



MDL



**CrossFire
Commander V6**

Quick Reference Guide

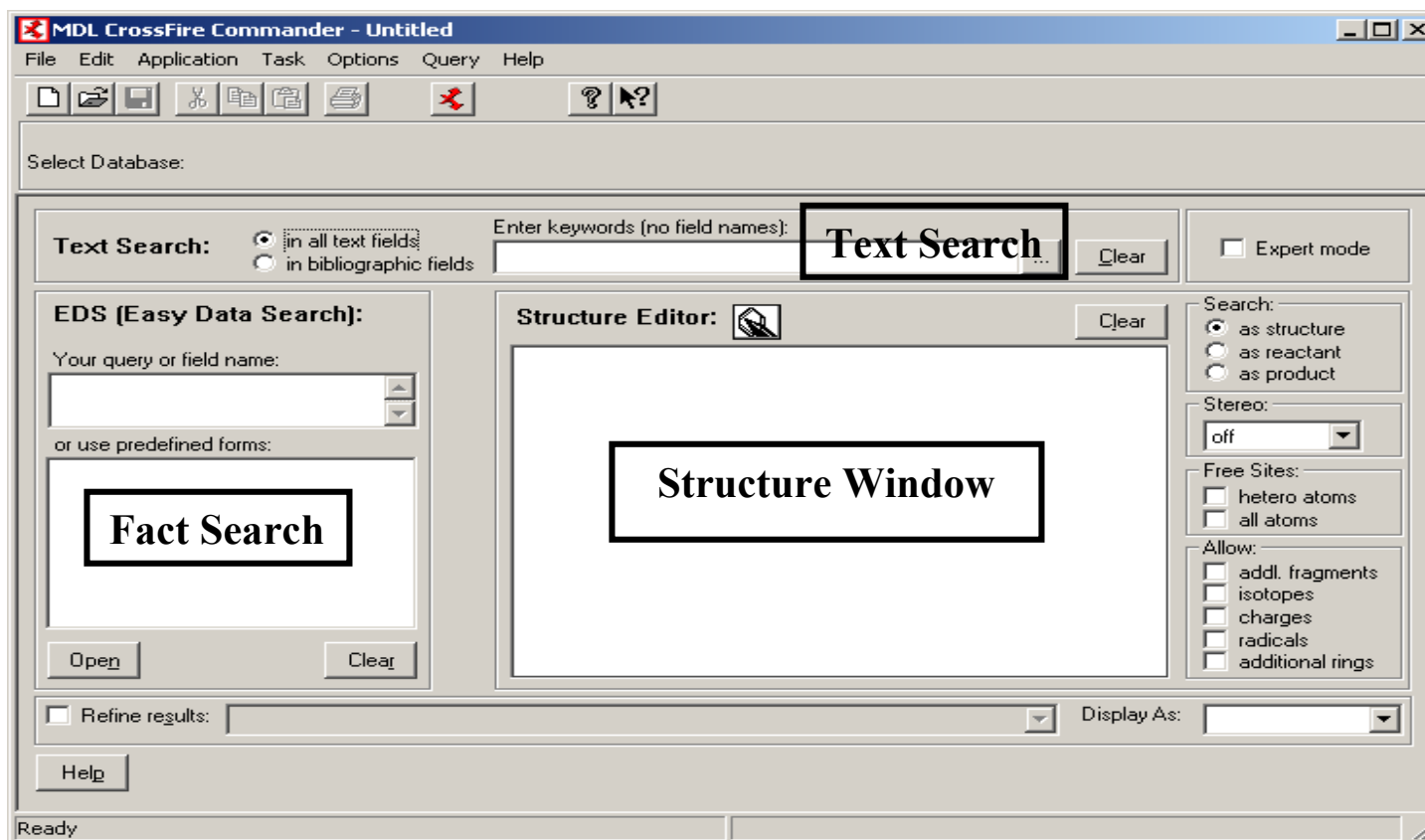
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03/2002

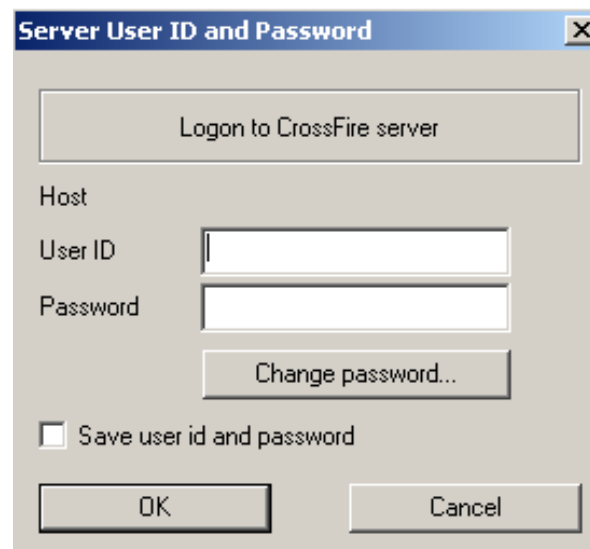
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1 Starting MDL CrossFire

- 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**”



- In Commander click the  -Button or select from Menu “**Application:CrossFire**”
- Fill in the login-box as required.



Server User ID and Password

Logon to CrossFire server

Host

User ID

Password

Change password...

