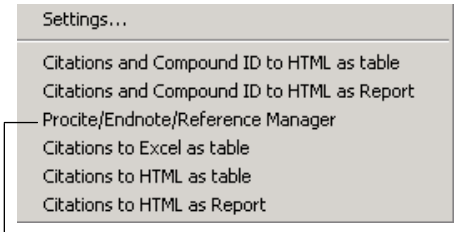
5.2 Exports

Hitsets and Hits can be exported to various targets. Clicking "Export Hits" in the button bar opens a menu with items depending on the context of the hitset:

Export Settings in a Substance Context (including predefined settings)

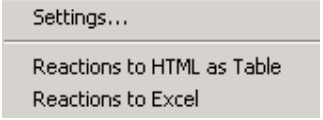


Export Settings in a Citation Context (including predefined settings)



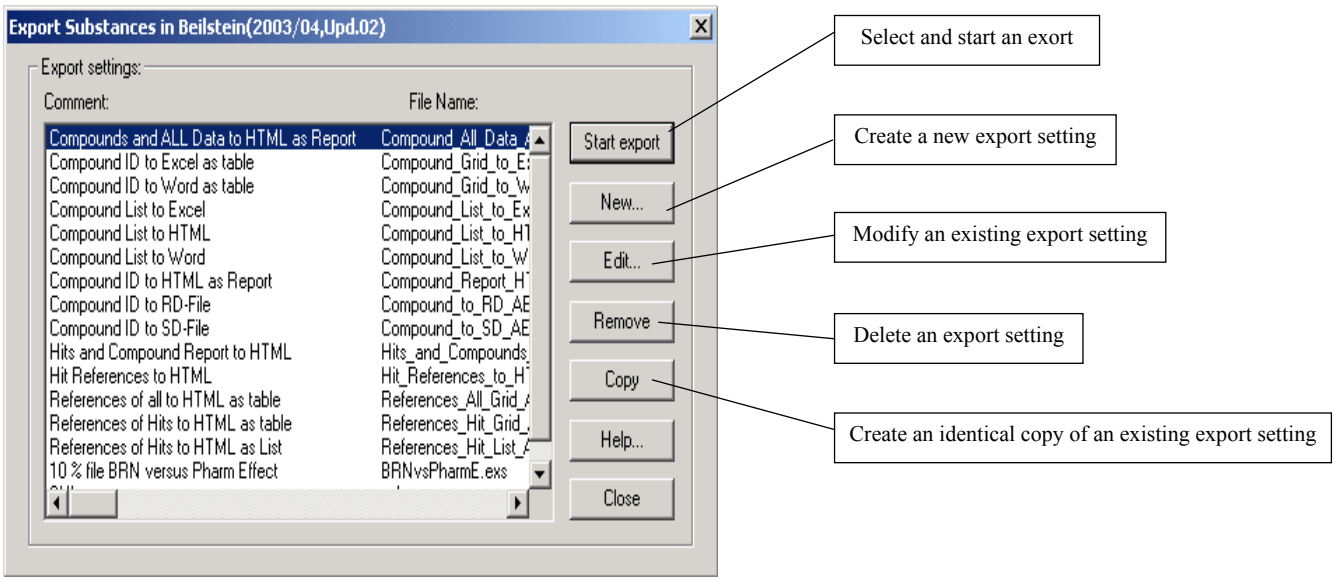
Note: the export setting to Reference Manager Software creates a file that can be imported into a Reference Manager, not in its native Format!

