Quick Reference Guide

03/2002

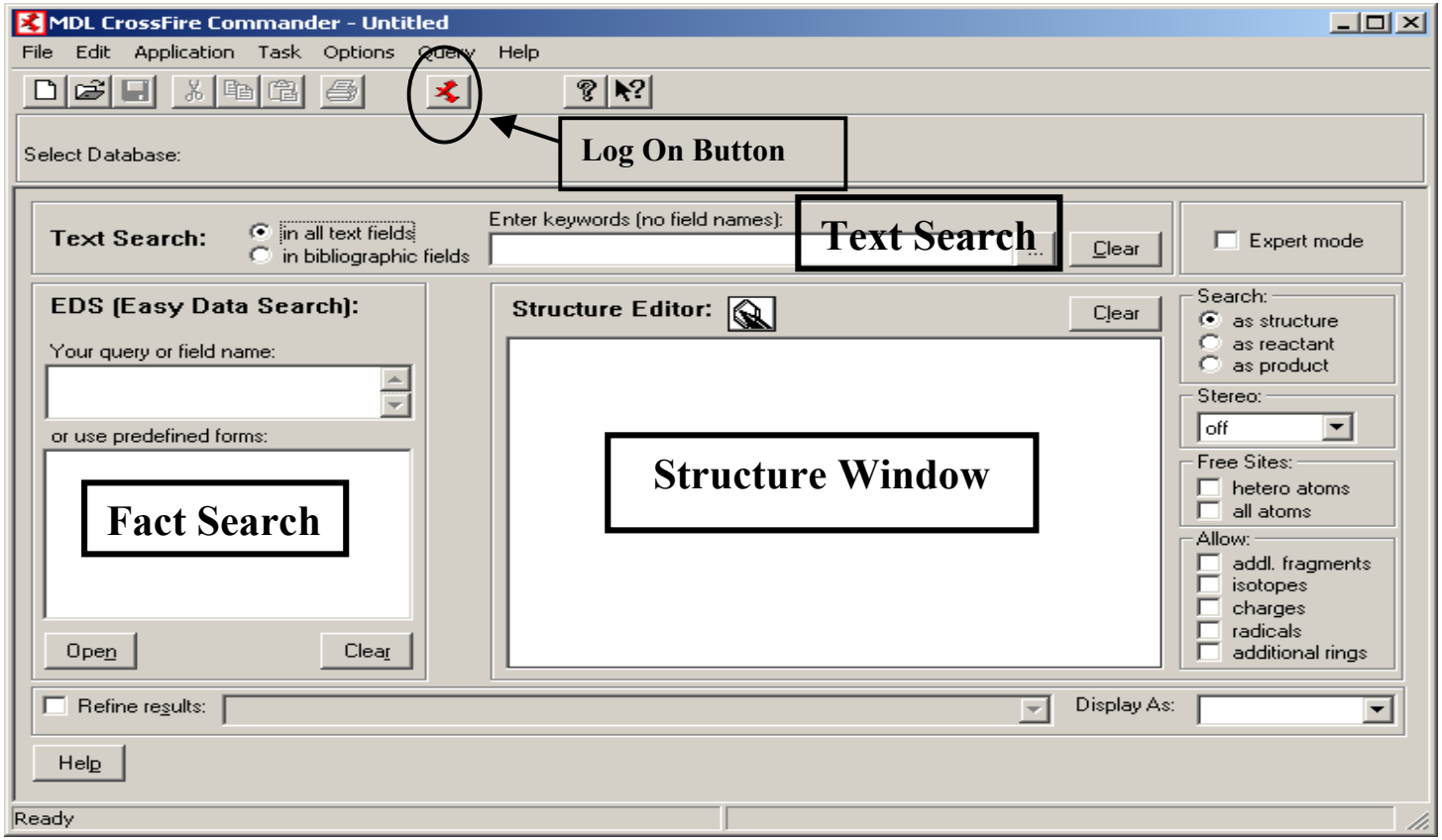
1 Getting Started

Welcome to MDL CrossFire Commander V6 SP1. This guide demonstrates briefly the use of the features to create queries and to view the result.

1.1 Logon

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 V6**"

The Commander Window looks like this:



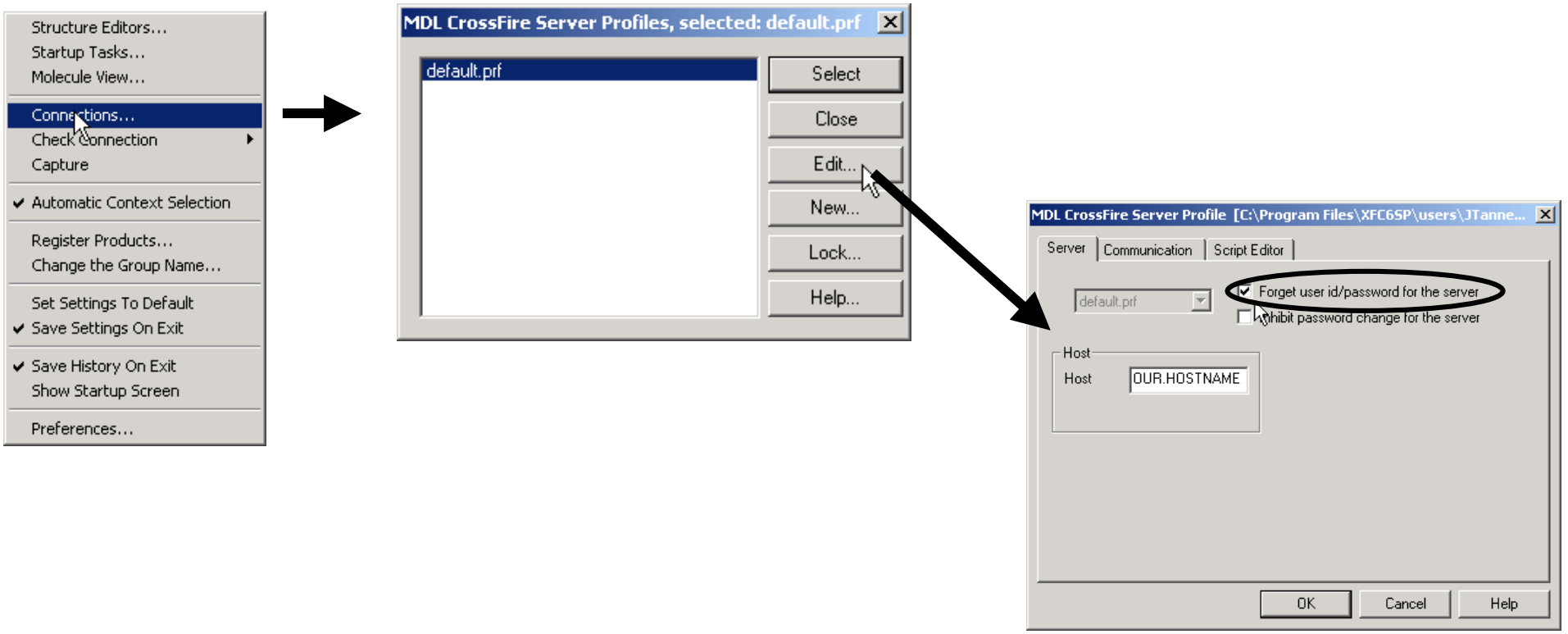
- In Commander click the  -Button or select from Menu "**Application:CrossFire**"

- Fill in the login-box as required.

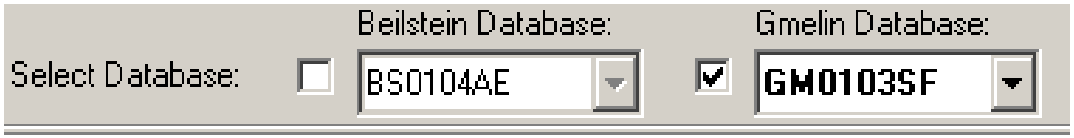
Click the checkbox if you want your user ID and your password to be saved. You will not be asked anymore for them after clicking the box.

If you need to change your password or enter a new password after you have saved it please proceed the following path:

Select Menu "**Options:Connections..**" and select the profil of which the password is to be changed. Click "**Edit**" and select the checkbox "**Forget user id/password for the server**". Click "**Ok**".
You will now be asked for your ID and password upon Logon again.



1.2 Database Selection



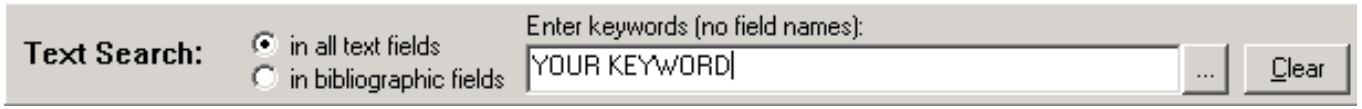
Select Database: These Listboxes select the Databases you will be searching in. Depending on your license you may select one or more (search over multiple database) databases by using the checkboxes. In the case of only one database being checked, the currently active database is displayed bold.
The abbreviation informs you about which version of the database is available:

XX YYYY ZZ

XX:	*BS* = Beilstein (organic Chemistry)		
	GM = Gmelin (inorganic Chemistry)		
YYYY:	Year (e.g. *01*) and update number (e.g. *04*)		
ZZ:	Specification	Beilstein	*PR* = Plus Reaction
			AB = Abstracts
			AE = EcoPharm
		Gmelin	*SF*= Structure&Facts

1.1.2 Search Options

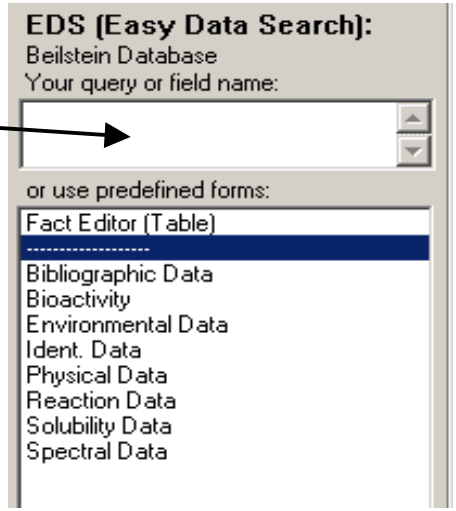
Text Search: Type in keywords, one ore more, to be searched in the basic index.
Example: “malaria”



Structure Editor: Draw and search for a structure as a molecular species or as component of a reaction.

Structures can be loaded as BCCOM-File or as SD-File using “**File:Open**”, “**File:Execute BCCOM**” or “**File:Execute Query List**”

Enter a **Factual Query** in the Text field, e.g. “bp > 100” or “Author is Maier”



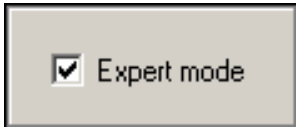
Use the **Fact Editor** (Table), the **Easy Data Search** (EDS) or the predefined forms to conduct a search for specific facts.

☞ Use a combination of these interfaces for improved search results

1.3 Expert Mode and Guided Mode

This guide describes the use of Commander in “Guided Mode” in which the Client interacts with the user to ensure a query according to the wish of the user.

If you do not want this interaction you can switch to “Expert Mode” by checking the corresponding checkbox. In this mode whatever was typed in is used directly as the query, it is designed for use by users with highly advanced knowledge of the CrossFire System.