Save user id and password

OK Cancel

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

1.1 General

1.1.1 Database Selection

	Beilstein Database:	Gmelin Database:
Select Database:	<input type="checkbox"/> BS0104AE	<input checked="" type="checkbox"/> GM0103SF

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:

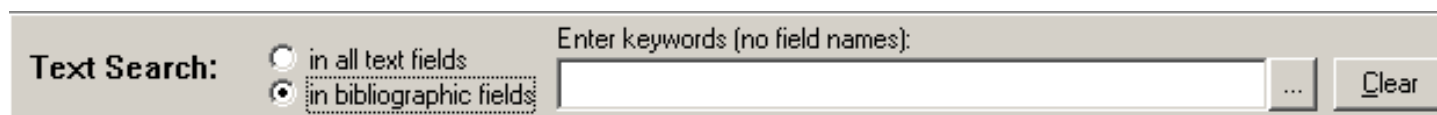
XX YYYY ZZ

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

1.1.2 Search Options

Text Search: Type in keywords, one or more, to be searched in the basic index.

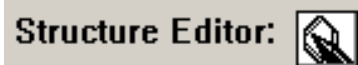
Example: “malaria”



The screenshot shows a search interface with the following elements:

- Text Search:** Label for the search section.
- in all text fields
- in bibliographic fields
- Enter keywords (no field names):
- Text input field for keywords.
- ... (More options button)
- Clear (button)

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

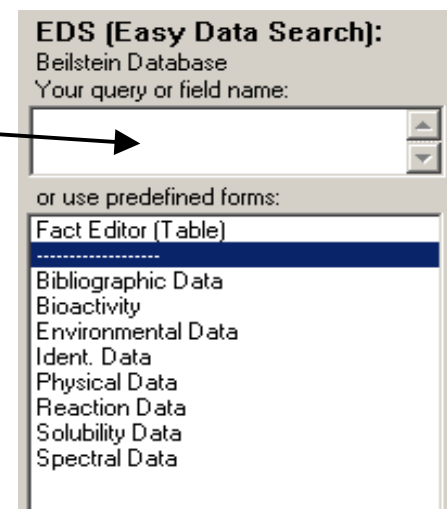


Structures can be loaded as BCCOM-File or as SD-File using “**File:Open**”, “**File:Execute BCCOM**” or “**File:Execute Query List**”

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.

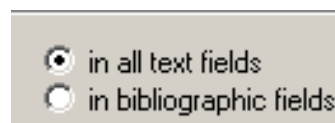
 Use a combination of these interfaces for improved search results



2 Search


2.1 Using the Text Search

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:



A screenshot of a search input field. The field is a rectangular box with a light gray border. Inside the box, the text "Enter keywords (no field names):" is displayed in a small, dark font at the top left. Below this text, the word "Malaria" is entered in a larger, black font. To the right of the text input area, there is a small, square button with three dots "..." inside it.

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.

Text Search in database Beilstein

Your query:
 malaria

Area searched:
 Preview of word occurrences in:

Words:	Substances	Reactions	Citations*
malaria	230	1	203
or			
protozoa	138	0	248

(Select by clicking column headings)

Options... Boolean operators: or
 Cascading searches: near, proximity, and
 Truncation: right

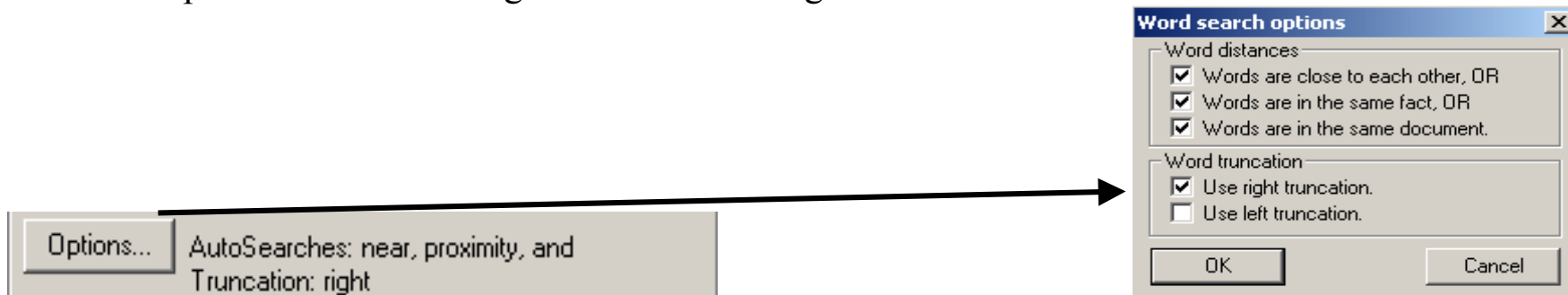
Help Cancel **Start Search**

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.