Export Settings in a Reaction Context (including predefined settings)



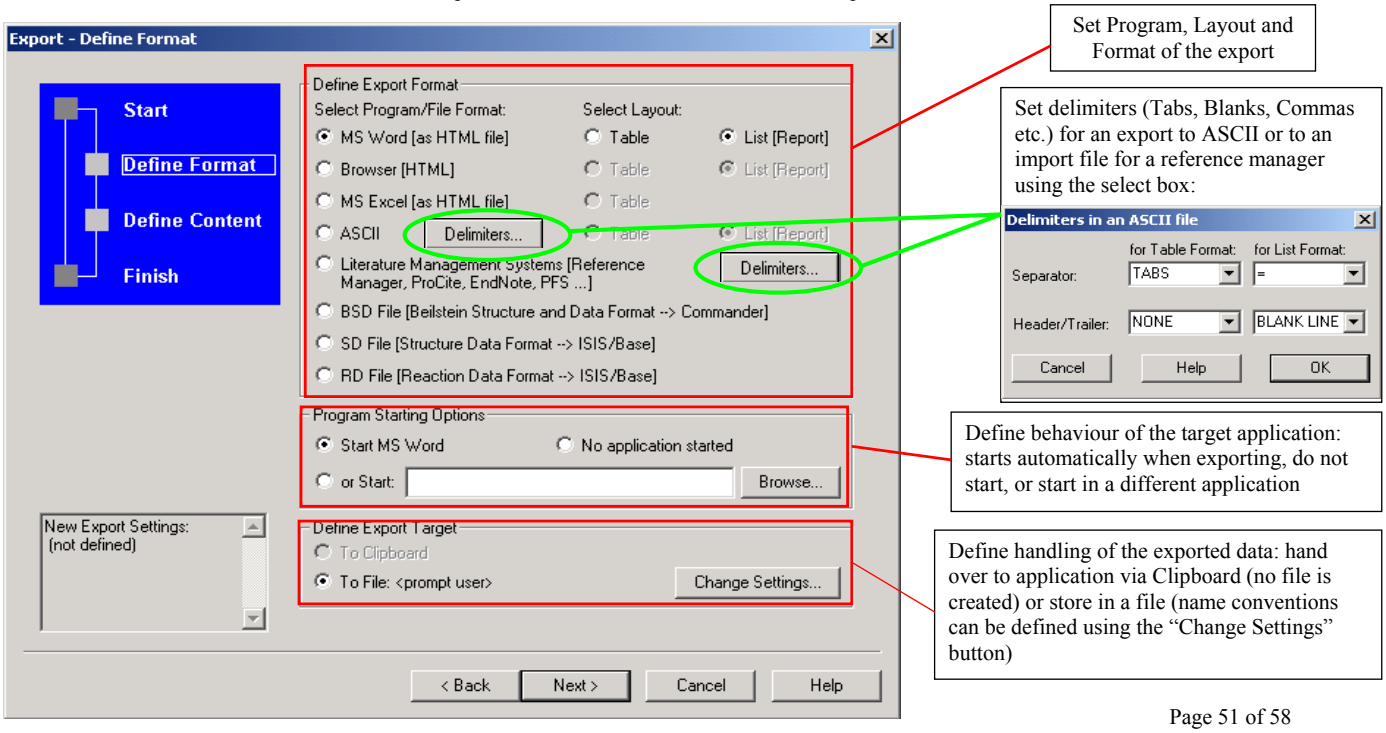
If you want to create your own export setting or change an existing one please select **"Settings…"**