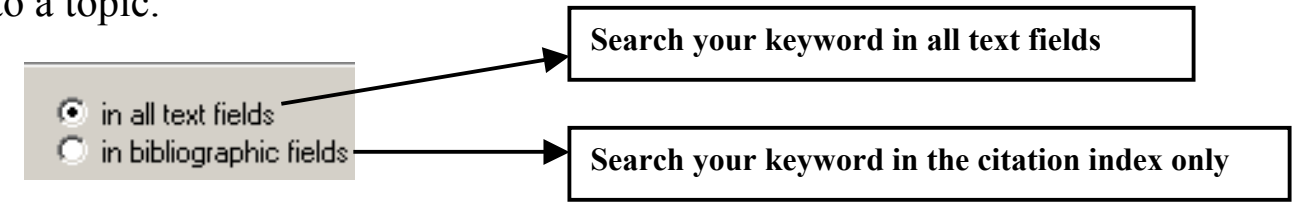


2 Search

2.1 Using the Text Search

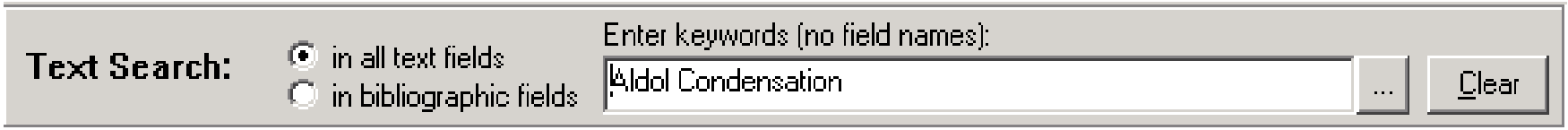
The Text Search is designed to search a keyword or expression against the basic index of the database. The result provides a general overview to a topic.

Select the level of your search:



The level determines the indexes which will be browsed with the text you enter in the query field. The Basic Index of the databases is searched for the words entered in the field.

Type your Keywords into the field, you can enter one or more words:

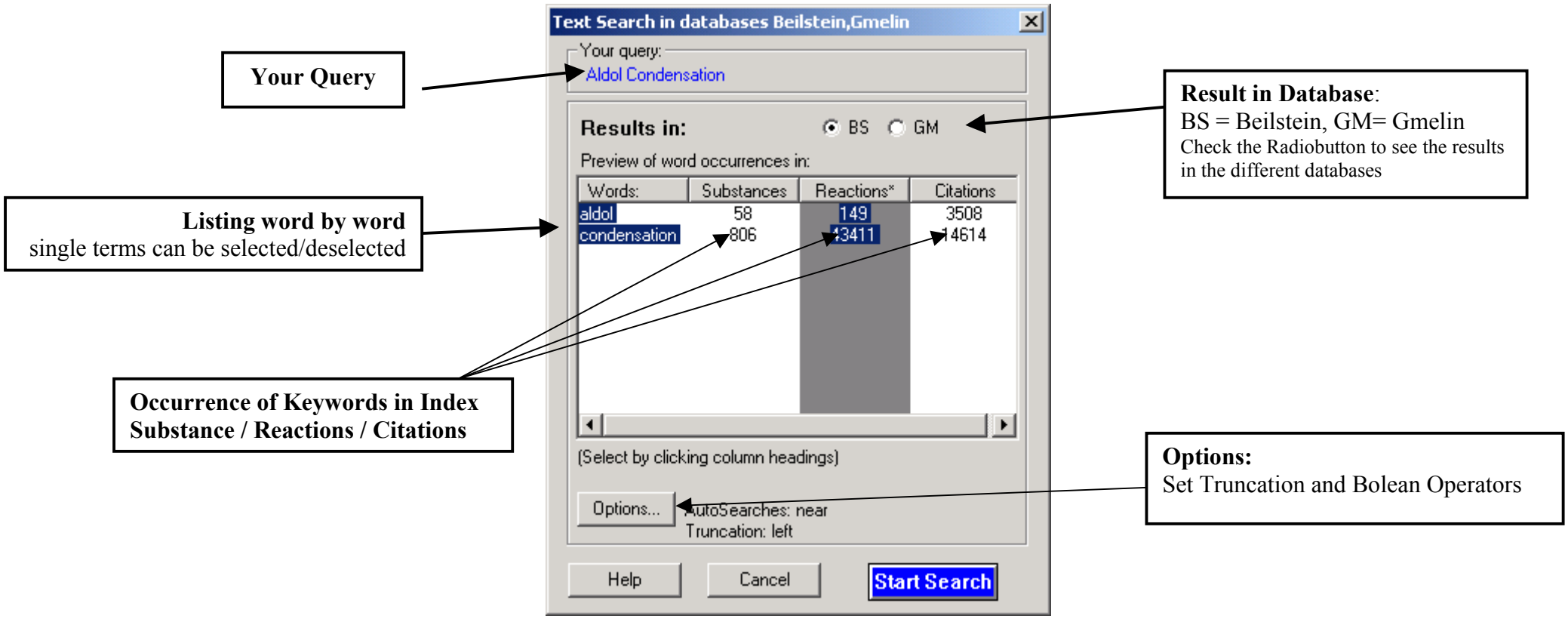


Examples: “Malaria” or “Antimalaria”, “Aldol Condensation”, “Cancer Treatment”, “Effect of Melatonin on sleep disorder”. We recommend to limit the search term to 5-6 words maximum.

Submit the query by carriage return or F7 or press “Start Search”. If more than one word is typed an AutoSearch search will be performed.

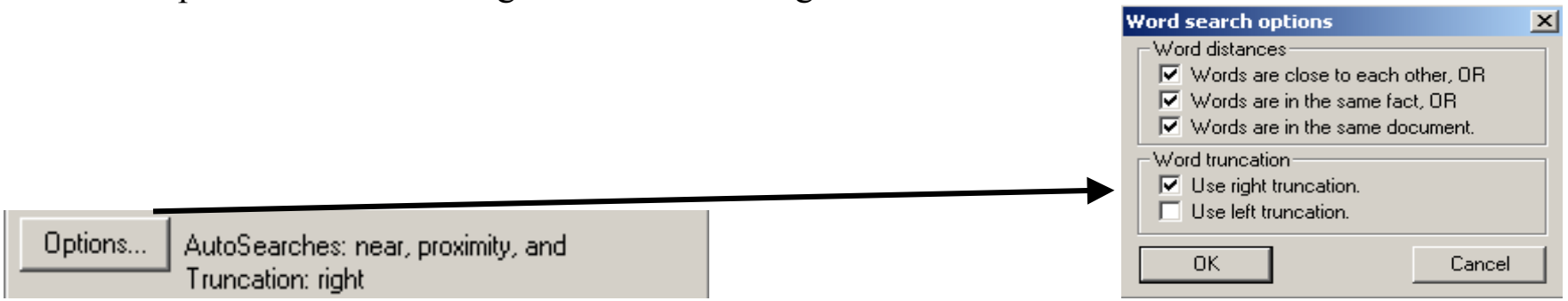
If you have selected “in bibliographic fields” only the Basic Index Citations will be searched. The result will be a list of references.

If you have selected “All Text Fields” you will be prompted to determine the context you want to apply for your search.



Choose “Substance”, “Reactions” or “Citations” to determine the context you want to be searched. The number of occurrences is shown for each word in the column of the context for each word separately. Choose the context you want by clicking the header.

Click the Options button to change the default settings:



Truncation:

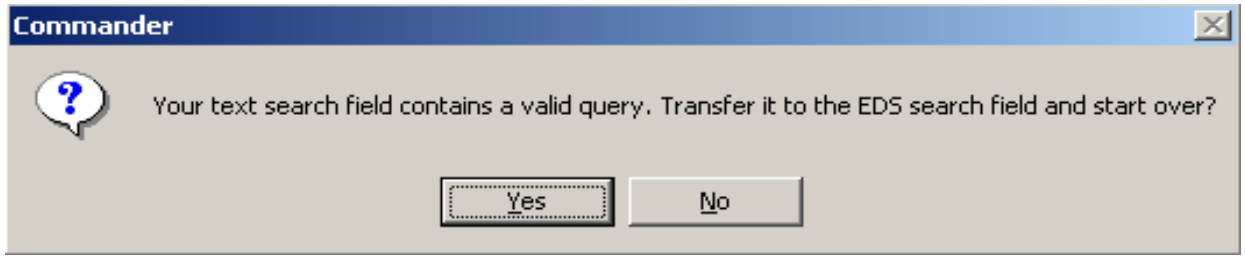
Truncation can be set off to search for an exact term.
A star at the end of the keyword can be used, it will switch on the option “Use right Truncation” automatically.

Note: Right Truncation will automatically suppress the word endings “-s” (for plural) and “-ing” to ensure the query regarding the structure of our databases.

Left Truncation will lead to a “> number” in the Information Box, correct numbers can’t be displayed for technical reasons

- For more sophisticated search Boolean operators can be used.

If a “query-like” text is introduced, for example “bp=100”, the user will be prompted:



If “Yes” is chosen Commander translates the Input into the Fact Editor Field. Please press “Start Search” again to submit your Query.

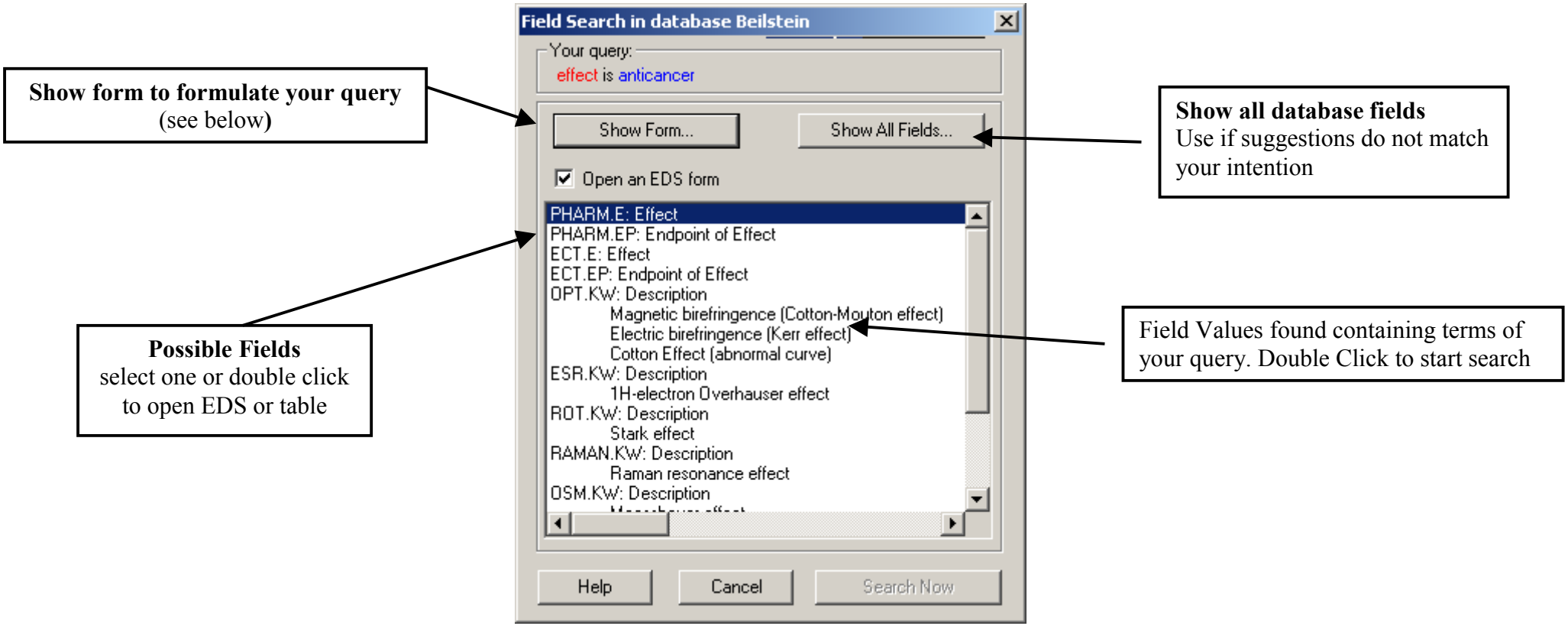
If “No” is chosen Commander will execute the entered text as a text search.