Important Notes for the use of the Text Search:

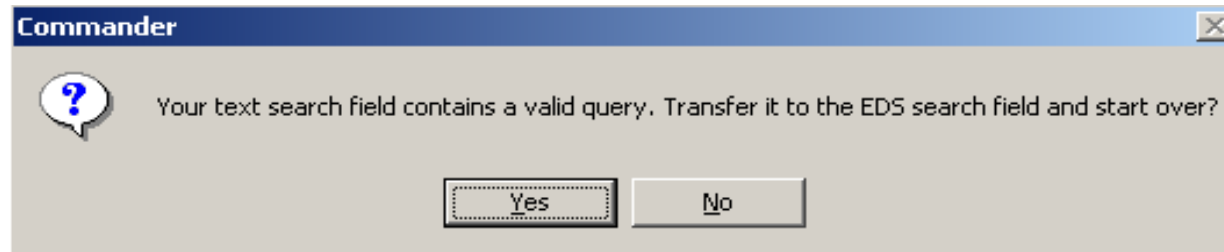
- CrossFire reads the input with “right truncation”, additional placeholders will be ignored in standard
- If more than one word is entered into the text search field the operators “near”, “proximity”, and “and” are used in AutoSearch (see Chapter 3.2)

Click the Options button to change the default settings:



- 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:

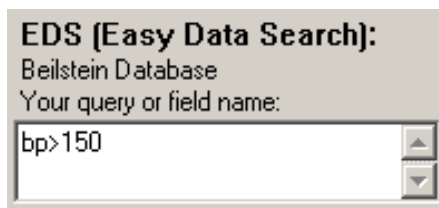


If “Yes” is chosen Commander translates the Input into the Fact Editor Field. Please press “Start Search” again to submit your Query.

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

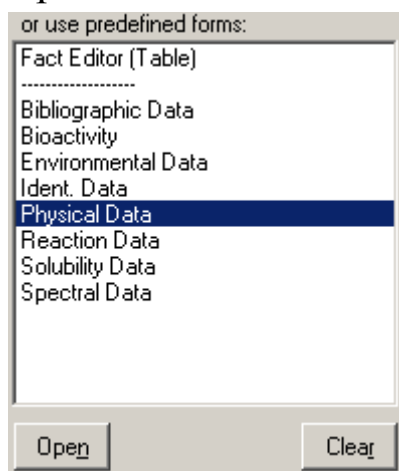
2.2 Using the Easy Data Search (EDS) or the Fact Editor

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



EDS [Easy Data Search]:
 Beilstein Database
 Your query or field name:
 bp>150

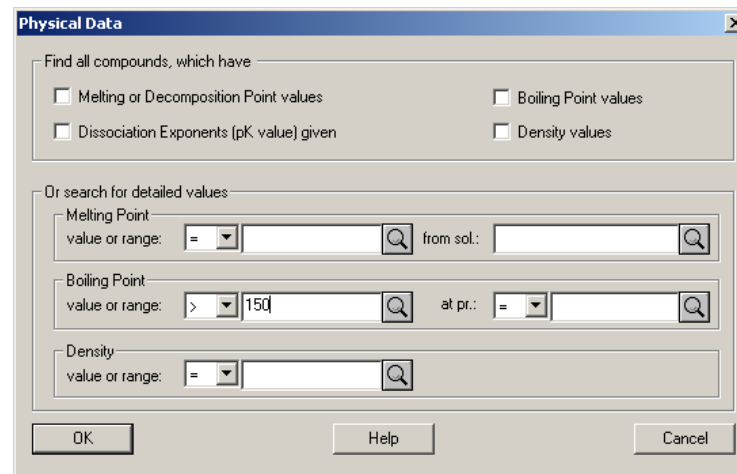
The lower field enables you to use predefined forms to start a factual search. Double Click or select and click "Open" to enter data:



or use predefined forms:

- Fact Editor (Table)
-
- Bibliographic Data
- Bioactivity
- Environmental Data
- Ident. Data
- Physical Data**
- Reaction Data
- Solubility Data
- Spectral Data

Open Clear



Physical Data

Find all compounds, which have

Melting or Decomposition Point values Boiling Point values

Dissociation Exponents (pK value) given Density values

Or search for detailed values

Melting Point
 value or range: = [] [] from sol.: [] []

Boiling Point
 value or range: > 150 [] [] at pr.: = [] []

Density
 value or range: = [] []

OK Help Cancel

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 **Structure Editor:**  or double click in the *Structure Editor Window* to open the Drawing tool.

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)

Please refer to the individual User Guides of the corresponding Editors on our web sites.

☞ Searches can only be started from Commander. Press “F7”-key or use the “**Start Search**” Button



to start your search.

2.4 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.

	Beilstein Database:	Gmelin Database:
Select Database:	<input checked="" type="checkbox"/> BS0104AE	<input checked="" type="checkbox"/> GM0103SF

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.

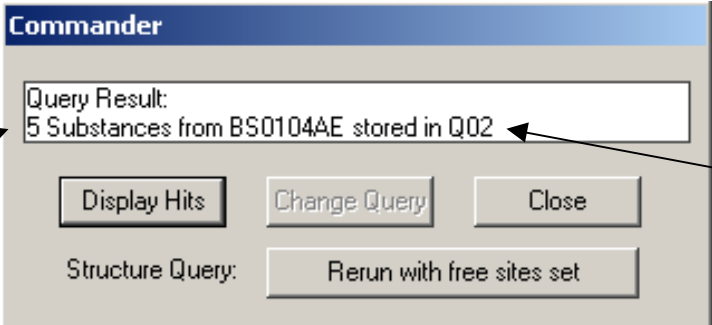
The results from each database will be displayed in parallel, in separate windows on a single screen, since different fields are connected with the content of each database.