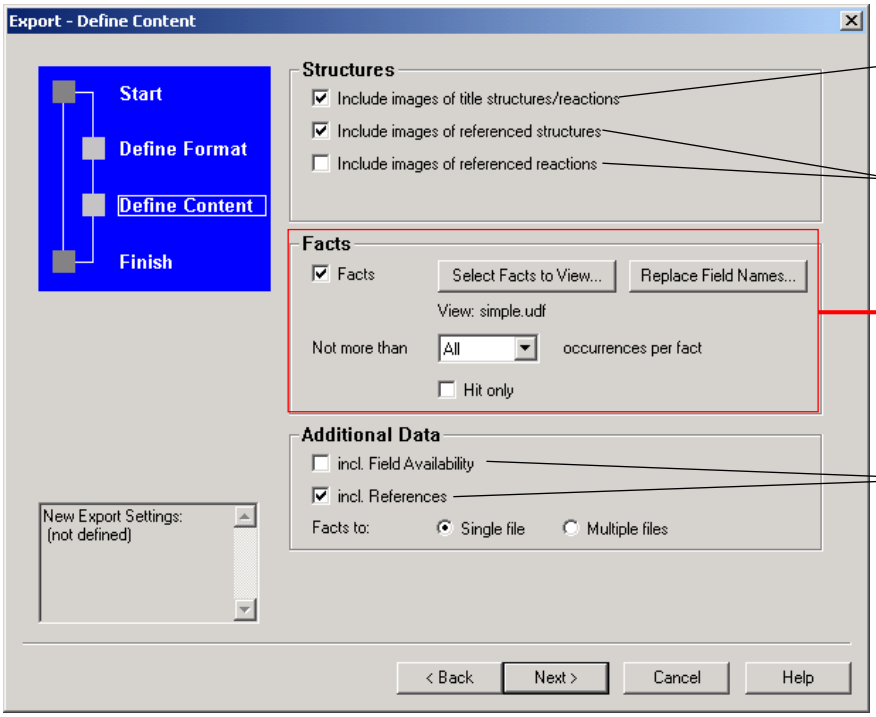
5.2.1 Creating/changing export settings



5.2.2 Prepare an export setting

After the first information screen a screen comes up which is used to select the format of the export:





Include image of the title compound or reaction. This is the one shown in the separate structure window of the detailed view

Include images of the compounds or reactions that are referenced in the data of the hit

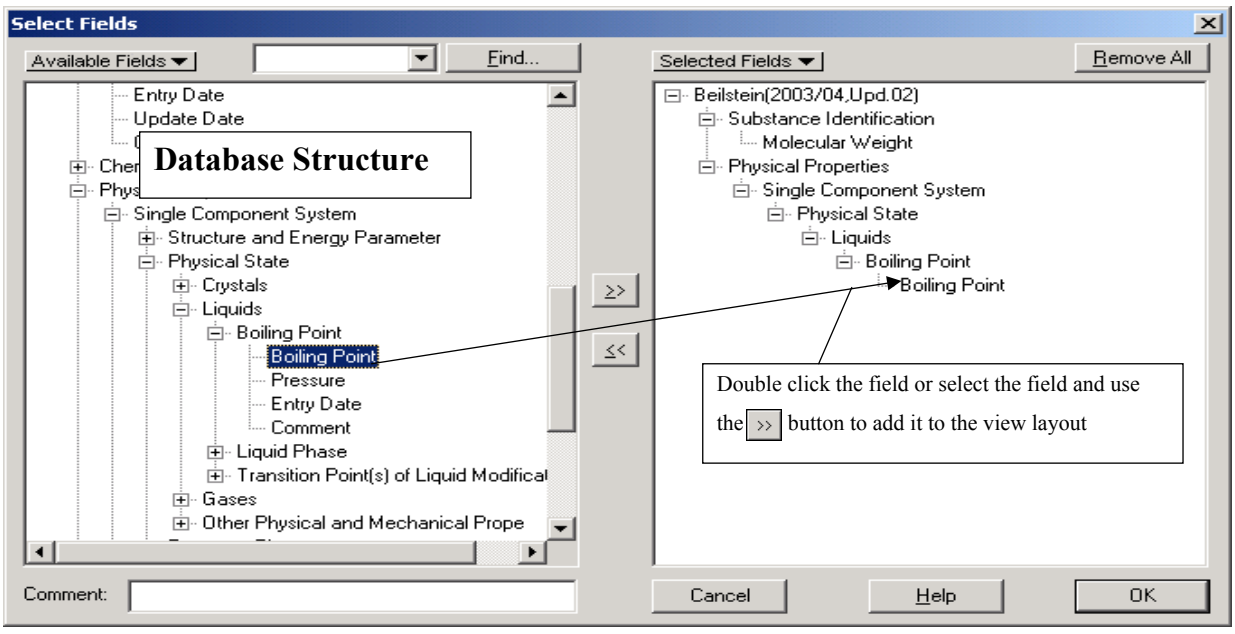
It is important that the "View" is defined. Please see next page

Please check if you want to include the Field Availability List and/or the List of References in the export

5.2.3 Selecting a "View"

It is important to define which data fields shall appear in an export. Click Select Facts to View... and "New" to define the fields for your export and select the fields from the datastructure.