2.2 Using the Easy Data Search (EDS) or the Fact Editor

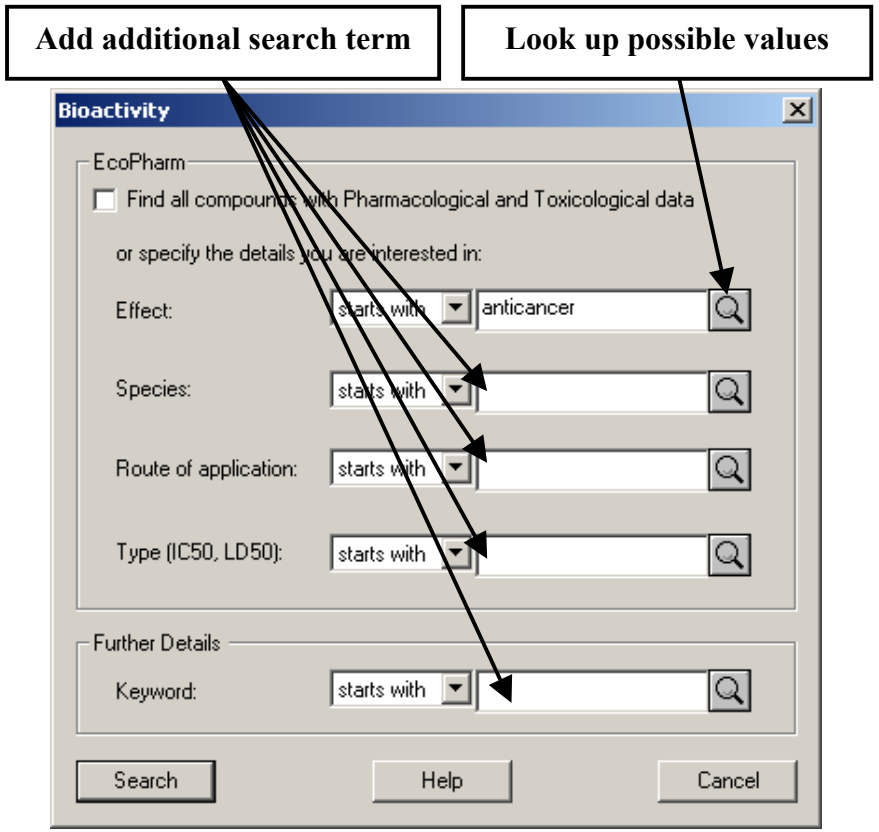
The upper field of the EDS is for expert search using the Commander's operators and field names:

It is possible to enter the query as a sentence like "Author is Mayer", "Effect is anticancer".

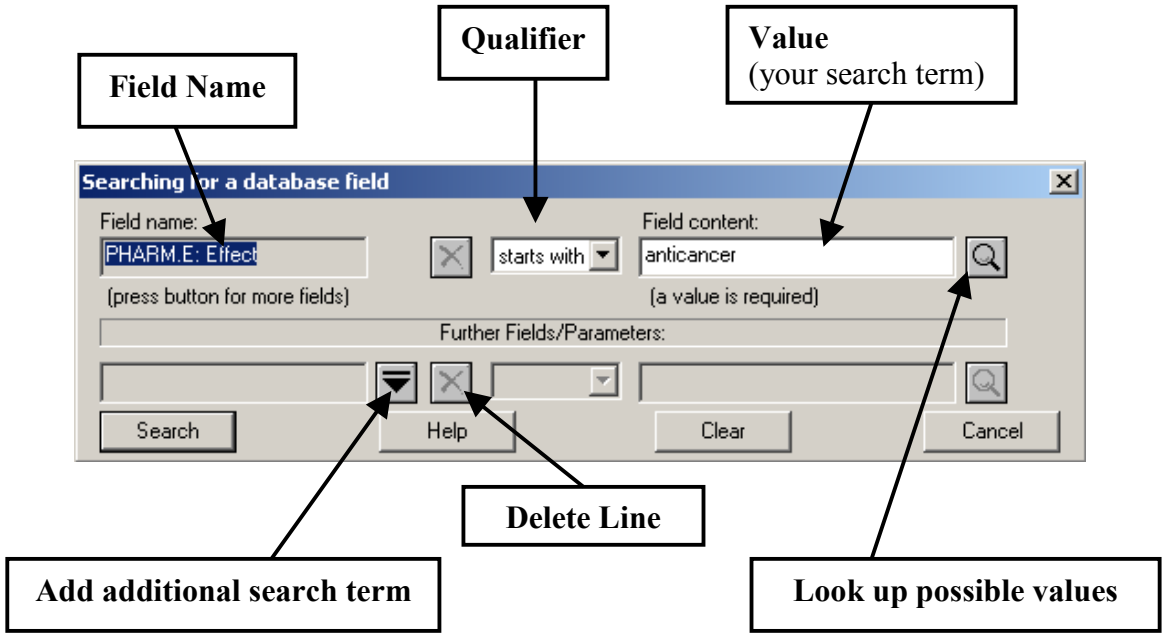
In this case Commander translates the sentence into the query language and will prompt the user if more than one field could be applied:



The button Show Form... transfers the selected field into a table for further refining. If "Open an EDS Form" is checked an EDS Form is used if available.



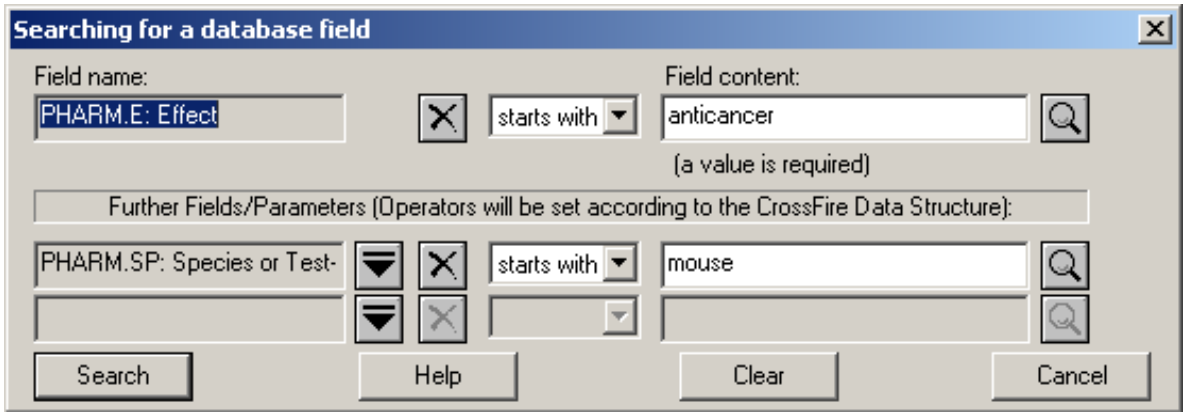
Translation into EDS Form



Translation into Table

A combination of sentences can be used as well, for example “effect is anticancer and species is mouse”. However, due to the complex structures of our databases it is not recommended.

Deselect “Open an EDS Form” and click “Show Form”.

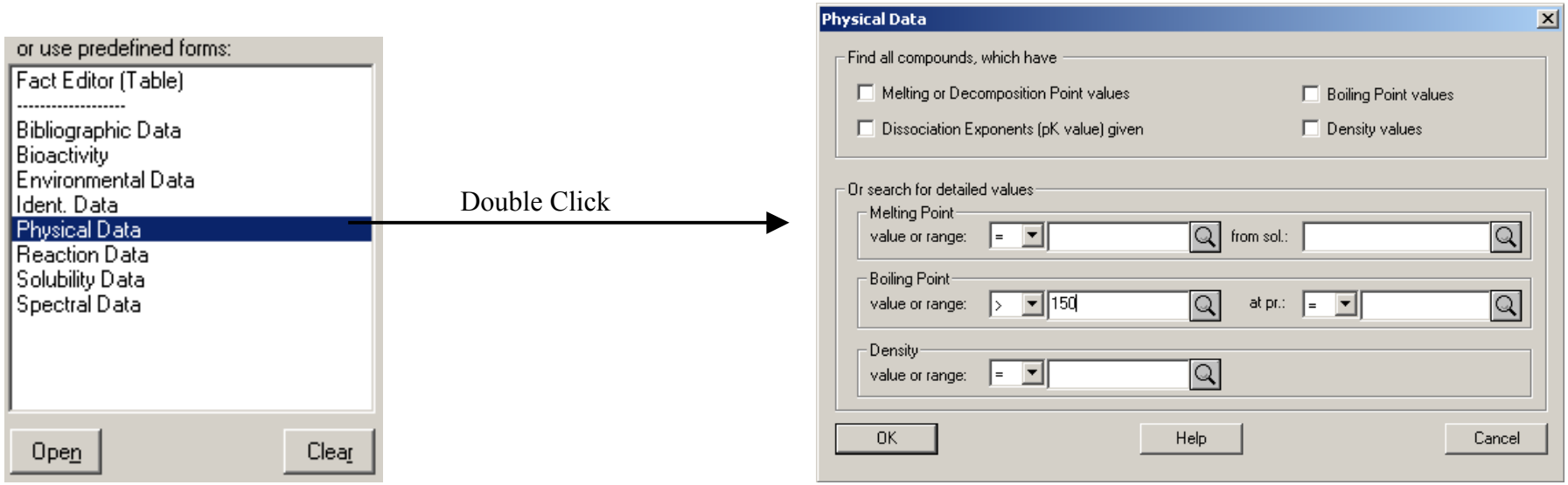


Successful Translation of a two sentence query

Note: Operators to connect the two sentences will be set by Commander according to the nature of the query. They can’t be changed.

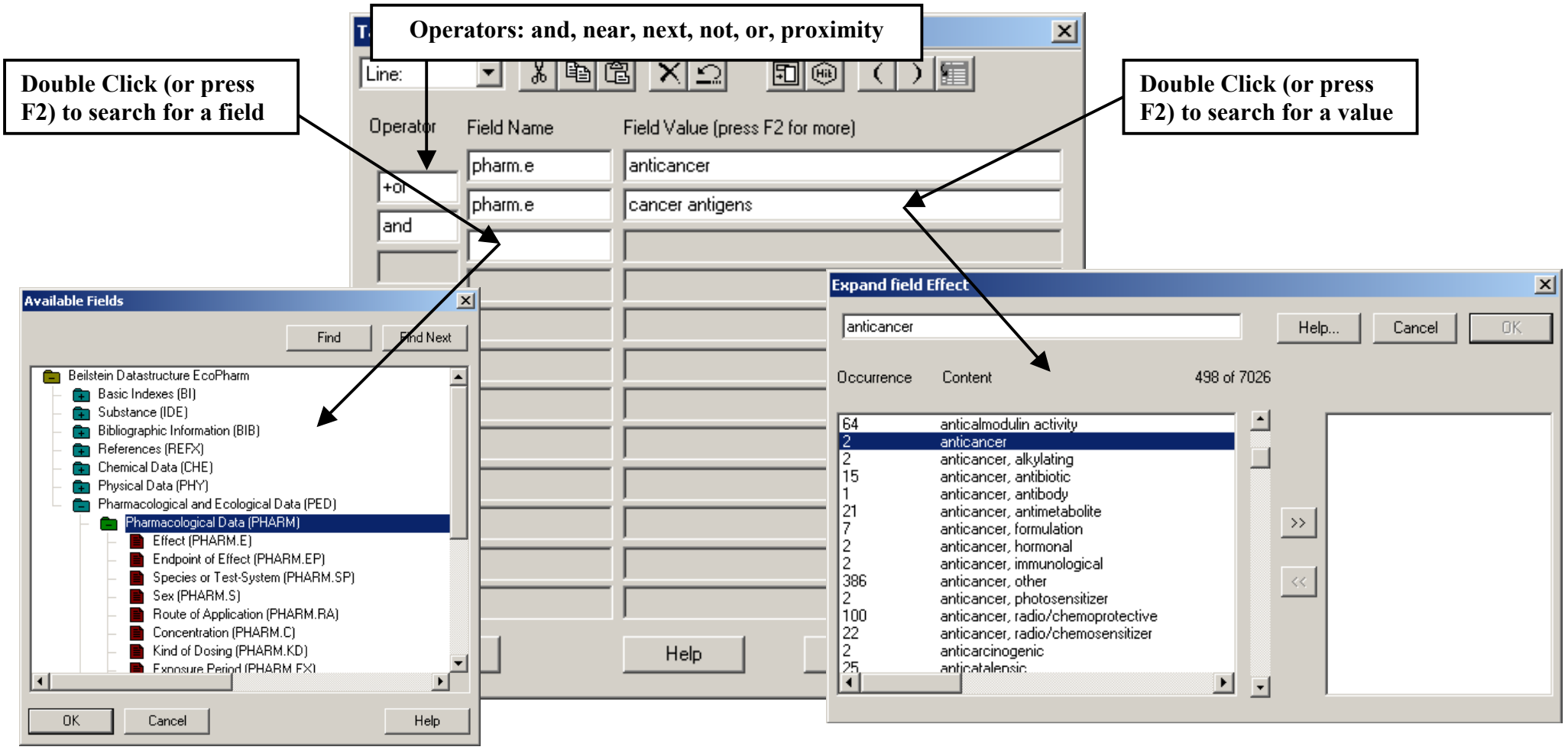
Use Predefined Forms:

The lower field enables you to use predefined forms to start a factual search. Double Click or select and click “Open” to enter data:



or double click “Fact Editor (Table) to search for specific values of specific Index Fields:

The Fact Editor Table displays the data structure of the selected Database and enables direct lookup of values for a field:



2.3 Using the Structure Editor

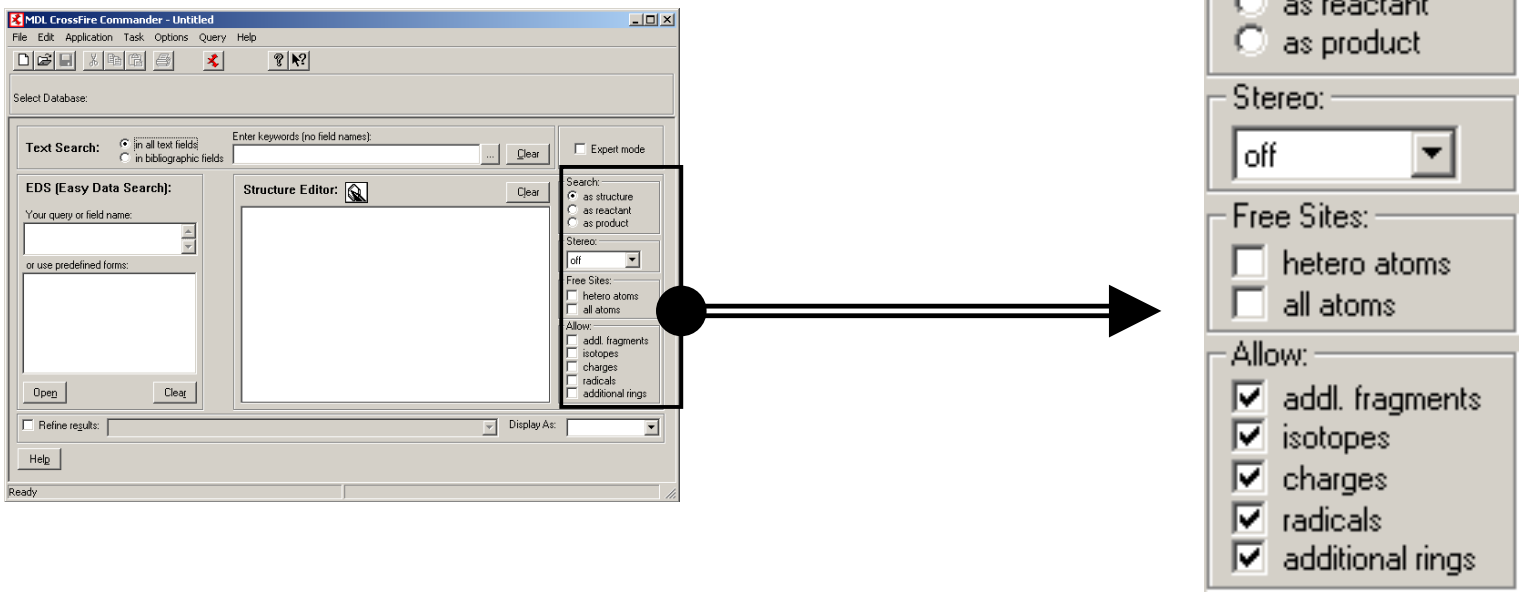
Two Structure Editors are available in this version: ISIS/Draw 2.4 (default) and the MDL CrossFire Structure Editor. You can select the tool of your choice at Menu "**Options: Structure Editors…**"

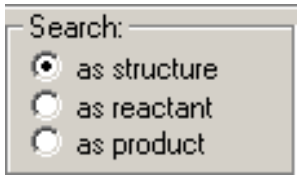
Press 

or double click in the *Structure Editor Window* to open the Drawing tool, and draw the structure or fragment, or the reaction or parts of a reaction you want to search for.

Go back to Commander by clicking on  (MDL ISIS Draw) or 

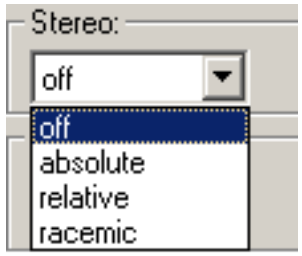
(MDL CrossFire Structure Editor). Once a structure is loaded in Commander general options for the search can be set on the right side of the screen



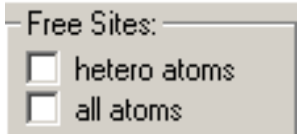


Select the role of the drawn structure:

- *as structure to retrieve data about the compound*
- *as reactant to view the reactivity of the compound*
- *as product to retrieve preparations of the compound*



Set stereochemistry options



Allow free sites on hetero atoms or all atoms.
No selection: exact search

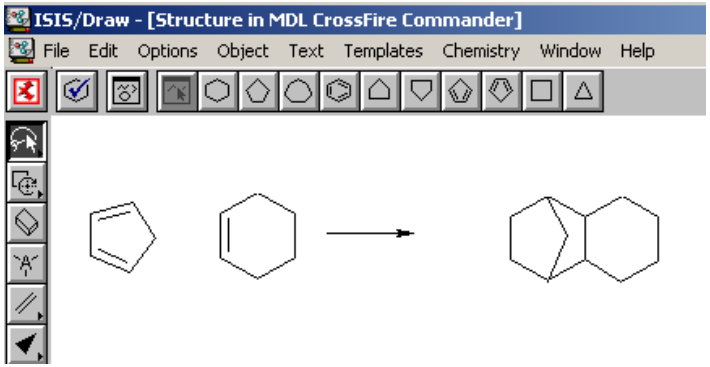
Use checkboxes to select the options you want to apply .

To toggle all options on/off hold CTRL and click one of the options

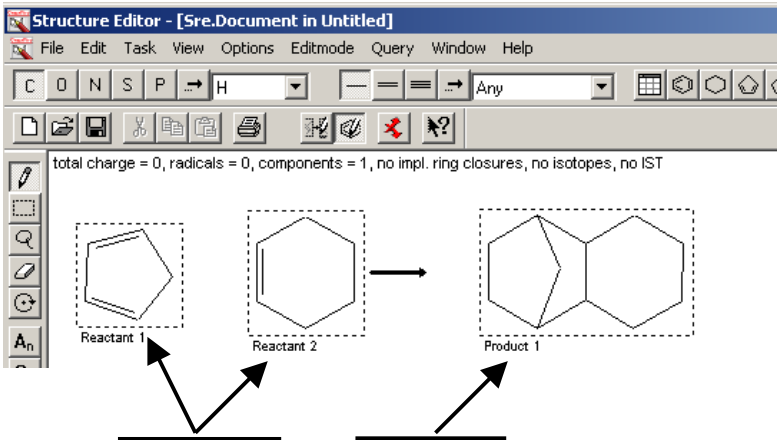
2.3.1 Reaction Search by Structure

Reactions are typically searched by structure. Full reactions, when starting material and product is known, can be searched by drawing the reaction in your preferred structure editor (see xxx)

Reaction Drawing in ISIS/Draw



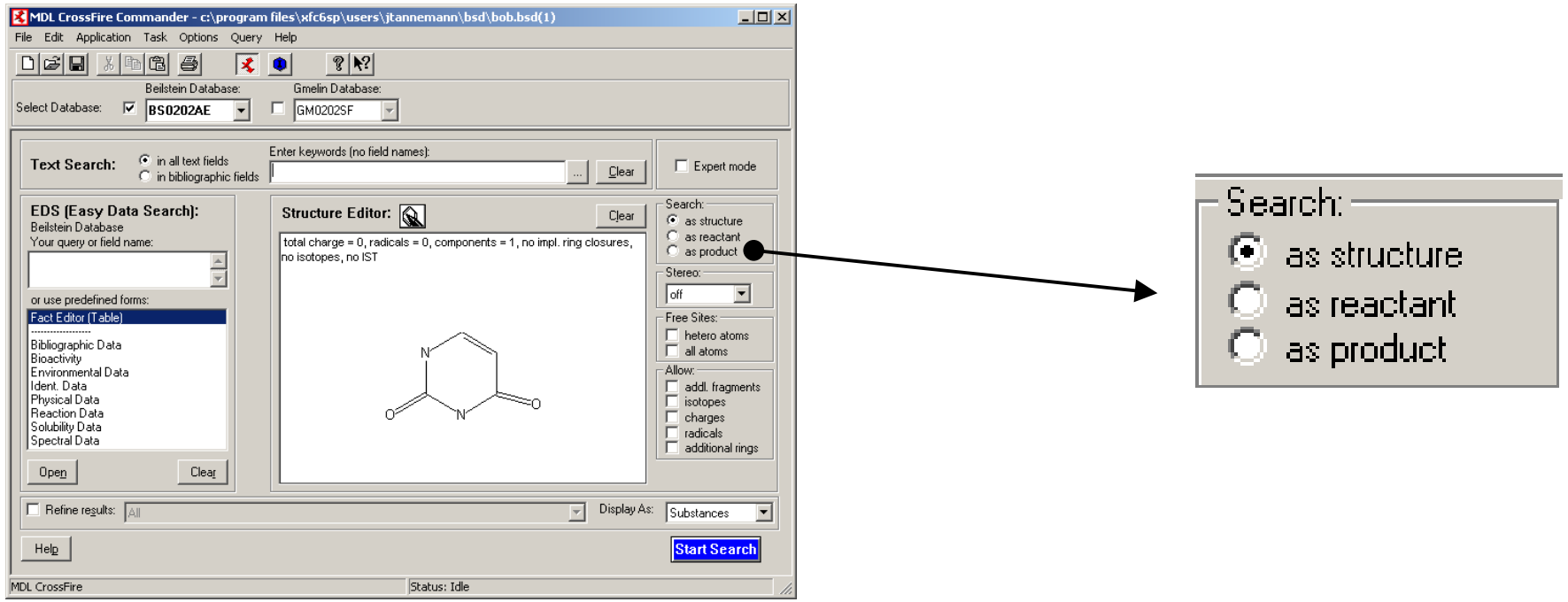
Reaction Drawing in CrossFire Structure Editor



Commander recognizes automatically the role of the structure as Reactant and Product by the position of the arrow.