3 Search Result

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

3.1 Query Result

The result of the search is displayed:



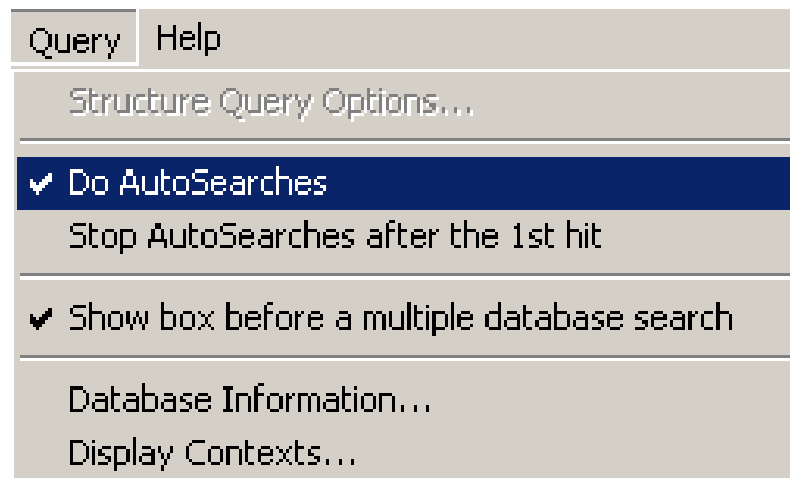
Number of found items

Hitset Number

3.2 AutoSearch

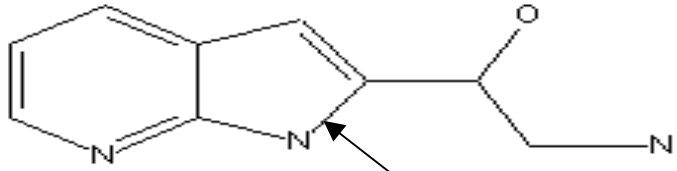
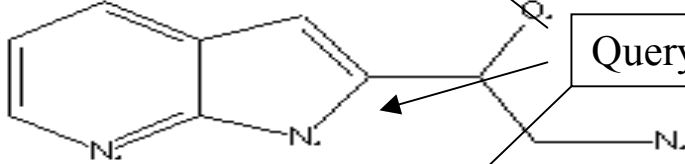

If “AutoSearch” is enabled Commander will refine the structure or the text entered as the query.

“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.

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

Select	Hits	Note	Query
01 <input type="checkbox"/>	0	Original Query	
02 <input checked="" type="checkbox"/>	5	Relax structural restraints: free sites on hetero atoms	
03 <input checked="" type="checkbox"/>	5	Relax structural restraints: free sites on all atoms	impl. free sites 

Information:
Variation of the Query

Hitset Number
Select Box
Number of Hits

Query used

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

3.3 Combined Search

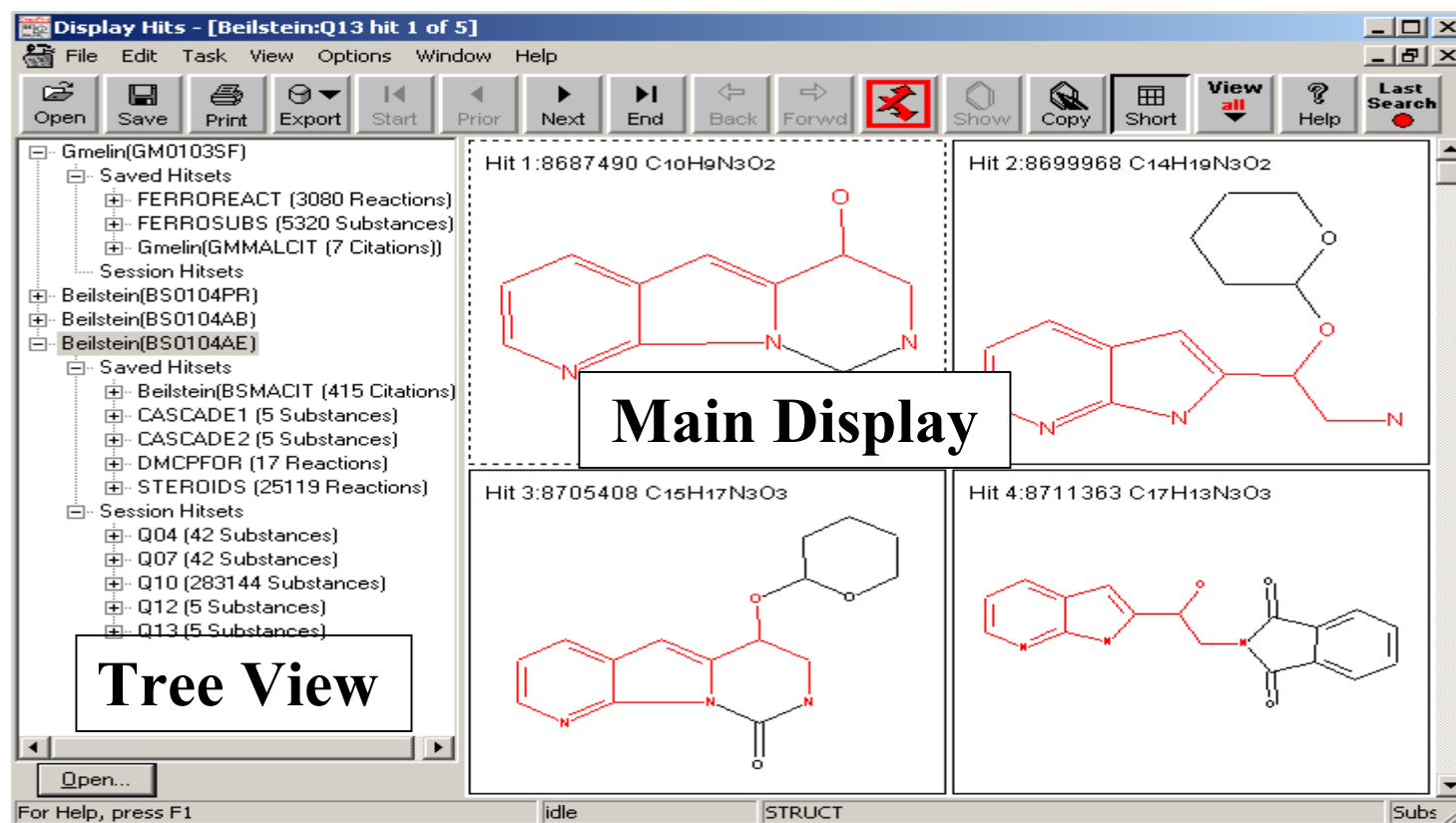
The result of a search in multiple Databases (combined search) is displayed in the same fashion.