Example: molecular weight and boiling points



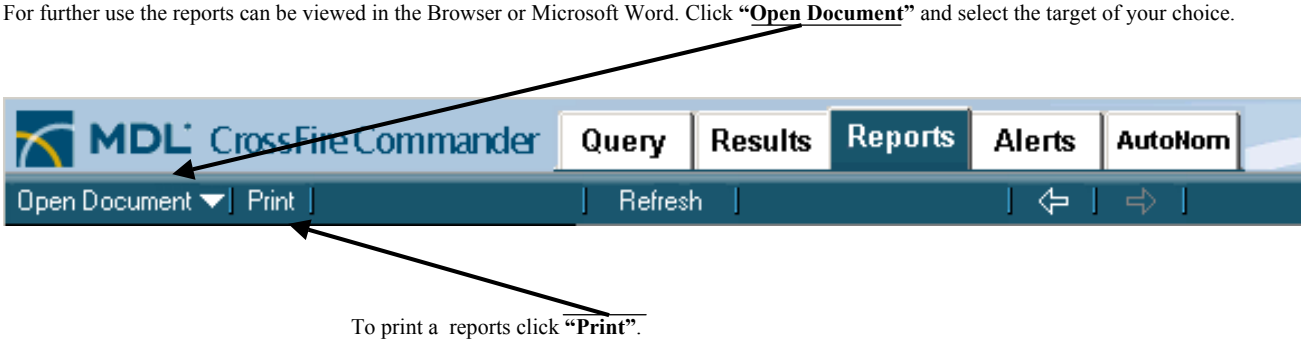
Double click the field or select the field and use the >> button to add it to the view layout