Half reactions can be drawn in similar way, however the structure options window described above can be used for more flexible query formulation:

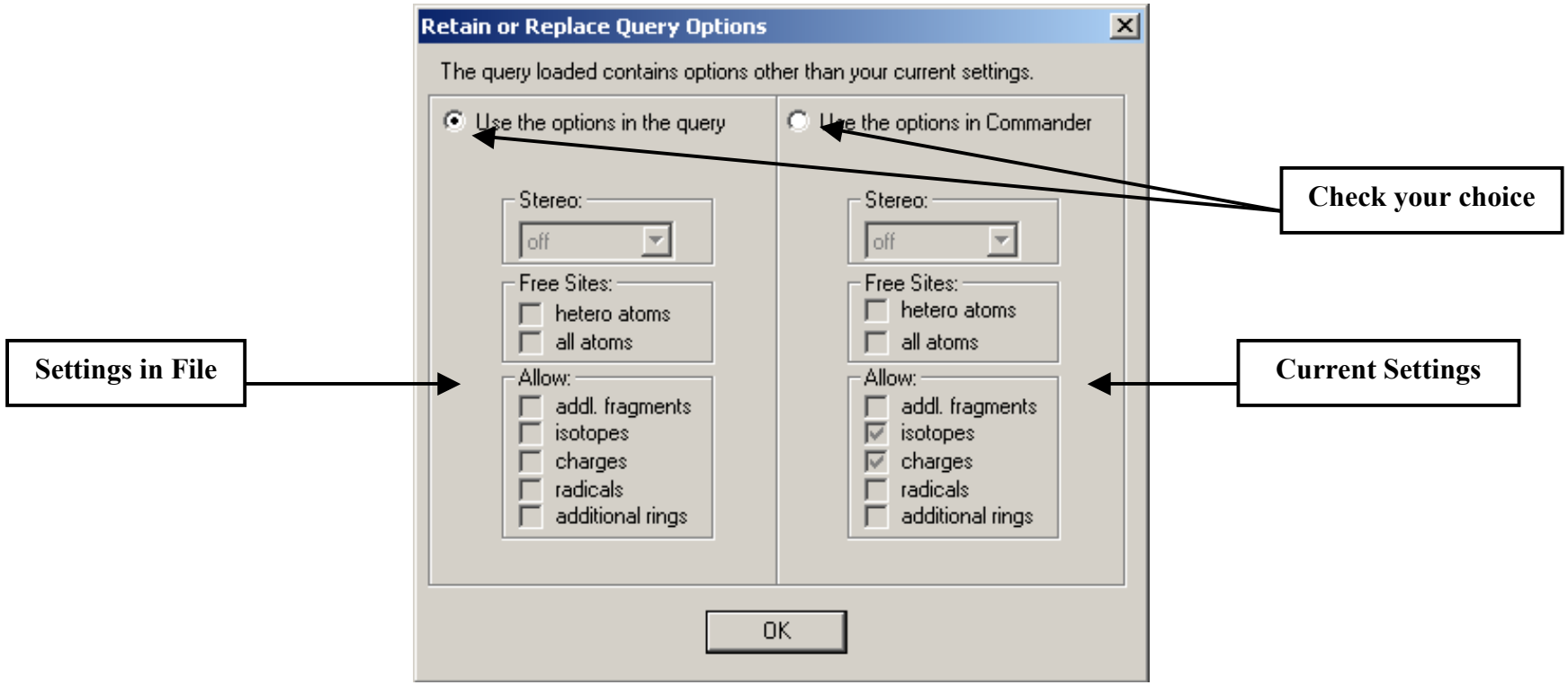
Draw a structure and load it into Commander. Select the role of the structure using the radio buttons.



2.4 Use a saved query

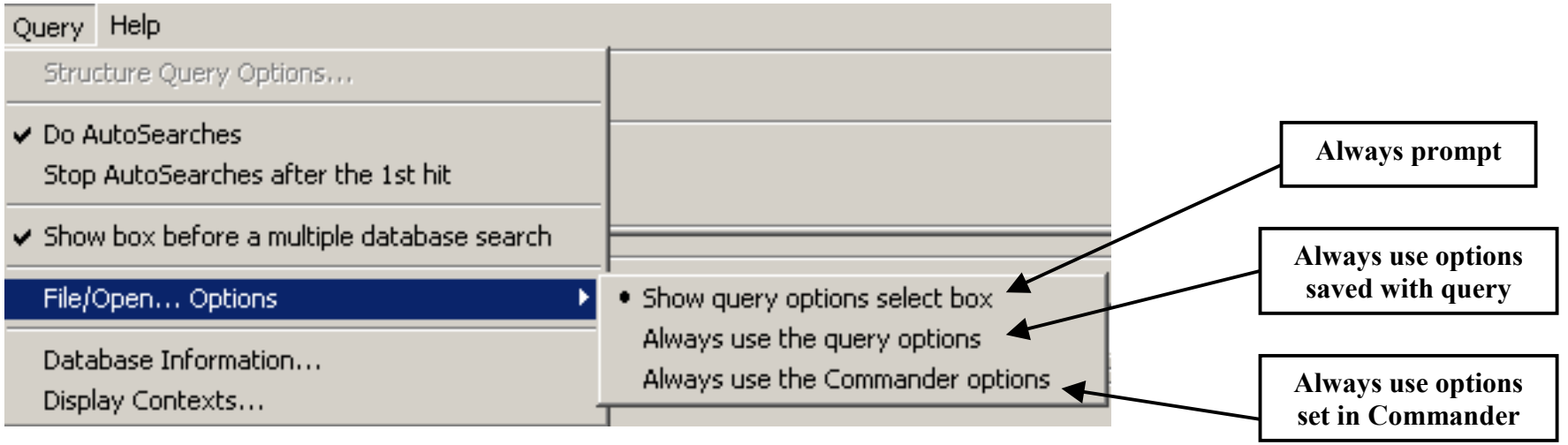
A query including all options can be saved for future use or as template using "**File:Save**" or "**File:Save as..**". from Commander. These can be text, fact or structure queries.

Using "**File:Open**" these can be loaded again into Commander. In case of a structure the options for the saved file can be different from the current settings. If this is the case Commander prompts you to select the options you want to apply:



The behavior of this prompt can be customized:

Use "**Query:File/Open…Options**" to select



2.5 Combined search

MDL CrossFire Commander V6 offers the unique opportunity cross search multiple Databases. Depending on your license you can choose MDL's Beilstein and Gmelin Databases; if available customer Databases can be included as well.

Click the checkbox of each Database to select or deselect it.

If more than one Database is selected the EDS are not active as they are specific for each single database. Therefore a multiple search can only be carried out with a structure and/or a text as query.

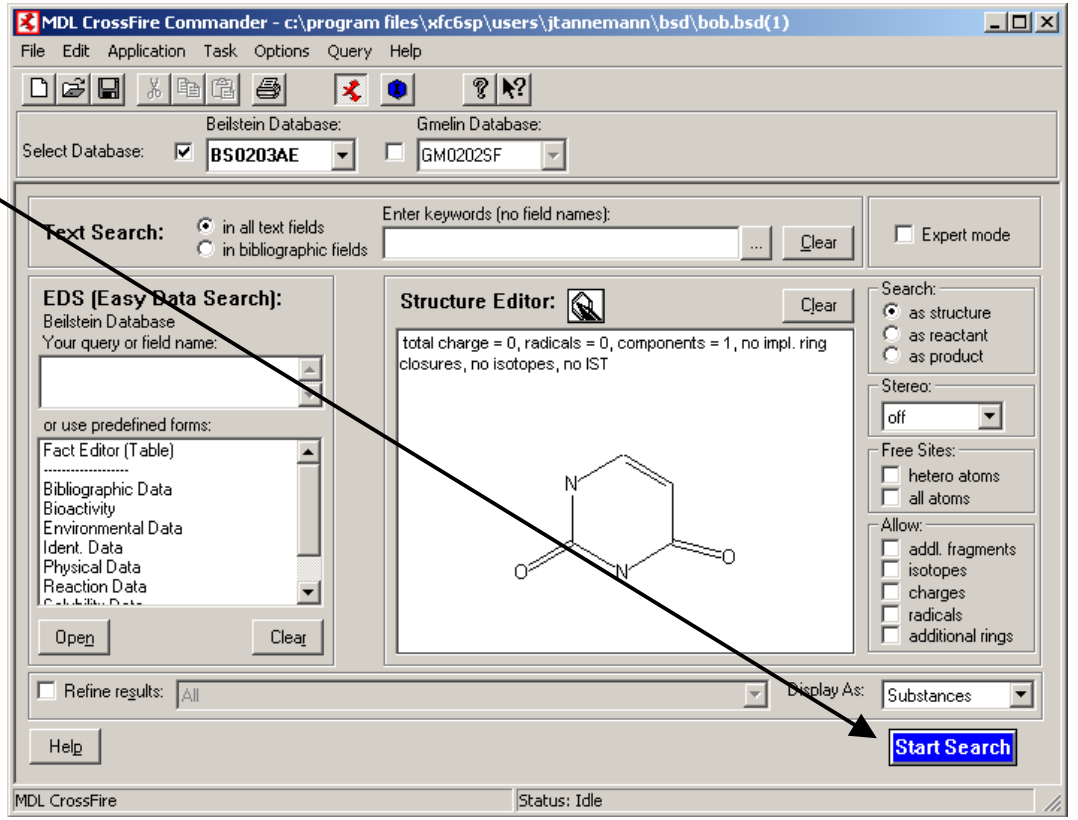
The results from each database will be displayed in parallel, in separate windows on a single screen, since different fields are connected with the content of each database.

2.6 Start Search

☞ **Searches can only be started from Commander.**

- use the "**Start Search"** Button
- Hit "Enter" on your keyboard
- Press F7

to start your search.

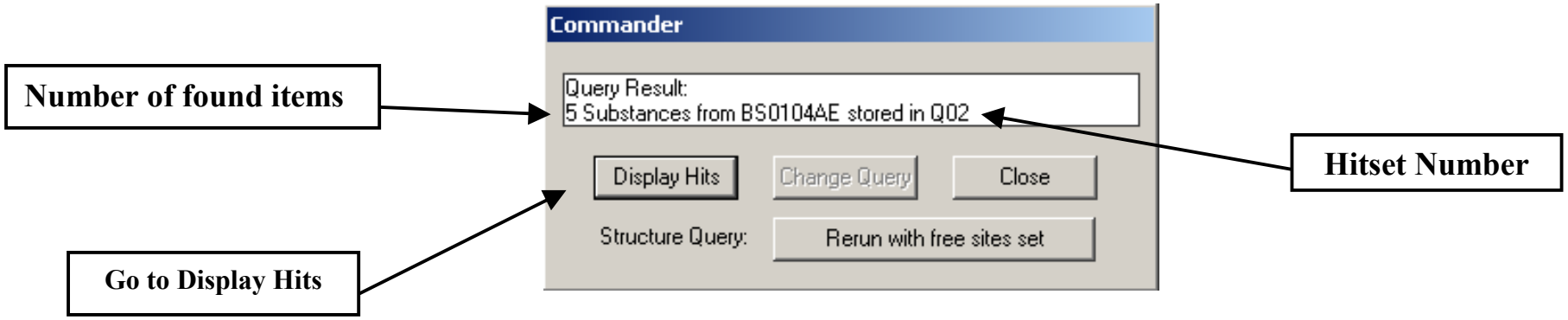


3 Search Options

Depending on the search option you used, Commander displays the result as described below. You always find a Button Change Query or Back to Query that enables you to rework your query when the result is insufficient.

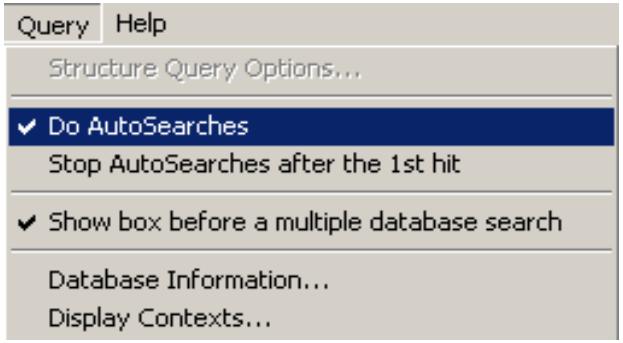
3.1 Query Result

The result of the search without further options is displayed like:



3.2 AutoSearch

If “AutoSearch” is enabled Commander will refine the structure or the text entered as the query step by step to find the closest hit. “AutoSearch” can be enabled/disabled in the Menu “**Query**”.