Select	Hits	Note	Query
01 <input checked="" type="checkbox"/>	415	Beilstein:	Factual Query: "malaria* or protozoa*"
02 <input checked="" type="checkbox"/>	7	Gmelin:	Factual Query: "malaria* or protozoa*"

Use the checkboxes to select the Hitsets for display.

4 Display Hits

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

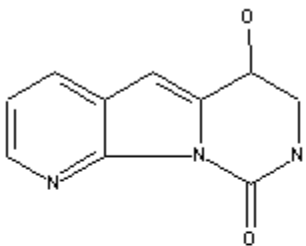
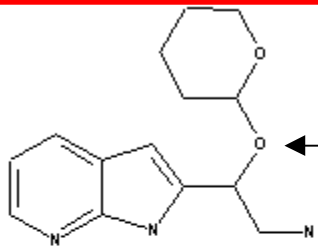
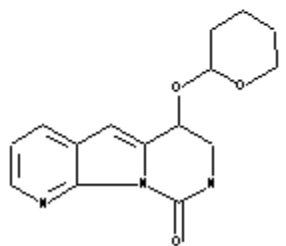
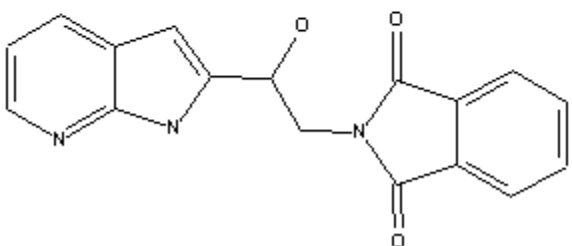


The screenshot shows the 'Display Hits' application window. The title bar reads 'Display Hits - [Beilstein:Q13 hit 1 of 5]'. The menu bar includes File, Edit, Task, View, Options, Window, and Help. The toolbar contains icons for Open, Save, Print, Export, Start, Prior, Next, End, Back, Forwd, a red 'X' icon, Show, Copy, Short, View all, Help, and Last Search. The left pane shows a 'Tree View' with a hierarchical list of search results, including 'Gmelin(GM0103SF)', 'Beilstein(BS0104PR)', 'Beilstein(BS0104AB)', 'Beilstein(BS0104AE)', and 'Beilstein(BSMACIT (415 Citations))'. The main display area is divided into four quadrants, each showing a chemical structure and its corresponding hit ID and formula: Hit 1: 8687490 C₁₀H₉N₃O₂, Hit 2: 8699968 C₁₄H₁₉N₃O₂, Hit 3: 8705408 C₁₅H₁₇N₃O₃, and Hit 4: 8711363 C₁₇H₁₃N₃O₃. A red 'X' icon in the toolbar is highlighted with a red box. The status bar at the bottom shows 'idle' and 'STRUCT'.