5.3 The Report Pane

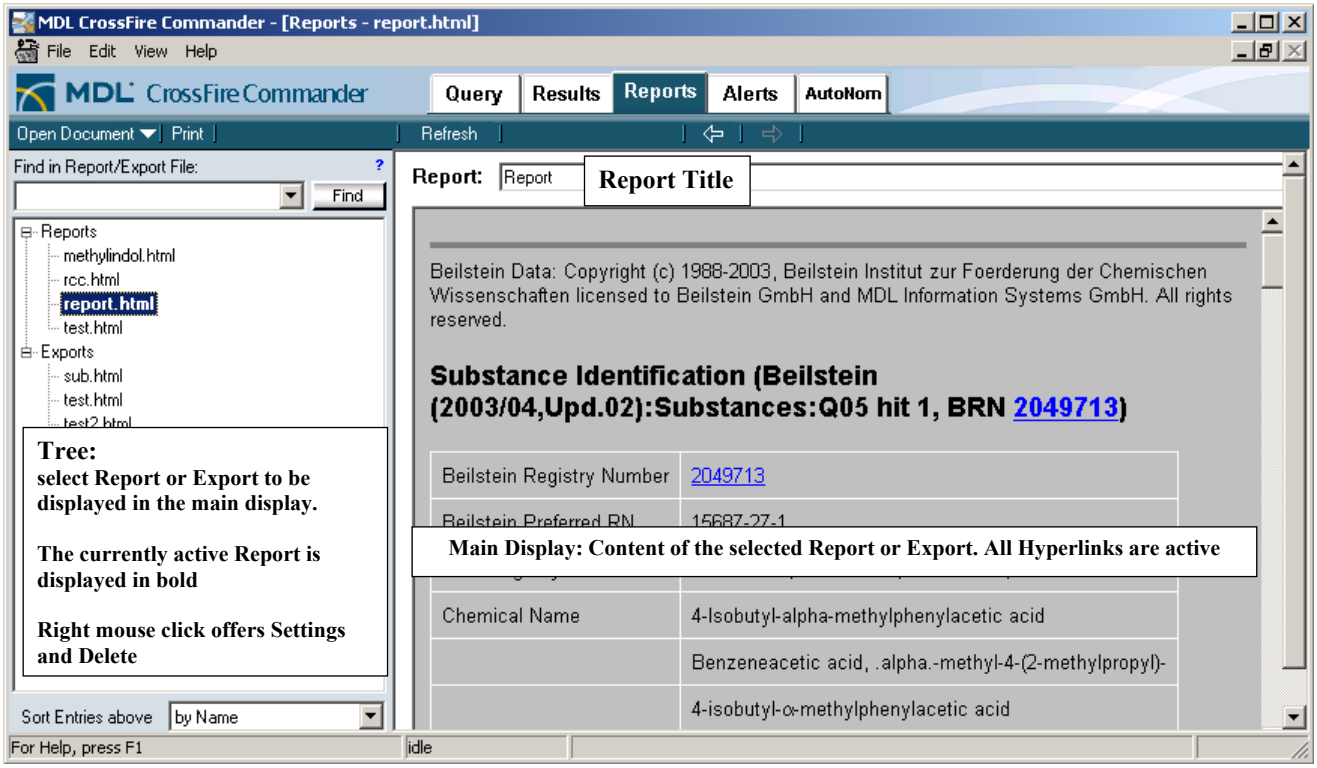
All reports are available in the first instance inside CrossFire Commander. This avoids any trouble with opening a report in the various Versions of Microsoft Office and Internet Explorer or other Browsers and the report can be viewed in a controlled environment.
In addition all exports in html-format are available in the report pane.

To access the report pane click the Reports Tab:

For further use the reports can be viewed in the Browser or Microsoft Word. Click **"Open Document"** and select the target of your choice.



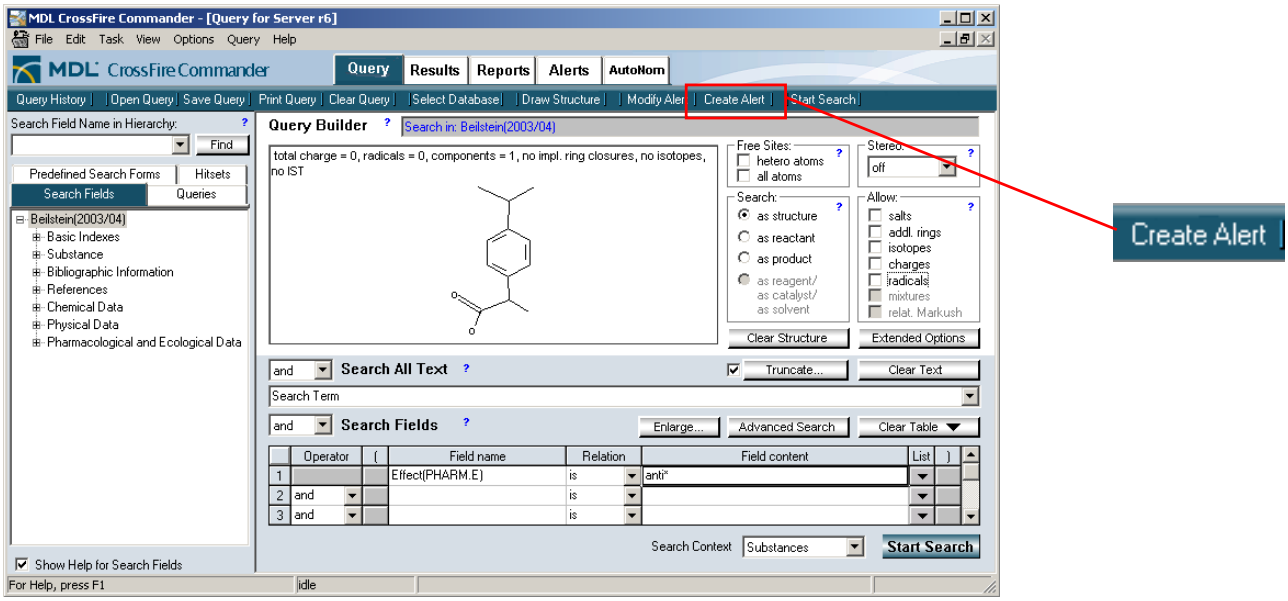
To print a reports click **"Print"**.