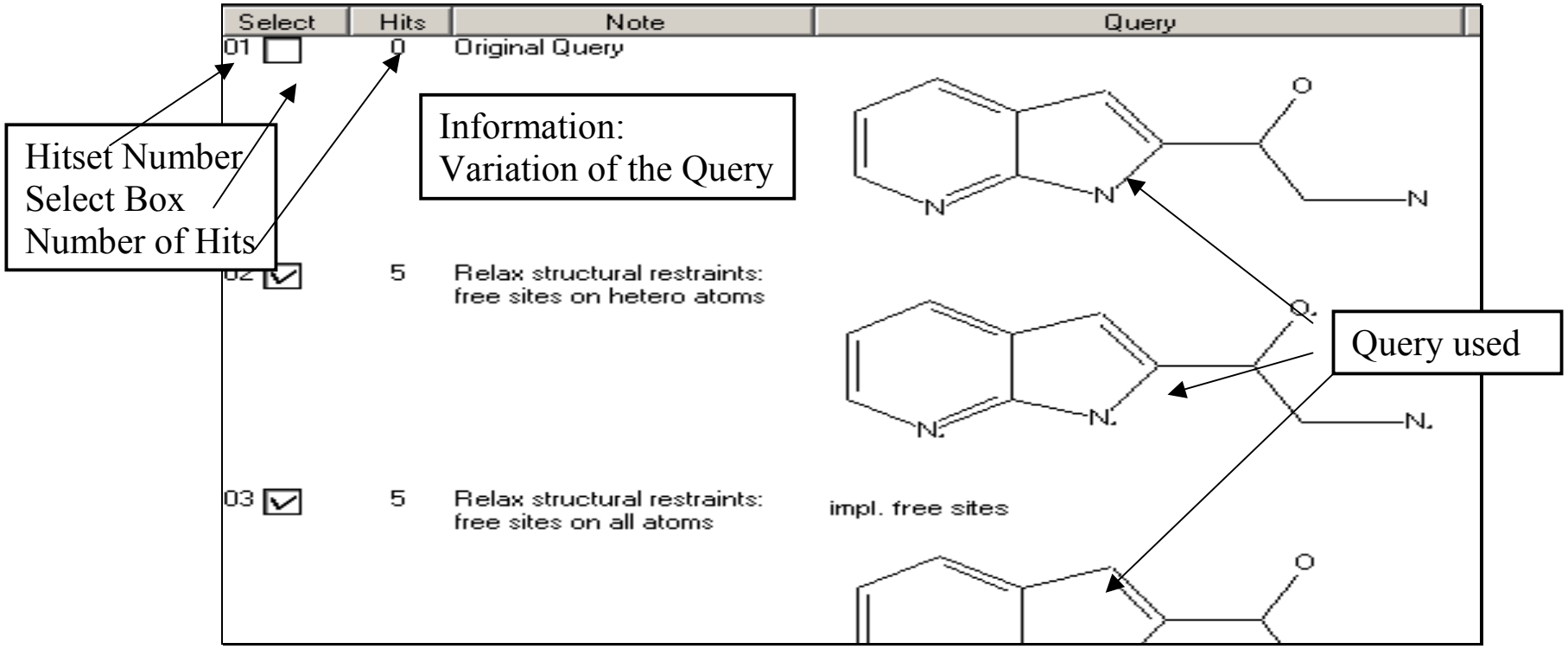


AutoSearch can be stopped after Commander found the first Hit. If this option is not selected Commander will use all possible variations of the query.

Variations when using a structure:
original query – free sites on hetero atoms – free sites on all atoms – allow additional rings

Variations when using a text search (more than one word):
Boolean Operators “near” – “proximity” – “and”

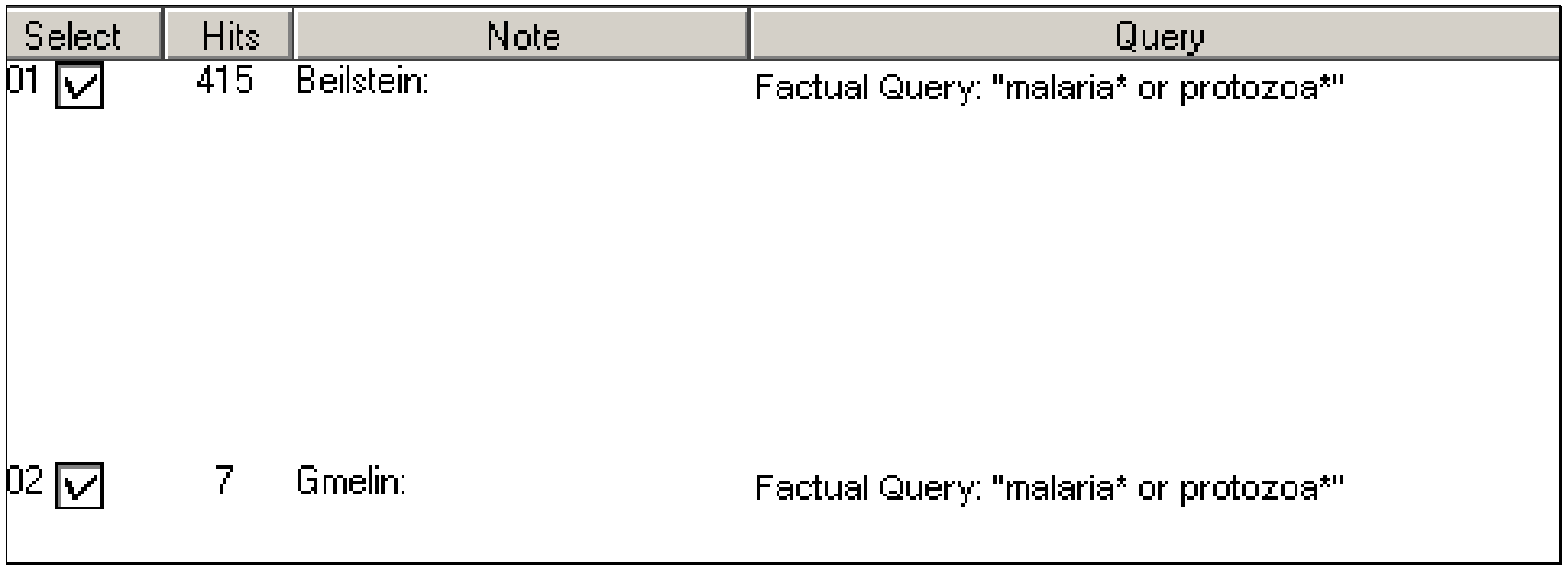
The result is displayed, including information on the variation of the query



Use the Checkboxes 02 ☑ to select one or more hitsets for display.

3.3 Combined Search

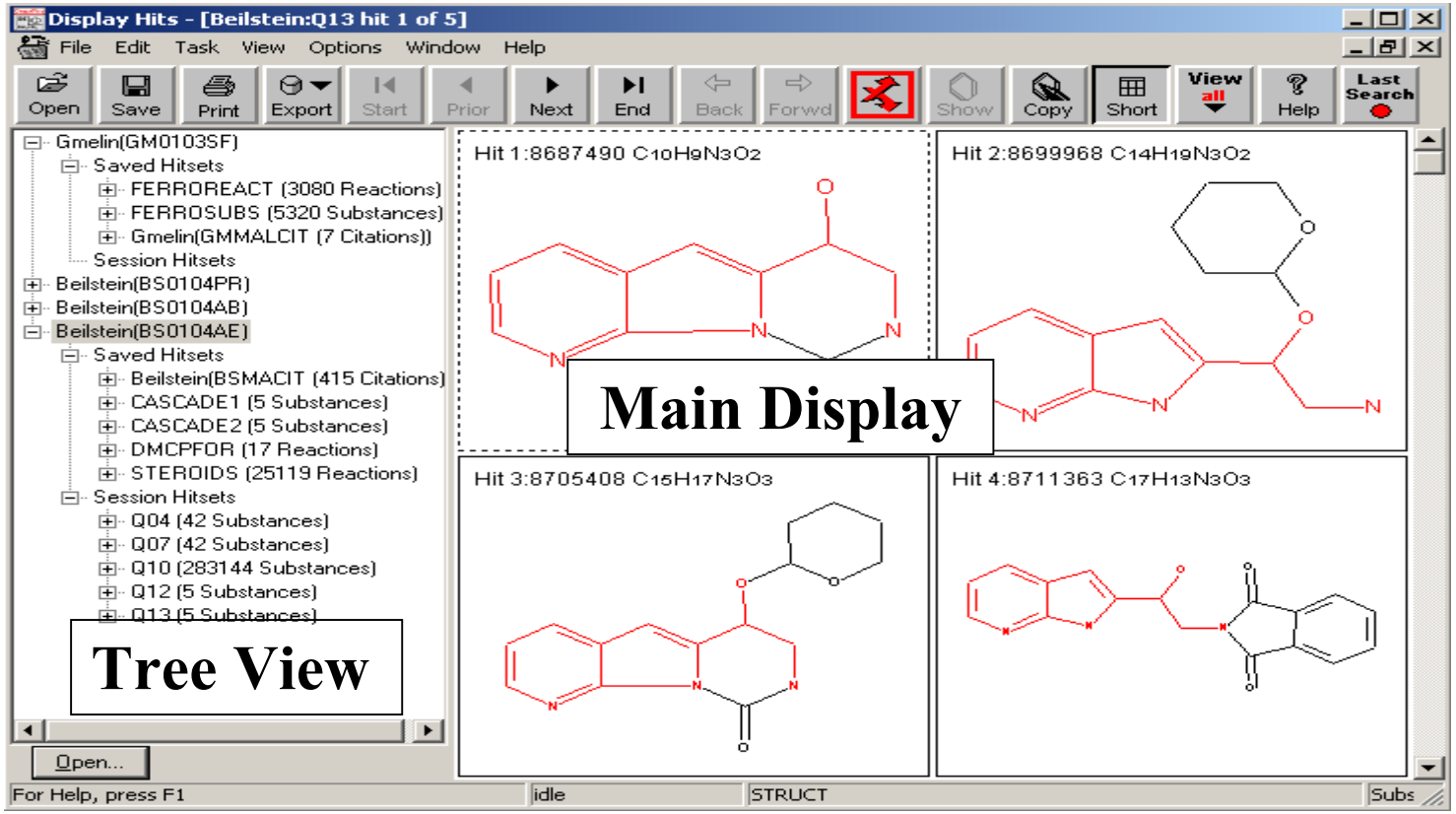
The result of a search in multiple Databases (combined search, see 1.1.1) is displayed in the same fashion.



Use the checkboxes to select the Hitsets for display.