4.1 Main Screen

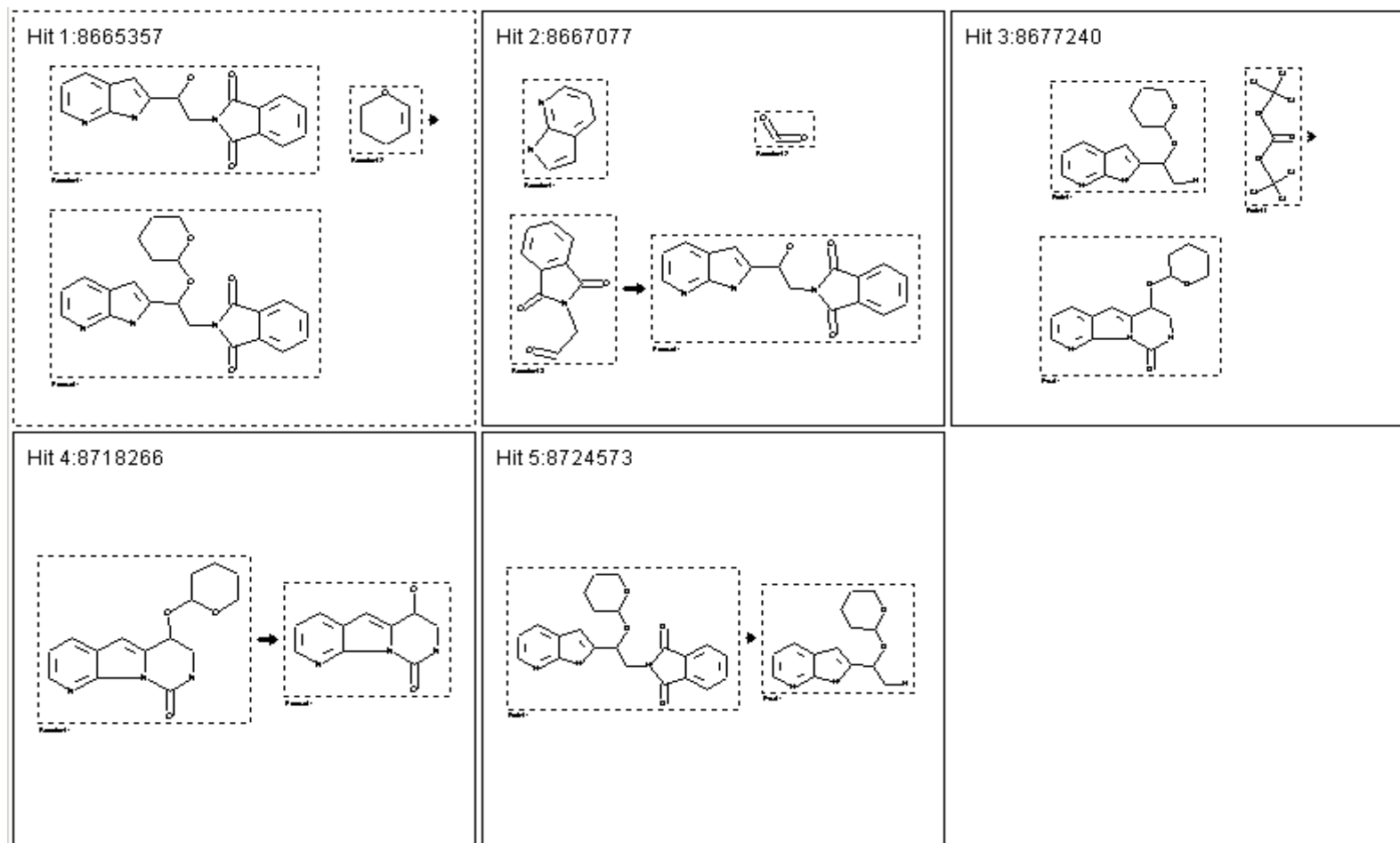
The main screen starts on default with the Short Display of the results. Depending on the query the hits are automatically displayed as

Structure

	BRN	Molecular Formula	
Hit 1:8687490 C ₁₀ H ₉ N ₃ O ₂			
			
Hit 2:8699968 C ₁₄ H ₁₉ N ₃ O ₂			
			Structure
Hit 3:8705408 C ₁₅ H ₁₇ N ₃ O ₃			
			
Hit 4:8711363 C ₁₇ H ₁₃ N ₃ O ₃			
			

Note:
If these are displayed in red: Biological Data are available!

as Reaction



-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.

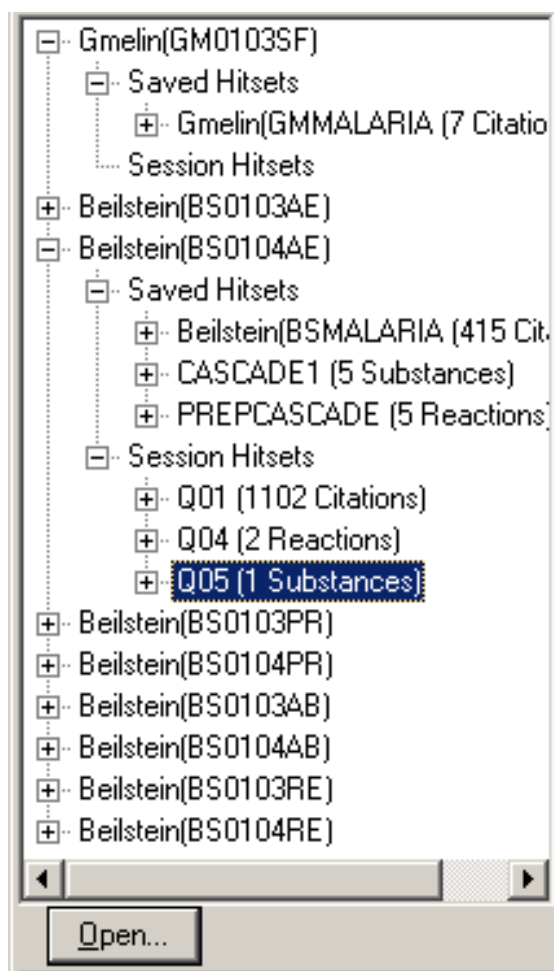
Hit 6:5528096 Journal; Hooper, M; Kirby, GC; Kulkarni, MM; Kulkarni, SN; Nagasampagi, BA; et al.; EJMCA5; Eur.J.Med.Chem.Chim.Ther.; EN; 25; 9; 1990; 717-723.



Short


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.