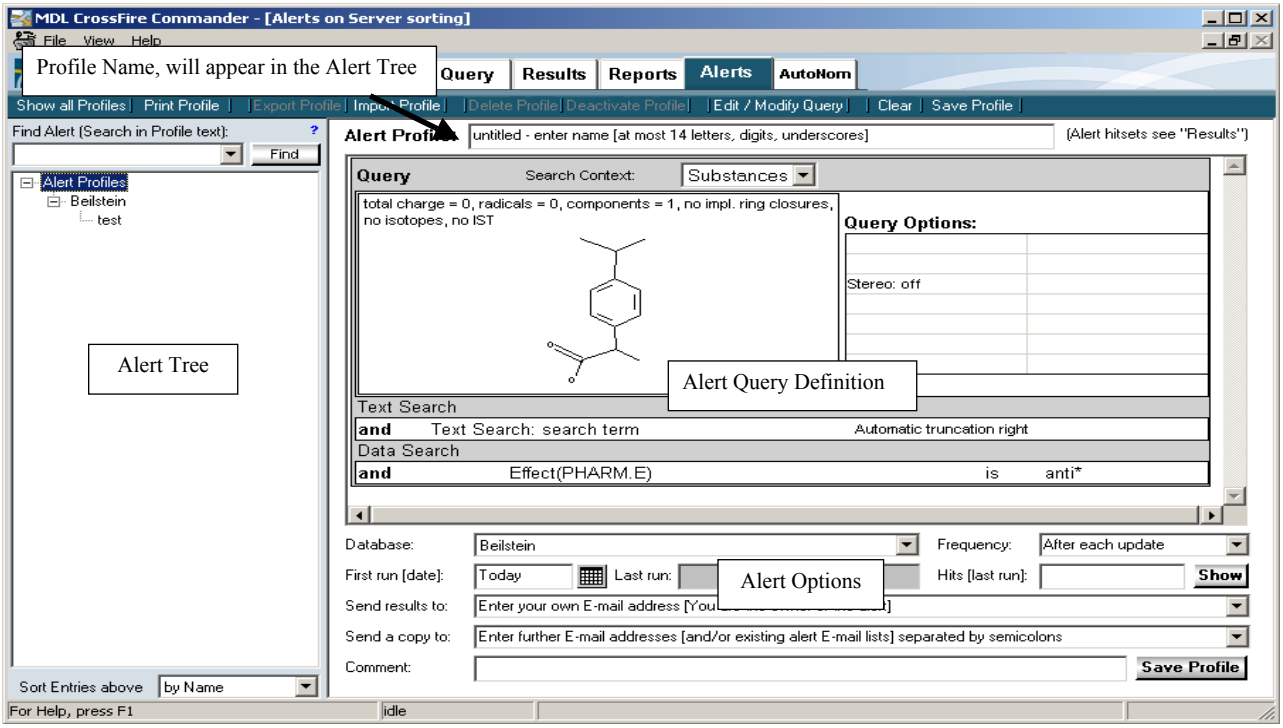
6 Alerts

MDL CrossFire Commander 7.0 offers an “Alert” feature (keep me posted feature). It is designed to retrieve results from a query that is run against the new data of an update.