4 Display Hits

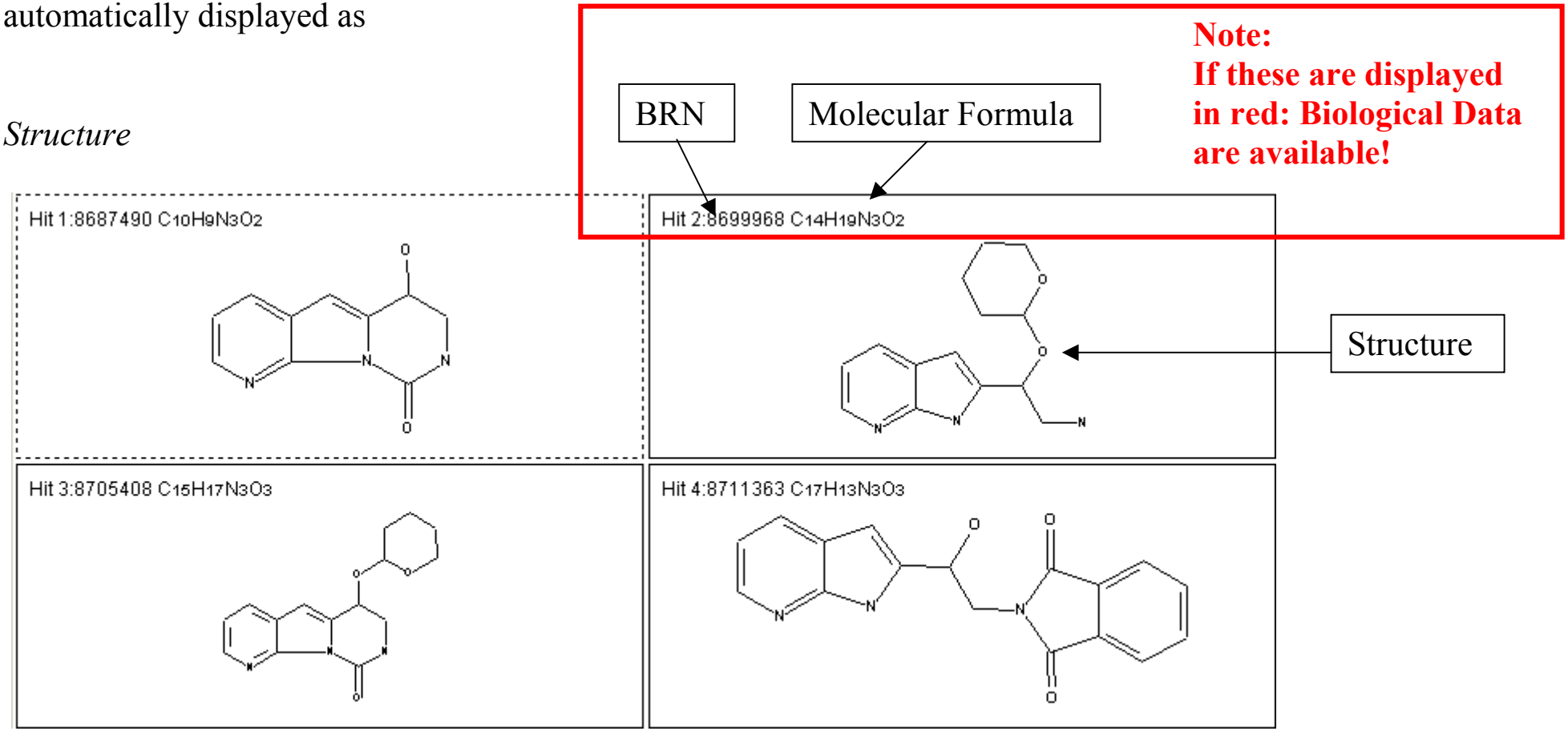
From the display of the query result click Display Hits or View to open “Display Hits”.



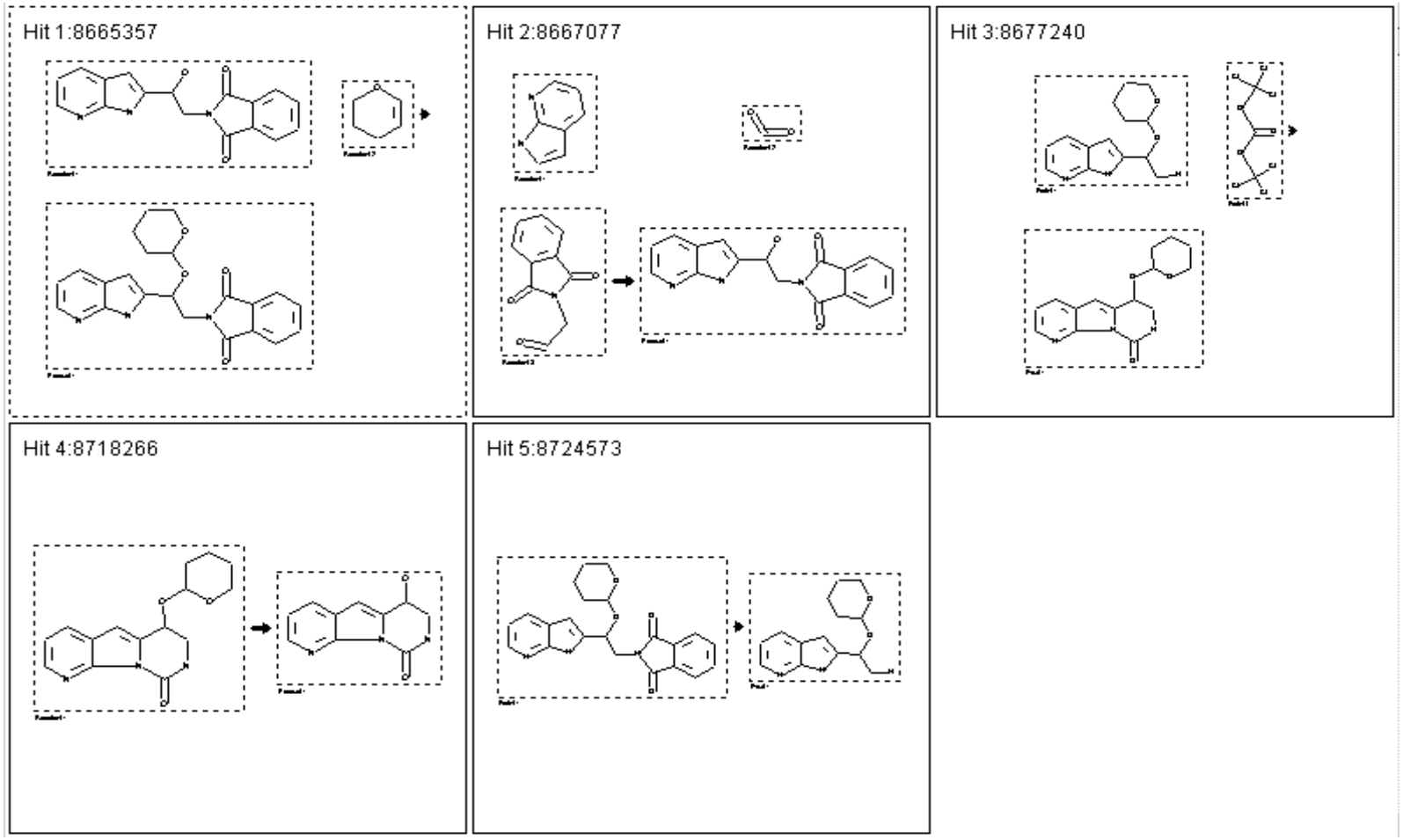
4.1 Main Screen

The main screen starts on default with the Short Display of the results. Depending on the query the hits are automatically displayed as

Structure

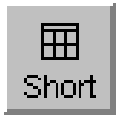


as Reaction


Hit 1:8665357
Hit 2:8667077
Hit 3:8677240
Hit 4:8718266
Hit 5:8724573

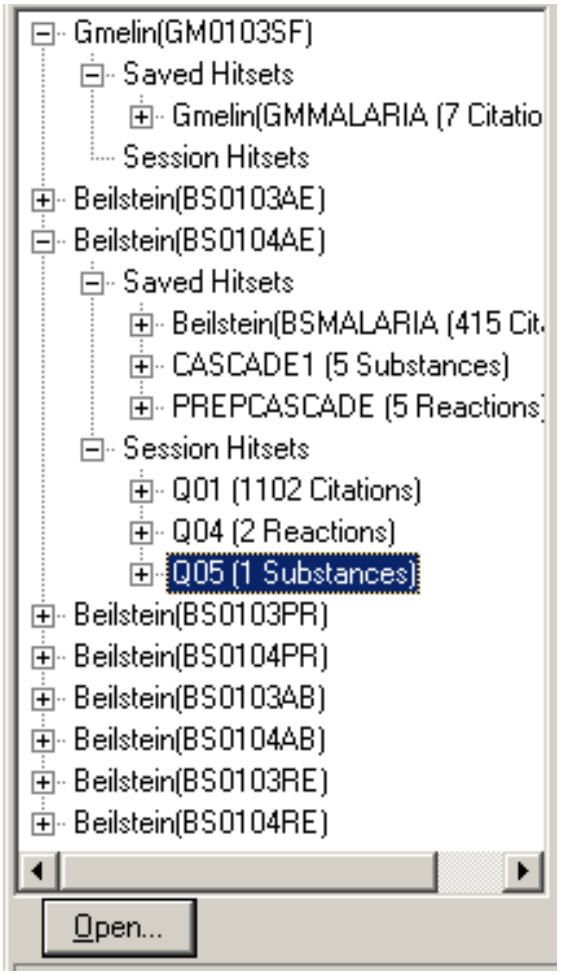
-or as citations

Hit 1:5500578	Journal; Pessi, Antonello; Bianchi, Elisabetta; Bonelli, Fabio; Chiappinelli, Lorella; JCCCAT; J.Chem.Soc.Chem.Commun.; EN; 1; 1990; 8-9.
Hit 2:5501252	Journal; Escande, C.; Chevalier, P.; Verdier, F.; Bourdon, R.; JPMSAE; J.Pharm.Sci.; EN; 79; 1; 1990; 23-27.
Hit 3:5503456	Journal; Narita, Mitsuaki; Takegahara, Hitoshi; Ono, Seiji; Sato, Hisaya; BCSJA8; Bull.Chem.Soc.Jpn.; EN; 63; 2; 1990; 484-488.
Hit 4:5509164	Journal; Jung, Mankil; Li, Xun; Bustos, Daniel A.; ElSohly, Hala N.; McChesney, James D.; Milhous, Wilbur K.; JMCMAR; J.Med. Chem.; EN; 33; 5; 1990; 1516-1518.
Hit 5:5525841	Journal; Mansor, S. M.; Ward, S. A.; Edwards, G.; Hoaksey, P. E.; Breckenridge, A. M.; JPPMAB; J.Pharm.Pharmacol.; EN; 42; 1990; 428-432.
Hit 6:5528096	Journal; Hooper, M; Kirby, GC; Kulkarni, MM; Kulkarni, SN; Nagasampagi, BA; et al.; EJMCA5; Eur.J.Med.Chem.Chim.Ther.; EN; 25; 9; 1990; 717-723.

Double Click the item you want to see or select it and click 

for details.

4.2 Tree View



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

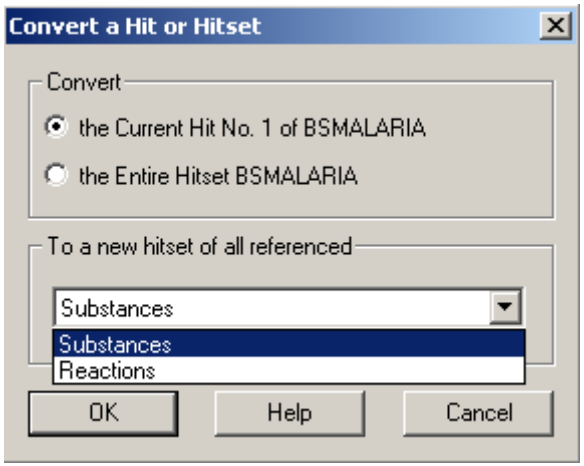
Select the Hitset you want to see and the main screen switches to Short Display.