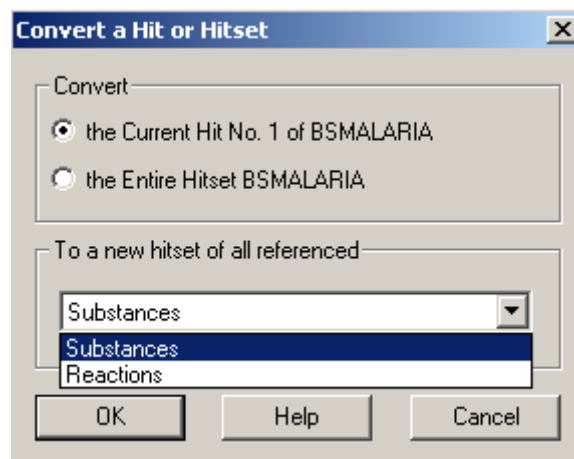
Click on  to drill down to details, ultimately to field level.

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

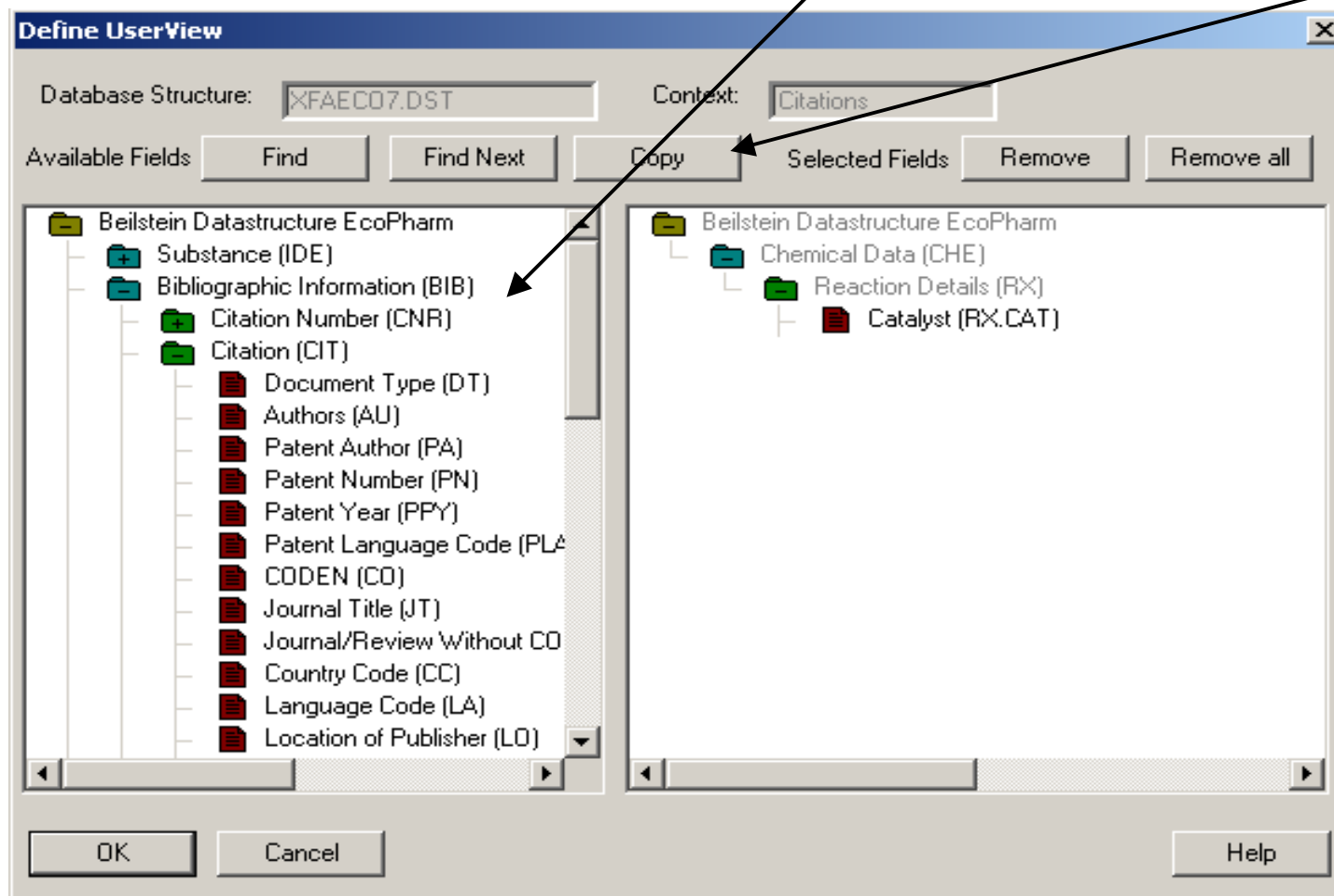


Define the view on the data:

- 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

Reaction 1 of 2			<input checked="" type="checkbox"/>	
Reaction ID	8713044			
Reactant BRN	8687490 1-hydroxy-2,3-dihydro-1H-3,4a,5-triaza-fluoren-4-one			
Product BRN	8682045 3H-3,4a,5-triaza-fluoren-4-one			




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.

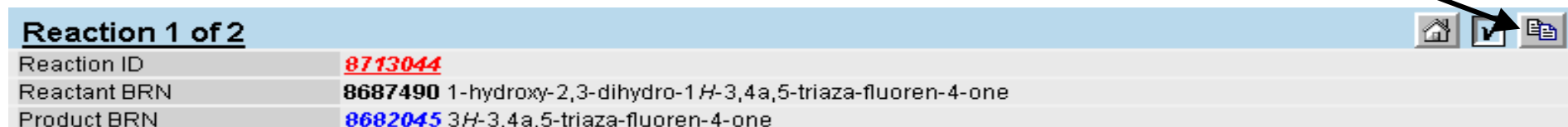
You will be prompted for the settings of your export. Choose one of the predefined settings for Export in various formats or “Settings..” to define your own.