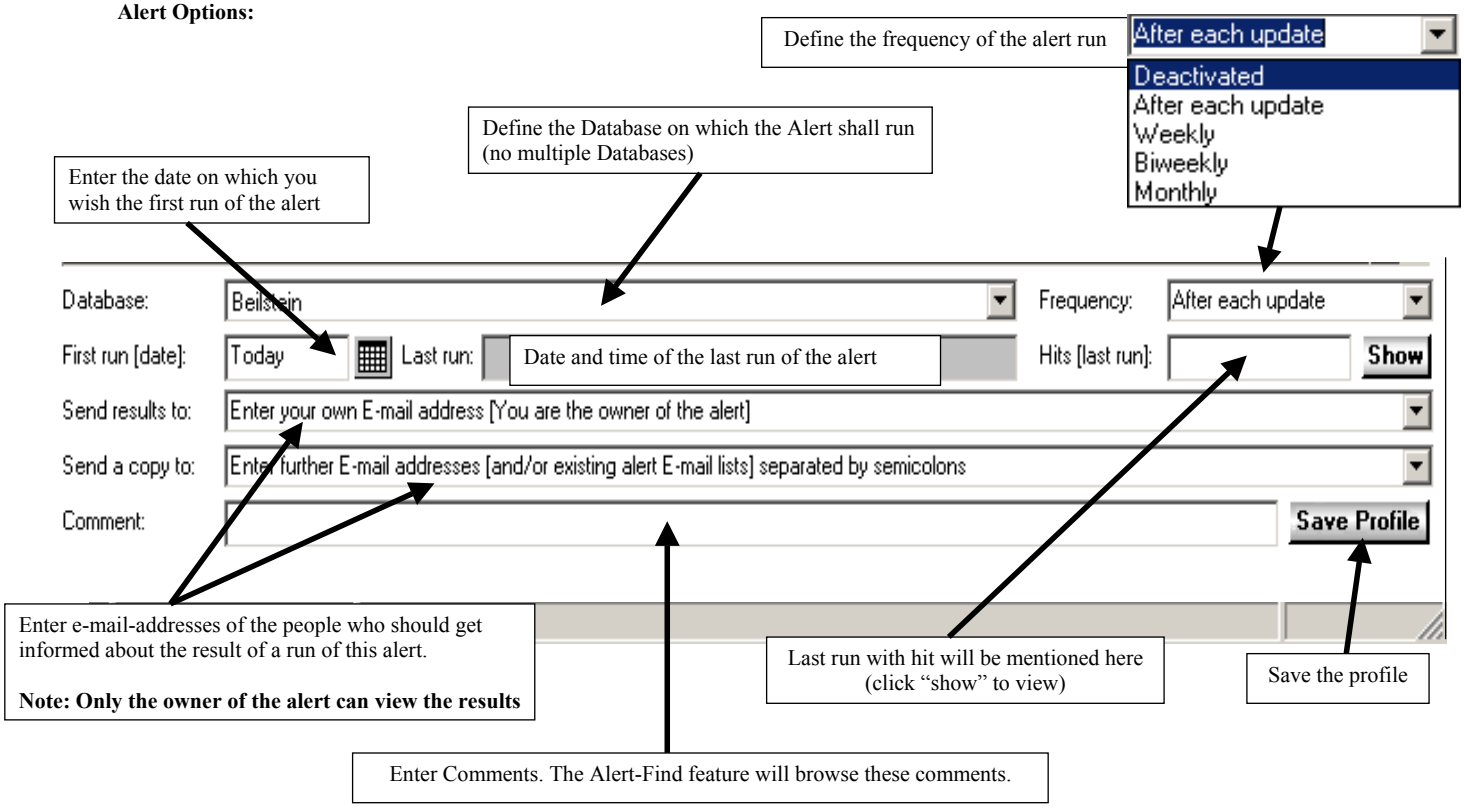
To create an Alert first create a Query in the Query Builder. In the button bar than click “Create Alert”



The query is then transferred into the Alert Window, where the Alert-Options must be set



Alert Options:



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