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

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

The Tree View can be used to change the context of a Hitset from the original to Citations, Reactions or Substances. Do a right click onto the Hitset and select "**Convert...**"

Choose the extent of the conversion and the context, which you want to put the hitset in (here converting a hitset in Citation Context to Substances or Reactions)



4.3 Function of the Buttons

The buttons in the Display Hits window have the following functions:

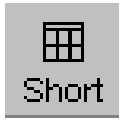
Export selected data. Select from predefined Export definition or create your own (choose Settings in Drop down menu)

Goto First / Previous / Next / Last hit of the selected hitset

Go to Commander. You can also press F7

Switch on/off Display of structure in Main Screen

Copy structure to Structure Editor (opens the Editor)



Toggle on/off Short Display

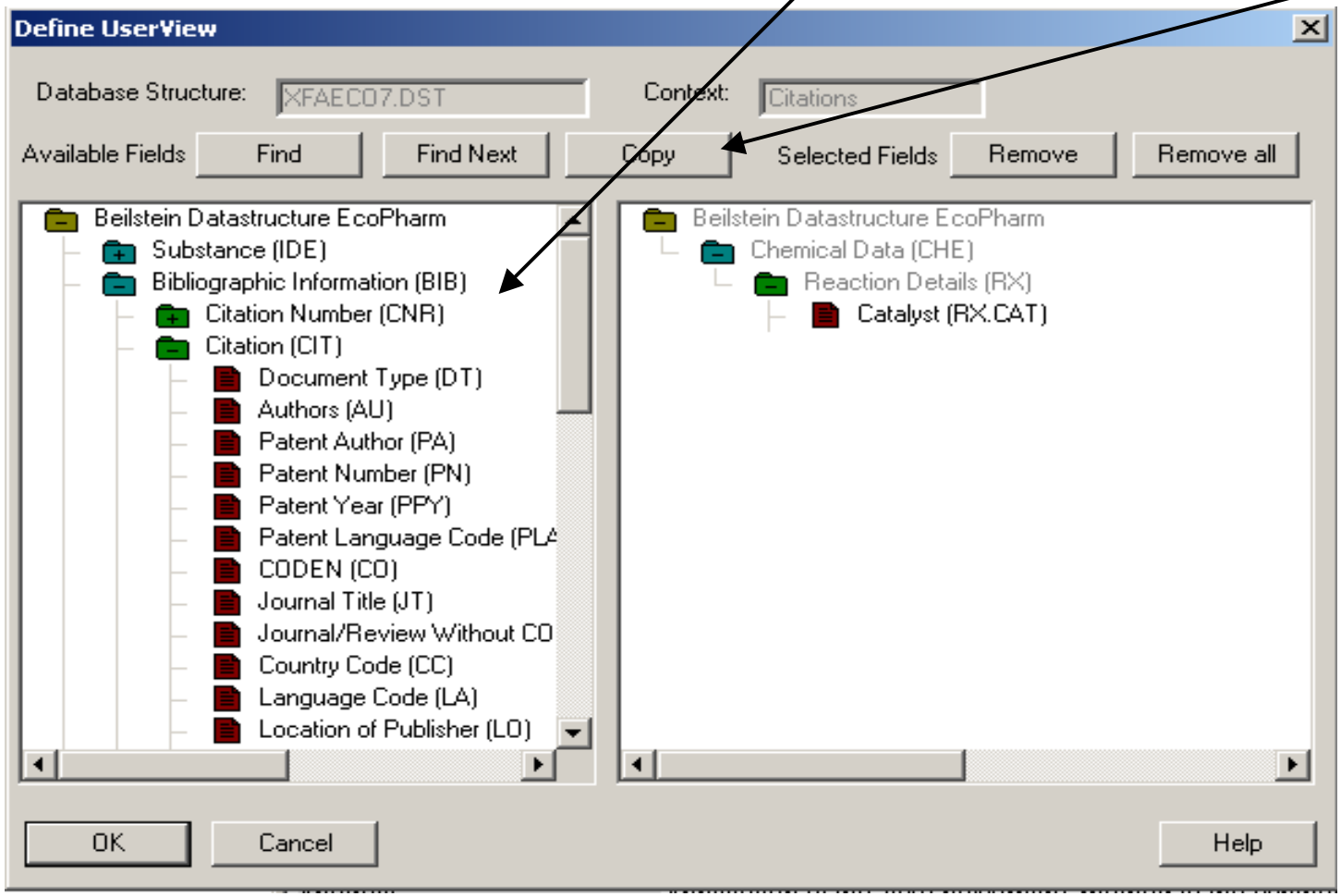
Click to view the search query used

Define the view on the data:

- Identification (Substance/Reaction/Reference and Field Availability List)
- All Fields
- Hit Only (Substance/ Reaction/Reference and Abstract)
- Define your own View File

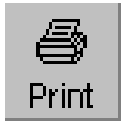
To define your own view click on Button “View” and select “Define…”. In the window which opens you will find your saved views. Select the View File and press “Apply”. Press “Edit” if you want to Edit the View File. Press “Remove” if you want to delete the View File.

To create a new one press “New…” Select the Field you want to apply in the left screen and press “Copy” to add it to the View File.



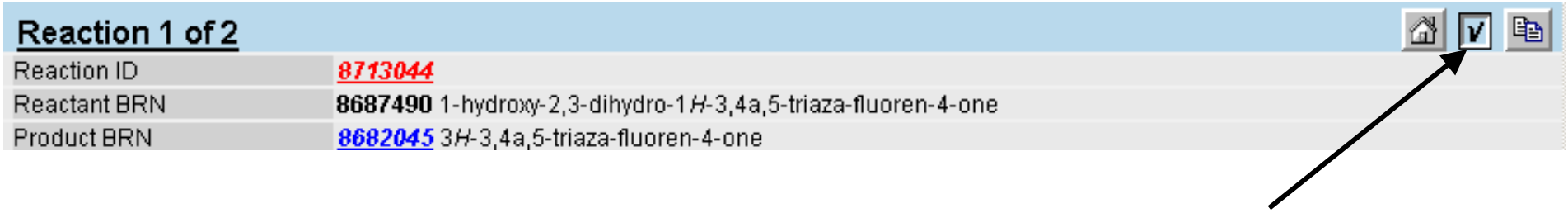
5. Print and Export

5.1 Printing

Choose “File:Print…” or [CTRL+P] or press 

and select the range you want to Print (Current Hit; Hit 1 – X). Select your options and the layout and press OK. Commander will print the View of the Main Screen (see 3.3.3) on your standard printer.

If you want to print only some facts from a hit, mark the desired detail at the check box on the top right



Select one or more facts and start printing as described above.

5.2 Export and Report

All information in your hits can be exported to other applications such as Microsoft Word, Microsoft Excel or your preferred HTML-Browser. You can export full hitsets, a range of hits or extract information from a hit.

Select the information and use the menu "**File:Export**" or the Button 

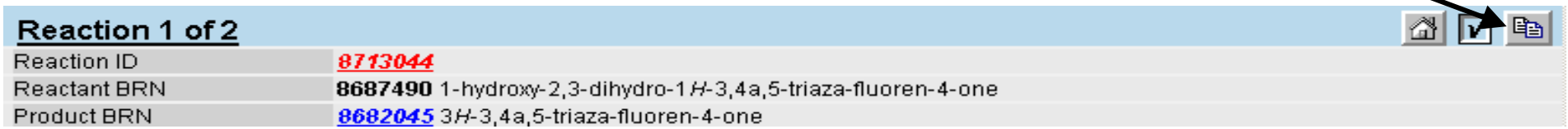
to define the format for export.

You will be prompted for the settings of your export. Choose one of the predefined settings for Export in various formats or "Settings.." to define your own.
The selected export destination will be opened with the export file when finished.

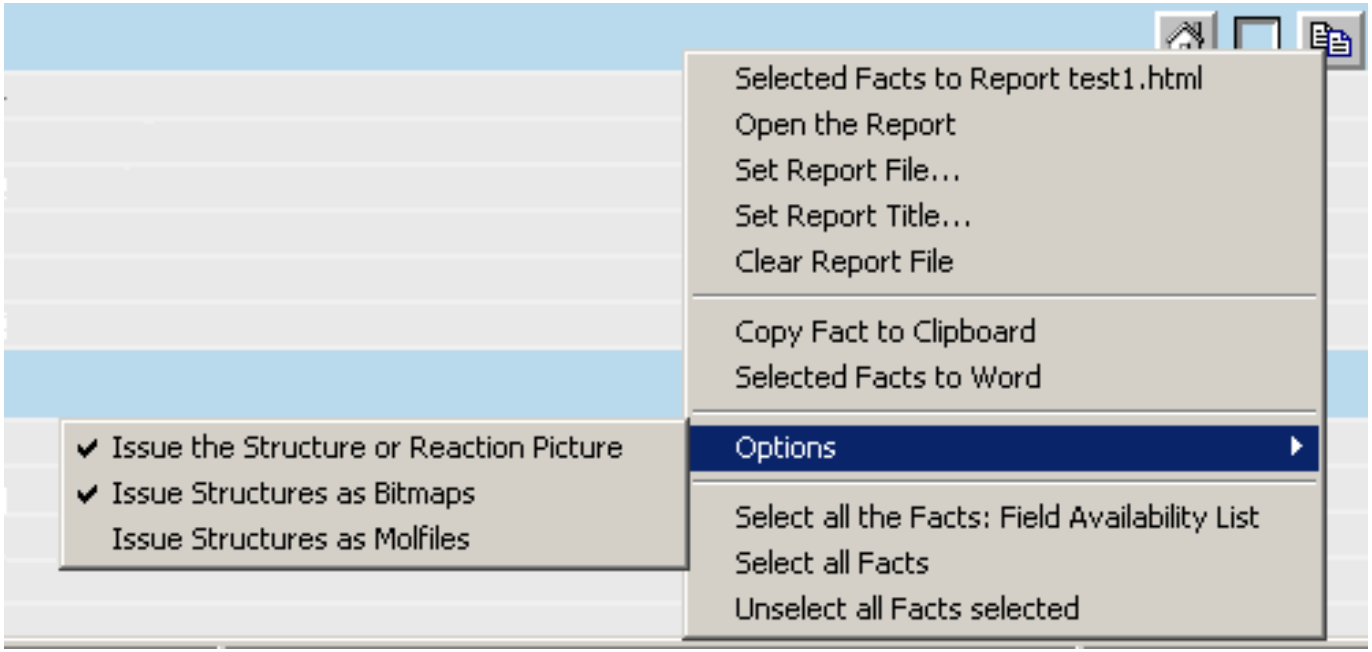
5.2.1 One Click Reporting

In the Full Display view, each field is equipped with a Title Bar on top that is used to select factual data (see 4.1) and to perform "One-Click-Reporting":

Button One-Click-Reporting



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



The selected fact will be added at the end of the defined report (see first row). Use the options to operate the Report function.
To view the report select “Open the Report”. To print the selected facts choose “Print” from the “File”-menu and check the range “Selected Facts”.

5.2.2 Reference Reporting

MDL Commander V6 offers the possibility to export reference lists in various ways:

- If a hit is in Substance context the last item of the tree of the substance is “Reference”. Select it and a deduplicated list of all references for this hit are displayed in the Main display. You can report, export and print it in the way described earlier.

- If you have a hitset in citation context you find a predefined export setting (see Chapter 5.2) for export of references to Endnote, Procite or other reference managing applications.

- From each hitset you can export a list of all references as HTML. You will find a predefined export setting if you click the “Export”-Button. A framed document is produced , in which you find the compounds you exported on the left side, select them by clicking on the hit number. The facts of this hit will be displayed in the right frame. On top of the frame you find a hyperlink “Reference List”. Clicking this link leads to a deduplicated list of all the references of the exported compounds.

6. Default Settings

Commander

General:

Application:	No Application
AutoSearch	Enabled
Stop AutoSearch after 1st Hit	Disabled
Save Password	Disabled
Startup Task	No Application
Expert Mode	Off
Save Settings on Exit	Enabled
Save History on Exit	Enabled
Automatic Context Selection	Enabled
Show Box before a multiple Database Search	Enabled
Show Startup Screen	Enabled
File/Open…Options	Show query options select box

Structure:

Structure Editor	MDL ISIS Draw
Options:	
Search	As structure
Stereo	Off
Free Sites: hetero atoms	Disabled
Free Sites: all atoms	Disabled
Allow addl. Fragments	Enabled
Allow isotopes	Enabled
Allow charges	Enabled
Allow radicals	Enabled
Allow additional rings	Enabled
Define Structure and Reaction View:	
Mean Bond Length	12 mm
Atom View	
Atom Symbol	Disabled
Without C	Enabled
C as Dot	Disabled
Atom Number	Disabled
Atom Attributes	
Number	Disabled

Mass	Enabled
Topology	Enabled
Charge	Enabled
Radical	Enabled
H-Count	Enabled
Free Sites	Enabled
Valency	Enabled
Attachement Points	Enabled
Attachement Number	Enabled
Stereo	Disabled
Bond Attributes	
Topology	Enabled
Stereo	Enabled
Site Number	Enabled
Reaction Attributes	
Atom Mapping	Enabled
Reaction Center	Disabled
New Bond Type	Enabled

Text Search:

Text Search	In all text fields

Options:

Words are close to each other	Enabled
Words are in the same fact	Enabled
Words are in the same document	Enabled
Use right truncation	Enabled
Use left truncation	Disabled

Display Hits

Short View	Enabled
Tree View	Enabled
Open Hitset in Short Display	Enabled
View	All
Save Settings on Exit	Enabled
Include Structures	Disabled
Include Field Availability	Enable
Selected Hits only	Disabled
Status Bar	Enabled

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