The selected export destination will be opened with the export file when finished.

5.2.1 One Click Reporting

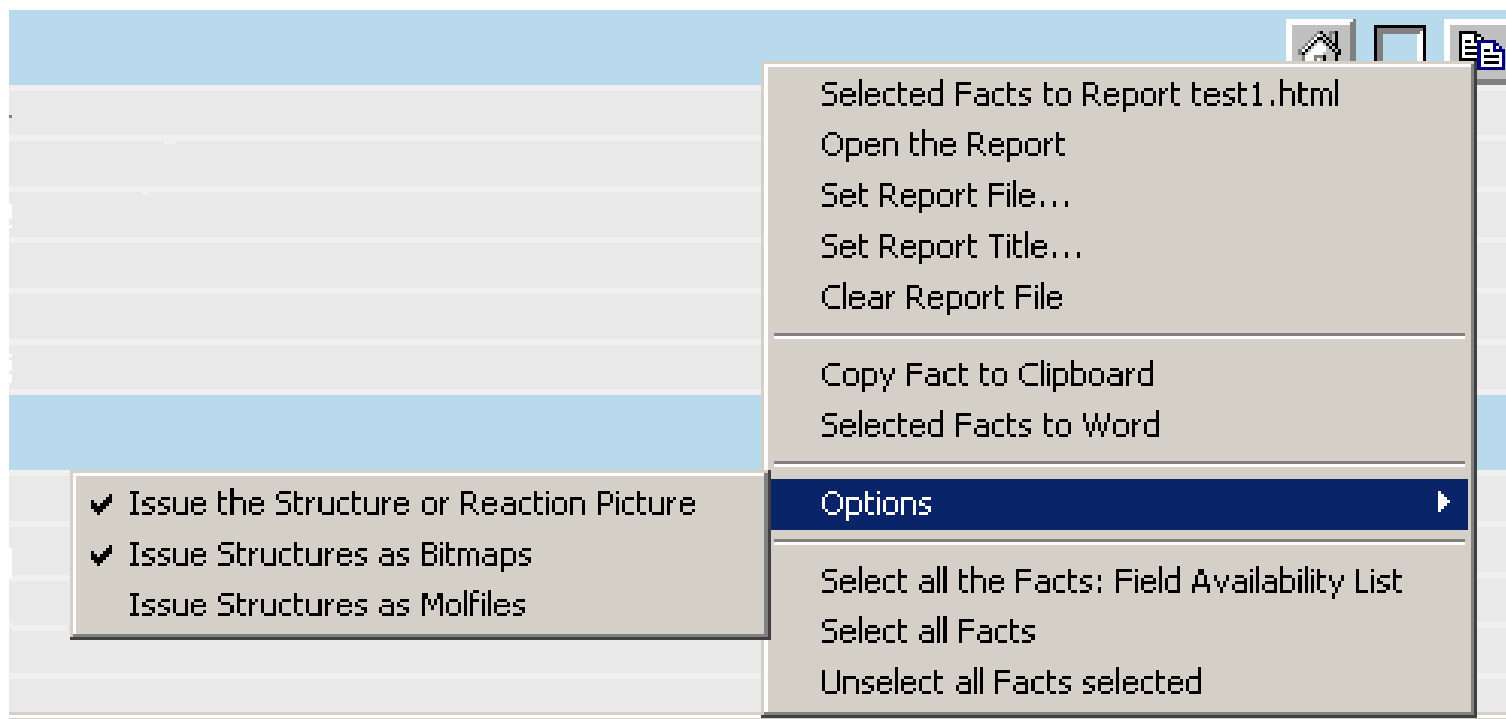
In the Full Display view, each field is equipped with a Title Bar on top that is used to select factual data (see 4.1) and to perform “One-Click-Reporting”:

Button One-Click-Reporting

A screenshot of a table with a light blue title bar. The title bar contains the text "Reaction 1 of 2" and three icons: a home icon, a checkmark icon, and a document icon. An arrow points from the text "Button One-Click-Reporting" to the checkmark icon. The table has three rows: "Reaction ID" with value "8713044", "Reactant BRN" with value "8687490 1-hydroxy-2,3-dihydro-1H-3,4a,5-triaza-fluoren-4-one", and "Product BRN" with value "8682045 3H-3,4a,5-triaza-fluoren-4-one".

Reaction 1 of 2	
Reaction ID	8713044
Reactant BRN	8687490 1-hydroxy-2,3-dihydro-1H-3,4a,5-triaza-fluoren-4-one
Product BRN	8682045 3H-3,4a,5-triaza-fluoren-4-one

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”.

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 1 st 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

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
Topoliogy	Enabled
Charge	Enabled

Radical	Enabled
H-Count	Enabled
Free Sites	Enabled
Valency	Enabled
Attachement Points	Enabled
Attachement Number	Enabled
Stereo	Disabled
<i>Bond Attributes</i>	
Topology	Enabled
Stereo	Enabled
Site Number	Enabled
<i>Reaction Attributes</i>	
Atom Mapping	Enabled
Reaction Center	Disabled
New Bond Type	Enabled
 <i>Text Search:</i>	
Text Search	In all text fields
<i>Options:</i>	
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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